



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:34 AM UTC

PDB ID : 1HLD / pdb_00001hld
Title : STRUCTURES OF HORSE LIVER ALCOHOL DEHYDROGENASE COM-
PLEXED WITH NAD⁺ AND SUBSTITUTED BENZYL ALCOHOLS
Authors : Ramaswamy, S.; Eklund, H.; Plapp, B.V.
Deposited on : 1993-11-23
Resolution : 2.10 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

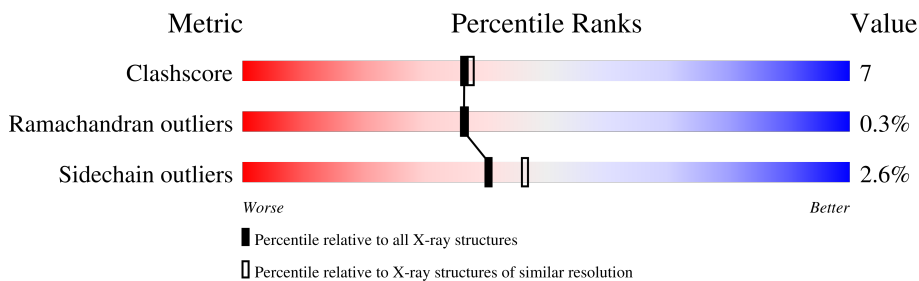
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	 79% 19% •
1	B	374	 81% 17% •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6100 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

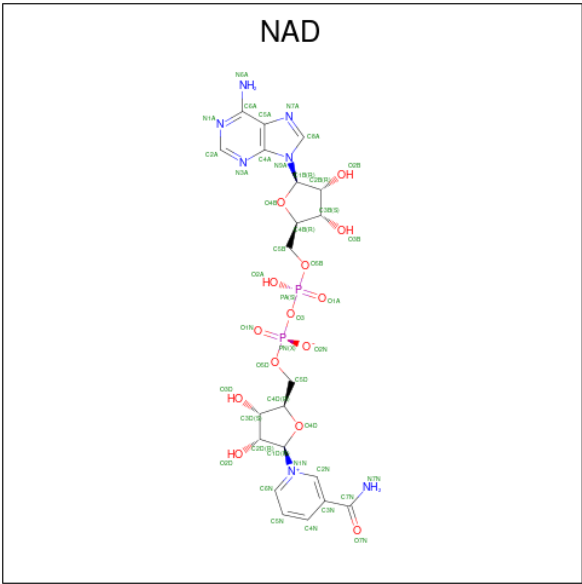
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

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

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

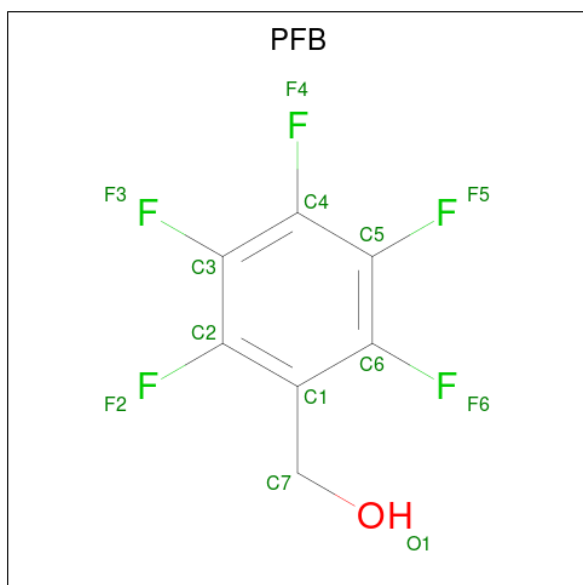
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



