



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:49 am BST

PDB ID : 1FDT
Title : HUMAN 17-BETA-HYDROXYSTEROID-DEHYDROGENASE TYPE 1
COMPLEXED WITH ESTRADIOL AND NADP+
Authors : Housset, D.; Breton, R.; Mazza, C.; Fontecilla-Camps, J.-C.
Deposited on : 1996-06-28
Resolution : 2.20 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)
Xtrriage (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) : 2.11

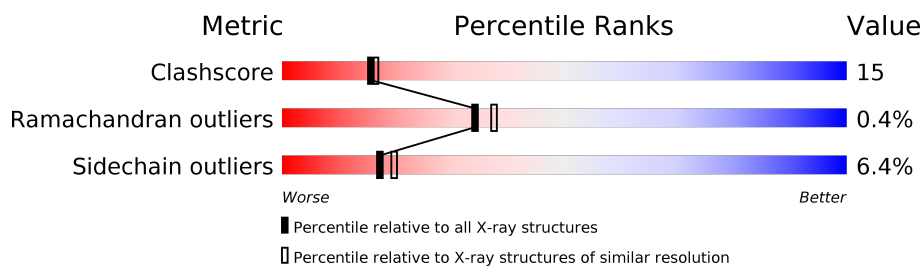
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	380	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2466 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 17-BETA-HYDROXYSTEROID-DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	2256	1433	399	411	13	0	10	0

There is a discrepancy between the modelled and reference sequences:

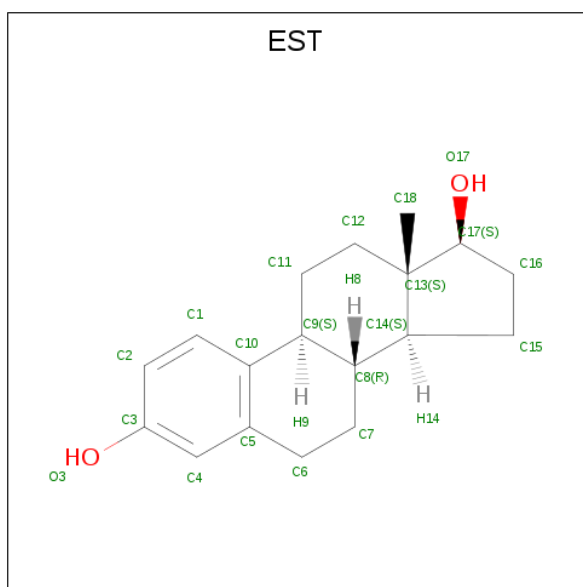
Chain	Residue	Modelled	Actual	Comment	Reference
A	301	ARG	ALA	CONFLICT	UNP P14061

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



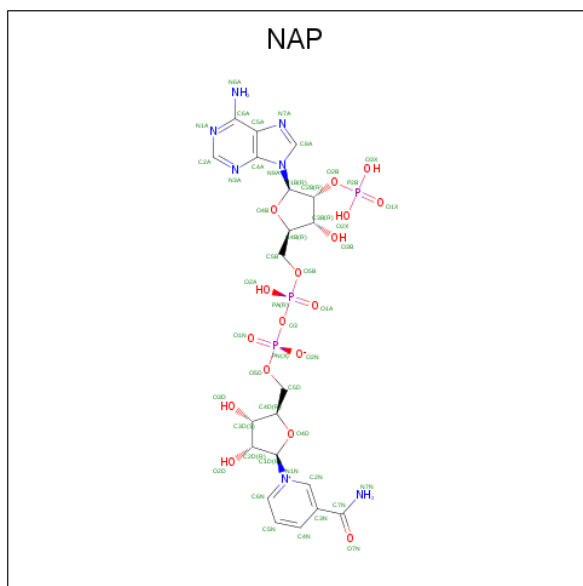
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is ESTRADIOL (three-letter code: EST) (formula: C₁₈H₂₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	18	2		

- Molecule 4 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	
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total 137	O 137	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.77Å 43.79Å 60.53Å 90.00° 99.47° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	84.8 (10.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.193 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2466	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

4 Model quality [i](#)

4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, EST, SO4

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	0.69	0/2302	0.86	5/3120 (0.2%)

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	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	GLY	N-CA-C	-5.95	98.22	113.10
1	A	244	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	262	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	31	LYS	N-CA-C	-5.40	96.43	111.00
1	A	68	ASP	CB-CG-OD1	5.22	123.00	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	HIS	Mainchain

4.2 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	2256	0	2300	66	0
2	A	5	0	0	1	0
3	A	20	0	24	2	0
4	A	48	0	23	14	0
5	A	137	0	0	5	0
All	All	2466	0	2347	69	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 15.

