wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 11:27 AM EDT

PDB ID	:	2J3K
Title	:	Crystal structure of Arabidopsis thaliana Double Bond Reductase (AT5G16970)-Ternary Complex II
Authors	:	Youn, B.; Kim, S.J.; Moinuddin, S.G.; Lee, C.; Bedgar, D.L.; Harper, A.R.; Davin, L.B.; Lewis, N.G.; Kang, C.
Deposited on	:	2006-08-22
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:

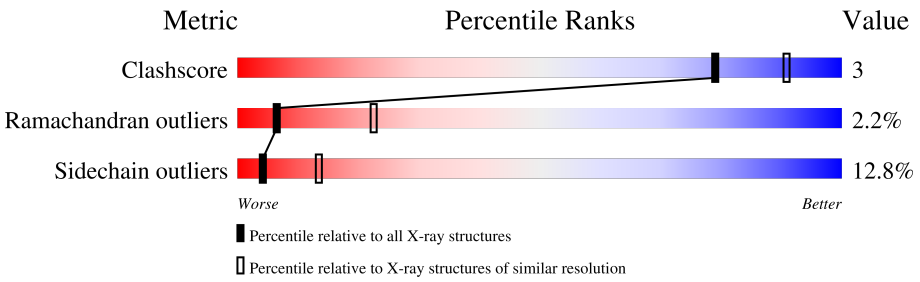
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	345	63% 27% 7% •
1	B	345	62% 31% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5556 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.

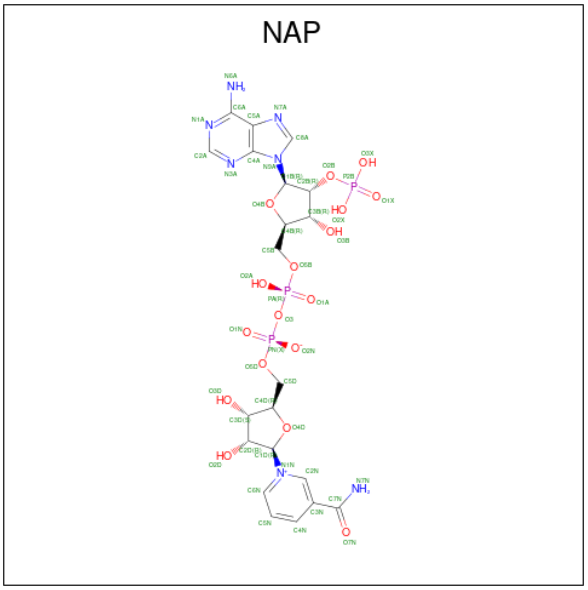
- Molecule 1 is a protein called NADPH-dependent oxidoreductase 2-alkenal reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	2623	1681	432	493	17	0	0	0
1	B	345	2681	1717	441	506	17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ASN	ILE	conflict	UNP Q39172
B	1279	ASN	ILE	conflict	UNP Q39172

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



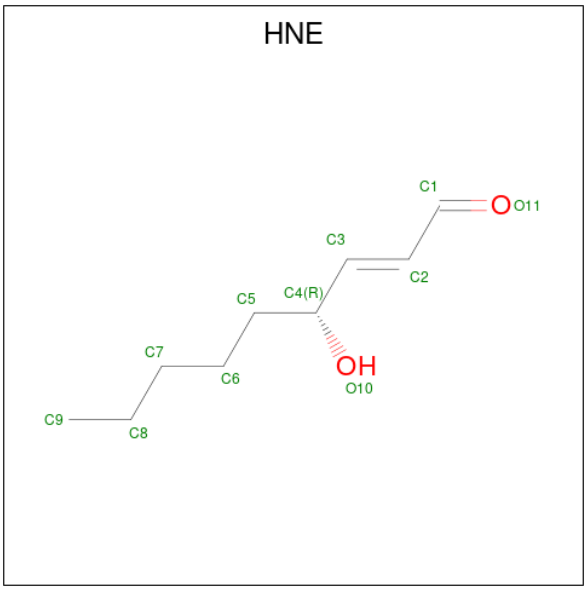
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is (2E,4R)-4-HYDROXYNON-2-ENAL (three-letter code: HNE) (formula: $C_9H_{16}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	11	9	2		0	0
3	B	1	11	9	2		0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	62	62	62	0	0
4	B	72	72	72	0	0

