wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 05:51 AM EDT

PDB ID	:	1OG6
Title	:	ydhF, an aldo-keto reductase from E.coli complexed with NADPH
Authors	:	Jeudy, S.; Abergel, C.; Claverie, J.M.
Deposited on	:	2003-04-24
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

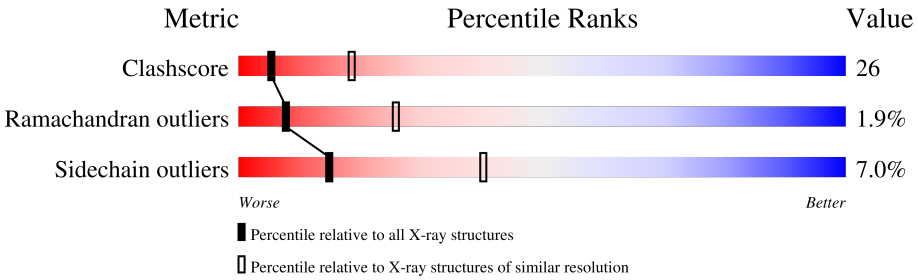
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 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	298	52% 43% .
1	B	298	49% 44% 6% .
1	C	298	49% 46% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7423 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.

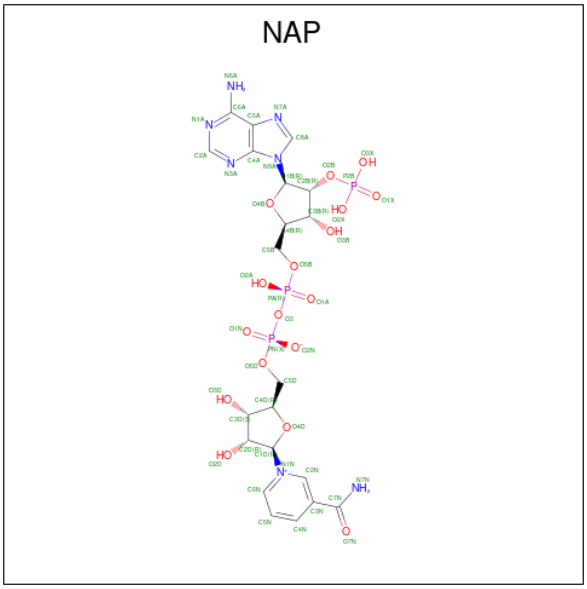
- Molecule 1 is a protein called HYPOTHETICAL OXIDOREDUCTASE YDHF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	1
			2362	1500	422	430	10			
1	B	294	Total	C	N	O	S	0	0	0
			2349	1493	418	428	10			
1	C	298	Total	C	N	O	S	0	0	0
			2369	1505	422	432	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	MET	conflict	UNP P76187
B	1	LEU	MET	conflict	UNP P76187
C	1	LEU	MET	conflict	UNP P76187

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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		
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	70	Total	O	0	0
			70	70		
3	B	76	Total	O	0	0
			76	76		
3	C	53	Total	O	0	0
			53	53		

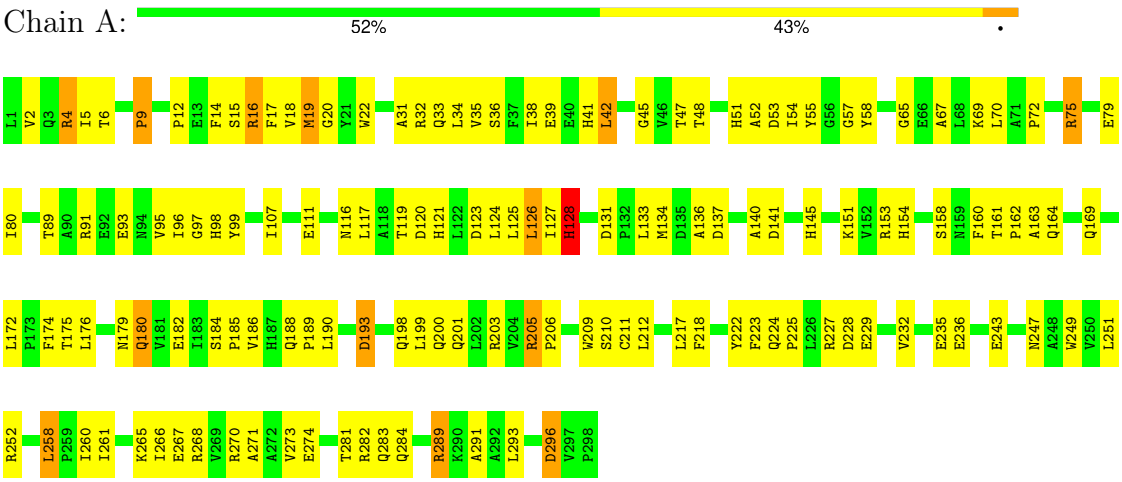
3 Residue-property plots (i)

