



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:47 AM UTC

PDB ID : 1HDY / pdb_00001hdy
Title : THREE-DIMENSIONAL STRUCTURES OF THREE HUMAN ALCOHOL DEHYDROGENASE VARIANTS: CORRELATIONS WITH THEIR FUNCTIONAL DIFFERENCES
Authors : Hurley, T.D.; Amzel, L.M.
Deposited on : 1993-10-15
Resolution : 2.50 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

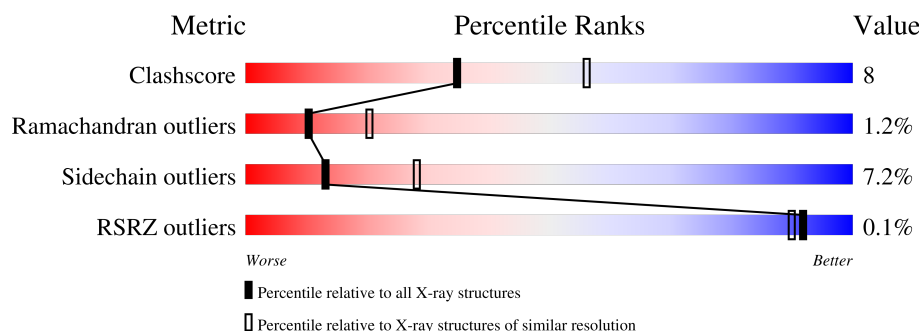
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	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
4	PYZ	A	378	-	-	X	-
4	PYZ	B	378	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5770 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.

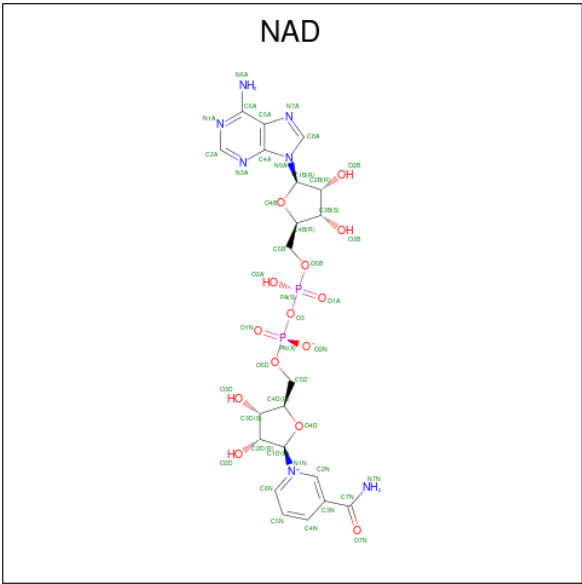
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2780	1770	472	516	22			
1	B	374	Total	C	N	O	S	0	0	0
			2780	1770	472	516	22			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

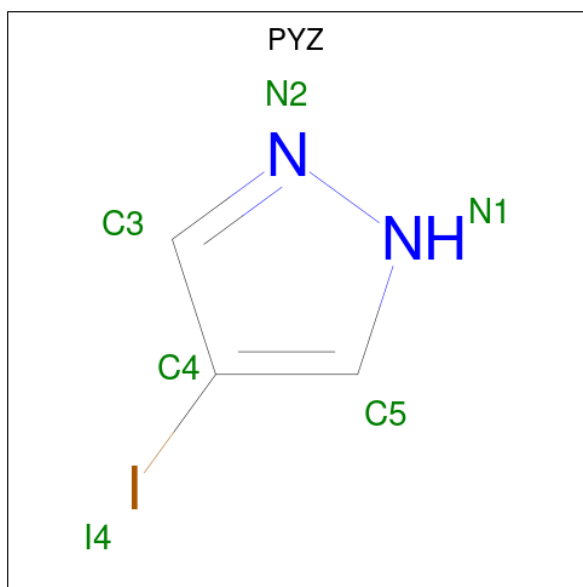
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is 4-iodOPYRAZOLE (CCD ID: PYZ) (formula: $C_3H_3IN_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	I	N	0	0
			6	3	1	2		
4	B	1	Total	C	I	N	0	0
			6	3	1	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl	0	0
			1 1		

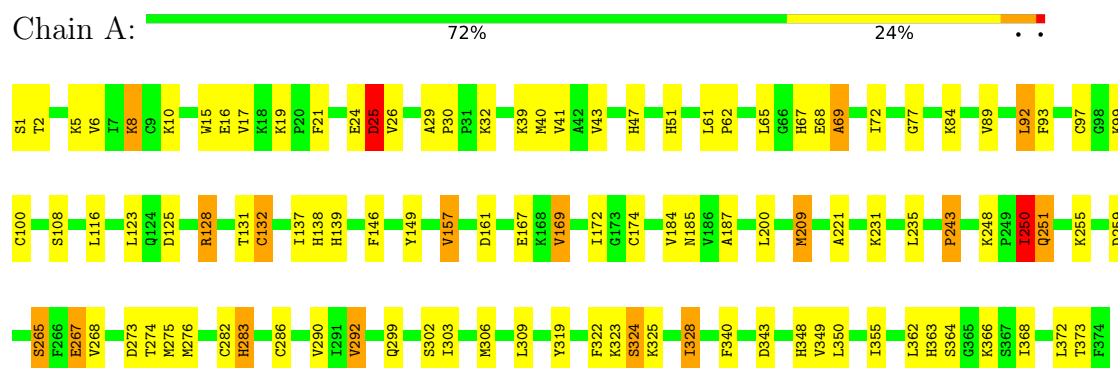
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	59	Total O	0	0
			59 59		
6	B	46	Total O	0	0
			46 46		