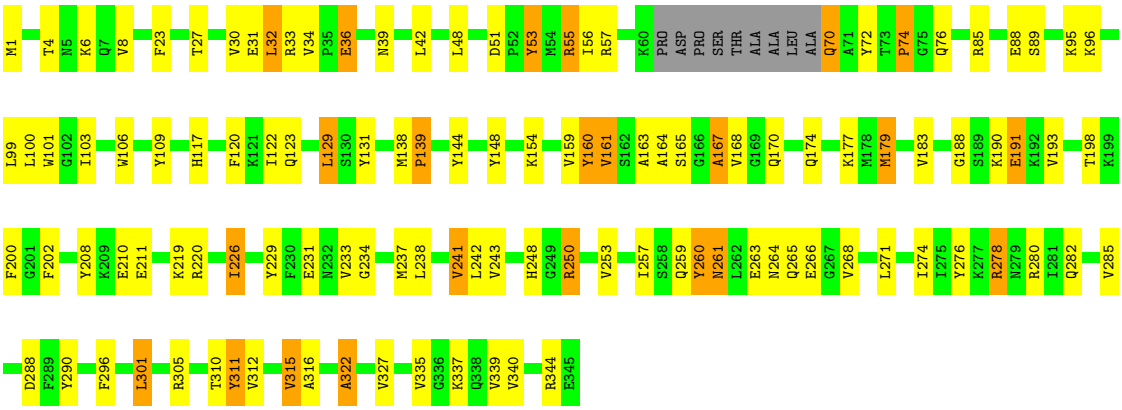
3 Residue-property plots (i)

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.

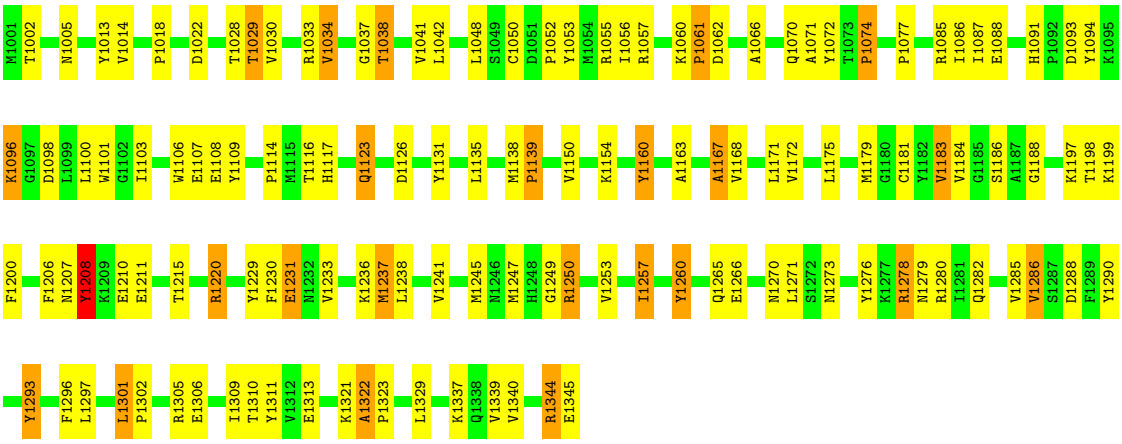
• Molecule 1: NADPH-dependent oxidoreductase 2-alkenal reductase

Chain A: 63% 27% 7% •



• Molecule 1: NADPH-dependent oxidoreductase 2-alkenal reductase

Chain B: 62% 31% 7%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.08Å 122.45Å 147.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	82.6 (15.00-2.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5556	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, HNE

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	1.30	4/2681 (0.1%)	2.09	107/3625 (3.0%)
1	B	1.29	2/2742 (0.1%)	2.10	116/3713 (3.1%)
All	All	1.30	6/5423 (0.1%)	2.10	223/7338 (3.0%)