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.

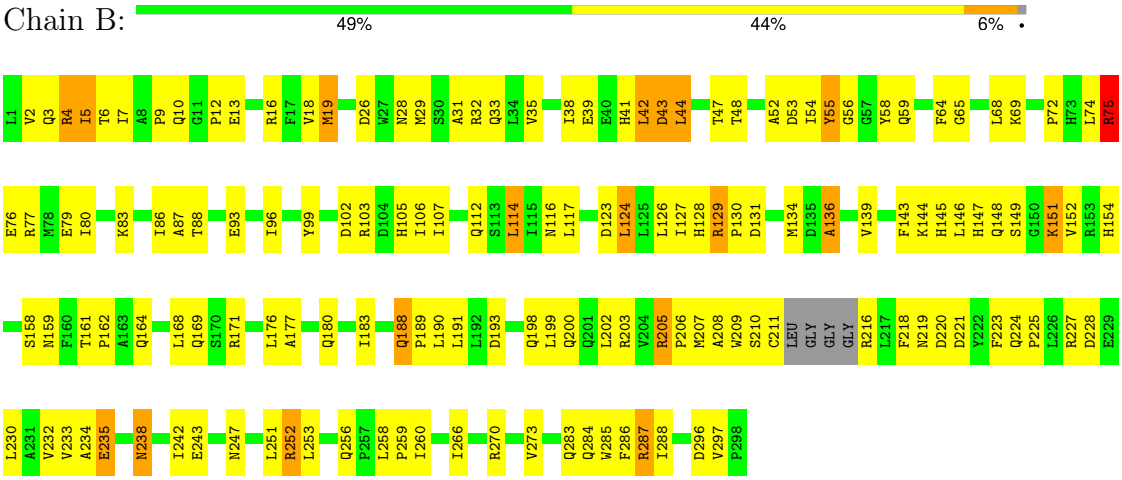
• Molecule 1: HYPOTHETICAL OXIDOREDUCTASE YDHF

Chain A:



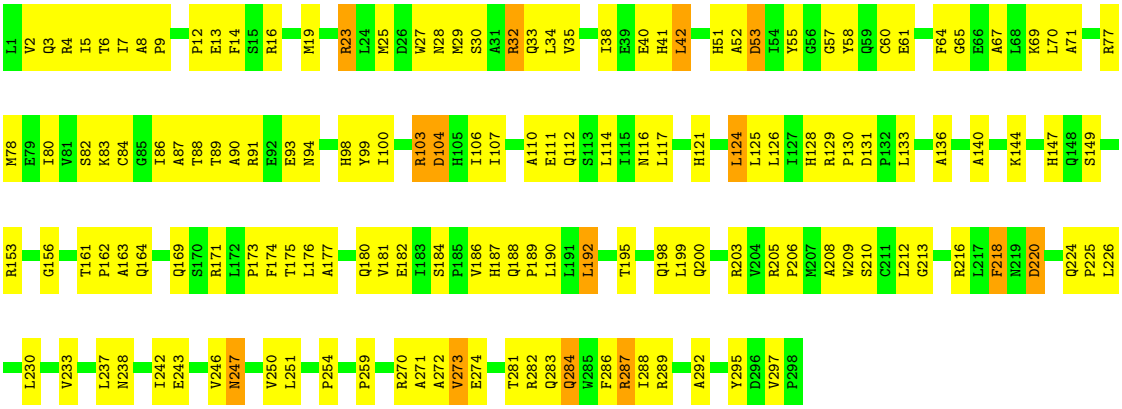
• Molecule 1: HYPOTHETICAL OXIDOREDUCTASE YDHF