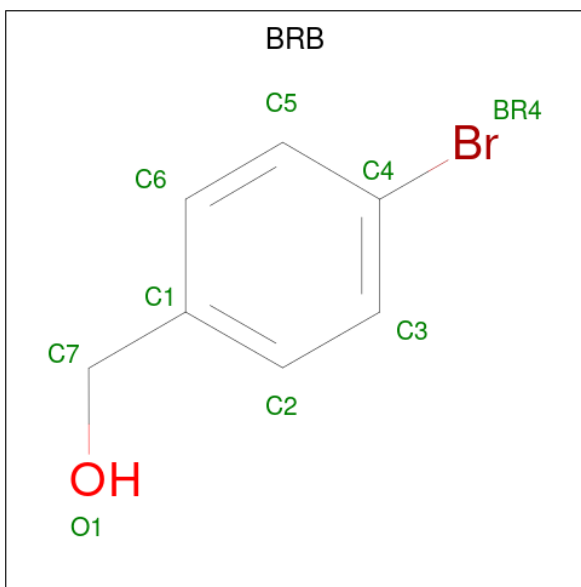
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is 2,3,4,5,6-PENTAFLUOROBENZYL ALCOHOL (CCD ID: PFB) (formula: $C_7H_3F_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			13	7	5	1		
4	B	1	Total	C	F	O	0	0
			13	7	5	1		

- Molecule 5 is PARA-BROMOBENZYL ALCOHOL (CCD ID: BRB) (formula: C_7H_7BrO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Br	C	O	0	0
			9	1	7	1		
5	B	1	Total	Br	C	O	0	0
			9	1	7	1		

- Molecule 6 is water.

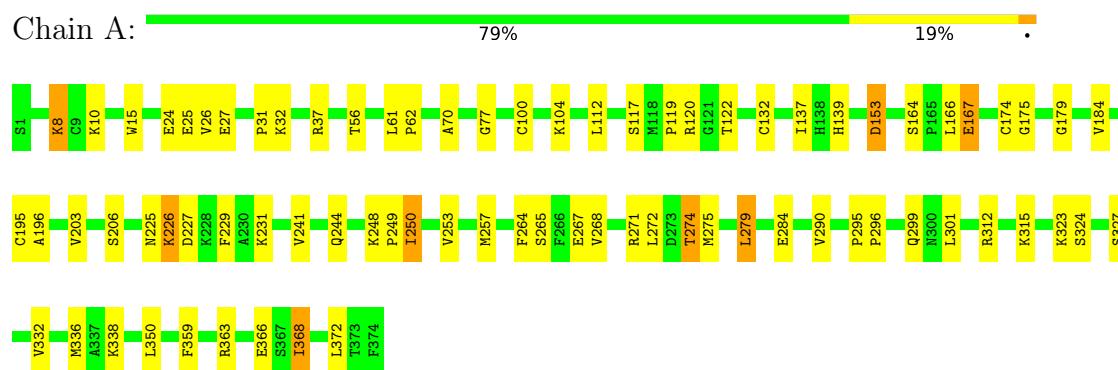
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	218	Total	O	0	0
			218	218		
6	B	176	Total	O	0	0
			176	176		

3 Residue-property plots

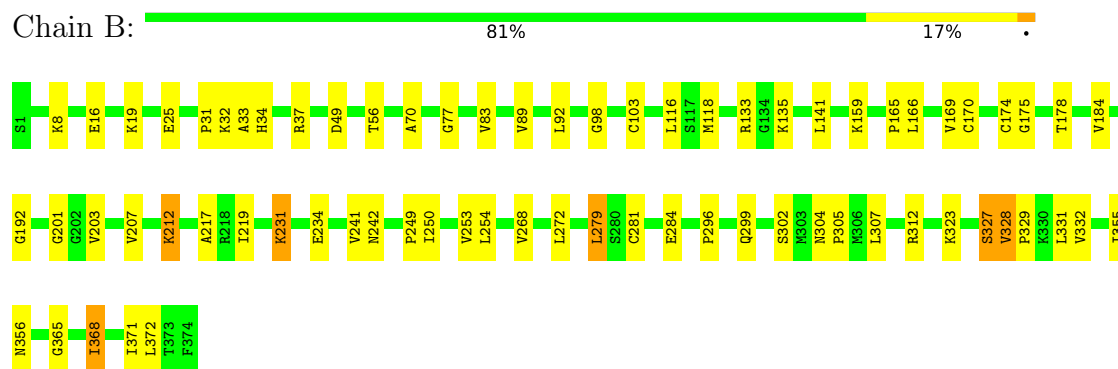
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: ALCOHOL DEHYDROGENASE



• Molecule 1: ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.10Å 180.70Å 44.30Å 90.00° 108.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6100	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, BRB, ZN, PFB

