



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:04 AM UTC

PDB ID : 1F8F / pdb_00001f8f
Title : CRYSTAL STRUCTURE OF BENZYL ALCOHOL DEHYDROGENASE
FROM ACINETOBACTER CALCOACETICUS
Authors : Beauchamp, J.C.; Gillooly, D.; Warwicker, J.; Fewson, C.A.; Laphorn, A.J.
Deposited on : 2000-06-30
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 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

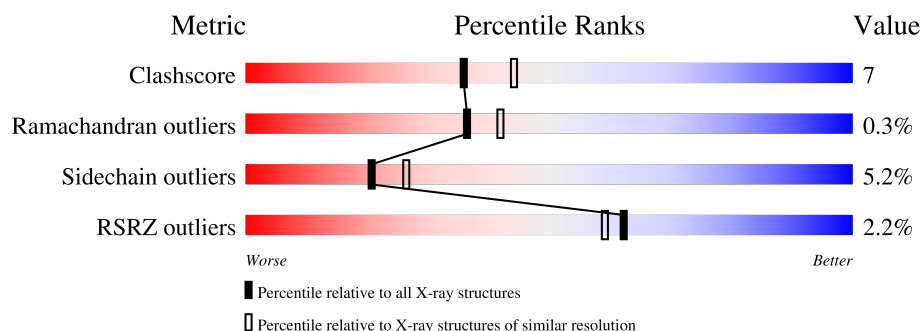
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	371	

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
5	EOH	A	374	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3040 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 BENZYL ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	1	0
			2672	1702	449	509	12			

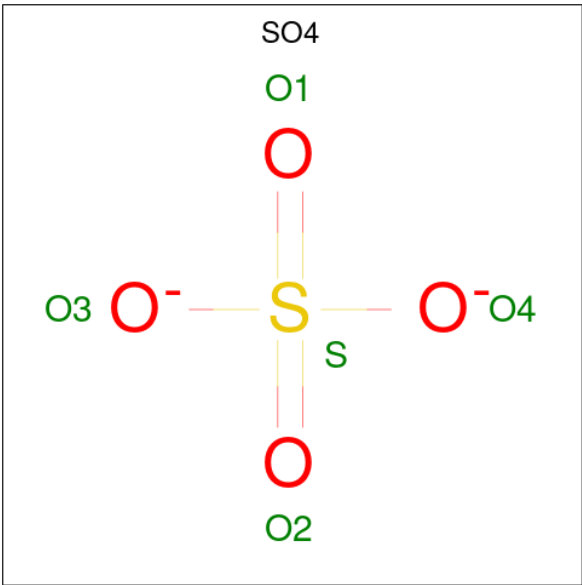
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	LYS	TYR	conflict	UNP Q59096
A	194	PHE	LEU	conflict	UNP Q59096
A	268	SER	ARG	conflict	UNP Q59096
A	359	ARG	HIS	conflict	UNP Q59096

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

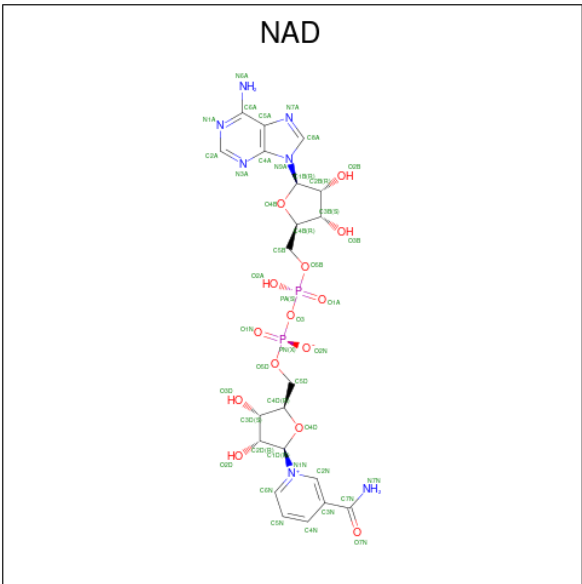
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