All (69) 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:37[B]:ARG:NH1	5:A:484:HOH:O	1.92	1.02
1:A:37[B]:ARG:CZ	5:A:484:HOH:O	2.10	0.99
1:A:146:LEU:HA	2:A:380:SO4:O2	1.83	0.78
1:A:90:ASN:HA	1:A:140:THR:HG23	1.65	0.77
1:A:94:GLY:HA3	1:A:195[A]:LYS:HB3	1.72	0.71
1:A:263:LEU:O	1:A:267:LEU:HG	1.95	0.66
1:A:37[A]:ARG:NH1	4:A:360:NAP:N7A	2.44	0.66
1:A:90:ASN:HA	1:A:140:THR:CG2	2.26	0.65
1:A:13:GLY:O	1:A:17:HIS:HD2	1.78	0.65
1:A:194[A]:GLU:C	1:A:195[A]:LYS:HG2	2.16	0.65
1:A:66:VAL:HG22	4:A:360:NAP:N1A	2.12	0.64
1:A:155:TYR:CG	1:A:195[A]:LYS:HE3	2.35	0.62
1:A:193[A]:MET:SD	1:A:197[A]:LEU:HD23	2.40	0.61
1:A:172:LEU:O	1:A:175:PRO:HD2	2.00	0.60
1:A:245:ARG:NH2	5:A:534:HOH:O	2.19	0.60
1:A:195[A]:LYS:O	1:A:196[A]:VAL:HG23	2.01	0.59
1:A:191[B]:ALA:O	1:A:193[B]:MET:N	2.38	0.57
1:A:269:ASP:HB3	5:A:438:HOH:O	2.04	0.56
1:A:35:THR:HG22	1:A:62:LEU:HB2	1.87	0.56
1:A:260:LEU:N	1:A:261:PRO:HD2	2.21	0.56
1:A:193[A]:MET:SD	1:A:197[A]:LEU:CD2	2.94	0.55
1:A:185:CYS:HB2	4:A:360:NAP:C5N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HA	4:A:360:NAP:O2X	2.07	0.55
1:A:90:ASN:OD1	1:A:140:THR:HG21	2.06	0.54
1:A:203:VAL:O	1:A:207:THR:HG22	2.08	0.54
1:A:260:LEU:O	1:A:264:ARG:HD3	2.09	0.53
1:A:131:ARG:HH11	1:A:131:ARG:HG3	1.73	0.52
1:A:152:ASN:ND2	1:A:195[A]:LYS:HZ2	2.06	0.52
1:A:16:LEU:HD23	1:A:16:LEU:C	2.30	0.52
1:A:197[A]:LEU:HD12	1:A:215:PHE:CZ	2.45	0.51
1:A:149:LEU:CD1	3:A:350:EST:H182	2.42	0.50
1:A:95:LEU:H	1:A:195[A]:LYS:NZ	2.09	0.50
1:A:190[B]:THR:O	1:A:191[B]:ALA:HB3	2.12	0.50
1:A:37[A]:ARG:CZ	4:A:360:NAP:N7A	2.72	0.49
1:A:257:GLU:HG2	1:A:260:LEU:HD22	1.93	0.49
1:A:9:GLY:HA2	4:A:360:NAP:H1B	1.96	0.47
1:A:16:LEU:HG	1:A:45:LEU:HD23	1.97	0.47
1:A:155:TYR:CD2	1:A:195[A]:LYS:HE3	2.51	0.46
1:A:95:LEU:H	1:A:195[A]:LYS:HZ3	1.64	0.46
1:A:37[B]:ARG:HG3	4:A:360:NAP:C6A	2.47	0.45
1:A:166:CYS:HB3	1:A:180:LEU:CD2	2.45	0.45
1:A:174:LEU:HB3	1:A:175:PRO:HD3	1.98	0.45
1:A:192[A]:PHE:C	1:A:194[A]:GLU:H	2.18	0.45
1:A:96:LEU:HD11	1:A:218:TYR:CE2	2.53	0.44
1:A:197[A]:LEU:HD12	1:A:215:PHE:HZ	1.83	0.43
1:A:260:LEU:HD13	5:A:451:HOH:O	2.18	0.43
1:A:140:THR:HB	1:A:240:PHE:HZ	1.84	0.43
1:A:68:ASP:O	1:A:72:VAL:HG23	2.19	0.43
1:A:77:GLU:HG2	1:A:78:ARG:N	2.34	0.43
1:A:152:ASN:HD22	1:A:195[A]:LYS:NZ	2.16	0.42
4:A:360:NAP:H52N	4:A:360:NAP:O5B	2.19	0.42
1:A:159:LYS:HA	1:A:159:LYS:HD3	1.67	0.42
1:A:195[B]:LYS:HD2	1:A:195[B]:LYS:HA	1.68	0.42
1:A:12:SER:O	4:A:360:NAP:PA	2.77	0.42
4:A:360:NAP:O5B	4:A:360:NAP:C5D	2.68	0.42
1:A:147:MET:HB2	1:A:275:TYR:CZ	2.54	0.42
1:A:152:ASN:ND2	1:A:195[A]:LYS:NZ	2.68	0.42
1:A:149:LEU:HD11	3:A:350:EST:H182	2.01	0.42
1:A:224:GLN:O	1:A:228:GLU:HG2	2.20	0.41
1:A:185:CYS:HB2	4:A:360:NAP:C6N	2.51	0.41
1:A:37[B]:ARG:HG3	4:A:360:NAP:N6A	2.34	0.41
1:A:194[A]:GLU:HG2	1:A:195[A]:LYS:HG2	2.03	0.41
1:A:281:ARG:HD2	1:A:281:ARG:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:CYS:HB3	1:A:180:LEU:HD22	2.03	0.40
1:A:12:SER:O	4:A:360:NAP:O1A	2.39	0.40
1:A:55:PRO:HA	1:A:56:PRO:HD3	1.93	0.40
1:A:188:VAL:HG22	1:A:236:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	293/327 (90%)	282 (96%)	9 (3%)	2 (1%)	22 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192[A]	PHE
1	A	192[B]	PHE