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	0.62	0/2837	1.01	10/3834 (0.3%)
1	B	0.59	1/2837 (0.0%)	1.03	16/3834 (0.4%)
All	All	0.60	1/5674 (0.0%)	1.02	26/7668 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	VAL	CA-CB	6.92	1.57	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	SER	N-CA-C	10.34	123.52	111.11
1	A	184	VAL	N-CA-C	8.00	118.80	110.72
1	B	284	GLU	N-CA-C	7.04	119.81	111.71
1	B	327	SER	N-CA-C	6.99	120.29	111.69
1	A	323	LYS	N-CA-C	-6.95	99.14	109.15
1	B	323	LYS	N-CA-C	-6.64	99.59	109.15
1	B	184	VAL	N-CA-C	6.37	117.16	110.72
1	B	304	ASN	CA-C-N	6.11	125.79	119.56
1	B	304	ASN	C-N-CA	6.11	125.79	119.56
1	A	284	GLU	N-CA-C	6.10	118.72	111.71
1	B	242	ASN	CA-C-N	5.96	125.64	119.56
1	B	242	ASN	C-N-CA	5.96	125.64	119.56
1	A	164	SER	N-CA-C	5.87	117.28	109.83
1	B	207	VAL	N-CA-C	-5.66	105.21	110.53
1	A	229	PHE	N-CA-C	5.57	117.03	111.07
1	B	8	LYS	N-CA-C	-5.53	100.17	109.07
1	A	139	HIS	N-CA-C	-5.52	102.58	110.59
1	B	118	MET	CA-C-N	5.40	125.32	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	MET	C-N-CA	5.40	125.32	119.76
1	A	327	SER	N-CA-C	5.39	119.80	112.04
1	B	25	GLU	N-CA-C	-5.36	100.51	109.24
1	A	368	ILE	N-CA-C	-5.33	98.25	109.34
1	B	49	ASP	N-CA-C	-5.12	105.77	111.36
1	B	201	GLY	N-CA-C	-5.08	105.34	112.60
1	B	368	ILE	N-CA-C	-5.05	98.84	109.34
1	A	250	ILE	N-CA-C	5.02	115.74	110.62

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	2785	0	2848	45	0
1	B	2785	0	2848	40	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
4	A	13	0	1	0	0
4	B	13	0	1	0	0
5	A	9	0	0	0	0
5	B	9	0	1	0	0
6	A	218	0	0	4	0
6	B	176	0	0	2	0
All	All	6100	0	5751	82	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 7.

