



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:24 PM UTC

PDB ID : 1F0X / pdb_00001f0x
Title : CRYSTAL STRUCTURE OF D-LACTATE DEHYDROGENASE, A PERIPHERAL MEMBRANE RESPIRATORY ENZYME.
Authors : Dym, O.; Pratt, E.A.; Ho, C.; Eisenberg, D.
Deposited on : 2000-05-17
Resolution : 1.90 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

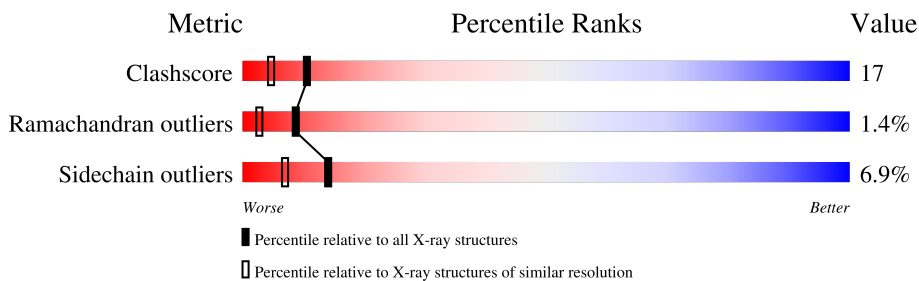
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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.

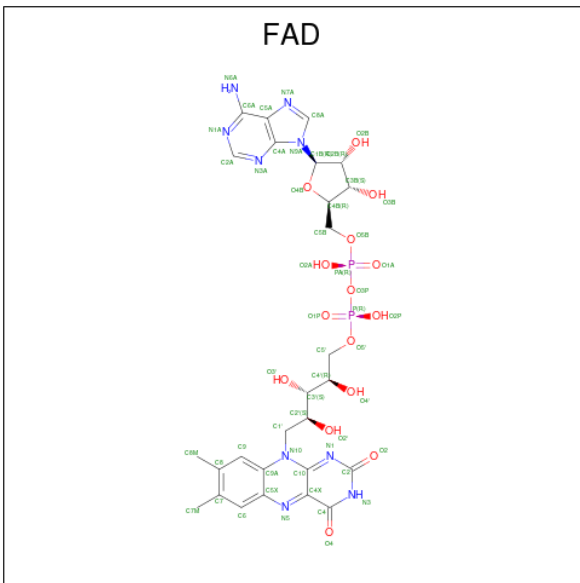
Mol	Chain	Length	Quality of chain
1	A	571	
1	B	571	

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 D-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total 3983	C 2515	N 706	O 748	S 14	0	0	0
1	B	502	Total 3983	C 2515	N 706	O 748	S 14	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	179	Total 179	O 179	0	0
3	B	142	Total 142	O 142	0	0

L1524	Q1524	G1417	LYS
Y1525	Y1525	G1417	THR
P1526	P1526	T1423	ASP
A1527	A1527	T1423	ALA
E1528	E1528	E1426	ALA
H1529	H1529	E1426	THR
N1530	N1530	S1423	ASP
		K1429	ALA
H1533	H1533	F1431	THR
L1534	L1534	L1432	ASP
		F1435	ALA
A1537	A1537	A1436	ALA
P1538	P1538	A1436	THR
E1539	E1539	A1440	ASP
T1540	T1540	A1440	ALA
L1541	L1541	Q1445	THR
Q1542	Q1542	Q1445	ASP
K1543	K1543	L1455	ALA
F1544	F1544	L1455	THR
Y1545	Y1545	L1456	ASP
		A1457	ALA
N1552	N1552	L1458	THR
		D1459	ASP
N1555	N1555	T1467	ALA
P1556	P1556	E1471	THR
		P1474	ASP
G1559	G1559	D1478	ALA
K1560	K1560	D1478	THR
T1561	T1561	L1481	ASP
		K1484	ALA
N1566	N1566	L1485	THR
W1567	W1567	H1489	ASP
GLN	GLN	F1490	ALA
GLU	GLU	Y1493	THR
VAL	VAL	H1496	ASP
GLU	GLU	Q1497	ALA
		D1498	THR
		Y1499	ASP
		V1505	ALA
		D1506	THR
		V1507	ASP
		H1508	ALA
		A1509	THR
		L1510	ASP
		K1511	ALA
		M1514	THR
		Q1520	ASP
			L1377
			P1378
			P1379
			R1380
			M1381
			K1382
			R1385
			H1390
			M1396
			A1397
			D1410
			K1413
			E1416

