



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:36 AM UTC

PDB ID : 2CF6 / pdb_00002cf6
Title : Crystal Structures of the Arabidopsis Cinnamyl Alcohol Dehydrogenases At-CAD5
Authors : Youn, B.; Camacho, R.; Moinuddin, S.G.; Lee, C.; Davin, L.B.; Lewis, N.G.; Kang, C.
Deposited on : 2006-02-16
Resolution : 2.60 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)
Xtrriage (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

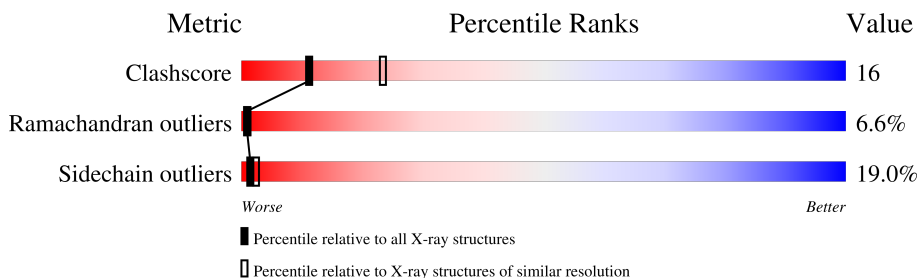
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	357	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2855 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.

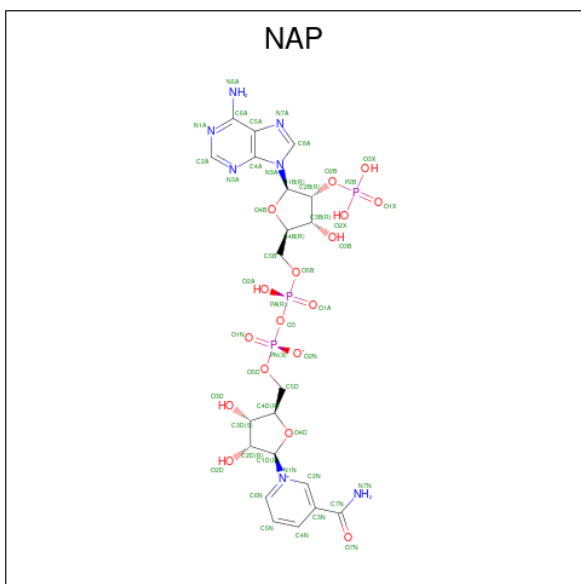
- Molecule 1 is a protein called CINNAMYL ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	352	2665	1686	450	507	22	0	0	0

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

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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total 140	O 140	0	0

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	54.71Å 54.71Å 303.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	93.2 (10.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.201 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2855	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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: NAP, ZN

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	0.90	12/2715 (0.4%)	1.89	72/3674 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	69	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	142	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	52	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	206	HIS	CD2-NE2	-6.48	1.30	1.37
1	A	174	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	205	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	48	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	194	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	255	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	205	HIS	CG-ND1	-5.41	1.32	1.38
1	A	256	HIS	CG-ND1	-5.16	1.32	1.38

