



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:26 pm BST

PDB ID : 2FVL
Title : Crystal structure of human 3-alpha hydroxysteroid/dihydrodiol dehydrogenase (AKR1C4) complexed with NADP+
Authors : Ugochukwu, E.; Smee, C.; Guo, K.; Lukacik, P.; Kavanagh, K.; Debreczeni, J.E.; von Delft, F.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.; Edwards, A.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2006-01-31
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

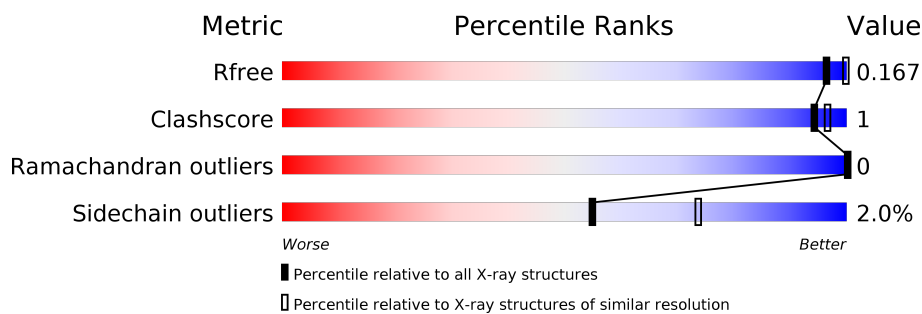
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	324	95%
1	B	324	95%
1	C	324	97%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8794 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.

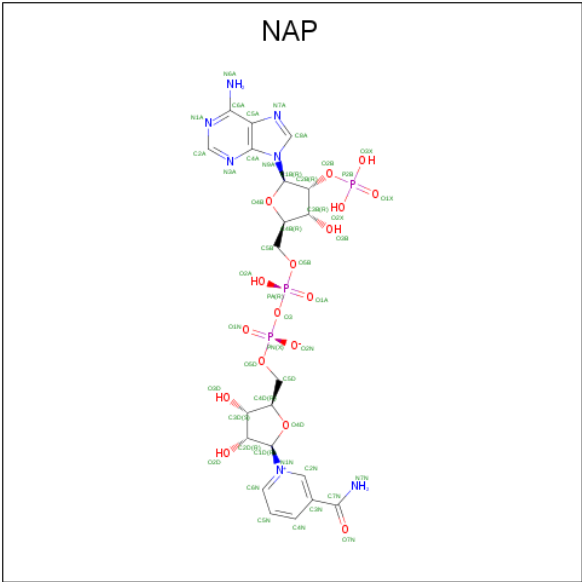
- Molecule 1 is a protein called Aldo-keto reductase family 1, member C4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	1	0
			2605	1678	438	473	16			
1	B	323	Total	C	N	O	S	0	0	0
			2602	1674	439	474	15			
1	C	323	Total	C	N	O	S	0	3	0
			2609	1680	438	476	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	CLONING ARTIFACT	GB 18088446
B	0	SER	-	CLONING ARTIFACT	GB 18088446
C	0	SER	-	CLONING ARTIFACT	GB 18088446

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	319	Total	O	0	0
			319	319		
3	B	229	Total	O	0	0
			229	229		
3	C	286	Total	O	0	0
			286	286		

3 Residue-property plots [i](#)

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. 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.

