



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:34 AM UTC

PDB ID : 1GYL / pdb_00001gyl
Title : INVOLVEMENT OF TYR24 AND TRP108 IN SUBSTRATE BINDING AND
SUBSTRATE SPECIFICITY OF GLYCOLATE OXIDASE
Authors : Lindqvist, Y.; Stenberg, K.
Deposited on : 1995-01-30
Resolution : 3.00 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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

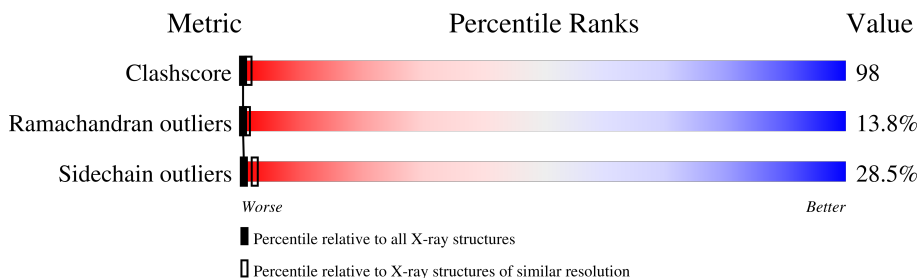
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	369	
1	B	369	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5436 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.

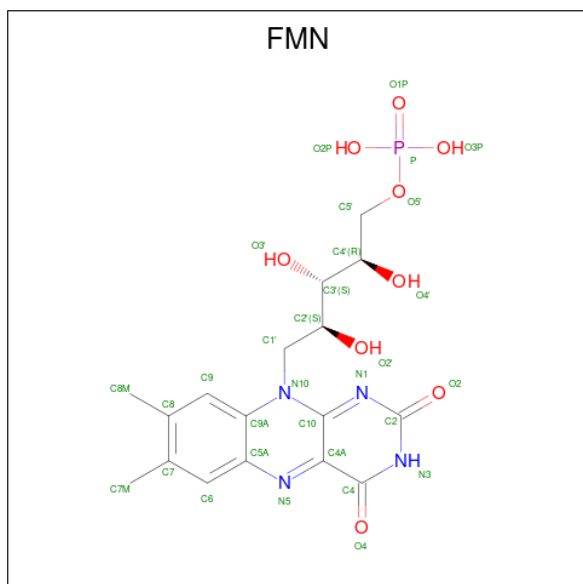
- Molecule 1 is a protein called GLYCOLATE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2708	1726	474	495	13			
1	B	350	Total	C	N	O	S	0	0	0
			2695	1718	471	493	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	PHE	TYR	conflict	UNP P05414
B	24	PHE	TYR	conflict	UNP P05414

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 3 is water.

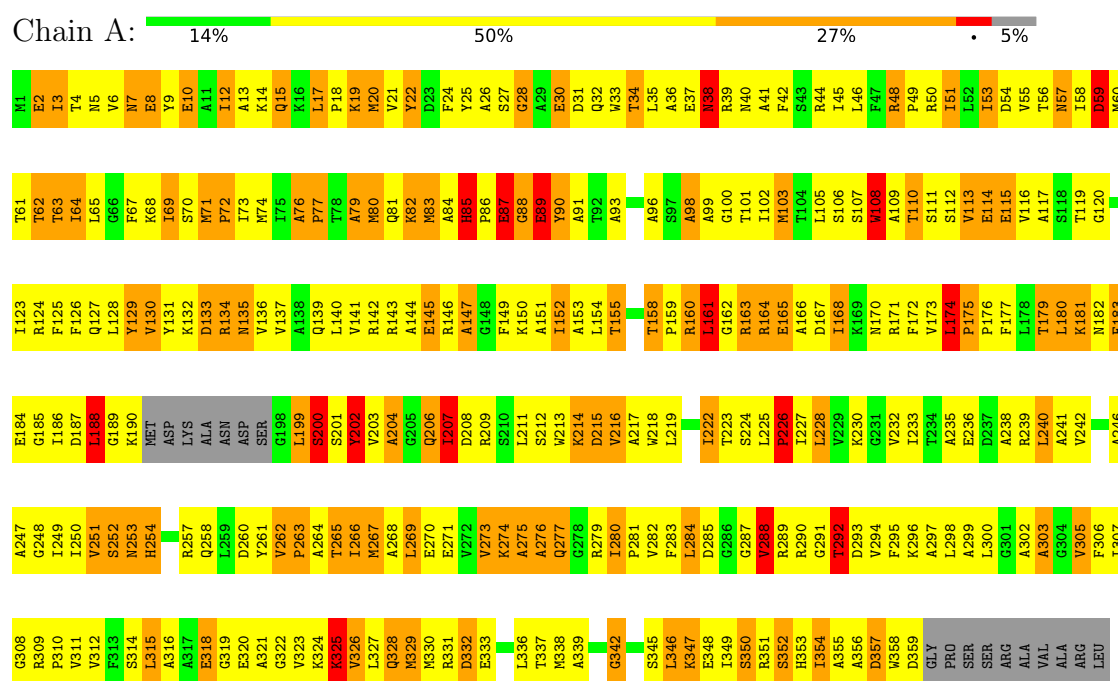
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		