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	4
1	B	0	6
All	All	0	10

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	TYR	CG-CD2	5.48	1.46	1.39
1	A	53	TYR	CG-CD1	5.25	1.46	1.39
1	A	148	TYR	CG-CD2	5.22	1.46	1.39
1	B	1276	TYR	CG-CD2	5.11	1.45	1.39
1	B	1053	TYR	CG-CD1	5.04	1.45	1.39

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	ARG	NE-CZ-NH1	11.99	126.29	120.30
1	A	72	TYR	CB-CG-CD1	-11.74	113.95	121.00
1	A	312	VAL	CG1-CB-CG2	-11.06	93.20	110.90
1	B	1055	ARG	NE-CZ-NH1	10.61	125.61	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1253	VAL	CG1-CB-CG2	-10.44	94.20	110.90

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	TYR	Sidechain
1	A	260	TYR	Sidechain
1	A	322	ALA	Peptide
1	A	34	VAL	Peptide
1	B	1034	VAL	Peptide

5.2 Too-close contacts (i)

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	2623	0	2594	15	0
1	B	2681	0	2648	15	0
2	A	48	0	25	6	0
2	B	48	0	25	5	0
3	A	11	0	16	1	0
3	B	11	0	16	0	0
4	A	62	0	0	0	0
4	B	72	0	0	1	0
All	All	5556	0	5324	30	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 3.

The worst 5 of 30 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:208:TYR:HE2	2:A:1346:NAP:O3X	1.43	1.02
1:A:174:GLN:HE22	1:A:310:THR:H	1.41	0.68
1:A:208:TYR:CE2	2:A:1346:NAP:O3X	2.36	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1208:TYR:OH	2:B:2346:NAP:O3X	2.15	0.64
1:A:208:TYR:HE2	2:A:1346:NAP:P2B	2.24	0.61

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	332/345 (96%)	293 (88%)	34 (10%)	5 (2%)	10 33
1	B	343/345 (99%)	305 (89%)	28 (8%)	10 (3%)	4 15
All	All	675/690 (98%)	598 (89%)	62 (9%)	15 (2%)	6 22

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	322	ALA
1	B	1034	VAL
1	B	1096	LYS
1	B	1167	ALA

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	283/289 (98%)	247 (87%)	36 (13%)	4 14
1	B	289/289 (100%)	252 (87%)	37 (13%)	4 13
All	All	572/578 (99%)	499 (87%)	73 (13%)	4 13

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1237	MET
1	B	1323	PRO
1	B	1247	MET
1	B	1288	ASP
1	A	242	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1005	ASN
1	B	1007	GLN
1	B	1207	ASN
1	B	1170	GLN
1	A	246	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	HNE	A	1347	-	10,10,10	1.48	2 (20%)	9,10,10	1.23	1 (11%)
2	NAP	B	2346	-	46,52,52	1.71	11 (23%)	61,80,80	2.46	17 (27%)
3	HNE	B	2347	-	10,10,10	1.47	2 (20%)	9,10,10	1.22	1 (11%)
2	NAP	A	1346	-	46,52,52	2.04	9 (19%)	61,80,80	2.35	12 (19%)

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	HNE	A	1347	-	-	6/9/9/9	-
2	NAP	B	2346	-	-	13/31/67/67	0/5/5/5
3	HNE	B	2347	-	-	6/9/9/9	-
2	NAP	A	1346	-	-	16/31/67/67	0/5/5/5

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1346	NAP	PN-O3	6.64	1.66	1.59
2	A	1346	NAP	C2N-N1N	6.29	1.41	1.35
2	B	2346	NAP	C2N-N1N	5.42	1.40	1.35
2	A	1346	NAP	PA-O3	4.59	1.64	1.59
2	B	2346	NAP	O4B-C1B	4.02	1.46	1.40