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.01Å 74.19Å 102.00Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	18.00 – 1.90	Depositor
% Data completeness (in resolution range)	96.5 (18.00-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8393	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: FAD

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	1.09	12/4072 (0.3%)	1.51	63/5511 (1.1%)
1	B	1.07	7/4072 (0.2%)	1.41	49/5511 (0.9%)
All	All	1.08	19/8144 (0.2%)	1.46	112/11022 (1.0%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1528	GLU	CD-OE1	13.78	1.51	1.25
1	A	173	MET	SD-CE	-13.50	1.45	1.79
1	B	1173	MET	SD-CE	-12.72	1.47	1.79
1	A	77	ALA	N-CA	11.80	1.61	1.46
1	A	528	GLU	CD-OE1	10.13	1.44	1.25

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	TYR	CA-C-N	-31.43	87.39	119.76
1	A	525	TYR	C-N-CA	-31.43	87.39	119.76
1	B	1525	TYR	CA-C-N	-24.74	93.11	119.83
1	B	1525	TYR	C-N-CA	-24.74	93.11	119.83
1	A	377	LEU	C-N-CD	-18.31	80.32	120.60

There are no chirality outliers.

There are no planarity outliers.

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	3983	0	3900	137	2
1	B	3983	0	3900	125	2
2	A	53	0	31	6	0
2	B	53	0	31	6	0
3	A	179	0	0	4	0
3	B	142	0	0	8	0
All	All	8393	0	7862	267	2

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 17.

The worst 5 of 267 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:1285:GLN:O	1:B:1288:VAL:HG12	1.52	1.09
1:B:1076:ALA:O	1:B:1077:ALA:HB3	1.47	1.09
1:A:76:ALA:O	1:A:77:ALA:HB3	1.41	1.08
1:A:212:LYS:HD2	1:B:1520:GLN:HE22	1.17	1.08
1:A:285:GLN:O	1:A:288:VAL:HG12	1.55	1.07

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASP:OD1	1:B:1010:LYS:NZ[1_445]	2.01	0.19
1:A:238:ASP:N	1:B:1010:LYS:NZ[1_445]	2.19	0.01

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	498/571 (87%)	474 (95%)	16 (3%)	8 (2%)	7	2
1	B	498/571 (87%)	474 (95%)	18 (4%)	6 (1%)	10	4
All	All	996/1142 (87%)	948 (95%)	34 (3%)	14 (1%)	9	3

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	LYS
1	A	378	PRO
1	B	1274	LYS
1	B	1378	PRO
1	A	77	ALA

5.3.2 Protein sidechains ⓘ

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	421/484 (87%)	392 (93%)	29 (7%)	14	7
1	B	421/484 (87%)	392 (93%)	29 (7%)	14	7
All	All	842/968 (87%)	784 (93%)	58 (7%)	14	7

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	567	TRP
1	B	1493	TYR
1	B	1136	ARG
1	B	1474	PRO
1	B	1413	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1190	HIS

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Mol	Chain	Res	Type
1	B	1433	HIS
1	B	1201	GLN
1	B	1311	HIS
1	B	1519	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](#)

2 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	$\# Z > 2$
2	FAD	B	1600	-	58,58,58	3.18	29 (50%)	85,89,89	1.67	13 (15%)
2	FAD	A	600	-	58,58,58	3.21	19 (32%)	85,89,89	1.62	14 (16%)

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	FAD	B	1600	-	-	3/34/50/50	0/6/6/6
2	FAD	A	600	-	-	2/34/50/50	0/6/6/6

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	P-O3P	-13.52	1.44	1.59
2	B	1600	FAD	C5'-C4'	-12.85	1.34	1.51
2	A	600	FAD	C5'-C4'	-11.42	1.36	1.51
2	B	1600	FAD	P-O3P	-11.13	1.47	1.59
2	A	600	FAD	C2'-C3'	-6.78	1.41	1.53