All (82) 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:B:272:LEU:HD11	1:B:299:GLN:HB3	1.59	0.84
1:B:241:VAL:HG11	1:B:250:ILE:HD11	1.59	0.84
1:B:170:CYS:SG	1:B:371:ILE:HD12	2.21	0.80
1:B:212:LYS:HE3	1:B:212:LYS:HA	1.65	0.76
1:B:296:PRO:HB2	1:B:299:GLN:HG3	1.70	0.73
1:A:253:VAL:HG12	1:A:257:MET:HE3	1.76	0.66
1:A:132:CYS:HB3	1:A:137:ILE:HD11	1.77	0.65
1:A:153:ASP:HB3	6:A:2193:HOH:O	1.96	0.64
1:B:241:VAL:CG1	1:B:250:ILE:HD11	2.27	0.62
1:B:92:LEU:HA	6:B:2022:HOH:O	1.99	0.62
1:B:327:SER:O	1:B:331:LEU:HG	2.02	0.59
1:A:10:LYS:HA	1:A:24:GLU:O	2.03	0.58
1:A:8:LYS:HE2	1:A:27:GLU:HG2	1.84	0.58
1:B:56:THR:HG23	1:B:296:PRO:HA	1.87	0.56
1:A:295:PRO:HB2	6:A:2142:HOH:O	2.05	0.56
1:A:167:GLU:HB2	6:A:2290:HOH:O	2.06	0.56
1:A:301:LEU:HD23	1:B:305:PRO:HG3	1.87	0.56
1:B:133:ARG:HH11	1:B:135:LYS:HZ2	1.55	0.55
1:B:70:ALA:HB1	1:B:166:LEU:HD22	1.88	0.55
1:A:267:GLU:HG3	1:A:275:MET:HA	1.88	0.55
1:B:192:GLY:HA2	1:B:217:ALA:HB2	1.88	0.54
1:A:8:LYS:HZ2	1:A:8:LYS:HB3	1.73	0.54
1:A:272:LEU:HD11	1:A:299:GLN:HB3	1.89	0.54
1:A:167:GLU:H	1:A:167:GLU:CD	2.15	0.54
1:A:226:LYS:HG3	6:A:2386:HOH:O	2.08	0.54
1:A:8:LYS:NZ	1:A:25:GLU:HG2	2.24	0.53
1:A:8:LYS:CE	1:A:27:GLU:HG2	2.38	0.52
1:A:175:GLY:HA2	1:A:203:VAL:HG22	1.90	0.52
1:B:328:VAL:O	1:B:332:VAL:HG23	2.10	0.52
1:A:301:LEU:CD2	1:B:305:PRO:HG3	2.40	0.51
1:B:365:GLY:HA2	6:B:2029:HOH:O	2.11	0.51
1:B:133:ARG:HH11	1:B:135:LYS:NZ	2.09	0.50
1:A:359:PHE:HB3	1:A:363:ARG:CZ	2.42	0.50
1:A:241:VAL:HG11	1:A:250:ILE:HD11	1.94	0.49
1:A:100:CYS:HB2	1:A:112:LEU:HD12	1.95	0.48
1:B:231:LYS:O	1:B:234:GLU:HB3	2.11	0.48
1:B:83:VAL:HG12	1:B:159:LYS:HB2	1.96	0.48
1:A:231:LYS:HG2	1:A:368:ILE:CD1	2.44	0.47
1:A:70:ALA:HB1	1:A:166:LEU:HD22	1.95	0.47
1:A:290:VAL:HA	1:A:315:LYS:O	2.15	0.47
1:B:165:PRO:O	1:B:169:VAL:HG22	2.15	0.47
1:A:301:LEU:O	1:B:302:SER:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:VAL:O	1:A:336:MET:HG2	2.15	0.46
1:B:175:GLY:HA2	1:B:203:VAL:HG22	1.96	0.46
1:B:178:THR:HG21	3:B:901:NAD:C4N	2.46	0.46
1:B:89:VAL:HG12	1:B:159:LYS:HA	1.96	0.46
1:A:32:LYS:O	1:A:77:GLY:HA3	2.16	0.46
1:A:117:SER:C	1:A:119:PRO:HD3	2.41	0.46
1:B:328:VAL:N	1:B:329:PRO:HD2	2.31	0.46
1:B:16:GLU:HB2	1:B:19:LYS:HG3	1.99	0.45
1:B:254:LEU:HD12	1:B:281:CYS:SG	2.57	0.44
1:B:249:PRO:O	1:B:253:VAL:HG23	2.17	0.44
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.18	0.44
1:A:179:GLY:HA3	1:A:206:SER:HB2	2.00	0.44
1:B:116:LEU:HG	1:B:141:LEU:HD22	1.98	0.44
1:A:120:ARG:NH1	1:A:122:THR:OG1	2.51	0.44
1:B:92:LEU:CD2	1:B:328:VAL:HG21	2.47	0.44
1:A:56:THR:HG23	1:A:296:PRO:HA	2.01	0.43
1:A:279:LEU:HD22	1:A:312:ARG:HD3	1.99	0.43
1:A:31:PRO:HD3	1:A:37:ARG:HB2	2.01	0.43
1:A:350:LEU:O	1:A:372:LEU:HA	2.19	0.42
1:B:250:ILE:HD12	1:B:250:ILE:HA	1.87	0.42
1:A:26:VAL:HG12	1:A:132:CYS:HB2	2.01	0.42
1:B:32:LYS:O	1:B:77:GLY:HA3	2.19	0.42
1:B:231:LYS:HB2	1:B:231:LYS:NZ	2.33	0.42
1:A:338:LYS:HB3	1:A:338:LYS:HE2	1.84	0.42
1:B:212:LYS:HD2	1:B:219:ILE:HD12	2.02	0.42
1:B:279:LEU:HD22	1:B:312:ARG:HD3	2.02	0.42
1:B:31:PRO:HD3	1:B:37:ARG:HB2	2.02	0.42
1:A:195:CYS:HA	1:A:264:PHE:O	2.20	0.41
1:B:98:GLY:HA2	1:B:103:CYS:HB3	2.02	0.41
1:A:15:TRP:HA	1:A:62:PRO:HB3	2.02	0.41
1:A:225:ASN:ND2	1:A:227:ASP:H	2.19	0.41
1:A:231:LYS:HG2	1:A:368:ILE:HD11	2.03	0.41
1:A:248:LYS:HG3	1:A:249:PRO:HD2	2.02	0.41
1:A:301:LEU:HD12	1:A:301:LEU:C	2.46	0.41
1:B:231:LYS:HG2	1:B:368:ILE:CD1	2.51	0.41
1:B:33:ALA:O	1:B:34:HIS:HB2	2.22	0.40
1:A:61:LEU:HA	1:A:62:PRO:C	2.46	0.40
1:A:117:SER:O	1:A:119:PRO:HD3	2.21	0.40
1:B:355:ILE:HG23	1:B:356:ASN:N	2.36	0.40
1:A:196:ALA:O	1:A:265:SER:HA	2.21	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%)	354 (95%)	17 (5%)	1 (0%)	36	36
1	B	372/374 (100%)	352 (95%)	19 (5%)	1 (0%)	36	36
All	All	744/748 (100%)	706 (95%)	36 (5%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	CYS
1	B	174	CYS