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	GLU	N-CA-C	-9.07	98.97	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	LYS	N-CA-C	8.37	122.06	109.25
1	A	351	GLU	N-CA-C	-7.98	101.58	112.03
1	A	258	LEU	N-CA-C	7.96	121.05	111.82
1	A	127	ASN	CA-CB-CG	7.81	120.41	112.60
1	A	342	VAL	N-CA-C	7.67	125.29	109.34
1	A	215	LYS	N-CA-C	7.43	119.03	111.07
1	A	353	SER	N-CA-C	7.24	126.22	110.80
1	A	330	VAL	N-CA-C	7.04	117.15	110.53
1	A	177	LEU	N-CA-C	6.93	125.56	110.80
1	A	14	ALA	N-CA-C	6.87	119.68	108.55
1	A	182	LEU	N-CA-C	6.80	125.29	110.80
1	A	38	ASN	CA-CB-CG	6.67	119.27	112.60
1	A	31	GLU	CA-C-O	6.62	127.50	120.36
1	A	17	ASP	CA-C-N	6.60	128.09	119.84
1	A	17	ASP	C-N-CA	6.60	128.09	119.84
1	A	54	THR	CA-CB-OG1	-6.52	99.82	109.60
1	A	71	VAL	N-CA-C	6.48	118.73	108.89
1	A	348	VAL	CA-C-N	-6.41	113.65	122.30
1	A	348	VAL	C-N-CA	-6.41	113.65	122.30
1	A	286	PRO	N-CA-C	6.39	125.64	112.47
1	A	328	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	53	GLN	N-CA-C	-6.32	104.01	111.03
1	A	205	HIS	CA-CB-CG	6.24	120.04	113.80
1	A	356	ASP	N-CA-C	6.15	116.56	108.07
1	A	127	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	A	211	SER	N-CA-C	5.96	118.35	108.99
1	A	250	ASP	N-CA-C	5.86	118.46	108.02
1	A	287	LEU	CA-C-O	5.82	126.58	120.42
1	A	279	ASN	CA-CB-CG	5.78	118.38	112.60
1	A	31	GLU	N-CA-C	5.77	118.31	108.90
1	A	244	SER	N-CA-C	5.74	120.34	111.56
1	A	127	ASN	CB-CG-ND2	5.72	124.98	116.40
1	A	69	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	A	316	LYS	N-CA-C	-5.70	97.97	107.99
1	A	228	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	257	ALA	CA-C-O	5.59	126.85	120.54
1	A	137	LYS	N-CA-C	5.57	122.66	110.80
1	A	108	ARG	N-CA-C	-5.55	99.48	108.41
1	A	167	THR	CA-CB-OG1	-5.54	101.29	109.60
1	A	17	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	48	HIS	CB-CG-CD2	-5.44	124.12	131.20
1	A	256	HIS	CB-CG-CD2	-5.44	124.13	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	THR	O-C-N	5.41	127.86	122.12
1	A	32	THR	CA-C-O	5.38	128.20	120.51
1	A	54	THR	N-CA-CB	-5.36	101.44	110.49
1	A	178	LYS	CA-CB-CG	5.33	124.75	114.10
1	A	348	VAL	CB-CA-C	-5.32	103.86	111.31
1	A	206	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	A	122	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	55	LYS	CA-C-N	5.25	131.56	121.54
1	A	55	LYS	C-N-CA	5.25	131.56	121.54
1	A	309	MET	N-CA-C	5.20	117.62	111.33
1	A	343	ARG	CA-C-N	5.19	131.46	121.54
1	A	343	ARG	C-N-CA	5.19	131.46	121.54
1	A	270	LYS	N-CA-C	5.19	116.87	108.41
1	A	65	MET	N-CA-C	5.19	116.87	108.41
1	A	179	GLN	CA-C-N	5.18	125.16	120.03
1	A	179	GLN	C-N-CA	5.18	125.16	120.03
1	A	116	LYS	N-CA-C	5.14	119.25	112.25
1	A	279	ASN	N-CA-CB	5.12	119.49	110.37
1	A	290	LEU	N-CA-C	-5.12	105.35	111.03
1	A	108	ARG	CA-C-N	5.10	131.28	121.54
1	A	108	ARG	C-N-CA	5.10	131.28	121.54
1	A	324	VAL	CA-C-O	5.10	126.61	120.65
1	A	261	TYR	CA-CB-CG	-5.07	104.78	113.90
1	A	126	ILE	N-CA-CB	-5.05	102.89	111.23
1	A	180	PRO	N-CA-C	5.05	118.99	111.41
1	A	13	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	A	294	VAL	N-CA-C	5.04	115.23	108.17
1	A	168	VAL	N-CA-CB	-5.04	100.95	111.24
1	A	54	THR	CA-CB-CG2	5.01	119.01	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	SER	Peptide

5.2 Too-close contacts [i](#)

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	2665	0	2666	87	0
2	A	2	0	0	0	0
3	A	48	0	25	8	0
4	A	140	0	0	5	0
All	All	2855	0	2691	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 16.