- Molecule 1: Aldo-keto reductase family 1, member C4

Chain A:  95%



- Molecule 1: Aldo-keto reductase family 1, member C4

Chain B:  95%



- Molecule 1: Aldo-keto reductase family 1, member C4

Chain C:  97%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.01Å 166.01Å 194.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.73 – 2.40 32.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (32.73-2.40) 98.4 (32.73-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.166 , 0.205 0.170 , 0.167	Depositor DCC
R_{free} test set	1968 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.3	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	0.93	EDS
Total number of atoms	8794	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: 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	0.52	0/2671	0.70	3/3619 (0.1%)
1	B	0.49	0/2665	0.63	0/3612
1	C	0.52	0/2681	0.67	0/3637
All	All	0.51	0/8017	0.67	3/10868 (0.0%)

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	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ASP	N-CA-C	6.39	128.26	111.00
1	A	31	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	A	31	ARG	NE-CZ-NH1	-5.64	117.48	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	ALA	Peptide
1	A	71	ASP	Peptide
1	A	72	GLY	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	2605	0	2601	11	0
1	B	2602	0	2594	7	0
1	C	2609	0	2604	4	0
2	A	48	0	25	1	0
2	B	48	0	25	3	0
2	C	48	0	25	0	0
3	A	319	0	0	0	1
3	B	229	0	0	3	0
3	C	286	0	0	0	1
All	All	8794	0	7874	21	1

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 1.

All (21) 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:288:LEU:CD1	1:A:293[B]:MET:HE2	2.27	0.64
1:A:71:ASP:OD2	1:A:73:SER:OG	2.18	0.61
1:A:288:LEU:HD12	1:A:293[B]:MET:CE	2.32	0.60
1:A:270:LYS:O	2:A:1001:NAP:H8A	2.04	0.57
1:A:262:GLN:HB2	1:A:293[B]:MET:HE1	1.88	0.55
1:A:288:LEU:HD12	1:A:293[B]:MET:HE2	1.88	0.55
1:A:288:LEU:HD13	1:A:293[B]:MET:HE2	1.89	0.53
1:B:276:ARG:HG2	2:B:1003:NAP:C5A	2.40	0.52
1:B:270:LYS:O	2:B:1003:NAP:H8A	2.10	0.51
1:B:285:GLU:OE1	3:B:1124:HOH:O	2.19	0.51
1:B:276:ARG:HG2	2:B:1003:NAP:C6A	2.41	0.51
1:C:219:LEU:HD21	1:C:257:LEU:HD13	1.94	0.50
1:C:40:LEU:HD13	1:C:274:GLU:HG3	1.94	0.50
1:A:170:TYR:OH	1:C:322:GLU:HG3	2.14	0.47
1:A:70:ALA:O	1:A:71:ASP:HB2	2.15	0.47
1:B:196:TYR:CD2	1:B:301:ARG:HD2	2.51	0.45
1:A:19:LEU:HD23	1:A:281:ILE:HD12	2.00	0.43
1:C:185:LYS:HB2	1:C:186:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LYS:HE3	3:B:1156:HOH:O	2.19	0.42
1:B:31:ARG:HD3	3:B:1074:HOH:O	2.20	0.41
1:A:259:TYR:HA	1:A:293[B]:MET:CE	2.51	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1205:HOH:O	3:C:1248:HOH:O[5_555]	2.03	0.17

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	322/324 (99%)	312 (97%)	10 (3%)	0	100	100
1	B	321/324 (99%)	313 (98%)	8 (2%)	0	100	100
1	C	324/324 (100%)	316 (98%)	8 (2%)	0	100	100
All	All	967/972 (100%)	941 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	285/291 (98%)	279 (98%)	6 (2%)	53	72
1	B	285/291 (98%)	277 (97%)	8 (3%)	43	63
1	C	287/291 (99%)	284 (99%)	3 (1%)	76	88
All	All	857/873 (98%)	840 (98%)	17 (2%)	55	74

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	31	ARG
1	A	71	ASP
1	A	170	TYR
1	A	209	LYS
1	A	263	ARG
1	B	1	MET
1	B	31	ARG
1	B	32	ASN
1	B	63	LEU
1	B	109	ASP
1	B	170	TYR
1	B	281	ILE
1	B	294	LYS
1	C	109	ASP
1	C	200	SER
1	C	257	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

