WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 05:03 PM EST

PDB ID	:	1HDX
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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36
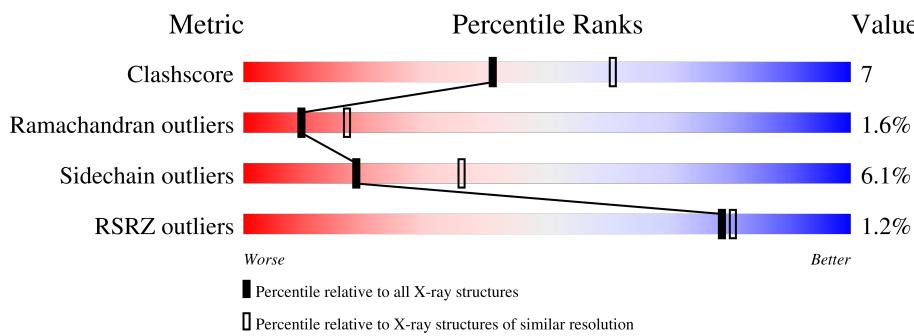
1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		1.6%
Sidechain outliers		6.1%
RSRZ outliers		1.2%

Worse   *Better*

▌Percentile relative to all X-ray structures

❙Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	.% 79% 19% •
1	B	374	.% 75% 22% ••

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	CXL	B	378	-	-	X	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 5779 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.
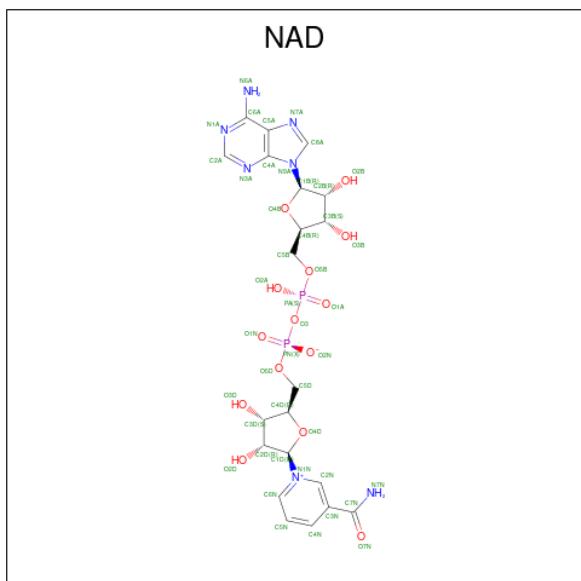
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2781	1770	473	516	22			
1	B	374	Total	C	N	O	S	0	0	0
			2781	1770	473	516	22			