4.3.2 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	243/258 (94%)	225 (93%)	18 (7%)	13 14

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	52	LEU
1	A	76	ARG
1	A	77	GLU
1	A	105	ASP
1	A	140	THR
1	A	192[A]	PHE
1	A	192[B]	PHE
1	A	195[A]	LYS
1	A	195[B]	LYS
1	A	197[A]	LEU
1	A	197[B]	LEU
1	A	204	LEU
1	A	241	LEU
1	A	244	LEU
1	A	263	LEU
1	A	264	ARG
1	A	273	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	42	GLN
1	A	123	GLN
1	A	152	ASN
1	A	224	GLN
1	A	231	GLN
1	A	274	ASN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 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
3	EST	A	350	-	23,23,23	0.71	1 (4%)	36,36,36	0.77	0
2	SO4	A	380	-	4,4,4	1.37	1 (25%)	6,6,6	2.40	3 (50%)
4	NAP	A	360	1	45,52,52	1.93	6 (13%)	56,80,80	1.68	14 (25%)

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	EST	A	350	-	-	-	0/4/4/4
4	NAP	A	360	1	-	13/31/67/67	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	360	NAP	P2B-O2B	-7.71	1.44	1.59
4	A	360	NAP	P2B-O2X	-5.94	1.31	1.54
4	A	360	NAP	C2N-N1N	4.05	1.39	1.35
4	A	360	NAP	P2B-O1X	-3.78	1.38	1.50
4	A	360	NAP	P2B-O3X	-3.00	1.43	1.54
2	A	380	SO4	O2-S	-2.19	1.34	1.46
4	A	360	NAP	C2D-C1D	-2.05	1.50	1.53
3	A	350	EST	C16-C17	2.02	1.57	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	360	NAP	N3A-C2A-N1A	-4.49	121.66	128.68
