



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2021 – 03:08 PM BST

PDB ID : 7NDW
Title : ThyX-FADH2 soaked with 20 mM Formaldehyde
Authors : Bou-Nader, C.; Pecqueur, L.; Hamdane, D.
Deposited on : 2021-02-02
Resolution : 2.00 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) : 2.23.1

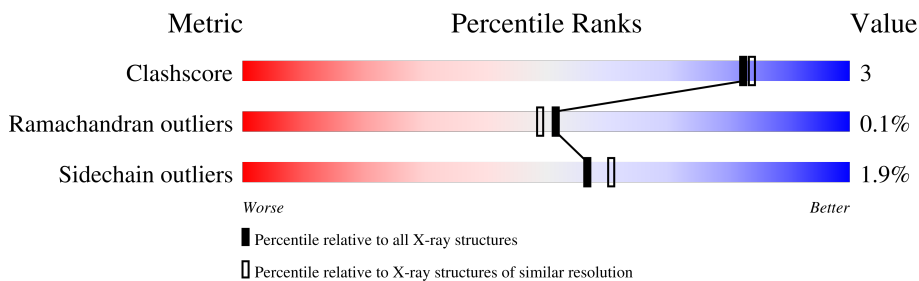
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	232	
1	B	232	
1	C	232	
1	D	232	

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7404 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 Flavin-dependent thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	Total 1717	C 1124	N 287	O 301	S 5	0	4	0
1	B	211	Total 1723	C 1125	N 290	O 303	S 5	0	2	0
1	C	216	Total 1745	C 1139	N 296	O 304	S 6	0	2	0
1	D	218	Total 1775	C 1159	N 302	O 309	S 5	0	1	0

There are 48 discrepancies between the modelled and reference sequences:

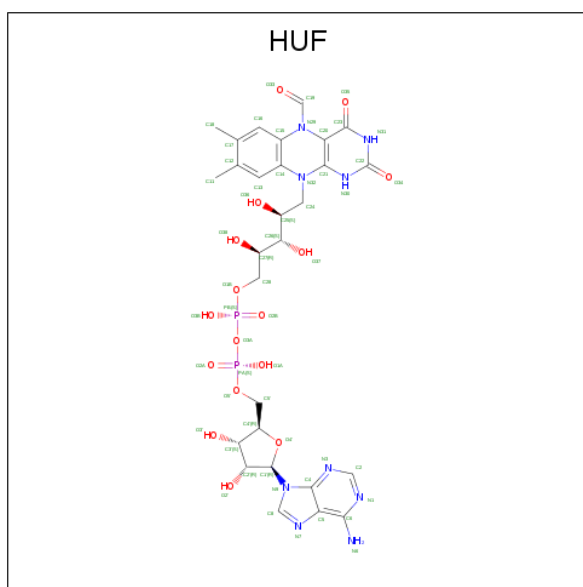
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9WYT0
A	-10	GLY	-	expression tag	UNP Q9WYT0
A	-9	SER	-	expression tag	UNP Q9WYT0
A	-8	ASP	-	expression tag	UNP Q9WYT0
A	-7	LYS	-	expression tag	UNP Q9WYT0
A	-6	ILE	-	expression tag	UNP Q9WYT0
A	-5	HIS	-	expression tag	UNP Q9WYT0
A	-4	HIS	-	expression tag	UNP Q9WYT0
A	-3	HIS	-	expression tag	UNP Q9WYT0
A	-2	HIS	-	expression tag	UNP Q9WYT0
A	-1	HIS	-	expression tag	UNP Q9WYT0
A	0	HIS	-	expression tag	UNP Q9WYT0
B	-11	MET	-	initiating methionine	UNP Q9WYT0
B	-10	GLY	-	expression tag	UNP Q9WYT0
B	-9	SER	-	expression tag	UNP Q9WYT0
B	-8	ASP	-	expression tag	UNP Q9WYT0
B	-7	LYS	-	expression tag	UNP Q9WYT0
B	-6	ILE	-	expression tag	UNP Q9WYT0
B	-5	HIS	-	expression tag	UNP Q9WYT0
B	-4	HIS	-	expression tag	UNP Q9WYT0
B	-3	HIS	-	expression tag	UNP Q9WYT0

Continued on next page...

Continued from previous page...