3 Residue-property plots

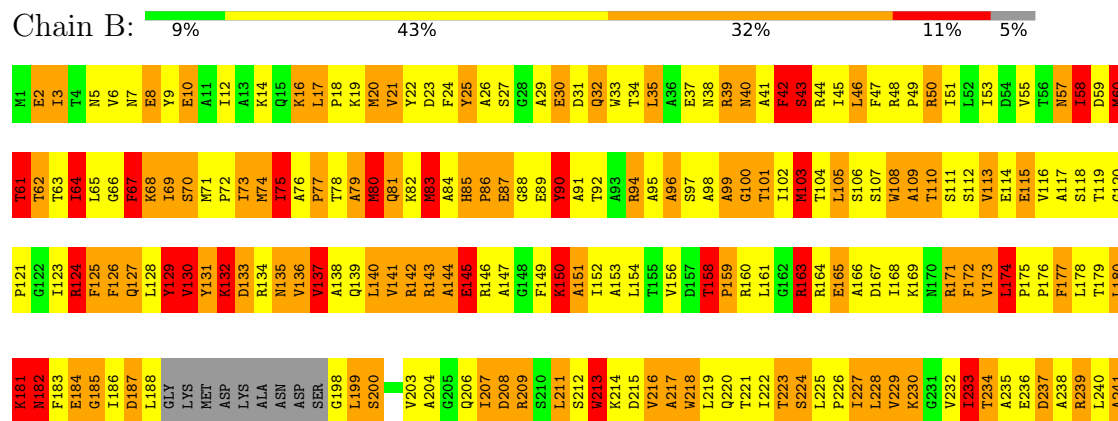
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: GLYCOLATE OXIDASE



• Molecule 1: GLYCOLATE OXIDASE



V242	A303	SER
Q243	G304	ARG
H244	V305	ALA
G245	F306	VAL
A246	I307	ALA
A247	G308	ARG
G248	R309	LEU
I249	P310	
I250	V311	
V251	F312	
S252	F313	
N253	S314	
H254	L315	
G255	A316	
A256	A317	
R257	E318	
Q258	G319	
L259	E320	
D260	A321	
Y261	G322	
V262	V323	
P263	K324	
A264	K325	
T265	V326	
I266	I327	
N267	Q328	
A268	M329	
L269	M330	
E270	R331	
E271	D332	
V272	F333	
V273	F334	
K274	E335	
A275	L336	
A276	T337	
Q277	M338	
G278	A339	
R279	L340	
I280	S341	
P281	G342	
V282	C343	
F283	R344	
L284	S345	
D285	L346	
	K347	
	E348	
V288	I349	
R289	S350	
R290	R351	
G291	S352	
T292	H353	
D293	I354	
V294	A355	
F295	A356	
K296	D357	
A297	W358	
L298	D359	
A299	GLY	
L300	PRO	
G301	SER	
A302		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	145.50Å 145.50Å 100.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.254 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5436	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: FMN

