



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:15 AM EDT

PDB ID : 8REP / pdb\_00008rep  
Title : Crystal structure of oxidized ThyX-Y91F mutant  
Authors : Pecqueur, L.; Hamdane, D.  
Deposited on : 2023-12-12  
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](mailto: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>.

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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)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

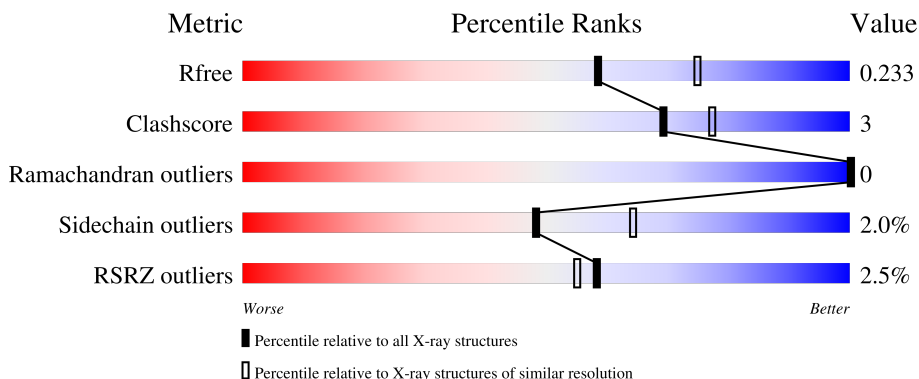
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	3% 81% 11% 7%
1	B	232	% 86% 6% 7%
1	C	232	3% 84% 7% 8%
1	D	232	2% 84% 7% 8%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7398 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	215	Total 1761	C 1150	N 295	O 311	S 5	0	0	0
1	B	215	Total 1746	C 1143	N 295	O 303	S 5	0	0	0
1	C	214	Total 1724	C 1130	N 288	O 301	S 5	0	0	0
1	D	213	Total 1756	C 1145	N 302	O 304	S 5	0	0	0

There are 52 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
A	91	PHE	TYR	engineered mutation	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

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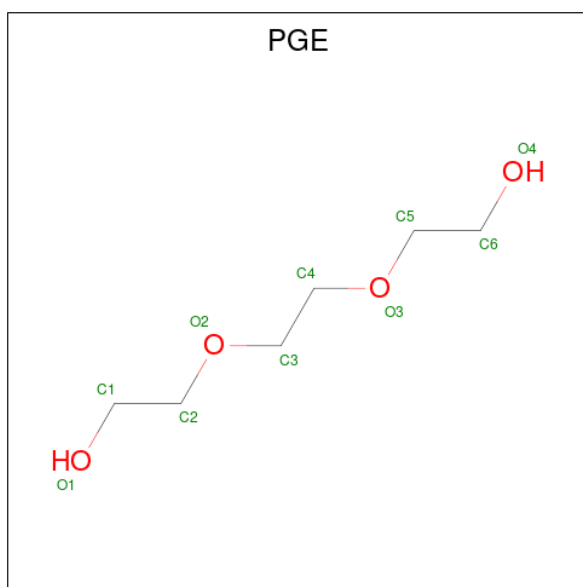
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q9WYT0
B	-2	HIS	-	expression tag	UNP Q9WYT0
B	-1	HIS	-	expression tag	UNP Q9WYT0
B	0	HIS	-	expression tag	UNP Q9WYT0
B	91	PHE	TYR	engineered mutation	UNP Q9WYT0
C	-11	MET	-	initiating methionine	UNP Q9WYT0
C	-10	GLY	-	expression 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
C	91	PHE	TYR	engineered mutation	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
D	91	PHE	TYR	engineered mutation	UNP Q9WYT0

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



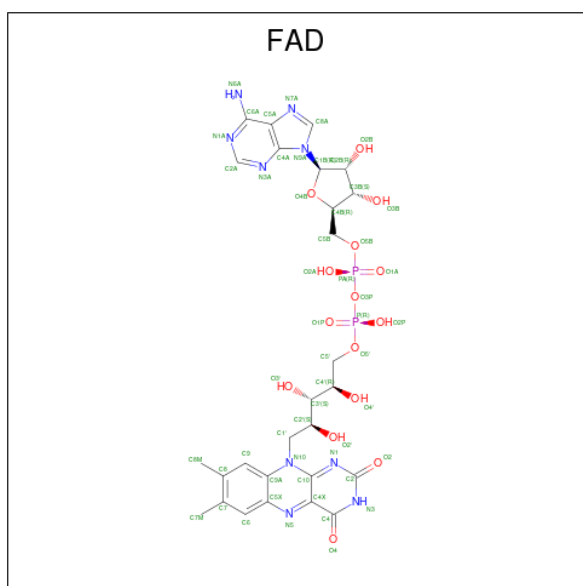
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