- Molecule 2 is ZINC ION (three-letter code: 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 (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).
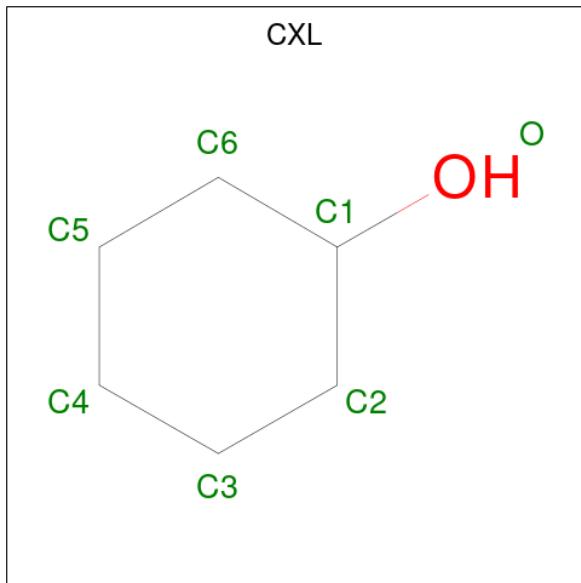
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is CYCLOHEXANOL (three-letter code: CXL) (formula: $C_6H_{12}O$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	6	1		
4	B	1	Total	C	O	0	0
			7	6	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
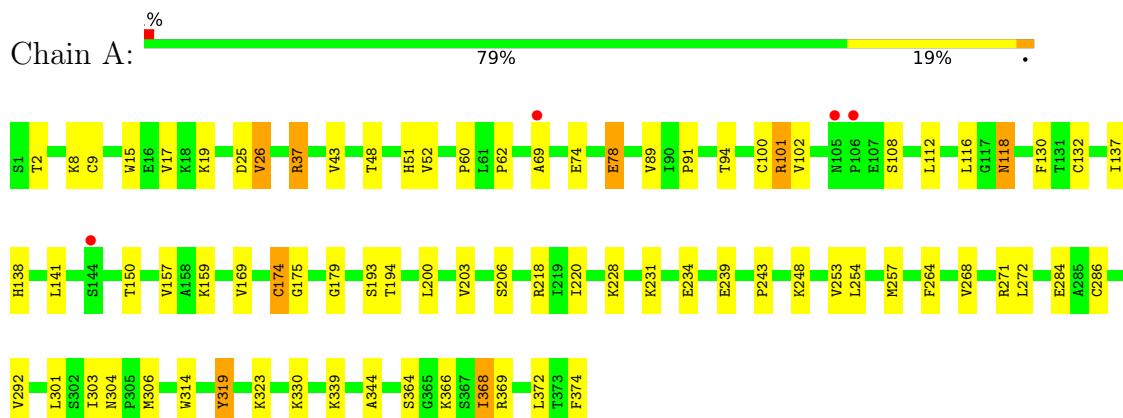
- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	63	Total	O	0	0
			63	63		
6	B	47	Total	O	0	0
			47	47		
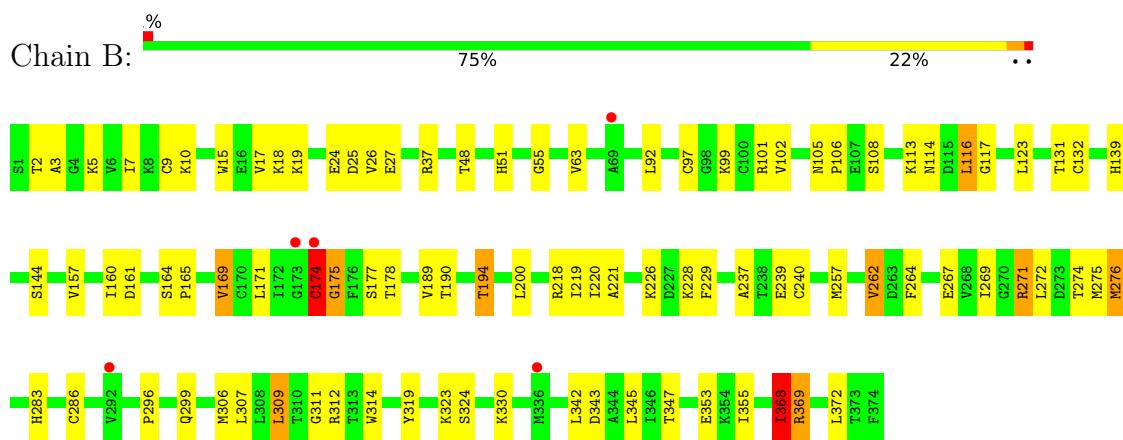
3 Residue-property plots ⓘ

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	54.58Å 44.94Å 94.30Å 92.29° 103.37° 68.97°	Depositor
Resolution (Å)	7.00 – 2.50 28.15 – 2.37	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.50) 65.7 (28.15-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.21 (at 2.36Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available) 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 81.6	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5779	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, ZN, NAD, CXL

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	0.77	1/2833 (0.0%)	1.40	18/3833 (0.5%)
1	B	0.73	1/2833 (0.0%)	1.36	13/3833 (0.3%)
All	All	0.75	2/5666 (0.0%)	1.38	31/7666 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	VAL	CA-CB	5.08	1.65	1.54
1	B	63	VAL	CA-CB	5.07	1.65	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	A	37	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	314	TRP	CD1-CG-CD2	8.61	113.18	106.30
1	A	37	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	A	319	TYR	CB-CG-CD2	-7.82	116.31	121.00
1	A	314	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	B	368	ILE	N-CA-C	-7.56	90.58	111.00
1	B	15	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	B	314	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	B	15	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	B	314	TRP	CD1-CG-CD2	6.88	111.81	106.30
1	A	15	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	A	15	TRP	CE2-CD2-CG	-6.79	101.87	107.30
1	B	169	VAL	CG1-CB-CG2	-6.52	100.47	110.90
1	A	257	MET	CA-CB-CG	6.24	123.91	113.30
1	A	101	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	368	ILE	N-CA-C	-5.96	94.91	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	37	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	323	LYS	N-CA-C	-5.83	95.27	111.00
1	B	271	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	101	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	369	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	271	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	218	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	52	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	B	314	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	B	194	THR	CA-CB-CG2	5.32	119.84	112.40
1	B	101	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	319	TYR	CB-CG-CD1	5.09	124.06	121.00
1	A	314	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	B	323	LYS	N-CA-C	-5.04	97.38	111.00

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	2781	0	2856	35	0
1	B	2781	0	2856	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	26	3	0
3	B	44	0	26	1	0
4	A	7	0	12	0	0
4	B	7	0	12	7	0
5	B	1	0	0	0	0
6	A	63	0	0	1	0
6	B	47	0	0	2	0
All	All	5779	0	5788	81	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 7.