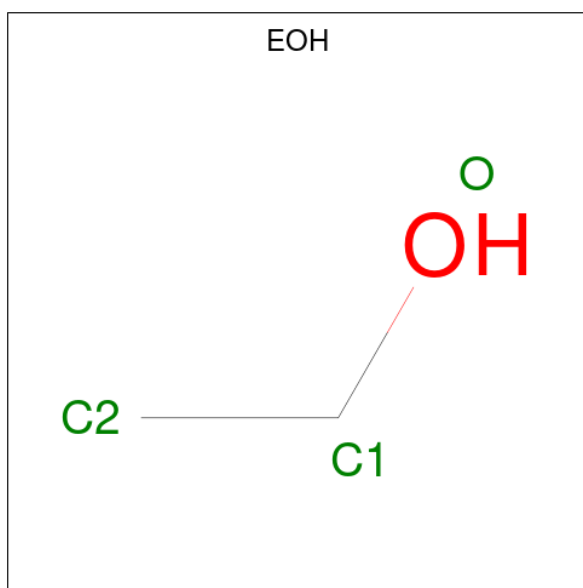
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 5 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	2	1		

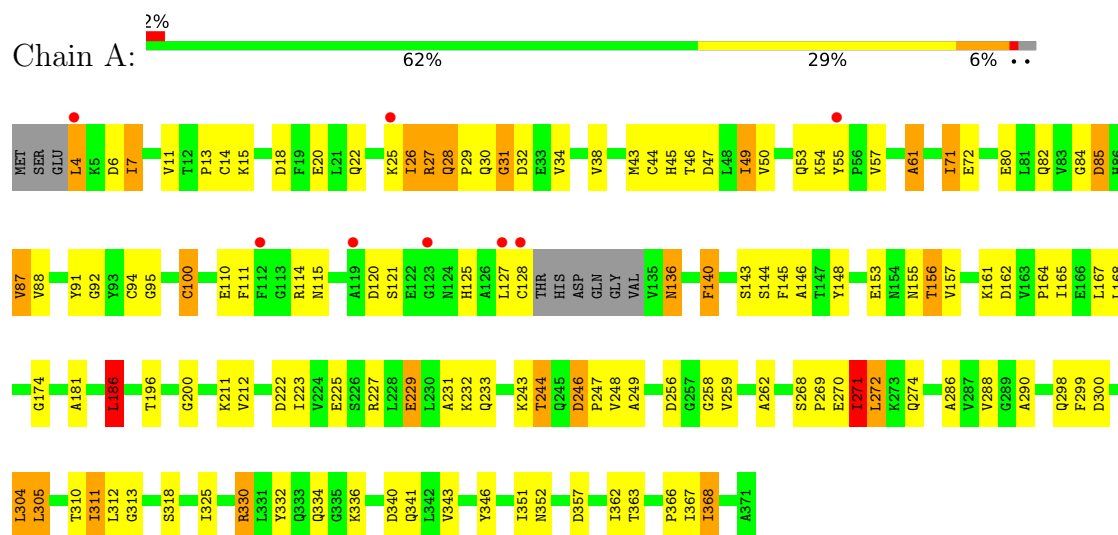
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	309	Total	O	0	0
			309	309		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: BENZYL ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.29Å 96.98Å 103.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-2.20) 91.5 (20.00-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.263 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3040	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, NAD, EOH

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	0.89	0/2722	2.25	113/3693 (3.1%)

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	2

There are no bond length outliers.

