



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:14 PM UTC

PDB ID : 1BW9 / pdb_00001bw9
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 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

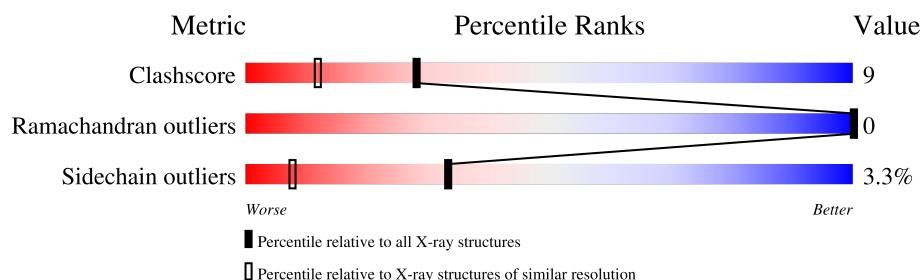
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (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 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	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
			Total	C	N	O	S			
1	A	350	2551	1573	450	516	12	0	9	0

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
			Total	C	N	O	S			
2	B	347	2521	1558	447	505	11	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

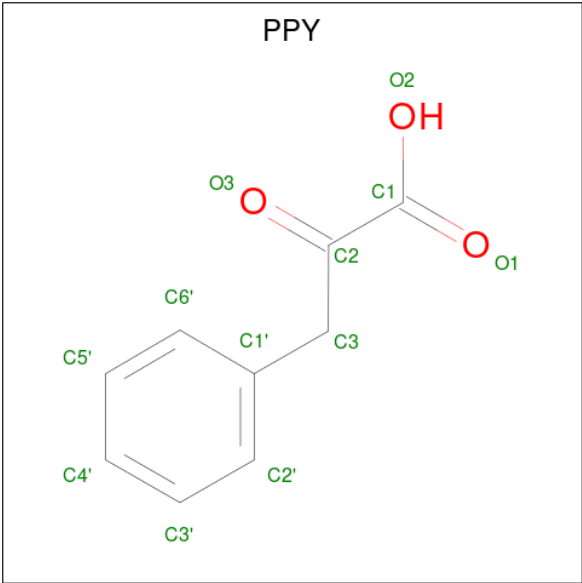
Chain	Residue	Modelled	Actual	Comment	Reference
B	419	LYS	ARG	SEE REMARK 999	UNP Q59771
B	420	MET	GLU	SEE REMARK 999	UNP Q59771

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is 3-PHENYLPYRUVIC ACID (CCD ID: 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		

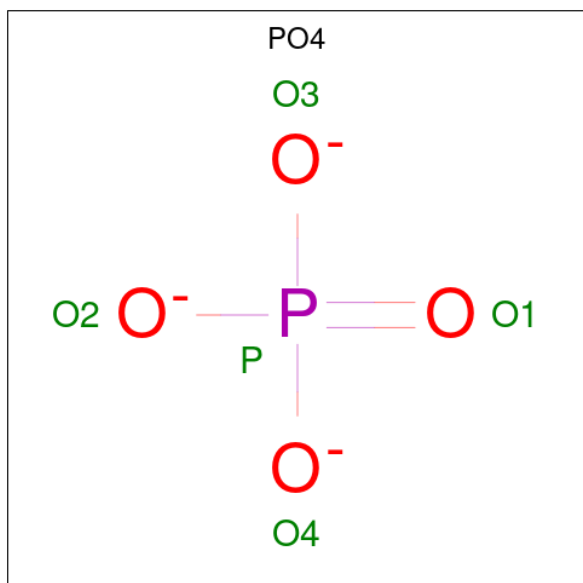
- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