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1600	FAD	C4'-C3'-C2'	-7.61	100.91	113.57
2	A	600	FAD	C4'-C3'-C2'	-5.61	104.23	113.57
2	A	600	FAD	O5B-PA-O1A	-5.33	87.82	108.94
2	B	1600	FAD	O5B-PA-O1A	-4.85	89.70	108.94
2	A	600	FAD	O4B-C4B-C5B	-4.60	94.60	109.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	PA-O3P-P-O2P
2	B	1600	FAD	PA-O3P-P-O2P
2	B	1600	FAD	O4B-C4B-C5B-O5B
2	B	1600	FAD	PA-O3P-P-O1P
2	A	600	FAD	O4B-C4B-C5B-O5B

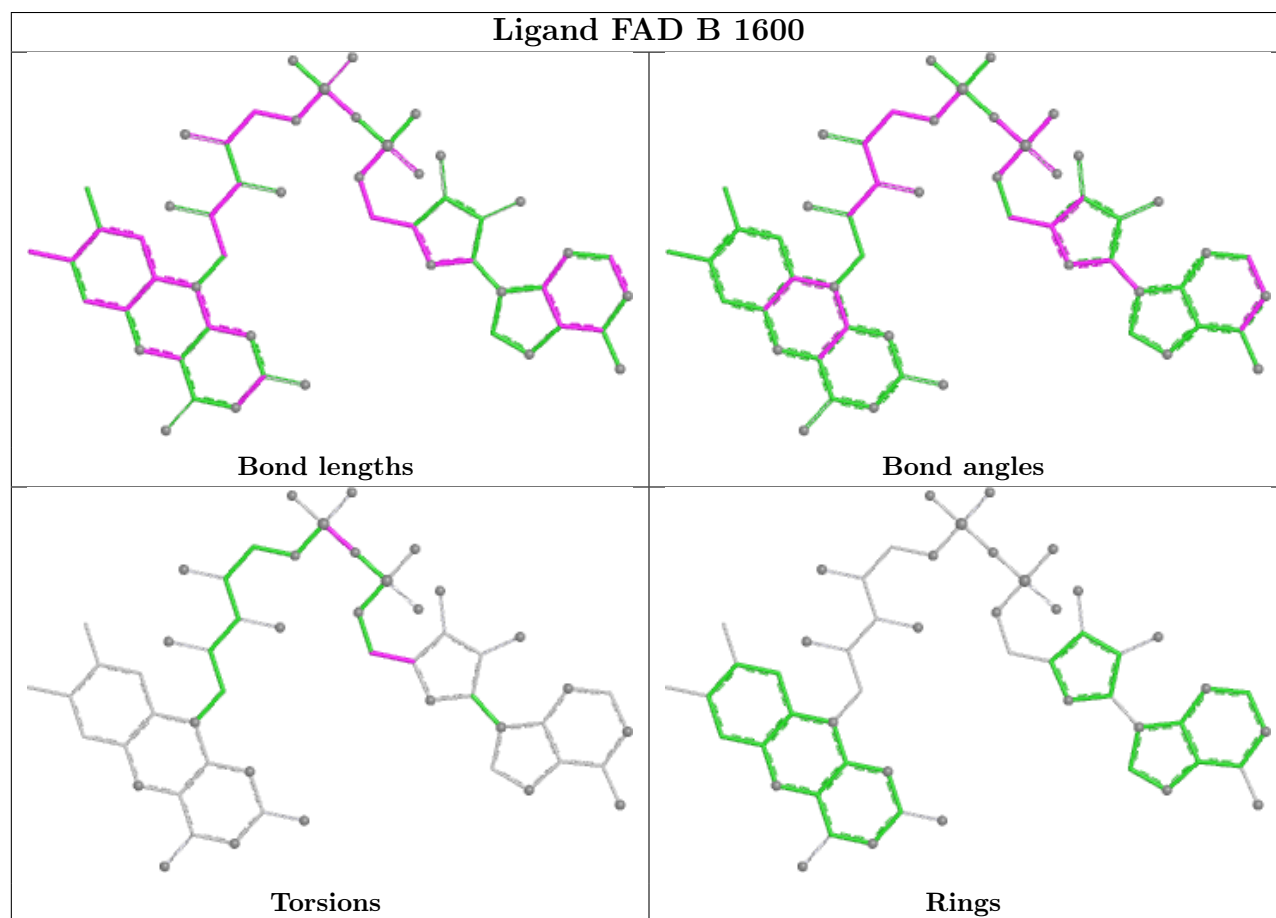
There are no ring outliers.