Chain B:



• Molecule 1: HYPOTHETICAL OXIDOREDUCTASE YDHF

Chain C:


L1 V2 Q3 R4 I5 T6 I7 A8 P9 P12 E13 F14 S15 R16 M19 R23 L24 M25 D26 W27 N28 M29 S30 A31 R32 Q33 L34 V35 I38 E39 E40 H41 L42 H51 A52 D53 I54 Y55 G56 G57 Y58 Q59 C60 E61 F64 G65 E66 A67 L68 K69 L70 A71 R77
M78 E79 I80 V81 S82 K83 C84 G85 I86 A87 T88 T89 A90 R91 E92 E93 N94 H98 Y99 I100 R103 D104 H105 I106 I107 A110 E111 Q112 S113 L114 I115 N116 L117 H121 L124 L125 L126 I127 H128 R129 P130 D131 P132 L133 A136 A140 K144 H147 Q148 S149
R153 G156 T161 P162 A163 Q164 Q169 S170 R171 L172 P173 F174 T175 L176 A177 Q180 V181 E182 I183 S184 P185 V186 H187 Q188 P189 L190 L191 L192 T195 Q198 L199 Q200 R203 V204 R205 P206 M207 A208 W209 S210 C211 L212 G213 R216 L217 F218 N219 D220 Q224 P225 L226
L230 V233 L237 N238 I242 E243 V246 N247 V250 L251 P254 P259 R270 A271 A272 V273 E274 T281 R282 Q283 Q284 W285 F286 R287 I288 R289 A292 Y295 D296 V297 P298

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	174.53Å 174.53Å 97.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.91 – 2.80	Depositor
% Data completeness (in resolution range)	99.7 (29.91-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7423	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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: 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	0.36	0/2414	0.65	0/3278
1	B	0.37	0/2401	0.64	0/3259
1	C	0.36	0/2422	0.65	0/3288
All	All	0.36	0/7237	0.65	0/9825

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	2362	0	2355	123	0
1	B	2349	0	2341	124	0
1	C	2369	0	2362	146	0
2	A	48	0	25	8	0
2	B	48	0	25	7	0
2	C	48	0	25	5	0
3	A	70	0	0	4	0
3	B	76	0	0	6	0
3	C	53	0	0	13	0
All	All	7423	0	7133	375	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 26.

The worst 5 of 375 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:C:161:THR:HB	1:C:164:GLN:HG3	1.40	1.02
1:A:95:VAL:H	1:C:283:GLN:NE2	1.60	1.00
1:A:210:SER:H	2:A:1298:NAP:H51N	1.28	0.96
1:B:75:ARG:HD3	1:B:75:ARG:O	1.67	0.94
1:C:88:THR:HG22	1:C:90:ALA:H	1.33	0.92

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	296/298 (99%)	266 (90%)	24 (8%)	6 (2%)	7	24
1	B	290/298 (97%)	258 (89%)	26 (9%)	6 (2%)	7	23
1	C	296/298 (99%)	260 (88%)	31 (10%)	5 (2%)	9	29
All	All	882/894 (99%)	784 (89%)	81 (9%)	17 (2%)	8	26

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	53	ASP
1	B	75	ARG
1	B	136	ALA
1	C	3	GLN

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	252/253 (100%)	236 (94%)	16 (6%)	18	46
1	B	252/253 (100%)	233 (92%)	19 (8%)	13	37
1	C	253/253 (100%)	235 (93%)	18 (7%)	14	39
All	All	757/759 (100%)	704 (93%)	53 (7%)	15	40

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	151	LYS
1	C	19	MET
1	C	220	ASP
1	B	205	ARG
1	B	243	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3	GLN
1	C	145	HIS
1	C	10	GLN
1	C	105	HIS
1	C	154	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	1299	-	46,52,52	2.12	11 (23%)	61,80,80	2.60	20 (32%)
2	NAP	B	1299	-	46,52,52	2.12	11 (23%)	61,80,80	2.58	22 (36%)
2	NAP	A	1298	-	46,52,52	2.24	12 (26%)	61,80,80	2.58	21 (34%)