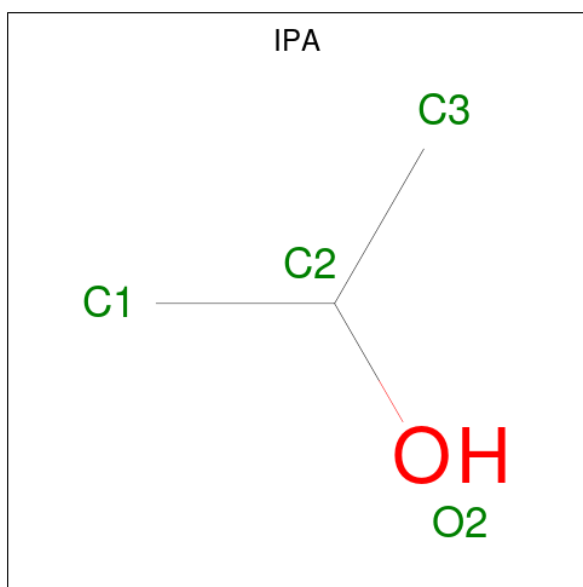
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O P 5 4 1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: 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 (CCD ID: IPA) (formula: C_3H_8O).



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.

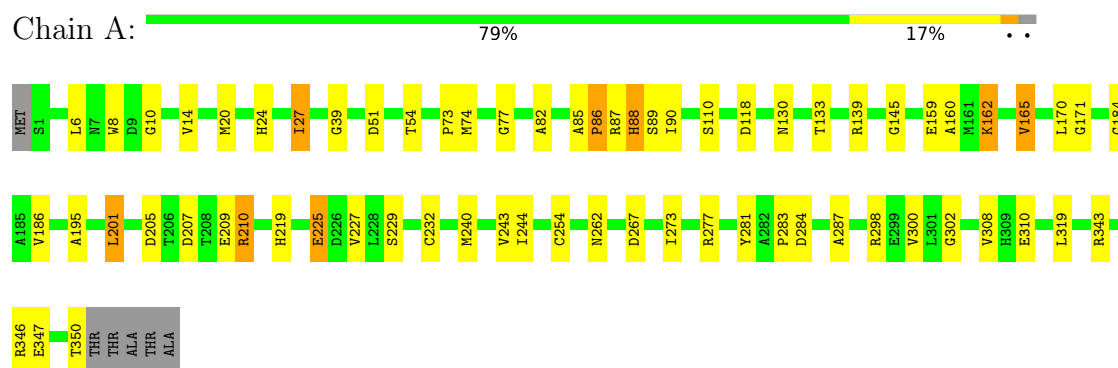
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	519	Total	O	0	0
			519	519		
10	B	502	Total	O	0	0
			502	502		

3 Residue-property plots

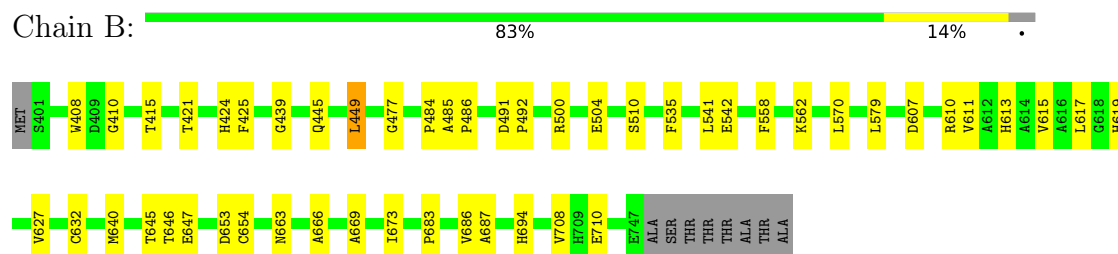
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: PHENYLALANINE DEHYDROGENASE