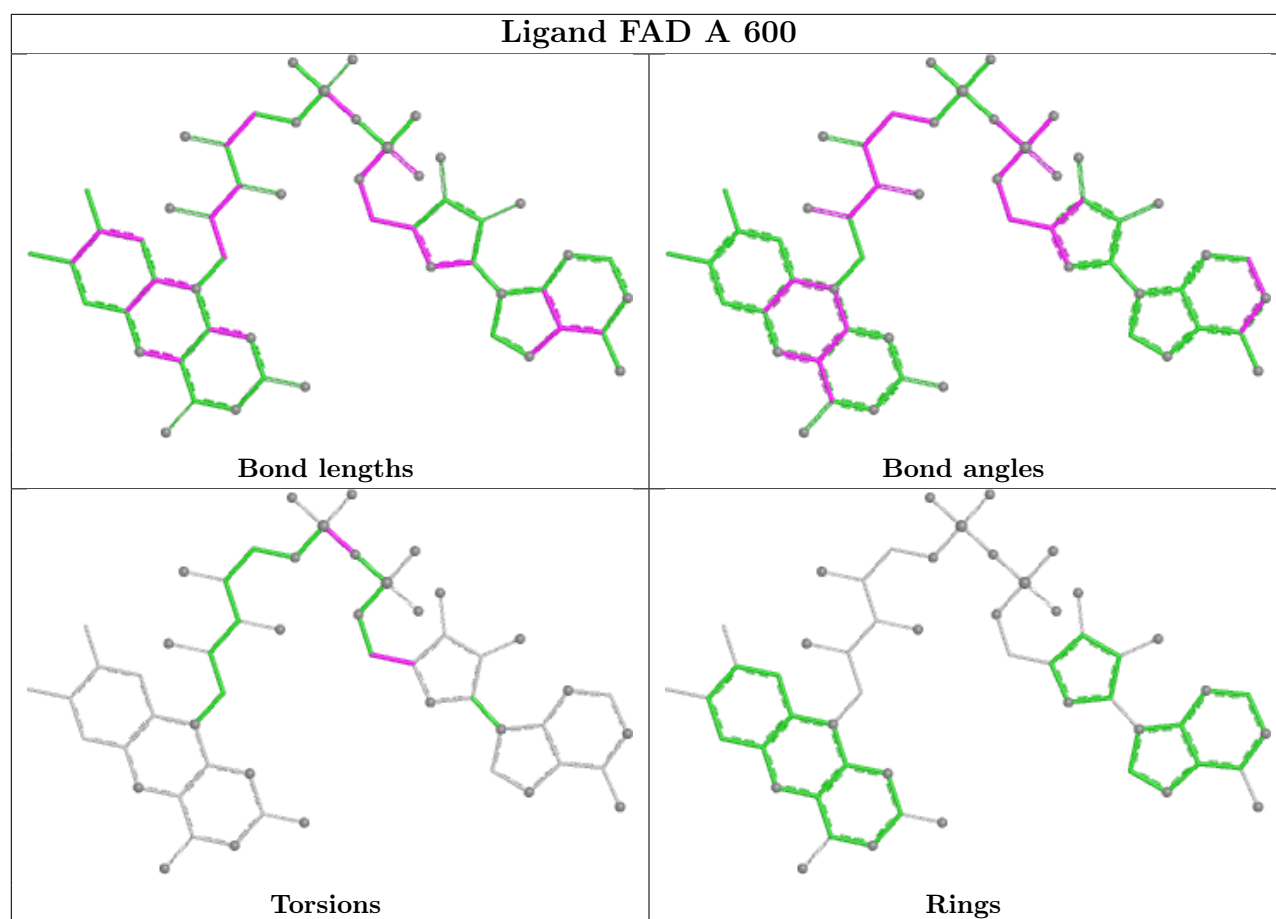
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1600	FAD	6	0
2	A	600	FAD	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 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.