



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:04 AM UTC

PDB ID : 3BTO / pdb_00003bto
Title : HORSE LIVER ALCOHOL DEHYDROGENASE COMPLEXED TO NADH
AND (1S,3S)3-BUTYLTHIOLANE 1-OXIDE
Authors : Ramaswamy, S.; Plapp, B.V.
Deposited on : 1996-11-08
Resolution : 1.66 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

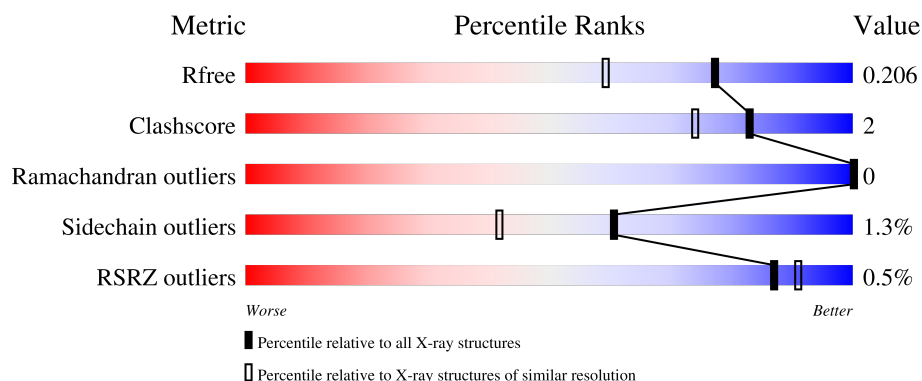
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

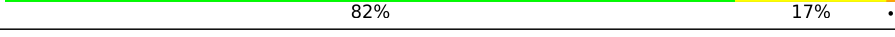
The reported resolution of this entry is 1.66 Å.

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))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	
1	C	374	
1	D	374	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12979 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.

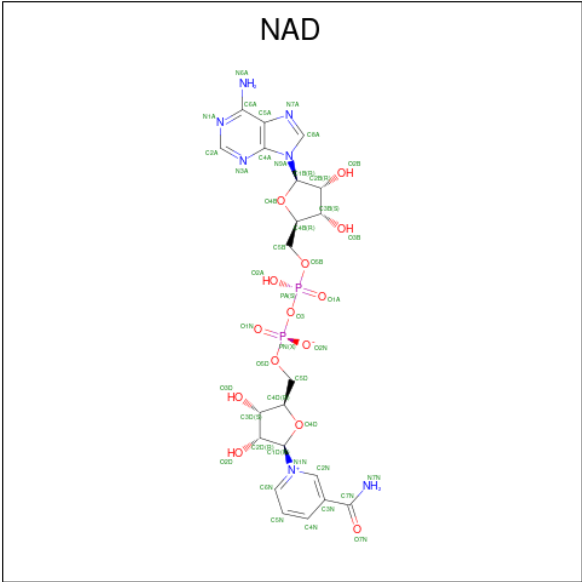
- Molecule 1 is a protein called LIVER ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	B	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	C	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	D	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			

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

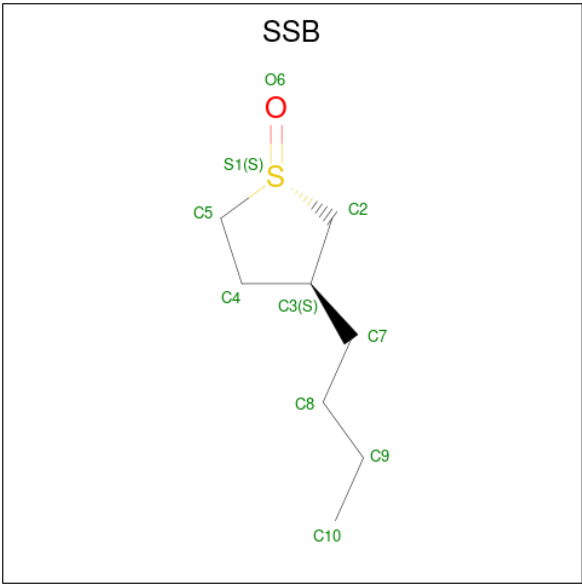
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- 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	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

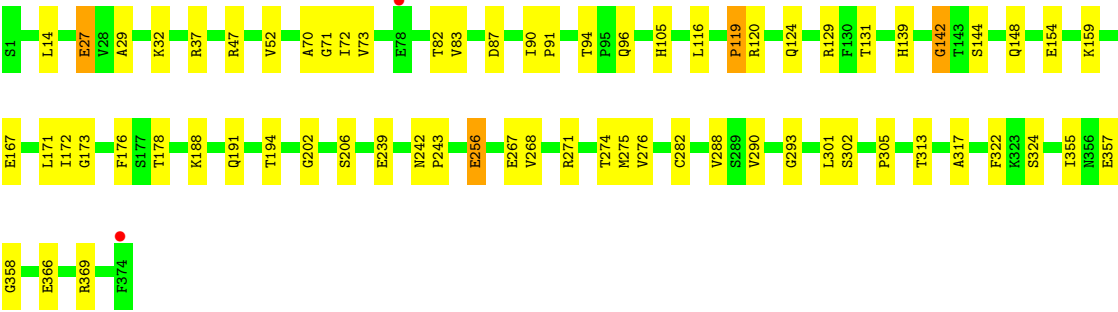
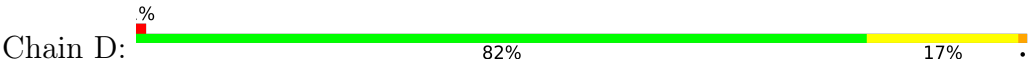
- Molecule 4 is 3-BUTYLTHIOLANE 1-OXIDE (CCD ID: SSB) (formula: C₈H₁₆OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 10 8 1 1	0	0
4	B	1	Total C O S 10 8 1 1	0	0
4	C	1	Total C O S 10 8 1 1	0	0
4	D	1	Total C O S 10 8 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	376	Total O 376 376	0	0
5	B	437	Total O 437 437	0	0
5	C	406	Total O 406 406	0	0
5	D	396	Total O 396 396	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.93Å 180.20Å 86.80Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.66 20.00 – 1.66	Depositor EDS
% Data completeness (in resolution range)	89.8 (20.00-1.66) 89.6 (20.00-1.66)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 1.66Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.223 0.175 , 0.206	Depositor DCC
R_{free} test set	1554 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	10.9	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12979	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1322e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SSB, 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	1.18	3/2837 (0.1%)	1.98	80/3834 (2.1%)
1	B	1.21	1/2837 (0.0%)	1.96	81/3834 (2.1%)
1	C	1.08	1/2837 (0.0%)	1.82	45/3834 (1.2%)
1	D	1.14	0/2837	1.90	65/3834 (1.7%)
All	All	1.15	5/11348 (0.0%)	1.91	271/15336 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	316	GLY	N-CA	6.55	1.51	1.45
1	A	42	ALA	CA-C	6.36	1.60	1.52
1	A	316	GLY	N-CA	6.33	1.51	1.45
1	A	328	VAL	CA-C	5.39	1.57	1.52
1	B	69	ALA	N-CA	5.34	1.52	1.46

