



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:50 am GMT

PDB ID : 2CF6
Title : CRYSTAL STRUCTURES OF THE ARABIDOPSIS CINNAMYL ALCOHOL DEHYDROGENASES ATCAD5
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

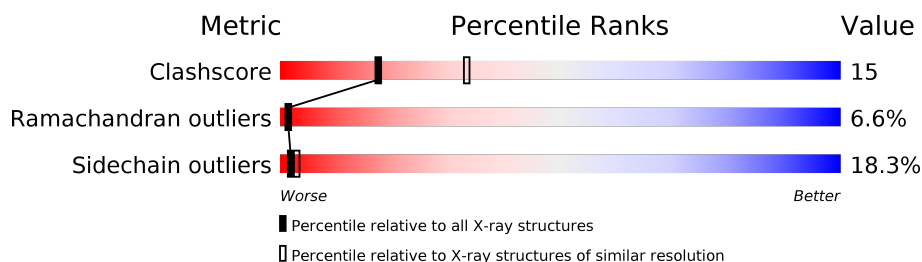
1 Overall quality at a glance

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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

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.

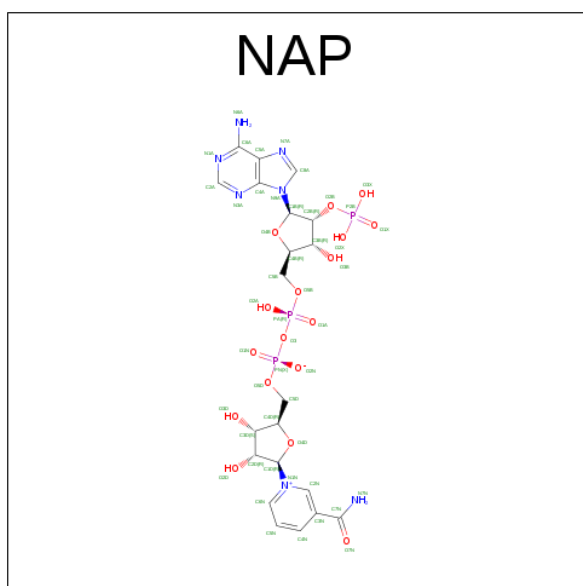
- Molecule 1 is a protein called CINNAMYL ALCOHOL DEHYDROGENASE.

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

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 4 is water.

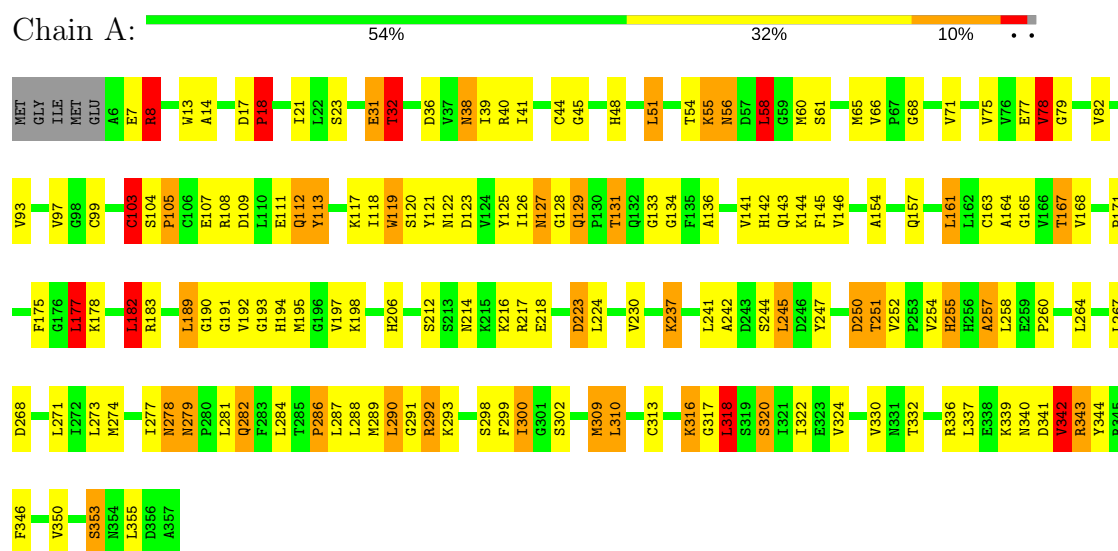
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total 140	O 140	0	0

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: CINNAMYL 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 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.	Xtriage
Total number of atoms	2855	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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: ZN, NAP

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	0.68	0/2715	1.53	31/3674 (0.8%)