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)
1:A:117:LYS:HZ2	1:A:119:TRP:HE1	1.28	0.81
1:A:48:HIS:HA	1:A:51:LEU:HD12	1.62	0.81
1:A:183:ARG:HG2	1:A:206:HIS:HB3	1.66	0.78
1:A:117:LYS:NZ	1:A:119:TRP:HE1	1.84	0.76
1:A:336:ARG:HA	1:A:339:LYS:HG2	1.67	0.76
1:A:127:ASN:ND2	1:A:129:GLN:H	1.87	0.72
1:A:71:VAL:HG23	1:A:93:VAL:HG13	1.72	0.71
1:A:154:ALA:HB3	1:A:157:GLN:HB2	1.73	0.70
1:A:212:SER:HG	3:A:450:NAP:P2B	2.15	0.70
1:A:93:VAL:HB	1:A:146:VAL:HG12	1.74	0.70
1:A:99:CYS:HG	1:A:145:PHE:HZ	1.41	0.69
1:A:127:ASN:HD22	1:A:129:GLN:H	1.40	0.69
1:A:250:ASP:HB2	1:A:273:LEU:HA	1.77	0.67
1:A:103:CYS:SG	1:A:105:PRO:HB2	2.36	0.65
1:A:127:ASN:HD22	1:A:128:GLY:N	1.95	0.64
1:A:212:SER:OG	3:A:450:NAP:O2X	2.16	0.63
1:A:118:ILE:HD13	1:A:125:TYR:HA	1.81	0.62
1:A:32:THR:HA	1:A:36:ASP:HB2	1.82	0.62
1:A:105:PRO:HB3	1:A:113:TYR:O	2.00	0.62
1:A:195:MET:SD	1:A:198:LYS:NZ	2.71	0.62
1:A:14:ALA:HB2	1:A:66:VAL:HG22	1.82	0.61
1:A:99:CYS:SG	1:A:145:PHE:HZ	2.23	0.61
1:A:175:PHE:HB2	1:A:177:LEU:HD22	1.84	0.60
1:A:44:CYS:SG	1:A:45:GLY:N	2.74	0.59
1:A:178:LYS:HE2	1:A:203:MET:HE2	1.85	0.59
1:A:112:GLN:NE2	1:A:112:GLN:H	2.01	0.58
1:A:142:HIS:HD2	1:A:144:LYS:H	1.53	0.57
1:A:68:GLY:HA3	1:A:134:GLY:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PRO:O	1:A:55:LYS:HA	2.06	0.55
1:A:141:VAL:HG12	1:A:142:HIS:H	1.71	0.55
1:A:112:GLN:H	1:A:112:GLN:HE21	1.54	0.54
1:A:99:CYS:HB2	4:A:2134:HOH:O	2.07	0.53
1:A:342:VAL:HG12	1:A:346:PHE:CE1	2.43	0.53
1:A:157:GLN:HE22	1:A:320:SER:H	1.58	0.52
1:A:194:HIS:ND1	1:A:224:LEU:HD21	2.25	0.52
1:A:278:ASN:HD22	1:A:278:ASN:H	1.57	0.52
1:A:121:TYR:HA	1:A:131:THR:O	2.10	0.51
1:A:163:CYS:SG	1:A:164:ALA:N	2.84	0.51
1:A:141:VAL:HG12	1:A:142:HIS:N	2.25	0.51
1:A:53:GLN:HB3	1:A:65:MET:HE1	1.92	0.50
1:A:161:LEU:HA	1:A:165:GLY:HA3	1.93	0.50
1:A:177:LEU:HG	1:A:247:TYR:CD1	2.47	0.50
1:A:251:THR:HG22	4:A:2084:HOH:O	2.10	0.50
1:A:167:THR:OG1	3:A:450:NAP:H4N	2.12	0.50
1:A:254:VAL:HG22	1:A:255:HIS:H	1.77	0.50