All (271) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ALA	O-C-N	11.42	136.24	123.33
1	A	328	VAL	O-C-N	11.28	128.08	120.07
1	A	30	PRO	N-CA-CB	11.05	109.38	103.19
1	A	324	SER	CA-C-O	-9.34	110.52	120.42
1	D	37	ARG	CA-C-O	9.33	130.60	120.43
1	D	90	ILE	CA-C-N	9.29	129.06	119.76
1	D	90	ILE	C-N-CA	9.29	129.06	119.76
1	B	59	THR	O-C-N	9.25	129.04	121.83
1	A	342	LEU	CA-C-O	9.16	128.94	118.77
1	D	256	GLU	CB-CG-CD	9.07	128.02	112.60
1	A	70	ALA	O-C-N	8.96	133.45	123.33
1	B	30	PRO	N-CA-CB	8.82	108.13	103.19
1	A	148	GLN	O-C-N	-8.57	112.19	122.22
1	A	315	LYS	O-C-N	8.51	132.88	123.10
1	D	324	SER	O-C-N	8.51	131.85	122.15
1	B	120	ARG	CA-CB-CG	8.32	130.75	114.10
1	A	42	ALA	CA-C-O	-8.23	111.78	120.99
1	B	291	ILE	O-C-N	8.22	132.97	122.94
1	A	84	ARG	O-C-N	-8.17	116.48	121.71
1	A	291	ILE	O-C-N	8.10	132.83	122.94
1	A	59	THR	O-C-N	8.09	127.51	121.85
1	B	69	ALA	CA-C-O	7.98	129.85	121.31
1	A	43	THR	CA-C-O	7.93	130.29	120.54
1	B	353	GLU	CB-CG-CD	7.82	125.89	112.60
1	A	342	LEU	O-C-N	-7.78	113.78	122.34
1	B	176	PHE	CA-CB-CG	-7.65	106.15	113.80
1	B	43	THR	CA-C-O	7.59	129.71	120.60
1	A	177	SER	O-C-N	7.59	130.16	122.12
1	A	332	VAL	O-C-N	7.48	129.13	121.87
1	A	315	LYS	CA-C-N	-7.38	112.58	122.03
1	A	315	LYS	C-N-CA	-7.38	112.58	122.03
1	B	173	GLY	CA-C-O	-7.36	110.81	119.50
1	B	70	ALA	O-C-N	7.36	131.64	123.33
1	B	328	VAL	O-C-N	7.35	125.29	120.07
1	B	84	ARG	O-C-N	-7.34	117.01	121.71
1	A	332	VAL	CA-C-O	-7.33	113.33	120.95
1	A	84	ARG	CA-C-O	7.24	127.16	120.50
1	D	91	PRO	N-CA-CB	7.23	110.07	103.34
1	D	29	ALA	CA-C-O	7.19	128.82	120.69
1	A	317	ALA	O-C-N	7.16	131.08	123.42
1	A	117	SER	N-CA-C	7.15	118.72	111.07
1	A	292	VAL	CA-C-N	7.13	126.77	119.92
1	A	292	VAL	C-N-CA	7.13	126.77	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	315	LYS	CA-C-N	-7.13	112.90	122.03
1	C	315	LYS	C-N-CA	-7.13	112.90	122.03
1	A	324	SER	O-C-N	7.11	130.26	122.15
1	A	203	VAL	CA-C-O	-7.08	113.13	120.71
1	C	324	SER	O-C-N	7.01	129.66	122.09
1	C	52	VAL	O-C-N	6.99	129.03	121.83
1	B	64	ILE	O-C-N	6.96	132.99	122.76
1	D	37	ARG	O-C-N	-6.91	115.47	123.27
1	D	293	GLY	CA-C-O	6.89	129.34	121.90
1	C	293	GLY	CA-C-O	6.84	129.50	121.71
1	D	206	SER	CA-C-O	-6.83	113.31	120.55
1	B	177	SER	O-C-N	6.81	129.09	122.07
1	A	305	PRO	N-CA-CB	6.79	109.80	103.41
1	B	138	HIS	O-C-N	6.78	130.85	122.86
1	B	305	PRO	N-CA-CB	6.75	109.76	103.41
1	B	337	ALA	O-C-N	-6.74	113.74	122.37
1	D	206	SER	O-C-N	6.72	129.24	122.12
1	B	299	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	D	96	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	D	96	GLN	CG-CD-OE1	6.68	134.17	120.80
1	C	96	GLN	OE1-CD-NE2	-6.67	115.93	122.60
1	B	42	ALA	O-C-N	6.66	131.21	123.41
1	A	29	ALA	CA-C-N	6.65	124.52	119.66
1	A	29	ALA	C-N-CA	6.65	124.52	119.66
1	C	157	VAL	CA-C-O	-6.58	113.86	120.90
1	D	154	GLU	O-C-N	6.58	129.92	122.22
1	D	52	VAL	O-C-N	6.56	128.59	121.83
1	B	220	ILE	CA-C-N	-6.56	115.21	121.57
1	B	220	ILE	C-N-CA	-6.56	115.21	121.57
1	C	96	GLN	CG-CD-OE1	6.53	133.87	120.80
1	A	333	ALA	CA-C-O	6.47	127.62	120.82
1	A	42	ALA	CA-C-N	-6.42	110.63	121.94
1	A	42	ALA	C-N-CA	-6.42	110.63	121.94
1	D	324	SER	CA-C-O	-6.42	113.61	120.42
1	A	164	SER	CA-C-N	6.36	127.78	119.84
1	A	164	SER	C-N-CA	6.36	127.78	119.84
1	B	29	ALA	CA-C-N	6.36	124.30	119.66
1	B	29	ALA	C-N-CA	6.36	124.30	119.66
1	D	144	SER	O-C-N	-6.35	115.26	123.32
1	A	203	VAL	O-C-N	6.33	130.20	121.84
1	D	302	SER	O-C-N	-6.33	115.77	123.30
1	D	148	GLN	OE1-CD-NE2	6.32	128.92	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	293	GLY	O-C-N	-6.31	115.15	122.91
1	C	34	HIS	CA-CB-CG	-6.30	107.50	113.80
1	C	358	GLY	CA-C-O	-6.28	114.22	121.00
1	D	139	HIS	O-C-N	6.28	129.97	122.94
1	C	120	ARG	N-CA-C	-6.27	105.76	113.41
1	C	317	ALA	O-C-N	6.27	130.13	123.42
1	B	296	PRO	N-CA-CB	6.25	108.90	103.27
1	A	207	VAL	O-C-N	6.25	128.19	121.94
1	B	315	LYS	O-C-N	6.25	130.29	123.10
1	C	324	SER	CA-C-O	-6.21	114.30	120.70
1	D	87	ASP	CA-C-O	-6.21	114.20	121.16
1	A	304	ASN	CA-C-N	6.20	126.32	119.87
1	A	304	ASN	C-N-CA	6.20	126.32	119.87
1	A	279	LEU	O-C-N	6.20	129.22	122.15
1	B	304	ASN	CA-C-N	6.20	126.31	119.87
1	B	304	ASN	C-N-CA	6.20	126.31	119.87
1	B	165	PRO	N-CA-CB	6.18	109.74	103.25
1	A	24	GLU	CB-CG-CD	-6.18	102.10	112.60
1	A	328	VAL	CA-C-O	-6.18	113.60	118.85
1	D	87	ASP	O-C-N	6.18	130.43	122.89
1	C	90	ILE	CA-C-N	6.16	126.10	119.76
1	C	90	ILE	C-N-CA	6.16	126.10	119.76
1	B	292	VAL	CA-C-O	-6.13	114.76	120.34
1	D	94	THR	O-C-N	6.12	128.88	121.29
1	B	343	ASP	O-C-N	-6.11	114.65	120.70
1	A	311	GLY	O-C-N	6.10	130.63	122.70
1	A	34	HIS	CA-CB-CG	-6.10	107.70	113.80
1	A	327	SER	CA-C-O	6.04	126.95	120.24
1	B	21	PHE	O-C-N	6.04	129.99	122.86
1	D	120	ARG	N-CA-C	-6.02	106.47	113.88
1	C	47	ARG	O-C-N	-6.01	115.19	122.22
1	C	124	GLN	OE1-CD-NE2	5.99	128.59	122.60
1	B	38	ILE	N-CA-C	5.98	116.55	108.17
1	B	203	VAL	CA-C-O	-5.96	114.34	120.71
1	B	110	PHE	CA-C-O	5.95	130.49	122.51
1	B	34	HIS	CA-CB-CG	-5.94	107.86	113.80
1	D	176	PHE	CA-CB-CG	-5.94	107.86	113.80
1	A	67	HIS	CA-CB-CG	-5.92	107.88	113.80
1	C	317	ALA	CA-C-O	-5.91	114.91	121.23
1	B	189	VAL	O-C-N	5.85	128.46	122.79
1	A	207	VAL	CA-C-O	-5.84	115.19	121.27
1	B	164	SER	CA-C-N	5.84	127.14	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	SER	C-N-CA	5.84	127.14	119.84
1	B	315	LYS	CA-C-N	-5.82	114.58	122.03
1	B	315	LYS	C-N-CA	-5.82	114.58	122.03
1	D	29	ALA	O-C-N	-5.80	114.93	121.43
1	B	327	SER	CA-C-N	-5.79	116.59	120.24
1	B	327	SER	C-N-CA	-5.79	116.59	120.24
1	C	170	CYS	CA-C-O	-5.78	113.73	120.20
1	B	332	VAL	CA-C-O	-5.78	115.05	121.17
1	A	69	ALA	CA-C-O	5.77	127.48	121.31
