



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:14 PM UTC

PDB ID : 1HDZ / pdb_00001hdz
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

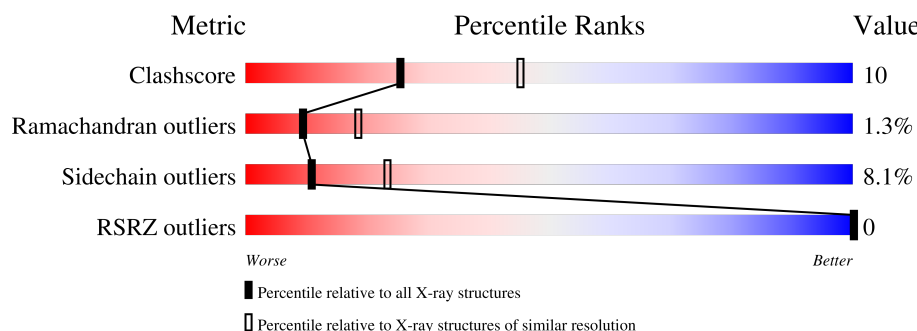
1 Overall quality at a glance

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	 66% 28% 5%
1	B	374	 63% 29% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5724 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
			2774	1766	470	516	22			
1	B	374	Total	C	N	O	S	0	0	0
			2774	1766	470	516	22			

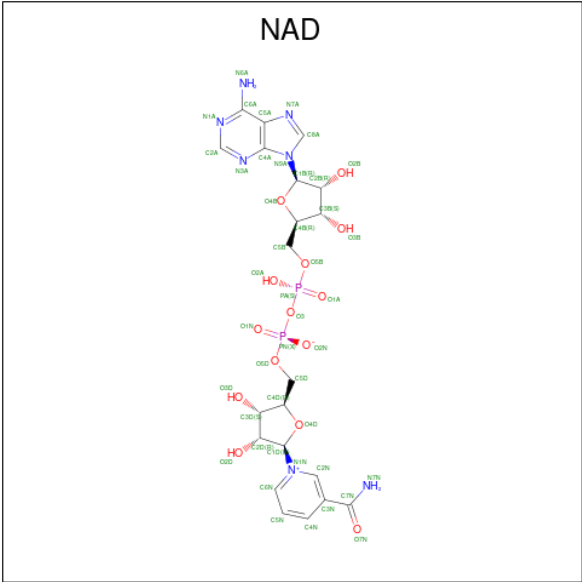
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLY	ARG	conflict	UNP P00325
B	47	GLY	ARG	conflict	UNP P00325

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

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

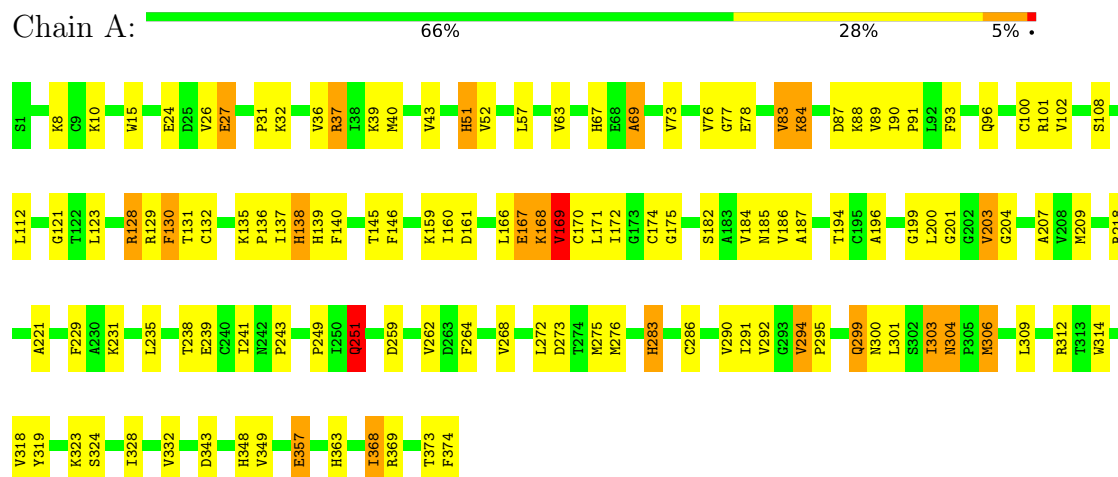
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	45	Total	O	0	0
			45	45		
5	B	38	Total	O	0	0
			38	38		

