



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 01:34 am BST

PDB ID : 1BW9
Title : PHENYLALANINE DEHYDROGENASE STRUCTURE IN TERNARY COMPLEX WITH NAD⁺ AND PHENYLPYRUVATE
Authors : Vanhooke, J.L.; Thoden, J.B.; Brunhuber, N.M.W.; Blanchard, J.L.; Holden, H.M.
Deposited on : 1998-10-01
Resolution : 1.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

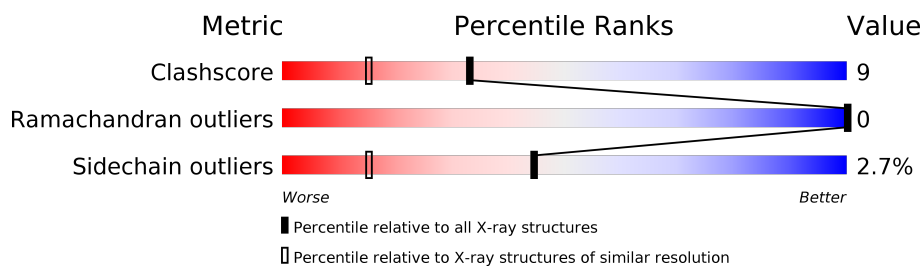
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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 on 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	356	
2	B	356	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	EDO	B	874	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6225 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 PHENYLALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	9	0
			2551	1573	450	516	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	ARG	SEE REMARK 999	UNP Q59771
A	20	MET	GLU	SEE REMARK 999	UNP Q59771
A	48	ASN	GLN	SEE REMARK 999	UNP Q59771

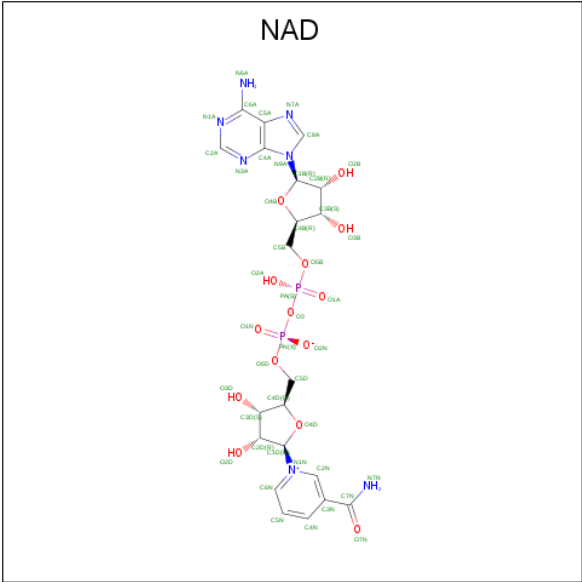
- Molecule 2 is a protein called PHENYLALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	347	Total	C	N	O	S	0	4	0
			2521	1558	447	505	11			

There are 2 discrepancies between the modelled and reference sequences:

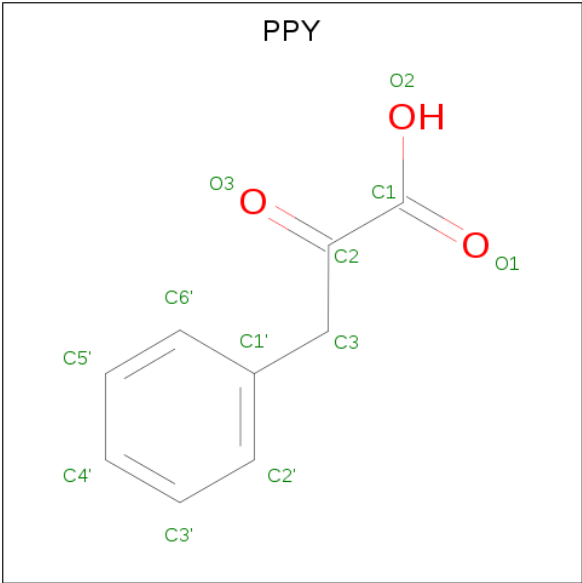
Chain	Residue	Modelled	Actual	Comment	Reference
B	419	LYS	ARG	SEE REMARK 999	UNP Q59771
B	420	MET	GLU	SEE REMARK 999	UNP Q59771

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: 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
			27	10	5	10	2		

- Molecule 4 is 3-PHENYLPYRUVIC ACID (three-letter code: PPY) (formula: C₉H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	9	3		
4	B	1	Total	C	O	0	0
			12	9	3		