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

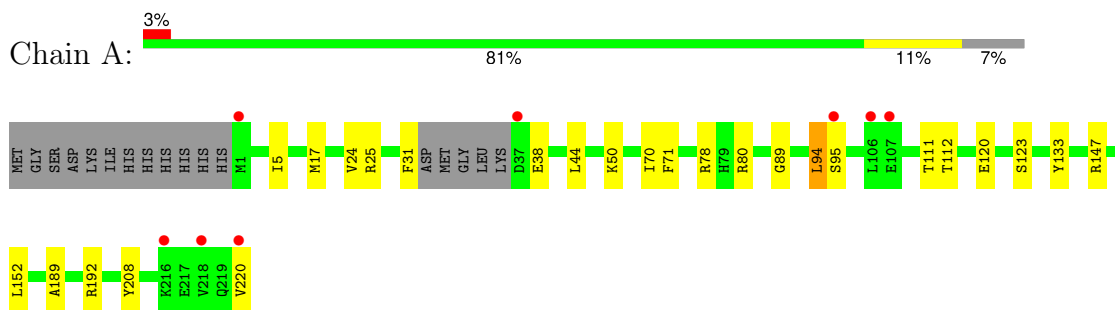
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	24	Total O 24 24	0	0
6	B	22	Total O 22 22	0	0
6	C	31	Total O 31 31	0	0
6	D	22	Total O 22 22	0	0

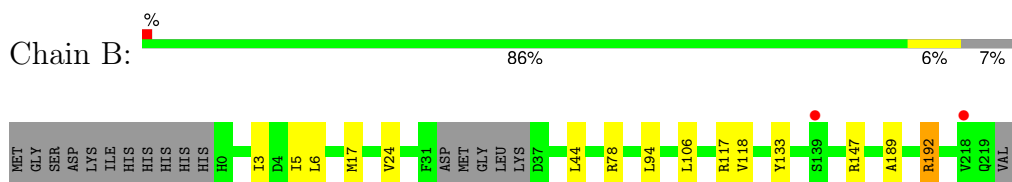
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

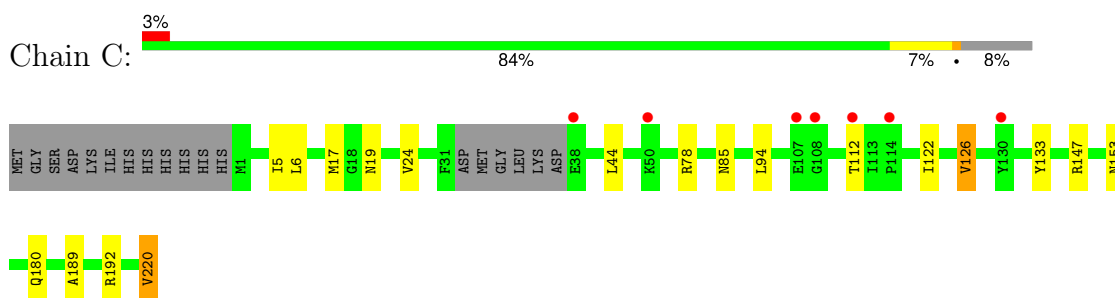
- Molecule 1: Flavin-dependent thymidylate synthase



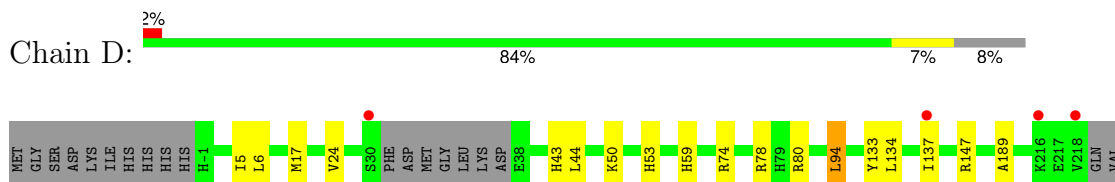
- Molecule 1: Flavin-dependent thymidylate synthase