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
2	NAP	A	1001	-	45,52,52	1.47	5 (11%)	56,80,80	1.24	3 (5%)
2	NAP	B	1003	-	45,52,52	1.38	5 (11%)	56,80,80	1.18	4 (7%)
2	NAP	C	1002	-	45,52,52	1.44	7 (15%)	56,80,80	1.37	7 (12%)

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
2	NAP	A	1001	-	-	1/31/67/67	0/5/5/5
2	NAP	B	1003	-	-	5/31/67/67	0/5/5/5
2	NAP	C	1002	-	-	11/31/67/67	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1002	NAP	C2N-N1N	5.30	1.41	1.35
2	A	1001	NAP	C2N-N1N	5.25	1.41	1.35
2	B	1003	NAP	C2N-N1N	4.40	1.40	1.35
2	A	1001	NAP	O4B-C1B	4.35	1.47	1.41
2	B	1003	NAP	O4D-C1D	4.01	1.46	1.41
2	B	1003	NAP	O4B-C1B	3.66	1.46	1.41
2	A	1001	NAP	P2B-O1X	3.27	1.61	1.50
2	C	1002	NAP	P2B-O1X	2.95	1.60	1.50
2	C	1002	NAP	O4D-C1D	2.93	1.45	1.41
2	B	1003	NAP	P2B-O1X	2.93	1.60	1.50
2	B	1003	NAP	C6N-N1N	2.45	1.41	1.35
2	C	1002	NAP	O5D-C5D	-2.36	1.35	1.44
2	A	1001	NAP	C6N-N1N	2.27	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1002	NAP	P2B-O3X	-2.26	1.46	1.54
2	C	1002	NAP	O4B-C1B	2.22	1.44	1.41
2	A	1001	NAP	O4D-C1D	2.18	1.44	1.41
2	C	1002	NAP	C6N-N1N	2.15	1.40	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	NAP	N3A-C2A-N1A	-4.62	121.45	128.68
2	B	1003	NAP	N3A-C2A-N1A	-3.85	122.67	128.68
2	C	1002	NAP	O4D-C4D-C5D	-3.79	96.90	109.37
2	C	1002	NAP	N3A-C2A-N1A	-3.73	122.85	128.68
2	B	1003	NAP	C6N-N1N-C2N	-3.19	119.07	121.97
2	A	1001	NAP	C6N-N1N-C2N	-2.98	119.25	121.97
2	C	1002	NAP	C6N-N1N-C2N	-2.79	119.43	121.97
2	B	1003	NAP	O2B-P2B-O1X	-2.76	98.73	109.39
2	C	1002	NAP	O2N-PN-O5D	2.67	120.13	107.75
2	C	1002	NAP	O5D-PN-O1N	-2.29	100.11	109.07
2	A	1001	NAP	C5B-C4B-C3B	-2.25	106.76	115.18
2	C	1002	NAP	O3X-P2B-O2X	2.21	116.09	107.64
2	C	1002	NAP	O5B-C5B-C4B	2.04	116.01	108.99
2	B	1003	NAP	C5B-C4B-C3B	-2.02	107.62	115.18

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1002	NAP	C5B-O5B-PA-O1A
2	C	1002	NAP	C5B-O5B-PA-O3
2	C	1002	NAP	O4B-C4B-C5B-O5B
2	C	1002	NAP	C3B-C4B-C5B-O5B
2	C	1002	NAP	O4D-C4D-C5D-O5D
2	A	1001	NAP	PA-O3-PN-O5D
2	B	1003	NAP	PA-O3-PN-O5D
2	C	1002	NAP	PA-O3-PN-O5D
2	B	1003	NAP	C2B-O2B-P2B-O2X
2	C	1002	NAP	C5D-O5D-PN-O3
2	C	1002	NAP	PN-O3-PA-O2A
2	C	1002	NAP	C5B-O5B-PA-O2A
2	B	1003	NAP	C4D-C5D-O5D-PN
2	B	1003	NAP	C5B-O5B-PA-O3
2	C	1002	NAP	PN-O3-PA-O1A