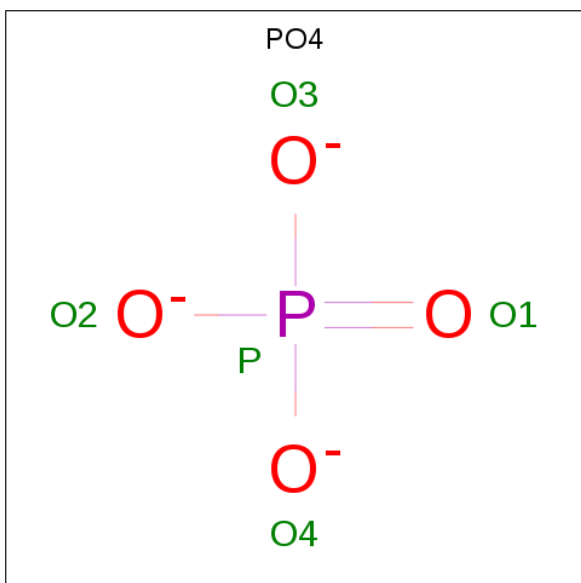
- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total K 2 2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Na 2 2	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



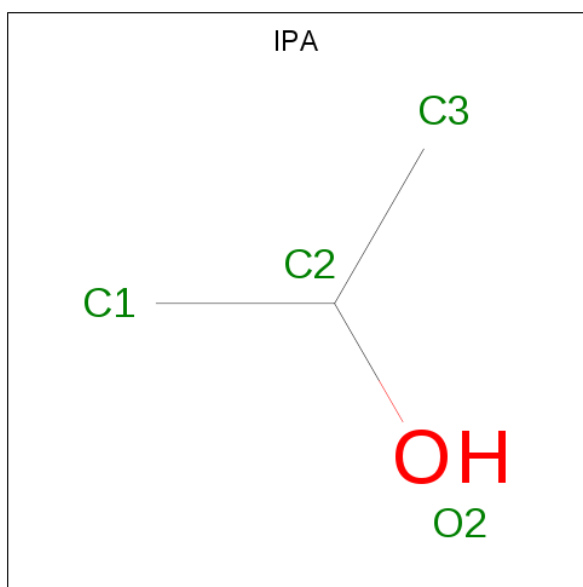
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O P 5 4 1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	3	1		
9	B	1	Total	C	O	0	0
			4	3	1		
9	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	519	Total	O	0	0
			519	519		
10	B	502	Total	O	0	0
			502	502		

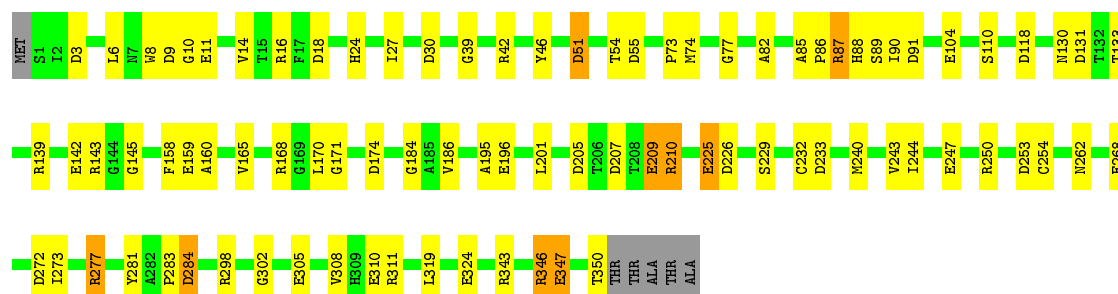
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

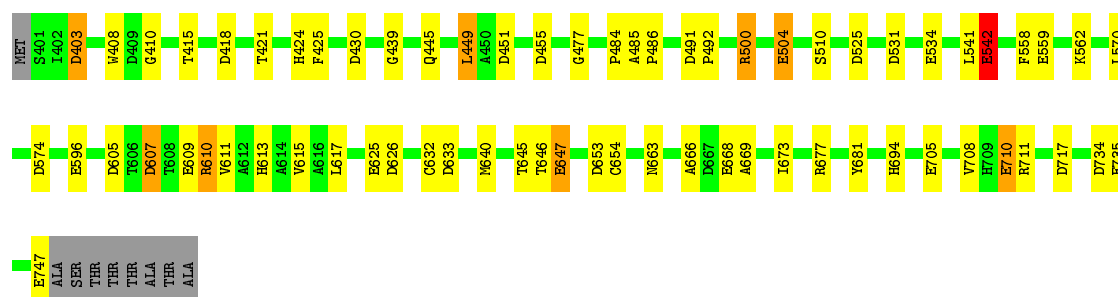
• Molecule 1: PHENYLALANINE DEHYDROGENASE

