



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:45 AM UTC

PDB ID : 3HUD / pdb_00003hud
Title : THE STRUCTURE OF HUMAN BETA 1 BETA 1 ALCOHOL DEHYDROGENASE: CATALYTIC EFFECTS OF NON-ACTIVE-SITE SUBSTITUTIONS
Authors : Hurley, T.D.; Bosron, W.F.; Hamilton, J.A.; Amzel, L.M.
Deposited on : 1993-01-04
Resolution : 3.20 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

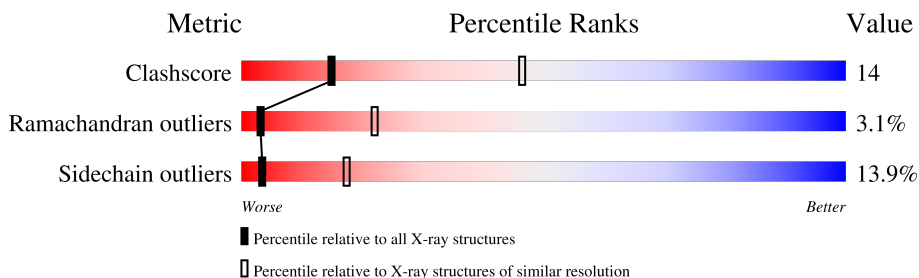
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5654 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.

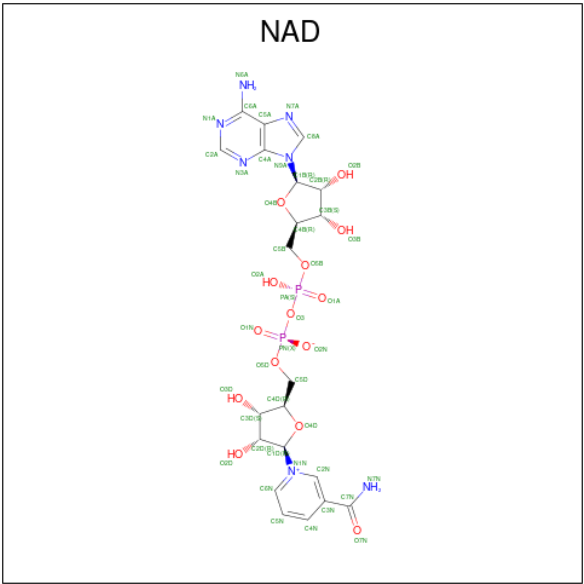
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

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 (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).



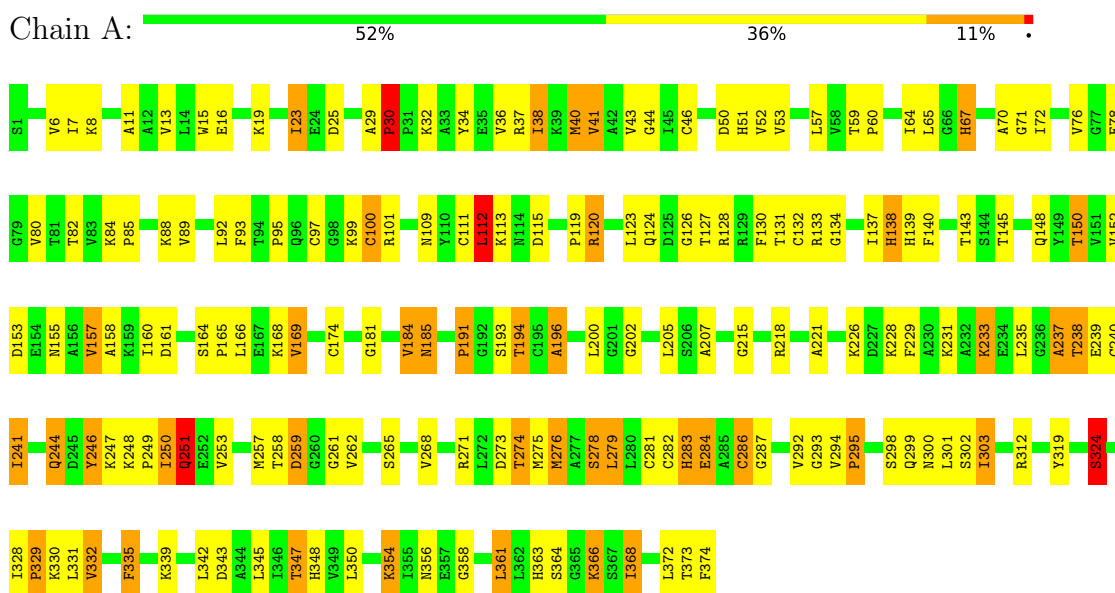
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

3 Residue-property plots

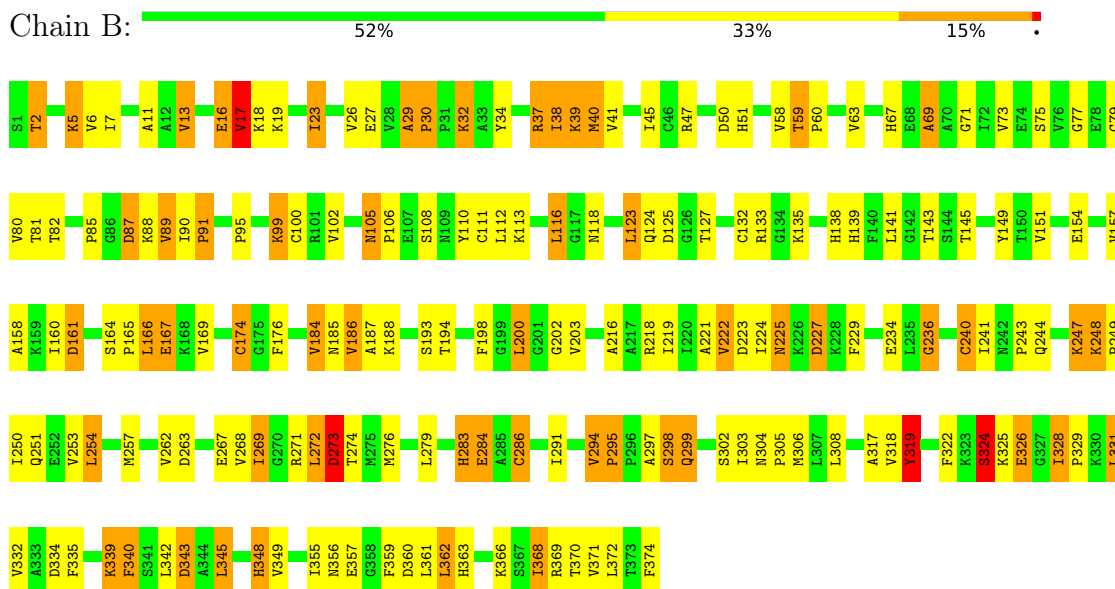
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