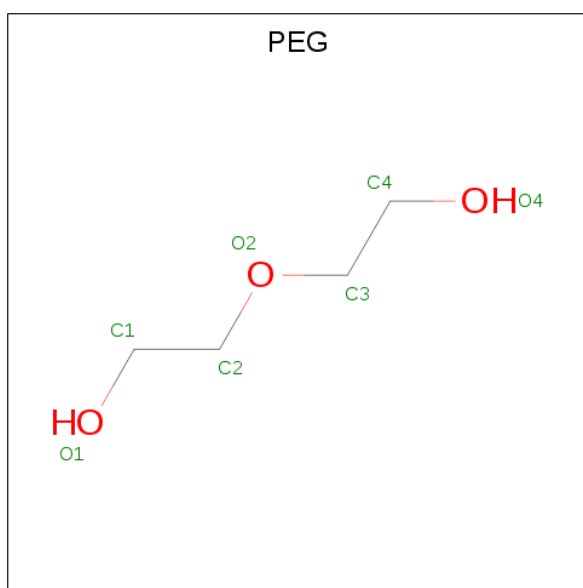
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q9WYT0
B	-1	HIS	-	expression tag	UNP Q9WYT0
B	0	HIS	-	expression tag	UNP Q9WYT0
C	-11	MET	-	initiating methionine	UNP Q9WYT0
C	-10	GLY	-	expression tag	UNP Q9WYT0
C	-9	SER	-	expression tag	UNP Q9WYT0
C	-8	ASP	-	expression tag	UNP Q9WYT0
C	-7	LYS	-	expression tag	UNP Q9WYT0
C	-6	ILE	-	expression tag	UNP Q9WYT0
C	-5	HIS	-	expression tag	UNP Q9WYT0
C	-4	HIS	-	expression tag	UNP Q9WYT0
C	-3	HIS	-	expression tag	UNP Q9WYT0
C	-2	HIS	-	expression tag	UNP Q9WYT0
C	-1	HIS	-	expression tag	UNP Q9WYT0
C	0	HIS	-	expression tag	UNP Q9WYT0
D	-11	MET	-	initiating methionine	UNP Q9WYT0
D	-10	GLY	-	expression tag	UNP Q9WYT0
D	-9	SER	-	expression tag	UNP Q9WYT0
D	-8	ASP	-	expression tag	UNP Q9WYT0
D	-7	LYS	-	expression tag	UNP Q9WYT0
D	-6	ILE	-	expression tag	UNP Q9WYT0
D	-5	HIS	-	expression tag	UNP Q9WYT0
D	-4	HIS	-	expression tag	UNP Q9WYT0
D	-3	HIS	-	expression tag	UNP Q9WYT0
D	-2	HIS	-	expression tag	UNP Q9WYT0
D	-1	HIS	-	expression tag	UNP Q9WYT0
D	0	HIS	-	expression tag	UNP Q9WYT0

- Molecule 2 is [[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2R,3S,4S)-5-[5-methanoyl-7,8-dimethyl-2,4-bis(oxidanylidene)-1H-benzog]pteridin-10-yl]-2,3,4-tris(oxidanyl)pentyl] hydrogen phosphate (three-letter code: HUF) (formula: C₂₈H₃₅N₉O₁₆P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	55	28	9	16	2	0	0
2	B	1	55	28	9	16	2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



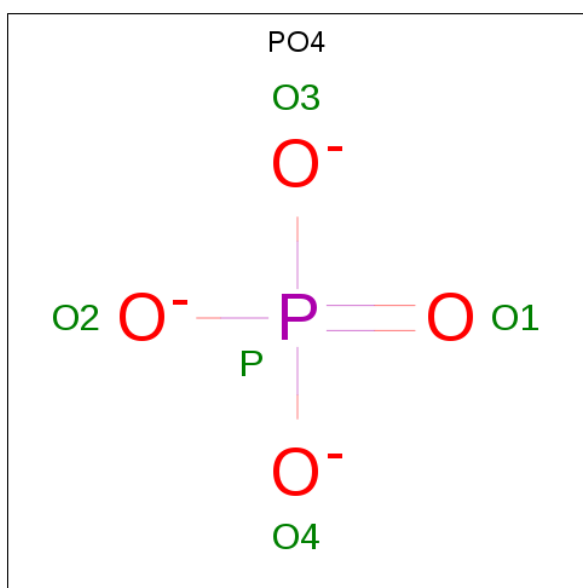
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	7	4	3	0	0
3	B	1	7	4	3	0	0

Continued on next page...

Continued from previous page...

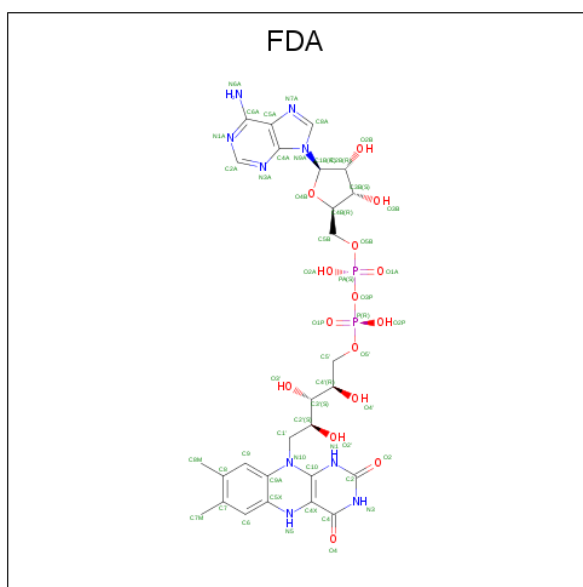
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