2	A	380	SO4	O4-S-O2	-3.99	88.49	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	360	NAP	O5B-C5B-C4B	-3.93	95.48	108.99
4	A	360	NAP	C3D-C2D-C1D	3.72	106.58	100.98
2	A	380	SO4	O4-S-O3	3.33	123.28	109.06
4	A	360	NAP	O2B-C2B-C1B	2.82	120.25	110.10
4	A	360	NAP	O5D-C5D-C4D	2.74	118.42	108.99
4	A	360	NAP	C3N-C7N-N7N	-2.65	114.57	117.75
4	A	360	NAP	O2B-P2B-O1X	2.61	119.48	109.39
4	A	360	NAP	C4A-C5A-N7A	-2.44	106.86	109.40
4	A	360	NAP	C5A-C6A-N6A	2.35	123.93	120.35
4	A	360	NAP	O4B-C4B-C5B	2.30	116.95	109.37
4	A	360	NAP	C2B-C3B-C4B	2.29	106.97	101.99
4	A	360	NAP	O3D-C3D-C2D	2.26	119.14	111.82
4	A	360	NAP	C3N-C2N-N1N	-2.09	118.39	120.43
4	A	360	NAP	O2D-C2D-C1D	-2.07	103.20	110.85
2	A	380	SO4	O4-S-O1	2.03	119.88	109.31

There are no chirality outliers.

All (13) torsion outliers are listed below:

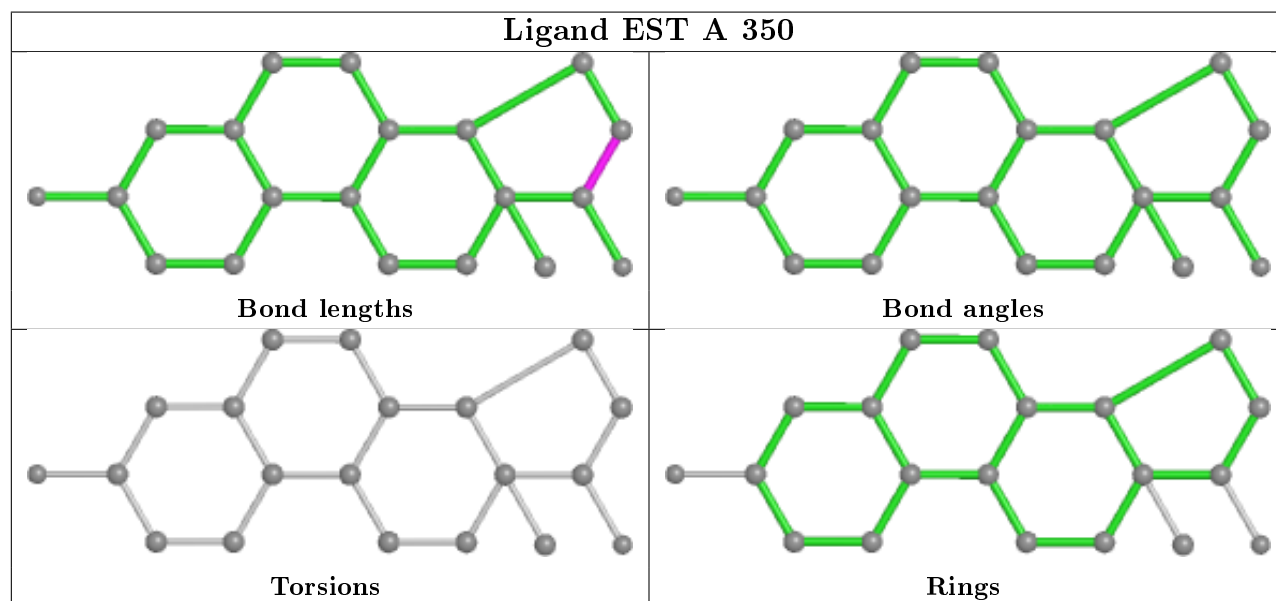
Mol	Chain	Res	Type	Atoms
4	A	360	NAP	C5B-O5B-PA-O1A
4	A	360	NAP	O4B-C4B-C5B-O5B
4	A	360	NAP	C1B-C2B-O2B-P2B
4	A	360	NAP	C5D-O5D-PN-O3
4	A	360	NAP	C5D-O5D-PN-O1N
4	A	360	NAP	C5D-O5D-PN-O2N
4	A	360	NAP	C3B-C4B-C5B-O5B
4	A	360	NAP	PN-O3-PA-O5B
4	A	360	NAP	C5B-O5B-PA-O3
4	A	360	NAP	C4B-C5B-O5B-PA
4	A	360	NAP	C5B-O5B-PA-O2A
4	A	360	NAP	C3D-C4D-C5D-O5D
4	A	360	NAP	O4D-C4D-C5D-O5D