• Molecule 1: ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.59Å 45.05Å 93.86Å 91.93° 102.50° 68.82°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5654	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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, 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	1.05	10/2833 (0.4%)	1.98	73/3833 (1.9%)
1	B	1.07	12/2833 (0.4%)	2.06	95/3833 (2.5%)
All	All	1.06	22/5666 (0.4%)	2.02	168/7666 (2.2%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	HIS	CD2-NE2	-6.92	1.30	1.37
1	B	30	PRO	CA-C	6.91	1.55	1.51
1	B	348	HIS	CD2-NE2	-6.84	1.30	1.37
1	B	51	HIS	CD2-NE2	-6.83	1.30	1.37
1	B	138	HIS	CD2-NE2	-6.75	1.30	1.37
1	A	348	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	67	HIS	CD2-NE2	-6.72	1.30	1.37
1	B	363	HIS	CD2-NE2	-6.55	1.30	1.37
1	B	283	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	363	HIS	CD2-NE2	-6.32	1.30	1.37
1	B	139	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	283	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	303	ILE	CA-CB	6.19	1.63	1.54
1	B	67	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	138	HIS	CD2-NE2	-5.88	1.31	1.37
1	B	67	HIS	CG-ND1	-5.56	1.32	1.38
1	A	328	ILE	CA-CB	5.35	1.57	1.53
1	B	295	PRO	CA-C	5.31	1.54	1.51
1	A	139	HIS	CD2-NE2	-5.29	1.32	1.37
1	B	138	HIS	CG-ND1	-5.22	1.32	1.38
1	A	23	ILE	CA-CB	5.16	1.59	1.53
1	B	45	ILE	CA-CB	5.14	1.60	1.54