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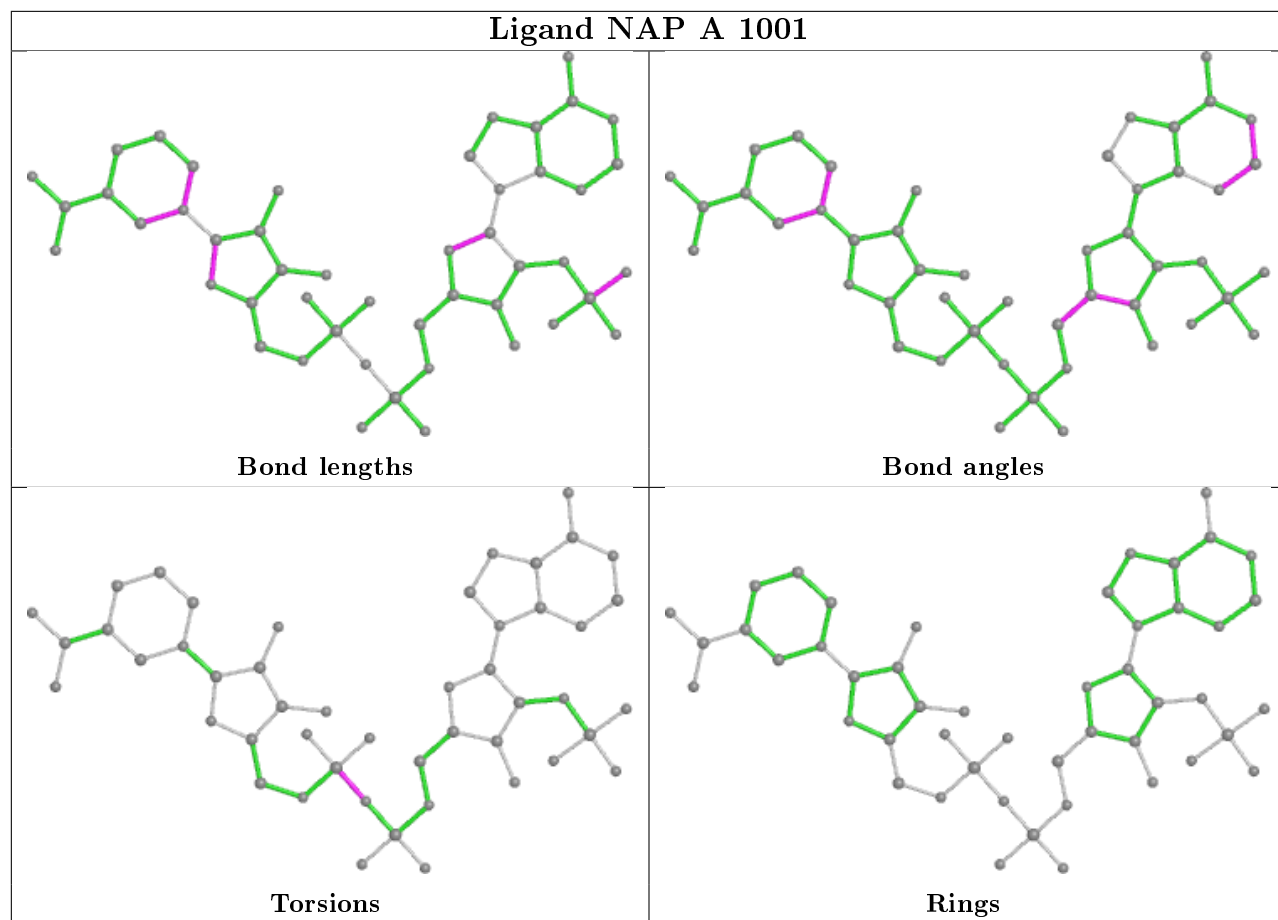
Mol	Chain	Res	Type	Atoms
2	C	1002	NAP	PA-O3-PN-O2N
2	B	1003	NAP	C5B-O5B-PA-O1A