1	D	305	PRO	N-CA-CB	5.76	108.83	103.41
1	D	29	ALA	CA-C-N	5.76	123.81	119.66
1	D	29	ALA	C-N-CA	5.76	123.81	119.66
1	B	43	THR	O-C-N	-5.76	116.36	123.33
1	A	266	PHE	O-C-N	-5.75	116.58	123.31
1	C	43	THR	CA-C-N	-5.75	115.42	122.15
1	C	43	THR	C-N-CA	-5.75	115.42	122.15
1	C	110	PHE	CA-C-O	5.75	129.36	122.41
1	D	242	ASN	CA-C-N	5.73	125.58	119.28
1	D	242	ASN	C-N-CA	5.73	125.58	119.28
1	D	194	THR	CA-C-O	5.72	126.61	120.38
1	D	322	PHE	CA-CB-CG	5.72	119.52	113.80
1	B	297	ASP	O-C-N	5.70	129.92	122.97
1	C	279	LEU	O-C-N	5.69	127.93	122.07
1	B	170	CYS	CA-C-O	-5.69	113.67	120.10
1	B	186	VAL	CA-C-O	-5.69	113.64	121.15
1	A	143	THR	CA-C-O	-5.68	112.38	120.51
1	C	139	HIS	O-C-N	5.66	129.31	122.68
1	D	290	VAL	O-C-N	5.66	129.13	123.18
1	C	50	ASP	O-C-N	-5.65	116.13	122.12
1	B	337	ALA	CA-C-N	5.65	130.59	122.40
1	B	337	ALA	C-N-CA	5.65	130.59	122.40
1	D	47	ARG	O-C-N	-5.64	115.62	122.22
1	A	191	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	B	173	GLY	O-C-N	5.64	129.05	122.68
1	D	119	PRO	N-CA-CB	5.62	108.33	103.27
1	B	133	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	B	151	VAL	O-C-N	5.62	129.33	123.26
1	B	70	ALA	CA-C-O	-5.62	114.70	120.99
1	A	71	GLY	CA-C-O	5.61	126.66	121.38
1	D	202	GLY	O-C-N	5.61	127.58	122.19
1	A	201	GLY	O-C-N	-5.61	117.41	122.96
1	C	275	MET	N-CA-C	-5.59	105.26	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	THR	CA-C-O	-5.59	114.34	119.76
1	A	150	THR	O-C-N	-5.58	115.93	122.96
1	A	186	VAL	CA-C-O	-5.58	113.79	121.15
1	B	334	ASP	O-C-N	-5.58	116.21	122.12
1	B	178	THR	CA-C-O	-5.56	115.16	121.00
1	A	123	MET	CA-C-O	-5.56	116.17	122.01
1	D	73	VAL	O-C-N	5.56	129.05	122.66
1	D	313	THR	O-C-N	5.55	129.90	123.30
1	B	342	LEU	O-C-N	-5.54	115.78	122.48
1	D	70	ALA	CA-C-O	-5.53	115.15	121.40
1	B	69	ALA	N-CA-CB	-5.53	102.50	111.24
1	A	229	PHE	N-CA-C	5.52	117.38	111.36
1	C	91	PRO	O-C-N	5.52	129.71	123.03
1	D	14	LEU	O-C-N	-5.49	116.52	123.05
1	B	201	GLY	O-C-N	-5.49	117.93	122.92
1	B	312	ARG	CA-C-O	5.46	127.34	121.55
1	D	282	CYS	O-C-N	5.45	129.16	123.06
1	D	369	ARG	O-C-N	5.45	129.72	123.29
1	D	276	VAL	O-C-N	-5.44	116.23	121.83
1	B	356	ASN	CA-CB-CG	-5.42	107.18	112.60
1	C	52	VAL	CA-C-O	-5.42	115.11	120.85
1	C	176	PHE	CA-CB-CG	-5.41	108.39	113.80
1	D	293	GLY	O-C-N	-5.41	115.89	122.76
1	A	352	PHE	O-C-N	-5.40	116.39	122.12
1	A	148	GLN	OE1-CD-NE2	5.40	128.00	122.60
1	B	177	SER	CA-C-N	-5.39	113.53	120.65
1	B	177	SER	C-N-CA	-5.39	113.53	120.65
1	C	315	LYS	O-C-N	5.39	129.30	123.10
1	D	142	GLY	O-C-N	-5.38	116.18	122.31
1	C	296	PRO	N-CA-CB	5.37	108.11	103.27
1	A	311	GLY	CA-C-O	-5.34	111.28	120.57
1	A	333	ALA	O-C-N	-5.34	116.57	122.07
1	C	157	VAL	O-C-N	5.34	129.28	123.09
1	B	190	THR	CA-C-O	5.32	128.16	121.66
1	B	148	GLN	OE1-CD-NE2	5.32	127.92	122.60
1	A	345	LEU	CA-C-N	-5.31	115.97	122.93
1	A	345	LEU	C-N-CA	-5.31	115.97	122.93
1	B	342	LEU	CA-C-O	5.31	124.65	118.97
1	B	350	LEU	CA-C-O	5.30	125.38	120.50
1	C	119	PRO	N-CA-CB	5.30	107.89	103.17
1	D	358	GLY	CA-C-O	-5.29	115.30	120.75
1	D	243	PRO	N-CA-CB	5.29	109.10	103.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ALA	CA-C-O	-5.29	115.07	120.99
1	A	92	LEU	CA-C-O	-5.27	114.82	120.46
1	B	332	VAL	O-C-N	5.27	127.07	121.91
1	B	350	LEU	O-C-N	-5.27	118.34	121.71
1	C	9	CYS	CA-C-O	-5.26	115.68	121.31
1	C	360	ASP	CA-CB-CG	5.26	117.86	112.60
1	D	288	VAL	O-C-N	5.25	128.87	123.20
1	D	52	VAL	CA-C-O	-5.25	115.28	120.85
1	A	51	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	B	67	HIS	CA-CB-CG	-5.25	108.55	113.80
1	A	138	HIS	O-C-N	5.25	129.05	122.86
1	D	275	MET	O-C-N	5.25	127.47	122.07
1	A	87	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	40	MET	CG-SD-CE	5.24	112.43	100.90
1	C	302	SER	CA-C-O	5.24	126.02	120.36
1	C	67	HIS	CA-CB-CG	-5.24	108.56	113.80
1	A	176	PHE	CA-CB-CG	-5.23	108.57	113.80
1	D	172	ILE	O-C-N	-5.23	115.20	122.05
1	D	124	GLN	OE1-CD-NE2	5.23	127.83	122.60
1	C	290	VAL	O-C-N	5.22	128.90	123.26
1	D	105	HIS	CA-C-N	5.22	125.02	119.28
1	D	105	HIS	C-N-CA	5.22	125.02	119.28
1	B	83	VAL	O-C-N	5.21	128.91	123.02
1	B	92	LEU	O-C-N	5.21	129.69	123.13
1	B	175	GLY	O-C-N	5.20	127.17	122.18
1	C	73	VAL	O-C-N	5.20	127.97	122.67
1	A	64	ILE	O-C-N	5.20	130.40	122.76
1	A	337	ALA	CA-C-N	5.20	129.52	122.19
1	A	337	ALA	C-N-CA	5.20	129.52	122.19
1	B	68	GLU	CG-CD-OE1	5.20	130.35	118.40
1	C	369	ARG	O-C-N	5.18	129.38	123.27
1	C	161	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	268	VAL	CA-C-O	5.16	127.23	120.78
1	A	201	GLY	CA-C-O	5.14	127.32	121.92
1	A	86	GLY	O-C-N	5.14	128.71	122.60
1	C	288	VAL	O-C-N	5.12	128.57	123.10
1	D	72	ILE	O-C-N	-5.11	117.66	123.18
1	D	173	GLY	CA-C-N	-5.11	111.77	121.54
1	D	173	GLY	C-N-CA	-5.11	111.77	121.54
1	D	313	THR	CA-C-O	-5.11	114.84	120.36
1	B	42	ALA	CA-C-N	-5.09	113.61	122.37
1	B	42	ALA	C-N-CA	-5.09	113.61	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	MET	O-C-N	5.09	127.32	122.07
1	A	239	GLU	CA-C-O	-5.09	115.65	121.40
1	A	249	PRO	N-CA-CB	5.09	107.73	103.25
1	C	323	LYS	N-CA-C	-5.09	102.11	109.59
1	B	219	ILE	CA-C-O	5.08	124.74	120.22
1	B	110	PHE	O-C-N	-5.07	116.19	122.83
1	C	353	GLU	CB-CG-CD	5.05	121.19	112.60
1	A	63	VAL	O-C-N	5.05	128.33	122.82
1	D	178	THR	CA-C-O	-5.05	115.52	120.82
1	D	27	GLU	O-C-N	5.04	129.24	123.29
1	A	68	GLU	CA-C-O	-5.04	114.22	120.57
1	A	165	PRO	N-CA-CB	5.04	108.54	103.25
1	D	82	THR	N-CA-C	5.03	119.57	113.38
1	B	64	ILE	CA-C-O	-5.03	114.91	120.74
1	D	317	ALA	O-C-N	5.03	128.80	123.42
1	A	145	THR	OG1-CB-CG2	5.03	119.35	109.30
1	D	355	ILE	CA-C-O	-5.01	115.84	121.05
1	D	267	GLU	O-C-N	5.00	128.93	123.22