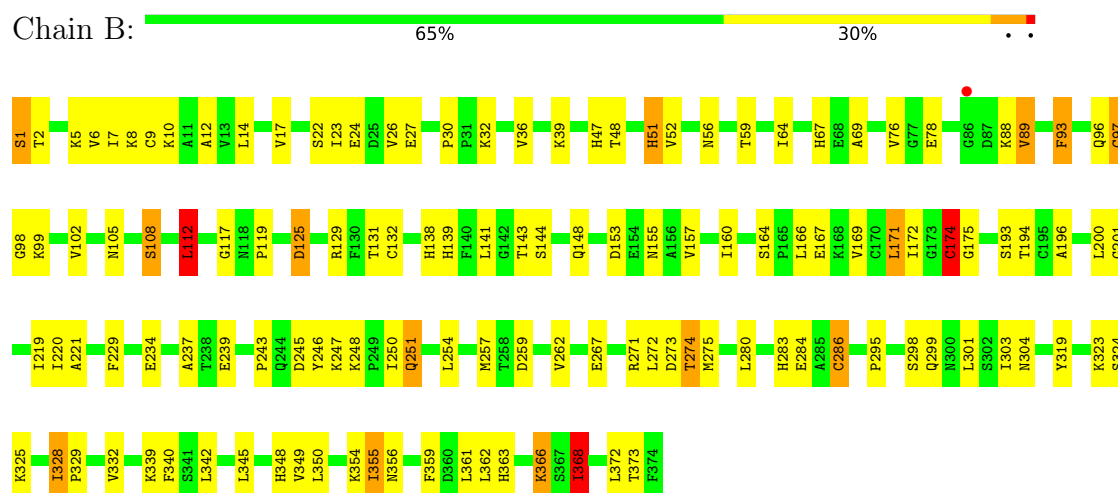
3 Residue-property plots

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 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: ALCOHOL DEHYDROGENASE



• Molecule 1: ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.36Å 44.89Å 93.85Å 92.65° 103.21° 68.77°	Depositor
Resolution (Å)	7.00 – 2.50 7.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.50) 76.1 (7.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.31Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.185 , (Not available) 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 92.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5770	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.99	9/2833 (0.3%)	1.79	50/3834 (1.3%)
1	B	0.94	11/2833 (0.4%)	1.75	56/3834 (1.5%)
All	All	0.96	20/5666 (0.4%)	1.77	106/7668 (1.4%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	HIS	CD2-NE2	-7.61	1.29	1.37
1	B	283	HIS	CD2-NE2	-7.31	1.29	1.37
1	B	67	HIS	CD2-NE2	-7.17	1.29	1.37
1	B	138	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	348	HIS	CD2-NE2	-6.32	1.30	1.37
1	B	47	HIS	CG-ND1	-6.23	1.31	1.38
1	A	363	HIS	CD2-NE2	-6.23	1.31	1.37
1	A	283	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	328	ILE	CA-CB	6.20	1.57	1.54
1	B	47	HIS	CD2-NE2	-5.96	1.31	1.37
1	B	363	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	139	HIS	CD2-NE2	-5.84	1.31	1.37
1	B	348	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	138	HIS	CD2-NE2	-5.73	1.31	1.37
1	A	51	HIS	CD2-NE2	-5.62	1.31	1.37
1	B	30	PRO	CA-C	5.52	1.54	1.51
1	A	47	HIS	CG-ND1	-5.47	1.32	1.38
1	B	51	HIS	CD2-NE2	-5.25	1.32	1.37
1	B	138	HIS	CG-ND1	-5.02	1.32	1.38
1	B	250	ILE	CA-CB	5.00	1.60	1.54