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	64.30Å 110.20Å 113.40Å 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, PO4, K, NA, NAD, EDO, PPY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.06	1/2625 (0.0%)	1.39	9/3577 (0.3%)
2	B	1.11	0/2579	1.38	7/3512 (0.2%)
All	All	1.09	1/5204 (0.0%)	1.38	16/7089 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	ASP	CG-OD2	5.43	1.35	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	VAL	N-CA-C	7.26	117.98	110.36
2	B	627	VAL	N-CA-C	6.86	117.56	110.36
1	A	287	ALA	N-CA-C	6.29	118.14	111.28
1	A	267	ASP	CA-CB-CG	-6.21	106.39	112.60
2	B	686	VAL	N-CA-C	-6.18	105.70	111.45
1	A	201	LEU	N-CA-C	6.13	119.23	109.24
2	B	687	ALA	N-CA-C	5.99	117.81	111.28
1	A	300	VAL	CB-CA-C	-5.97	105.77	111.44
1	A	219	HIS	CA-CB-CG	-5.93	107.87	113.80
2	B	535	PHE	N-CA-C	5.91	119.86	110.70
2	B	653	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	88	HIS	CA-CB-CG	5.67	119.47	113.80
1	A	27	ILE	N-CA-CB	5.39	119.16	111.82
2	B	619	HIS	CA-CB-CG	-5.30	108.50	113.80
2	B	683	PRO	N-CA-CB	5.18	107.85	103.19
1	A	86	PRO	N-CA-CB	5.13	107.81	103.19

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	52	0
2	B	2521	0	2473	32	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	7	0
10	B	502	0	0	2	0
All	All	6225	0	5062	92	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 (92) 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:346:ARG:C	1:A:350:THR:HG22	2.14	0.73
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:243:VAL:HG23	1:A:244:ILE:HG13	1.76	0.67
1:A:73:PRO:C	1:A:74[A]:MET:HG2	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:613:HIS:CD2	2:B:617:LEU:HD11	2.29	0.66
3:A:360:NAD:H6N	3:A:360:NAD:O5D	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:8:TRP:CH2	1:A:10:GLY:HA3	2.34	0.62
1:A:225:GLU:N	1:A:225:GLU:OE1	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
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
1:A:225:GLU:H	1:A:225:GLU:CD	2.10	0.52
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: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:24:HIS:HB2	1:A:82:ALA:HB3	1.97	0.47
1:A:284:ASP:HB3	10:A:634:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:159:GLU:CD	1:A:162:LYS:HE2	2.43	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
3:A:360:NAD:C6N	8:B:874:EDO:H12	2.48	0.43
10:A:610:HOH:O	9:B:860:IPA:H33	2.18	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:20:MET:HE2	10:A:569:HOH:O	2.18	0.42
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
2:B:542:GLU:H	2:B:542:GLU:CD	2.29	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:51:ASP:C	1:A:54[B]:THR:HG22	2.46	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

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	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%)	254 (96%)	12 (4%)	24	4
2	B	260/261 (100%)	253 (97%)	7 (3%)	39	12
All	All	526/522 (101%)	507 (96%)	19 (4%)	33	6

All (19) 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	162	LYS
1	A	165	VAL
1	A	209	GLU
1	A	210	ARG

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Mol	Chain	Res	Type
1	A	225	GLU
1	A	229	SER
1	A	240	MET
1	A	310	GLU
2	B	445	GLN
2	B	449	LEU
2	B	510	SER
2	B	570	LEU
2	B	579	LEU
2	B	640	MET
2	B	647	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	48	ASN
1	A	71	ASN
1	A	88	HIS
1	A	181	GLN
1	A	200	GLN
2	B	600	GLN
2	B	613	HIS
2	B	663	ASN
2	B	694	HIS
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 oligosaccharides in this entry.