All (81) 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:116:LEU:HB3	4:B:378:CXL:H41	1.42	0.99
1:B:116:LEU:CD2	4:B:378:CXL:H62	1.93	0.98
1:B:116:LEU:HD22	4:B:378:CXL:H62	1.51	0.92
1:A:116:LEU:HD23	1:A:141:LEU:HD22	1.53	0.88
1:A:8:LYS:HE2	1:A:25:ASP:HB3	1.60	0.82
1:B:272:LEU:HD11	1:B:299:GLN:HB3	1.61	0.81
1:B:116:LEU:HD23	4:B:378:CXL:H62	1.66	0.77
1:B:178:THR:HG21	3:B:377:NAD:C4N	2.18	0.73
1:A:231:LYS:HD2	1:A:344:ALA:HB1	1.71	0.72
1:B:26:VAL:HG12	1:B:132:CYS:HB2	1.72	0.72
1:B:194:THR:HG22	1:B:262:VAL:HG12	1.72	0.71
1:B:116:LEU:CB	4:B:378:CXL:H41	2.23	0.66
1:B:116:LEU:HB3	4:B:378:CXL:C4	2.25	0.61
1:A:175:GLY:HA2	1:A:203:VAL:HG22	1.85	0.58
1:A:108:SER:OG	1:B:286:CYS:HB3	2.04	0.58
1:A:26:VAL:HG12	1:A:132:CYS:HB2	1.85	0.58
1:A:89:VAL:HG12	1:A:159:LYS:HA	1.86	0.57
1:A:200:LEU:O	1:A:228:LYS:HE2	2.07	0.55
1:A:193:SER:HG	1:A:264:PHE:HE2	1.54	0.55
1:B:102:VAL:HG13	1:B:108:SER:HB2	1.89	0.55
1:B:92:LEU:HD13	1:B:324:SER:HB2	1.90	0.54
1:B:200:LEU:O	1:B:228:LYS:HD2	2.08	0.54
1:B:307:LEU:O	1:B:312:ARG:HD2	2.08	0.53
1:B:272:LEU:HD23	1:B:275:MET:CE	2.40	0.52
1:A:69:ALA:O	1:A:91:PRO:HD2	2.10	0.52
1:B:369:ARG:HA	6:B:605:HOH:O	2.11	0.51
1:B:296:PRO:HB2	1:B:299:GLN:NE2	2.27	0.50
1:B:7:ILE:O	1:B:27:GLU:HA	2.13	0.49
1:A:272:LEU:HD22	1:A:301:LEU:HG	1.93	0.48
1:B:345:LEU:O	1:B:368:ILE:HB	2.14	0.48
1:B:17:VAL:HG12	1:B:18:LYS:HG3	1.96	0.48
1:A:268:VAL:HG12	3:A:377:NAD:H52N	1.96	0.47
1:B:174:CYS:SG	1:B:175:GLY:N	2.87	0.47
1:B:10:LYS:HA	1:B:24:GLU:O	2.15	0.47
1:A:100:CYS:HB2	1:A:112:LEU:HD12	1.97	0.47
1:A:94:THR:OG1	1:A:116:LEU:HD11	2.14	0.47
1:B:19:LYS:HA	1:B:19:LYS:HD3	1.68	0.47
1:A:248:LYS:HG3	1:A:253:VAL:HG23	1.96	0.46
1:B:171:LEU:HD12	1:B:342:LEU:HB3	1.97	0.46
1:A:130:PHE:HB2	1:A:137:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:PHE:CD1	1:B:240:CYS:HB3	2.51	0.45
1:A:364:SER:HB2	1:A:366:LYS:HD3	1.97	0.45
1:B:200:LEU:HD11	1:B:221:ALA:HB1	1.97	0.45
1:A:43:VAL:HG13	1:A:374:PHE:HE1	1.80	0.45
1:B:226:LYS:HG2	1:B:229:PHE:CE2	2.51	0.45
1:B:55:GLY:HA2	6:B:604:HOH:O	2.16	0.45
1:B:5:LYS:HD3	1:B:5:LYS:HA	1.80	0.45
1:A:48:THR:O	1:A:51:HIS:HB2	2.17	0.45
1:A:102:VAL:HG13	1:A:108:SER:HB3	1.99	0.45
1:B:306:MET:SD	1:B:309:LEU:HD22	2.57	0.45
1:B:9:CYS:O	1:B:25:ASP:HA	2.16	0.45
1:A:9:CYS:O	1:A:25:ASP:HA	2.16	0.44
1:A:292:VAL:O	3:A:377:NAD:H2N	2.17	0.44
1:A:62:PRO:O	1:A:138:HIS:HB2	2.18	0.43
1:B:116:LEU:HD22	4:B:378:CXL:C6	2.37	0.43
1:B:218:ARG:HH22	1:B:257:MET:HG2	1.84	0.43
1:A:179:GLY:HA3	1:A:206:SER:HB2	2.01	0.43
1:B:347:THR:HG21	1:B:368:ILE:HG12	2.01	0.43
1:B:105:ASN:HA	1:B:106:PRO:HD3	1.89	0.43
1:B:139:HIS:HA	1:B:144:SER:OG	2.18	0.43
1:A:60:PRO:HD3	6:A:404:HOH:O	2.18	0.43
1:A:118:ASN:HD22	1:A:118:ASN:HA	1.71	0.42
1:A:78:GLU:H	1:A:78:GLU:HG3	1.70	0.42
1:B:220:ILE:HG12	1:B:239:GLU:HG3	2.02	0.42
1:B:219:ILE:HB	1:B:237:ALA:HA	2.01	0.42
1:A:304:ASN:OD1	1:A:306:MET:HB2	2.20	0.41
1:B:161:ASP:HB3	1:B:164:SER:OG	2.20	0.41
1:A:174:CYS:SG	3:A:377:NAD:H5N	2.60	0.41
1:B:355:ILE:HG13	1:B:372:LEU:HD11	2.02	0.41
1:A:19:LYS:HA	1:A:19:LYS:HD3	1.88	0.41
1:A:220:ILE:HG21	1:A:254:LEU:HD21	2.03	0.41
1:B:276:MET:HA	1:B:276:MET:CE	2.50	0.41
1:B:48:THR:HA	1:B:51:HIS:CD2	2.56	0.41
1:B:123:LEU:HD23	1:B:123:LEU:HA	1.93	0.41
1:A:286:CYS:HB3	1:B:108:SER:HB3	2.03	0.40
1:B:114:ASN:HB2	1:B:116:LEU:HD12	2.02	0.40
1:B:189:VAL:HA	1:B:264:PHE:CE2	2.56	0.40
1:A:43:VAL:HG22	1:A:372:LEU:HB2	2.04	0.40
1:A:37:ARG:HD2	1:A:74:GLU:OE1	2.22	0.40
1:A:43:VAL:HG12	1:A:69:ALA:HB2	2.03	0.40
1:B:164:SER:HA	1:B:165:PRO:HD2	1.89	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	372/374 (100%)	346 (93%)	24 (6%)	2 (0%)	29	48
1	B	372/374 (100%)	338 (91%)	24 (6%)	10 (3%)	5	7
All	All	744/748 (100%)	684 (92%)	48 (6%)	12 (2%)	9	17