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ARG	CD-NE-CZ	34.55	172.76	124.40
1	A	270	GLU	CB-CG-CD	11.32	131.85	112.60
1	A	186	LEU	CA-C-O	9.95	130.95	120.70
1	A	47	ASP	CA-CB-CG	9.92	122.52	112.60
1	A	186	LEU	O-C-N	-9.50	111.83	122.09
1	A	114	ARG	NE-CZ-NH2	9.45	127.71	119.20
1	A	211	LYS	N-CA-CB	9.45	123.77	110.07
1	A	91	TYR	CA-C-N	9.35	130.62	122.29
1	A	91	TYR	C-N-CA	9.35	130.62	122.29
1	A	343	VAL	N-CA-C	9.31	122.58	108.71
1	A	155	ASN	CA-CB-CG	9.08	121.68	112.60
1	A	186	LEU	CA-C-N	8.69	136.04	122.93
1	A	186	LEU	C-N-CA	8.69	136.04	122.93
1	A	27	ARG	CD-NE-CZ	8.63	136.49	124.40
1	A	111	PHE	CA-C-O	-8.50	111.72	121.07
1	A	71	ILE	CA-C-N	8.35	135.81	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ILE	C-N-CA	8.35	135.81	122.11
1	A	88	VAL	O-C-N	-8.28	114.48	123.18
1	A	94	CYS	CA-C-O	-8.27	111.06	120.24
1	A	168	LEU	N-CA-C	8.18	123.25	113.28
1	A	352	ASN	OD1-CG-ND2	8.05	130.65	122.60
1	A	300	ASP	CA-CB-CG	7.97	120.57	112.60
1	A	57	VAL	N-CA-C	-7.95	101.79	108.63
1	A	111	PHE	O-C-N	-7.82	113.72	122.08
1	A	18	ASP	CA-CB-CG	7.66	120.26	112.60
1	A	341	GLN	OE1-CD-NE2	7.66	130.26	122.60
1	A	6	ASP	CA-CB-CG	7.62	120.22	112.60
1	A	223	ILE	N-CA-CB	7.53	121.29	112.33
1	A	110	GLU	CB-CG-CD	7.37	125.14	112.60
1	A	223	ILE	CB-CA-C	-7.30	102.74	110.62
1	A	325	ILE	N-CA-CB	7.15	116.03	110.45
1	A	298	GLN	CA-C-O	-7.14	113.09	121.16
1	A	312	LEU	N-CA-C	7.12	121.13	109.24
1	A	164	PRO	CA-C-O	-7.10	113.58	121.32
1	A	330	ARG	NE-CZ-NH2	7.09	125.58	119.20
1	A	352	ASN	CA-CB-CG	-7.01	105.59	112.60
1	A	227	ARG	CD-NE-CZ	6.98	134.17	124.40
1	A	346	TYR	CA-C-O	-6.89	113.39	121.46
1	A	318	SER	CA-C-N	-6.68	110.74	123.29
1	A	318	SER	C-N-CA	-6.68	110.74	123.29
1	A	243	LYS	CA-C-N	6.63	133.74	122.26
1	A	243	LYS	C-N-CA	6.63	133.74	122.26
1	A	54	LYS	CA-C-N	6.58	137.85	121.80
1	A	54	LYS	C-N-CA	6.58	137.85	121.80
1	A	311	ILE	CA-CB-CG1	6.48	121.41	110.40
1	A	61	ALA	N-CA-C	6.42	118.30	108.42
1	A	49	ILE	CA-C-O	-6.40	112.29	120.03
1	A	244	THR	N-CA-CB	-6.39	101.00	110.53
1	A	120	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	212	VAL	CA-C-O	-6.27	114.43	120.95
1	A	38	VAL	N-CA-C	6.22	117.08	109.30
1	A	313	GLY	CA-C-O	-6.19	115.20	120.89
1	A	115	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	A	85	ASP	CA-C-N	6.09	130.78	122.19
1	A	85	ASP	C-N-CA	6.09	130.78	122.19
1	A	244	THR	N-CA-C	6.00	120.76	113.38
1	A	196	THR	CA-C-O	-5.98	113.75	120.32
1	A	305	LEU	CB-CA-C	5.97	120.83	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	268	SER	CA-C-O	5.93	123.71	119.32
1	A	181	ALA	CA-C-O	5.87	126.77	120.55
1	A	22	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	A	156	THR	CA-C-N	5.82	130.55	122.93
1	A	156	THR	C-N-CA	5.82	130.55	122.93
1	A	167	LEU	N-CA-CB	-5.79	100.95	110.40
1	A	368	ILE	CB-CG1-CD1	5.76	125.89	113.80
1	A	200	GLY	CA-C-O	-5.71	115.93	121.92
1	A	249	ALA	O-C-N	5.68	128.62	122.15
1	A	290	ALA	N-CA-C	5.68	118.71	110.14
1	A	162	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	144	SER	N-CA-C	5.63	119.24	112.93
1	A	157	VAL	CA-C-O	5.63	127.27	120.74
1	A	258	GLY	CA-C-O	-5.62	115.67	121.91
1	A	92	GLY	CA-C-O	5.61	125.63	120.81
1	A	165	ILE	O-C-N	-5.60	114.71	122.05
1	A	94	CYS	O-C-N	5.56	129.46	122.23
1	A	125	HIS	CA-C-O	-5.51	114.93	121.16
1	A	288	VAL	O-C-N	-5.51	116.10	122.17
1	A	256	ASP	CA-C-O	-5.48	115.34	122.14
1	A	140	PHE	N-CA-C	-5.45	105.26	112.24
1	A	351	ILE	CA-C-O	-5.45	115.28	120.95
1	A	271	ILE	CA-C-O	5.40	126.08	120.25
1	A	231	ALA	CA-C-N	5.37	127.47	120.28