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	PRO	N-CA-C	12.28	125.68	110.70
1	B	139	HIS	CA-CB-CG	12.20	126.00	113.80
1	B	30	PRO	N-CA-C	10.97	121.00	110.47
1	A	127	THR	N-CA-C	10.65	125.29	109.95
1	B	374	PHE	CA-CB-CG	-10.64	103.16	113.80
1	A	368	ILE	N-CA-C	-9.37	89.85	109.34
1	B	123	LEU	N-CA-C	-9.29	96.78	110.52
1	A	155	ASN	CA-CB-CG	9.07	121.67	112.60
1	B	161	ASP	CA-CB-CG	8.98	121.58	112.60
1	A	82	THR	N-CA-C	8.98	122.03	111.71
1	A	300	ASN	CA-CB-CG	8.78	121.38	112.60
1	B	317	ALA	N-CA-C	8.74	121.81	108.52
1	A	67	HIS	CB-CG-CD2	-8.68	119.92	131.20
1	B	225	ASN	OD1-CG-ND2	-8.50	114.10	122.60
1	B	298	SER	N-CA-C	8.36	122.92	111.39
1	B	200	LEU	N-CA-C	8.22	120.31	110.44
1	B	185	ASN	CA-CB-CG	8.22	120.82	112.60
1	B	368	ILE	N-CA-C	-8.18	92.32	109.34
1	B	105	ASN	CB-CA-C	-8.18	96.28	109.69
1	B	99	LYS	N-CA-C	7.99	121.08	111.82
1	B	184	VAL	N-CA-C	7.94	119.67	110.62
1	B	295	PRO	O-C-N	-7.94	117.66	121.31
1	A	93	PHE	CA-CB-CG	7.84	121.64	113.80
1	A	348	HIS	CA-CB-CG	7.83	121.63	113.80
1	A	29	ALA	N-CA-C	7.76	119.55	109.93
1	A	161	ASP	CA-CB-CG	7.60	120.20	112.60
1	B	82	THR	N-CA-C	7.50	120.12	111.11
1	B	273	ASP	CA-CB-CG	7.48	120.08	112.60
1	B	356	ASN	OD1-CG-ND2	-7.42	115.19	122.60
1	B	51	HIS	CB-CG-CD2	-7.40	121.58	131.20
1	B	225	ASN	CB-CG-ND2	7.35	127.42	116.40
1	A	328	ILE	CA-C-O	-7.32	112.63	118.85
1	A	343	ASP	N-CA-C	7.27	121.25	112.38
1	B	359	PHE	CA-CB-CG	-7.17	106.63	113.80
1	A	99	LYS	N-CA-C	6.99	121.97	113.38
1	B	135	LYS	N-CA-C	-6.96	99.62	110.14
1	A	109	ASN	CA-CB-CG	6.95	119.55	112.60
1	B	294	VAL	CA-C-N	6.93	124.72	119.66
1	B	294	VAL	C-N-CA	6.93	124.72	119.66
1	A	184	VAL	N-CA-CB	-6.93	103.07	110.62
1	A	139	HIS	CA-CB-CG	6.87	120.67	113.80
1	A	238	THR	N-CA-C	-6.84	97.28	110.56
1	B	184	VAL	N-CA-CB	-6.83	101.93	110.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	PRO	N-CA-C	6.82	119.02	110.70
1	B	244	GLN	N-CA-C	6.82	119.55	111.71
1	A	335	PHE	N-CA-C	-6.78	103.58	110.97
1	B	118	ASN	CA-CB-CG	-6.72	105.88	112.60
1	A	113	LYS	N-CA-C	-6.70	103.30	113.89
1	A	259	ASP	CA-C-O	6.69	130.08	120.51
1	B	2	THR	N-CA-C	-6.68	102.42	112.04
1	A	29	ALA	CA-C-N	6.65	127.22	120.38
1	A	29	ALA	C-N-CA	6.65	127.22	120.38
1	B	60	PRO	N-CA-C	6.62	120.80	110.80
1	A	247	LYS	N-CA-C	-6.61	104.85	113.12
1	A	226	LYS	N-CA-C	6.60	120.59	112.54
1	A	279	LEU	N-CA-C	-6.59	104.88	113.12
1	A	250	ILE	CA-C-O	-6.56	112.58	120.78
1	B	13	VAL	N-CA-C	6.55	118.24	108.54
1	B	17	VAL	CB-CA-C	-6.54	101.46	111.08
1	B	116	LEU	N-CA-C	-6.54	102.81	111.24
1	B	304	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	A	193	SER	N-CA-C	6.48	124.61	110.80
1	B	222	VAL	N-CA-CB	-6.46	103.71	110.95
1	B	362	LEU	N-CA-C	-6.45	103.87	111.03
1	A	361	LEU	N-CA-C	-6.44	104.35	111.82
1	B	348	HIS	CB-CG-CD2	-6.43	122.84	131.20
1	B	263	ASP	CA-CB-CG	6.40	119.00	112.60
1	B	125	ASP	N-CA-C	6.38	120.53	112.87
1	A	246	TYR	N-CA-C	6.34	119.96	110.14
1	A	191	PRO	N-CA-C	-6.33	101.24	110.80
1	B	158	ALA	CA-C-O	6.32	127.41	120.71
1	B	357	GLU	CA-CB-CG	6.29	126.69	114.10
1	A	88	LYS	CA-CB-CG	-6.29	101.52	114.10
1	A	366	LYS	CA-C-O	6.25	125.88	118.69
1	B	91	PRO	CA-C-O	-6.23	114.16	121.95
1	A	278	SER	CA-CB-OG	6.22	123.55	111.10
1	A	312	ARG	CB-CG-CD	-6.17	97.10	111.30
1	B	283	HIS	N-CA-C	6.16	123.93	110.80
1	B	343	ASP	CA-CB-CG	6.16	118.75	112.60
1	B	29	ALA	CA-C-N	6.13	124.13	119.66
1	B	29	ALA	C-N-CA	6.13	124.13	119.66
1	B	87	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	51	HIS	CB-CG-ND1	6.09	131.83	122.70
1	B	326	GLU	N-CA-C	6.07	120.45	111.04
1	A	51	HIS	CB-CG-CD2	-6.02	123.37	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	PRO	N-CA-C	6.02	120.70	110.95
1	B	339	LYS	N-CA-C	6.01	118.62	111.71
1	A	72	ILE	N-CA-CB	-5.95	101.03	111.39
1	A	332	VAL	N-CA-C	-5.95	104.52	111.00
1	A	32	LYS	CB-CG-CD	-5.93	97.67	111.30
1	A	123	LEU	N-CA-C	-5.92	100.25	109.72
1	B	304	ASN	CA-C-N	5.91	127.23	119.84
1	B	304	ASN	C-N-CA	5.91	127.23	119.84
1	B	244	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	A	356	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	115	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	291	ILE	N-CA-C	-5.86	99.97	108.87
1	B	127	THR	O-C-N	-5.84	116.44	123.03
1	B	176	PHE	CA-C-N	5.78	129.48	120.82
1	B	176	PHE	C-N-CA	5.78	129.48	120.82
1	B	247	LYS	CA-C-O	5.75	125.91	119.41
1	B	58	VAL	N-CA-C	-5.74	101.32	108.89
1	B	186	VAL	N-CA-C	5.71	121.22	109.34
1	B	299	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	A	100	CYS	N-CA-C	5.70	118.25	110.55
1	B	16	GLU	CB-CG-CD	5.67	122.24	112.60
1	B	69	ALA	N-CA-C	5.64	116.00	108.38
1	A	46	CYS	O-C-N	-5.63	116.62	123.10
1	A	67	HIS	CB-CG-ND1	5.62	131.14	122.70
1	B	343	ASP	N-CA-C	-5.62	105.05	111.07
1	B	47	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	A	164	SER	N-CA-C	5.59	116.74	109.64
1	B	99	LYS	CA-CB-CG	5.58	125.26	114.10
1	A	89	VAL	O-C-N	5.57	129.32	123.02
1	B	138	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	A	153	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	185	ASN	CB-CA-C	-5.54	100.68	111.03
1	B	5	LYS	O-C-N	5.53	129.86	122.73
1	B	127	THR	N-CA-C	5.52	118.97	110.42
1	A	339	LYS	N-CA-C	5.52	120.07	113.23
1	B	88	LYS	N-CA-C	-5.50	101.50	109.59
1	A	207	ALA	N-CA-C	-5.46	105.41	111.36
1	A	67	HIS	CA-CB-CG	5.45	119.25	113.80
1	A	148	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	B	127	THR	N-CA-CB	-5.42	102.10	110.56
1	B	39	LYS	N-CA-C	-5.42	100.41	109.24
1	B	158	ALA	N-CA-C	5.41	118.30	109.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LYS	CA-C-O	-5.39	116.02	120.71
1	B	299	GLN	CA-C-O	5.39	126.23	120.46
1	A	133	ARG	N-CA-C	-5.37	99.17	108.52
1	A	52	VAL	N-CA-C	-5.37	105.62	110.82
1	A	157	VAL	CB-CA-C	5.35	118.55	110.63
1	A	251	GLN	N-CA-CB	5.35	119.27	110.39
1	A	237	ALA	N-CA-C	5.35	118.07	110.10
1	B	244	GLN	CG-CD-NE2	5.34	124.41	116.40
1	A	23	ILE	N-CA-C	-5.34	99.92	107.98
1	B	124	GLN	CB-CG-CD	5.33	121.67	112.60
1	B	328	ILE	N-CA-CB	-5.32	107.15	110.50
1	A	273	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	138	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	A	196	ALA	N-CA-C	-5.26	99.86	108.76
1	B	360	ASP	N-CA-C	-5.25	105.47	111.14
1	A	347	THR	CA-CB-OG1	5.24	117.46	109.60
1	B	188	LYS	CA-CB-CG	5.23	124.55	114.10
1	A	41	VAL	N-CA-C	-5.21	107.50	111.62
1	B	63	VAL	N-CA-C	5.20	116.51	108.44
1	B	187	ALA	N-CA-C	-5.18	105.81	111.82
1	B	324	SER	N-CA-C	5.18	121.83	110.80
1	B	248	LYS	N-CA-CB	-5.17	103.30	110.29
1	B	299	GLN	CB-CA-C	5.16	119.20	110.79
1	B	59	THR	CA-CB-OG1	-5.15	101.88	109.60
1	A	347	THR	N-CA-C	5.13	119.81	113.50
1	B	302	SER	N-CA-C	-5.13	100.05	108.41
1	A	329	PRO	CA-C-N	5.12	127.41	120.65
1	A	329	PRO	C-N-CA	5.12	127.41	120.65
1	B	248	LYS	CA-C-N	5.12	125.36	119.83
1	B	248	LYS	C-N-CA	5.12	125.36	119.83
1	B	50	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	286	CYS	O-C-N	-5.11	115.79	122.59
1	B	366	LYS	CA-C-O	5.11	125.25	119.27
1	A	38	ILE	N-CA-CB	-5.10	103.04	112.43
1	A	15	TRP	CA-CB-CG	5.10	123.28	113.60
1	B	295	PRO	N-CA-C	5.08	115.35	110.47
1	B	89	VAL	N-CA-CB	-5.08	102.53	111.93
1	B	222	VAL	O-C-N	-5.08	117.14	122.83
1	B	319	TYR	N-CA-C	5.02	118.37	111.54
1	B	284	GLU	N-CA-C	5.01	121.48	110.80
1	A	251	GLN	CA-CB-CG	5.01	124.12	114.10

