



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:48 am BST

PDB ID : 1P0F
Title : Crystal Structure of the Binary Complex: NADP(H)-Dependent Vertebrate Alcohol Dehydrogenase (ADH8) with the cofactor NADP
Authors : Rosell, A.; Valencia, E.; Pares, X.; Fita, I.; Farres, J.; Ochoa, W.F.
Deposited on : 2003-04-10
Resolution : 1.80 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

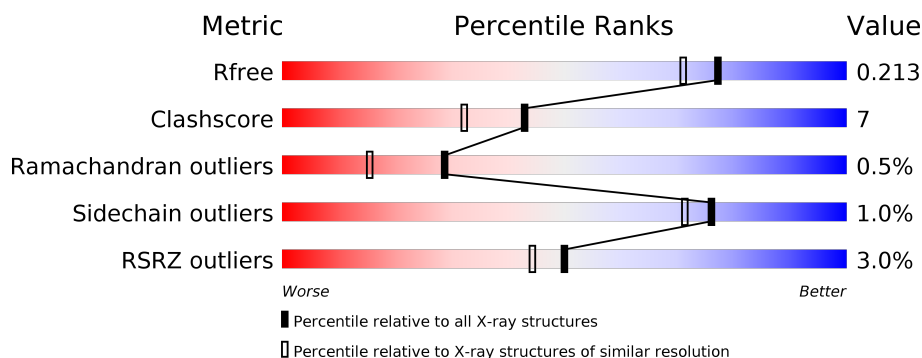
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 $\leq 5\%$. 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	373	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>13%</div> </div> </div>
1	B	373	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5963 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 NADP-dependent ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2727	1728	457	517	25			
1	B	372	Total	C	N	O	S	0	0	0
			2727	1728	457	517	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1141	MET	VAL	CONFLICT	UNP O57380
B	2141	MET	VAL	CONFLICT	UNP O57380

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

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

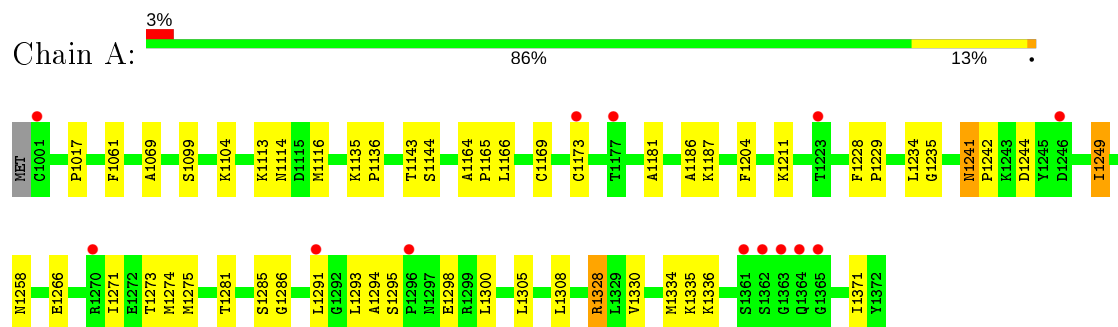
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total 215	O 215	0	0
5	B	182	Total 182	O 182	0	0

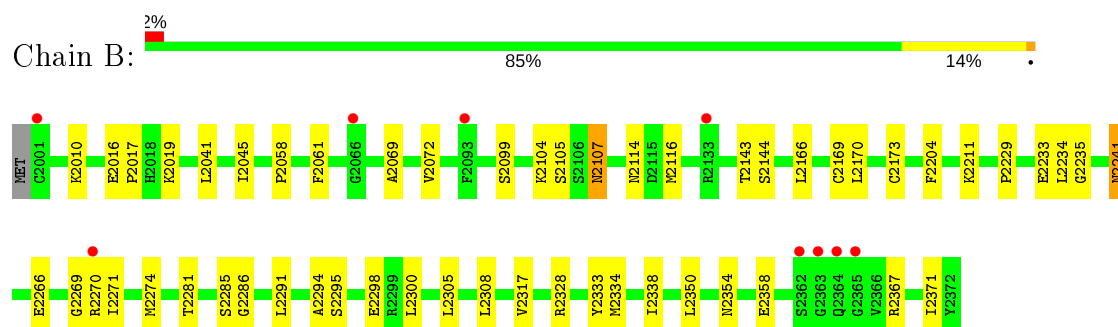
3 Residue-property plots [i](#)