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	C	1299	-	-	12/31/67/67	0/5/5/5
2	NAP	B	1299	-	-	6/31/67/67	0/5/5/5
2	NAP	A	1298	-	-	7/31/67/67	0/5/5/5

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1298	NAP	C2N-N1N	7.97	1.43	1.35
2	C	1299	NAP	C2N-N1N	6.75	1.42	1.35
2	B	1299	NAP	C2N-N1N	6.49	1.42	1.35
2	B	1299	NAP	C4N-C3N	5.57	1.47	1.39
2	A	1298	NAP	C4N-C3N	5.26	1.47	1.39

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1299	NAP	O3X-P2B-O1X	-7.85	80.25	110.83
2	B	1299	NAP	O3X-P2B-O1X	-7.80	80.45	110.83
2	A	1298	NAP	O5D-PN-O1N	-7.59	78.86	108.94
2	C	1299	NAP	O5D-PN-O1N	-7.53	79.07	108.94
2	B	1299	NAP	O5D-PN-O1N	-7.38	79.67	108.94

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1298	NAP	O4D-C1D-N1N-C2N
2	A	1298	NAP	O4D-C1D-N1N-C6N
2	A	1298	NAP	C2D-C1D-N1N-C2N
2	A	1298	NAP	C2D-C1D-N1N-C6N
2	B	1299	NAP	O4D-C1D-N1N-C2N

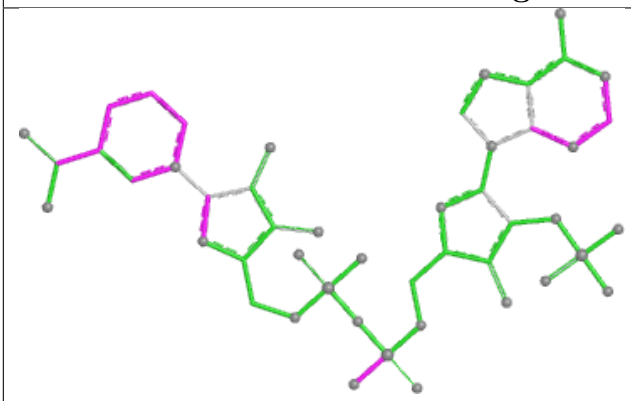
There are no ring outliers.

3 monomers are involved in 20 short contacts:

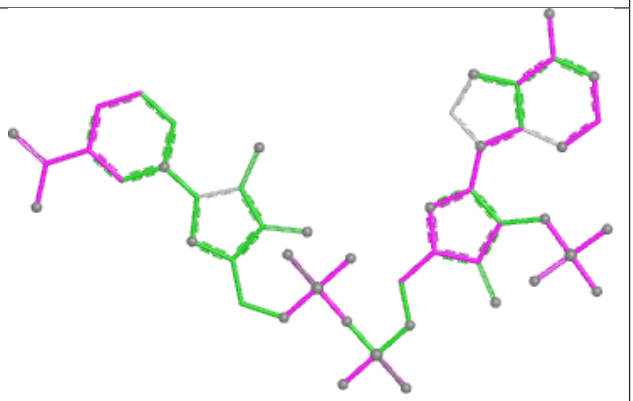
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1299	NAP	5	0
2	B	1299	NAP	7	0
2	A	1298	NAP	8	0

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 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.