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	77	0
1	B	2781	0	2856	82	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	26	5	0
3	B	44	0	26	4	0
All	All	5654	0	5764	157	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 14.

All (157) 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:92:LEU:HD13	1:A:324:SER:HB2	1.25	1.14
1:B:269:ILE:HD12	1:B:274:THR:HG21	1.49	0.95
1:A:174:CYS:SG	3:A:377:NAD:H5N	2.14	0.87
1:B:174:CYS:SG	3:B:377:NAD:H5N	2.19	0.82
1:B:143:THR:HG22	1:B:145:THR:HG23	1.65	0.77
1:A:282:CYS:HB2	1:A:287:GLY:HA3	1.69	0.75
1:A:120:ARG:HH12	1:A:126:GLY:HA2	1.53	0.72
1:A:43:VAL:HG23	1:A:374:PHE:HE2	1.56	0.70
1:A:292:VAL:O	3:A:377:NAD:H2N	1.92	0.69
1:B:355:ILE:HA	1:B:372:LEU:HD21	1.75	0.68
1:A:92:LEU:HD13	1:A:324:SER:CB	2.15	0.67
1:B:80:VAL:HG22	1:B:154:GLU:HG3	1.77	0.67
1:A:233:LYS:HA	1:A:237:ALA:HB3	1.77	0.66
1:B:348:HIS:CD2	1:B:361:LEU:HD21	2.30	0.66
1:A:7:ILE:HG13	1:A:37:ARG:NH1	2.11	0.66
1:B:348:HIS:HB2	1:B:370:THR:HG23	1.77	0.65
1:A:350:LEU:HD23	1:A:354:LYS:HB3	1.78	0.65
1:B:110:TYR:HE1	1:B:116:LEU:HD22	1.60	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:CYS:SG	1:B:133:ARG:HD2	2.37	0.64
1:B:221:ALA:HB3	1:B:240:CYS:HB3	1.79	0.64
1:A:345:LEU:O	1:A:368:ILE:HB	1.98	0.63
1:B:95:PRO:HG3	1:B:113:LYS:HB2	1.81	0.62
1:A:70:ALA:HB1	1:A:166:LEU:HD22	1.82	0.61
1:B:100:CYS:HB2	1:B:112:LEU:HD22	1.82	0.61
1:B:194:THR:HG22	1:B:262:VAL:HG23	1.83	0.61
1:A:11:ALA:O	1:A:23:ILE:HA	2.01	0.61
1:A:275:MET:HE1	1:A:295:PRO:HB3	1.82	0.61
1:A:97:CYS:HB3	1:A:111:CYS:SG	2.42	0.59
1:A:6:VAL:HG22	1:A:30:PRO:HD2	1.86	0.58
1:A:92:LEU:HD21	1:A:158:ALA:HB2	1.86	0.58
1:A:194:THR:HG23	1:A:218:ARG:HB2	1.85	0.58
1:A:143:THR:O	1:A:150:THR:HG21	2.04	0.57
1:A:229:PHE:CD1	1:A:240:CYS:HB3	2.40	0.56
1:B:26:VAL:HG12	1:B:132:CYS:HB2	1.87	0.56
1:B:69:ALA:O	1:B:90:ILE:HG23	2.06	0.56
1:A:258:THR:HG21	1:A:262:VAL:HA	1.88	0.56
1:B:37:ARG:HG2	1:B:151:VAL:HG22	1.88	0.55
1:B:95:PRO:HG2	1:B:111:CYS:HB3	1.89	0.55
1:B:248:LYS:HG2	1:B:253:VAL:HG23	1.88	0.54
1:A:160:ILE:HG21	1:A:332:VAL:HG21	1.91	0.53
1:B:73:VAL:HB	1:B:85:PRO:HA	1.89	0.53
1:B:200:LEU:HD21	1:B:221:ALA:HB1	1.91	0.53
1:A:246:TYR:CE2	1:A:253:VAL:HG11	2.43	0.53
1:B:38:ILE:HD12	1:B:40:MET:HE1	1.91	0.52
1:A:120:ARG:NH1	1:A:126:GLY:HA2	2.24	0.52
1:B:342:LEU:HA	1:B:345:LEU:HD12	1.92	0.52
1:A:43:VAL:HG21	1:A:145:THR:O	2.10	0.52
1:A:38:ILE:HD11	1:A:157:VAL:HG21	1.92	0.51
1:B:116:LEU:HD11	1:B:318:VAL:HG11	1.93	0.51
1:B:219:ILE:HD12	1:B:236:GLY:O	2.10	0.51
1:B:5:LYS:HA	1:B:30:PRO:HG3	1.92	0.51
1:B:161:ASP:HB3	1:B:164:SER:OG	2.11	0.51
1:A:364:SER:HB2	1:A:366:LYS:HE2	1.92	0.51
1:B:174:CYS:SG	3:B:377:NAD:C5N	2.97	0.51
1:A:174:CYS:SG	3:A:377:NAD:C5N	2.94	0.50
1:B:271:ARG:HB3	1:B:273:ASP:OD1	2.10	0.50
1:A:249:PRO:HB2	1:A:251:GLN:OE1	2.12	0.50
1:B:222:VAL:HG22	1:B:241:ILE:HG12	1.92	0.50
1:B:250:ILE:O	1:B:254:LEU:HD12	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:CYS:SG	1:A:112:LEU:HD22	2.52	0.50
1:A:101:ARG:HH11	1:B:283:HIS:CD2	2.29	0.50
1:B:11:ALA:O	1:B:23:ILE:HA	2.10	0.50
1:B:91:PRO:HB2	1:B:143:THR:HG23	1.94	0.50
1:B:34:TYR:CE1	1:B:79:GLY:HA3	2.47	0.50
1:A:181:GLY:O	1:A:185:ASN:HB2	2.12	0.49
1:A:294:VAL:HB	3:A:377:NAD:O2D	2.11	0.49
1:B:16:GLU:HG2	1:B:17:VAL:H	1.76	0.49
1:A:194:THR:HG21	1:A:258:THR:HG23	1.94	0.49
1:A:200:LEU:HD21	1:A:221:ALA:HB1	1.94	0.49
1:B:271:ARG:HB2	1:B:274:THR:OG1	2.12	0.49
1:B:41:VAL:HG11	1:B:166:LEU:HD12	1.94	0.49
1:A:268:VAL:HG22	1:A:292:VAL:HB	1.93	0.49
1:B:32:LYS:O	1:B:77:GLY:HA3	2.13	0.49
1:A:347:THR:HG21	1:A:368:ILE:HG12	1.94	0.49
1:B:250:ILE:HA	1:B:253:VAL:HB	1.95	0.49
1:A:40:MET:HB3	1:A:374:PHE:CD2	2.48	0.49