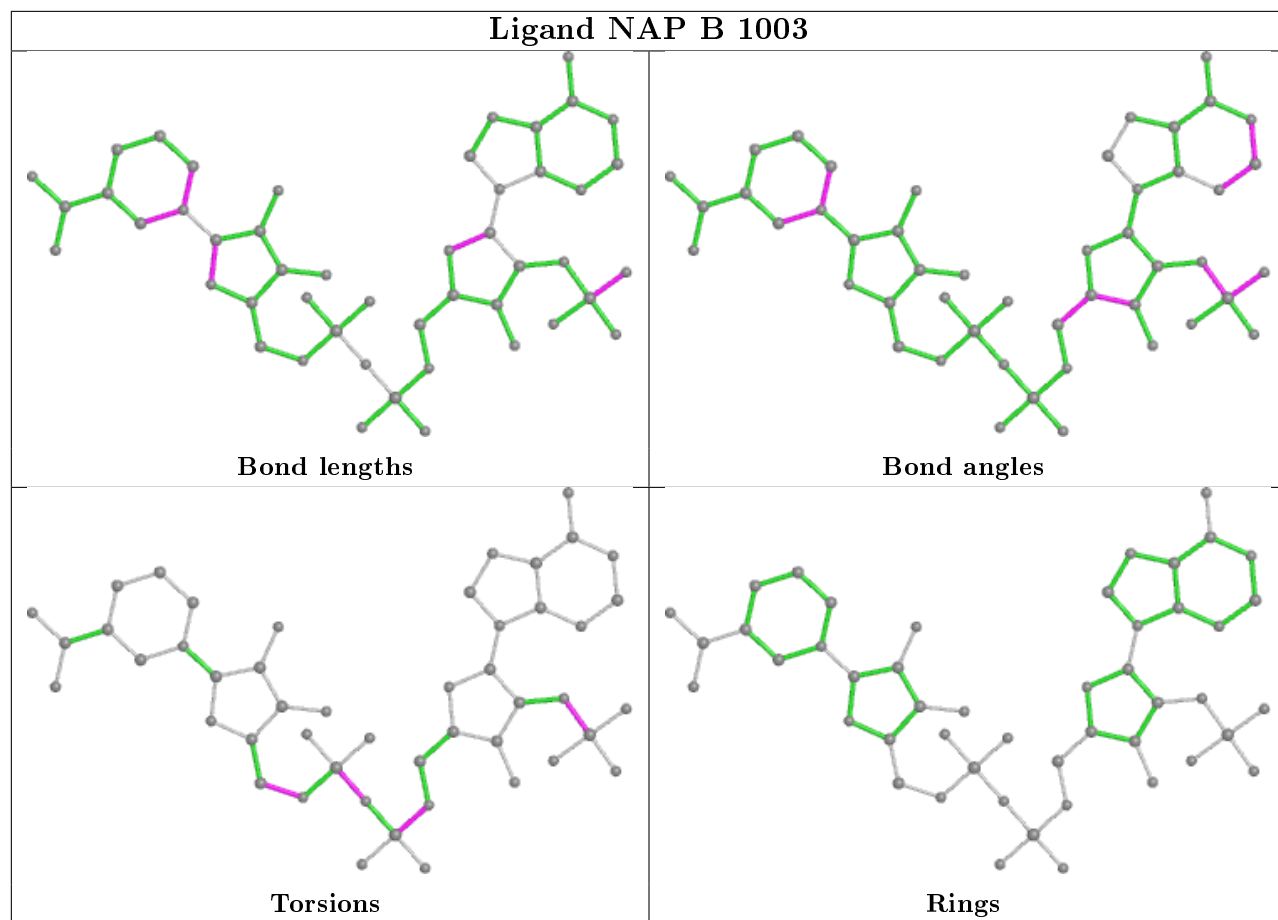
There are no ring outliers.