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	CYS
1	A	284	GLU
1	B	3	ALA
1	B	97	CYS
1	B	117	GLY
1	B	169	VAL
1	B	175	GLY
1	B	311	GLY
1	B	368	ILE
1	A	368	ILE
1	B	269	ILE
1	B	160	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%)	288 (94%)	17 (6%)	21	40
1	B	305/305 (100%)	285 (93%)	20 (7%)	16	32
All	All	610/610 (100%)	573 (94%)	37 (6%)	18	36

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	VAL
1	A	78	GLU
1	A	101	ARG
1	A	118	ASN
1	A	150	THR
1	A	157	VAL
1	A	169	VAL
1	A	174	CYS
1	A	194	THR
1	A	234	GLU
1	A	239	GLU
1	A	243	PRO
1	A	303	ILE
1	A	319	TYR
1	A	330	LYS
1	A	339	LYS
1	B	2	THR
1	B	99	LYS
1	B	113	LYS
1	B	116	LEU
1	B	131	THR
1	B	157	VAL
1	B	174	CYS
1	B	177	SER
1	B	190	THR
1	B	262	VAL
1	B	267	GLU
1	B	271	ARG
1	B	274	THR
1	B	276	MET
1	B	283	HIS
1	B	309	LEU
1	B	319	TYR
1	B	330	LYS

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Mol	Chain	Res	Type
1	B	343	ASP
1	B	353	GLU