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 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: NADP-dependent ALCOHOL DEHYDROGENASE



• Molecule 1: NADP-dependent ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.16Å 79.50Å 91.84Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.25 – 1.80	Depositor EDS
% Data completeness (in resolution range)	55.4 (30.00-1.80) 98.1 (29.25-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.219 0.189 , 0.213	Depositor DCC
R_{free} test set	7418 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5963	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: GOL, 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	0.29	0/2773	0.58	0/3751
1	B	0.28	0/2773	0.58	0/3751
All	All	0.29	0/5546	0.58	0/7502

There are no bond length outliers.

There are no bond angle outliers.

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	2727	0	2798	38	0
1	B	2727	0	2798	38	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	48	0	25	2	0
3	B	48	0	25	2	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	215	0	0	5	0
5	B	182	0	0	4	0
All	All	5963	0	5662	76	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 (76) 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:1294:ALA:HB2	5:A:270:HOH:O	1.77	0.84
1:B:2294:ALA:HB2	5:B:429:HOH:O	1.77	0.84
1:A:1114:ASN:HD22	1:A:1116:MET:H	1.27	0.82
1:B:2274:MET:HE3	5:B:429:HOH:O	1.79	0.81
1:A:1295:SER:HB3	1:A:1298:GLU:HG3	1.62	0.81
1:B:2114:ASN:HD22	1:B:2116:MET:H	1.36	0.72
1:B:2305:LEU:HD23	1:B:2308:LEU:HD12	1.73	0.71
1:A:1305:LEU:HD23	1:A:1308:LEU:HD12	1.75	0.69
1:B:2354:ASN:O	1:B:2358:GLU:HG3	1.94	0.68
1:A:1166:LEU:HD13	1:A:1371:ILE:HD12	1.75	0.68
1:A:1241:ASN:HB3	1:A:1244:ASP:OD2	1.94	0.67
1:B:2105:SER:OG	1:B:2107:ASN:ND2	2.29	0.65
1:B:2271:ILE:HG23	1:B:2300:LEU:HD12	1.82	0.61
1:B:2017:PRO:HG3	1:B:2061:PHE:CZ	2.37	0.60
5:A:380:HOH:O	1:B:2308:LEU:HD11	2.03	0.58
1:B:2291:LEU:O	3:B:3292:NAP:H2N	2.03	0.58
1:A:1330:VAL:HG12	1:A:1334:MET:HE1	1.86	0.57
1:A:1291:LEU:O	3:A:4292:NAP:H2N	2.05	0.57
1:A:1143:THR:O	1:A:1144:SER:HB2	2.05	0.57
1:A:1069:ALA:HA	1:A:1169:CYS:HB2	1.85	0.56
1:B:2099:SER:O	1:B:2104:LYS:HE3	2.06	0.55
1:B:2170:LEU:HD22	1:B:2367:ARG:HG2	1.88	0.55
1:A:1271:ILE:HG23	1:A:1300:LEU:HD12	1.89	0.54
1:B:2229:PRO:O	1:B:2233:GLU:HG3	2.08	0.54
1:B:2010:LYS:HD2	1:B:2350:LEU:HD23	1.90	0.54
1:A:1114:ASN:ND2	1:A:1116:MET:H	2.01	0.53
1:A:1274:MET:HE3	5:A:270:HOH:O	2.09	0.53
1:A:1017:PRO:HG3	1:A:1061:PHE:CZ	2.44	0.53
3:A:4292:NAP:H52A	3:A:4292:NAP:H52N	1.91	0.52
1:B:2045:ILE:N	1:B:2045:ILE:HD12	2.25	0.52