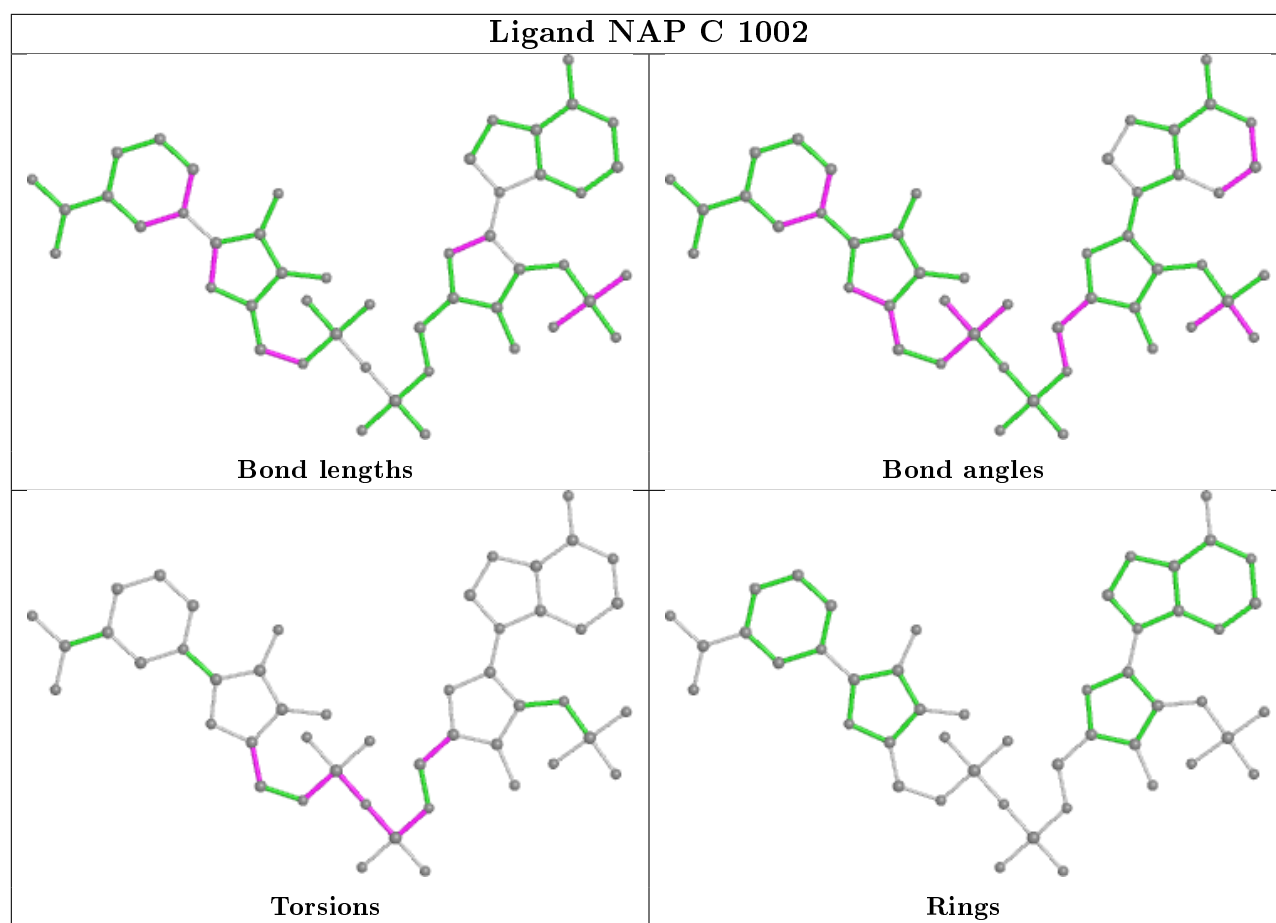
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAP	1	0
2	B	1003	NAP	3	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