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%)	298 (97%)	10 (3%)	34	38
1	B	308/308 (100%)	302 (98%)	6 (2%)	50	58
All	All	616/616 (100%)	600 (97%)	16 (3%)	40	46

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

Mol	Chain	Res	Type
1	A	8	LYS
1	A	104	LYS
1	A	153	ASP
1	A	167	GLU

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Mol	Chain	Res	Type
1	A	226	LYS
1	A	244	GLN
1	A	268	VAL
1	A	274	THR
1	A	279	LEU
1	A	366	GLU
1	B	212	LYS
1	B	231	LYS
1	B	268	VAL
1	B	279	LEU
1	B	307	LEU
1	B	372	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	225	ASN
1	B	225	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	A	801	-	46,48,48	1.39	7 (15%)	64,73,73	2.00	17 (26%)
5	BRB	B	1004	2,4	9,9,9	3.57	3 (33%)	11,11,11	1.46	3 (27%)
4	PFB	A	1001	5,2	13,13,13	2.63	5 (38%)	19,19,19	1.59	5 (26%)
5	BRB	A	1003	2,4	9,9,9	2.93	3 (33%)	11,11,11	1.36	2 (18%)
4	PFB	B	1002	5,2	13,13,13	3.07	7 (53%)	19,19,19	2.14	5 (26%)
3	NAD	B	901	-	46,48,48	1.41	5 (10%)	64,73,73	2.01	12 (18%)