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	SER	N-CA-C	15.92	128.11	111.07
1	B	259	ASP	CA-CB-CG	12.42	125.02	112.60
1	B	125	ASP	CA-CB-CG	9.31	121.91	112.60
1	A	368	ILE	N-CA-C	-8.88	90.87	109.34
1	A	67	HIS	CB-CG-CD2	-8.69	119.90	131.20
1	B	323	LYS	N-CA-C	-8.28	95.84	108.67
1	B	340	PHE	CA-CB-CG	8.02	121.82	113.80
1	A	259	ASP	CA-CB-CG	7.74	120.34	112.60
1	B	193	SER	N-CA-C	7.60	120.13	110.33
1	B	69	ALA	N-CA-C	7.49	119.53	108.14
1	B	93	PHE	CA-CB-CG	7.40	121.20	113.80
1	B	273	ASP	CA-CB-CG	7.37	119.97	112.60
1	B	201	GLY	N-CA-C	-7.28	102.76	112.81
1	A	323	LYS	N-CA-C	-7.17	98.28	109.25
1	B	283	HIS	CB-CG-CD2	-7.16	121.89	131.20
1	A	92	LEU	N-CA-C	7.12	120.34	108.73
1	A	350	LEU	O-C-N	-7.02	117.22	121.71
1	B	324	SER	N-CA-C	6.91	122.70	111.37
1	B	67	HIS	CB-CG-CD2	-6.91	122.22	131.20
1	B	30	PRO	O-C-N	-6.82	118.17	121.31
1	A	128	ARG	CB-CG-CD	-6.80	95.65	111.30
1	A	362	LEU	N-CA-C	-6.79	103.33	111.69
1	B	356	ASN	OD1-CG-ND2	-6.70	115.90	122.60
1	A	169	VAL	N-CA-CB	-6.66	100.24	111.23
1	B	359	PHE	CA-CB-CG	-6.65	107.15	113.80
1	A	116	LEU	N-CA-C	-6.64	104.81	113.12
1	A	267	GLU	CB-CG-CD	6.45	123.56	112.60
1	B	250	ILE	N-CA-C	6.44	117.97	110.62
1	A	184	VAL	N-CA-C	6.42	119.12	111.09
1	B	59	THR	N-CA-C	-6.42	102.44	108.22
1	B	112	LEU	N-CA-C	6.42	120.69	112.34
1	B	155	ASN	OD1-CG-ND2	-6.42	116.18	122.60
1	A	299	GLN	CA-CB-CG	-6.40	101.29	114.10
1	A	343	ASP	N-CA-C	6.35	119.01	111.33
1	A	69	ALA	N-CA-C	6.30	117.80	108.60
1	A	283	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	A	340	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	125	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	229	PHE	N-CA-C	6.12	117.95	111.28
1	B	23	ILE	N-CA-C	-6.11	98.41	107.51
1	A	273	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	99	LYS	N-CA-C	6.09	120.88	113.38
1	A	8	LYS	CA-CB-CG	-6.08	101.94	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	SER	N-CA-C	6.01	116.96	109.57
1	A	146	PHE	CA-CB-CG	6.00	119.80	113.80
1	A	251	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	B	234	GLU	CA-CB-CG	5.97	126.05	114.10
1	B	349	VAL	N-CA-C	-5.85	99.79	108.45
1	B	298	SER	N-CA-C	5.84	119.98	112.86
1	A	19	LYS	CA-C-N	5.83	126.16	119.92
1	A	19	LYS	C-N-CA	5.83	126.16	119.92
1	A	209	MET	CG-SD-CE	-5.83	88.08	100.90
1	A	138	HIS	CB-CG-CD2	-5.82	123.63	131.20
1	B	56	ASN	CB-CG-ND2	5.82	125.13	116.40
1	B	108	SER	N-CA-C	5.76	119.05	110.52
1	A	132	CYS	N-CA-C	-5.72	98.57	108.69
1	B	105	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	100	CYS	CA-CB-SG	5.70	127.50	114.40
1	A	67	HIS	CB-CG-ND1	5.68	131.23	122.70
1	A	51	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	B	89	VAL	N-CA-CB	-5.66	100.87	111.62
1	A	93	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	247	LYS	N-CA-C	-5.63	106.18	113.16
1	A	123	LEU	N-CA-C	-5.61	101.70	110.17
1	B	14	LEU	N-CA-C	-5.60	99.60	108.73
1	B	52	VAL	N-CA-C	-5.58	104.92	111.00
1	A	349	VAL	N-CA-C	-5.55	100.13	108.12
1	A	251	GLN	CG-CD-NE2	5.55	124.72	116.40
1	A	41	VAL	N-CA-C	-5.53	107.42	111.90
1	A	185	ASN	CA-CB-CG	5.51	118.11	112.60
1	B	284	GLU	N-CA-C	5.43	118.70	111.75
1	A	184	VAL	CA-C-O	-5.41	114.62	120.47
1	B	362	LEU	N-CA-C	-5.41	105.29	111.14
1	B	283	HIS	CB-CG-ND1	5.41	130.81	122.70
1	A	292	VAL	N-CA-C	-5.39	107.57	112.96
1	B	245	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	161	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	304	ASN	N-CA-C	-5.38	101.77	109.24
1	B	368	ILE	N-CA-C	-5.36	98.19	109.34
1	B	8	LYS	N-CA-C	-5.35	99.73	108.76
1	A	283	HIS	CB-CG-ND1	5.34	130.71	122.70
1	B	328	ILE	CA-C-N	5.33	124.51	118.97
1	B	328	ILE	C-N-CA	5.33	124.51	118.97
1	A	348	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	A	84	LYS	N-CA-C	-5.30	102.44	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ILE	CA-CB-CG2	5.28	119.48	110.50
1	A	355	ILE	N-CA-C	5.24	116.59	110.62
1	B	39	LYS	N-CA-C	-5.21	100.24	108.73
1	B	64	ILE	N-CA-C	-5.18	100.28	107.80
1	B	30	PRO	N-CA-C	5.18	115.44	110.47
1	B	119	PRO	N-CA-C	5.17	119.00	111.03
1	A	185	ASN	CB-CA-C	-5.16	99.97	109.15
1	B	246	TYR	N-CA-C	5.15	118.46	110.17
1	B	339	LYS	CA-CB-CG	-5.13	103.84	114.10
1	A	25	ASP	N-CA-C	-5.12	100.39	108.73
1	B	56	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	322	PHE	N-CA-C	5.08	117.84	109.76
1	B	1	SER	N-CA-C	-5.08	96.78	111.00
1	A	29	ALA	CA-C-N	5.07	123.36	119.66
1	A	29	ALA	C-N-CA	5.07	123.36	119.66
1	B	295	PRO	N-CA-C	5.02	116.83	110.70
1	B	259	ASP	CA-C-N	-5.01	117.46	123.08
1	B	259	ASP	C-N-CA	-5.01	117.46	123.08
1	B	248	LYS	CA-C-N	5.01	124.92	119.76
1	B	248	LYS	C-N-CA	5.01	124.92	119.76
1	B	138	HIS	CB-CG-CD2	-5.00	124.69	131.20

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	2780	0	2850	40	0
1	B	2780	0	2850	39	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	26	7	0
3	B	44	0	26	5	0
4	A	6	0	2	4	0
4	B	6	0	2	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	59	0	0	0	0
6	B	46	0	0	2	0
All	All	5770	0	5756	85	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 8.

