Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 08:01 AM EDT

PDB ID	:	1DOH
Title	:	STRUCTURE OF TRIHYDROXYNAPHTHALENE REDUCTASE IN COMPLEX WITH NADPH AND 4-NITRO-INDEN-1-ONE
Authors	:	Liao, D.I.; Basarab, G.S.; Gatenby, A.A.; Jordan, D.B.
Deposited on	:	1999-12-20
Resolution	:	2.10 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:

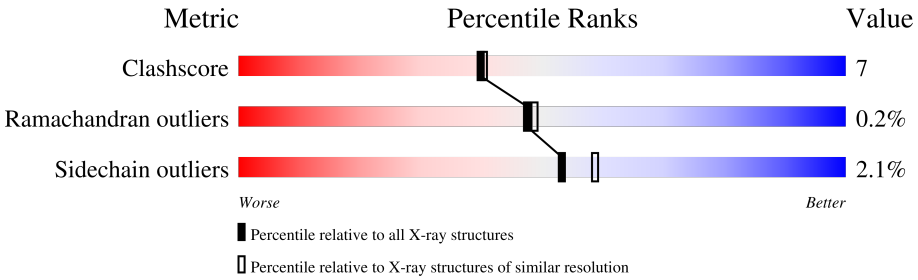
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	283	81% 16%
1	B	283	81% 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4596 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.

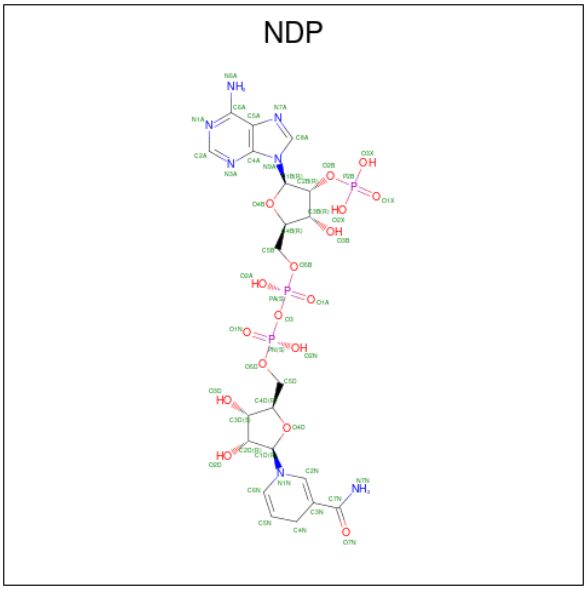
- Molecule 1 is a protein called TRIHYDROXYNAPHTHALENE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2036	1279	357	385	15			
1	B	271	Total	C	N	O	S	0	0	0
			2021	1270	354	382	15			

There are 6 discrepancies between the modelled and reference sequences:

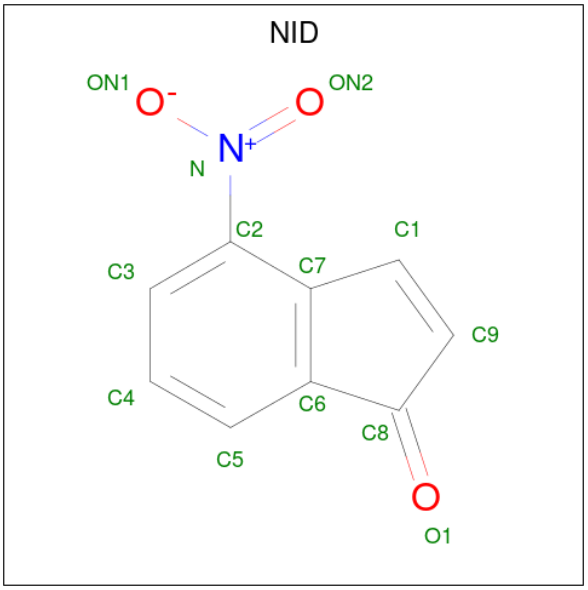
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	VAL	SER	engineered mutation	UNP Q12634
A	242	GLN	ALA	engineered mutation	UNP Q12634
A	247	ARG	HIS	engineered mutation	UNP Q12634
B	241	VAL	SER	engineered mutation	UNP Q12634
B	242	GLN	ALA	engineered mutation	UNP Q12634
B	247	ARG	HIS	engineered mutation	UNP Q12634