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	GLY	Mainchain
1	B	12	ALA	Mainchain
1	C	107	GLU	Mainchain
1	D	71	GLY	Mainchain

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	2785	0	2848	16	0
1	B	2785	0	2848	10	0
1	C	2785	0	2848	12	0
1	D	2785	0	2848	14	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	44	0	25	1	0
3	B	44	0	25	1	0
3	C	44	0	26	2	0
3	D	44	0	25	1	0
4	A	10	0	16	1	0
4	B	10	0	16	1	0
4	C	10	0	16	1	0
4	D	10	0	16	1	0
5	A	376	0	0	5	0
5	B	437	0	0	3	0
5	C	406	0	0	6	0
5	D	396	0	0	6	0
All	All	12979	0	11557	55	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 2.

All (55) 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:D:167:GLU:OE2	5:D:548:HOH:O	1.72	1.06
1:D:357:GLU:HG2	5:D:770:HOH:O	1.78	0.82
1:C:120:ARG:HB2	5:C:1041:HOH:O	1.94	0.67
1:D:167:GLU:HG3	5:D:766:HOH:O	1.96	0.66
1:A:230:ALA:O	1:A:234:GLU:HG3	1.99	0.63
1:A:248:LYS:HE2	5:A:745:HOH:O	1.98	0.63
1:A:39:LYS:NZ	5:A:601:HOH:O	2.31	0.62
1:C:234:GLU:HG2	5:C:1125:HOH:O	1.98	0.62
1:C:32:LYS:HE3	5:C:1029:HOH:O	2.01	0.60
1:D:32:LYS:HE3	1:D:129:ARG:CZ	2.35	0.56
1:D:119:PRO:HG3	5:D:769:HOH:O	2.05	0.56
1:B:118:MET:HG2	5:B:611:HOH:O	2.06	0.55
1:A:88:LYS:HD3	1:A:166:LEU:HD21	1.88	0.54
1:C:330:LYS:HG3	5:C:1078:HOH:O	2.06	0.54
1:B:116:LEU:HG	1:B:141:LEU:HD22	1.88	0.54
1:B:279:LEU:HD22	1:B:312:ARG:HD3	1.91	0.52
3:D:377:NAD:C3N	4:D:378:SSB:H22	2.39	0.52
1:A:17:GLU:OE2	1:B:338:LYS:NZ	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:LEU:HD22	1:C:312:ARG:HD3	1.93	0.51
1:D:167:GLU:H	1:D:167:GLU:CD	2.19	0.51
1:C:347:THR:HG21	5:C:1175:HOH:O	2.11	0.50
3:B:377:NAD:C3N	4:B:378:SSB:H22	2.44	0.48
3:A:377:NAD:C3N	4:A:378:SSB:H22	2.43	0.48
3:C:377:NAD:C3N	4:C:378:SSB:H22	2.43	0.48
1:B:61:LEU:HB3	1:B:62:PRO:HA	1.95	0.48
1:A:138:HIS:HE1	5:A:730:HOH:O	1.96	0.47
1:C:26:VAL:HG12	1:C:132:CYS:HB2	1.96	0.47
1:C:178:THR:HG21	3:C:377:NAD:C4N	2.45	0.47
1:A:199:GLY:O	1:A:204:GLY:HA3	2.15	0.46
1:D:366:GLU:O	1:D:366:GLU:HG2	2.15	0.46
1:A:248:LYS:HB2	1:A:249:PRO:HD2	1.98	0.45
1:C:83:VAL:HG12	1:C:159:LYS:HB2	1.98	0.45
1:D:271:ARG:HB2	1:D:274:THR:OG1	2.17	0.45
1:A:68:GLU:OE2	1:A:174:CYS:HB3	2.17	0.45
1:B:299:GLN:NE2	5:B:728:HOH:O	2.50	0.44
1:C:357:GLU:HG3	5:C:1024:HOH:O	2.17	0.44
1:B:142:GLY:HA2	5:B:618:HOH:O	2.18	0.43
1:A:306:MET:HE2	1:A:306:MET:HA	2.00	0.43
1:C:301:LEU:C	1:C:301:LEU:HD12	2.42	0.43
1:A:116:LEU:HG	1:A:141:LEU:HD22	2.00	0.42
1:A:350:LEU:O	1:A:372:LEU:HA	2.20	0.42
1:A:350:LEU:HB3	1:A:351:PRO:HD2	2.02	0.42
1:B:369:ARG:HH11	1:B:369:ARG:HD3	1.71	0.42
1:A:336:MET:HE3	5:A:644:HOH:O	2.19	0.42
1:C:70:ALA:HB1	1:C:166:LEU:HD22	2.01	0.42
1:D:142:GLY:HA2	5:D:617:HOH:O	2.20	0.41
1:A:142:GLY:HA2	5:A:672:HOH:O	2.21	0.41
1:A:56:THR:HG23	1:A:296:PRO:HA	2.03	0.41
1:D:171:LEU:HD23	1:D:171:LEU:HA	1.91	0.41
1:D:83:VAL:HG12	1:D:159:LYS:HB2	2.02	0.41
1:B:271:ARG:HB2	1:B:274:THR:OG1	2.21	0.41
1:D:301:LEU:C	1:D:301:LEU:HD12	2.46	0.41
1:D:27:GLU:HB2	1:D:131:THR:OG1	2.21	0.40
1:B:306:MET:HA	1:B:306:MET:HE2	2.03	0.40
1:D:188:LYS:HD2	5:D:695:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/374 (100%)	360 (97%)	12 (3%)	0	100	100
1	B	372/374 (100%)	360 (97%)	12 (3%)	0	100	100
1	C	372/374 (100%)	361 (97%)	11 (3%)	0	100	100
1	D	372/374 (100%)	361 (97%)	11 (3%)	0	100	100
All	All	1488/1496 (100%)	1442 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/308 (100%)	305 (99%)	3 (1%)	68	52
1	B	308/308 (100%)	303 (98%)	5 (2%)	55	34
1	C	308/308 (100%)	305 (99%)	3 (1%)	68	52
1	D	308/308 (100%)	303 (98%)	5 (2%)	55	34
All	All	1232/1232 (100%)	1216 (99%)	16 (1%)	61	42

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	84	ARG

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Mol	Chain	Res	Type
1	A	268	VAL
1	B	40	MET
1	B	164	SER
1	B	268	VAL
1	B	279	LEU
1	B	309	LEU
1	C	268	VAL
1	C	279	LEU
1	C	330	LYS
1	D	116	LEU
1	D	191	GLN
1	D	239	GLU
1	D	256	GLU
1	D	268	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	ASN
1	A	300	ASN
1	B	138	HIS
1	B	299	GLN
1	D	300	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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	C	377	-	46,48,48	2.17	18 (39%)	64,73,73	2.31	18 (28%)
4	SSB	C	378	2	9,10,10	1.27	1 (11%)	8,12,12	0.98	0
4	SSB	B	378	2	9,10,10	1.51	1 (11%)	8,12,12	1.32	2 (25%)
3	NAD	B	377	-	46,48,48	2.31	16 (34%)	64,73,73	2.70	21 (32%)
3	NAD	A	377	-	46,48,48	2.23	17 (36%)	64,73,73	2.48	16 (25%)
3	NAD	D	377	-	46,48,48	2.22	20 (43%)	64,73,73	2.66	19 (29%)
4	SSB	D	378	2	9,10,10	1.06	0	8,12,12	1.22	0
4	SSB	A	378	2	9,10,10	1.50	1 (11%)	8,12,12	1.43	2 (25%)

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	C	377	-	-	4/30/62/62	0/5/5/5
4	SSB	C	378	2	-	0/4/13/13	0/1/1/1
4	SSB	B	378	2	-	0/4/13/13	0/1/1/1
3	NAD	B	377	-	-	4/30/62/62	0/5/5/5
3	NAD	A	377	-	-	4/30/62/62	0/5/5/5
3	NAD	D	377	-	-	6/30/62/62	0/5/5/5
4	SSB	D	378	2	-	0/4/13/13	0/1/1/1
4	SSB	A	378	2	-	0/4/13/13	0/1/1/1