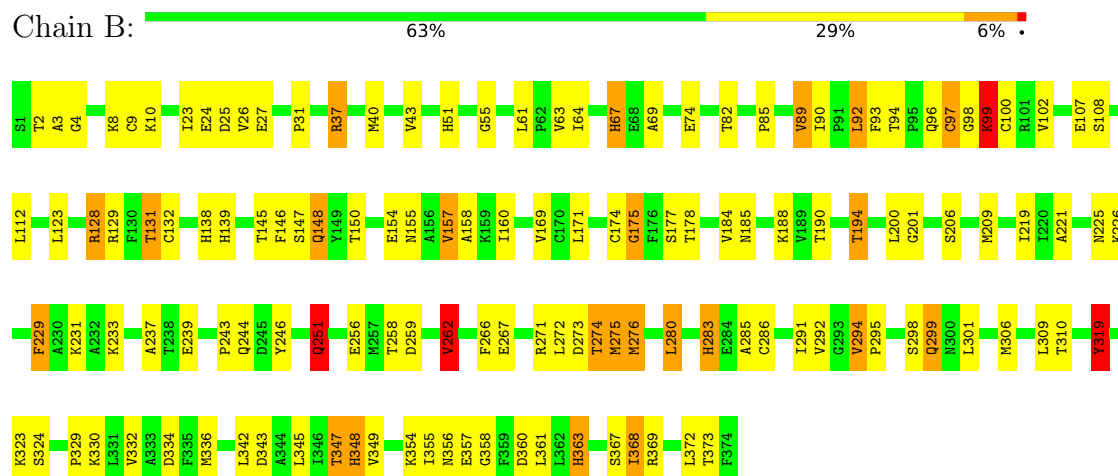
3 Residue-property plots

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	53.56Å 44.26Å 93.01Å 92.36° 103.63° 68.84°	Depositor
Resolution (Å)	7.00 – 2.50 7.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.50) 82.2 (7.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.39Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.194 , (Not available) 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5724	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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: CL, 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	1.06	9/2826 (0.3%)	1.77	49/3824 (1.3%)
1	B	1.01	8/2826 (0.3%)	1.79	60/3824 (1.6%)
All	All	1.04	17/5652 (0.3%)	1.78	109/7648 (1.4%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	283	HIS	CD2-NE2	-7.75	1.29	1.37
1	B	67	HIS	CD2-NE2	-7.40	1.29	1.37
1	B	348	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	283	HIS	CD2-NE2	-6.75	1.30	1.37
1	A	67	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	138	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	348	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	51	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	363	HIS	CD2-NE2	-6.32	1.30	1.37
1	B	139	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	139	HIS	CD2-NE2	-6.08	1.31	1.37
1	B	51	HIS	CD2-NE2	-5.94	1.31	1.37
1	B	363	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	363	HIS	CG-ND1	-5.59	1.32	1.38
1	B	157	VAL	CA-CB	5.46	1.62	1.54
1	B	63	VAL	CA-CB	5.43	1.63	1.55
1	A	63	VAL	CA-CB	5.03	1.62	1.55

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	SER	N-CA-C	12.00	123.91	111.07
1	A	332	VAL	N-CA-C	-9.76	101.35	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	LYS	N-CA-C	-9.57	95.53	109.59
1	A	51	HIS	CB-CG-CD2	-8.91	119.62	131.20
1	B	69	ALA	N-CA-C	8.24	120.67	108.14
1	A	299	GLN	OE1-CD-NE2	-8.20	114.41	122.60
1	A	259	ASP	CA-CB-CG	8.12	120.72	112.60
1	A	323	LYS	N-CA-C	-8.12	96.09	108.67
1	A	368	ILE	N-CA-C	-8.11	92.47	109.34
1	A	51	HIS	CB-CG-ND1	7.79	134.38	122.70
1	B	259	ASP	CA-CB-CG	7.77	120.37	112.60
1	B	348	HIS	CB-CG-CD2	-7.70	121.19	131.20
1	B	299	GLN	OE1-CD-NE2	-7.58	115.02	122.60
1	A	251	GLN	OE1-CD-NE2	-7.51	115.09	122.60
1	B	89	VAL	N-CA-CB	-7.49	97.92	111.92
1	B	368	ILE	N-CA-C	-7.37	94.01	109.34
1	B	273	ASP	CA-CB-CG	7.27	119.87	112.60
1	A	207	ALA	N-CA-C	-7.27	103.29	111.14
1	B	201	GLY	N-CA-C	-7.23	102.14	112.55
1	A	87	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	69	ALA	N-CA-C	7.14	119.03	108.60
1	B	177	SER	CA-CB-OG	-7.10	96.89	111.10
1	A	294	VAL	CA-C-N	7.10	124.77	119.66
1	A	294	VAL	C-N-CA	7.10	124.77	119.66
1	A	273	ASP	CA-CB-CG	6.94	119.54	112.60
1	B	184	VAL	N-CA-C	6.91	117.66	110.62
1	A	324	SER	N-CA-C	6.87	122.70	111.37
1	B	262	VAL	N-CA-CB	-6.87	98.47	110.49
1	B	262	VAL	CB-CA-C	6.60	120.74	111.63
1	B	61	LEU	O-C-N	-6.56	115.30	121.20
1	B	275	MET	CG-SD-CE	-6.48	86.65	100.90
1	A	168	LYS	N-CA-C	-6.44	103.49	112.12
1	B	294	VAL	CA-C-N	6.40	124.27	119.66
1	B	294	VAL	C-N-CA	6.40	124.27	119.66
1	B	123	LEU	N-CA-C	-6.33	101.10	110.46
1	B	348	HIS	CB-CG-ND1	6.27	132.10	122.70
1	B	64	ILE	N-CA-C	-6.26	98.73	107.80