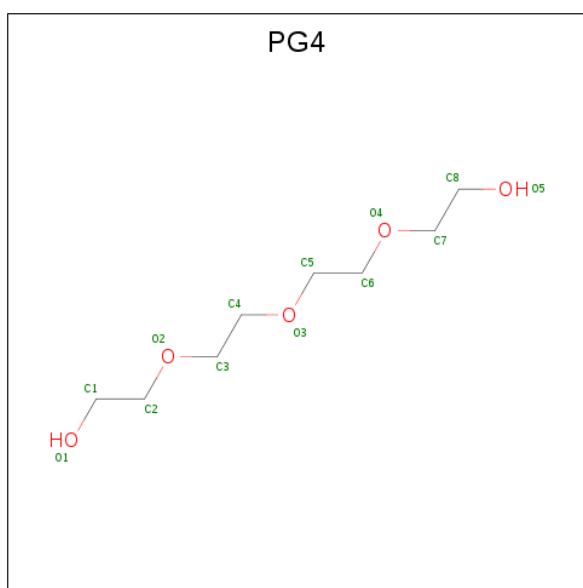
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	31	Total 31	O 31	0	0
7	B	32	Total 32	O 32	0	0
7	C	46	Total 46	O 46	0	0
7	D	42	Total 42	O 42	0	0

4 Data and refinement statistics

Xtrriage (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	54.96Å 116.78Å 141.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.98 - 2.00	Depositor
% Data completeness (in resolution range)	98.4 (44.98-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.270 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7404	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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: FDA, PG4, PEG, HUF, PO4

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	0.52	0/1762	0.65	0/2393
1	B	0.54	0/1770	0.66	0/2399
1	C	0.52	0/1794	0.63	0/2436
1	D	0.52	0/1825	0.65	0/2480
All	All	0.53	0/7151	0.65	0/9708

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	1717	0	1653	13	0
1	B	1723	0	1682	12	0
1	C	1745	0	1683	8	0
1	D	1775	0	1717	12	0
2	A	55	0	0	0	0
2	B	55	0	0	0	0
3	A	7	0	10	0	0
3	B	14	0	20	1	0
3	D	28	0	40	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	1	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	C	53	0	33	1	0
5	D	53	0	33	0	0
6	C	13	0	18	0	0
7	A	31	0	0	1	0
7	B	32	0	0	1	0
7	C	46	0	0	1	0
7	D	42	0	0	1	0
All	All	7404	0	6889	36	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.

All (36) 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:125[B]:ILE:HD11	1:D:132:THR:HG21	1.30	1.05
1:A:17:MET:HB2	1:B:17:MET:HB2	1.50	0.92
1:C:17:MET:HB2	1:D:17:MET:HB2	1.57	0.85
1:A:133:TYR:CE1	1:A:147:ARG:HG2	2.18	0.77
1:C:173:LEU:HD13	5:C:301:FDA:H5'1	1.78	0.66
1:A:125[B]:ILE:CD1	1:D:132:THR:HG21	2.18	0.63
1:C:137:ILE:HD11	1:C:143:ARG:HA	1.82	0.61
1:D:19:ASN:HB2	7:D:424:HOH:O	2.00	0.61
1:B:68:ALA:HB1	1:B:72[B]:VAL:HG12	1.84	0.59
1:D:53:HIS:HA	3:D:303:PEG:H32	1.85	0.58
1:A:125[A]:ILE:HG21	1:D:149:VAL:HB	1.85	0.58
1:B:137:ILE:HD11	1:B:143:ARG:HA	1.86	0.56
1:D:103:PRO:HB3	1:D:115:PRO:HB2	1.88	0.55
1:D:169:ASN:HB2	3:D:305:PEG:H22	1.87	0.55
1:B:68:ALA:HB1	1:B:72[B]:VAL:CG1	2.36	0.54
1:A:89:GLY:HA3	3:D:304:PEG:H21	1.90	0.54
1:A:133:TYR:HE1	1:A:147:ARG:HG2	1.71	0.54
1:A:137:ILE:HD11	1:A:143:ARG:HA	1.90	0.54
1:A:121:LYS:O	1:A:125[B]:ILE:HD12	2.09	0.53
1:B:19:ASN:HB2	7:B:407:HOH:O	2.11	0.50
1:B:102:SER:H	3:B:303:PEG:H32	1.77	0.50
1:B:118:VAL:HG13	1:C:136:LEU:HD22	1.94	0.50
1:A:143:ARG:O	1:A:147:ARG:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:PRO:HB3	1:C:115:PRO:HB2	1.97	0.47
1:C:19:ASN:HB2	7:C:406:HOH:O	2.14	0.46
1:A:136:LEU:HD22	1:D:118:VAL:HG13	1.96	0.45
1:D:122:ILE:O	1:D:126:VAL:HG13	2.17	0.45
1:B:149:VAL:HB	1:C:125:ILE:HG21	1.99	0.43
1:D:145:VAL:O	1:D:148:ILE:HG12	2.20	0.42
1:B:90:ARG:HG3	4:B:302:PO4:O4	2.20	0.41
1:D:-1:HIS:HD2	1:D:197:LYS:NZ	2.18	0.41
1:B:125:ILE:HG21	1:C:149:VAL:HB	2.02	0.41
1:B:122:ILE:O	1:B:126:VAL:HG13	2.21	0.40
1:A:19:ASN:HB2	7:A:407:HOH:O	2.21	0.40
1:A:147:ARG:HB3	3:D:304:PEG:H22	2.02	0.40
1:B:5:ILE:HD11	1:B:189:ALA:HB2	2.03	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	208/232 (90%)	202 (97%)	5 (2%)	1 (0%)	29	23
1	B	207/232 (89%)	200 (97%)	7 (3%)	0	100	100
1	C	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
1	D	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
All	All	846/928 (91%)	824 (97%)	21 (2%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	VAL