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	377	NAD	PA-O3	-6.79	1.52	1.59
3	C	377	NAD	PN-O3	6.31	1.66	1.59
3	B	377	NAD	C7N-N7N	5.89	1.43	1.33
3	A	377	NAD	O4D-C1D	5.61	1.48	1.40
3	D	377	NAD	PN-O3	5.60	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	377	NAD	C2A-N3A	5.33	1.43	1.33
3	A	377	NAD	C7N-N7N	5.15	1.42	1.33
3	B	377	NAD	C2A-N3A	4.49	1.41	1.33
3	C	377	NAD	C2A-N3A	4.40	1.41	1.33
3	A	377	NAD	C2A-N3A	4.26	1.41	1.33
3	A	377	NAD	C4N-C3N	4.18	1.45	1.39
3	A	377	NAD	PA-O3	-4.10	1.55	1.59
3	B	377	NAD	C4N-C3N	3.80	1.45	1.39
3	D	377	NAD	O4D-C4D	3.79	1.53	1.45
3	B	377	NAD	C2N-C3N	-3.78	1.33	1.39
3	C	377	NAD	O4D-C4D	3.74	1.53	1.45
3	C	377	NAD	C2N-N1N	3.68	1.39	1.35
3	D	377	NAD	C2N-N1N	3.60	1.38	1.35
3	D	377	NAD	C3N-C7N	3.59	1.55	1.50
3	B	377	NAD	O2B-C2B	-3.42	1.34	1.43
3	B	377	NAD	C5A-N7A	-3.41	1.32	1.39
3	C	377	NAD	C3N-C7N	3.40	1.55	1.50
3	D	377	NAD	C4N-C3N	3.35	1.44	1.39
3	A	377	NAD	O3B-C3B	3.33	1.51	1.43
3	A	377	NAD	O2B-C2B	-3.32	1.34	1.43
3	D	377	NAD	PA-O3	-3.28	1.56	1.59
3	D	377	NAD	C5A-N7A	-3.22	1.33	1.39
4	A	378	SSB	C2-C3	3.20	1.59	1.52
3	A	377	NAD	C6N-N1N	3.06	1.42	1.35
3	C	377	NAD	O4D-C1D	3.03	1.44	1.40
3	C	377	NAD	C4A-N9A	3.02	1.44	1.37
3	A	377	NAD	PN-O3	-3.00	1.56	1.59
3	B	377	NAD	PN-O3	2.96	1.62	1.59
3	A	377	NAD	C5A-C6A	2.90	1.49	1.41
3	C	377	NAD	C5A-N7A	-2.88	1.33	1.39
4	B	378	SSB	C2-C3	2.85	1.58	1.52
3	C	377	NAD	C5A-C6A	2.84	1.48	1.41
3	C	377	NAD	C4N-C3N	2.82	1.43	1.39
3	B	377	NAD	C5A-C6A	2.80	1.48	1.41
3	D	377	NAD	C5A-C6A	2.77	1.48	1.41
3	D	377	NAD	C5N-C4N	2.71	1.43	1.38
3	D	377	NAD	O2D-C2D	-2.70	1.36	1.43
3	A	377	NAD	C4A-N9A	2.70	1.43	1.37
3	A	377	NAD	C6N-C5N	-2.69	1.33	1.38
3	A	377	NAD	C4A-N3A	2.66	1.39	1.34
3	D	377	NAD	C7N-N7N	2.64	1.37	1.33
3	D	377	NAD	O4D-C1D	2.64	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	378	SSB	C2-C3	2.61	1.58	1.52
3	A	377	NAD	C2N-C3N	-2.61	1.34	1.39
3	C	377	NAD	O4B-C4B	2.59	1.50	1.45
3	D	377	NAD	C2N-C3N	-2.57	1.34	1.39
3	C	377	NAD	C4A-N3A	2.51	1.39	1.34
3	C	377	NAD	O2B-C2B	-2.46	1.36	1.43
3	B	377	NAD	O4B-C4B	2.46	1.50	1.45
3	A	377	NAD	C5A-N7A	-2.46	1.34	1.39
3	B	377	NAD	C6N-N1N	2.45	1.40	1.35
3	B	377	NAD	O4D-C1D	2.43	1.44	1.40
3	D	377	NAD	C4A-N9A	2.39	1.42	1.37
3	B	377	NAD	C3N-C7N	2.35	1.54	1.50
3	C	377	NAD	PN-O2N	-2.35	1.44	1.55
3	B	377	NAD	C3D-C4D	2.28	1.58	1.53
3	B	377	NAD	O4D-C4D	2.28	1.50	1.45
3	C	377	NAD	C2N-C3N	-2.26	1.35	1.39
3	C	377	NAD	C7N-N7N	2.26	1.37	1.33
3	C	377	NAD	C5N-C4N	2.23	1.42	1.38
3	D	377	NAD	PN-O2N	-2.23	1.45	1.55
3	D	377	NAD	O4B-C4B	2.21	1.49	1.45
3	A	377	NAD	O4B-C4B	2.20	1.49	1.45
3	C	377	NAD	O2D-C2D	-2.19	1.37	1.43
3	D	377	NAD	O2B-C2B	-2.15	1.37	1.43
3	B	377	NAD	O5D-C5D	2.08	1.52	1.44
3	A	377	NAD	O4D-C4D	2.08	1.49	1.45
3	D	377	NAD	C4A-N3A	2.02	1.38	1.34
3	D	377	NAD	C3B-C4B	2.02	1.58	1.53

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	377	NAD	C5N-C4N-C3N	-9.36	111.17	120.36
3	B	377	NAD	C5N-C4N-C3N	-9.13	111.39	120.36
3	A	377	NAD	C5N-C4N-C3N	-8.43	112.08	120.36
3	D	377	NAD	C2A-N1A-C6A	8.25	132.29	118.73
3	B	377	NAD	O7N-C7N-C3N	8.20	129.62	119.60
3	D	377	NAD	C2N-C3N-C4N	7.75	127.27	118.26
3	B	377	NAD	C2A-N1A-C6A	7.12	130.43	118.73
3	C	377	NAD	C5N-C4N-C3N	-7.10	113.38	120.36
3	A	377	NAD	C2A-N1A-C6A	7.03	130.29	118.73
3	C	377	NAD	C2N-C3N-C4N	7.02	126.43	118.26
3	C	377	NAD	C2A-N1A-C6A	6.65	129.66	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	377	NAD	N3A-C2A-N1A	-6.40	118.89	128.58
3	B	377	NAD	C2N-C3N-C4N	6.05	125.30	118.26
3	B	377	NAD	N3A-C2A-N1A	-5.93	119.61	128.58
3	A	377	NAD	O7N-C7N-C3N	5.83	126.73	119.60
3	A	377	NAD	C2N-C3N-C4N	5.09	124.18	118.26
3	A	377	NAD	C3N-C7N-N7N	-4.94	111.65	117.74
3	A	377	NAD	N3A-C2A-N1A	-4.81	121.31	128.58
3	A	377	NAD	C6N-C5N-C4N	4.75	126.30	119.45
3	C	377	NAD	N3A-C2A-N1A	-4.69	121.48	128.58
3	B	377	NAD	C3N-C7N-N7N	-4.59	112.09	117.74
3	B	377	NAD	C6N-C5N-C4N	4.58	126.06	119.45
3	C	377	NAD	C4A-N9A-C8A	-4.12	101.42	105.74
3	A	377	NAD	C1B-N9A-C8A	4.05	136.09	127.09
3	B	377	NAD	C2B-C3B-C4B	4.02	110.37	102.61
3	C	377	NAD	C6N-N1N-C2N	3.90	125.19	121.88
3	D	377	NAD	C4A-N9A-C8A	-3.89	101.65	105.74
3	D	377	NAD	O2A-PA-O1A	3.88	130.47	112.44
3	D	377	NAD	C6N-N1N-C2N	3.81	125.12	121.88
3	A	377	NAD	C4A-N9A-C8A	-3.73	101.82	105.74
3	D	377	NAD	O3-PA-O1A	-3.73	99.48	110.70
3	A	377	NAD	C2B-C3B-C4B	3.72	109.80	102.61
3	D	377	NAD	C6N-C5N-C4N	3.55	124.56	119.45
3	D	377	NAD	O4B-C1B-N9A	-3.29	101.77	108.09
3	D	377	NAD	N6A-C6A-N1A	3.28	125.68	118.38
3	B	377	NAD	C4A-N9A-C8A	-3.23	102.34	105.74
3	B	377	NAD	N6A-C6A-N1A	3.19	125.49	118.38
3	C	377	NAD	O2A-PA-O1A	3.12	126.94	112.44
3	C	377	NAD	C4B-O4B-C1B	-3.11	102.60	109.47
3	C	377	NAD	O4B-C1B-N9A	-3.08	102.17	108.09
3	D	377	NAD	C1B-N9A-C8A	3.07	133.90	127.09
3	B	377	NAD	O7N-C7N-N7N	-3.02	118.25	122.62
3	C	377	NAD	C1B-N9A-C8A	2.95	133.64	127.09
3	D	377	NAD	C2B-C3B-C4B	2.92	108.25	102.61
3	B	377	NAD	C1B-N9A-C8A	2.90	133.54	127.09
3	A	377	NAD	N6A-C6A-N1A	2.89	124.81	118.38
3	D	377	NAD	C5A-C6A-N1A	-2.81	110.37	117.51
3	A	377	NAD	O2B-C2B-C3B	2.80	120.80	111.82
3	B	377	NAD	C6N-N1N-C1D	-2.78	114.27	119.73
3	B	377	NAD	C2D-C3D-C4D	2.75	107.93	102.61
3	C	377	NAD	C2B-C3B-C4B	2.75	107.91	102.61
3	D	377	NAD	C5N-C6N-N1N	-2.74	116.64	120.38
3	A	377	NAD	C2D-C3D-C4D	2.70	107.82	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	377	NAD	C5A-C6A-N1A	-2.60	110.91	117.51
3	D	377	NAD	C4B-O4B-C1B	-2.58	103.77	109.47
3	C	377	NAD	C5A-C6A-N1A	-2.56	111.01	117.51
4	A	378	SSB	C7-C3-C2	-2.53	107.63	115.42
3	B	377	NAD	C5N-C6N-N1N	-2.48	116.99	120.38
3	C	377	NAD	C3B-C2B-C1B	-2.47	96.79	101.46
3	C	377	NAD	N6A-C6A-N1A	2.45	123.82	118.38
3	B	377	NAD	C3B-C2B-C1B	-2.40	96.93	101.46
3	B	377	NAD	O2B-C2B-C3B	2.35	119.37	111.82
3	C	377	NAD	C6N-C5N-C4N	2.33	122.81	119.45
3	D	377	NAD	O4D-C4D-C3D	-2.27	100.65	105.15
4	A	378	SSB	C7-C3-C4	-2.25	106.96	115.45
3	D	377	NAD	C3B-C2B-C1B	-2.22	97.27	101.46
4	B	378	SSB	C7-C3-C2	-2.19	108.69	115.42
3	D	377	NAD	O3D-C3D-C4D	2.16	117.28	111.08
4	B	378	SSB	C7-C3-C4	-2.14	107.35	115.45
3	C	377	NAD	C5D-C4D-C3D	2.14	122.91	115.21
3	B	377	NAD	C5A-C6A-N1A	-2.13	112.10	117.51
3	B	377	NAD	C4N-C3N-C7N	-2.12	115.29	121.06
3	C	377	NAD	O4B-C4B-C5B	-2.08	102.67	109.33
3	B	377	NAD	O2A-PA-O5B	-2.06	98.23	107.57
3	A	377	NAD	C4D-O4D-C1D	2.04	111.79	109.92
3	C	377	NAD	O3-PA-O1A	-2.03	104.60	110.70
3	B	377	NAD	C2N-N1N-C1D	2.02	123.59	119.13
3	A	377	NAD	O4B-C4B-C3B	-2.00	101.18	105.15