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	118	ASN
1	A	138	HIS
1	A	283	HIS
1	A	348	HIS
1	B	244	GLN
1	B	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
3	NAD	A	377	-	42,48,48	2.11	7 (16%)	50,73,73	1.53	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	CXL	B	378	-	7,7,7	1.32	1 (14%)	8,8,8	0.63	0
4	CXL	A	378	-	7,7,7	1.33	2 (28%)	8,8,8	0.99	1 (12%)
3	NAD	B	377	-	42,48,48	2.01	6 (14%)	50,73,73	1.73	12 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	377	-	-	13/26/62/62	0/5/5/5
4	CXL	B	378	-	-	-	0/1/1/1
4	CXL	A	378	-	-	-	0/1/1/1
3	NAD	B	377	-	-	14/26/62/62	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	377	NAD	C3N-C7N	-10.99	1.34	1.50
3	B	377	NAD	C3N-C7N	-10.48	1.34	1.50
3	A	377	NAD	C2N-C3N	-3.43	1.33	1.39
3	B	377	NAD	C2N-C3N	-2.95	1.34	1.39
3	B	377	NAD	C4N-C3N	-2.92	1.34	1.39
3	A	377	NAD	C4N-C3N	-2.62	1.34	1.39
4	B	378	CXL	C6-C1	2.62	1.57	1.51
3	B	377	NAD	C5N-C4N	-2.60	1.33	1.38
3	A	377	NAD	C4A-N3A	-2.58	1.32	1.35
3	A	377	NAD	C5N-C4N	-2.55	1.33	1.38
3	B	377	NAD	C2N-N1N	-2.54	1.31	1.35
4	A	378	CXL	C6-C1	2.49	1.57	1.51
3	B	377	NAD	C5A-N7A	-2.38	1.31	1.39
3	A	377	NAD	C3D-C4D	-2.10	1.47	1.53
3	A	377	NAD	C5A-N7A	-2.05	1.32	1.39
4	A	378	CXL	C2-C1	2.01	1.56	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	377	NAD	O4B-C1B-C2B	-4.56	100.26	106.93
3	B	377	NAD	O7N-C7N-N7N	-4.39	116.34	122.58
3	A	377	NAD	C3N-C7N-N7N	3.99	122.54	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	377	NAD	N3A-C2A-N1A	-3.99	122.45	128.68
3	B	377	NAD	C3N-C7N-N7N	3.42	121.85	117.75
3	A	377	NAD	O7N-C7N-N7N	-3.31	117.88	122.58
3	B	377	NAD	N3A-C2A-N1A	-3.31	123.51	128.68
3	A	377	NAD	O2D-C2D-C3D	-3.02	102.06	111.82
3	B	377	NAD	O4D-C1D-C2D	-2.93	102.64	106.93
3	B	377	NAD	O2D-C2D-C3D	-2.84	102.65	111.82
3	B	377	NAD	C3B-C2B-C1B	2.77	105.16	100.98
3	B	377	NAD	C6N-N1N-C2N	-2.74	119.47	121.97
3	A	377	NAD	PN-O3-PA	2.72	142.17	132.83
3	A	377	NAD	C5A-C6A-N6A	2.46	124.09	120.35
3	B	377	NAD	O3D-C3D-C4D	-2.45	103.95	111.05
3	B	377	NAD	C5D-C4D-C3D	-2.37	106.30	115.18
3	B	377	NAD	O3B-C3B-C4B	-2.29	104.42	111.05
3	A	377	NAD	O3D-C3D-C4D	-2.26	104.51	111.05
3	A	377	NAD	C2N-C3N-C4N	2.19	120.74	118.26
4	A	378	CXL	C5-C4-C3	2.09	117.60	111.18
3	A	377	NAD	C2A-N1A-C6A	2.09	122.32	118.75
3	B	377	NAD	C2N-C3N-C4N	2.00	120.53	118.26

There are no chirality outliers.

All (27) 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-O2A
3	A	377	NAD	C5B-O5B-PA-O3
3	A	377	NAD	PN-O3-PA-O5B
3	A	377	NAD	PA-O3-PN-O5D
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	C5B-O5B-PA-O1A
3	B	377	NAD	C5D-O5D-PN-O3
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	C3B-C4B-C5B-O5B

