



Full wwPDB X-ray Structure Validation Report

Dec 9, 2023 – 09:49 am GMT

PDB ID : 2BXV
Title : Dual binding mode of a novel series of DHODH inhibitors
Authors : Baumgartner, R.; Walloschek, M.; Karlik, M.; Gotschlich, A.; Tasler, S.; Mies, J.; Leban, J.
Deposited on : 2005-07-27
Resolution : 2.15 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, 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) : 2.36

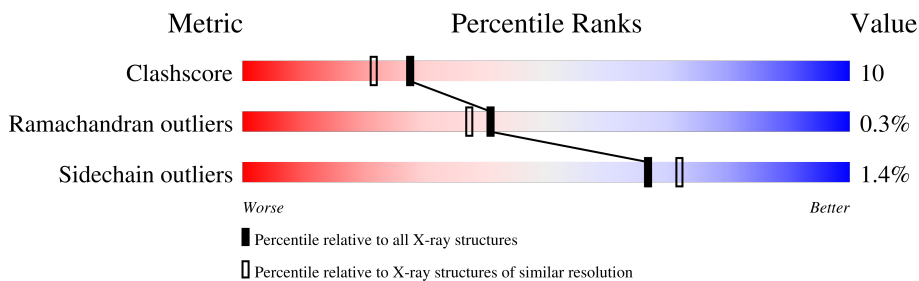
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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	367	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3028 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 DIHYDROOROTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	360	2755	1729	507	514	5	0	2	0

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



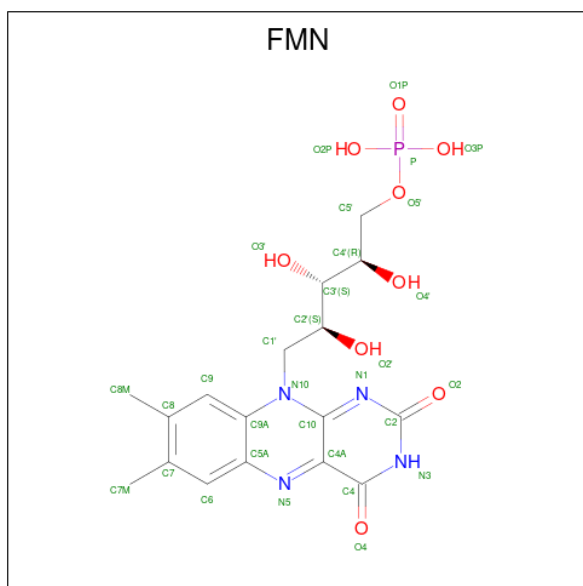
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



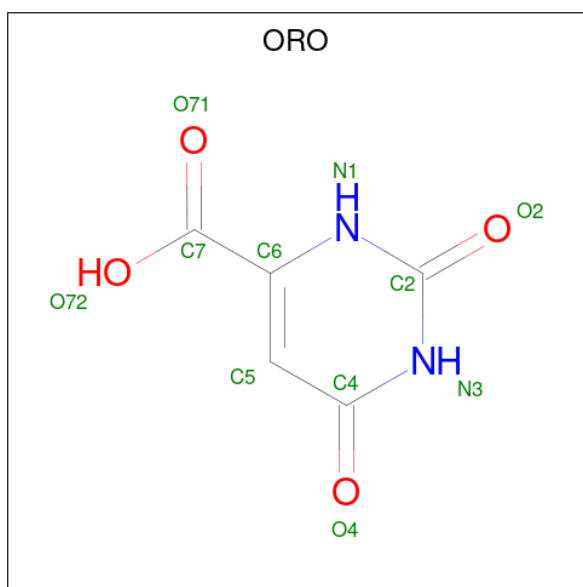
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



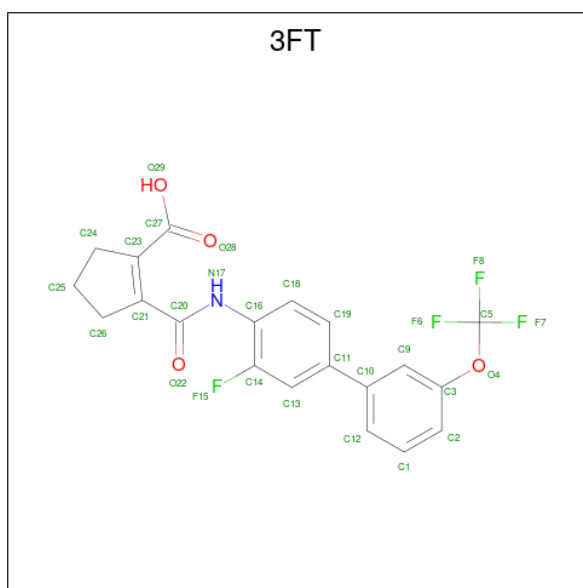
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 5 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	11	5	2	4	0	0