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	173/207 (84%)	170 (98%)	3 (2%)	60	65
1	B	176/207 (85%)	173 (98%)	3 (2%)	60	65
1	C	175/207 (84%)	171 (98%)	4 (2%)	50	53
1	D	180/207 (87%)	175 (97%)	5 (3%)	43	44
All	All	704/828 (85%)	689 (98%)	15 (2%)	57	57

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	38	GLU
1	A	53	HIS
1	B	38[A]	GLU
1	B	38[B]	GLU
1	B	147	ARG
1	C	42	ARG
1	C	87	LEU
1	C	147[A]	ARG
1	C	147[B]	ARG
1	D	2	LYS
1	D	37	ASP
1	D	87	LEU
1	D	95	SER
1	D	147	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	B	53	HIS
1	D	-1	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](#)

15 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	PEG	B	303	-	6,6,6	0.23	0	5,5,5	0.22	0
2	HUF	A	301	-	51,60,60	1.66	7 (13%)	58,92,92	3.02	8 (13%)
5	FDA	C	301	-	51,58,58	2.15	9 (17%)	60,89,89	2.47	13 (21%)
5	FDA	D	301	-	51,58,58	2.11	7 (13%)	60,89,89	2.18	10 (16%)
4	PO4	C	302	-	4,4,4	2.47	1 (25%)	6,6,6	0.86	0
2	HUF	B	301	-	51,60,60	1.71	7 (13%)	58,92,92	3.15	7 (12%)
3	PEG	A	302	-	6,6,6	0.12	0	5,5,5	0.07	0
6	PG4	C	303	-	12,12,12	0.22	0	11,11,11	0.23	0
4	PO4	D	302	-	4,4,4	2.35	1 (25%)	6,6,6	0.52	0
3	PEG	B	304	-	6,6,6	0.12	0	5,5,5	0.11	0
3	PEG	D	304	-	6,6,6	0.25	0	5,5,5	0.17	0
4	PO4	B	302	-	4,4,4	2.44	1 (25%)	6,6,6	0.40	0
3	PEG	D	305	-	6,6,6	0.19	0	5,5,5	0.08	0
3	PEG	D	306	-	6,6,6	0.12	0	5,5,5	0.09	0
3	PEG	D	303	-	6,6,6	0.33	0	5,5,5	0.23	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
3	PEG	B	303	-	-	2/4/4/4	-
2	HUF	A	301	-	-	2/30/52/52	0/6/6/6
5	FDA	C	301	-	-	8/30/50/50	0/6/6/6
5	FDA	D	301	-	-	8/30/50/50	0/6/6/6
2	HUF	B	301	-	-	3/30/52/52	0/6/6/6
3	PEG	A	302	-	-	2/4/4/4	-
6	PG4	C	303	-	-	3/10/10/10	-
3	PEG	B	304	-	-	3/4/4/4	-
3	PEG	D	304	-	-	2/4/4/4	-
3	PEG	D	305	-	-	1/4/4/4	-
3	PEG	D	306	-	-	3/4/4/4	-
3	PEG	D	303	-	-	1/4/4/4	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	301	FDA	C4X-C10	10.62	1.49	1.38
5	C	301	FDA	C4X-C10	10.34	1.49	1.38
2	A	301	HUF	C20-N29	5.87	1.48	1.38
2	B	301	HUF	C20-N29	5.50	1.47	1.38
2	A	301	HUF	C15-N29	5.35	1.47	1.38
2	B	301	HUF	C15-N29	5.33	1.47	1.38
5	C	301	FDA	C4-C4X	5.19	1.50	1.41
2	B	301	HUF	C23-C20	4.82	1.49	1.41
5	D	301	FDA	C4-C4X	4.80	1.49	1.41
5	C	301	FDA	C9A-C5X	4.42	1.51	1.42
5	D	301	FDA	C9A-N10	4.23	1.44	1.38
2	B	301	HUF	C14-N32	4.18	1.44	1.38
5	C	301	FDA	C8-C7	4.15	1.51	1.40
4	B	302	PO4	P-O1	4.11	1.60	1.50
4	C	302	PO4	P-O1	4.11	1.60	1.50
5	D	301	FDA	C9A-C5X	3.93	1.50	1.42
5	C	301	FDA	C9A-N10	3.92	1.43	1.38
4	D	302	PO4	P-O1	3.85	1.59	1.50
5	D	301	FDA	C8-C7	3.82	1.50	1.40
2	A	301	HUF	C21-N30	3.78	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	HUF	C14-N32	3.69	1.43	1.38
2	A	301	HUF	C23-N31	3.65	1.39	1.33
2	A	301	HUF	C23-C20	3.57	1.47	1.41
2	B	301	HUF	C23-N31	3.51	1.39	1.33
2	B	301	HUF	C21-N30	3.48	1.37	1.33
5	D	301	FDA	C5A-C4A	2.93	1.48	1.40
5	C	301	FDA	C5A-C4A	2.78	1.48	1.40
2	A	301	HUF	O33-C19	2.66	1.42	1.23
5	D	301	FDA	C2-N1	-2.57	1.33	1.38
2	B	301	HUF	O33-C19	2.51	1.41	1.23
5	C	301	FDA	C2-N1	-2.13	1.33	1.38
5	C	301	FDA	C4X-N5	2.05	1.36	1.33
5	C	301	FDA	O4B-C1B	2.03	1.43	1.41