1	A	96	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	B	185	ASN	CA-CB-CG	6.17	118.77	112.60
1	A	184	VAL	N-CA-C	6.15	118.74	111.05
1	B	334	ASP	CA-CB-CG	6.13	118.73	112.60
1	B	251	GLN	CB-CA-C	-6.11	101.28	110.88
1	B	93	PHE	CA-CB-CG	6.08	119.89	113.80
1	B	299	GLN	CG-CD-NE2	6.07	125.51	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	B	23	ILE	N-CA-C	-5.90	99.81	108.54
1	A	185	ASN	CB-CA-C	-5.90	99.74	109.65
1	B	229	PHE	N-CA-C	5.88	117.69	111.28
1	B	82	THR	N-CA-C	5.88	120.58	113.41
1	A	146	PHE	CA-CB-CG	5.86	119.66	113.80
1	B	155	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	A	169	VAL	N-CA-CB	-5.85	101.58	111.23
1	A	185	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	161	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	348	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	A	349	VAL	N-CA-C	-5.75	99.84	108.12
1	B	356	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	A	343	ASP	N-CA-C	5.71	119.05	111.75
1	A	67	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	B	280	LEU	N-CA-C	5.62	118.18	111.71
1	B	51	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	B	298	SER	N-CA-C	5.60	119.36	111.52
1	A	8	LYS	N-CA-C	-5.58	99.81	108.90
1	A	203	VAL	N-CA-C	-5.58	105.67	111.58
1	B	67	HIS	CB-CG-CD2	-5.54	123.99	131.20
1	B	258	THR	N-CA-C	5.53	119.67	111.87
1	B	256	GLU	CA-CB-CG	-5.52	103.06	114.10
1	A	300	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	251	GLN	CG-CD-NE2	5.50	124.65	116.40
1	A	15	TRP	CG-CD2-CE3	5.49	139.39	133.90
1	B	55	GLY	N-CA-C	-5.42	107.56	115.63
1	B	225	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	B	96	GLN	N-CA-C	-5.40	99.58	108.49
1	B	343	ASP	N-CA-C	5.30	117.47	111.11
1	A	201	GLY	N-CA-C	-5.29	104.47	112.41
1	A	84	LYS	N-CA-C	-5.28	100.97	109.58
1	A	121	GLY	N-CA-C	-5.27	107.53	115.32
1	B	148	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	A	264	PHE	CA-C-O	-5.24	114.69	120.24
1	B	8	LYS	N-CA-C	-5.23	100.37	108.90
1	B	266	PHE	O-C-N	-5.23	117.20	123.27
1	A	37	ARG	N-CA-C	-5.22	100.66	109.07
1	A	357	GLU	N-CA-C	-5.22	105.77	111.82
1	B	92	LEU	CA-C-O	-5.22	114.78	120.36
1	B	206	SER	N-CA-C	-5.21	105.67	112.23
1	B	246	TYR	N-CA-C	5.21	118.08	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	CYS	CA-C-N	5.20	128.02	120.79
1	B	100	CYS	C-N-CA	5.20	128.02	120.79
1	A	93	PHE	CA-CB-CG	5.20	119.00	113.80
1	B	319	TYR	N-CA-C	5.20	118.92	112.47
1	A	259	ASP	CA-C-O	5.20	127.58	121.40
1	B	347	THR	N-CA-CB	-5.18	102.49	110.42
1	A	15	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	B	146	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	229	PHE	N-CA-C	5.12	116.87	111.28
1	A	27	GLU	N-CA-C	-5.11	101.36	109.59
1	B	37	ARG	N-CA-C	-5.10	100.85	109.07
1	B	349	VAL	N-CA-C	-5.10	100.77	108.12
1	A	304	ASN	N-CA-C	-5.10	102.15	109.24
1	A	123	LEU	N-CA-C	-5.08	102.49	110.17
1	B	251	GLN	N-CA-CB	5.08	117.38	110.01
1	B	267	GLU	O-C-N	-5.05	117.04	123.05
1	B	360	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	57	LEU	N-CA-C	-5.04	100.08	108.34
1	A	299	GLN	CG-CD-NE2	5.03	123.95	116.40
1	B	99	LYS	N-CA-C	5.02	121.10	114.12
1	B	43	VAL	N-CA-C	5.01	115.34	108.12
1	B	129	ARG	N-CA-C	-5.01	105.90	112.41
1	A	130	PHE	O-C-N	5.01	129.38	123.27