1:B:2270:ARG:O	1:B:2274:MET:HG3	2.09	0.52
1:B:2058:PRO:HG3	5:B:425:HOH:O	2.08	0.51
1:B:2241:ASN:HD22	1:B:2241:ASN:C	2.13	0.51
1:B:2143:THR:O	1:B:2144:SER:HB2	2.09	0.51
1:A:1241:ASN:HD22	1:A:1241:ASN:C	2.14	0.51
1:B:2328:ARG:HH11	1:B:2328:ARG:HG2	1.76	0.51
1:A:1017:PRO:HG3	1:A:1061:PHE:CE1	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1242:PRO:HG3	1:A:1249:ILE:HG13	1.94	0.50
1:A:1113:LYS:HE2	5:A:397:HOH:O	2.11	0.49
1:B:2204:PHE:HD2	1:B:2234:LEU:HD12	1.77	0.48
1:A:1330:VAL:HG12	1:A:1334:MET:CE	2.43	0.48
1:B:2328:ARG:HG2	1:B:2328:ARG:NH1	2.29	0.48
1:B:2017:PRO:HG3	1:B:2061:PHE:CE1	2.48	0.48
1:A:1334:MET:HE3	5:A:204:HOH:O	2.15	0.47
1:A:1266:GLU:HG2	1:A:1273:THR:HG22	1.96	0.47
1:A:1181:ALA:CB	1:A:1291:LEU:HD11	2.45	0.47
1:A:1308:LEU:O	1:B:2317:VAL:HG23	2.15	0.46
1:B:2069:ALA:HA	1:B:2169:CYS:HB2	1.96	0.46
1:B:2041:LEU:HD11	1:B:2072:VAL:HG23	1.97	0.46
1:A:1204:PHE:HD2	1:A:1234:LEU:HD12	1.80	0.45
3:B:3292:NAP:H52A	3:B:3292:NAP:H52N	1.98	0.45
1:B:2114:ASN:ND2	1:B:2116:MET:HB2	2.32	0.45
1:A:1211:LYS:HD2	1:A:1235:GLY:HA2	1.99	0.44
1:B:2170:LEU:CD2	1:B:2367:ARG:HG2	2.48	0.44
1:B:2333:TYR:HA	1:B:2338:ILE:HG13	2.00	0.43
1:A:1099:SER:O	1:A:1104:LYS:HE3	2.18	0.43
1:A:1114:ASN:ND2	1:A:1116:MET:HB2	2.33	0.43
1:A:1275:MET:SD	1:A:1300:LEU:HD11	2.58	0.43
1:A:1135:LYS:HA	1:A:1136:PRO:HD3	1.91	0.43
1:B:2211:LYS:HD2	1:B:2235:GLY:HA2	2.01	0.43
1:B:2295:SER:HB2	1:B:2298:GLU:HG3	2.01	0.43
1:A:1293:LEU:N	1:A:1293:LEU:HD12	2.34	0.42
1:A:1186:ALA:O	1:A:1187:LYS:HB2	2.20	0.42
1:A:1328:ARG:O	1:A:1328:ARG:HD3	2.20	0.42
1:B:2166:LEU:HD13	1:B:2371:ILE:HD12	2.02	0.42
1:A:1293:LEU:HG	1:B:2308:LEU:CD1	2.49	0.42
1:A:1164:ALA:HA	1:A:1165:PRO:HD3	1.91	0.41
1:B:2016:GLU:OE2	1:B:2019:LYS:HG3	2.21	0.41
1:B:2269:GLY:C	5:B:429:HOH:O	2.59	0.41
1:B:2281:THR:HB	1:B:2286:GLY:HA3	2.02	0.41
1:A:1204:PHE:CD2	1:A:1234:LEU:HD12	2.56	0.41
1:A:1335:LYS:O	1:A:1336:LYS:HB2	2.21	0.40
1:A:1281:THR:HB	1:A:1286:GLY:HA3	2.02	0.40
1:B:2334:MET:HB2	1:B:2334:MET:HE2	1.97	0.40
1:A:1228:PHE:HB2	1:A:1229:PRO:HD3	2.03	0.40
1:B:2266:GLU:HG3	1:B:2274:MET:HA	2.03	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	370/373 (99%)	357 (96%)	11 (3%)	2 (0%)	29	15
1	B	370/373 (99%)	358 (97%)	10 (3%)	2 (0%)	29	15
All	All	740/746 (99%)	715 (97%)	21 (3%)	4 (0%)	29	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1285	SER
1	B	2173	CYS
1	B	2285	SER
1	A	1173	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	300/301 (100%)	296 (99%)	4 (1%)	69	62
1	B	300/301 (100%)	298 (99%)	2 (1%)	84	81
All	All	600/602 (100%)	594 (99%)	6 (1%)	76	71