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	HUF	O33-C19-N29	-16.27	106.44	124.60
2	A	301	HUF	O33-C19-N29	-14.37	108.56	124.60
2	A	301	HUF	C23-N31-C22	13.71	126.72	115.14
2	B	301	HUF	C23-N31-C22	13.65	126.67	115.14
5	D	301	FDA	C4-N3-C2	8.60	122.40	115.14
5	C	301	FDA	C4-C4X-C10	-7.91	114.72	119.95
5	C	301	FDA	C4-N3-C2	7.81	121.74	115.14
5	C	301	FDA	C1'-N10-C9A	7.47	124.17	118.29
2	B	301	HUF	C20-C23-N31	-7.45	113.24	123.43
2	A	301	HUF	C20-C23-N31	-7.26	113.50	123.43
5	C	301	FDA	C4X-N5-C5X	5.97	122.74	116.77
5	D	301	FDA	C4-C4X-C10	-5.75	116.14	119.95
5	C	301	FDA	C4-C4X-N5	5.42	124.80	118.60
5	D	301	FDA	C1'-N10-C9A	5.38	122.52	118.29
5	D	301	FDA	C4X-N5-C5X	4.87	121.64	116.77
5	C	301	FDA	N3A-C2A-N1A	-4.66	121.39	128.68
2	A	301	HUF	C24-N32-C14	4.22	121.61	118.29
5	D	301	FDA	C4-C4X-N5	4.12	123.30	118.60
2	A	301	HUF	C20-N29-C15	-4.06	113.10	122.12
5	D	301	FDA	N3A-C2A-N1A	-4.03	122.37	128.68
5	D	301	FDA	C4X-C4-N3	-3.97	118.00	123.43
2	B	301	HUF	C20-N29-C15	-3.94	113.36	122.12
5	C	301	FDA	O4'-C4'-C3'	3.69	118.07	109.10
5	C	301	FDA	O4'-C4'-C5'	-3.40	102.28	109.92
2	B	301	HUF	C24-N32-C14	3.31	120.90	118.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	HUF	C16-C15-N29	-3.30	117.85	121.68
5	D	301	FDA	C9A-N10-C10	-3.28	117.61	121.91
2	A	301	HUF	C16-C15-N29	-3.28	117.88	121.68
5	C	301	FDA	C4X-C4-N3	-3.07	119.24	123.43
5	C	301	FDA	C2A-N1A-C6A	2.94	123.79	118.75
5	D	301	FDA	O2'-C2'-C3'	2.78	115.85	109.10
5	C	301	FDA	C1'-N10-C10	-2.76	115.94	118.41
5	D	301	FDA	C2A-N1A-C6A	2.69	123.36	118.75
2	A	301	HUF	O5'-PA-O2A	2.40	118.43	109.07
5	C	301	FDA	O5'-C5'-C4'	-2.28	103.27	109.36
2	B	301	HUF	C5-C6-N6	2.17	123.65	120.35
2	A	301	HUF	C5-C6-N6	2.16	123.63	120.35
5	C	301	FDA	C5'-C4'-C3'	-2.14	108.07	112.20

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	FDA	C2'-C3'-C4'-O4'
5	C	301	FDA	C2'-C3'-C4'-C5'
5	C	301	FDA	O3'-C3'-C4'-O4'
5	C	301	FDA	O3'-C3'-C4'-C5'
5	C	301	FDA	C3'-C4'-C5'-O5'
5	C	301	FDA	O4'-C4'-C5'-O5'
5	C	301	FDA	C5'-O5'-P-O3P
5	D	301	FDA	C2'-C1'-N10-C9A
5	D	301	FDA	C1'-C2'-C3'-O3'
5	D	301	FDA	C1'-C2'-C3'-C4'
5	D	301	FDA	O2'-C2'-C3'-O3'
5	D	301	FDA	O2'-C2'-C3'-C4'
5	D	301	FDA	C3'-C4'-C5'-O5'
5	D	301	FDA	O4'-C4'-C5'-O5'
3	D	306	PEG	O2-C3-C4-O4
3	B	303	PEG	O2-C3-C4-O4
3	D	306	PEG	O1-C1-C2-O2
3	B	304	PEG	O2-C3-C4-O4
3	D	304	PEG	C4-C3-O2-C2
3	A	302	PEG	C1-C2-O2-C3
3	A	302	PEG	C4-C3-O2-C2
6	C	303	PG4	C8-C7-O4-C6
2	A	301	HUF	PA-O3A-PB-O3B
6	C	303	PG4	C1-C2-O2-C3

Continued on next page...

Continued from previous page...