1:B:254:LEU:HA	1:B:257:MET:HE3	1.95	0.49
1:B:164:SER:HB3	1:B:169:VAL:HG21	1.94	0.48
1:A:65:LEU:HA	1:A:140:PHE:CB	2.43	0.48
1:B:102:VAL:HG13	1:B:108:SER:HB2	1.96	0.48
1:B:73:VAL:HG23	1:B:87:ASP:O	2.14	0.48
1:B:203:VAL:HG12	3:B:377:NAD:O2N	2.14	0.47
1:B:223:ASP:OD1	3:B:377:NAD:H1B	2.13	0.47
1:A:295:PRO:HD2	1:B:306:MET:HE2	1.95	0.47
1:A:6:VAL:HG22	1:A:30:PRO:CD	2.43	0.47
1:A:248:LYS:HG3	1:A:253:VAL:HG22	1.96	0.47
1:A:100:CYS:HB2	1:A:112:LEU:HD23	1.97	0.47
1:B:334:ASP:HB3	1:B:339:LYS:HG2	1.96	0.47
1:A:128:ARG:HD2	1:A:138:HIS:HA	1.96	0.47
1:B:91:PRO:HA	1:B:157:VAL:HG23	1.96	0.47
1:A:16:GLU:HB2	1:A:19:LYS:HB2	1.97	0.46
1:B:39:LYS:HG3	1:B:149:TYR:CZ	2.51	0.46
1:A:7:ILE:HD12	1:A:37:ARG:HD2	1.97	0.46
1:A:218:ARG:HA	1:A:238:THR:HG21	1.98	0.46
1:B:331:LEU:HD23	1:B:340:PHE:CZ	2.50	0.46
1:B:7:ILE:O	1:B:27:GLU:HA	2.16	0.46
1:A:271:ARG:HG3	1:A:274:THR:OG1	2.15	0.46
1:B:16:GLU:HB3	1:B:19:LYS:CG	2.46	0.46
1:A:276:MET:HG2	1:A:301:LEU:HD22	1.98	0.46
1:B:345:LEU:O	1:B:368:ILE:HB	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:GLY:HA2	1:A:361:LEU:HD12	1.99	0.45
1:B:16:GLU:HG2	1:B:17:VAL:N	2.32	0.45
1:A:283:HIS:HB3	1:A:286:CYS:SG	2.57	0.45
1:B:335:PHE:HB2	1:B:340:PHE:HE1	1.81	0.45
1:A:160:ILE:CG2	1:A:332:VAL:HG21	2.47	0.44
1:B:193:SER:H	1:B:216:ALA:HA	1.82	0.44
1:A:41:VAL:HG23	1:A:71:GLY:HA2	1.99	0.44
1:A:241:ILE:HD12	1:A:250:ILE:HD11	1.98	0.44
1:B:40:MET:HA	1:B:40:MET:HE3	1.99	0.44
1:B:34:TYR:HA	1:B:80:VAL:HG23	2.00	0.44
1:B:328:ILE:O	1:B:332:VAL:HG23	2.17	0.44
1:B:37:ARG:CG	1:B:151:VAL:HG22	2.48	0.44
1:A:293:GLY:HA2	3:A:377:NAD:H1D	2.00	0.43
1:B:39:LYS:O	1:B:71:GLY:HA3	2.19	0.43
1:B:272:LEU:HD21	1:B:299:GLN:O	2.18	0.43
1:B:319:TYR:O	1:B:322:PHE:HB2	2.19	0.43
1:B:326:GLU:O	1:B:329:PRO:HD2	2.18	0.43
1:B:91:PRO:HG3	1:B:145:THR:HG21	2.00	0.43
1:A:41:VAL:HG21	1:A:166:LEU:CD1	2.49	0.43
1:A:43:VAL:HG12	1:A:44:GLY:N	2.33	0.43
1:A:60:PRO:HB2	1:A:138:HIS:CE1	2.54	0.43
1:B:34:TYR:HE1	1:B:79:GLY:HA3	1.83	0.42
1:A:274:THR:O	1:A:278:SER:HB3	2.19	0.42
1:B:6:VAL:HG22	1:B:29:ALA:HA	2.01	0.42
1:A:65:LEU:HA	1:A:140:PHE:HB3	2.00	0.42
1:A:200:LEU:O	1:A:228:LYS:HE2	2.20	0.42
1:B:17:VAL:O	1:B:19:LYS:HE3	2.19	0.42
1:B:34:TYR:O	1:B:154:GLU:HB2	2.20	0.42
1:B:349:VAL:HA	1:B:371:VAL:O	2.19	0.42
1:A:132:CYS:HB2	1:A:137:ILE:HD11	2.01	0.42
1:B:369:ARG:HA	1:B:369:ARG:HD3	1.72	0.42
1:B:223:ASP:HB3	1:B:229:PHE:HE1	1.85	0.42
1:A:130:PHE:HB2	1:A:137:ILE:HB	2.01	0.42
1:A:165:PRO:CG	1:A:335:PHE:HE2	2.33	0.42
1:A:169:VAL:HG21	1:A:332:VAL:HG13	2.02	0.41
1:A:248:LYS:HB3	1:A:248:LYS:HE2	1.79	0.41
1:A:244:GLN:HE21	1:A:244:GLN:HB2	1.74	0.41
1:A:261:GLY:HA2	1:A:281:CYS:O	2.19	0.41
1:B:294:VAL:HA	1:B:295:PRO:HD2	1.94	0.41
1:B:335:PHE:HB2	1:B:340:PHE:CE1	2.55	0.41
1:A:191:PRO:HA	1:A:215:GLY:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PHE:O	1:B:269:ILE:HG13	2.20	0.41
1:A:50:ASP:HA	1:A:53:VAL:HG12	2.02	0.41
1:B:224:ILE:HG13	1:B:225:ASN:N	2.35	0.41
1:A:34:TYR:HA	1:A:80:VAL:HG22	2.02	0.41
1:A:36:VAL:HG11	1:A:157:VAL:HG11	2.03	0.41
1:A:76:VAL:HB	1:A:80:VAL:HB	2.02	0.41
1:A:283:HIS:O	1:A:287:GLY:N	2.51	0.41
1:B:105:ASN:HA	1:B:106:PRO:HD3	1.85	0.41
1:A:8:LYS:HE3	1:A:25:ASP:HB3	2.01	0.41
1:B:194:THR:HG23	1:B:218:ARG:HB2	2.03	0.41
1:B:123:LEU:HA	1:B:123:LEU:HD23	1.79	0.40
1:B:164:SER:HA	1:B:165:PRO:HD2	1.96	0.40
1:A:196:ALA:HB2	1:A:262:VAL:HG11	2.02	0.40
1:A:231:LYS:O	1:A:235:LEU:HG	2.21	0.40
1:B:241:ILE:HD11	1:B:250:ILE:HD11	2.03	0.40
1:B:167:GLU:CD	1:B:167:GLU:H	2.29	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%)	317 (85%)	44 (12%)	11 (3%)	3	23
1	B	372/374 (100%)	311 (84%)	49 (13%)	12 (3%)	3	21
All	All	744/748 (100%)	628 (84%)	93 (12%)	23 (3%)	3	22