- Molecule 1: Flavin-dependent thymidylate synthase



- Molecule 1: Flavin-dependent thymidylate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.92Å 116.80Å 142.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.53 – 2.20 43.53 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (43.53-2.20) 97.5 (43.53-2.20)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.20Å)	Xtrriage
Refinement program	BUSTER 2.10.4	Depositor
R, $R_{free}$	0.222 , 0.241 0.209 , 0.233	Depositor DCC
$R_{free}$ test set	2310 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtrriage
Anisotropy	0.089	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 35.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7398	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: PEG, PG4, FAD, PGE

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	0.66	0/1809	1.01	2/2454 (0.1%)
1	B	0.68	0/1795	1.00	0/2438
1	C	0.66	0/1772	1.01	0/2409
1	D	0.67	0/1805	1.03	0/2447
All	All	0.67	0/7181	1.01	2/9748 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	THR	CA-C-N	5.17	127.20	120.28
1	A	111	THR	C-N-CA	5.17	127.20	120.28

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	1761	0	1708	18	0
1	B	1746	0	1687	8	0
1	C	1724	0	1659	13	0
1	D	1756	0	1721	15	0
2	A	26	0	36	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	13	0	18	0	0
3	A	10	0	14	0	0
3	B	10	0	14	1	0
3	D	20	0	28	6	0
4	A	53	0	31	1	0
4	B	53	0	31	1	0
4	C	53	0	31	1	0
4	D	53	0	31	1	0
5	D	21	0	30	1	0
6	A	24	0	0	0	0
6	B	22	0	0	0	0
6	C	31	0	0	1	0
6	D	22	0	0	0	0
All	All	7398	0	7039	50	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 (50) 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:17:MET:HB2	1:B:17:MET:HB2	1.57	0.87
1:C:17:MET:HB2	1:D:17:MET:HB2	1.61	0.83
1:B:78:ARG:HH12	4:B:302:FAD:C2	2.02	0.72
3:B:301:PGE:H1	1:C:180:GLN:OE1	1.99	0.62
1:A:152:LEU:HD13	3:D:301:PGE:H42	1.82	0.61
1:A:70:ILE:HD11	2:A:302:PG4:H12	1.83	0.61
1:D:50:LYS:NZ	3:D:303:PGE:O3	2.29	0.60
1:A:50:LYS:HD2	2:A:301:PG4:H62	1.85	0.58
1:A:89:GLY:HA2	2:A:302:PG4:H22	1.88	0.56
1:A:50:LYS:HZ2	2:A:301:PG4:H72	1.71	0.56
1:C:5:ILE:HD11	1:C:189:ALA:HB2	1.88	0.55
2:A:302:PG4:H11	1:D:74:ARG:HH12	1.71	0.54
1:D:5:ILE:HD11	1:D:189:ALA:HB2	1.90	0.54
1:D:50:LYS:HZ1	3:D:303:PGE:C4	2.20	0.54
1:D:5:ILE:HG22	1:D:6:LEU:HG	1.89	0.53
1:C:122:ILE:O	1:C:126:VAL:HG13	2.08	0.53
1:B:5:ILE:HD11	1:B:189:ALA:HB2	1.91	0.53
1:D:78:ARG:HH12	4:D:305:FAD:C2	2.22	0.52
1:A:24:VAL:HG13	1:A:44:LEU:HD23	1.93	0.50
1:A:94:LEU:HD21	2:A:302:PG4:H21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:TYR:CE1	1:D:147:ARG:HG3	2.46	0.50
1:B:3:ILE:HD11	1:B:192:ARG:HG2	1.93	0.50
1:C:5:ILE:HG22	1:C:6:LEU:HG	1.94	0.49
1:A:133:TYR:CE1	1:A:147:ARG:HG3	2.47	0.49
1:C:24:VAL:HG13	1:C:44:LEU:HD23	1.95	0.49
1:A:78:ARG:HH22	4:A:304:FAD:C2	2.25	0.49
1:C:133:TYR:CE1	1:C:147:ARG:HG3	2.48	0.48
1:D:24:VAL:HG13	1:D:44:LEU:HD23	1.95	0.48
1:A:208:TYR:OH	2:A:301:PG4:H31	2.14	0.48
1:D:94:LEU:HD21	3:D:301:PGE:H22	1.96	0.48
1:B:24:VAL:HG13	1:B:44:LEU:HD23	1.96	0.47
1:D:53:HIS:HA	5:D:306:PEG:H31	1.96	0.47
1:B:133:TYR:CE1	1:B:147:ARG:HG3	2.50	0.46
1:C:85:ASN:ND2	1:D:59:HIS:NE2	2.57	0.46
1:A:50:LYS:HZ2	2:A:301:PG4:C7	2.29	0.46
1:A:71:PHE:HB2	3:D:301:PGE:H6	1.97	0.46
1:A:192:ARG:HD3	1:A:220:VAL:OXT	2.15	0.46
1:D:43:HIS:CE1	3:D:303:PGE:H62	2.51	0.45
1:C:192:ARG:HD3	1:C:220:VAL:OXT	2.16	0.45
1:A:80:ARG:HB3	1:D:80:ARG:HB3	1.98	0.45
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.99	0.44
1:A:50:LYS:NZ	2:A:301:PG4:H72	2.34	0.43
1:C:19:ASN:HB2	6:C:410:HOH:O	2.19	0.43
1:B:5:ILE:HG22	1:B:6:LEU:HG	1.99	0.42
1:C:78:ARG:HH12	4:C:302:FAD:C2	2.32	0.41
1:C:192:ARG:HB2	1:C:220:VAL:HG22	2.03	0.41
1:B:106:LEU:HD21	1:B:118:VAL:HG11	2.03	0.41
1:A:25:ARG:HD3	1:A:31:PHE:HA	2.02	0.41
1:C:126:VAL:HG11	1:C:153:ASN:HD21	1.86	0.41
1:D:134:LEU:HA	1:D:137:ILE:CG1	2.51	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	211/232 (91%)	206 (98%)	5 (2%)	0	100	100
1	B	211/232 (91%)	207 (98%)	4 (2%)	0	100	100
1	C	210/232 (90%)	206 (98%)	4 (2%)	0	100	100
1	D	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
All	All	841/928 (91%)	824 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	181/207 (87%)	175 (97%)	6 (3%)	33	45
1	B	177/207 (86%)	174 (98%)	3 (2%)	53	69
1	C	174/207 (84%)	170 (98%)	4 (2%)	44	59
1	D	182/207 (88%)	181 (100%)	1 (0%)	81	90
All	All	714/828 (86%)	700 (98%)	14 (2%)	48	64