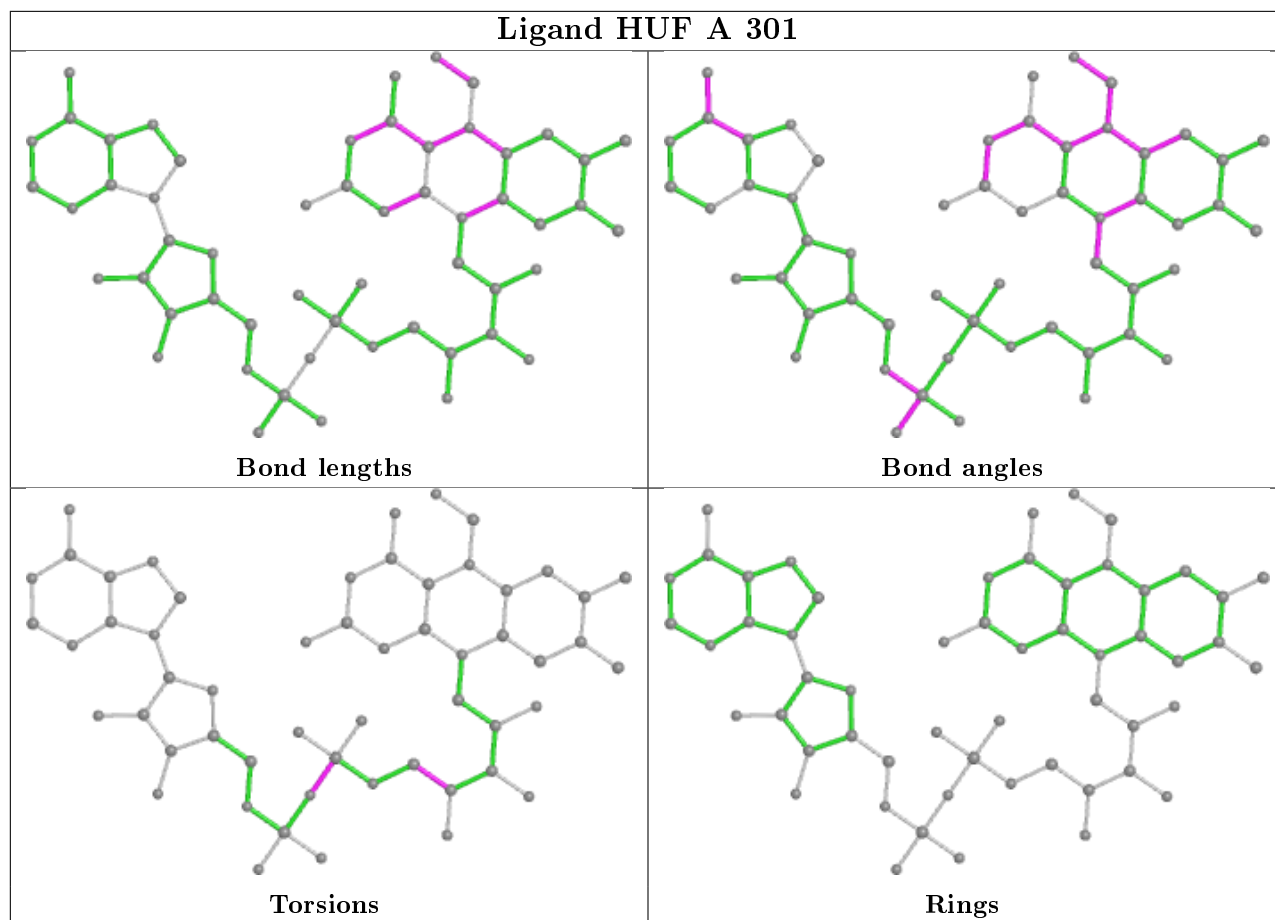
Mol	Chain	Res	Type	Atoms
3	B	303	PEG	C4-C3-O2-C2
5	C	301	FDA	C5'-O5'-P-O1P
3	B	304	PEG	C1-C2-O2-C3
3	D	304	PEG	C1-C2-O2-C3
3	D	303	PEG	C1-C2-O2-C3
3	D	306	PEG	C4-C3-O2-C2
2	B	301	HUF	PA-O3A-PB-O3B
3	D	305	PEG	O2-C3-C4-O4
3	B	304	PEG	C4-C3-O2-C2
2	A	301	HUF	O38-C27-C28-O1B
2	B	301	HUF	PA-O3A-PB-O2B
5	D	301	FDA	PA-O3P-P-O1P
2	B	301	HUF	O38-C27-C28-O1B
6	C	303	PG4	C4-C3-O2-C2