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	0.95	1/2756 (0.0%)	1.67	63/3729 (1.7%)
1	B	1.01	5/2743 (0.2%)	1.70	85/3713 (2.3%)
All	All	0.98	6/5499 (0.1%)	1.68	148/7442 (2.0%)

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	1
1	B	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	MET	SD-CE	6.43	1.95	1.79
1	B	20	MET	SD-CE	6.41	1.95	1.79
1	B	200	SER	CA-C	5.93	1.57	1.52
1	B	262	VAL	CA-CB	5.62	1.61	1.53
1	B	251	VAL	CA-CB	5.55	1.60	1.54

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ALA	N-CA-C	-14.55	93.57	112.93
1	B	60	MET	N-CA-C	-13.02	95.61	112.93
1	A	120	GLY	CA-C-N	12.55	135.53	119.84
1	A	120	GLY	C-N-CA	12.55	135.53	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	PHE	N-CA-C	-12.49	96.56	113.18

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	TYR	Sidechain
1	B	90	TYR	Sidechain

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	2708	0	2771	422	0
1	B	2695	0	2755	712	0
2	A	31	0	19	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	5436	0	5545	1072	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 98.

The worst 5 of 1072 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:B:235:ALA:HA	1:B:238:ALA:HB3	1.18	1.14
1:A:80:MET:HG2	1:A:110:THR:HG23	1.27	1.14
1:B:82:LYS:HB2	1:B:178:LEU:HD11	1.22	1.13
1:B:227:ILE:HB	1:B:246:ALA:HB1	1.17	1.09
1:B:165:GLU:HA	1:B:168:ILE:HB	1.16	1.09

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	279/369 (76%)	190 (68%)	55 (20%)	34 (12%)	0	1
1	B	346/369 (94%)	203 (59%)	91 (26%)	52 (15%)	0	0
All	All	625/738 (85%)	393 (63%)	146 (23%)	86 (14%)	0	1

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	19	LYS
1	A	89	GLU
1	A	200	SER
1	A	207	ILE

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	281/294 (96%)	213 (76%)	68 (24%)	1	4
1	B	280/294 (95%)	188 (67%)	92 (33%)	0	1
All	All	561/588 (95%)	401 (72%)	160 (28%)	0	2

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	180	LEU

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Mol	Chain	Res	Type
1	B	284	LEU
1	B	208	ASP
1	B	244	HIS
1	B	324	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	40	ASN
1	B	81	GLN
1	B	277	GLN
1	B	135	ASN
1	A	139	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	FMN	A	370	-	33,33,33	3.12	14 (42%)	48,50,50	2.14	20 (41%)

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	FMN	A	370	-	-	7/18/18/18	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	370	FMN	C5'-C4'	12.27	1.68	1.51
2	A	370	FMN	C4'-C3'	5.78	1.63	1.53
2	A	370	FMN	C10-N1	4.66	1.42	1.33
2	A	370	FMN	C4A-N5	4.33	1.40	1.30
2	A	370	FMN	C1'-N10	-3.70	1.38	1.47

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	370	FMN	C4A-C10-N10	4.46	122.86	116.48
2	A	370	FMN	C9-C9A-N10	-4.19	116.22	121.85
2	A	370	FMN	C4A-C10-N1	-4.11	114.50	124.59
2	A	370	FMN	C10-N1-C2	3.99	125.48	116.85
2	A	370	FMN	O2'-C2'-C3'	3.40	117.20	109.25