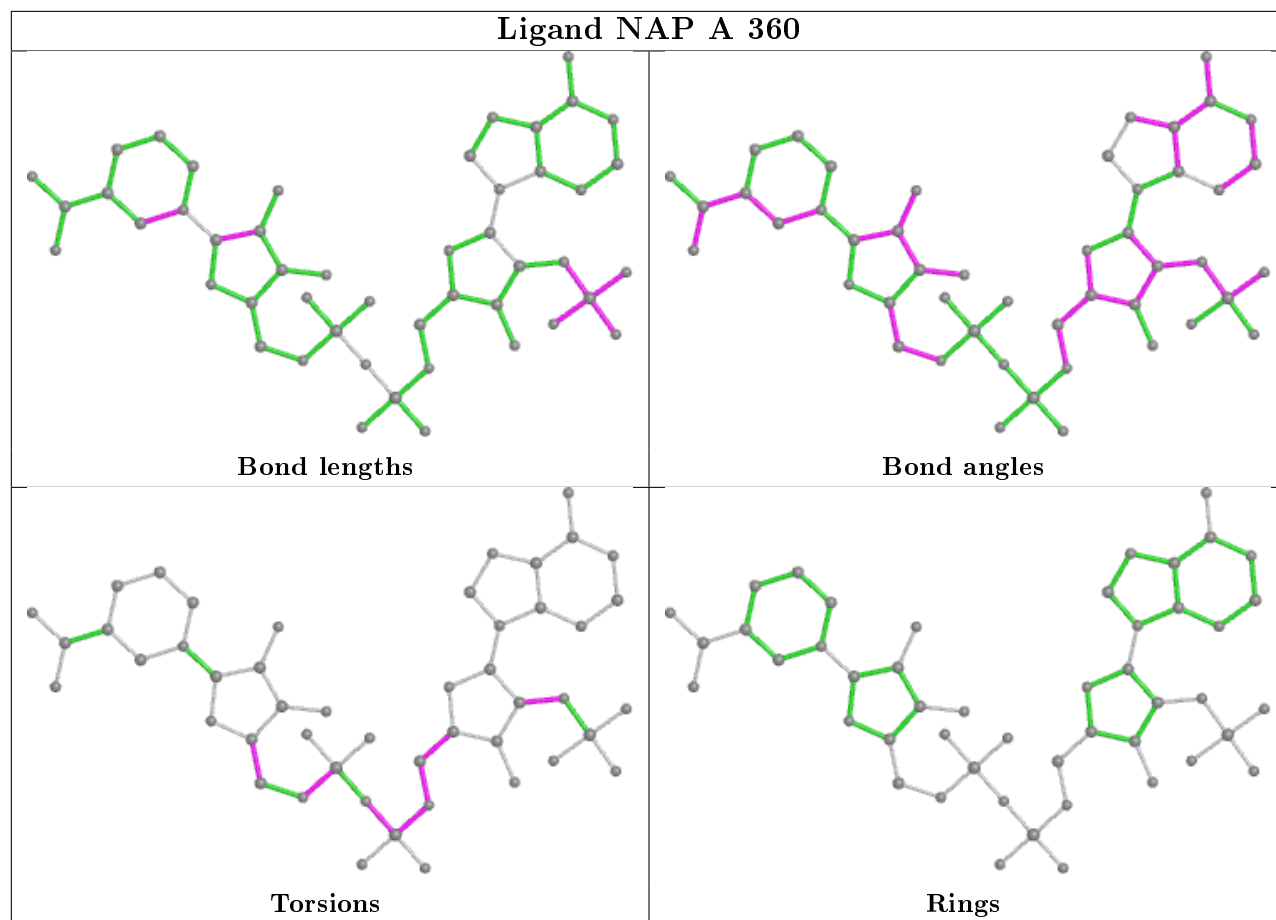
There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	350	EST	2	0
2	A	380	SO4	1	0
4	A	360	NAP	14	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.





4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

5.4 Ligands

EDS was not executed - this section is therefore empty.

5.5 Other polymers

EDS was not executed - this section is therefore empty.