1:A:7:GLU:CA	1:A:31:GLU:HG2	2.41	0.49
1:A:193:GLY:O	1:A:197:VAL:HG23	2.13	0.48
1:A:190:GLY:HA2	1:A:194:HIS:HD2	1.77	0.48
1:A:38:ASN:HB3	1:A:77:GLU:HB3	1.95	0.48
1:A:65:MET:HE3	1:A:122:ASN:HB2	1.94	0.48
1:A:267:LEU:HA	1:A:291:GLY:O	2.12	0.48
1:A:287:LEU:O	1:A:290:LEU:HB3	2.13	0.48
1:A:288:LEU:HA	1:A:293:LYS:HB2	1.96	0.47
1:A:56:ASN:HA	1:A:61:SER:HB2	1.96	0.47
1:A:212:SER:OG	3:A:450:NAP:P2B	2.72	0.47
1:A:257:ALA:HA	1:A:282:GLN:HE22	1.81	0.46
1:A:153:MET:HE2	1:A:157:GLN:HB3	1.99	0.45
1:A:268:ASP:HA	1:A:292:ARG:O	2.17	0.45
1:A:58:LEU:HD13	1:A:60:MET:HB2	1.99	0.45
1:A:192:VAL:HG23	3:A:450:NAP:O2N	2.16	0.45
1:A:255:HIS:HB2	1:A:279:ASN:HD22	1.82	0.45
1:A:97:VAL:HG21	1:A:120:SER:HA	1.98	0.44
1:A:316:LYS:O	1:A:318:LEU:HD22	2.18	0.44
1:A:161:LEU:HD12	1:A:310:LEU:HD12	2.00	0.44
1:A:75:VAL:HG21	4:A:2036:HOH:O	2.17	0.44
1:A:78:VAL:HG13	1:A:82:VAL:HB	1.99	0.44
1:A:165:GLY:HA2	1:A:195:MET:HG3	2.00	0.44
1:A:182:LEU:H	1:A:182:LEU:HD12	1.82	0.44
1:A:78:VAL:HG22	1:A:82:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:HG23	1:A:237:LYS:HB3	2.01	0.43
1:A:277:ILE:HG21	1:A:281:LEU:HD21	2.01	0.43
1:A:214:ASN:O	1:A:217:ARG:HB2	2.19	0.43
1:A:30:ARG:HH21	1:A:36:ASP:CG	2.27	0.42
1:A:41:ILE:HD12	1:A:136:ALA:O	2.19	0.42
1:A:113:TYR:CE2	1:A:299:PHE:HB3	2.54	0.42
1:A:171:PRO:HG3	1:A:274:MET:HE1	2.01	0.42
1:A:212:SER:OG	3:A:450:NAP:O3X	2.38	0.42
1:A:300:ILE:H	3:A:450:NAP:H72N	1.68	0.41
1:A:104:SER:HA	1:A:107:GLU:HB2	2.01	0.41
1:A:177:LEU:H	1:A:177:LEU:HD13	1.85	0.41
1:A:189:LEU:O	1:A:216:LYS:HD3	2.21	0.41
1:A:284:LEU:HB2	1:A:287:LEU:HG	2.03	0.41
3:A:450:NAP:H6N	3:A:450:NAP:H2D	1.73	0.41
1:A:258:LEU:HD11	1:A:281:LEU:HB3	2.03	0.40
1:A:65:MET:CE	1:A:122:ASN:HB2	2.51	0.40
1:A:163:CYS:HB2	4:A:2135:HOH:O	2.21	0.40
1:A:192:VAL:HG12	4:A:2084:HOH:O	2.20	0.40
1:A:338:GLU:C	1:A:340:ASN:H	2.30	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	350/357 (98%)	276 (79%)	51 (15%)	23 (7%)	1 1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PRO
1	A	56	ASN