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	2774	0	2846	58	0
1	B	2774	0	2846	54	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	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	45	0	0	0	0
5	B	38	0	0	0	0
All	All	5724	0	5744	109	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 10.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ALA:HB2	1:A:290:VAL:HG21	1.62	0.81
1:B:348:HIS:HD2	1:B:361:LEU:HD13	1.47	0.80
1:A:73:VAL:HG21	1:A:83:VAL:HG11	1.65	0.78
1:B:178:THR:HG21	3:B:377:NAD:C4N	2.14	0.77
1:A:171:LEU:HD21	1:A:369:ARG:HG3	1.68	0.76
1:B:26:VAL:HG12	1:B:132:CYS:HB2	1.67	0.76
1:B:97:CYS:SG	1:B:99:LYS:HE3	2.25	0.75
1:B:90:ILE:HD12	1:B:160:ILE:HG21	1.71	0.73
1:B:251:GLN:HG2	1:B:280:LEU:HB2	1.75	0.69
1:A:306:MET:HE3	1:A:309:LEU:HD23	1.72	0.69
1:A:36:VAL:HG22	1:A:76:VAL:HG12	1.75	0.67
1:A:209:MET:HE2	1:A:235:LEU:HD22	1.78	0.66
1:A:276:MET:HA	1:A:276:MET:HE3	1.79	0.65
1:A:272:LEU:HD11	1:A:299:GLN:HB3	1.82	0.61
1:B:347:THR:HG21	1:B:368:ILE:H	1.66	0.61
1:A:174:CYS:SG	3:A:377:NAD:H5N	2.41	0.60
1:B:94:THR:HB	1:B:319:TYR:CD2	2.37	0.60
1:B:94:THR:HB	1:B:319:TYR:HD2	1.66	0.60
1:A:283:HIS:CD2	1:A:286:CYS:SG	2.95	0.59
1:B:347:THR:HG22	1:B:369:ARG:O	2.02	0.59
1:B:306:MET:SD	1:B:309:LEU:HD23	2.43	0.59
1:A:108:SER:OG	1:B:286:CYS:HB3	2.03	0.58
1:B:275:MET:HE2	1:B:291:ILE:HG23	1.86	0.57
1:A:69:ALA:O	1:A:91:PRO:HD2	2.04	0.57
1:B:10:LYS:HA	1:B:24:GLU:O	2.05	0.57
1:A:73:VAL:HG21	1:A:83:VAL:CG1	2.35	0.56
1:B:102:VAL:HG13	1:B:108:SER:HB2	1.87	0.56
1:A:26:VAL:HG12	1:A:132:CYS:HB2	1.87	0.55
1:B:272:LEU:HD11	1:B:299:GLN:HB3	1.87	0.55
1:A:102:VAL:HG13	1:A:108:SER:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:MET:HE1	1:B:345:LEU:HD11	1.88	0.54
1:A:32:LYS:O	1:A:77:GLY:HA3	2.08	0.54
1:A:171:LEU:CD2	1:A:369:ARG:HG3	2.36	0.53
1:B:174:CYS:SG	1:B:175:GLY:N	2.81	0.53
1:A:304:ASN:OD1	1:A:306:MET:HB2	2.09	0.53
1:B:348:HIS:NE2	1:B:361:LEU:HD22	2.24	0.53
1:A:43:VAL:HG22	1:A:69:ALA:HB2	1.90	0.53
1:A:90:ILE:HD11	1:A:169:VAL:HG13	1.91	0.52
1:B:271:ARG:HB2	1:B:274:THR:OG1	2.10	0.52
1:A:251:GLN:NE2	1:A:251:GLN:H	2.09	0.51
1:B:355:ILE:HG13	1:B:372:LEU:HD11	1.93	0.51
1:B:27:GLU:HB2	1:B:131:THR:OG1	2.10	0.50
1:A:272:LEU:HD22	1:A:301:LEU:HG	1.92	0.50
1:A:275:MET:HE1	1:A:295:PRO:HG3	1.93	0.50
1:B:283:HIS:HD2	1:B:285:ALA:H	1.59	0.50
1:A:275:MET:HE2	1:A:291:ILE:HG23	1.93	0.50
1:B:251:GLN:HG2	1:B:280:LEU:CB	2.41	0.50
1:B:219:ILE:HB	1:B:237:ALA:HA	1.94	0.50
1:A:175:GLY:HA2	1:A:203:VAL:HG22	1.94	0.50
1:A:90:ILE:HG13	1:A:160:ILE:HD13	1.95	0.49
1:B:194:THR:HG22	1:B:262:VAL:HG22	1.94	0.49
1:A:128:ARG:HD3	1:A:138:HIS:HA	1.93	0.49
1:A:199:GLY:O	1:A:204:GLY:HA3	2.13	0.49
1:B:160:ILE:HB	1:B:332:VAL:HG11	1.94	0.48
1:B:354:LYS:HA	1:B:354:LYS:HE2	1.96	0.47
1:B:229:PHE:O	1:B:233:LYS:HG3	2.13	0.47
1:B:292:VAL:O	3:B:377:NAD:H2N	2.14	0.47
1:A:88:LYS:HD3	1:A:166:LEU:HD21	1.96	0.47
1:A:306:MET:HE3	1:A:309:LEU:HB3	1.96	0.47
1:B:200:LEU:HD11	1:B:221:ALA:HB1	1.97	0.47
1:B:174:CYS:SG	3:B:377:NAD:H5N	2.55	0.47
1:B:348:HIS:CD2	1:B:361:LEU:HD13	2.38	0.46
1:B:294:VAL:HA	1:B:295:PRO:HD3	1.78	0.46
1:A:69:ALA:HA	1:A:170:CYS:HB2	1.98	0.46
1:B:171:LEU:HD12	1:B:342:LEU:HB3	1.98	0.46
1:B:9:CYS:HB2	1:B:148:GLN:OE1	2.15	0.46
1:B:9:CYS:O	1:B:25:ASP:HA	2.16	0.45
1:A:172:ILE:HG22	1:A:328:ILE:HG23	1.98	0.45
1:B:271:ARG:O	1:B:275:MET:HG3	2.16	0.45
1:A:10:LYS:HA	1:A:24:GLU:O	2.17	0.45
1:A:292:VAL:O	3:A:377:NAD:H2N	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ARG:HG2	1:B:138:HIS:HA	1.99	0.45
1:A:129:ARG:NH1	1:A:129:ARG:HG2	2.32	0.44
1:B:31:PRO:HD3	1:B:37:ARG:HB2	2.00	0.44
1:B:40:MET:HG3	1:B:147:SER:O	2.17	0.44
1:A:312:ARG:HH11	1:A:312:ARG:HD2	1.70	0.43
1:A:89:VAL:HG12	1:A:159:LYS:HA	2.00	0.43
1:A:43:VAL:HG23	1:A:374:PHE:HE1	1.83	0.43
1:A:100:CYS:HB2	1:A:112:LEU:HD12	1.99	0.43
1:A:128:ARG:O	1:A:129:ARG:NH1	2.51	0.43
1:A:303:ILE:HG21	1:A:314:TRP:CH2	2.53	0.43
1:A:294:VAL:HA	1:A:295:PRO:HD3	1.73	0.43
1:B:330:LYS:HB3	1:B:330:LYS:HE3	1.89	0.43
1:A:196:ALA:HB2	1:A:262:VAL:HG11	2.00	0.43
1:B:92:LEU:HA	1:B:319:TYR:OH	2.18	0.43
1:B:158:ALA:HB1	1:B:329:PRO:HD3	2.00	0.43
1:A:31:PRO:HD3	1:A:37:ARG:HB2	2.01	0.43
1:A:51:HIS:CD2	3:A:377:NAD:HO2N	2.37	0.42
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.83	0.42
1:A:52:VAL:HG21	1:A:140:PHE:CE1	2.54	0.42
1:A:182:SER:O	1:A:186:VAL:HB	2.19	0.42
1:B:40:MET:HE3	1:B:150:THR:HG22	2.02	0.42
1:A:241:ILE:HD13	1:A:241:ILE:HG21	1.86	0.42
1:A:101:ARG:HD3	1:B:283:HIS:CE1	2.56	0.41
1:A:309:LEU:HD21	1:B:294:VAL:HG22	2.01	0.41
1:B:154:GLU:O	1:B:157:VAL:HG12	2.21	0.41
1:B:231:LYS:HD3	1:B:231:LYS:HA	1.85	0.41
1:B:272:LEU:HD22	1:B:301:LEU:HG	2.02	0.41
1:A:200:LEU:HD21	1:A:221:ALA:HB1	2.03	0.41
1:B:358:GLY:HA2	1:B:361:LEU:HD12	2.03	0.41
1:A:130:PHE:HB2	1:A:137:ILE:HB	2.02	0.41
1:B:276:MET:HA	1:B:276:MET:CE	2.51	0.41
1:A:135:LYS:HA	1:A:136:PRO:HD3	1.98	0.40
1:A:40:MET:HB3	1:A:374:PHE:CE1	2.56	0.40
1:A:167:GLU:H	1:A:167:GLU:CD	2.29	0.40
1:A:218:ARG:HA	1:A:238:THR:HG21	2.03	0.40
1:B:94:THR:H	1:B:319:TYR:HE2	1.68	0.40
1:B:347:THR:HG21	1:B:368:ILE:N	2.33	0.40
1:A:69:ALA:HB3	1:A:145:THR:HG21	2.03	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%)	339 (91%)	32 (9%)	1 (0%)	36	55
1	B	372/374 (100%)	332 (89%)	31 (8%)	9 (2%)	4	8
All	All	744/748 (100%)	671 (90%)	63 (8%)	10 (1%)	9	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	ALA
1	B	169	VAL
1	B	175	GLY
1	B	363	HIS
1	B	97	CYS
1	B	145	THR
1	B	67	HIS
1	A	368	ILE
1	B	4	GLY
1	B	98	GLY