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	801	-	-	6/30/62/62	0/5/5/5
5	BRB	B	1004	2,4	-	0/2/2/2	0/1/1/1
4	PFB	A	1001	5,2	-	0/2/2/2	0/1/1/1
5	BRB	A	1003	2,4	-	0/2/2/2	0/1/1/1
4	PFB	B	1002	5,2	-	1/2/2/2	0/1/1/1
3	NAD	B	901	-	-	3/30/62/62	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1004	BRB	BR4-C4	-9.60	1.71	1.90
4	B	1002	PFB	C7-C1	-8.73	1.42	1.51
5	A	1003	BRB	BR4-C4	-7.76	1.75	1.90
4	A	1001	PFB	C7-C1	-7.02	1.44	1.51
3	B	901	NAD	C2N-N1N	5.32	1.40	1.35
3	A	801	NAD	C2N-N1N	4.26	1.39	1.35
3	B	901	NAD	O4D-C1D	3.69	1.45	1.40
3	A	801	NAD	PA-O3	-3.48	1.55	1.59
3	A	801	NAD	C5A-N7A	-3.45	1.32	1.39
4	A	1001	PFB	F5-C5	-3.38	1.30	1.34
3	B	901	NAD	C5A-N7A	-3.37	1.32	1.39
5	B	1004	BRB	C7-C1	-3.34	1.40	1.51
4	B	1002	PFB	F2-C2	-3.00	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	PFB	F3-C3	-2.98	1.30	1.34
4	B	1002	PFB	F5-C5	-2.81	1.30	1.34
4	A	1001	PFB	F6-C6	-2.80	1.30	1.34
4	B	1002	PFB	F3-C3	-2.78	1.30	1.34
5	A	1003	BRB	C3-C2	2.78	1.43	1.38
4	B	1002	PFB	C5-C4	2.75	1.42	1.38
3	B	901	NAD	C6N-N1N	2.71	1.41	1.35
4	A	1001	PFB	F2-C2	-2.48	1.31	1.34
5	A	1003	BRB	C7-C1	-2.44	1.43	1.51
4	B	1002	PFB	F4-C4	-2.42	1.31	1.34
3	A	801	NAD	C6N-N1N	2.39	1.40	1.35
3	A	801	NAD	O4D-C1D	2.26	1.43	1.40
3	B	901	NAD	PN-O3	-2.17	1.57	1.59
3	A	801	NAD	PN-O3	-2.13	1.57	1.59
5	B	1004	BRB	C3-C2	2.12	1.42	1.38
3	A	801	NAD	C4A-N9A	-2.11	1.33	1.37
4	B	1002	PFB	C6-C5	2.08	1.41	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	NAD	N3A-C4A-N9A	6.92	138.94	127.17
3	B	901	NAD	C5A-C4A-N3A	-6.76	117.41	126.72
3	A	801	NAD	N3A-C4A-N9A	5.65	136.77	127.17
3	A	801	NAD	C5A-C4A-N3A	-5.26	119.47	126.72
3	A	801	NAD	N3A-C2A-N1A	-4.96	121.08	128.58
4	B	1002	PFB	C7-C1-C2	-4.88	116.15	121.81
4	B	1002	PFB	C6-C1-C2	4.76	121.51	115.91
3	B	901	NAD	N3A-C2A-N1A	-4.67	121.52	128.58
4	B	1002	PFB	C1-C6-C5	-4.49	117.23	122.36
3	B	901	NAD	C6A-C5A-C4A	3.90	122.50	117.18
3	A	801	NAD	C6A-C5A-N7A	-3.85	124.66	132.09
3	B	901	NAD	C6A-C5A-N7A	-3.68	124.99	132.09
3	A	801	NAD	C6A-C5A-C4A	3.62	122.12	117.18
3	B	901	NAD	C2A-N3A-C4A	3.57	120.56	111.83
4	A	1001	PFB	C7-C1-C6	-3.54	117.70	121.81
3	A	801	NAD	C4B-O4B-C1B	-3.49	101.77	109.47
3	B	901	NAD	C4A-N9A-C8A	3.31	109.22	105.74
4	A	1001	PFB	C6-C1-C2	3.30	119.79	115.91
3	A	801	NAD	O4B-C1B-N9A	3.22	114.27	108.09
3	A	801	NAD	C2A-N1A-C6A	3.19	123.96	118.73
3	A	801	NAD	C4A-N9A-C8A	3.17	109.07	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	NAD	O2A-PA-O5B	3.15	121.84	107.57
5	B	1004	BRB	BR4-C4-C5	2.99	123.37	119.30
3	A	801	NAD	C4D-O4D-C1D	-2.94	107.23	109.92
3	A	801	NAD	C2A-N3A-C4A	2.88	118.86	111.83
3	A	801	NAD	O5B-PA-O1A	-2.84	97.69	108.94
3	B	901	NAD	N9A-C8A-N7A	-2.69	110.11	113.94
5	A	1003	BRB	C5-C4-C3	-2.65	117.32	121.33
4	A	1001	PFB	C6-C5-C4	2.54	122.11	119.53
3	B	901	NAD	C4D-O4D-C1D	-2.41	107.72	109.92
3	A	801	NAD	N9A-C8A-N7A	-2.40	110.53	113.94
5	B	1004	BRB	C5-C4-C3	-2.35	117.77	121.33
3	B	901	NAD	O4B-C1B-N9A	2.33	112.57	108.09
4	A	1001	PFB	C1-C6-C5	-2.30	119.73	122.36
3	A	801	NAD	C4A-C5A-N7A	2.29	113.20	110.58
3	B	901	NAD	O7N-C7N-N7N	2.27	125.90	122.62
4	A	1001	PFB	C1-C2-C3	-2.27	119.76	122.36
4	B	1002	PFB	F6-C6-C1	2.16	122.53	119.36
5	A	1003	BRB	BR4-C4-C5	2.15	122.22	119.30
5	B	1004	BRB	C2-C3-C4	2.12	121.72	119.18
4	B	1002	PFB	F4-C4-C5	2.09	123.42	119.27
3	B	901	NAD	O3D-C3D-C2D	-2.05	105.24	111.82
3	A	801	NAD	O4B-C4B-C5B	2.05	115.90	109.33
3	A	801	NAD	N6A-C6A-N1A	2.05	122.94	118.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