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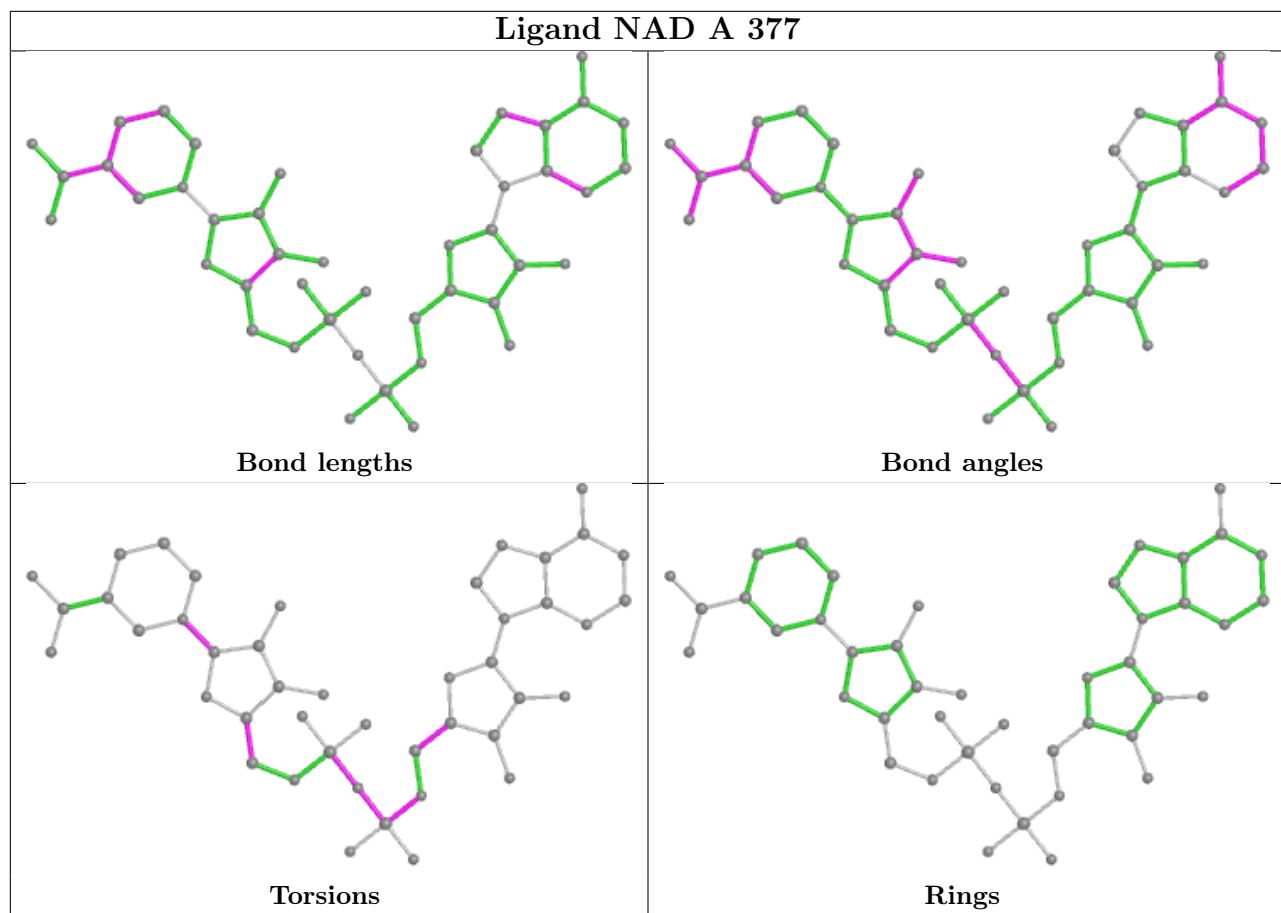
Mol	Chain	Res	Type	Atoms
3	B	377	NAD	O4D-C4D-C5D-O5D
3	B	377	NAD	C3D-C4D-C5D-O5D
3	B	377	NAD	C5B-O5B-PA-O3
3	A	377	NAD	O4D-C4D-C5D-O5D
3	B	377	NAD	C5B-O5B-PA-O2A
3	B	377	NAD	C5D-O5D-PN-O1N
3	B	377	NAD	PA-O3-PN-O2N
3	B	377	NAD	O4B-C4B-C5B-O5B
3	A	377	NAD	PN-O3-PA-O1A
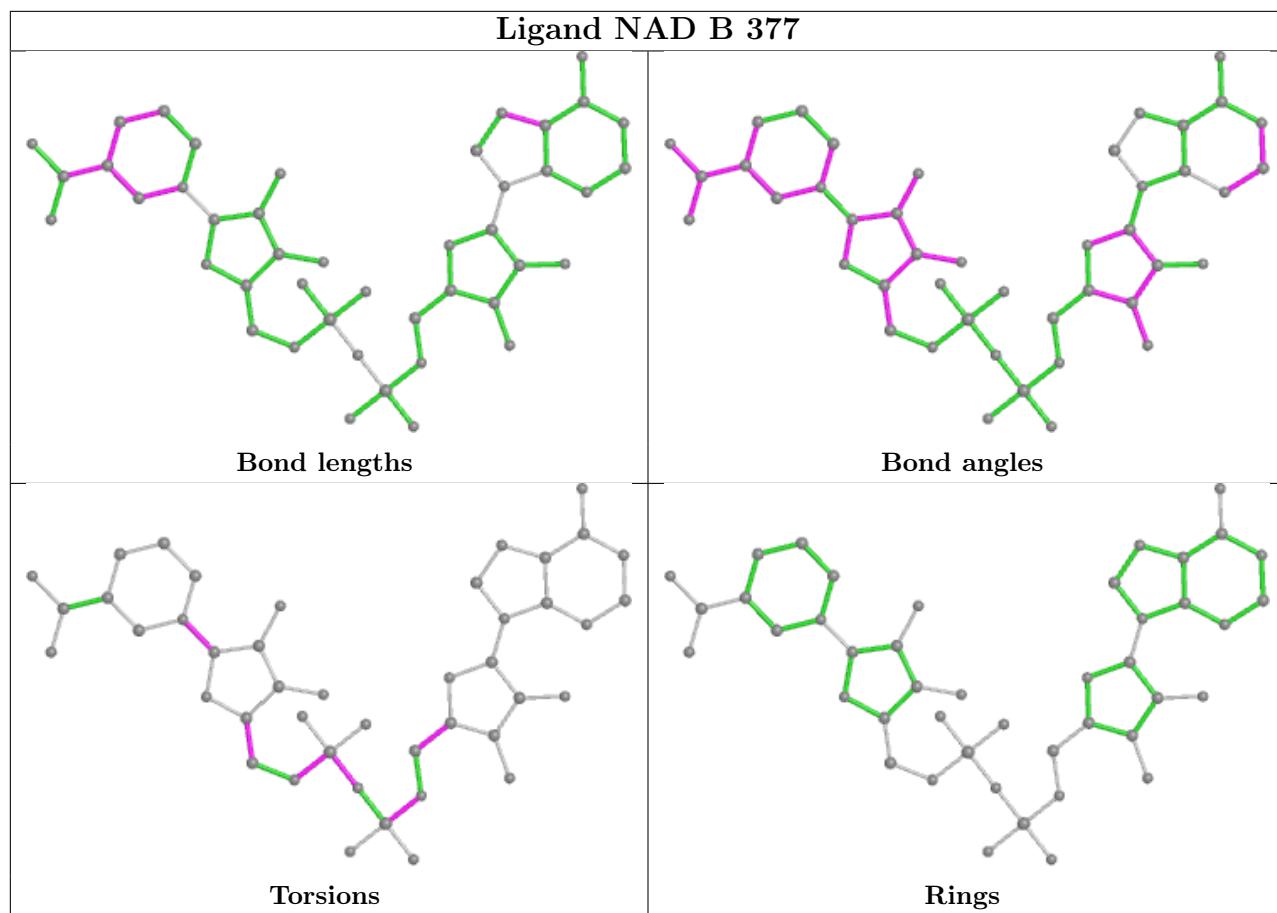
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	377	NAD	3	0
4	B	378	CXL	7	0
3	B	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 then 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.