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	304/304 (100%)	281 (92%)	23 (8%)	12	26
1	B	304/304 (100%)	278 (91%)	26 (9%)	10	21
All	All	608/608 (100%)	559 (92%)	49 (8%)	11	23

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	39	LYS
1	A	78	GLU
1	A	83	VAL
1	A	84	LYS
1	A	128	ARG
1	A	131	THR
1	A	167	GLU
1	A	168	LYS
1	A	169	VAL
1	A	194	THR
1	A	231	LYS
1	A	239	GLU
1	A	243	PRO
1	A	249	PRO
1	A	251	GLN
1	A	268	VAL
1	A	303	ILE
1	A	306	MET
1	A	318	VAL
1	A	319	TYR
1	A	357	GLU
1	A	373	THR
1	B	2	THR
1	B	74	GLU
1	B	85	PRO
1	B	89	VAL
1	B	99	LYS
1	B	107	GLU
1	B	112	LEU
1	B	128	ARG
1	B	131	THR
1	B	188	LYS
1	B	190	THR
1	B	194	THR
1	B	226	LYS
1	B	239	GLU
1	B	243	PRO
1	B	244	GLN
1	B	251	GLN
1	B	262	VAL
1	B	274	THR

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Mol	Chain	Res	Type
1	B	276	MET
1	B	310	THR
1	B	319	TYR
1	B	336	MET
1	B	357	GLU
1	B	367	SER
1	B	373	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	A	251	GLN
1	A	283	HIS
1	A	348	HIS
1	B	124	GLN
1	B	155	ASN
1	B	244	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	B	377	-	46,48,48	2.14	9 (19%)	64,73,73	1.78	14 (21%)
3	NAD	A	377	-	46,48,48	2.28	12 (26%)	64,73,73	1.69	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
3	NAD	B	377	-	-	12/30/62/62	0/5/5/5
3	NAD	A	377	-	-	16/30/62/62	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	377	NAD	C3N-C7N	-10.54	1.34	1.50
3	A	377	NAD	C3N-C7N	-10.38	1.35	1.50
3	A	377	NAD	C5A-N7A	-4.66	1.30	1.39
3	B	377	NAD	C5A-N7A	-4.43	1.31	1.39
3	A	377	NAD	PN-O3	-4.01	1.55	1.59
3	A	377	NAD	C4A-N9A	-3.56	1.30	1.37
3	B	377	NAD	C4A-N9A	-3.43	1.30	1.37
3	B	377	NAD	C4N-C3N	-3.26	1.34	1.39
3	A	377	NAD	C2N-C3N	-3.23	1.33	1.39
3	B	377	NAD	C5N-C4N	-3.18	1.33	1.38
3	A	377	NAD	C2N-N1N	-2.89	1.31	1.35
3	A	377	NAD	C5N-C4N	-2.81	1.34	1.38
3	A	377	NAD	PA-O3	-2.74	1.56	1.59
3	B	377	NAD	C2N-C3N	-2.61	1.34	1.39
3	A	377	NAD	C8A-N9A	-2.58	1.33	1.37
3	B	377	NAD	C8A-N9A	-2.53	1.33	1.37
3	A	377	NAD	C4N-C3N	-2.22	1.36	1.39
3	B	377	NAD	C3D-C4D	-2.18	1.47	1.53
3	A	377	NAD	C3D-C4D	-2.04	1.47	1.53
3	A	377	NAD	C5A-C4A	-2.02	1.35	1.39
3	B	377	NAD	C2N-N1N	-2.02	1.32	1.35