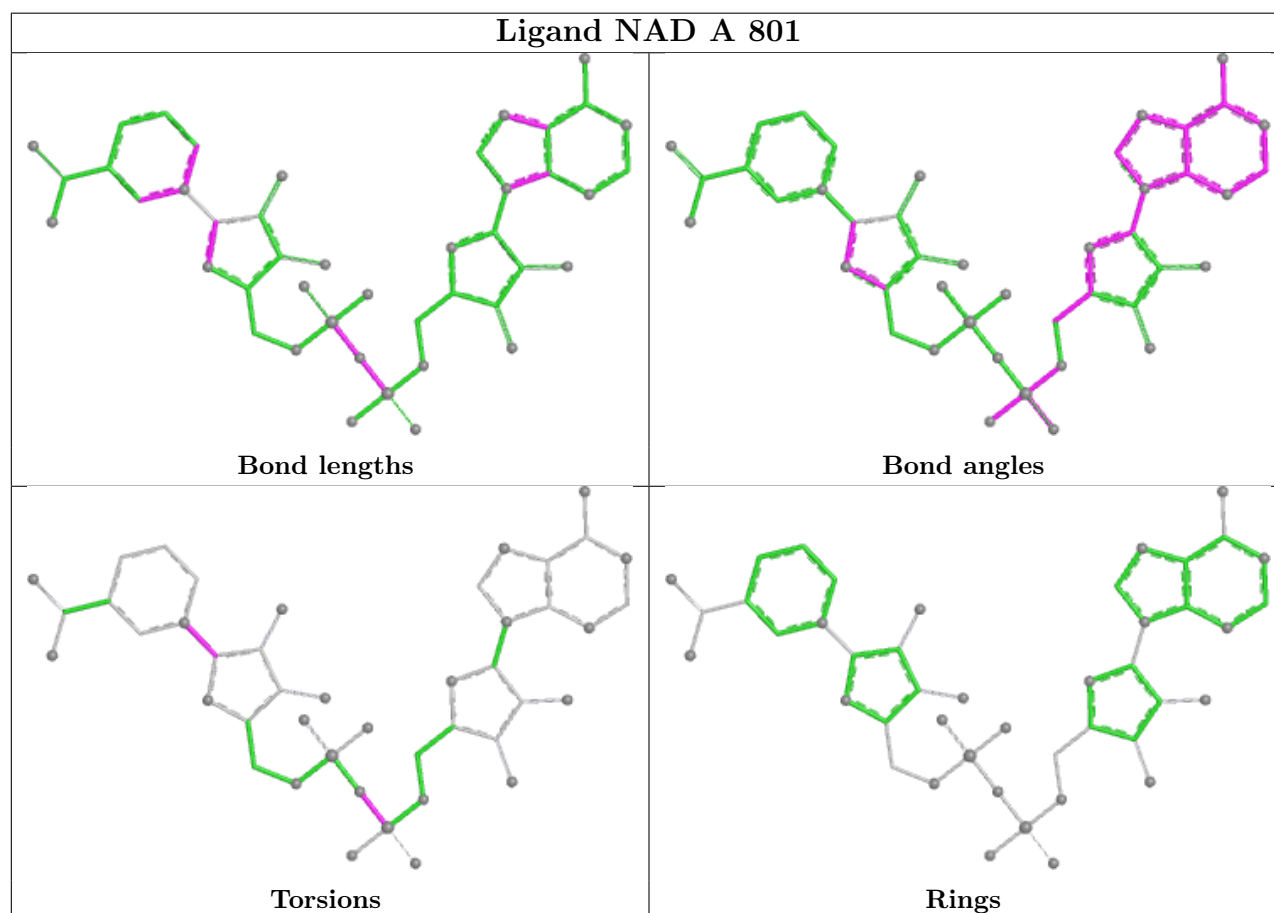
Mol	Chain	Res	Type	Atoms
3	A	801	NAD	O4D-C1D-N1N-C2N
3	A	801	NAD	O4D-C1D-N1N-C6N
3	A	801	NAD	C2D-C1D-N1N-C2N
3	B	901	NAD	O4D-C1D-N1N-C2N
3	B	901	NAD	O4D-C1D-N1N-C6N
3	B	901	NAD	C2D-C1D-N1N-C2N
3	A	801	NAD	PN-O3-PA-O1A
3	A	801	NAD	C2D-C1D-N1N-C6N
4	B	1002	PFB	C2-C1-C7-O1
3	A	801	NAD	PN-O3-PA-O2A