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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		

- Molecule 3 is 4-NITRO-INDEN-1-ONE (three-letter code: NID) (formula: $C_9H_5NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	210	Total	O	0	0
			210	210		
4	B	207	Total	O	0	0
			207	207		

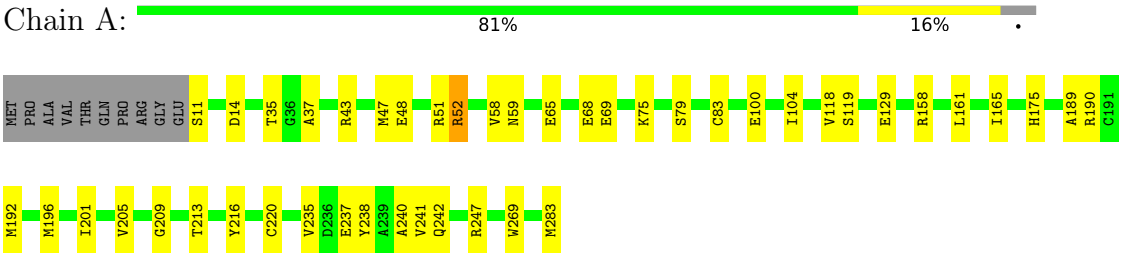
3 Residue-property plots (i)

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. 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.

Note EDS was not executed.

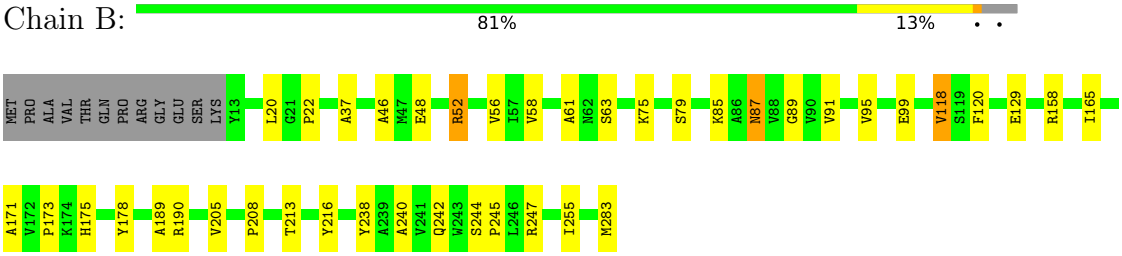
• Molecule 1: TRIHYDROXYNAPHTHALENE REDUCTASE

Chain A:



• Molecule 1: TRIHYDROXYNAPHTHALENE REDUCTASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.80Å 142.80Å 72.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	97.0 (8.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.205 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4596	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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: NID, NDP

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	0.49	0/2068	0.70	1/2790 (0.0%)
1	B	0.50	0/2053	0.69	0/2771
All	All	0.49	0/4121	0.70	1/5561 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	209	GLY	N-CA-C	-5.24	100.01	113.10