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	377	NAD	O7N-C7N-N7N	-4.71	115.81	122.62
3	A	377	NAD	O7N-C7N-N7N	-4.69	115.84	122.62
3	A	377	NAD	O2N-PN-O3	4.55	119.57	107.27
3	B	377	NAD	C3N-C7N-N7N	4.11	122.80	117.74
3	B	377	NAD	O2N-PN-O3	3.97	118.02	107.27
3	B	377	NAD	C5D-C4D-C3D	-3.80	101.52	115.21
3	A	377	NAD	N3A-C2A-N1A	-3.45	123.36	128.58
3	B	377	NAD	O4B-C1B-C2B	-3.38	99.37	106.62
3	A	377	NAD	C3N-C7N-N7N	3.33	121.84	117.74
3	B	377	NAD	C6N-N1N-C2N	-3.29	119.08	121.88
3	B	377	NAD	C5A-C4A-N3A	-3.25	122.24	126.72
3	B	377	NAD	N3A-C2A-N1A	-3.04	123.98	128.58
3	B	377	NAD	O2D-C2D-C3D	-3.03	102.09	111.82
3	B	377	NAD	C6A-C5A-C4A	3.02	121.30	117.18
3	A	377	NAD	C5A-C4A-N3A	-2.94	122.67	126.72
3	A	377	NAD	C5D-C4D-C3D	-2.92	104.71	115.21
3	A	377	NAD	O2D-C2D-C3D	-2.85	102.67	111.82
3	A	377	NAD	C6A-C5A-C4A	2.72	120.89	117.18
3	B	377	NAD	O4D-C4D-C5D	2.69	117.96	109.33
3	A	377	NAD	O3D-C3D-C4D	-2.53	103.82	111.08
3	B	377	NAD	C6A-C5A-N7A	-2.48	127.30	132.09
3	B	377	NAD	O2A-PA-O3	2.48	113.97	107.27
3	A	377	NAD	O2A-PA-O3	2.38	113.70	107.27
3	A	377	NAD	C6A-C5A-N7A	-2.25	127.76	132.09
3	A	377	NAD	C2N-C3N-C4N	2.24	120.86	118.26
3	B	377	NAD	O3D-C3D-C4D	-2.20	104.75	111.08
3	A	377	NAD	C6N-N1N-C2N	-2.19	120.01	121.88
3	A	377	NAD	C6N-N1N-C1D	2.02	123.70	119.73

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	377	NAD	C5B-O5B-PA-O1A
3	A	377	NAD	C5D-O5D-PN-O3
3	A	377	NAD	C5D-O5D-PN-O2N
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-O1N
3	B	377	NAD	C5D-O5D-PN-O2N
3	B	377	NAD	O4D-C4D-C5D-O5D

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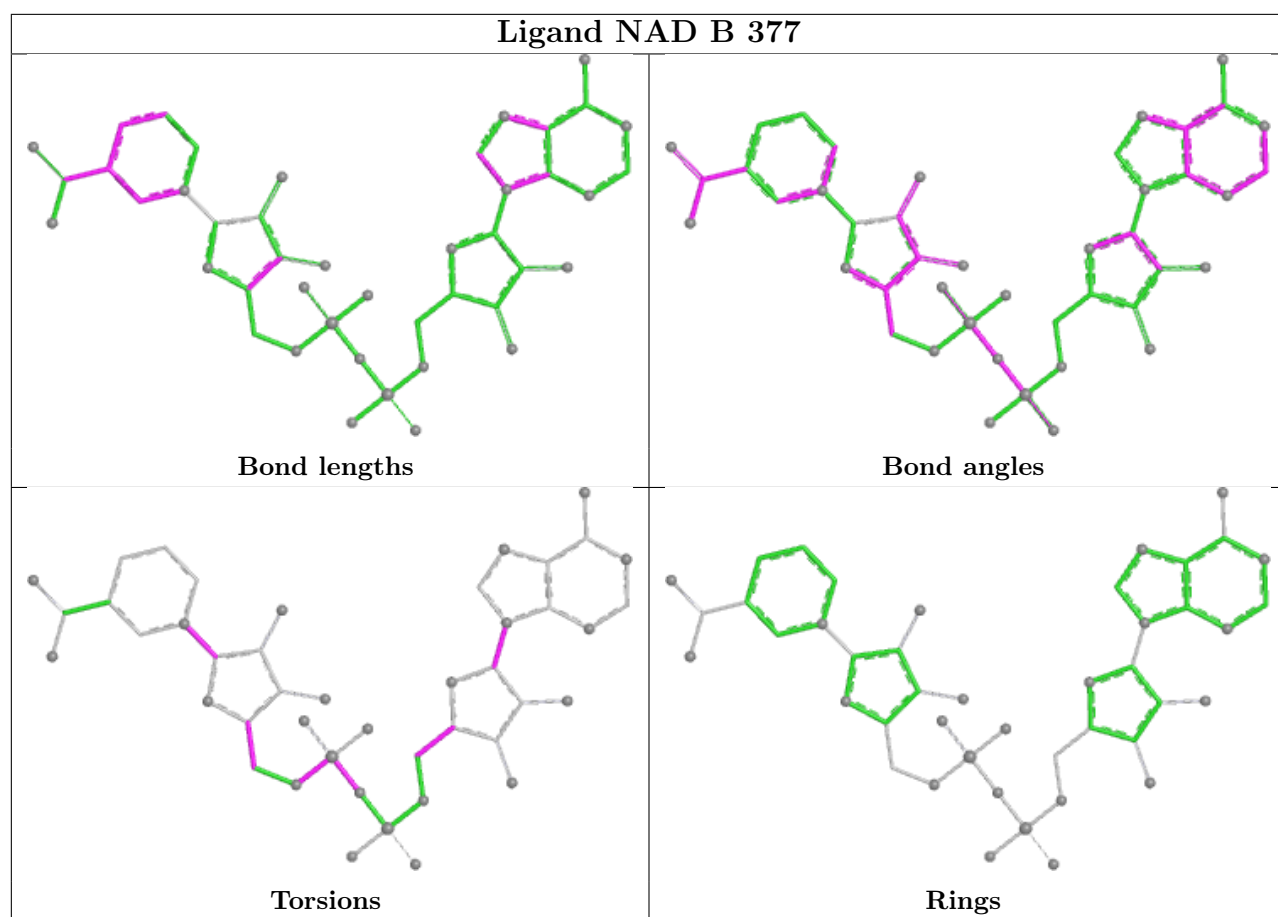
Mol	Chain	Res	Type	Atoms
3	B	377	NAD	O4D-C1D-N1N-C6N
3	B	377	NAD	C2D-C1D-N1N-C2N
3	A	377	NAD	O4D-C4D-C5D-O5D
3	B	377	NAD	C3D-C4D-C5D-O5D
3	A	377	NAD	C3B-C4B-C5B-O5B
3	A	377	NAD	O4B-C4B-C5B-O5B
3	A	377	NAD	C3D-C4D-C5D-O5D
3	A	377	NAD	C2B-C1B-N9A-C8A
3	B	377	NAD	PA-O3-PN-O2N
3	A	377	NAD	C5B-O5B-PA-O2A
3	A	377	NAD	C5B-O5B-PA-O3
3	B	377	NAD	C5D-O5D-PN-O3
3	B	377	NAD	C2D-C1D-N1N-C6N
3	B	377	NAD	O4D-C1D-N1N-C2N
3	A	377	NAD	PA-O3-PN-O1N
3	A	377	NAD	PA-O3-PN-O2N
3	B	377	NAD	C2B-C1B-N9A-C8A
3	B	377	NAD	O4B-C4B-C5B-O5B