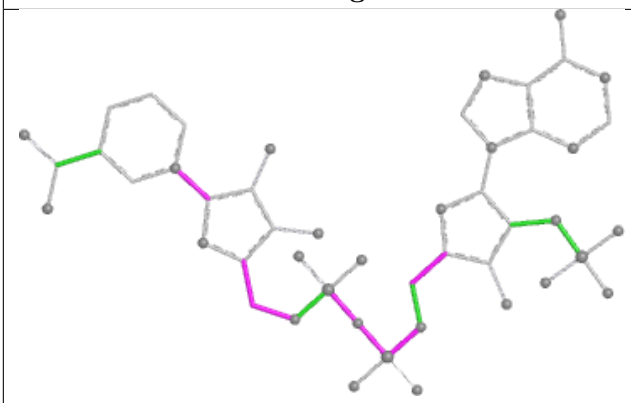
Ligand NAP C 1299



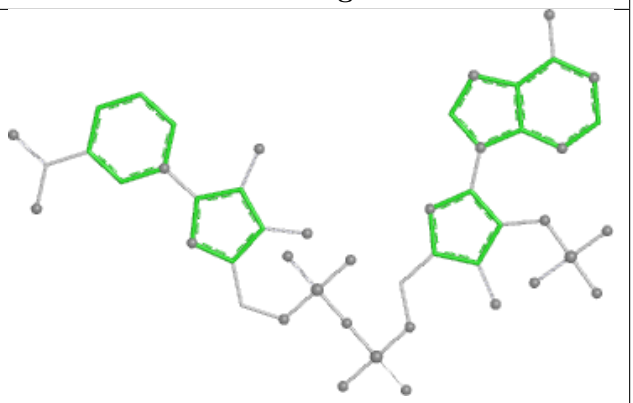
Bond lengths



Bond angles

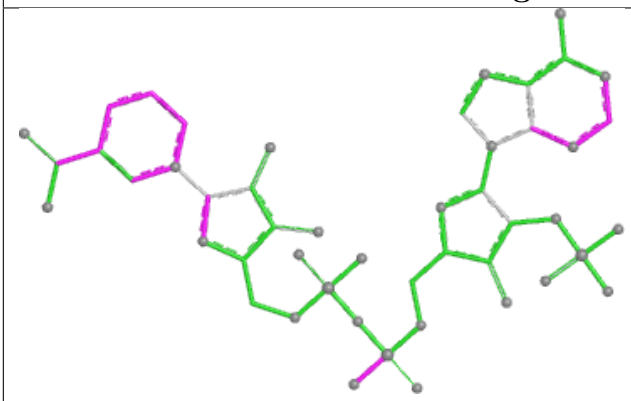


Torsions

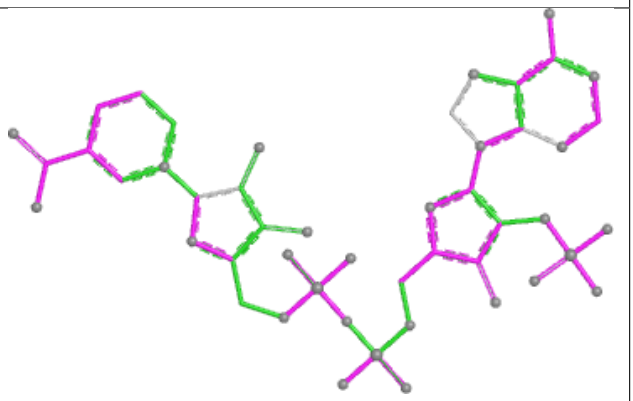


Rings