1	A	231	ALA	C-N-CA	5.37	127.47	120.28
1	A	20	GLU	CA-CB-CG	5.34	124.78	114.10
1	A	246	ASP	CA-C-N	5.33	124.66	118.85
1	A	246	ASP	C-N-CA	5.33	124.66	118.85
1	A	87	VAL	CA-C-O	5.32	126.89	121.63
1	A	80	GLU	CA-CB-CG	5.31	124.72	114.10
1	A	227	ARG	NH1-CZ-NH2	-5.30	112.41	119.30
1	A	340	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	44	CYS	CA-C-O	5.27	127.28	121.11
1	A	136	ASN	CA-CB-CG	-5.25	107.35	112.60
1	A	259	VAL	N-CA-CB	-5.24	101.32	110.49
1	A	114	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	A	157	VAL	N-CA-C	5.21	115.27	107.51
1	A	92	GLY	O-C-N	-5.18	120.08	123.35
1	A	262	ALA	N-CA-C	5.18	117.06	109.24
1	A	310	THR	CA-C-O	5.18	125.95	120.36
1	A	7	ILE	N-CA-C	5.17	115.62	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	VAL	CA-C-O	5.17	126.64	121.17
1	A	146	ALA	CA-C-O	5.16	126.75	121.23
1	A	336	LYS	CA-C-N	-5.12	117.77	122.28
1	A	336	LYS	C-N-CA	-5.12	117.77	122.28
1	A	222	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	100	CYS	CA-C-O	-5.11	115.14	120.55
1	A	174	GLY	N-CA-C	5.10	118.85	112.73
1	A	366	PRO	CA-C-N	5.08	130.46	122.84
1	A	366	PRO	C-N-CA	5.08	130.46	122.84
1	A	153	GLU	CA-C-O	-5.08	115.17	120.55
1	A	45	HIS	CA-CB-CG	-5.05	108.75	113.80
1	A	332	TYR	CA-C-O	-5.04	115.51	120.70
1	A	247	PRO	O-C-N	-5.04	115.94	122.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	LEU	Mainchain
1	A	367	ILE	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	2672	0	2715	39	0
2	A	2	0	0	0	0
3	A	10	0	0	0	0
4	A	44	0	26	1	0
5	A	3	0	6	2	0
6	A	309	0	0	1	0
All	All	3040	0	2747	40	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 (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLY:HA2	1:A:100:CYS:HB3	1.68	0.76
1:A:271:ILE:HD13	1:A:274:GLN:NE2	2.02	0.75
1:A:330:ARG:O	1:A:334:GLN:HG3	1.94	0.68
4:A:375:NAD:H4N	5:A:374:EOH:H11	1.84	0.60
1:A:145:PHE:CE1	1:A:368:ILE:HD13	2.38	0.58
1:A:357:ASP:HB3	1:A:362:ILE:HD11	1.88	0.56
1:A:11:VAL:O	1:A:13:PRO:HD3	2.08	0.53
1:A:26:ILE:HD12	1:A:127:LEU:CD2	2.38	0.53
1:A:84:GLY:O	1:A:161:LYS:NZ	2.43	0.52
1:A:7:ILE:HG21	1:A:148:TYR:HB2	1.92	0.52
1:A:95:GLY:HA2	1:A:100:CYS:CB	2.41	0.51
1:A:299:PHE:HE2	1:A:304:LEU:HD22	1.74	0.51
1:A:14:CYS:O	1:A:15:LYS:C	2.54	0.50
1:A:71:ILE:HD12	1:A:85:ASP:HB2	1.93	0.50
1:A:49:ILE:C	1:A:49:ILE:HD12	2.37	0.49
1:A:61:ALA:HB2	1:A:136:ASN:HB2	1.93	0.49
1:A:43:MET:HE3	1:A:368:ILE:HD11	1.94	0.49
1:A:30:GLN:O	1:A:31:GLY:C	2.56	0.48
1:A:87:VAL:HG11	1:A:156:THR:HG22	1.95	0.48
1:A:271:ILE:HD13	1:A:274:GLN:HE22	1.75	0.48
1:A:271:ILE:HD13	1:A:274:GLN:HE21	1.78	0.47
1:A:46:THR:HA	1:A:49:ILE:HG13	1.96	0.46
1:A:28:GLN:HB3	1:A:29:PRO:HD2	1.99	0.44
1:A:27:ARG:HG3	1:A:28:GLN:O	2.17	0.44
1:A:225:GLU:O	1:A:229:GLU:HG2	2.16	0.44
1:A:311:ILE:HD13	1:A:311:ILE:HG21	1.74	0.44
1:A:121:SER:HB2	6:A:580:HOH:O	2.18	0.44
1:A:140:PHE:CZ	5:A:374:EOH:H12	2.53	0.43
1:A:272:LEU:C	1:A:272:LEU:HD23	2.45	0.42
1:A:53:GLN:C	1:A:55:TYR:H	2.25	0.42
1:A:299:PHE:CE2	1:A:304:LEU:HD22	2.54	0.42
1:A:186:LEU:HD21	1:A:286:ALA:HB2	2.02	0.41
1:A:229:GLU:O	1:A:233:GLN:HG3	2.19	0.41
1:A:49:ILE:HD12	1:A:50:VAL:N	2.35	0.41
1:A:362:ILE:HD12	1:A:363:THR:OG1	2.20	0.41
1:A:246:ASP:OD1	1:A:246:ASP:C	2.64	0.41
1:A:4:LEU:C	1:A:4:LEU:HD12	2.46	0.41
1:A:271:ILE:HA	1:A:274:GLN:HE21	1.86	0.41
1:A:244:THR:O	1:A:244:THR:HG22	2.21	0.40
1:A:72:GLU:O	1:A:72:GLU:HG3	2.21	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	359/371 (97%)	339 (94%)	19 (5%)	1 (0%)	36	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLY