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2346	NAP	C4B-O4B-C1B	-9.90	100.86	109.92
2	A	1346	NAP	O5D-C5D-C4D	7.74	135.34	108.99
2	A	1346	NAP	C4D-O4D-C1D	7.53	116.82	109.92
2	B	2346	NAP	O4B-C1B-N9A	6.03	116.74	108.75
2	A	1346	NAP	N3A-C2A-N1A	-5.92	120.63	128.67

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1346	NAP	C5B-O5B-PA-O3
2	A	1346	NAP	C3B-C4B-C5B-O5B
2	A	1346	NAP	C5D-O5D-PN-O3
2	A	1346	NAP	C5D-O5D-PN-O1N
2	A	1346	NAP	C4D-C5D-O5D-PN

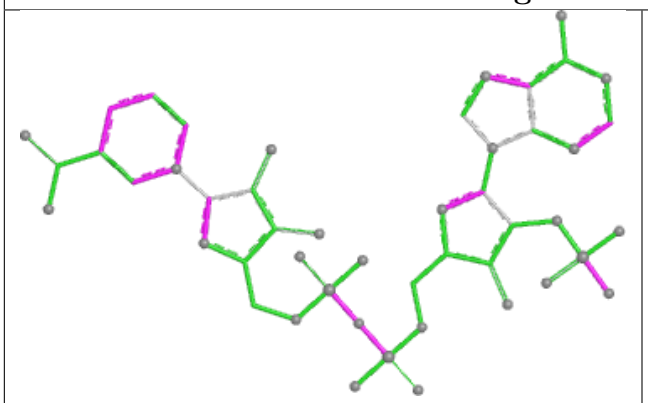
There are no ring outliers.

3 monomers are involved in 12 short contacts:

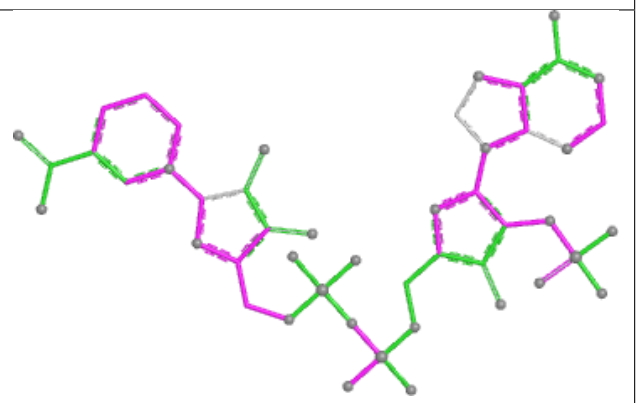
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1347	HNE	1	0
2	B	2346	NAP	5	0
2	A	1346	NAP	6	0

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.