All (85) 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)
3:B:377:NAD:C4N	4:B:378:PYZ:N2	2.17	1.08
3:A:377:NAD:C5N	4:A:378:PYZ:N2	2.31	0.94
3:A:377:NAD:H4N	4:A:378:PYZ:N2	1.92	0.83
1:B:26:VAL:HG12	1:B:132:CYS:HB2	1.69	0.73
3:B:377:NAD:C5N	4:B:378:PYZ:N2	2.52	0.72
1:B:93:PHE:HB2	1:B:141:LEU:HD13	1.72	0.71
1:B:251:GLN:HG2	1:B:280:LEU:HB2	1.77	0.66
1:A:243:PRO:HG3	1:A:250:ILE:HG13	1.77	0.66
1:B:361:LEU:HD22	1:B:366:LYS:HD2	1.78	0.66
1:A:292:VAL:O	3:A:377:NAD:H2N	1.96	0.64
1:A:200:LEU:HD21	1:A:221:ALA:HB1	1.81	0.63
1:B:172:ILE:HG22	1:B:328:ILE:HG23	1.84	0.59
1:A:265:SER:OG	1:A:282:CYS:HB3	2.03	0.58
1:A:17:VAL:HG23	1:A:61:LEU:HD11	1.85	0.58
1:B:160:ILE:HB	1:B:332:VAL:HG11	1.88	0.56
1:B:354:LYS:HA	1:B:354:LYS:HE2	1.87	0.56
1:B:36:VAL:HG22	1:B:76:VAL:HG12	1.88	0.56
1:B:200:LEU:HD11	1:B:221:ALA:HB1	1.87	0.55
1:B:272:LEU:HD11	1:B:299:GLN:HB3	1.89	0.55
1:B:117:GLY:HA2	6:B:630:HOH:O	2.07	0.54
1:B:96:GLN:HB3	1:B:325:LYS:HB2	1.90	0.54
1:A:6:VAL:HG22	1:A:30:PRO:HD3	1.90	0.54
1:A:172:ILE:HG22	1:A:328:ILE:HG23	1.91	0.53
1:A:16:GLU:HA	1:A:61:LEU:HD13	1.90	0.53
1:A:15:TRP:HA	1:A:62:PRO:HB3	1.91	0.53
1:B:171:LEU:HB2	1:B:342:LEU:HD13	1.91	0.53
1:B:9:CYS:HB2	1:B:148:GLN:HB2	1.91	0.52
1:A:92:LEU:HD13	1:A:324:SER:HB2	1.91	0.52
3:A:377:NAD:C3N	4:A:378:PYZ:N2	2.67	0.52
1:A:364:SER:HB2	1:A:366:LYS:NZ	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:377:NAD:C4N	4:A:378:PYZ:C3	2.82	0.51
1:A:283:HIS:ND1	1:A:286:CYS:SG	2.84	0.51
1:A:306:MET:SD	1:A:309:LEU:HD23	2.51	0.50
1:A:43:VAL:HG23	1:A:69:ALA:HB2	1.93	0.50
1:A:324:SER:O	1:A:328:ILE:HG12	2.12	0.50
1:B:102:VAL:HG13	1:B:108:SER:HB2	1.94	0.50
3:B:377:NAD:C3N	4:B:378:PYZ:N2	2.73	0.49
1:A:26:VAL:HG12	1:A:132:CYS:HB2	1.93	0.49
1:A:8:LYS:HE2	1:A:25:ASP:HB3	1.94	0.49
1:B:88:LYS:HD2	1:B:166:LEU:HD21	1.94	0.49
1:A:209:MET:HE2	1:A:235:LEU:HD13	1.94	0.49
1:B:220:ILE:HD13	1:B:257:MET:HE3	1.95	0.48
1:A:89:VAL:HB	1:A:157:VAL:HG23	1.96	0.48
1:A:302:SER:HA	1:B:301:LEU:O	2.13	0.48
1:B:219:ILE:HB	1:B:237:ALA:HA	1.96	0.47
1:A:132:CYS:HB3	1:A:137:ILE:HD11	1.96	0.46
1:A:267:GLU:HG3	1:A:275:MET:HG2	1.97	0.46
1:B:6:VAL:HG13	1:B:27:GLU:HB3	1.97	0.46
1:B:196:ALA:HB2	1:B:262:VAL:HG11	1.97	0.46
1:B:139:HIS:HA	1:B:144:SER:OG	2.15	0.46
1:B:1:SER:O	1:B:5:LYS:HD3	2.16	0.45
1:A:43:VAL:HG12	1:A:372:LEU:HB2	1.99	0.45
1:A:364:SER:HB2	1:A:366:LYS:HZ3	1.81	0.45
1:B:350:LEU:O	1:B:372:LEU:HA	2.17	0.45
1:B:12:ALA:HA	1:B:22:SER:O	2.17	0.45
3:B:377:NAD:H4N	4:B:378:PYZ:N2	2.23	0.45
1:B:174:CYS:SG	3:B:377:NAD:H5N	2.56	0.45
1:A:231:LYS:HD3	1:A:231:LYS:HA	1.69	0.44
1:B:271:ARG:HB2	1:B:274:THR:OG1	2.17	0.44
1:B:153:ASP:HB3	6:B:631:HOH:O	2.16	0.44
1:A:174:CYS:SG	3:A:377:NAD:H5N	2.58	0.43
1:B:2:THR:HB	1:B:7:ILE:HD11	1.99	0.43
1:A:21:PHE:HZ	1:A:65:LEU:HD12	1.84	0.43
1:A:209:MET:HE2	1:A:235:LEU:HD22	2.01	0.43
1:B:10:LYS:HA	1:B:24:GLU:O	2.19	0.43
1:A:276:MET:HE3	1:A:303:ILE:HG22	2.00	0.42
1:B:345:LEU:O	1:B:368:ILE:HB	2.19	0.42
1:A:68:GLU:HB2	1:A:174:CYS:HB3	2.00	0.42
1:B:220:ILE:HG21	1:B:257:MET:HE1	2.00	0.42
1:A:5:LYS:HE3	1:A:5:LYS:HB3	1.86	0.42
1:B:48:THR:O	1:B:51:HIS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LYS:HD2	1:A:99:LYS:C	2.45	0.41
1:A:39:LYS:HG2	1:A:149:TYR:CE1	2.55	0.41
1:A:286:CYS:HB3	1:B:108:SER:HB3	2.01	0.41
1:A:32:LYS:O	1:A:77:GLY:HA3	2.20	0.41
1:A:10:LYS:HA	1:A:24:GLU:O	2.21	0.41
1:B:350:LEU:HB2	1:B:372:LEU:HD23	2.02	0.41
1:A:97:CYS:SG	1:A:99:LYS:HE3	2.60	0.41
1:A:128:ARG:HD3	1:A:137:ILE:O	2.21	0.41
1:B:220:ILE:HD13	1:B:257:MET:CE	2.51	0.41
1:A:187:ALA:HB2	1:A:290:VAL:HG21	2.02	0.41
1:B:32:LYS:HE3	1:B:129:ARG:CZ	2.51	0.41
1:B:267:GLU:HG3	1:B:275:MET:HA	2.03	0.41
3:A:377:NAD:H6N	3:A:377:NAD:H2D	1.90	0.40
1:A:108:SER:OG	1:B:286:CYS:HB3	2.21	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	372/374 (100%)	341 (92%)	31 (8%)	0	100	100
1	B	372/374 (100%)	338 (91%)	25 (7%)	9 (2%)	4	8
All	All	744/748 (100%)	679 (91%)	56 (8%)	9 (1%)	10	20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	CYS
1	B	97	CYS
1	B	125	ASP
1	B	286	CYS