Ligand NAD A 377

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 377

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	374/374 (100%)	-0.64	4 (1%)	80	82	8, 25, 43, 58	0
1	B	374/374 (100%)	-0.46	5 (1%)	77	79	9, 32, 54, 69	0
All	All	748/748 (100%)	-0.55	9 (1%)	79	80	8, 28, 49, 69	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	69	ALA	3.2
1	B	336	MET	2.5
1	B	174	CYS	2.5
1	A	69	ALA	2.2
1	B	173	GLY	2.1
1	A	106	PRO	2.1
1	A	144	SER	2.1
1	A	105	ASN	2.1
1	B	292	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.
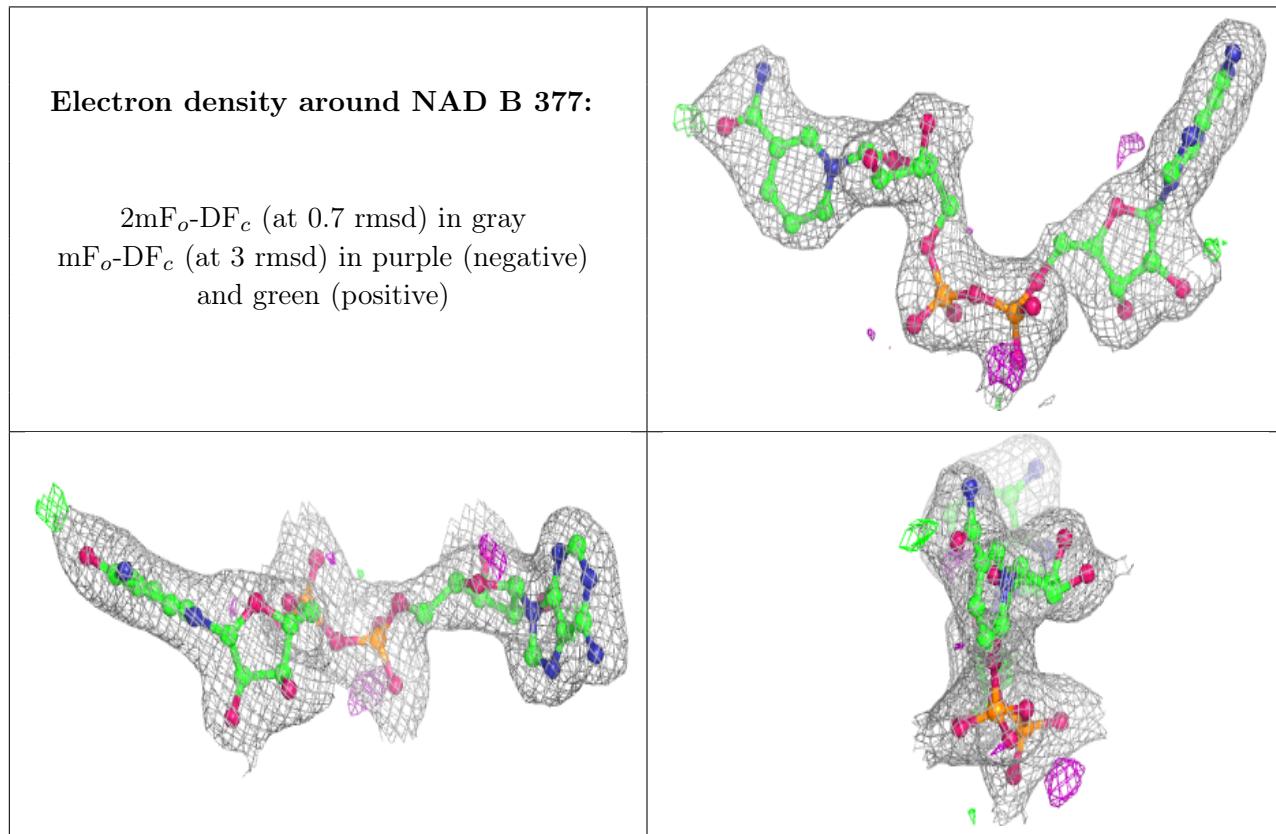
6.4 Ligands ⓘ