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1241	ASN
1	A	1249	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1258	ASN
1	A	1328	ARG
1	B	2107	ASN
1	B	2241	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1114	ASN
1	A	1184	ASN
1	A	1241	ASN
1	A	1258	ASN
1	A	1297	ASN
1	B	2107	ASN
1	B	2114	ASN
1	B	2184	ASN
1	B	2241	ASN
1	B	2258	ASN
1	B	2297	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	GOL	B	8002	2	5,5,5	0.15	0	5,5,5	0.53	0
3	NAP	A	4292	-	45,52,52	2.06	12 (26%)	56,80,80	1.83	12 (21%)
3	NAP	B	3292	-	45,52,52	2.10	11 (24%)	56,80,80	1.84	13 (23%)
4	GOL	A	8001	-	5,5,5	0.13	0	5,5,5	0.46	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	GOL	B	8002	2	-	2/4/4/4	-
3	NAP	A	4292	-	-	6/31/67/67	0/5/5/5
3	NAP	B	3292	-	-	5/31/67/67	0/5/5/5
4	GOL	A	8001	-	-	2/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3292	NAP	C2N-N1N	6.55	1.42	1.35
3	A	4292	NAP	C2N-N1N	5.91	1.42	1.35
3	A	4292	NAP	C4N-C3N	4.77	1.47	1.39
3	B	3292	NAP	C4N-C3N	4.68	1.47	1.39
3	B	3292	NAP	C2A-N3A	4.46	1.39	1.32
3	B	3292	NAP	O4D-C1D	4.40	1.47	1.41
3	A	4292	NAP	C2A-N3A	4.29	1.39	1.32
3	A	4292	NAP	O4D-C1D	4.14	1.46	1.41
3	B	3292	NAP	C2A-N1A	3.91	1.41	1.33
3	A	4292	NAP	C2A-N1A	3.83	1.41	1.33
3	A	4292	NAP	C6N-N1N	3.48	1.43	1.35
3	A	4292	NAP	C2D-C1D	-3.42	1.48	1.53
3	B	3292	NAP	C6N-N1N	3.38	1.43	1.35
3	B	3292	NAP	C2D-C1D	-3.34	1.48	1.53
3	B	3292	NAP	C4A-N3A	2.77	1.39	1.35
3	A	4292	NAP	C4A-N3A	2.69	1.39	1.35