5.3.2 Protein sidechains [i](#)

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	287/294 (98%)	272 (95%)	15 (5%)	21	26

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	25	LYS
1	A	26	ILE
1	A	28	GLN
1	A	34	VAL
1	A	82	GLN
1	A	128	CYS
1	A	143	SER
1	A	229	GLU
1	A	232	LYS

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Mol	Chain	Res	Type
1	A	269	PRO
1	A	271	ILE
1	A	272	LEU
1	A	304	LEU
1	A	305	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	82	GLN
1	A	99	GLN
1	A	274	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	NAD	A	375	-	46,48,48	1.42	6 (13%)	64,73,73	1.88	9 (14%)
3	SO4	A	376	-	4,4,4	0.73	0	6,6,6	0.28	0
3	SO4	A	377	-	4,4,4	0.77	0	6,6,6	0.43	0
5	EOH	A	374	-	2,2,2	0.13	0	1,1,1	0.45	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	NAD	A	375	-	-	4/30/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	375	NAD	C3N-C7N	4.60	1.57	1.50
4	A	375	NAD	PA-O3	3.73	1.63	1.59
4	A	375	NAD	C6N-N1N	3.53	1.43	1.35
4	A	375	NAD	C7N-N7N	3.04	1.38	1.33
4	A	375	NAD	O4D-C1D	2.46	1.44	1.40
4	A	375	NAD	C4N-C3N	2.42	1.43	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	375	NAD	C5N-C4N-C3N	-9.21	111.31	120.36
4	A	375	NAD	C5N-C6N-N1N	-5.68	112.64	120.38
4	A	375	NAD	C4D-O4D-C1D	-4.80	105.53	109.92
4	A	375	NAD	C6N-C5N-C4N	4.25	125.57	119.45
4	A	375	NAD	C2N-C3N-C4N	2.28	120.91	118.26
4	A	375	NAD	C3N-C7N-N7N	-2.19	115.04	117.74
4	A	375	NAD	O7N-C7N-N7N	2.16	125.74	122.62
4	A	375	NAD	C6N-N1N-C2N	-2.11	120.08	121.88
4	A	375	NAD	C5D-C4D-C3D	2.08	122.69	115.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	375	NAD	O4D-C1D-N1N-C2N