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	O4D-C1D-N1N-C2N
3	B	377	NAD	O4D-C1D-N1N-C6N
3	B	377	NAD	C2D-C1D-N1N-C2N
3	C	377	NAD	O4D-C1D-N1N-C2N
3	C	377	NAD	O4D-C1D-N1N-C6N
3	C	377	NAD	C2D-C1D-N1N-C2N
3	C	377	NAD	C2D-C1D-N1N-C6N
3	D	377	NAD	C5B-O5B-PA-O1A

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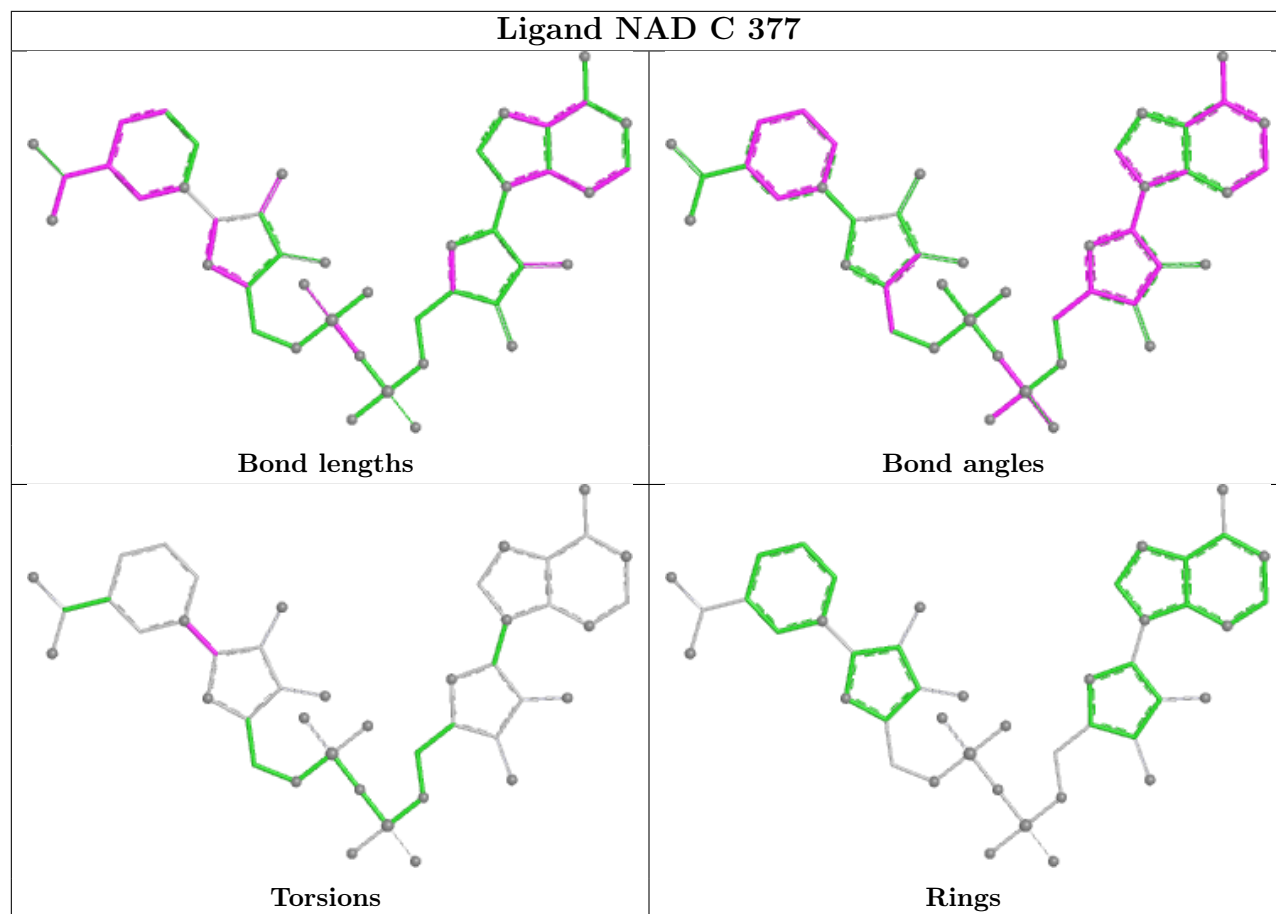
Mol	Chain	Res	Type	Atoms
3	D	377	NAD	O4D-C1D-N1N-C2N
3	D	377	NAD	O4D-C1D-N1N-C6N
3	D	377	NAD	C2D-C1D-N1N-C2N
3	D	377	NAD	C2D-C1D-N1N-C6N
3	B	377	NAD	C2D-C1D-N1N-C6N
3	D	377	NAD	O4B-C4B-C5B-O5B

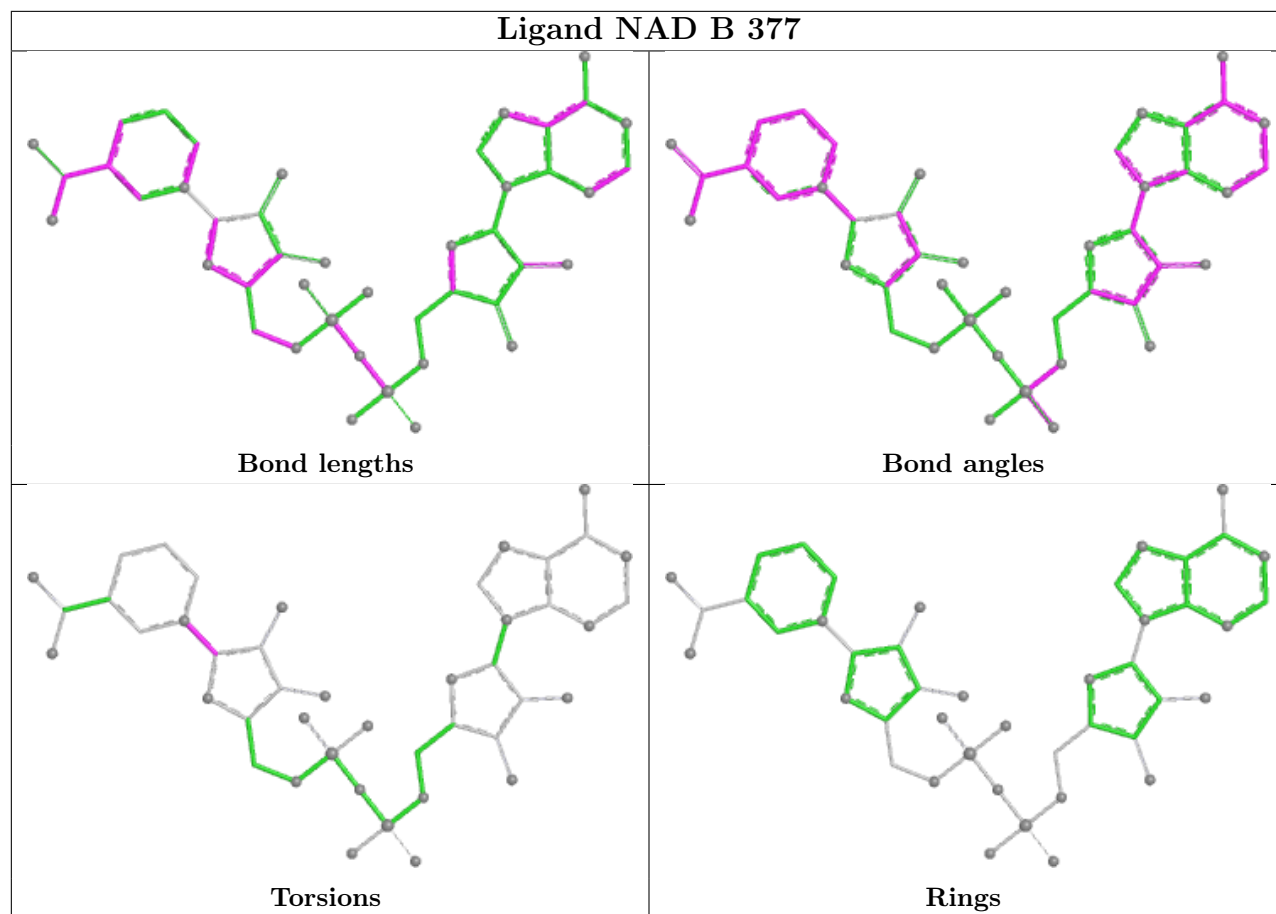
There are no ring outliers.