3	B	3292	NAP	PA-O1A	-2.58	1.41	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4292	NAP	PA-O1A	-2.49	1.42	1.50
3	B	3292	NAP	O4B-C4B	2.45	1.50	1.45
3	A	4292	NAP	O4B-C4B	2.39	1.50	1.45
3	A	4292	NAP	C3N-C7N	2.25	1.54	1.50
3	B	3292	NAP	C3N-C7N	2.18	1.53	1.50
3	A	4292	NAP	C3D-C4D	2.04	1.58	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4292	NAP	O5D-PN-O1N	-6.25	84.66	109.07
3	B	3292	NAP	O5D-PN-O1N	-5.91	85.99	109.07
3	B	3292	NAP	O2N-PN-O5D	-4.55	86.60	107.75
3	B	3292	NAP	C5A-C6A-N6A	4.45	127.12	120.35
3	A	4292	NAP	C5A-C6A-N6A	4.43	127.09	120.35
3	A	4292	NAP	O2N-PN-O5D	-4.40	87.31	107.75
3	B	3292	NAP	N3A-C2A-N1A	-3.68	122.93	128.68
3	A	4292	NAP	N3A-C2A-N1A	-3.66	122.96	128.68
3	B	3292	NAP	C1B-N9A-C4A	-3.13	121.15	126.64
3	B	3292	NAP	C3N-C7N-N7N	3.00	121.35	117.75
3	A	4292	NAP	C1B-N9A-C4A	-2.88	121.57	126.64
3	B	3292	NAP	O5B-C5B-C4B	-2.84	99.21	108.99
3	A	4292	NAP	O2A-PA-O1A	2.84	126.27	112.24
3	B	3292	NAP	O2A-PA-O1A	2.81	126.12	112.24
3	A	4292	NAP	C2N-C3N-C4N	2.71	121.33	118.26
3	B	3292	NAP	O7N-C7N-C3N	-2.69	116.41	119.63
3	A	4292	NAP	O5B-C5B-C4B	-2.61	100.02	108.99
3	B	3292	NAP	C2N-C3N-C4N	2.57	121.17	118.26
3	A	4292	NAP	C3N-C7N-N7N	2.55	120.81	117.75
3	B	3292	NAP	O3X-P2B-O2X	2.37	116.69	107.64
3	A	4292	NAP	O7N-C7N-C3N	-2.36	116.81	119.63
3	B	3292	NAP	O2N-PN-O1N	2.33	123.76	112.24
3	A	4292	NAP	O3X-P2B-O2X	2.30	116.43	107.64
3	A	4292	NAP	O2N-PN-O1N	2.29	123.57	112.24
3	B	3292	NAP	C3N-C2N-N1N	-2.19	118.28	120.43