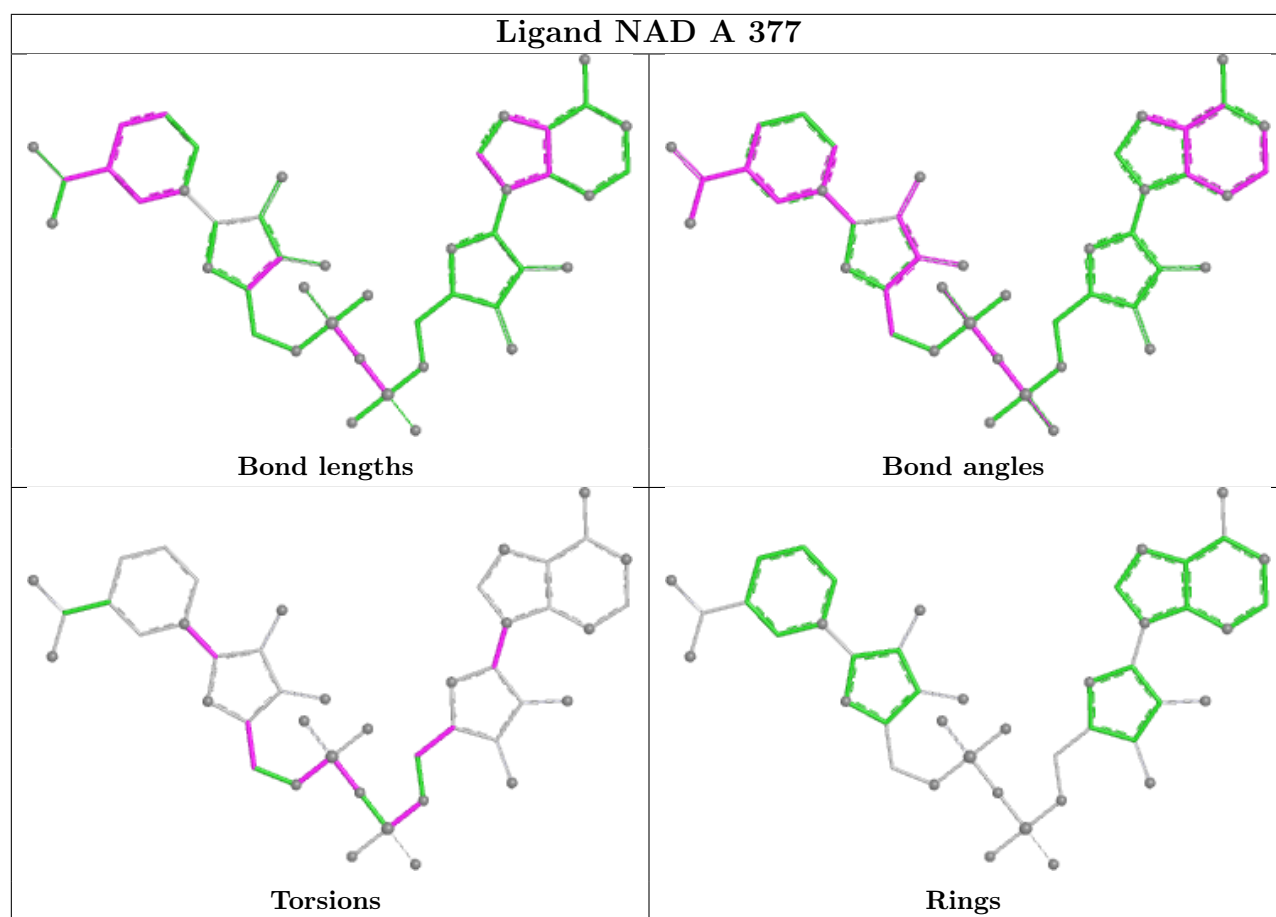
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	377	NAD	3	0
3	A	377	NAD	3	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%)	-0.81	0 100 100	5, 24, 42, 62	0
1	B	374/374 (100%)	-0.64	0 100 100	6, 31, 52, 59	0
All	All	748/748 (100%)	-0.73	0 100 100	5, 27, 48, 62	0

There are no RSRZ outliers to report.