- Molecule 6 is 2-([3-FLUORO-3'-(TRIFLUOROMETHOXY)BIPHENYL-4-YL]AMINO)CARBONYL)CYCLOPENT-1-ENE-1-CARBOXYLIC ACID (three-letter code: 3FT) (formula: C₂₀H₁₅F₄NO₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
6	A	1	29	20	4	1	4	0	0

- Molecule 7 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	193	Total 193	O 193	0	0

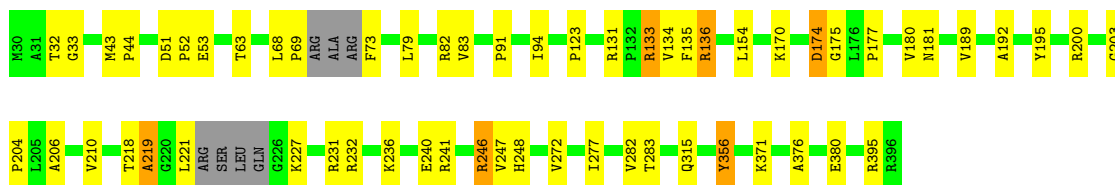
3 Residue-property plots [i](#)

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: DIHYDROOROTATE DEHYDROGENASE

Chain A:  82% 14% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.65Å 90.65Å 123.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 2.15	Depositor
% Data completeness (in resolution range)	99.2 (19.94-2.15)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3028	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: ORO, FMN, ACT, SO4, 3FT

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	0.27	0/2808	0.58	0/3791

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.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136[A]	ARG	Sidechain
1	A	136[B]	ARG	Sidechain

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	2755	0	2812	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
3	A	4	0	3	0	0
4	A	31	0	19	0	0
5	A	11	0	3	0	0
6	A	29	0	14	2	0
7	A	193	0	0	6	0
All	All	3028	0	2851	57	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 10.