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	2036	0	2051	29	0
1	B	2021	0	2033	32	0
2	A	48	0	26	0	0
2	B	48	0	26	5	0
3	A	13	0	5	1	0
3	B	13	0	5	2	0
4	A	210	0	0	3	0
4	B	207	0	0	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4596	0	4146	61	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 (61) 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:B:87:ASN:ND2	2:B:501:NDP:H62A	1.78	0.82
1:B:165:ILE:HG21	1:B:283:MET:HE3	1.62	0.81
1:A:165:ILE:HD13	1:A:283:MET:HE2	1.67	0.75
1:B:118:VAL:HG22	4:B:709:HOH:O	1.87	0.74
1:B:189:ALA:HB2	1:B:205:VAL:HG23	1.69	0.72
1:B:48:GLU:O	1:B:52:ARG:HG2	1.95	0.67
1:A:240:ALA:HB3	4:B:687:HOH:O	1.94	0.66
1:A:48:GLU:O	1:A:52:ARG:HG2	1.95	0.66
1:A:189:ALA:HB2	1:A:205:VAL:HG23	1.77	0.66
1:A:75:LYS:HA	1:A:79:SER:O	1.97	0.65
1:B:165:ILE:HD13	1:B:283:MET:HE3	1.83	0.59
1:A:68:GLU:OE1	1:A:83:CYS:SG	2.60	0.59
1:B:190:ARG:NH2	4:B:603:HOH:O	2.36	0.59
1:B:213:THR:H	1:B:216:TYR:HB3	1.69	0.57
1:A:165:ILE:HG21	1:A:283:MET:CE	2.34	0.57
1:B:165:ILE:HD13	1:B:283:MET:CE	2.34	0.57
1:B:118:VAL:CG2	4:B:709:HOH:O	2.51	0.55
1:A:190:ARG:NH2	4:A:587:HOH:O	2.39	0.55
1:A:189:ALA:HB2	1:A:205:VAL:CG2	2.37	0.55
2:B:501:NDP:H41N	3:B:503:NID:C8	2.38	0.54
1:B:208:PRO:HG2	2:B:501:NDP:C5N	2.39	0.53
1:B:87:ASN:HD22	2:B:501:NDP:H62A	1.57	0.52
1:B:91:VAL:O	1:B:95:VAL:HG23	2.10	0.52
1:A:189:ALA:CB	1:A:205:VAL:HG23	2.40	0.52
1:B:189:ALA:HB2	1:B:205:VAL:CG2	2.40	0.52
1:B:99:GLU:HG2	4:B:627:HOH:O	2.11	0.51
1:A:238:TYR:CE2	1:A:242:GLN:HG3	2.47	0.50
1:B:87:ASN:ND2	1:B:89:GLY:H	2.09	0.50
1:A:35:THR:HA	1:A:59:ASN:HB3	1.94	0.50
1:A:241:VAL:HG23	4:B:687:HOH:O	2.12	0.49
1:B:37:ALA:HB3	1:B:58:VAL:HG13	1.94	0.49
1:A:11:SER:HA	1:A:14:ASP:OD1	2.13	0.49
1:A:196:MET:HE1	1:A:201:ILE:HG21	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:HG2	4:A:538:HOH:O	2.13	0.48
1:B:240:ALA:O	1:B:247:ARG:HA	2.13	0.48
1:A:283:MET:CE	3:A:502:NID:H4	2.44	0.48
1:A:65:GLU:O	1:A:69:GLU:HG3	2.14	0.47
1:A:161:LEU:HD11	1:A:192:MET:CE	2.44	0.47
1:A:52:ARG:HA	1:B:22:PRO:HG3	1.96	0.47
1:A:43:ARG:O	1:A:47:MET:HG2	2.16	0.46
1:B:120:PHE:CE1	4:B:709:HOH:O	2.66	0.46
1:B:208:PRO:HB3	1:B:255:ILE:CD1	2.45	0.46
1:B:75:LYS:HA	1:B:79:SER:O	2.17	0.45
2:B:501:NDP:H52A	4:B:543:HOH:O	2.16	0.45
1:A:220:CYS:SG	1:A:235:VAL:HG11	2.56	0.45
1:B:89:GLY:HA3	4:B:537:HOH:O	2.16	0.45
1:A:100:GLU:O	1:A:104:ILE:HG13	2.17	0.45
1:B:283:MET:HE1	3:B:503:NID:H4	2.00	0.44
1:A:51:ARG:NH2	1:B:20:LEU:HD13	2.33	0.44
1:B:171:ALA:O	1:B:173:PRO:HD3	2.18	0.44
1:B:238:TYR:CE2	1:B:242:GLN:HG3	2.54	0.42
1:B:61:ALA:O	1:B:85:LYS:HE3	2.19	0.42
1:B:244:SER:HA	1:B:245:PRO:HD3	1.89	0.42
1:B:175:HIS:CE1	1:B:178:TYR:HD2	2.37	0.42
1:B:46:ALA:HB1	1:B:56:VAL:HG11	2.01	0.41
1:A:118:VAL:HG22	1:A:119:SER:H	1.85	0.41
1:A:37:ALA:HB3	1:A:58:VAL:HG13	2.03	0.41
1:A:240:ALA:O	1:A:247:ARG:HA	2.21	0.41
1:A:158:ARG:NH2	4:A:507:HOH:O	2.54	0.40
1:A:213:THR:H	1:A:216:TYR:HB3	1.86	0.40
1:B:175:HIS:CE1	1:B:178:TYR:CD2	3.10	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	271/283 (96%)	264 (97%)	7 (3%)	0	100 100
1	B	269/283 (95%)	258 (96%)	10 (4%)	1 (0%)	34 32
All	All	540/566 (95%)	522 (97%)	17 (3%)	1 (0%)	47 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	SER