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	3292	NAP	O4D-C1D-N1N-C2N
3	B	3292	NAP	O4D-C1D-N1N-C6N

Continued on next page...

Continued from previous page...

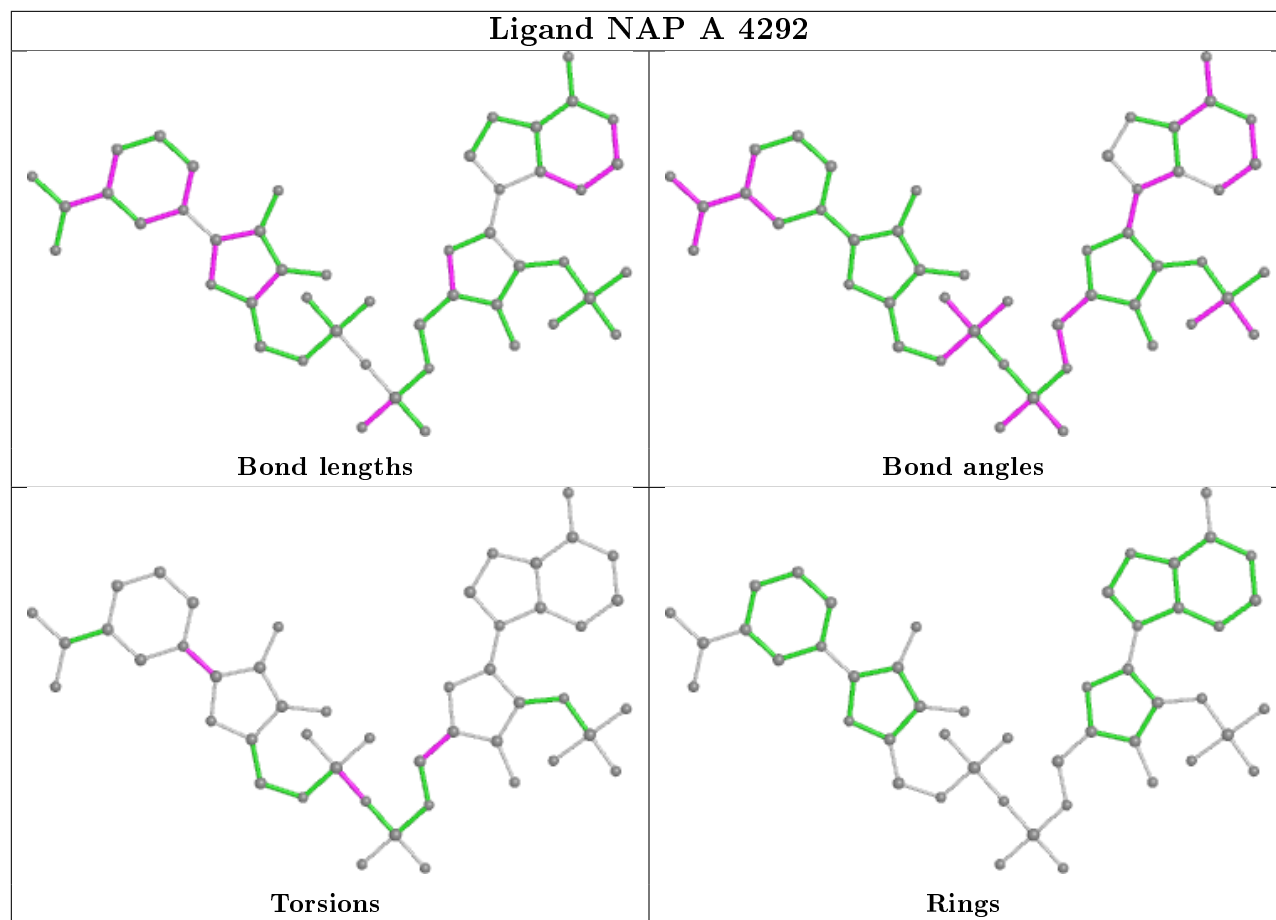
Mol	Chain	Res	Type	Atoms
3	B	3292	NAP	C2D-C1D-N1N-C2N
3	B	3292	NAP	C2D-C1D-N1N-C6N
4	B	8002	GOL	O1-C1-C2-C3
3	A	4292	NAP	O4D-C1D-N1N-C2N
3	A	4292	NAP	O4D-C1D-N1N-C6N
3	A	4292	NAP	C2D-C1D-N1N-C2N
3	A	4292	NAP	C2D-C1D-N1N-C6N
4	A	8001	GOL	O1-C1-C2-C3
4	B	8002	GOL	O1-C1-C2-O2
4	A	8001	GOL	O1-C1-C2-O2
3	B	3292	NAP	O4B-C4B-C5B-O5B
3	A	4292	NAP	O4B-C4B-C5B-O5B
3	A	4292	NAP	PA-O3-PN-O2N