Chain A: 



• Molecule 2: PHENYLALANINE DEHYDROGENASE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.30 Å 110.20 Å 113.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50	Depositor
% Data completeness (in resolution range)	94.0 (30.00-1.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6225	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, NAD, NA, K, EDO, PPY, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.91	13/2625 (0.5%)	1.28	36/3577 (1.0%)
2	B	0.93	13/2579 (0.5%)	1.27	32/3512 (0.9%)
All	All	0.92	26/5204 (0.5%)	1.28	68/7089 (1.0%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	GLU	CD-OE1	7.90	1.34	1.25
1	A	104	GLU	CD-OE1	6.99	1.33	1.25
2	B	625	GLU	CD-OE1	6.83	1.33	1.25
2	B	504	GLU	CD-OE1	6.66	1.32	1.25
2	B	647	GLU	CD-OE1	6.62	1.32	1.25
2	B	705	GLU	CD-OE1	6.54	1.32	1.25
1	A	347	GLU	CD-OE1	6.21	1.32	1.25
1	A	142	GLU	CD-OE2	6.15	1.32	1.25
2	B	710	GLU	CD-OE1	6.06	1.32	1.25
1	A	196	GLU	CD-OE2	5.90	1.32	1.25
1	A	11	GLU	CD-OE1	5.74	1.31	1.25
1	A	324	GLU	CD-OE1	5.71	1.31	1.25
2	B	668	GLU	CD-OE1	5.66	1.31	1.25
1	A	159	GLU	CD-OE2	5.66	1.31	1.25
1	A	209	GLU	CD-OE1	5.64	1.31	1.25
1	A	305	GLU	CD-OE1	5.63	1.31	1.25
1	A	310	GLU	CD-OE2	5.63	1.31	1.25
1	A	225	GLU	CD-OE1	5.58	1.31	1.25
2	B	747	GLU	CD-OE1	5.49	1.31	1.25
2	B	609	GLU	CD-OE1	5.47	1.31	1.25
1	A	268	GLU	CD-OE1	5.41	1.31	1.25
2	B	534	GLU	CD-OE1	5.40	1.31	1.25
2	B	542	GLU	CD-OE1	5.35	1.31	1.25
2	B	596	GLU	CD-OE2	5.33	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	735	GLU	CD-OE1	5.16	1.31	1.25
2	B	559	GLU	CD-OE2	5.01	1.31	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	681	TYR	CB-CG-CD2	-8.35	115.99	121.00
1	A	277	ARG	NE-CZ-NH1	8.33	124.47	120.30
2	B	525	ASP	CB-CG-OD1	-7.93	111.16	118.30
1	A	233	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	87	ARG	NE-CZ-NH1	7.35	123.98	120.30
2	B	711	ARG	NE-CZ-NH1	7.19	123.90	120.30
2	B	418	ASP	CB-CG-OD1	-7.13	111.89	118.30
2	B	633	ASP	CB-CG-OD1	-6.98	112.02	118.30
2	B	455[A]	ASP	CB-CG-OD2	6.93	124.54	118.30
2	B	455[B]	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	233	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	A	226	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	A	18	ASP	CB-CG-OD1	-6.82	112.16	118.30
2	B	418	ASP	CB-CG-OD2	6.80	124.42	118.30
2	B	430	ASP	CB-CG-OD1	6.71	124.33	118.30
1	A	46	TYR	CB-CG-CD2	-6.54	117.08	121.00
2	B	455[A]	ASP	CB-CG-OD1	-6.54	112.42	118.30
2	B	455[B]	ASP	CB-CG-OD1	-6.54	112.42	118.30
1	A	16	ARG	NE-CZ-NH2	-6.53	117.04	120.30
2	B	500	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	91[A]	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	A	91[B]	ASP	CB-CG-OD2	-6.37	112.57	118.30
2	B	430	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	42	ARG	NE-CZ-NH1	6.31	123.45	120.30
2	B	605	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	30	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	158	PHE	CB-CG-CD2	-6.10	116.53	120.80
2	B	734	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	A	311	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	277	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	B	451	ASP	CB-CG-OD1	-5.85	113.03	118.30
2	B	717	ASP	CB-CG-OD2	5.84	123.56	118.30
2	B	633	ASP	CB-CG-OD2	5.81	123.53	118.30
2	B	626	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	A	51	ASP	CB-CG-OD1	-5.72	113.15	118.30
2	B	653	ASP	CB-CG-OD1	-5.72	113.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ASP	CB-CG-OD2	-5.72	113.16	118.30
2	B	734	ASP	CB-CG-OD2	5.61	123.35	118.30
2	B	531	ASP	CB-CG-OD2	5.53	123.28	118.30
2	B	677	ARG	NE-CZ-NH1	5.51	123.06	120.30
2	B	653	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	531	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	346	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	B	607	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	143	ARG	NE-CZ-NH1	5.47	123.04	120.30
2	B	610	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	253	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	168	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	272	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	250	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	284	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	9[A]	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	9[B]	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	3	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	226	ASP	CB-CG-OD2	5.36	123.12	118.30
2	B	607	ASP	CB-CG-OD1	-5.31	113.52	118.30
2	B	717	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	A	9[A]	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	A	9[B]	ASP	CB-CG-OD1	-5.25	113.58	118.30
2	B	403	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	18	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	174	ASP	CB-CG-OD1	-5.22	113.60	118.30
2	B	626	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	55[A]	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	55[B]	ASP	CB-CG-OD1	5.10	122.89	118.30
2	B	574	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	131	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	174	ASP	CB-CG-OD2	5.00	122.81	118.30