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	213/221 (96%)	209 (98%)	4 (2%)	57 63
1	B	211/221 (96%)	206 (98%)	5 (2%)	49 53
All	All	424/442 (96%)	415 (98%)	9 (2%)	53 59

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	129	GLU
1	A	175	HIS
1	A	269	TRP
1	B	52	ARG
1	B	87	ASN
1	B	118	VAL
1	B	129	GLU
1	B	158	ARG

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	175	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	62	ASN
1	B	87	ASN
1	B	175	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

4 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	NDP	A	500	-	45,52,52	1.49	5 (11%)	53,80,80	1.26	4 (7%)
3	NID	A	502	-	12,14,14	1.87	1 (8%)	12,20,20	2.18	5 (41%)
3	NID	B	503	-	12,14,14	1.69	2 (16%)	12,20,20	2.23	4 (33%)
2	NDP	B	501	-	45,52,52	1.48	5 (11%)	53,80,80	1.30	4 (7%)

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	NDP	A	500	-	-	9/30/77/77	0/5/5/5
3	NID	A	502	-	-	0/2/13/13	0/2/2/2
3	NID	B	503	-	-	0/2/13/13	0/2/2/2
2	NDP	B	501	-	-	6/30/77/77	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NID	C2-N	-5.33	1.36	1.45
2	A	500	NDP	C4N-C3N	-5.06	1.40	1.49
3	B	503	NID	C2-N	-4.57	1.37	1.45
2	B	501	NDP	C6N-C5N	4.42	1.41	1.33
2	A	500	NDP	C6N-C5N	4.41	1.41	1.33
2	B	501	NDP	C4N-C3N	-4.38	1.41	1.49
2	A	500	NDP	C4N-C5N	-3.05	1.40	1.48
2	B	501	NDP	C4N-C5N	-2.84	1.41	1.48
2	B	501	NDP	C7N-C3N	2.60	1.54	1.48
2	B	501	NDP	C2A-N3A	2.57	1.36	1.32
2	A	500	NDP	C2A-N3A	2.50	1.36	1.32
2	A	500	NDP	C5A-N7A	-2.08	1.32	1.39
3	B	503	NID	C7-C1	2.03	1.52	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	NID	C3-C2-N	4.84	121.64	116.47
2	B	501	NDP	N3A-C2A-N1A	-4.81	121.17	128.68
2	A	500	NDP	N3A-C2A-N1A	-4.61	121.47	128.68
3	A	502	NID	C3-C2-N	4.40	121.17	116.47
3	A	502	NID	C7-C6-C8	-4.05	105.53	108.90
3	B	503	NID	C7-C6-C8	-3.80	105.74	108.90
3	B	503	NID	C6-C7-C2	2.93	120.69	116.80
3	A	502	NID	C6-C7-C2	2.58	120.23	116.80
2	A	500	NDP	C4A-C5A-N7A	2.46	111.96	109.40
2	B	501	NDP	O3B-C3B-C2B	-2.38	104.41	111.17
3	B	503	NID	C3-C2-C7	-2.37	117.56	120.67
2	B	501	NDP	C4A-C5A-N7A	2.23	111.72	109.40
2	A	500	NDP	O3B-C3B-C2B	-2.10	105.22	111.17
2	B	501	NDP	O4B-C1B-C2B	-2.08	102.98	106.59
3	A	502	NID	C3-C2-C7	-2.07	117.96	120.67
2	A	500	NDP	O5B-C5B-C4B	2.06	116.08	108.99
3	A	502	NID	C4-C3-C2	2.03	122.08	118.61