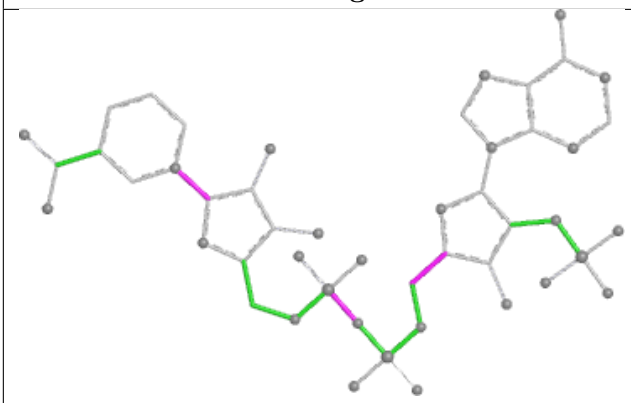
Ligand NAP B 1299



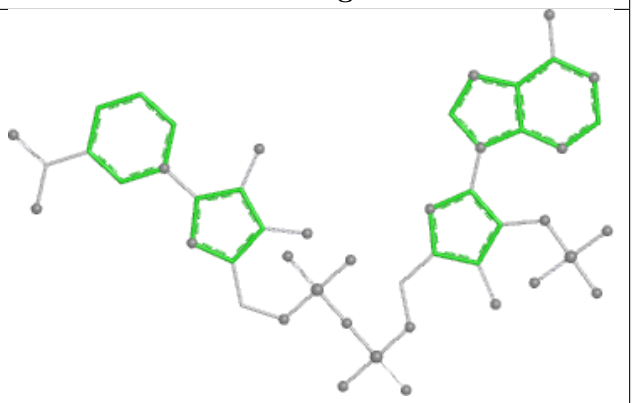
Bond lengths



Bond angles

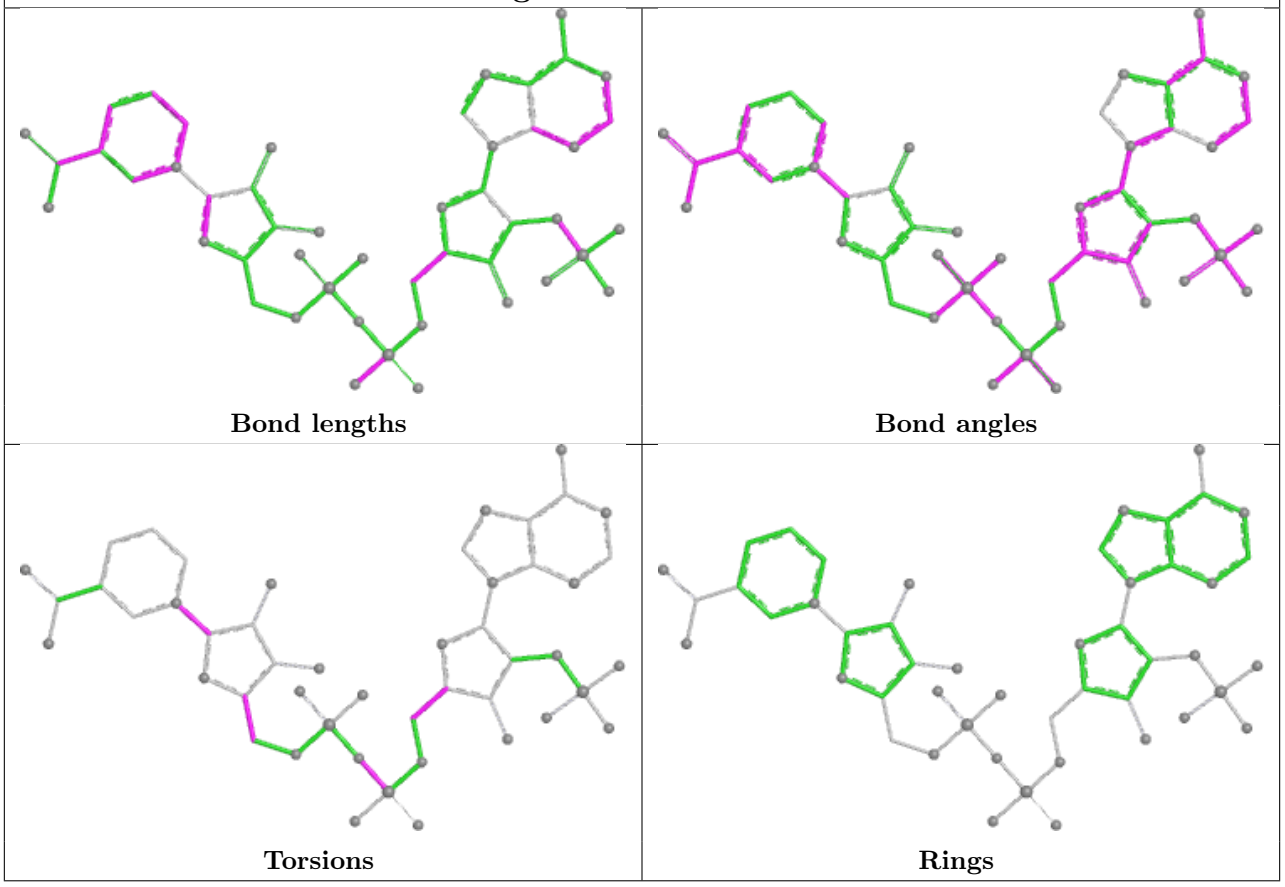


Torsions



Rings

Ligand NAP A 1298



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.