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	2551	0	2488	49	0
2	B	2521	0	2473	31	0
3	A	44	0	26	11	0
3	B	27	0	12	4	0
4	A	12	0	7	3	0
4	B	12	0	7	0	0
5	B	2	0	0	0	0
6	B	2	0	0	0	0
7	B	5	0	0	0	0
8	B	12	0	18	6	0
9	B	16	0	31	4	0
10	A	519	0	0	6	0
10	B	502	0	0	2	0
All	All	6225	0	5062	88	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 9.

All (88) 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)
2:B:663:ASN:HD22	9:B:862:IPA:H11	1.35	0.91
1:A:186:VAL:CG2	8:B:874:EDO:H11	2.07	0.85
1:A:186:VAL:HG21	8:B:874:EDO:H11	1.60	0.83
2:B:663:ASN:ND2	9:B:862:IPA:H11	1.99	0.77
1:A:346:ARG:O	1:A:350:THR:HG22	1.86	0.76
1:A:347:GLU:HA	1:A:350:THR:CG2	2.20	0.71
2:B:491:ASP:HB2	2:B:492:PRO:HD2	1.75	0.69
1:A:347:GLU:HA	1:A:350:THR:HG23	1.74	0.69
1:A:346:ARG:C	1:A:350:THR:HG22	2.14	0.68
1:A:243:VAL:HG23	1:A:244:ILE:HG13	1.76	0.67
2:B:613:HIS:CD2	2:B:617:LEU:HD11	2.29	0.66
3:A:360:NAD:O5D	3:A:360:NAD:H6N	1.96	0.65
1:A:343:ARG:O	1:A:347:GLU:HG3	1.96	0.65
1:A:51:ASP:HA	1:A:54[B]:THR:HG22	1.79	0.63
1:A:73:PRO:C	1:A:74[A]:MET:HG2	2.19	0.62
1:A:8:TRP:CH2	1:A:10:GLY:HA3	2.34	0.62
1:A:225:GLU:OE1	1:A:225:GLU:N	2.32	0.62
2:B:610:ARG:NH1	3:B:760:NAD:O3B	2.29	0.62
2:B:710:GLU:HG2	10:B:1292:HOH:O	2.02	0.59
1:A:232:CYS:O	1:A:254:CYS:HA	2.03	0.59
1:A:8:TRP:CZ3	1:A:10:GLY:HA3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:632:CYS:O	2:B:654:CYS:HA	2.04	0.58
1:A:51:ASP:HA	1:A:54[B]:THR:CG2	2.33	0.58
1:A:39:GLY:HA3	1:A:77:GLY:O	2.04	0.57
1:A:87:ARG:HA	1:A:90:ILE:HD12	1.85	0.57
2:B:611:VAL:O	2:B:615:VAL:HG23	2.04	0.56
1:A:195:ALA:HB2	1:A:201:LEU:HD12	1.88	0.55
3:A:360:NAD:C5N	8:B:874:EDO:H12	2.37	0.55
1:A:54[B]:THR:HG21	10:A:409:HOH:O	2.05	0.54
1:A:6:LEU:HD22	10:A:568:HOH:O	2.06	0.54
1:A:51:ASP:CA	1:A:54[B]:THR:HG22	2.38	0.53
1:A:262[B]:ASN:OD1	3:A:360:NAD:H2N	2.09	0.53
2:B:485:ALA:HB1	2:B:486:PRO:HD2	1.91	0.53
2:B:542:GLU:OE1	2:B:542:GLU:N	2.39	0.52
1:A:165:VAL:HG13	1:A:170:LEU:HB2	1.91	0.51
2:B:645:THR:HA	2:B:666:ALA:HB3	1.92	0.51
1:A:88:HIS:HD2	10:A:430:HOH:O	1.93	0.50
1:A:347:GLU:HA	1:A:350:THR:HG22	1.94	0.49
3:A:360:NAD:H72N	4:A:361:PPY:C1	2.26	0.49
2:B:500:ARG:O	2:B:504:GLU:HG3	2.13	0.49
1:A:85:ALA:HB1	1:A:86:PRO:HD2	1.94	0.49
1:A:73:PRO:O	1:A:74[A]:MET:HG2	2.12	0.48
2:B:439:GLY:HA3	2:B:477:GLY:O	2.13	0.48