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Mol	Chain	Res	Type
1	A	109	ASP
1	A	177	LEU
1	A	182	LEU
1	A	342	VAL
1	A	32	THR
1	A	79	GLY
1	A	133	GLY
1	A	223	ASP
1	A	242	ALA
1	A	255	HIS
1	A	279	ASN
1	A	300	ILE
1	A	317	GLY
1	A	353	SER
1	A	54	THR
1	A	58	LEU
1	A	191	GLY
1	A	264	LEU
1	A	343	ARG
1	A	8	ARG
1	A	340	ASN

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	295/300 (98%)	239 (81%)	56 (19%)	1 2

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	17	ASP
1	A	18	PRO
1	A	21	ILE
1	A	28	THR

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Mol	Chain	Res	Type
1	A	32	THR
1	A	39	ILE
1	A	46	ILE
1	A	78	VAL
1	A	93	VAL
1	A	103	CYS
1	A	105	PRO
1	A	108	ARG
1	A	111	GLU
1	A	112	GLN
1	A	126	ILE
1	A	127	ASN
1	A	129	GLN
1	A	131	THR
1	A	141	VAL
1	A	143	GLN
1	A	161	LEU
1	A	167	THR
1	A	168	VAL
1	A	177	LEU
1	A	189	LEU
1	A	218	GLU
1	A	223	ASP
1	A	237	LYS
1	A	241	LEU
1	A	244	SER
1	A	245	LEU
1	A	250	ASP
1	A	251	THR
1	A	252	VAL
1	A	260	PRO
1	A	271	LEU
1	A	278	ASN
1	A	282	GLN
1	A	286	PRO
1	A	289	MET
1	A	290	LEU
1	A	302	SER
1	A	305	GLU
1	A	310	LEU
1	A	313	CYS
1	A	316	LYS

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Mol	Chain	Res	Type
1	A	318	LEU
1	A	320	SER
1	A	322	ILE
1	A	330	VAL
1	A	332	THR
1	A	338	GLU
1	A	341	ASP
1	A	343	ARG
1	A	350	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	112	GLN
1	A	127	ASN
1	A	142	HIS
1	A	143	GLN
1	A	157	GLN
1	A	278	ASN
1	A	279	ASN
1	A	282	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	NAP	A	450	-	50,52,52	1.88	9 (18%)	71,80,80	1.91	14 (19%)

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	NAP	A	450	-	-	12/35/67/67	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	450	NAP	C2N-N1N	5.98	1.41	1.35
3	A	450	NAP	P2B-O2B	5.98	1.70	1.59
3	A	450	NAP	PN-O3	5.18	1.65	1.59
3	A	450	NAP	C5A-N7A	-3.49	1.32	1.39
3	A	450	NAP	PA-O3	3.39	1.63	1.59
3	A	450	NAP	O4D-C1D	2.78	1.44	1.40
3	A	450	NAP	C6N-N1N	2.59	1.41	1.35
3	A	450	NAP	C3N-C7N	2.58	1.54	1.50
3	A	450	NAP	C4A-N9A	-2.05	1.33	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	450	NAP	C5A-C4A-N3A	-6.19	118.19	126.72
3	A	450	NAP	N3A-C4A-N9A	5.84	137.10	127.17
3	A	450	NAP	N3A-C2A-N1A	-4.54	121.71	128.58
3	A	450	NAP	O5D-C5D-C4D	4.44	124.13	108.99
3	A	450	NAP	C6A-C5A-C4A	3.68	122.20	117.18
3	A	450	NAP	O5B-C5B-C4B	3.65	121.41	108.99
3	A	450	NAP	C6A-C5A-N7A	-3.53	125.29	132.09
3	A	450	NAP	C2A-N3A-C4A	3.40	120.13	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	450	NAP	C2B-C3B-C4B	3.33	109.16	101.99
3	A	450	NAP	O2X-P2B-O2B	3.11	117.98	105.85
3	A	450	NAP	O4D-C4D-C5D	2.62	117.72	109.33
3	A	450	NAP	O4B-C4B-C5B	2.54	117.46	109.33
3	A	450	NAP	C6N-N1N-C2N	-2.51	119.74	121.88
3	A	450	NAP	O2B-P2B-O1X	-2.32	101.07	109.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