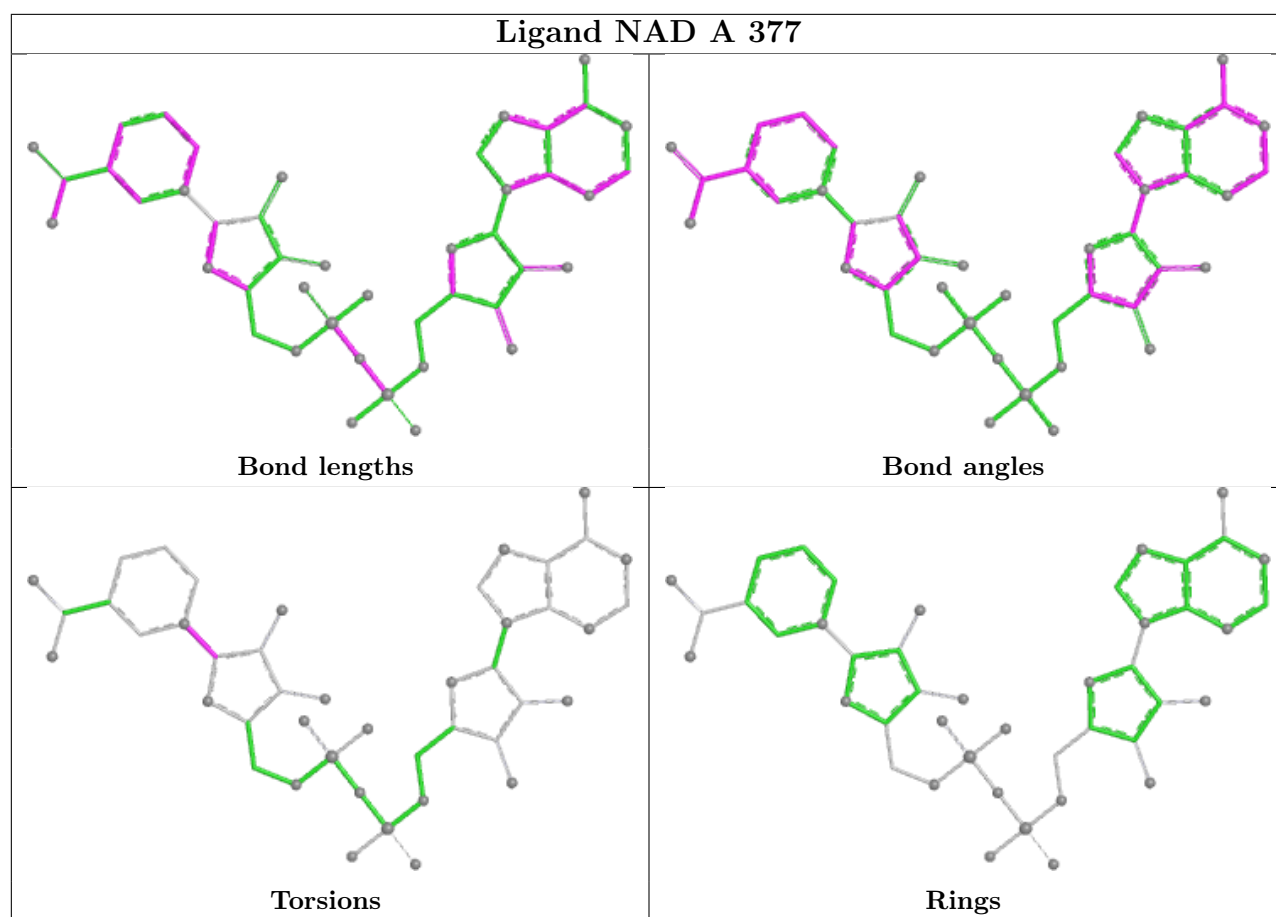
8 monomers are involved in 5 short contacts:

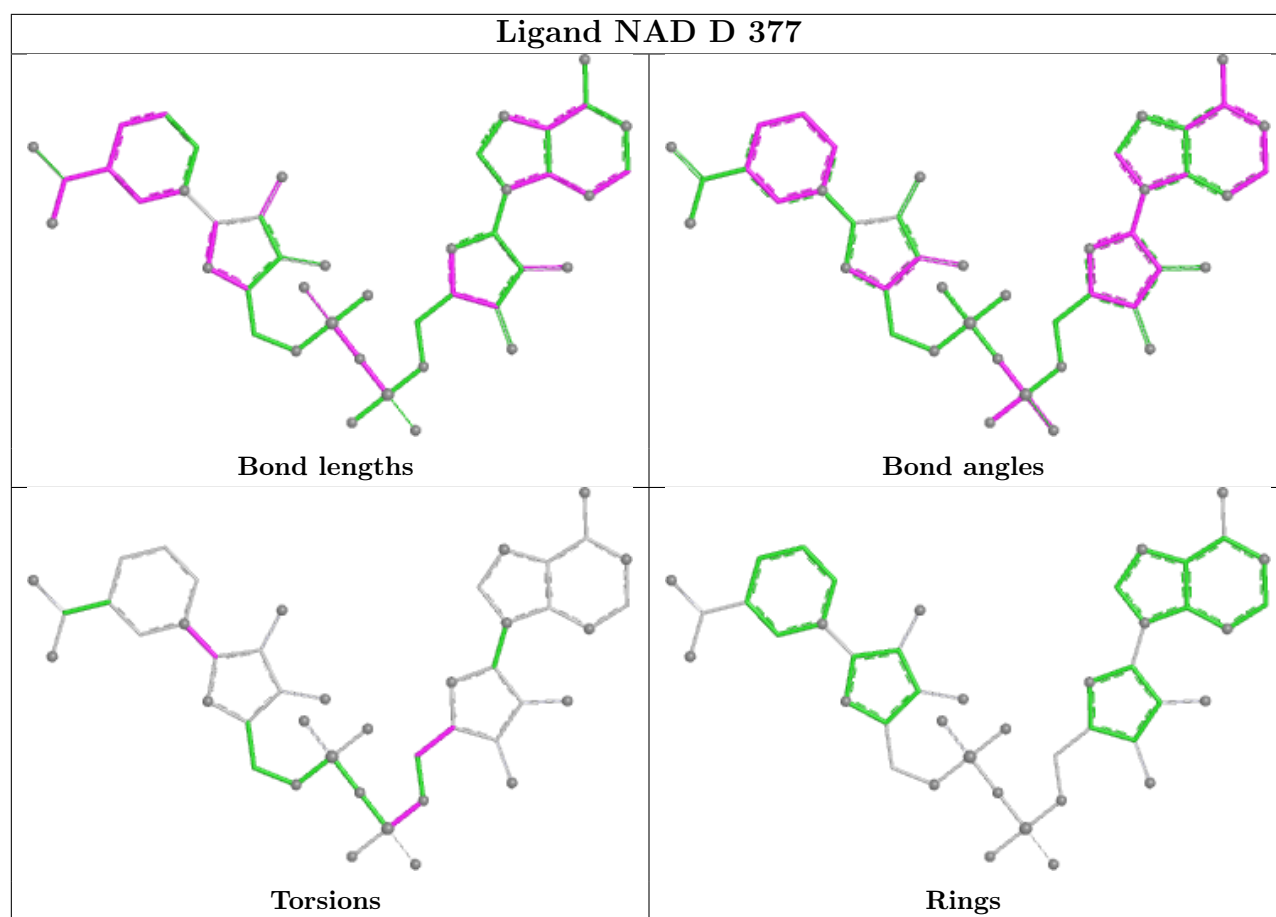
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	377	NAD	2	0
4	C	378	SSB	1	0
4	B	378	SSB	1	0
3	B	377	NAD	1	0
3	A	377	NAD	1	0
3	D	377	NAD	1	0
4	D	378	SSB	1	0
4	A	378	SSB	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.11	1 (0%) 90 93	6, 12, 23, 33	0
1	B	374/374 (100%)	-0.10	1 (0%) 90 93	5, 11, 21, 31	0
1	C	374/374 (100%)	0.16	3 (0%) 82 87	7, 13, 23, 33	0
1	D	374/374 (100%)	-0.05	2 (0%) 87 91	6, 13, 23, 35	0
All	All	1496/1496 (100%)	-0.03	7 (0%) 87 91	5, 12, 23, 35	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	84	ARG	3.5
1	A	336	MET	2.5
1	D	78	GLU	2.5
1	B	116	LEU	2.4
1	C	366	GLU	2.3
1	D	374	PHE	2.2
1	C	234	GLU	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 ⓘ