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

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	A	13	TRP	CD1-CG-CD2	8.02	112.71	106.30
1	A	13	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	A	119	TRP	CE2-CD2-CG	-7.28	101.48	107.30
1	A	119	TRP	CD1-CG-CD2	6.82	111.75	106.30
1	A	113	TYR	CB-CG-CD1	-6.79	116.93	121.00
1	A	58	LEU	CA-CB-CG	6.40	130.03	115.30
1	A	292	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	31	GLU	CA-C-N	-6.20	103.56	117.20
1	A	292	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	8	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	245	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	78	VAL	CA-CB-CG2	-5.97	101.95	110.90
1	A	257	ALA	CA-C-N	-5.89	104.25	117.20
1	A	355	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	353	SER	N-CA-C	5.64	126.22	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	324	VAL	CA-C-N	-5.49	105.12	117.20
1	A	177	LEU	N-CA-C	5.39	125.56	111.00
1	A	13	TRP	CG-CD2-CE3	5.33	138.69	133.90
1	A	182	LEU	N-CA-C	5.29	125.29	111.00
1	A	342	VAL	N-CA-C	5.29	125.29	111.00
1	A	286	PRO	N-CA-C	5.21	125.64	112.10
1	A	32	THR	CA-C-N	-5.21	105.79	116.20
1	A	318	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	178	LYS	CA-CB-CG	5.16	124.75	113.40
1	A	51	LEU	CA-CB-CG	5.13	127.11	115.30
1	A	344	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	A	103	CYS	CA-CB-SG	5.09	123.16	114.00
1	A	290	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	309	MET	CA-CB-CG	5.00	121.80	113.30

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 ⓘ

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	82	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	83	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 15.

All (83) 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: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:117:LYS:HZ2	1:A:119:TRP:HE1	1.36	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:112:GLN:H	1:A:112:GLN:NE2	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
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:HE21	1:A:112:GLN:H	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:H	1:A:278:ASN:HD22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:171:PRO:HG3	1:A:274:MET:HE1	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:182:LEU:HD12	1:A:182:LEU:H	1.82	0.44
1:A:165:GLY:HA2	1:A:195:MET:HG3	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:65:MET:HE3	1:A:122:ASN:HB2	1.99	0.43
1:A:78:VAL:HG22	1:A:82:VAL:HG11	1.99	0.43
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:113:TYR:CE2	1:A:299:PHE:HB3	2.54	0.42
1:A:41:ILE:HD12	1:A:136:ALA:O	2.19	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:HD13	1:A:177:LEU:H	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

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	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
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 ⓘ

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%)	241 (82%)	54 (18%)	2 3

All (54) 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	32	THR
1	A	38	ASN
1	A	39	ILE
1	A	55	LYS
1	A	78	VAL
1	A	103	CYS
1	A	105	PRO
1	A	108	ARG
1	A	111	GLU
1	A	112	GLN
1	A	123	ASP
1	A	126	ILE
1	A	127	ASN
1	A	129	GLN
1	A	131	THR
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

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Mol	Chain	Res	Type
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	298	SER
1	A	302	SER
1	A	309	MET
1	A	310	LEU
1	A	313	CYS
1	A	316	LYS
1	A	318	LEU
1	A	320	SER
1	A	322	ILE
1	A	330	VAL
1	A	332	THR
1	A	341	ASP
1	A	343	ARG
1	A	350	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) 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	157	GLN
1	A	278	ASN
1	A	279	ASN
1	A	282	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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	-	44,52,52	1.38	5 (11%)	51,80,80	1.86	9 (17%)

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	-	-	0/27/67/67	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	450	NAP	C6N-N1N	2.23	1.41	1.35
3	A	450	NAP	O4D-C1D	2.37	1.44	1.41
3	A	450	NAP	O4B-C1B	2.42	1.44	1.41
3	A	450	NAP	C3N-C7N	2.52	1.54	1.50
3	A	450	NAP	P2B-O2B	5.98	1.70	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	450	NAP	N3A-C2A-N1A	-8.21	121.71	128.86
3	A	450	NAP	O2B-P2B-O1X	-2.09	101.07	109.26
3	A	450	NAP	O4B-C4B-C5B	2.39	117.46	109.40
3	A	450	NAP	O4D-C4D-C5D	2.46	117.72	109.40
3	A	450	NAP	O2X-P2B-O2B	2.64	117.98	106.00
3	A	450	NAP	C2B-C3B-C4B	3.17	109.16	101.95
3	A	450	NAP	C4A-C5A-N7A	3.21	112.51	109.41
3	A	450	NAP	O5B-C5B-C4B	3.50	121.41	109.00
3	A	450	NAP	O5D-C5D-C4D	4.27	124.13	109.00

There are no chirality outliers.

There are no torsion outliers.

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

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.