5.6 Ligand geometry

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
4	PPY	A	361	-	12,12,12	2.21	3 (25%)	14,15,15	4.16	6 (42%)
8	EDO	B	874	-	3,3,3	0.36	0	2,2,2	0.39	0
9	IPA	B	863	-	3,3,3	0.27	0	3,3,3	0.51	0
8	EDO	B	873	-	3,3,3	0.38	0	2,2,2	0.27	0
9	IPA	B	862	-	3,3,3	0.84	0	3,3,3	1.32	0
7	PO4	B	880	5	4,4,4	1.58	1 (25%)	6,6,6	0.99	0
9	IPA	B	860	-	3,3,3	0.38	0	3,3,3	0.49	0
9	IPA	B	861	-	3,3,3	0.61	0	3,3,3	0.59	0
3	NAD	A	360	-	46,48,48	2.30	10 (21%)	64,73,73	2.65	11 (17%)
4	PPY	B	761	-	12,12,12	1.19	1 (8%)	14,15,15	1.08	2 (14%)
3	NAD	B	760	-	28,29,48	1.43	4 (14%)	43,45,73	1.43	7 (16%)
8	EDO	B	871	-	3,3,3	0.30	0	2,2,2	0.47	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
4	PPY	A	361	-	-	0/8/8/8	0/1/1/1
8	EDO	B	874	-	-	1/1/1/1	-
8	EDO	B	873	-	-	1/1/1/1	-
3	NAD	A	360	-	-	4/30/62/62	0/5/5/5
4	PPY	B	761	-	-	2/8/8/8	0/1/1/1
3	NAD	B	760	-	-	3/16/32/62	0/3/3/5
8	EDO	B	871	-	-	1/1/1/1	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	360	NAD	C2N-C3N	-8.65	1.25	1.39
3	A	360	NAD	C3N-C7N	-7.09	1.40	1.50
3	A	360	NAD	C4N-C3N	4.98	1.47	1.39
3	B	760	NAD	PA-O3	-4.71	1.54	1.59
4	A	361	PPY	C3-C2	-4.56	1.46	1.51
3	A	360	NAD	PN-O3	4.51	1.64	1.59
3	A	360	NAD	PA-O3	-4.46	1.54	1.59
4	A	361	PPY	O3-C2	-4.23	1.14	1.23
4	A	361	PPY	C3-C1'	-3.94	1.45	1.51
3	A	360	NAD	C2N-N1N	-3.45	1.31	1.35
4	B	761	PPY	C3-C2	-3.21	1.48	1.51
3	B	760	NAD	C2A-N1A	3.19	1.39	1.33
3	B	760	NAD	PN-O2N	2.47	1.64	1.54
3	B	760	NAD	C8A-N7A	2.39	1.36	1.31
3	A	360	NAD	C7N-N7N	2.29	1.37	1.33
3	A	360	NAD	C6N-N1N	2.27	1.40	1.35
3	A	360	NAD	C8A-N7A	2.11	1.35	1.31
7	B	880	PO4	P-O4	-2.11	1.48	1.54
3	A	360	NAD	C2A-N3A	-2.05	1.30	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	361	PPY	C1'-C3-C2	-12.97	92.12	113.56
3	A	360	NAD	C5N-C4N-C3N	-9.37	111.15	120.36
3	A	360	NAD	O7N-C7N-C3N	-7.53	110.39	119.60
3	A	360	NAD	C2N-C3N-C4N	7.49	126.97	118.26
3	A	360	NAD	C6N-N1N-C2N	7.40	128.17	121.88
3	A	360	NAD	C4N-C3N-C7N	-6.04	104.62	121.06
3	A	360	NAD	C5N-C6N-N1N	-5.92	112.31	120.38
3	A	360	NAD	C2N-N1N-C1D	-4.83	108.47	119.13
3	A	360	NAD	C3N-C7N-N7N	4.78	123.63	117.74
3	B	760	NAD	O2N-PN-O3	-4.17	90.64	104.64
4	A	361	PPY	C4'-C3'-C2'	-3.89	115.44	120.24
3	A	360	NAD	C6N-C5N-C4N	3.82	124.95	119.45
4	A	361	PPY	C3-C1'-C2'	-3.77	115.34	120.89
4	A	361	PPY	O3-C2-C1	-3.61	114.51	119.67
3	B	760	NAD	C1B-N9A-C8A	3.19	134.18	127.09
3	B	760	NAD	C4A-N9A-C1B	-3.05	119.50	126.63
3	A	360	NAD	C2N-C3N-C7N	3.01	128.16	119.46
3	B	760	NAD	O3B-C3B-C4B	-2.83	102.95	111.08
3	B	760	NAD	O3B-C3B-C2B	2.73	120.58	111.82
3	B	760	NAD	O4B-C4B-C5B	2.57	117.58	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	760	NAD	O5D-PN-O2N	2.56	117.41	107.80
4	A	361	PPY	O3-C2-C3	2.50	126.30	120.91
4	A	361	PPY	C5'-C4'-C3'	2.47	123.25	119.87
3	A	360	NAD	O7N-C7N-N7N	2.24	125.86	122.62
4	B	761	PPY	C1'-C3-C2	-2.17	109.97	113.56
4	B	761	PPY	O1-C1-C2	-2.15	119.14	121.81