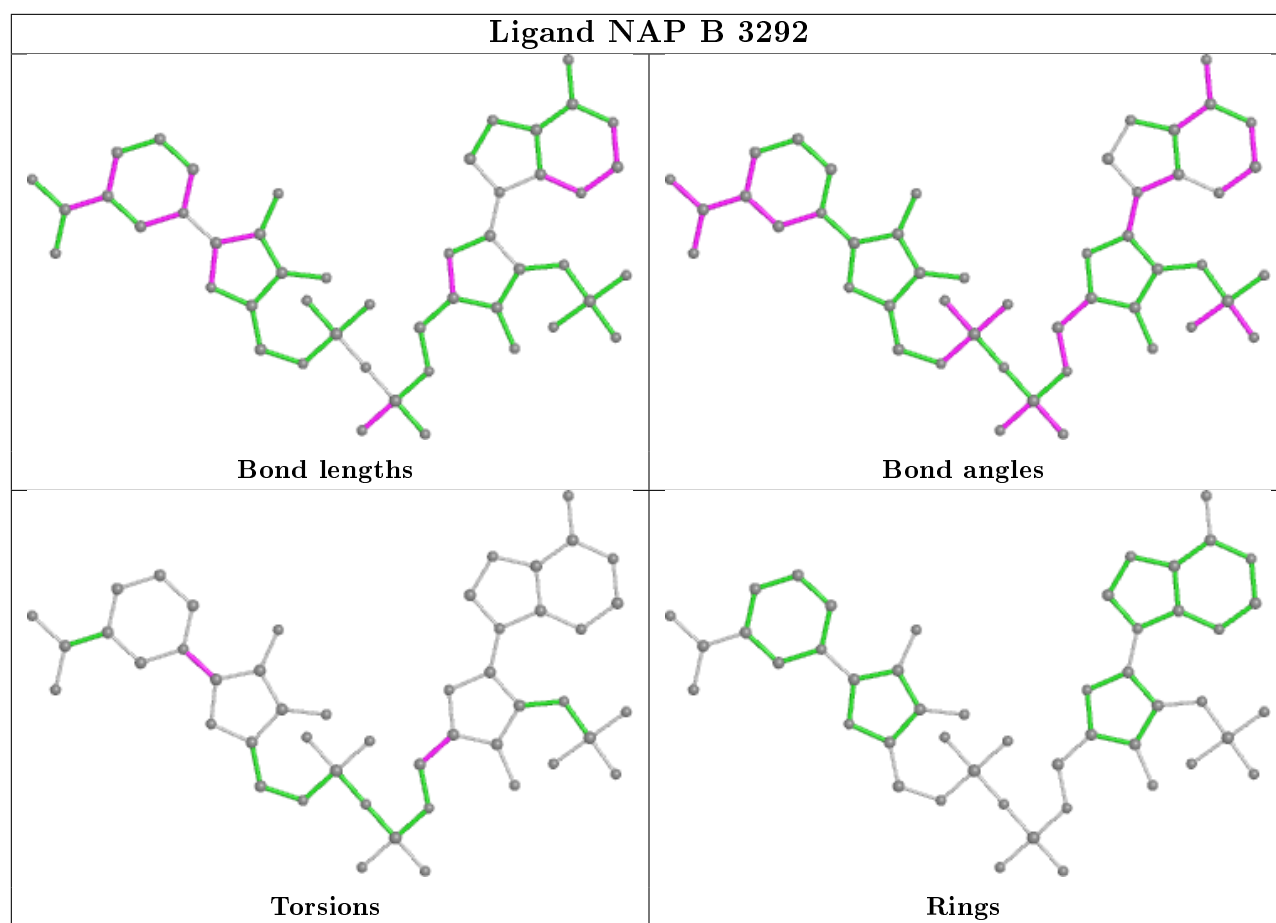
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4292	NAP	2	0
3	B	3292	NAP	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	372/373 (99%)	0.00	13 (3%) 44 38	13, 22, 38, 50	0
1	B	372/373 (99%)	0.04	9 (2%) 59 54	15, 24, 37, 52	0
All	All	744/746 (99%)	0.02	22 (2%) 50 44	13, 23, 38, 52	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1362	SER	5.9
1	B	2363	GLY	5.1
1	A	1246	ASP	4.8
1	B	2364	GLN	4.2
1	A	1364	GLN	3.8
1	A	1361	SER	3.7
1	A	1363	GLY	3.3
1	A	1001	CYS	2.9
1	B	2001	CYS	2.7
1	B	2362	SER	2.6
1	B	2133	ARG	2.5
1	B	2365	GLY	2.5
1	A	1173	CYS	2.4
1	A	1291	LEU	2.3
1	B	2066	GLY	2.2
1	B	2270	ARG	2.2
1	A	1270	ARG	2.2
1	A	1223	THR	2.2
1	B	2093	PHE	2.2
1	A	1177	THR	2.1
1	A	1296	PRO	2.0
1	A	1365	GLY	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 carbohydrates in this entry.