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	NDP	C5B-O5B-PA-O1A
2	A	500	NDP	C5B-O5B-PA-O3
2	A	500	NDP	O4B-C4B-C5B-O5B
2	B	501	NDP	C5B-O5B-PA-O1A
2	B	501	NDP	C5B-O5B-PA-O2A
2	B	501	NDP	C5B-O5B-PA-O3
2	A	500	NDP	C3B-C4B-C5B-O5B
2	A	500	NDP	PN-O3-PA-O2A
2	B	501	NDP	PN-O3-PA-O2A
2	A	500	NDP	C5B-O5B-PA-O2A
2	A	500	NDP	O4D-C1D-N1N-C6N
2	A	500	NDP	PN-O3-PA-O1A
2	B	501	NDP	O4D-C1D-N1N-C6N
2	A	500	NDP	C2B-O2B-P2B-O3X
2	B	501	NDP	C2D-C1D-N1N-C6N

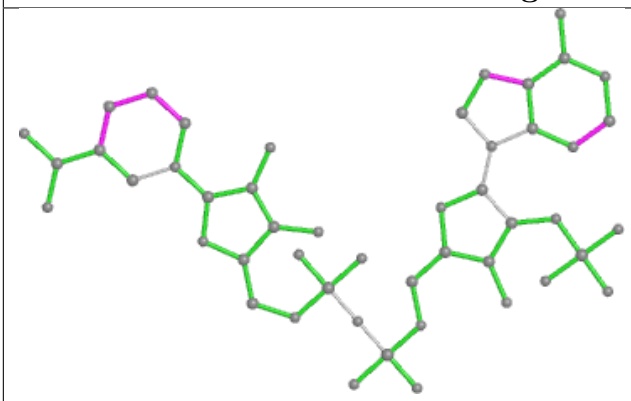
There are no ring outliers.

3 monomers are involved in 7 short contacts:

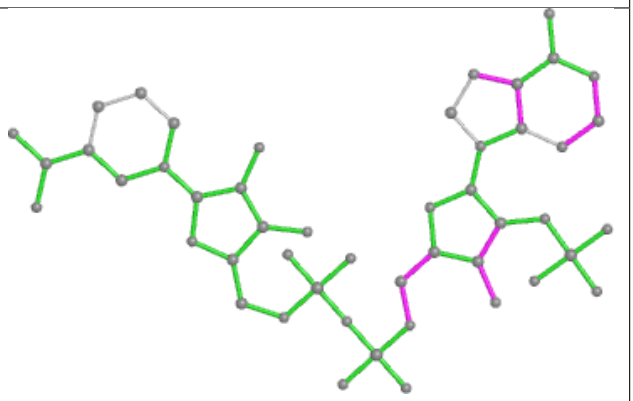
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NID	1	0
3	B	503	NID	2	0
2	B	501	NDP	5	0

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 then 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.