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	360	NAD	O4D-C1D-N1N-C6N
4	B	761	PPY	O2-C1-C2-C3
3	B	760	NAD	O4B-C4B-C5B-O5B
3	A	360	NAD	C2B-C1B-N9A-C8A
8	B	874	EDO	O1-C1-C2-O2
4	B	761	PPY	O3-C2-C3-C1'
3	A	360	NAD	O4D-C1D-N1N-C2N
8	B	871	EDO	O1-C1-C2-O2
8	B	873	EDO	O1-C1-C2-O2
3	B	760	NAD	C3B-C4B-C5B-O5B
3	B	760	NAD	PN-O3-PA-O2A
3	A	360	NAD	O4B-C4B-C5B-O5B

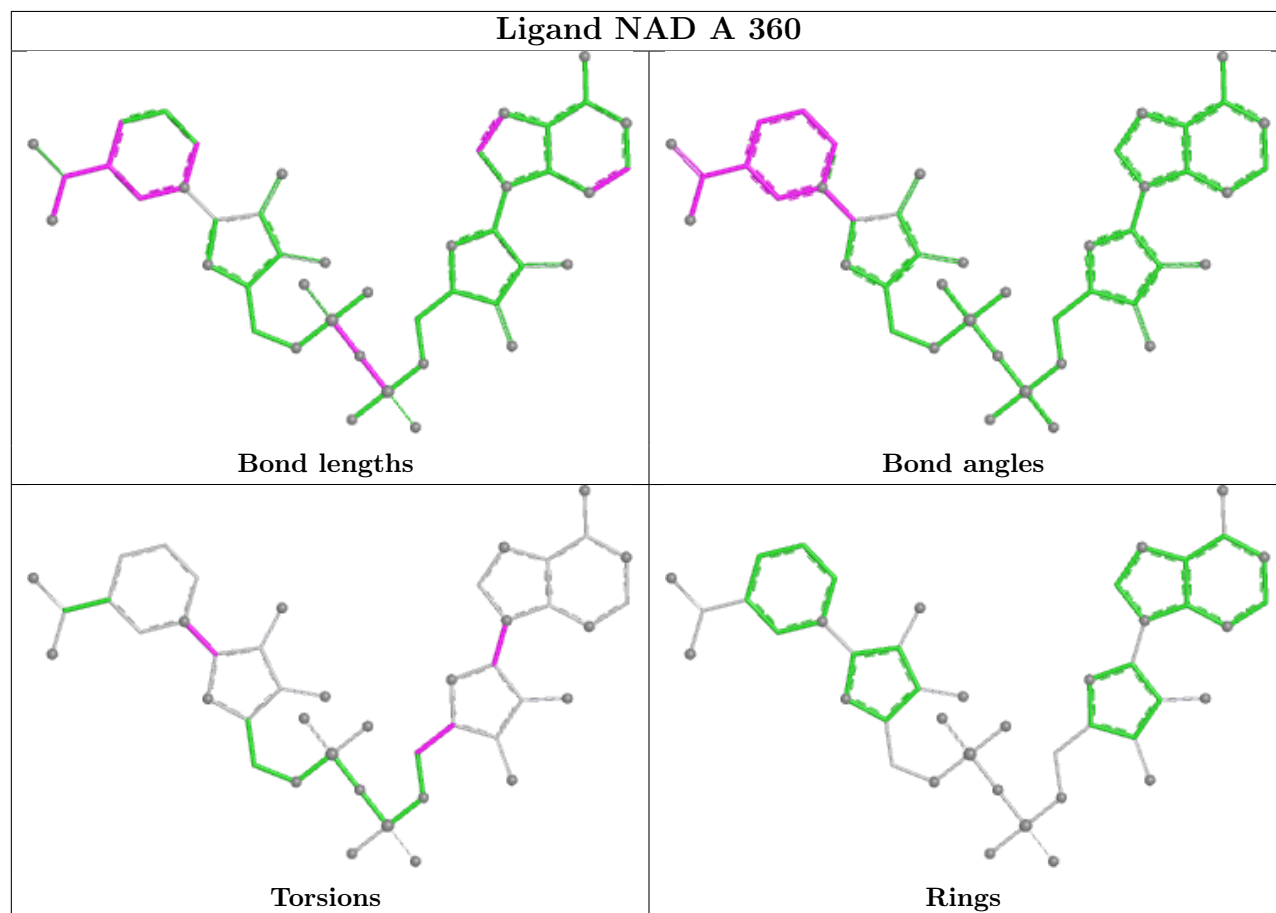
There are no ring outliers.