All (57) 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:33:GLY:HA2	1:A:69:PRO:HB2	1.62	0.80
1:A:232:ARG:NH1	1:A:232:ARG:HB2	2.05	0.70
1:A:134:VAL:HG22	1:A:136[B]:ARG:CG	2.25	0.67
1:A:33:GLY:CA	1:A:69:PRO:HB2	2.24	0.67
1:A:134:VAL:HG22	1:A:136[B]:ARG:HG3	1.76	0.67
1:A:395:ARG:HB3	7:A:2185:HOH:O	1.96	0.66
1:A:227:LYS:HZ2	1:A:231:ARG:HH22	1.43	0.65
1:A:246:ARG:HG3	7:A:2117:HOH:O	1.97	0.63
1:A:136[B]:ARG:CG	6:A:1401:3FT:H252	2.29	0.62
1:A:232:ARG:HB2	1:A:232:ARG:HH11	1.66	0.59
1:A:227:LYS:NZ	1:A:231:ARG:HH22	2.03	0.56
1:A:43:MET:HB2	1:A:44:PRO:HD3	1.88	0.56
1:A:53:GLU:OE2	1:A:133:ARG:HD3	2.06	0.56
1:A:32:THR:HB	7:A:2006:HOH:O	2.07	0.55
1:A:272:VAL:HG13	1:A:277:ILE:HB	1.87	0.55
1:A:247:VAL:HG22	7:A:2118:HOH:O	2.07	0.54
1:A:123:PRO:HA	1:A:154:LEU:HG	1.90	0.54
1:A:136[B]:ARG:CZ	1:A:136[B]:ARG:NH2	2.71	0.54
1:A:232:ARG:HH11	1:A:232:ARG:CB	2.22	0.51
1:A:135:PHE:C	1:A:136[B]:ARG:CG	2.79	0.51
1:A:282:VAL:HG12	1:A:283:THR:HG23	1.95	0.48
1:A:180:VAL:HG23	1:A:206:ALA:HB2	1.95	0.48
1:A:200:ARG:NH1	1:A:240:GLU:OE2	2.41	0.48
1:A:218:THR:O	1:A:219:ALA:C	2.53	0.47
1:A:282:VAL:HG12	1:A:283:THR:CG2	2.44	0.47
1:A:52:PRO:HA	1:A:136[A]:ARG:HH21	1.79	0.47
1:A:134:VAL:HG22	1:A:136[B]:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136[B]:ARG:HG2	6:A:1401:3FT:H252	1.97	0.47
1:A:247:VAL:HG23	1:A:248:HIS:CD2	2.50	0.47
1:A:79:LEU:O	1:A:91:PRO:HD3	2.15	0.47
1:A:135:PHE:N	1:A:136[B]:ARG:HG3	2.30	0.46
1:A:73:PHE:CD2	1:A:371:LYS:HE3	2.51	0.46
1:A:232:ARG:HD2	7:A:2106:HOH:O	2.16	0.46
1:A:189:VAL:HG12	1:A:189:VAL:O	2.16	0.46
1:A:282:VAL:CG1	1:A:283:THR:HG22	2.46	0.46
1:A:282:VAL:HG13	1:A:283:THR:HG22	1.99	0.45
1:A:356:TYR:C	1:A:356:TYR:CD2	2.90	0.45
1:A:170:LYS:O	1:A:174:ASP:HB2	2.17	0.45
1:A:227:LYS:NZ	1:A:231:ARG:NH2	2.64	0.45
1:A:195:TYR:OH	1:A:221:LEU:HD11	2.17	0.45
1:A:315:GLN:HA	1:A:315:GLN:OE1	2.16	0.45
1:A:180:VAL:CG2	1:A:206:ALA:HB2	2.47	0.44
1:A:181:ASN:HA	1:A:210:VAL:HB	2.01	0.43
1:A:136[B]:ARG:HD3	1:A:136[B]:ARG:NH1	2.33	0.43
1:A:82:ARG:O	1:A:83:VAL:HG13	2.20	0.42
1:A:241:ARG:HD2	1:A:241:ARG:C	2.39	0.42
1:A:203:GLY:N	1:A:204:PRO:CD	2.83	0.42
1:A:136[B]:ARG:NE	7:A:2050:HOH:O	2.54	0.41
1:A:94:ILE:HG23	1:A:94:ILE:O	2.21	0.41
1:A:192:ALA:HB1	1:A:236:LYS:HD3	2.02	0.41
1:A:376:ALA:O	1:A:380:GLU:HG3	2.21	0.41
1:A:51:ASP:HB2	1:A:52:PRO:HD2	2.03	0.40
1:A:63:THR:HA	1:A:68:LEU:HD21	2.01	0.40
1:A:175:GLY:C	1:A:177:PRO:HD3	2.42	0.40
1:A:131:ARG:HG2	1:A:133:ARG:HD2	2.02	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	356/367 (97%)	340 (96%)	15 (4%)	1 (0%)	41 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	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	292/296 (99%)	288 (99%)	4 (1%)	67 72

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ARG
1	A	174	ASP
1	A	246	ARG
1	A	356	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	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](#)

5 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
5	ORO	A	1400	-	9,11,11	2.00	3 (33%)	8,15,15	3.30	4 (50%)
6	3FT	A	1401	-	30,31,31	2.06	9 (30%)	37,45,45	1.37	8 (21%)
2	SO4	A	1397	-	4,4,4	0.26	0	6,6,6	0.05	0
4	FMN	A	1399	-	33,33,33	1.32	4 (12%)	48,50,50	1.29	5 (10%)
3	ACT	A	1398	-	3,3,3	0.99	0	3,3,3	1.39	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
4	FMN	A	1399	-	-	5/18/18/18	0/3/3/3
5	ORO	A	1400	-	-	4/4/4/4	0/1/1/1
6	3FT	A	1401	-	-	3/17/31/31	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1401	3FT	C13-C14	5.06	1.43	1.35
6	A	1401	3FT	C9-C3	4.48	1.45	1.37
6	A	1401	3FT	C16-C14	3.95	1.43	1.38
4	A	1399	FMN	C6-C5A	3.84	1.46	1.40
5	A	1400	ORO	C4-N3	3.49	1.39	1.33
5	A	1400	ORO	C6-N1	3.38	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1401	3FT	C19-C18	2.98	1.42	1.36
6	A	1401	3FT	C18-C16	2.89	1.44	1.39
6	A	1401	3FT	C2-C3	2.79	1.44	1.38
6	A	1401	3FT	O4-C5	2.72	1.47	1.31
4	A	1399	FMN	C9A-C5A	2.66	1.45	1.41
4	A	1399	FMN	C8-C7	2.51	1.47	1.40
6	A	1401	3FT	C1-C12	2.37	1.42	1.36
4	A	1399	FMN	C2-N3	2.19	1.44	1.39
6	A	1401	3FT	O29-C27	2.11	1.36	1.30
5	A	1400	ORO	C6-C7	2.04	1.53	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1400	ORO	C5-C4-N3	-7.83	114.94	124.08
5	A	1400	ORO	C6-C5-C4	3.40	118.93	116.73
6	A	1401	3FT	C13-C14-C16	-3.18	120.50	123.51
4	A	1399	FMN	C10-N1-C2	2.88	122.66	116.90
6	A	1401	3FT	O22-C20-N17	-2.81	117.92	123.92
6	A	1401	3FT	C16-N17-C20	2.62	134.11	126.80
6	A	1401	3FT	F15-C14-C16	2.59	120.75	117.50
5	A	1400	ORO	O72-C7-O71	2.51	128.91	123.35
4	A	1399	FMN	P-O5'-C5'	2.48	125.13	118.30
6	A	1401	3FT	O29-C27-O28	-2.46	117.97	123.61
4	A	1399	FMN	C4-C4A-N5	2.46	121.74	118.23
4	A	1399	FMN	C9A-C9-C8	2.46	124.26	119.30
6	A	1401	3FT	O22-C20-C21	-2.44	118.04	122.03
4	A	1399	FMN	C9-C9A-N10	2.15	124.74	121.84
5	A	1400	ORO	O72-C7-C6	-2.10	109.90	114.69
6	A	1401	3FT	C14-C13-C11	2.03	120.79	119.49
6	A	1401	3FT	C24-C23-C21	-2.01	109.61	111.31