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](#)

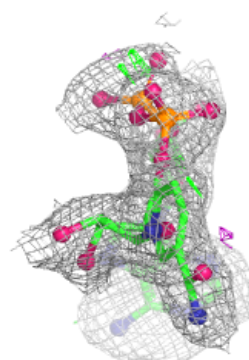
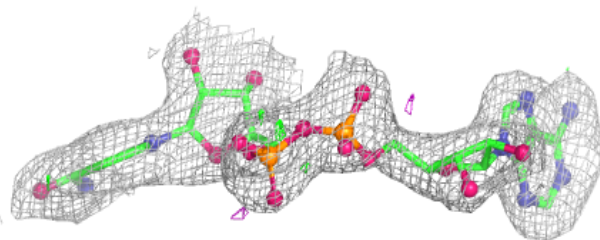
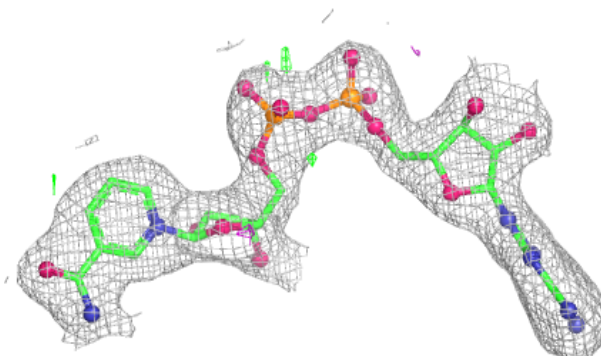
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

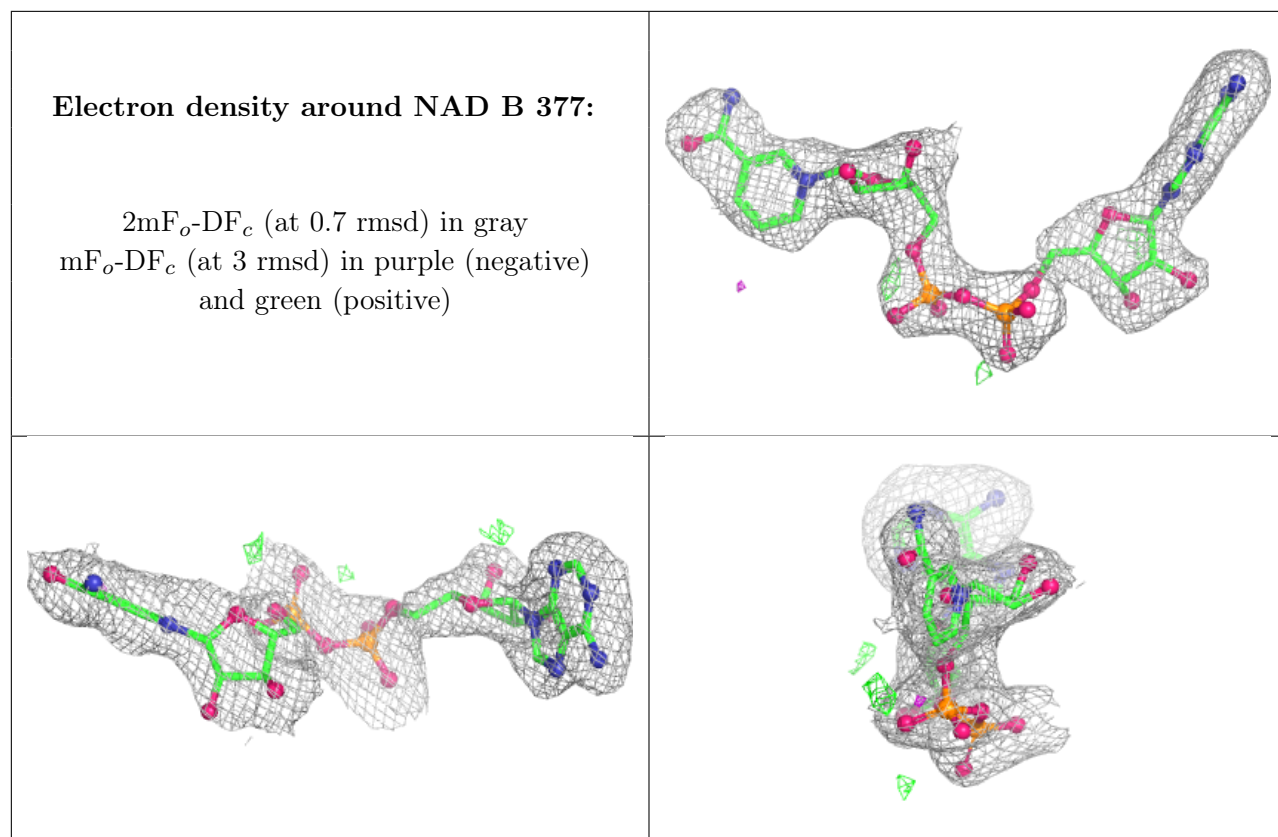
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	B	376	1/1	0.96	0.06	34,34,34,34	1
4	CL	B	601	1/1	0.96	0.08	42,42,42,42	0
2	ZN	A	375	1/1	0.97	0.02	35,35,35,35	0
3	NAD	A	377	44/44	0.97	0.05	2,17,23,32	0
3	NAD	B	377	44/44	0.97	0.05	8,26,38,42	0
2	ZN	A	376	1/1	0.97	0.08	26,26,26,26	1
2	ZN	B	375	1/1	0.98	0.04	29,29,29,29	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.