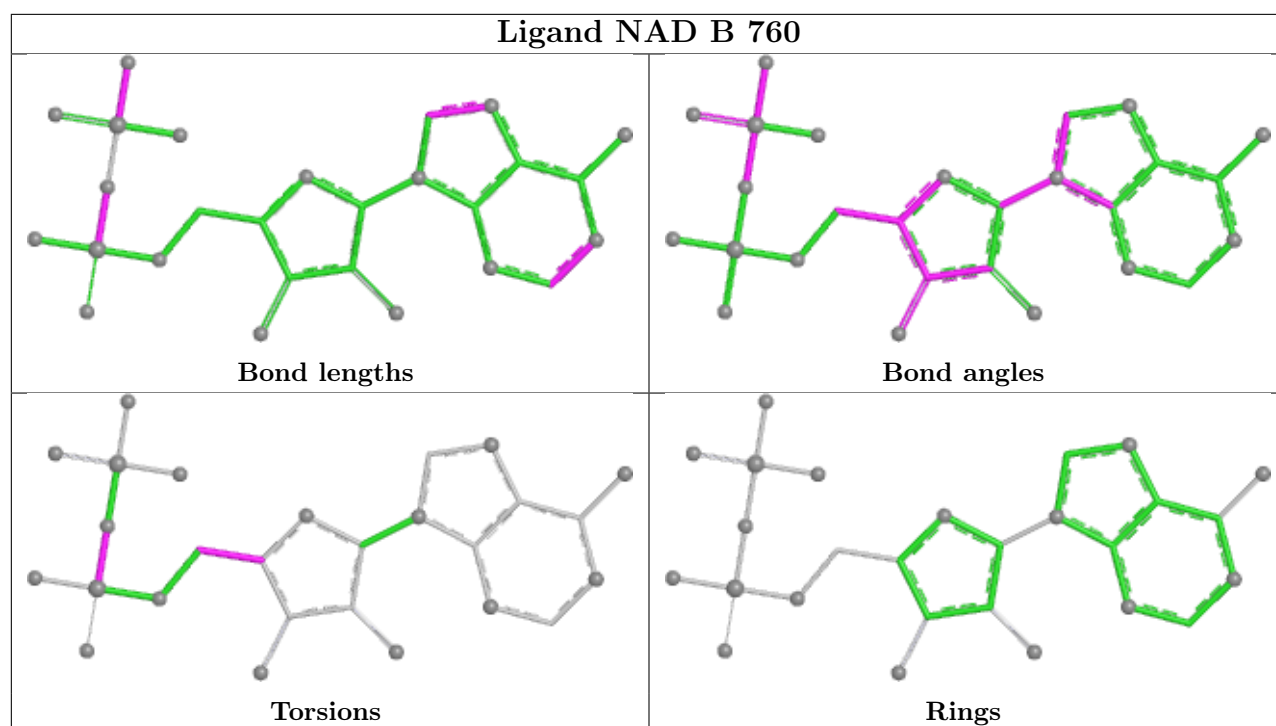
6 monomers are involved in 24 short contacts:

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