1:A:186:VAL:HG23	8:B:874:EDO:H11	1.93	0.48
1:A:225:GLU:H	1:A:225:GLU:CD	2.10	0.48
1:A:139:ARG:HB2	1:A:145:GLY:HA3	1.95	0.48
1:A:207:ASP:OD2	1:A:210:ARG:HD2	2.14	0.48
2:B:541:LEU:HB2	2:B:542:GLU:OE1	2.14	0.48
1:A:262[A]:ASN:OD1	3:A:360:NAD:H2N	2.13	0.48
2:B:610:ARG:NH1	3:B:760:NAD:H3B	2.29	0.47
1:A:284:ASP:HB3	10:A:634:HOH:O	2.15	0.47
1:A:24:HIS:HB2	1:A:82:ALA:HB3	1.97	0.47
2:B:613:HIS:NE2	2:B:617:LEU:HD11	2.30	0.46
4:A:361:PPY:C1	4:A:361:PPY:H2'	2.45	0.46
2:B:646[B]:THR:CG2	2:B:669:ALA:HB3	2.45	0.46
1:A:205:ASP:HA	3:A:360:NAD:C2A	2.46	0.46
2:B:646[A]:THR:HG23	2:B:673:ILE:CD1	2.46	0.46
1:A:184:GLY:HA3	3:A:360:NAD:O5B	2.16	0.46
2:B:491:ASP:HB2	2:B:492:PRO:CD	2.43	0.46
2:B:607:ASP:HB3	2:B:610:ARG:HD2	1.96	0.45
2:B:663:ASN:HD22	9:B:862:IPA:C1	2.19	0.45
2:B:694:HIS:HA	2:B:708:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:610:ARG:NH1	3:B:760:NAD:C3B	2.79	0.44
1:A:130:ASN:HA	1:A:133:THR:O	2.17	0.44
2:B:424:HIS:CG	2:B:449:LEU:CD1	3.00	0.44
2:B:558:PHE:O	2:B:562:LYS:HG3	2.18	0.44
2:B:646[B]:THR:HG21	2:B:669:ALA:HB3	2.00	0.44
1:A:118:ASP:HA	3:A:360:NAD:C4N	2.48	0.44
2:B:424:HIS:CG	2:B:449:LEU:HD11	2.52	0.44
1:A:273:ILE:O	1:A:277:ARG:HG3	2.18	0.43
1:A:298:ARG:HG2	1:A:308:VAL:HG21	2.01	0.43
10:A:610:HOH:O	9:B:860:IPA:H33	2.18	0.43
3:A:360:NAD:C6N	8:B:874:EDO:H12	2.48	0.43
1:A:347:GLU:CA	1:A:350:THR:HG22	2.48	0.43
2:B:408:TRP:CH2	2:B:410:GLY:HA3	2.53	0.43
2:B:415:THR:HA	2:B:425:PHE:O	2.19	0.43
1:A:160:ALA:HA	1:A:319:LEU:HD12	2.01	0.42
1:A:243:VAL:HG23	1:A:244:ILE:N	2.35	0.42
2:B:610:ARG:HH11	3:B:760:NAD:C3B	2.31	0.42
1:A:346:ARG:O	1:A:350:THR:N	2.53	0.42
8:B:874:EDO:H21	10:B:882:HOH:O	2.19	0.41
1:A:302:GLY:HA2	10:A:814:HOH:O	2.19	0.41
1:A:14:VAL:HB	1:A:27:ILE:HB	2.03	0.41
1:A:205:ASP:HA	3:A:360:NAD:N3A	2.35	0.41
1:A:281:TYR:CZ	1:A:283:PRO:HA	2.56	0.40
3:A:360:NAD:N7N	4:A:361:PPY:C1	2.84	0.40
2:B:421:THR:O	2:B:484:PRO:HG3	2.21	0.40
1:A:165:VAL:HG12	1:A:171:GLY:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/356 (100%)	351 (98%)	6 (2%)	0	100	100
2	B	350/356 (98%)	344 (98%)	6 (2%)	0	100	100
All	All	707/712 (99%)	695 (98%)	12 (2%)	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	266/261 (102%)	258 (97%)	8 (3%)	41	12
2	B	260/261 (100%)	252 (97%)	8 (3%)	40	11
All	All	526/522 (101%)	510 (97%)	16 (3%)	44	12