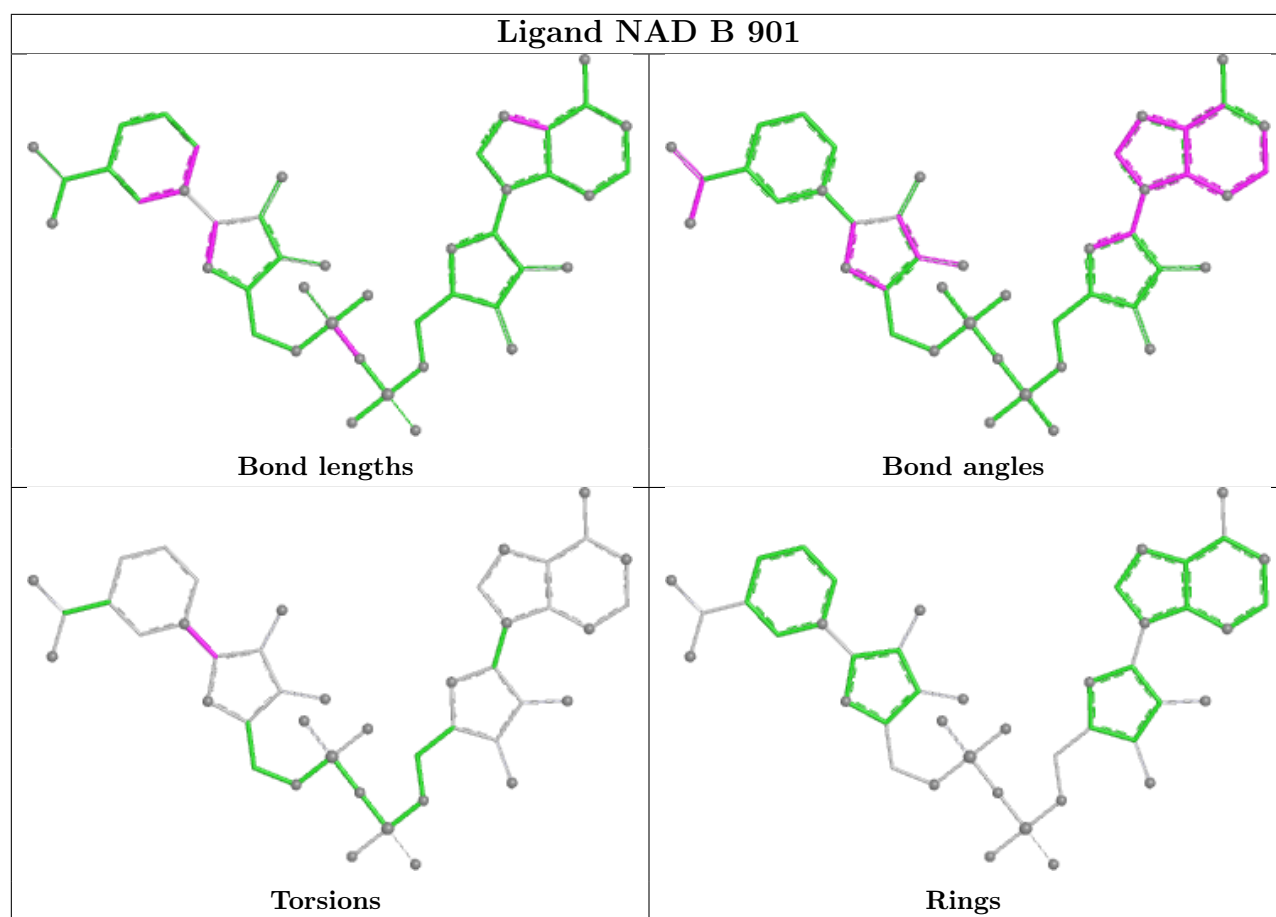
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	NAD	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

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.