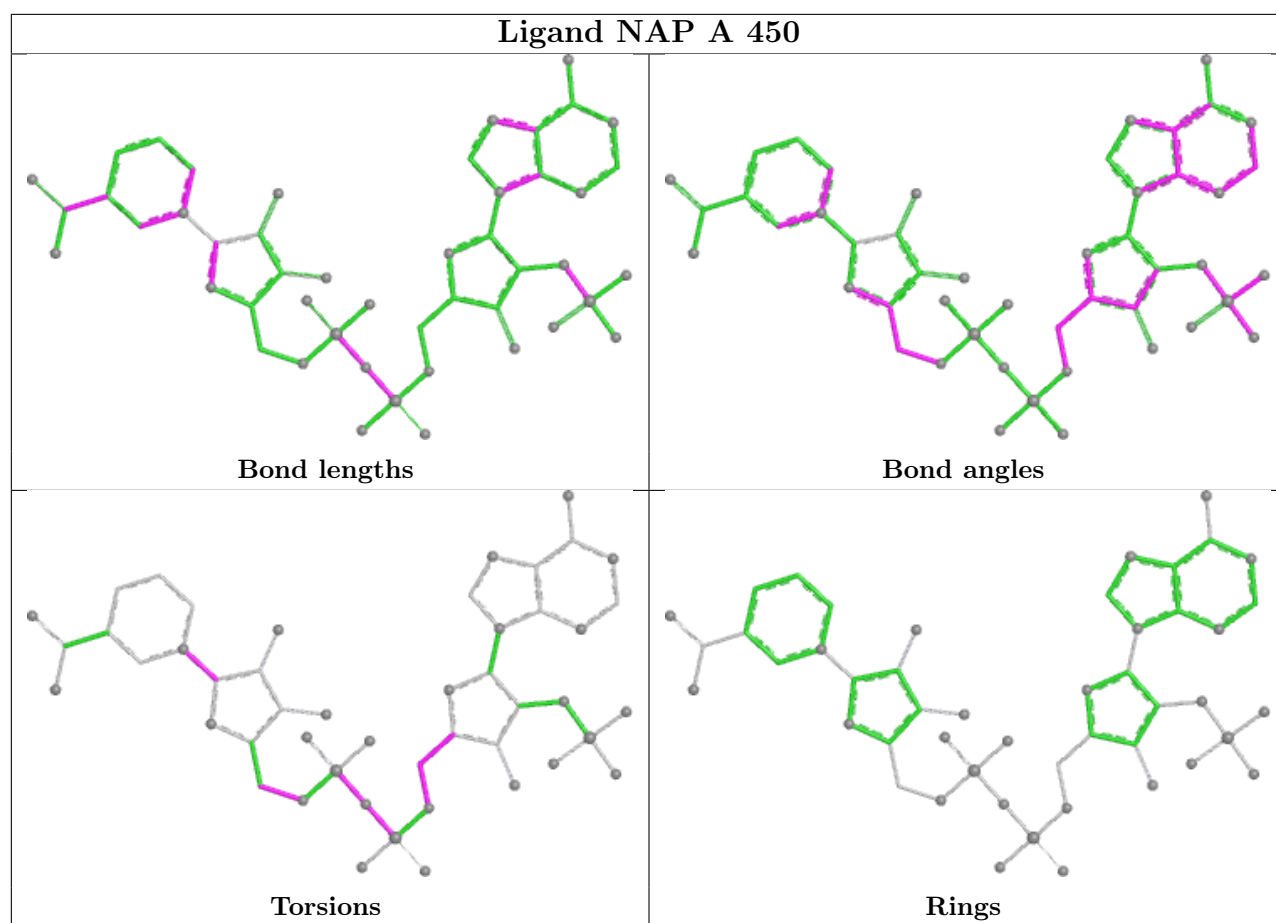
Mol	Chain	Res	Type	Atoms
3	A	450	NAP	C4B-C5B-O5B-PA
3	A	450	NAP	C3B-C4B-C5B-O5B
3	A	450	NAP	O4D-C1D-N1N-C2N
3	A	450	NAP	O4D-C1D-N1N-C6N
3	A	450	NAP	C2D-C1D-N1N-C2N
3	A	450	NAP	C2D-C1D-N1N-C6N
3	A	450	NAP	O4B-C4B-C5B-O5B
3	A	450	NAP	PN-O3-PA-O1A
3	A	450	NAP	PA-O3-PN-O5D
3	A	450	NAP	C4D-C5D-O5D-PN
3	A	450	NAP	PN-O3-PA-O2A
3	A	450	NAP	PA-O3-PN-O1N

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	450	NAP	8	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.