6.4 Ligands [i](#)

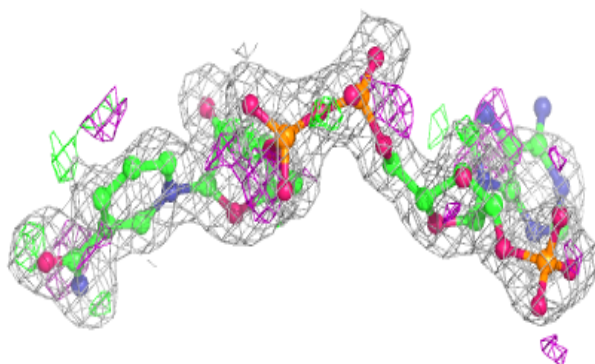
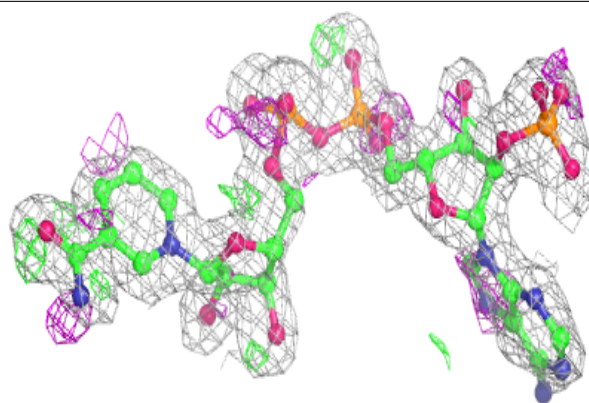
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	8001	6/6	0.55	0.37	43,49,50,51	0
4	GOL	B	8002	6/6	0.59	0.29	43,50,51,51	0
3	NAP	A	4292	48/48	0.85	0.16	24,30,48,50	0
3	NAP	B	3292	48/48	0.89	0.16	21,29,46,48	0
2	ZN	A	1502	1/1	0.99	0.04	28,28,28,28	0
2	ZN	B	2501	1/1	0.99	0.03	21,21,21,21	0
2	ZN	B	1503	1/1	0.99	0.02	33,33,33,33	0
2	ZN	A	2502	1/1	0.99	0.05	17,17,17,17	0

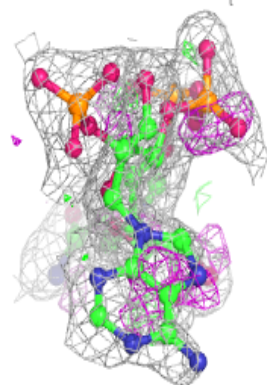
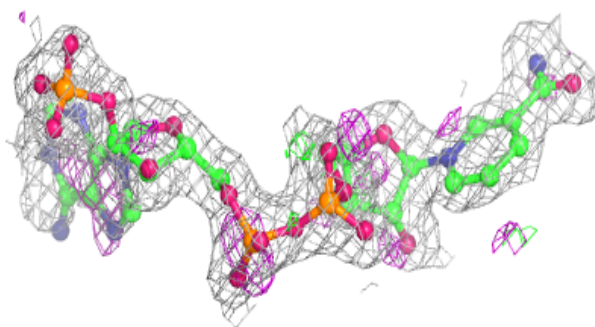
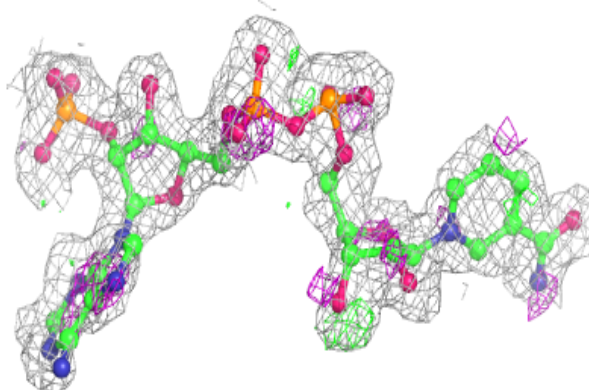
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAP A 4292:

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

**Electron density around NAP B 3292:**

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



6.5 Other polymers

There are no such residues in this entry.