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Mol	Chain	Res	Type
1	B	98	GLY
1	B	112	LEU
1	B	355	ILE
1	B	175	GLY
1	B	368	ILE

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	305/305 (100%)	285 (93%)	20 (7%)	15	32
1	B	305/305 (100%)	281 (92%)	24 (8%)	11	24
All	All	610/610 (100%)	566 (93%)	44 (7%)	13	28

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	THR
1	A	25	ASP
1	A	40	MET
1	A	72	ILE
1	A	131	THR
1	A	157	VAL
1	A	167	GLU
1	A	169	VAL
1	A	243	PRO
1	A	248	LYS
1	A	250	ILE
1	A	251	GLN
1	A	255	LYS
1	A	265	SER
1	A	268	VAL
1	A	274	THR
1	A	319	TYR

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Mol	Chain	Res	Type
1	A	325	LYS
1	A	373	THR
1	B	17	VAL
1	B	78	GLU
1	B	89	VAL
1	B	97	CYS
1	B	112	LEU
1	B	131	THR
1	B	143	THR
1	B	157	VAL
1	B	167	GLU
1	B	169	VAL
1	B	171	LEU
1	B	174	CYS
1	B	194	THR
1	B	239	GLU
1	B	243	PRO
1	B	251	GLN
1	B	254	LEU
1	B	274	THR
1	B	303	ILE
1	B	319	TYR
1	B	329	PRO
1	B	355	ILE
1	B	366	LYS
1	B	373	THR

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	56	ASN
1	A	118	ASN
1	A	251	GLN
1	A	300	ASN
1	A	348	HIS
1	B	251	GLN

5.3.3 RNA ⓘ

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 9 ligands modelled in this entry, 5 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$
4	PYZ	B	378	2	6,6,6	1.15	0	7,7,7	2.32	2 (28%)
3	NAD	A	377	4	46,48,48	2.24	8 (17%)	64,73,73	1.53	9 (14%)
3	NAD	B	377	-	46,48,48	2.18	9 (19%)	64,73,73	1.58	10 (15%)
4	PYZ	A	378	3,2	6,6,6	0.84	0	7,7,7	2.69	3 (42%)