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	CYS
1	B	284	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	286	CYS
1	A	124	GLN
1	A	284	GLU
1	A	298	SER
1	B	18	LYS
1	B	202	GLY
1	B	324	SER
1	A	67	HIS
1	A	324	SER
1	B	297	ALA
1	A	112	LEU
1	A	259	ASP
1	B	166	LEU
1	A	30	PRO
1	A	202	GLY
1	A	286	CYS
1	B	32	LYS
1	B	227	ASP
1	B	236	GLY
1	A	134	GLY
1	B	269	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%)	263 (86%)	42 (14%)	3	18
1	B	305/305 (100%)	262 (86%)	43 (14%)	3	17
All	All	610/610 (100%)	525 (86%)	85 (14%)	3	17

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	30	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	MET
1	A	57	LEU
1	A	59	THR
1	A	64	ILE
1	A	78	GLU
1	A	85	PRO
1	A	95	PRO
1	A	112	LEU
1	A	120	ARG
1	A	131	THR
1	A	150	THR
1	A	152	VAL
1	A	168	LYS
1	A	169	VAL
1	A	184	VAL
1	A	194	THR
1	A	205	LEU
1	A	233	LYS
1	A	239	GLU
1	A	241	ILE
1	A	244	GLN
1	A	251	GLN
1	A	257	MET
1	A	265	SER
1	A	274	THR
1	A	276	MET
1	A	279	LEU
1	A	284	GLU
1	A	299	GLN
1	A	302	SER
1	A	303	ILE
1	A	319	TYR
1	A	324	SER
1	A	329	PRO
1	A	330	LYS
1	A	331	LEU
1	A	342	LEU
1	A	354	LYS
1	A	372	LEU
1	A	373	THR
1	B	2	THR
1	B	13	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	17	VAL
1	B	23	ILE
1	B	37	ARG
1	B	38	ILE
1	B	40	MET
1	B	59	THR
1	B	75	SER
1	B	81	THR
1	B	89	VAL
1	B	99	LYS
1	B	141	LEU
1	B	160	ILE
1	B	167	GLU
1	B	184	VAL
1	B	186	VAL
1	B	227	ASP
1	B	234	GLU
1	B	240	CYS
1	B	243	PRO
1	B	247	LYS
1	B	249	PRO
1	B	251	GLN
1	B	254	LEU
1	B	267	GLU
1	B	268	VAL
1	B	272	LEU
1	B	273	ASP
1	B	276	MET
1	B	279	LEU
1	B	298	SER
1	B	303	ILE
1	B	305	PRO
1	B	308	LEU
1	B	319	TYR
1	B	324	SER
1	B	325	LYS
1	B	331	LEU
1	B	340	PHE
1	B	343	ASP
1	B	345	LEU
1	B	362	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	124	GLN
1	A	155	ASN
1	A	185	ASN
1	A	225	ASN
1	A	244	GLN
1	A	299	GLN
1	A	300	ASN
1	B	109	ASN
1	B	225	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 6 ligands modelled in this entry, 4 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	1.67	7 (15%)	64,73,73	1.80	12 (18%)
3	NAD	A	377	-	46,48,48	1.81	10 (21%)	64,73,73	1.72	11 (17%)