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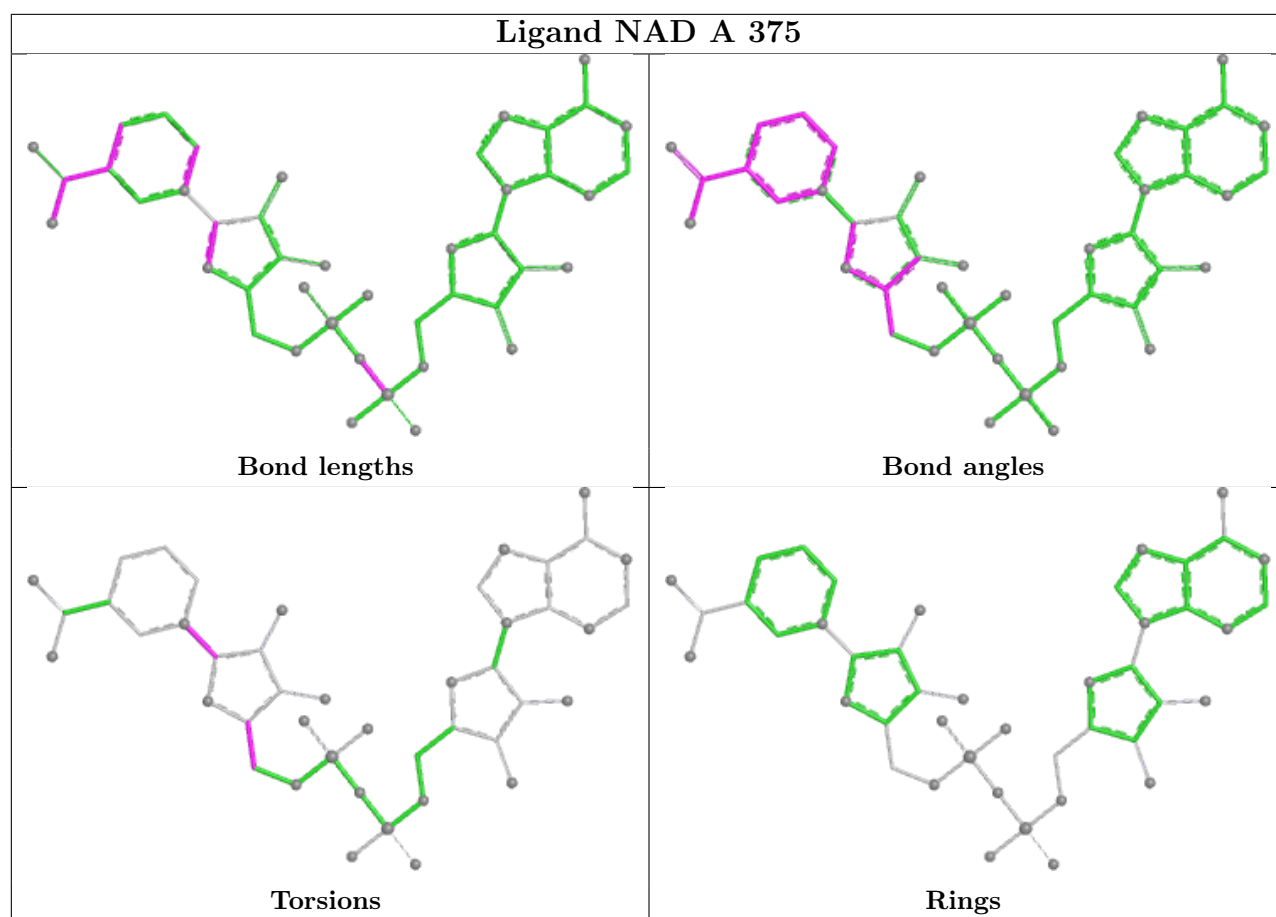
Mol	Chain	Res	Type	Atoms
4	A	375	NAD	O4D-C1D-N1N-C6N
4	A	375	NAD	C2D-C1D-N1N-C2N
4	A	375	NAD	O4D-C4D-C5D-O5D