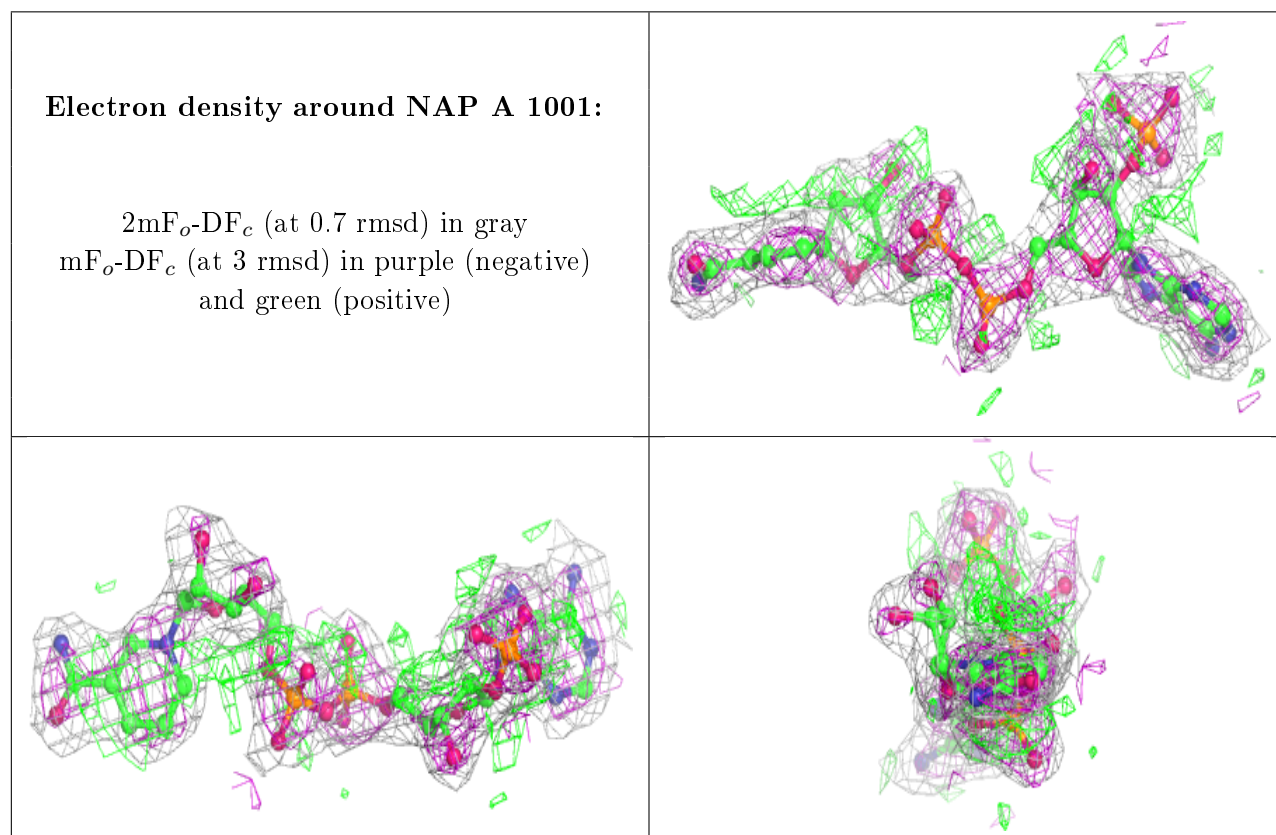
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