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

Mol	Chain	Res	Type
1	A	89[A]	SER
1	A	89[B]	SER
1	A	110[A]	SER
1	A	110[B]	SER
1	A	209	GLU
1	A	210	ARG
1	A	229	SER
1	A	240	MET
2	B	403	ASP
2	B	445	GLN
2	B	449	LEU
2	B	510	SER
2	B	542	GLU
2	B	570	LEU
2	B	640	MET
2	B	647	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	71	ASN
1	A	88	HIS
1	A	181	GLN
1	A	263	ASN
2	B	445	GLN
2	B	613	HIS
2	B	663	ASN
2	B	720	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
9	IPA	B	860	-	3,3,3	0.35	0	3,3,3	0.46	0
3	NAD	A	360	-	42,48,48	2.21	9 (21%)	50,73,73	2.96	13 (26%)
4	PPY	A	361	-	9,12,12	2.79	3 (33%)	10,15,15	3.90	4 (40%)
9	IPA	B	861	-	3,3,3	0.58	0	3,3,3	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	B	871	-	3,3,3	0.33	0	2,2,2	0.43	0
3	NAD	B	760	-	24,29,48	1.00	2 (8%)	29,45,73	1.77	8 (27%)
8	EDO	B	874	-	3,3,3	0.40	0	2,2,2	0.34	0
9	IPA	B	862	-	3,3,3	0.81	0	3,3,3	1.27	0
4	PPY	B	761	-	9,12,12	1.42	1 (11%)	10,15,15	0.98	1 (10%)
9	IPA	B	863	-	3,3,3	0.25	0	3,3,3	0.48	0
8	EDO	B	873	-	3,3,3	0.42	0	2,2,2	0.24	0
7	PO4	B	880	5	4,4,4	1.52	1 (25%)	6,6,6	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	360	-	-	4/26/62/62	0/5/5/5
4	PPY	A	361	-	-	2/4/8/8	0/1/1/1
8	EDO	B	871	-	-	1/1/1/1	-
3	NAD	B	760	-	-	2/12/32/62	0/3/3/5
8	EDO	B	874	-	-	1/1/1/1	-
4	PPY	B	761	-	-	2/4/8/8	0/1/1/1
8	EDO	B	873	-	-	1/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	360	NAD	C2N-C3N	-8.84	1.25	1.39
3	A	360	NAD	C3N-C7N	-7.01	1.40	1.50
4	A	361	PPY	C3-C2	-5.43	1.46	1.51
4	A	361	PPY	O3-C2	-4.88	1.14	1.22
3	A	360	NAD	C4N-C3N	4.47	1.47	1.39
4	A	361	PPY	C3-C1'	-3.90	1.45	1.51
4	B	761	PPY	C3-C2	-3.88	1.48	1.51
3	A	360	NAD	C2N-N1N	-3.09	1.31	1.35
3	B	760	NAD	C2A-N1A	3.06	1.39	1.33
3	A	360	NAD	C2D-C1D	-2.66	1.49	1.53
3	A	360	NAD	O4B-C1B	-2.54	1.37	1.41
3	B	760	NAD	PN-O2N	2.37	1.64	1.54
3	A	360	NAD	C4A-N3A	-2.23	1.32	1.35
3	A	360	NAD	C7N-N7N	2.21	1.37	1.33
3	A	360	NAD	C6N-N1N	2.09	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	880	PO4	P-O4	-2.03	1.48	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	361	PPY	C1'-C3-C2	-10.00	92.12	114.52
3	A	360	NAD	C5N-C4N-C3N	-7.77	111.15	120.34
3	A	360	NAD	O7N-C7N-C3N	-7.72	110.39	119.63
3	A	360	NAD	C2N-C3N-C4N	7.68	126.97	118.26
3	A	360	NAD	C6N-N1N-C2N	6.79	128.17	121.97
3	A	360	NAD	C4N-C3N-C7N	-6.14	104.62	121.04
3	A	360	NAD	C5N-C6N-N1N	-5.64	112.31	120.40
3	A	360	NAD	C3N-C2N-N1N	-4.91	115.63	120.43
3	A	360	NAD	C3N-C7N-N7N	4.90	123.63	117.75
3	A	360	NAD	C2N-N1N-C1D	-4.79	108.47	119.14
3	B	760	NAD	O2N-PN-O3	-4.17	90.64	104.64
3	B	760	NAD	C1B-N9A-C4A	-4.06	119.50	126.64
4	A	361	PPY	C3-C1'-C2'	-3.88	115.34	120.89
3	A	360	NAD	C6N-C5N-C4N	3.79	124.95	119.44
4	A	361	PPY	O3-C2-C3	3.52	126.30	120.75
4	A	361	PPY	C4'-C3'-C2'	-3.12	115.44	120.19
3	A	360	NAD	C2N-C3N-C7N	3.00	128.16	119.46
3	B	760	NAD	O3B-C3B-C4B	-2.80	102.95	111.05
3	B	760	NAD	C5A-C6A-N6A	2.78	124.57	120.35
3	B	760	NAD	O3B-C3B-C2B	2.71	120.58	111.82
3	B	760	NAD	O5D-PN-O2N	2.56	117.41	107.64
3	B	760	NAD	O4B-C4B-C5B	2.49	117.58	109.37
3	A	360	NAD	C1B-N9A-C4A	-2.44	122.35	126.64
3	A	360	NAD	O7N-C7N-N7N	2.31	125.86	122.58
3	B	760	NAD	PA-O3-PN	-2.11	125.58	132.83
4	B	761	PPY	C1'-C3-C2	-2.03	109.97	114.52