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	PYZ	B	378	2	-	-	0/1/1/1
3	NAD	A	377	4	-	12/30/62/62	0/5/5/5
3	NAD	B	377	-	-	9/30/62/62	0/5/5/5
4	PYZ	A	378	3,2	-	-	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	377	NAD	C3N-C7N	-11.20	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	377	NAD	C3N-C7N	-10.49	1.35	1.50
3	B	377	NAD	C5A-N7A	-4.82	1.30	1.39
3	A	377	NAD	C5A-N7A	-4.64	1.30	1.39
3	A	377	NAD	C4N-C3N	-4.28	1.32	1.39
3	B	377	NAD	C4A-N9A	-3.97	1.29	1.37
3	B	377	NAD	C4N-C3N	-3.61	1.33	1.39
3	A	377	NAD	C4A-N9A	-3.52	1.30	1.37
3	B	377	NAD	C5N-C4N	-3.28	1.33	1.38
3	A	377	NAD	C5N-C4N	-3.26	1.33	1.38
3	A	377	NAD	C2N-C3N	-3.06	1.34	1.39
3	A	377	NAD	C8A-N9A	-2.85	1.32	1.37
3	B	377	NAD	C2N-C3N	-2.64	1.34	1.39
3	B	377	NAD	C8A-N9A	-2.60	1.33	1.37
3	A	377	NAD	C2N-N1N	-2.41	1.32	1.35
3	B	377	NAD	C2N-N1N	-2.32	1.32	1.35
3	B	377	NAD	O4D-C1D	2.12	1.43	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	378	PYZ	C4-C3-N2	-5.53	107.52	111.81
4	B	378	PYZ	C4-C3-N2	-4.74	108.14	111.81
3	B	377	NAD	O2N-PN-O3	4.60	119.71	107.27
3	B	377	NAD	O7N-C7N-N7N	-4.46	116.18	122.62
3	A	377	NAD	O2N-PN-O3	4.24	118.73	107.27
3	A	377	NAD	C3N-C7N-N7N	3.96	122.61	117.74
3	A	377	NAD	N3A-C2A-N1A	-3.71	122.97	128.58
3	B	377	NAD	N3A-C2A-N1A	-3.45	123.36	128.58
3	B	377	NAD	C5A-C4A-N9A	3.25	109.35	105.81
3	B	377	NAD	O2A-PA-O3	3.15	115.78	107.27
3	B	377	NAD	C5A-C4A-N3A	-3.14	122.39	126.72
3	A	377	NAD	C5A-C4A-N3A	-3.01	122.57	126.72
4	B	378	PYZ	C5-C4-C3	2.99	107.95	105.11
4	A	378	PYZ	C5-C4-C3	2.97	107.93	105.11
3	A	377	NAD	C6N-N1N-C2N	-2.67	119.61	121.88
4	A	378	PYZ	C3-C4-I4	-2.54	124.36	127.92
3	B	377	NAD	C6N-N1N-C2N	-2.54	119.72	121.88
3	A	377	NAD	C6A-C5A-C4A	2.53	120.64	117.18
3	A	377	NAD	O7N-C7N-N7N	-2.51	118.99	122.62
3	B	377	NAD	C6A-C5A-C4A	2.50	120.59	117.18
3	A	377	NAD	C5A-C4A-N9A	2.46	108.49	105.81
3	B	377	NAD	O2D-C2D-C3D	-2.43	104.02	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	377	NAD	O3B-C3B-C2B	-2.41	104.08	111.82
3	B	377	NAD	O3D-C3D-C2D	-2.23	104.67	111.82

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	377	NAD	C5B-O5B-PA-O1A
3	A	377	NAD	C5B-O5B-PA-O3
3	A	377	NAD	PN-O3-PA-O5B
3	A	377	NAD	O4D-C1D-N1N-C2N
3	A	377	NAD	O4D-C1D-N1N-C6N
3	A	377	NAD	C2D-C1D-N1N-C2N
3	A	377	NAD	C2D-C1D-N1N-C6N
3	B	377	NAD	C5D-O5D-PN-O2N
3	B	377	NAD	O4D-C1D-N1N-C2N
3	B	377	NAD	O4D-C1D-N1N-C6N
3	B	377	NAD	C2D-C1D-N1N-C2N
3	B	377	NAD	C2D-C1D-N1N-C6N
3	A	377	NAD	O4B-C4B-C5B-O5B
3	A	377	NAD	C5B-O5B-PA-O2A
3	B	377	NAD	C5B-O5B-PA-O2A
3	A	377	NAD	PA-O3-PN-O2N
3	A	377	NAD	C3B-C4B-C5B-O5B
3	B	377	NAD	PA-O3-PN-O2N
3	B	377	NAD	O4B-C4B-C5B-O5B
3	B	377	NAD	PA-O3-PN-O1N
3	A	377	NAD	PA-O3-PN-O1N

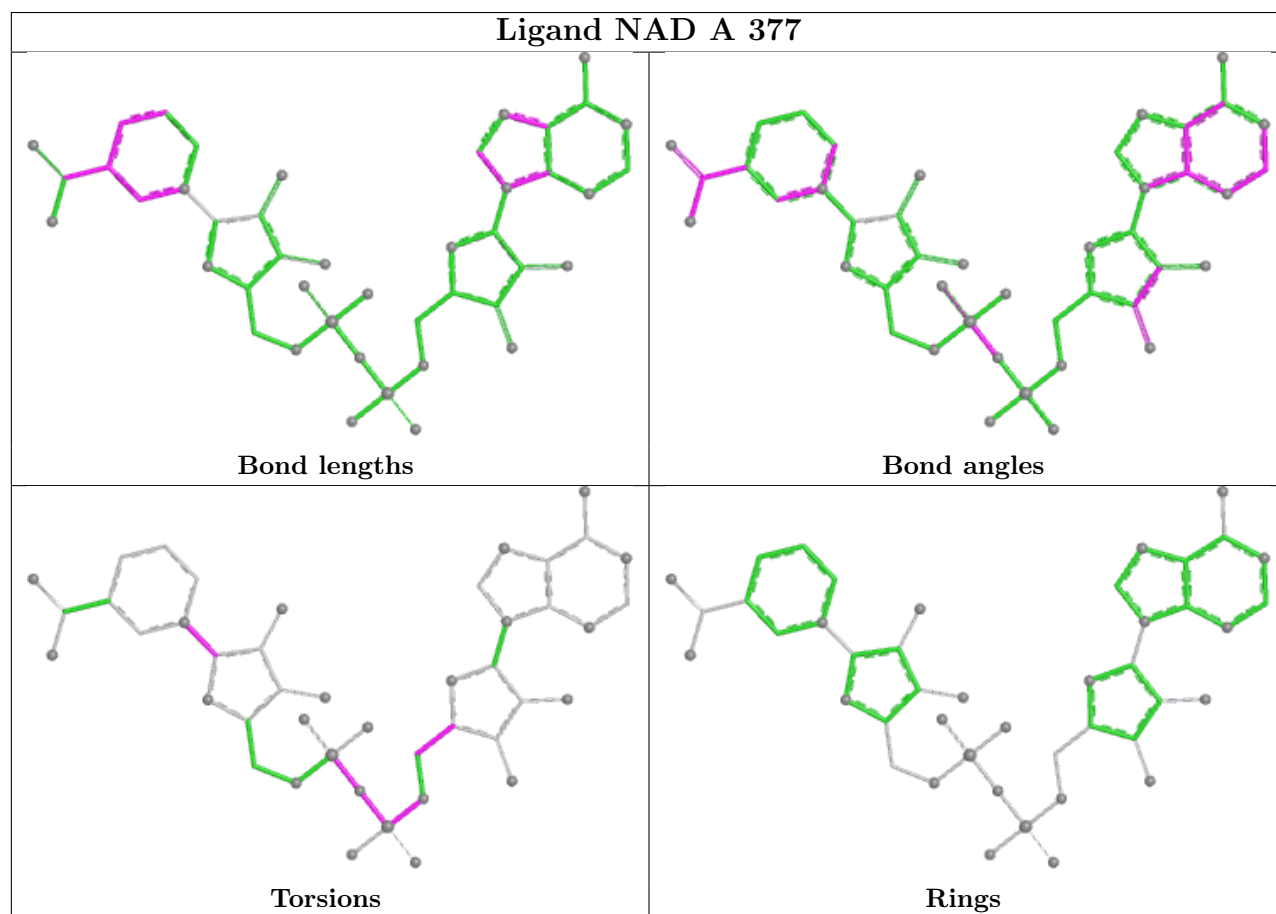
There are no ring outliers.