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	-	-	10/30/62/62	0/5/5/5
3	NAD	A	377	-	-	13/30/62/62	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	377	NAD	C3N-C7N	-6.15	1.41	1.50
3	A	377	NAD	C5A-N7A	-4.98	1.30	1.39
3	B	377	NAD	C3N-C7N	-4.67	1.43	1.50
3	B	377	NAD	C5A-N7A	-4.66	1.30	1.39
3	B	377	NAD	C4A-N9A	-3.62	1.30	1.37
3	A	377	NAD	C4A-N9A	-3.51	1.30	1.37
3	A	377	NAD	C2N-N1N	-3.45	1.31	1.35
3	B	377	NAD	O4D-C1D	3.04	1.44	1.40
3	A	377	NAD	C5A-C4A	-3.04	1.33	1.39
3	B	377	NAD	C8A-N9A	-3.01	1.32	1.37
3	B	377	NAD	C5A-C4A	-2.86	1.34	1.39
3	A	377	NAD	C8A-N9A	-2.80	1.32	1.37
3	A	377	NAD	C4A-N3A	-2.77	1.29	1.34
3	B	377	NAD	PN-O5D	2.60	1.69	1.59
3	A	377	NAD	C6A-N1A	-2.32	1.29	1.35
3	A	377	NAD	PA-O3	2.28	1.62	1.59
3	A	377	NAD	O4D-C4D	-2.22	1.40	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	377	NAD	O7N-C7N-N7N	-5.66	114.44	122.62
3	B	377	NAD	O7N-C7N-N7N	-5.20	115.11	122.62
3	B	377	NAD	O5D-C5D-C4D	4.86	125.54	108.99
3	A	377	NAD	C6A-C5A-C4A	4.39	123.17	117.18
3	A	377	NAD	C5A-C4A-N9A	4.29	110.48	105.81
3	B	377	NAD	C6A-C5A-C4A	4.16	122.86	117.18
3	B	377	NAD	C3N-C7N-N7N	4.11	122.80	117.74
3	A	377	NAD	C5A-C4A-N3A	-3.98	121.23	126.72
3	B	377	NAD	C5A-C4A-N9A	3.82	109.98	105.81
3	B	377	NAD	O2N-PN-O3	3.54	116.85	107.27
3	B	377	NAD	C6N-N1N-C2N	-3.47	118.93	121.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	377	NAD	C5A-C4A-N3A	-3.45	121.97	126.72
3	A	377	NAD	O7N-C7N-C3N	3.43	123.80	119.60
3	A	377	NAD	O4B-C1B-C2B	-3.07	100.04	106.62
3	B	377	NAD	C4D-O4D-C1D	2.91	112.59	109.92
3	A	377	NAD	C4A-N9A-C8A	-2.75	102.86	105.74
3	A	377	NAD	O2N-PN-O3	2.70	114.58	107.27
3	A	377	NAD	C6A-C5A-N7A	-2.63	127.02	132.09
3	A	377	NAD	C3N-C7N-N7N	2.48	120.80	117.74
3	B	377	NAD	C6A-C5A-N7A	-2.15	127.94	132.09
3	B	377	NAD	C5N-C6N-N1N	2.11	123.25	120.38
3	A	377	NAD	O3-PN-O1N	-2.03	104.61	110.70
3	B	377	NAD	O2D-C2D-C3D	-2.02	105.35	111.82

There are no chirality outliers.

All (23) torsion outliers are listed below:

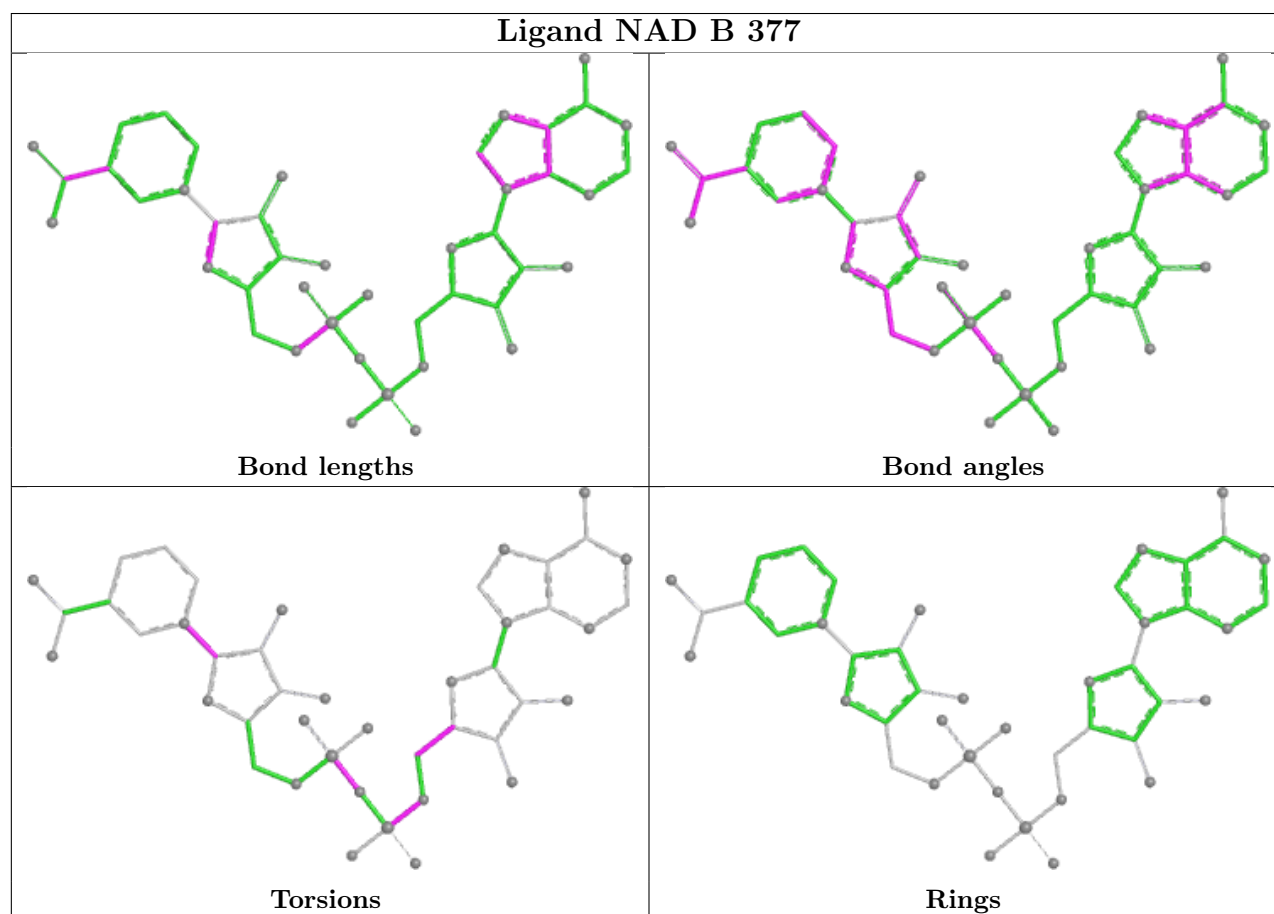
Mol	Chain	Res	Type	Atoms
3	A	377	NAD	C5B-O5B-PA-O1A
3	A	377	NAD	C5B-O5B-PA-O2A
3	A	377	NAD	C5B-O5B-PA-O3
3	A	377	NAD	O4D-C1D-N1N-C6N
3	A	377	NAD	C2D-C1D-N1N-C6N
3	B	377	NAD	C5B-O5B-PA-O1A
3	B	377	NAD	C5B-O5B-PA-O2A
3	B	377	NAD	C5B-O5B-PA-O3
3	B	377	NAD	O4D-C1D-N1N-C2N
3	B	377	NAD	O4D-C1D-N1N-C6N
3	B	377	NAD	C2D-C1D-N1N-C2N
3	B	377	NAD	C2D-C1D-N1N-C6N
3	B	377	NAD	C3B-C4B-C5B-O5B
3	B	377	NAD	O4B-C4B-C5B-O5B
3	A	377	NAD	PN-O3-PA-O1A
3	A	377	NAD	PN-O3-PA-O5B
3	A	377	NAD	C2B-C1B-N9A-C8A
3	A	377	NAD	PA-O3-PN-O1N
3	A	377	NAD	C2D-C1D-N1N-C2N
3	A	377	NAD	O4D-C1D-N1N-C2N
3	A	377	NAD	PA-O3-PN-O2N
3	A	377	NAD	O4B-C4B-C5B-O5B
3	B	377	NAD	PA-O3-PN-O1N