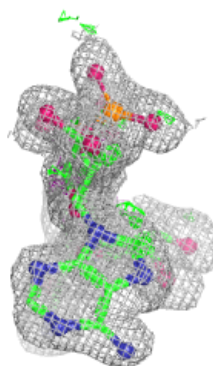
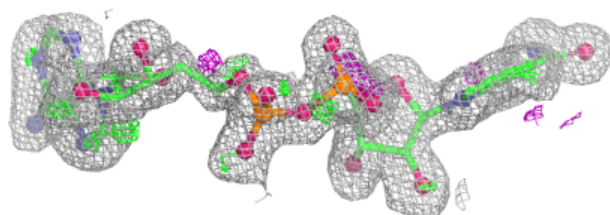
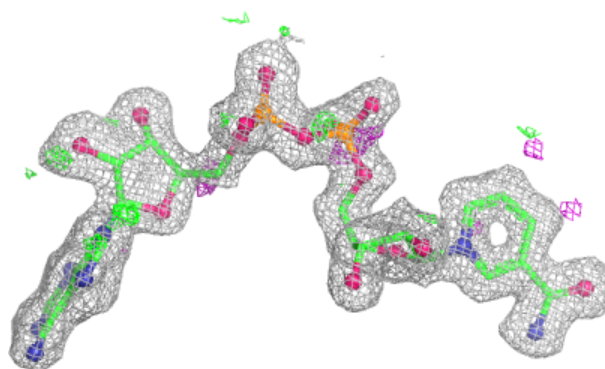
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SSB	C	378	10/10	0.91	0.12	12,15,18,20	0
4	SSB	D	378	10/10	0.94	0.10	14,16,20,21	0
3	NAD	C	377	44/44	0.95	0.07	7,11,17,21	0
4	SSB	B	378	10/10	0.96	0.09	6,13,16,18	0
3	NAD	A	377	44/44	0.96	0.06	3,12,17,19	0
4	SSB	A	378	10/10	0.96	0.08	5,13,17,19	0
2	ZN	B	376	1/1	0.97	0.03	11,11,11,11	0
2	ZN	C	375	1/1	0.97	0.04	12,12,12,12	0
3	NAD	D	377	44/44	0.98	0.05	4,10,13,15	0
2	ZN	C	376	1/1	0.98	0.03	10,10,10,10	0
2	ZN	A	375	1/1	0.98	0.03	10,10,10,10	0
3	NAD	B	377	44/44	0.98	0.05	4,9,14,18	0
2	ZN	B	375	1/1	0.98	0.03	10,10,10,10	0
2	ZN	D	376	1/1	0.99	0.02	11,11,11,11	0
2	ZN	A	376	1/1	0.99	0.02	9,9,9,9	0
2	ZN	D	375	1/1	0.99	0.02	12,12,12,12	0

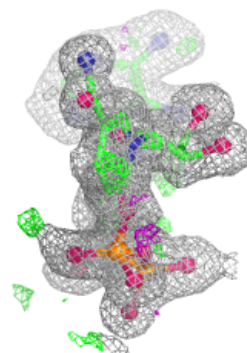
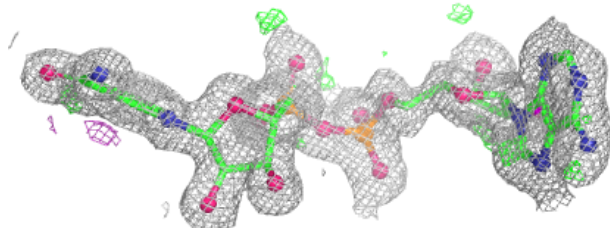
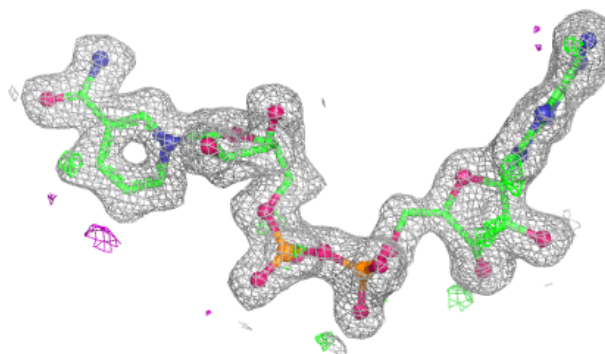
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD C 377:

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

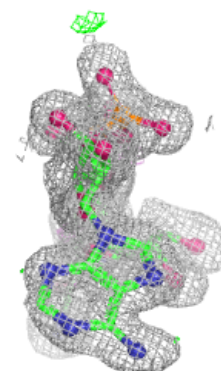
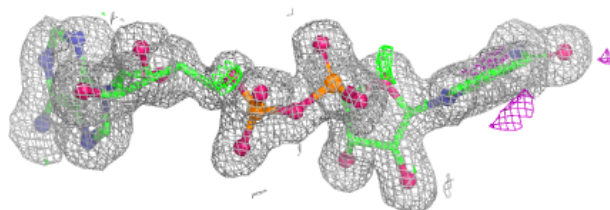
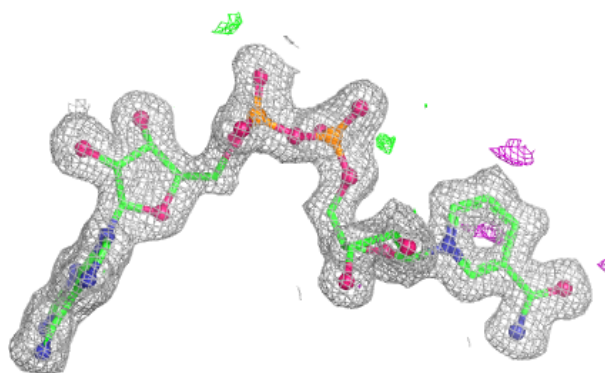
**Electron density around NAD A 377:**

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

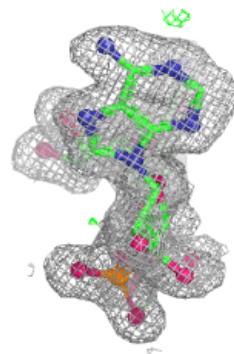
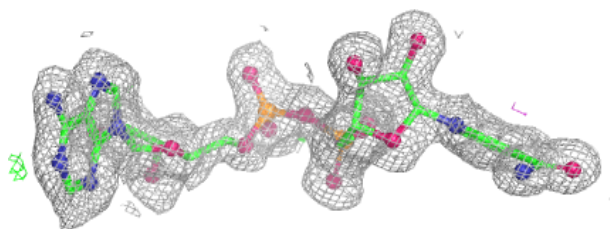
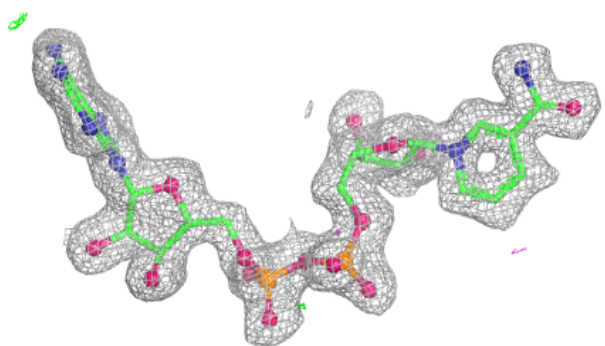


Electron density around NAD D 377:

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

**Electron density around NAD B 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.