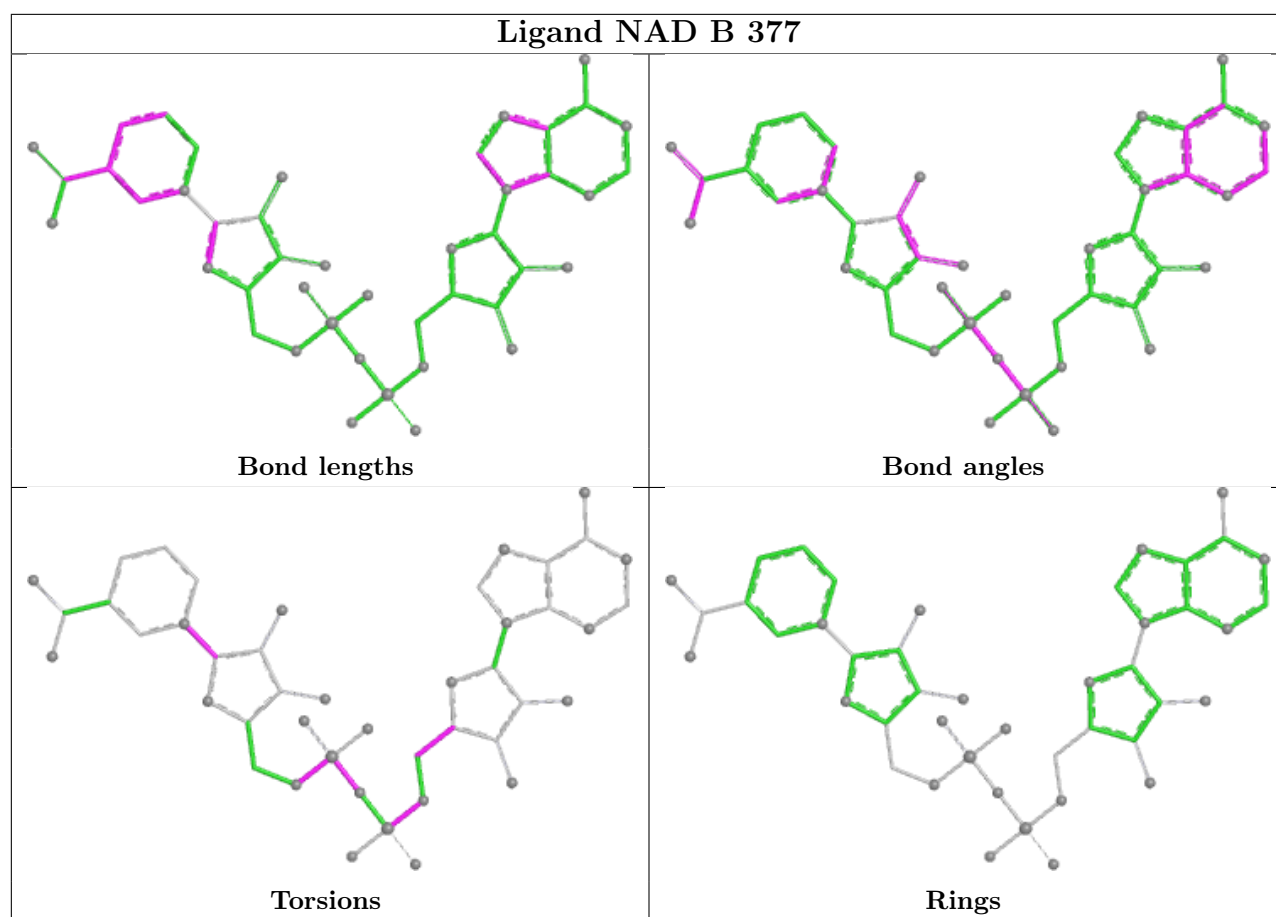
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	378	PYZ	4	0
3	A	377	NAD	7	0
3	B	377	NAD	5	0
4	A	378	PYZ	4	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	374/374 (100%)	-0.72	0 100 100	7, 23, 34, 43	0
1	B	374/374 (100%)	-0.57	1 (0%) 90 87	11, 29, 41, 44	0
All	All	748/748 (100%)	-0.65	1 (0%) 92 90	7, 26, 39, 44	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	GLY	2.1

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.