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	375	NAD	1	0
5	A	374	EOH	2	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	362/371 (97%)	-0.11	8 (2%) 62 59	17, 30, 60, 83	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	LEU	2.9
1	A	119	ALA	2.9
1	A	128	CYS	2.6
1	A	112	PHE	2.5
1	A	55	TYR	2.4
1	A	127	LEU	2.3
1	A	123	GLY	2.3
1	A	25	LYS	2.0

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](#)

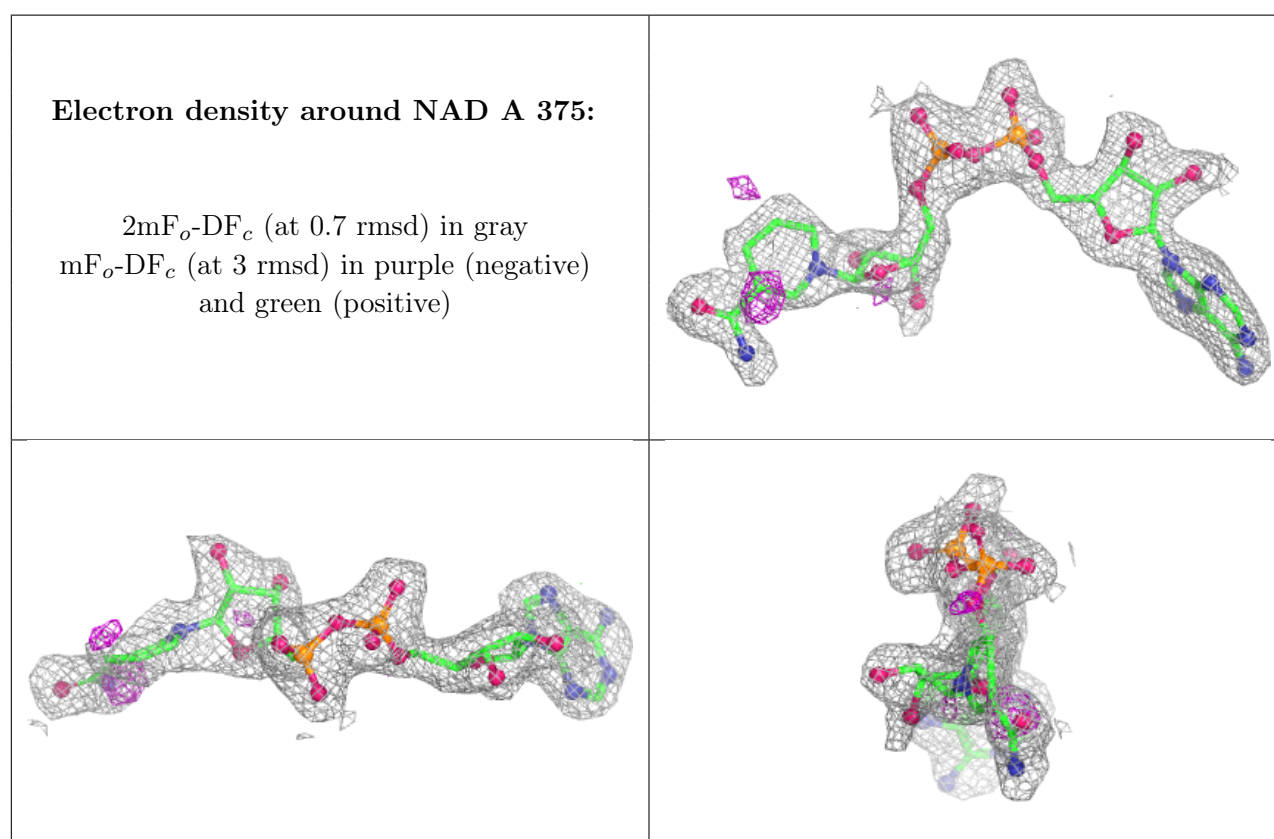
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
5	EOH	A	374	3/3	0.75	0.24	45,45,49,50	0
3	SO4	A	377	5/5	0.89	0.17	62,62,63,63	0
4	NAD	A	375	44/44	0.90	0.10	38,51,54,55	0
3	SO4	A	376	5/5	0.90	0.13	69,70,71,71	0
2	ZN	A	372	1/1	0.96	0.04	42,42,42,42	0
2	ZN	A	373	1/1	0.99	0.02	26,26,26,26	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.