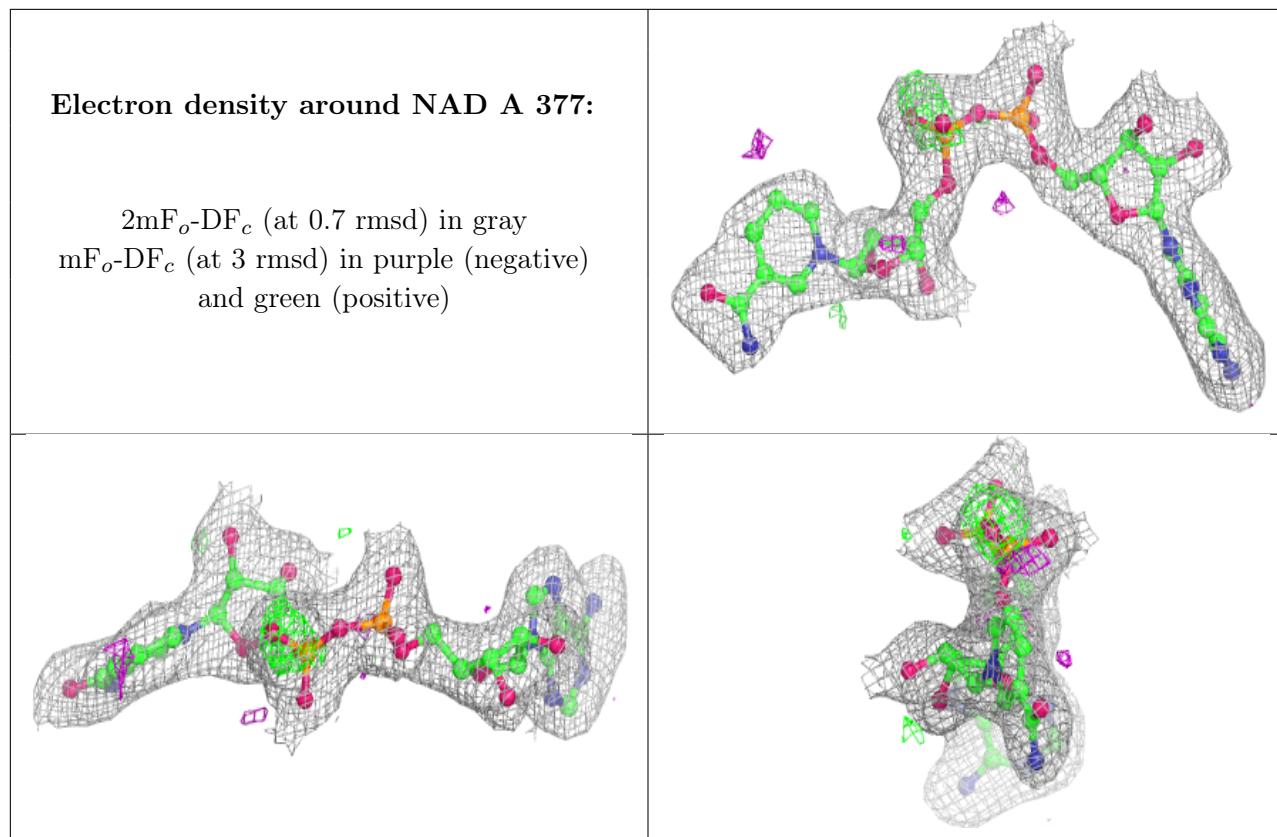
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	CXL	B	378	7/7	0.78	0.98	48,49,50,50	0
4	CXL	A	378	7/7	0.86	0.43	32,33,41,42	0
2	ZN	B	376	1/1	0.94	0.07	38,38,38,38	1
3	NAD	B	377	44/44	0.97	0.10	14,21,30,40	0
2	ZN	A	376	1/1	0.97	0.11	37,37,37,37	1
3	NAD	A	377	44/44	0.97	0.13	2,17,26,31	0
5	CL	B	601	1/1	0.98	0.26	47,47,47,47	1
2	ZN	A	375	1/1	0.99	0.02	29,29,29,29	0
2	ZN	B	375	1/1	1.00	0.03	31,31,31,31	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 B 377:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NAD A 377:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.