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	360	NAD	O4D-C1D-N1N-C6N
3	B	760	NAD	O4B-C4B-C5B-O5B
4	A	361	PPY	O3-C2-C3-C1'
8	B	874	EDO	O1-C1-C2-O2
4	B	761	PPY	C1-C2-C3-C1'
4	B	761	PPY	O3-C2-C3-C1'

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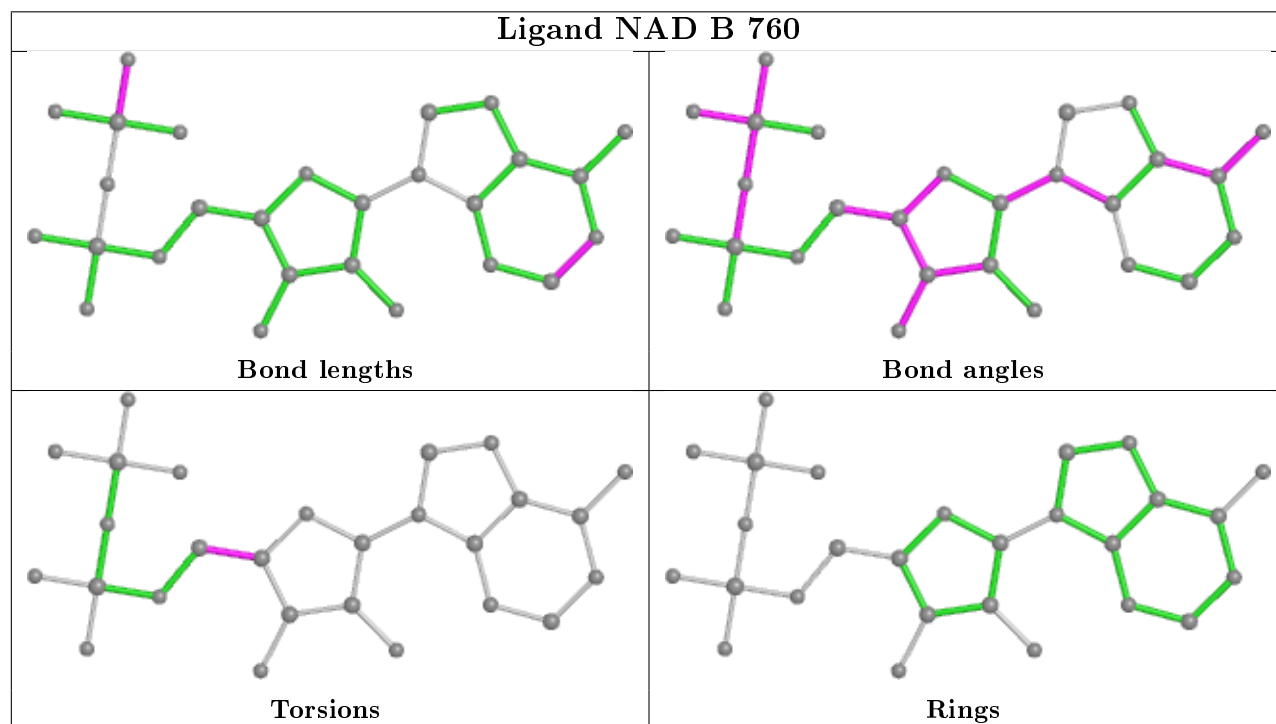
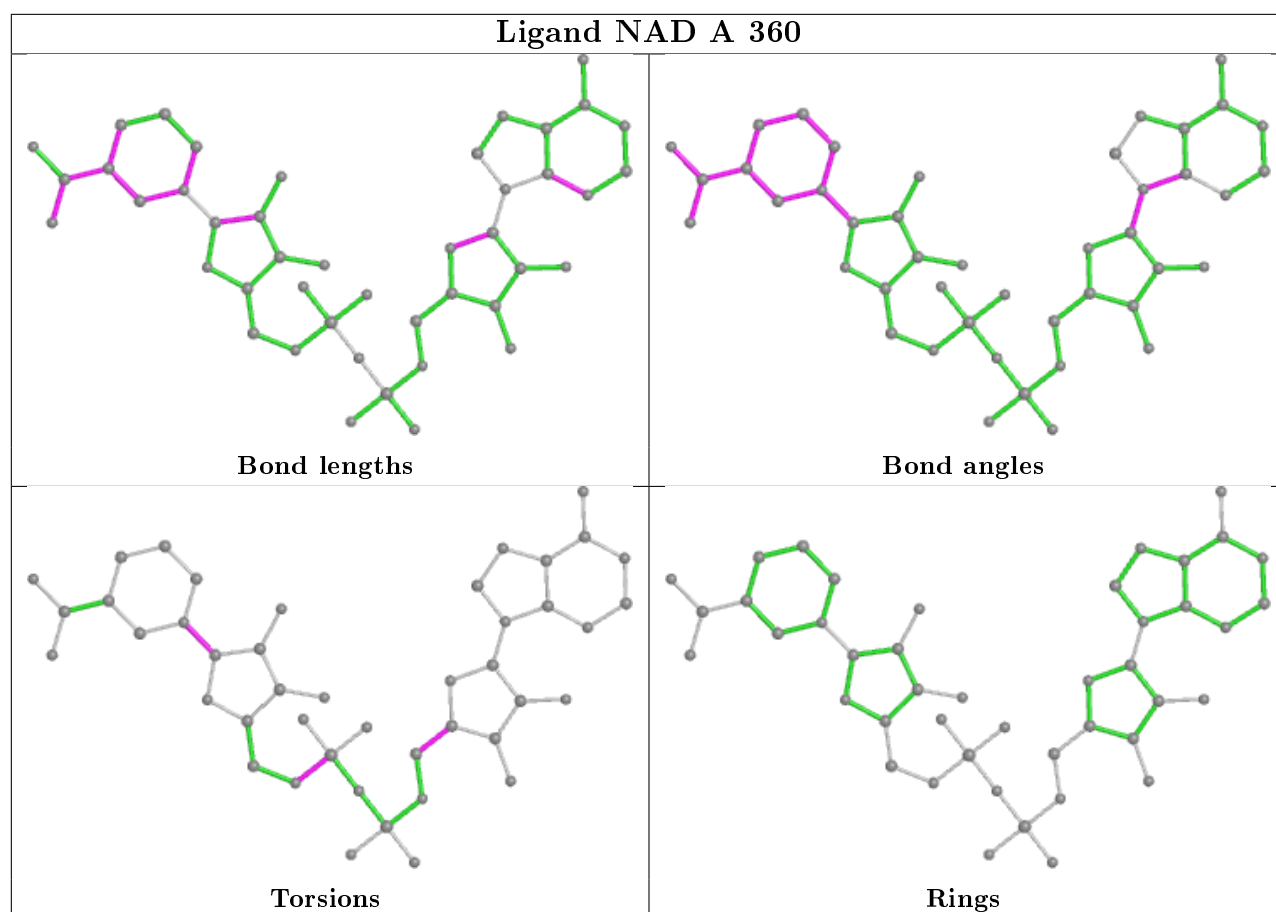
Mol	Chain	Res	Type	Atoms
4	A	361	PPY	C1-C2-C3-C1'
8	B	873	EDO	O1-C1-C2-O2
8	B	871	EDO	O1-C1-C2-O2
3	B	760	NAD	C3B-C4B-C5B-O5B
3	A	360	NAD	O4B-C4B-C5B-O5B
3	A	360	NAD	C5D-O5D-PN-O3
3	A	360	NAD	C5D-O5D-PN-O1N

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	860	IPA	1	0
3	A	360	NAD	11	0
4	A	361	PPY	3	0
3	B	760	NAD	4	0
8	B	874	EDO	6	0
9	B	862	IPA	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.