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

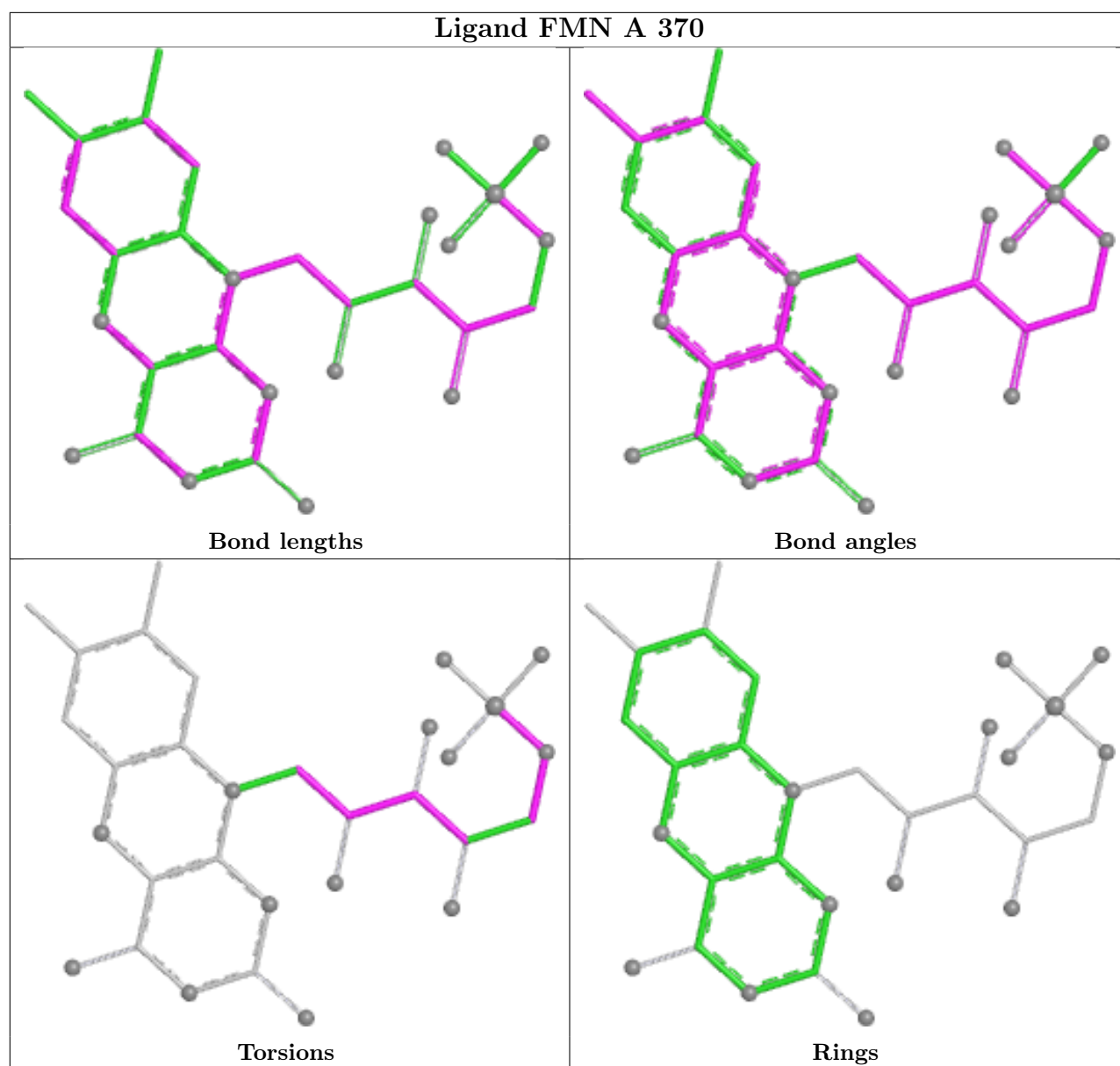
Mol	Chain	Res	Type	Atoms
2	A	370	FMN	C2'-C3'-C4'-O4'
2	A	370	FMN	O3'-C3'-C4'-O4'
2	A	370	FMN	O2'-C2'-C3'-O3'
2	A	370	FMN	O2'-C2'-C3'-C4'
2	A	370	FMN	C5'-O5'-P-O3P

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	370	FMN	5	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 [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.