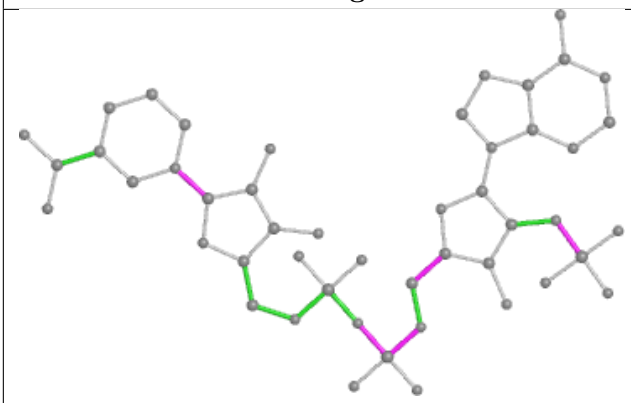
Ligand NDP A 500



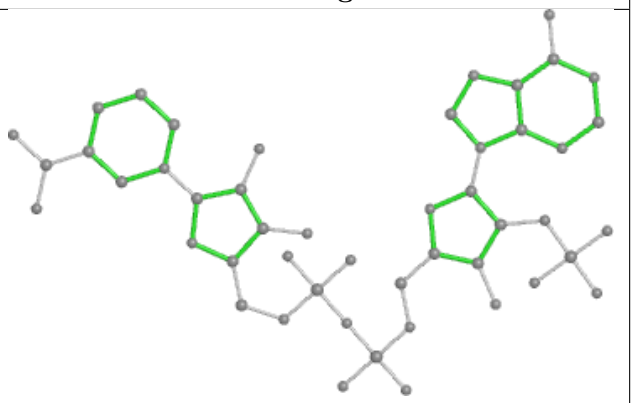
Bond lengths



Bond angles

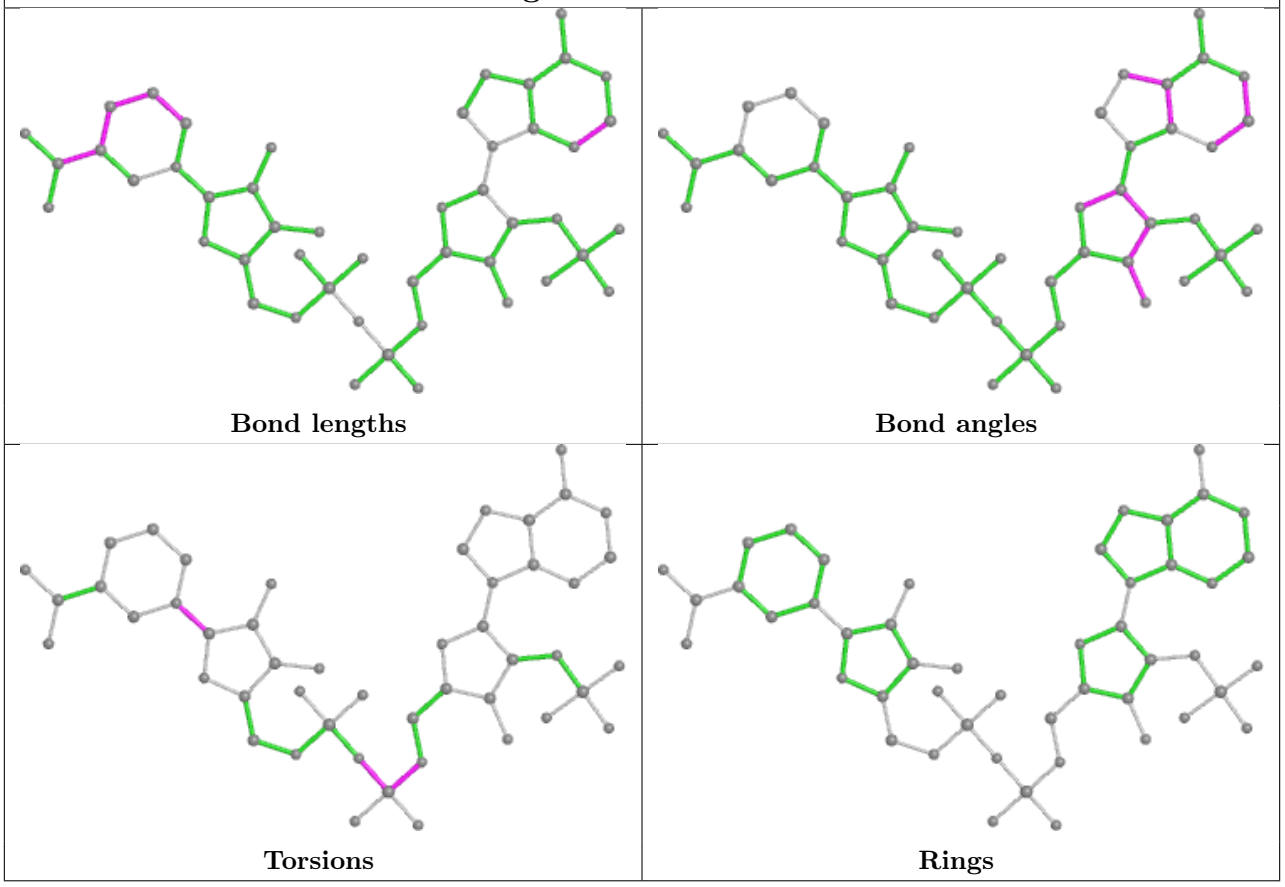


Torsions



Rings

Ligand NDP B 501



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.