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1400	ORO	N1-C6-C7-O71
5	A	1400	ORO	N1-C6-C7-O72
5	A	1400	ORO	C5-C6-C7-O71
5	A	1400	ORO	C5-C6-C7-O72
6	A	1401	3FT	N17-C20-C21-C23
4	A	1399	FMN	O3'-C3'-C4'-C5'

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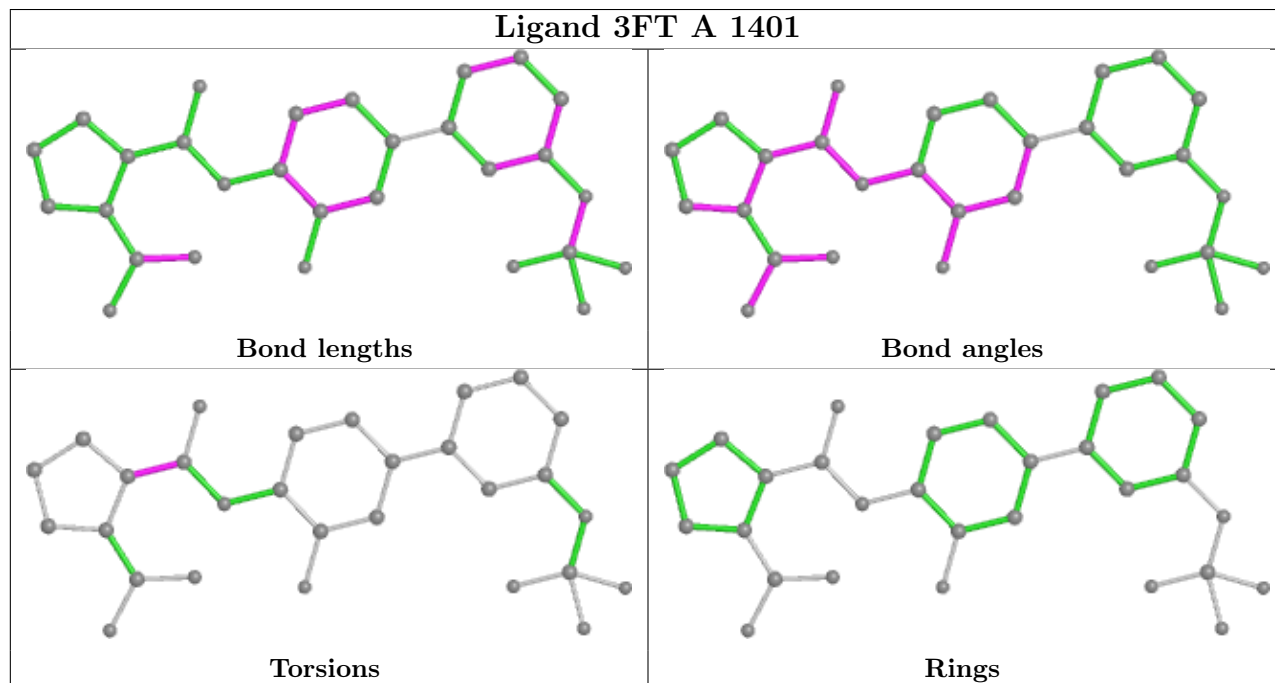
Mol	Chain	Res	Type	Atoms
4	A	1399	FMN	C2'-C3'-C4'-C5'
4	A	1399	FMN	C2'-C3'-C4'-O4'
4	A	1399	FMN	O3'-C3'-C4'-O4'
4	A	1399	FMN	C4'-C5'-O5'-P
6	A	1401	3FT	O22-C20-C21-C23
6	A	1401	3FT	O22-C20-C21-C26