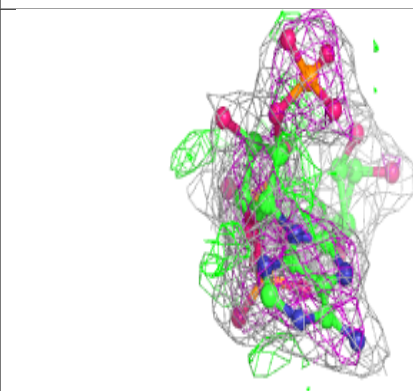
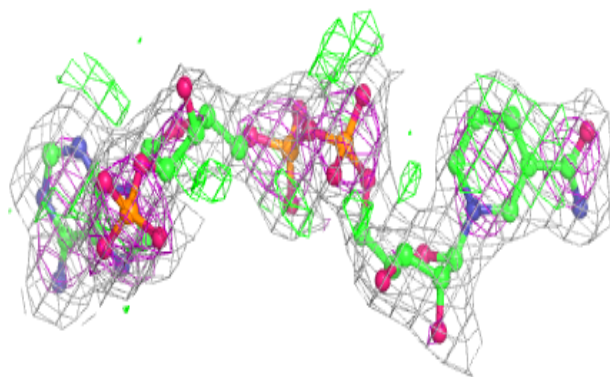
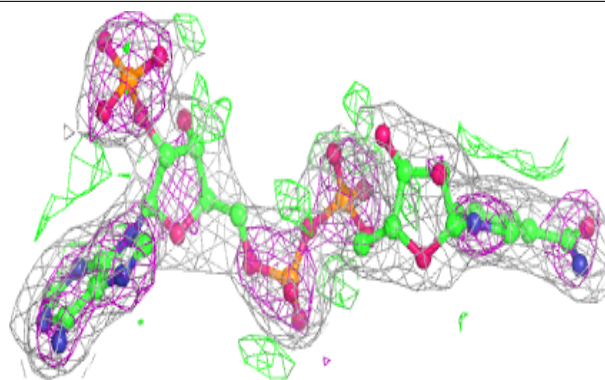
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

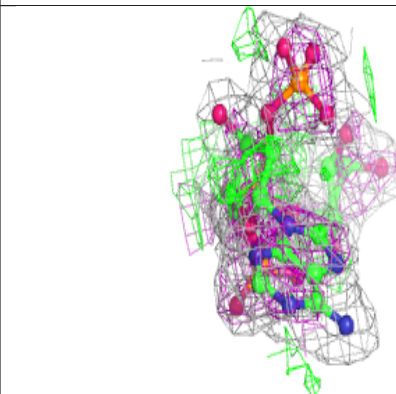
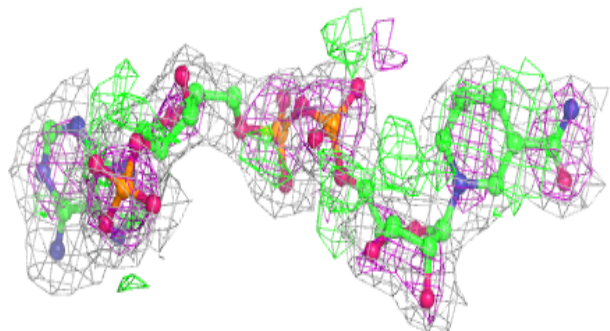
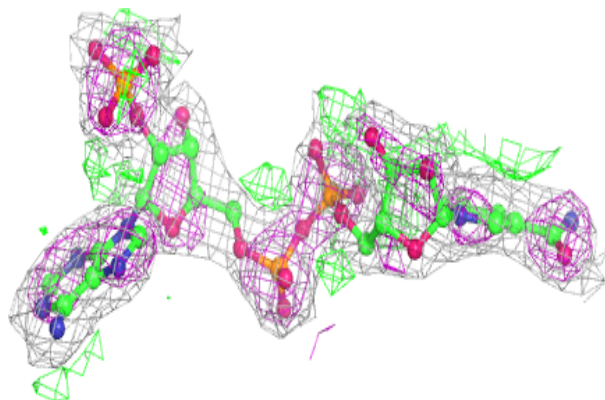


Electron density around NAP B 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAP C 1002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.