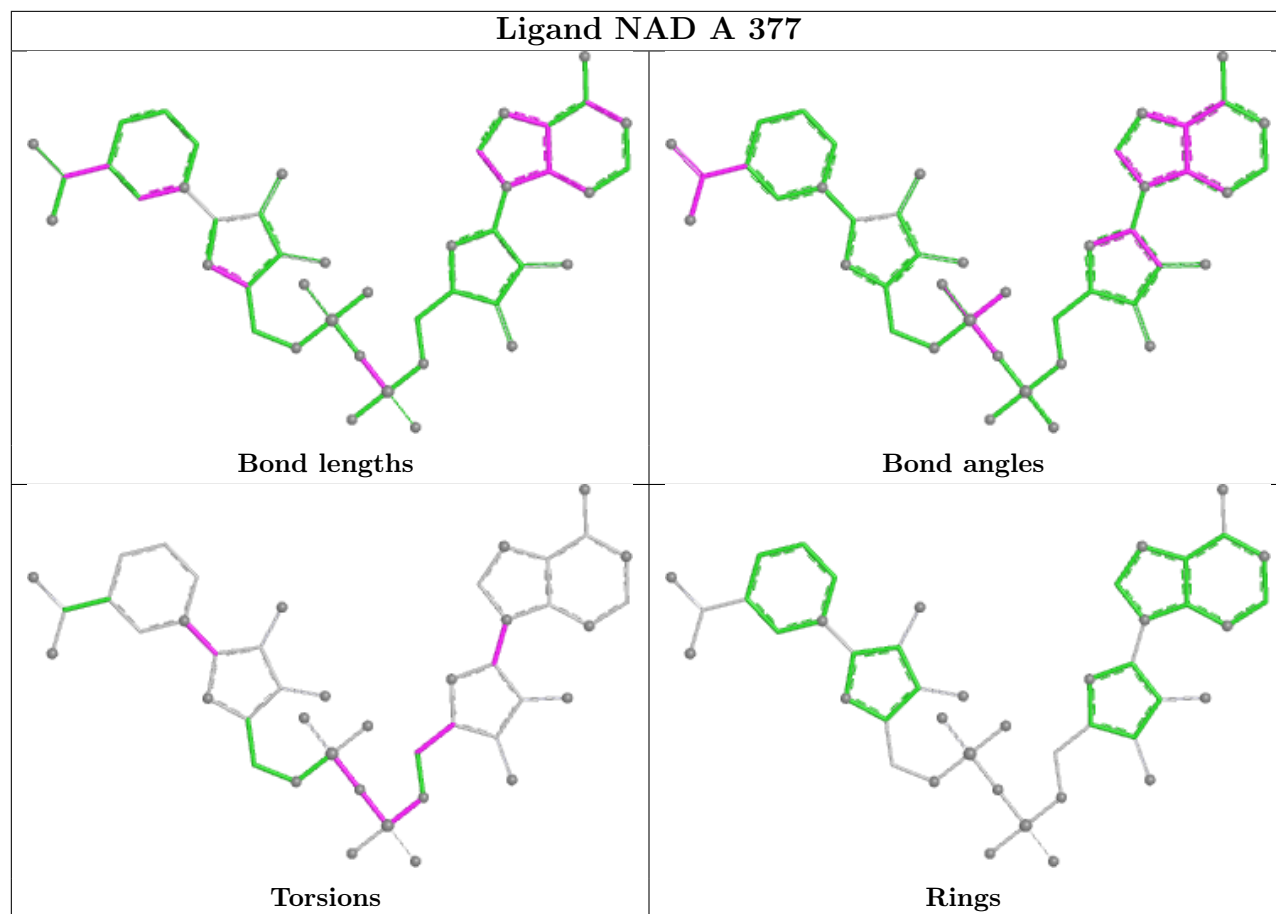
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	377	NAD	4	0
3	A	377	NAD	5	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.