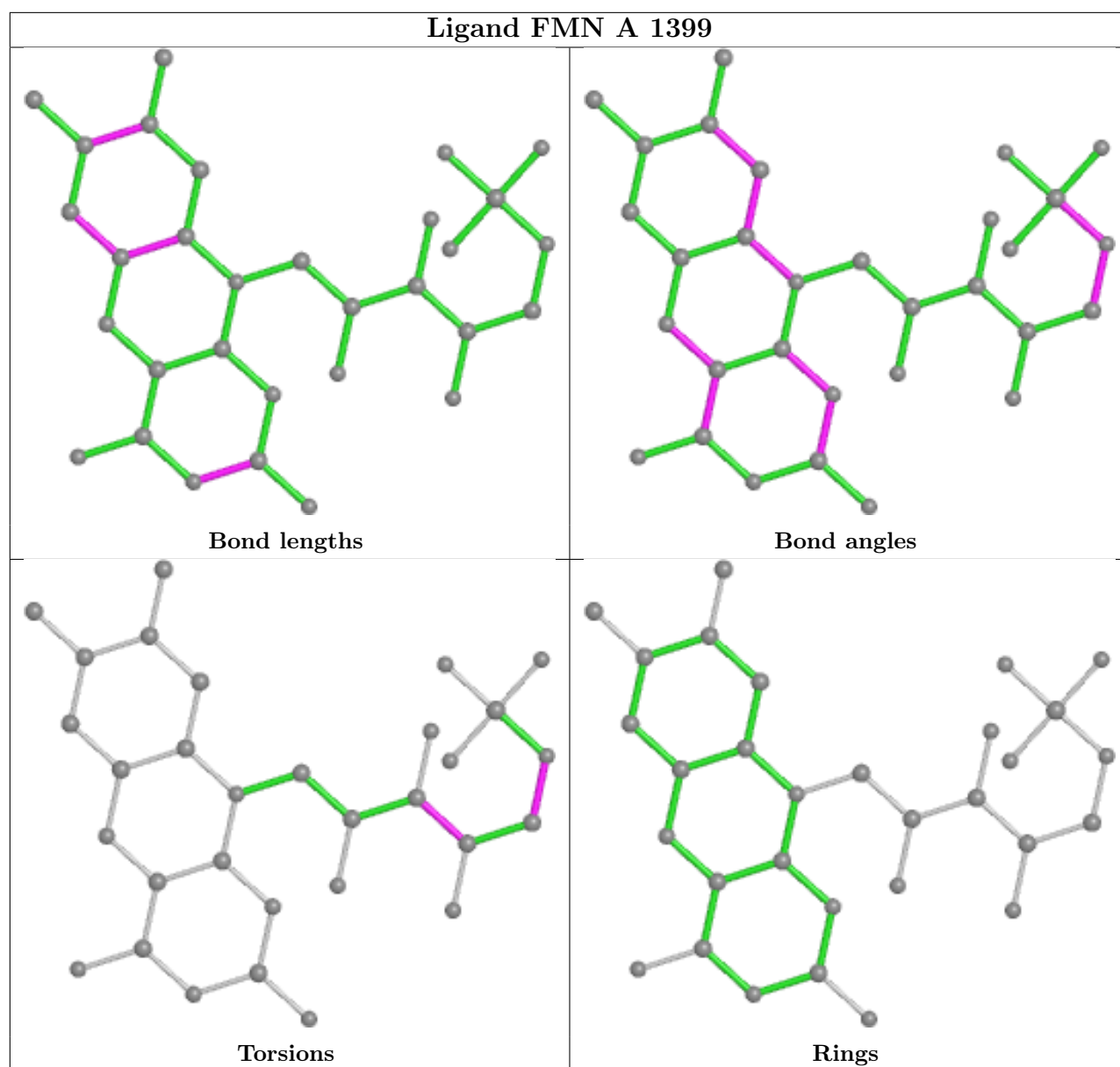
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1401	3FT	2	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.