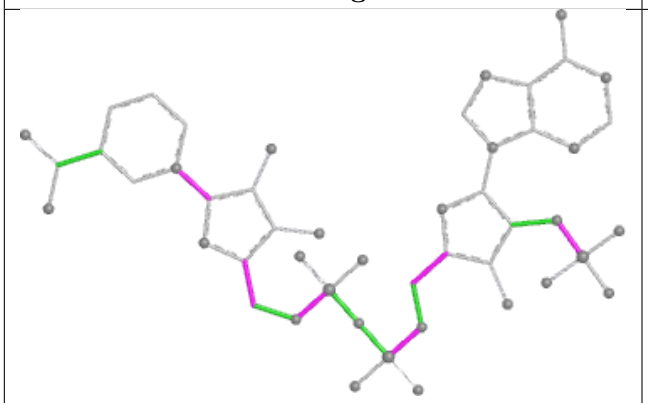
Ligand NAP B 2346



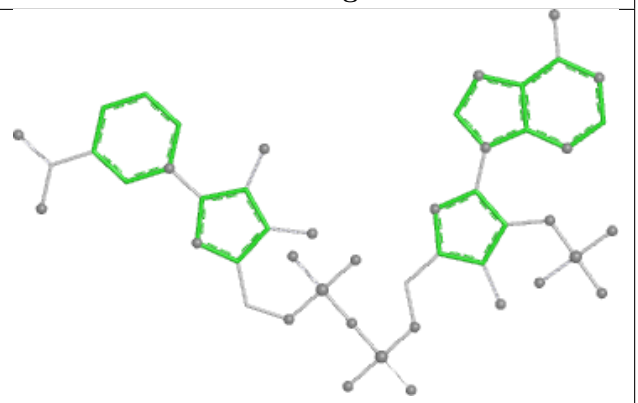
Bond lengths



Bond angles

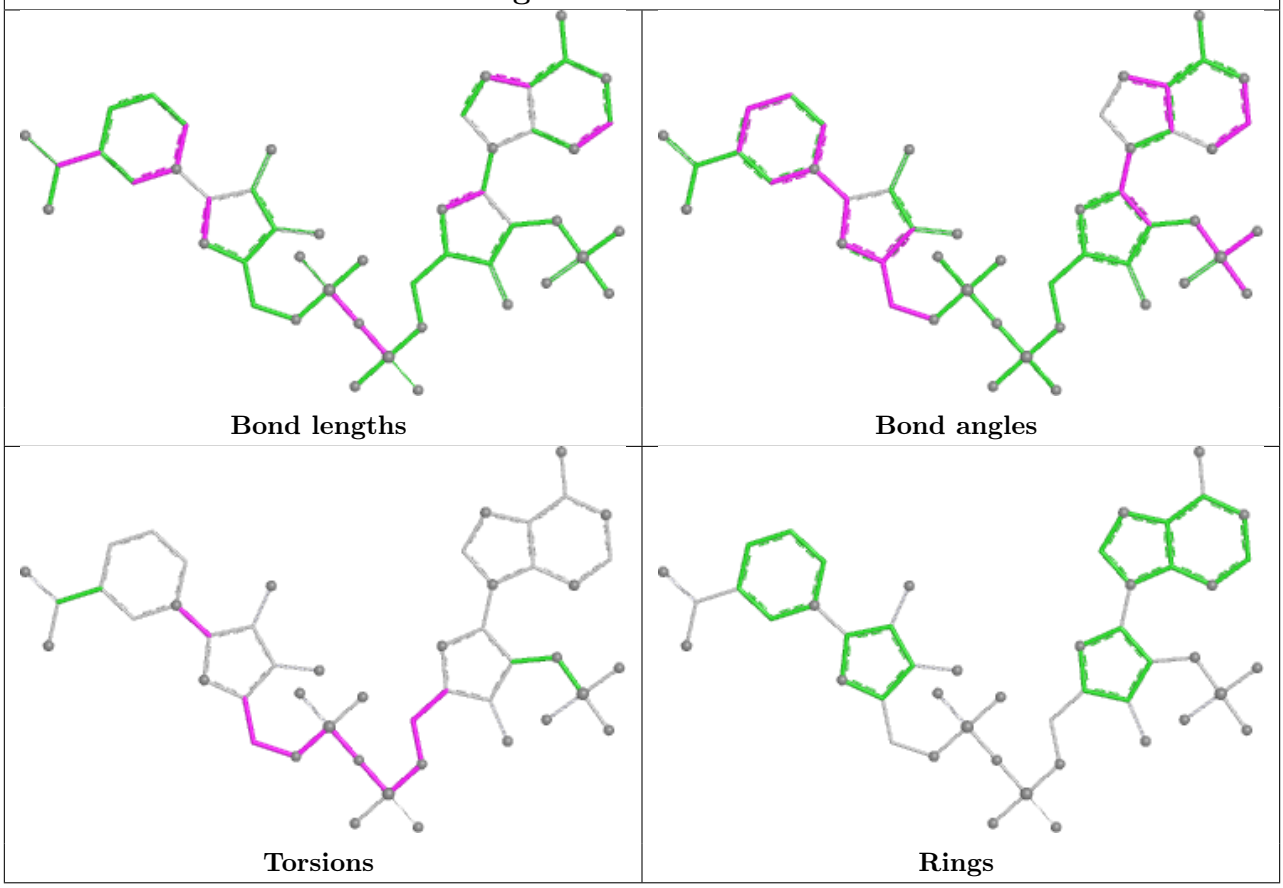


Torsions



Rings

Ligand NAP A 1346



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.