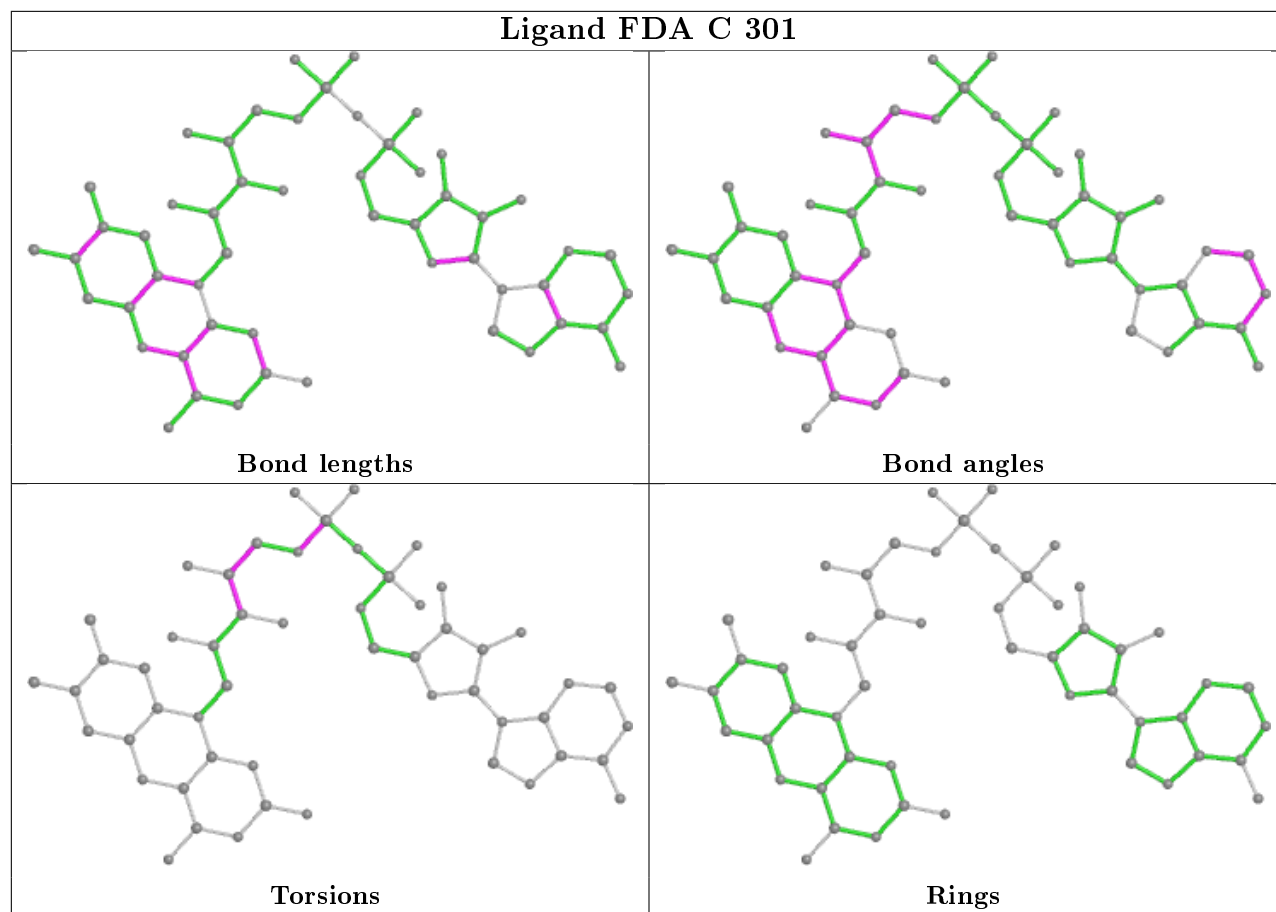
There are no ring outliers.

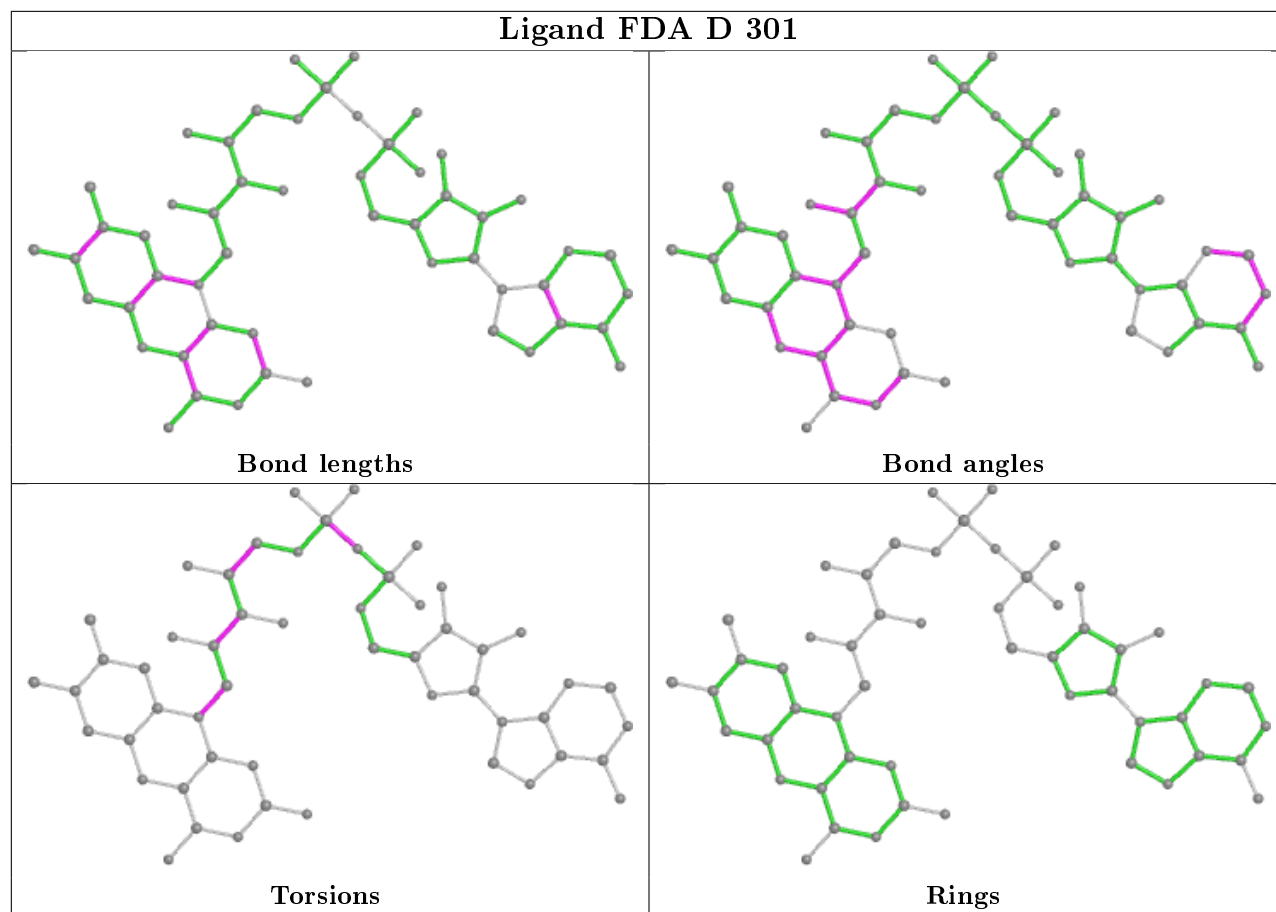
6 monomers are involved in 7 short contacts:

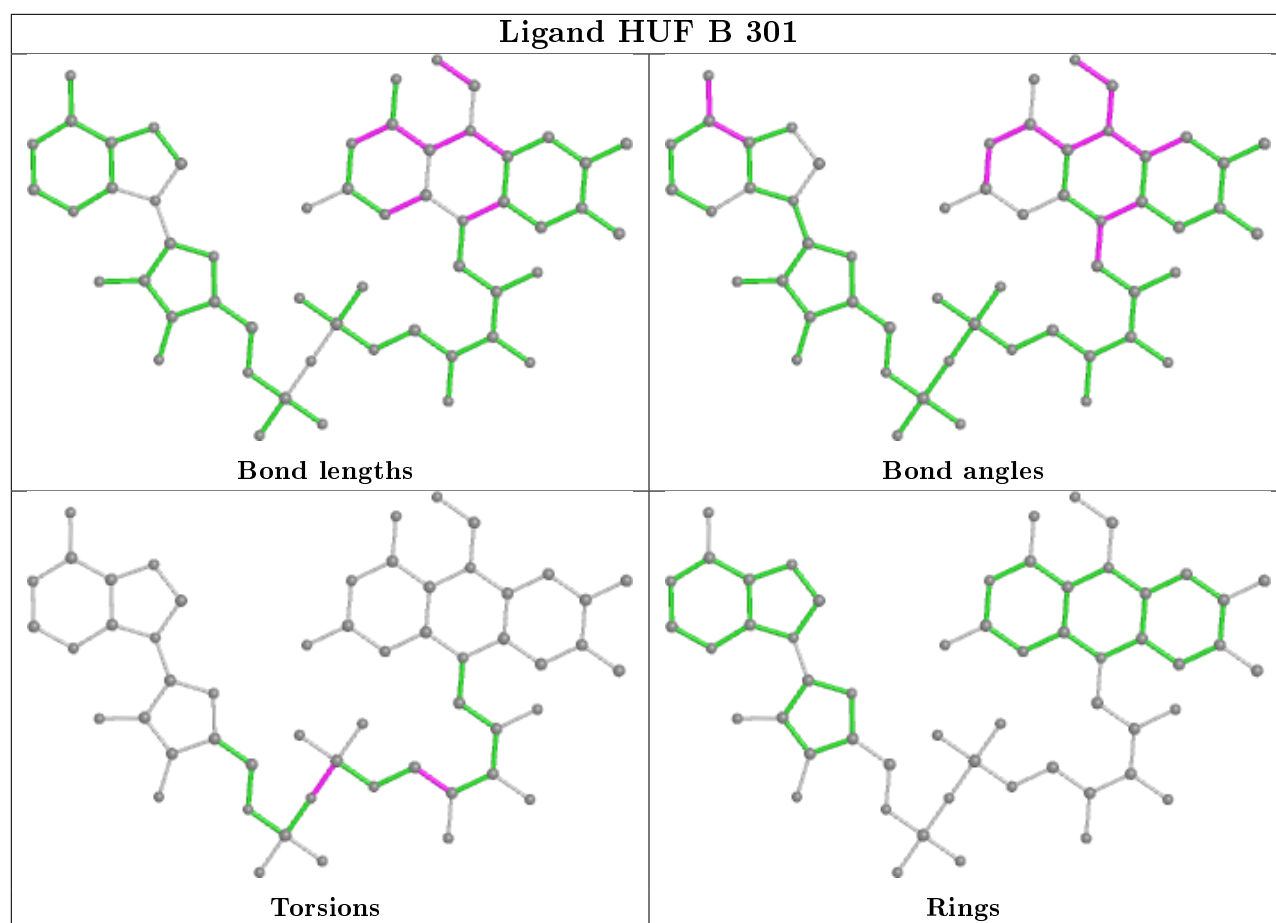
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	PEG	1	0
5	C	301	FDA	1	0
3	D	304	PEG	2	0
4	B	302	PO4	1	0
3	D	305	PEG	1	0
3	D	303	PEG	1	0

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

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.