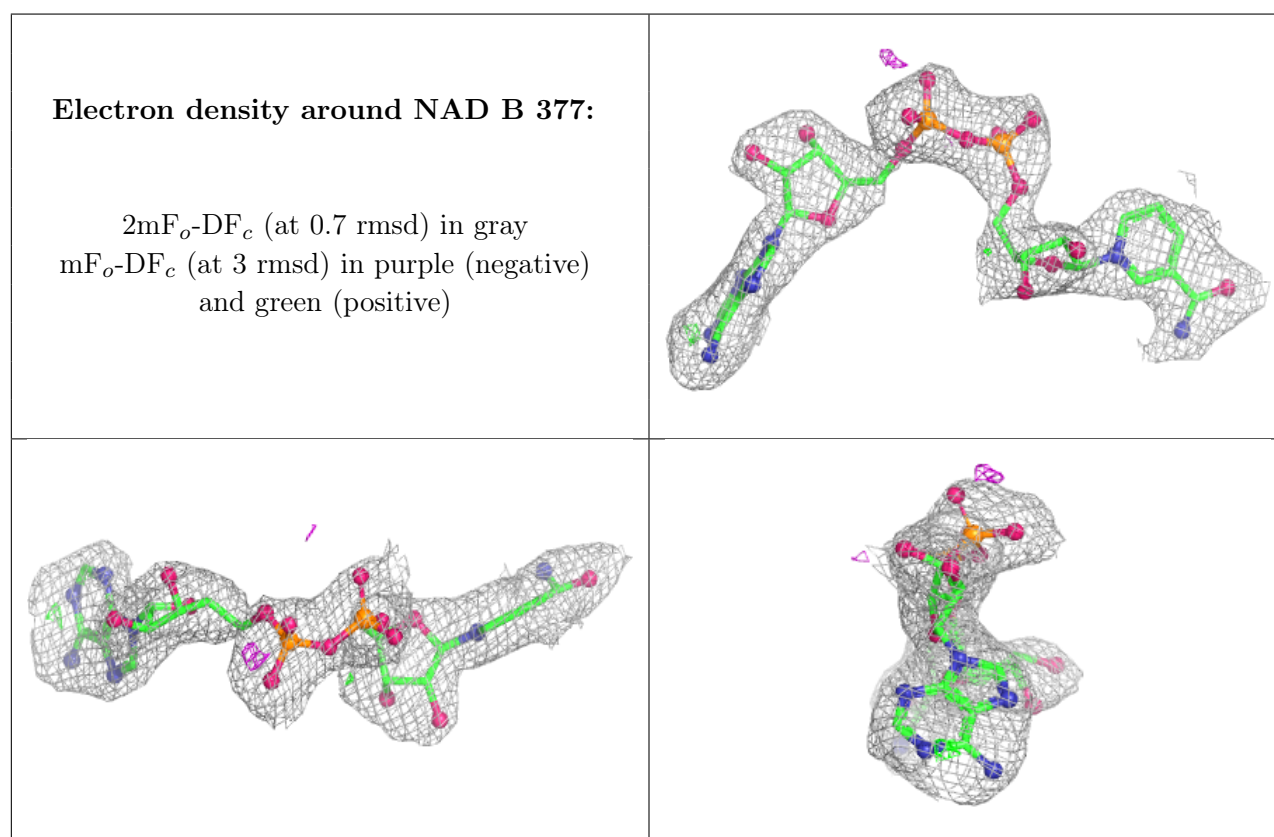
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CL	B	601	1/1	0.92	0.11	39,39,39,39	1
3	NAD	B	377	44/44	0.96	0.06	16,27,33,36	0
3	NAD	A	377	44/44	0.97	0.05	9,17,23,24	0
2	ZN	B	375	1/1	0.97	0.02	28,28,28,28	0

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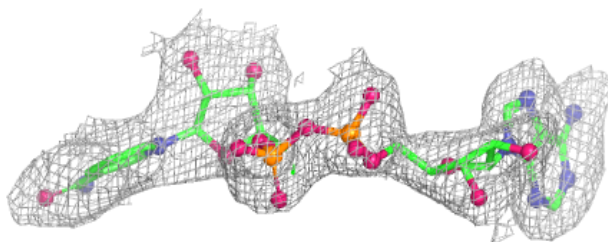
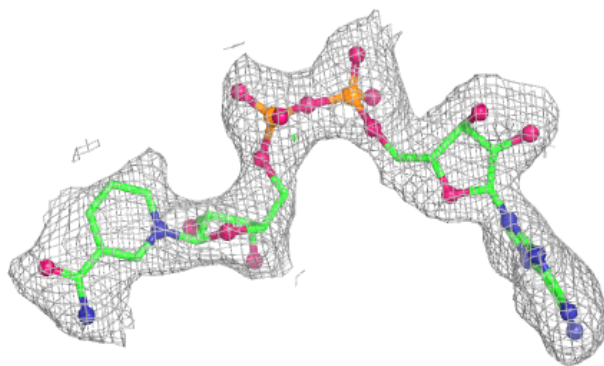
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	376	1/1	0.97	0.02	34,34,34,34	0
2	ZN	A	376	1/1	0.98	0.02	21,21,21,21	0
2	ZN	A	375	1/1	0.98	0.02	28,28,28,28	0
4	PYZ	B	378	6/6	1.00	0.04	17,23,23,33	0
4	PYZ	A	378	6/6	1.00	0.05	29,34,36,37	0

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 A 377:

$2mF_o-DF_c$ (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.