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	94	LEU
1	A	95	SER
1	A	112	THR
1	A	120	GLU
1	A	123	SER
1	B	94	LEU
1	B	117	ARG
1	B	192	ARG
1	C	94	LEU

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Mol	Chain	Res	Type
1	C	112	THR
1	C	126	VAL
1	C	220	VAL
1	D	94	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	51	HIS
1	C	153	ASN
1	D	0	HIS
1	D	53	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 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	$\# Z  > 2$
4	FAD	A	304	-	58,58,58	0.51	0	85,89,89	0.70	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PGE	A	303	-	9,9,9	0.25	0	8,8,8	0.50	0
3	PGE	D	301	-	9,9,9	0.11	0	8,8,8	0.19	0
3	PGE	B	301	-	9,9,9	0.16	0	8,8,8	0.18	0
5	PEG	D	304	-	6,6,6	0.10	0	5,5,5	0.19	0
4	FAD	C	302	-	58,58,58	0.63	1 (1%)	85,89,89	0.64	1 (1%)
2	PG4	A	302	-	12,12,12	0.23	0	11,11,11	0.22	0
4	FAD	D	305	-	58,58,58	0.53	0	85,89,89	0.74	4 (4%)
5	PEG	D	306	-	6,6,6	0.12	0	5,5,5	0.13	0
5	PEG	D	302	-	6,6,6	0.18	0	5,5,5	0.14	0
3	PGE	D	303	-	9,9,9	0.21	0	8,8,8	0.13	0
2	PG4	A	301	-	12,12,12	0.22	0	11,11,11	0.15	0
4	FAD	B	302	-	58,58,58	0.56	0	85,89,89	0.64	2 (2%)
2	PG4	C	301	-	12,12,12	0.14	0	11,11,11	0.15	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	FAD	A	304	-	-	1/34/50/50	0/6/6/6
3	PGE	A	303	-	-	5/7/7/7	-
3	PGE	D	301	-	-	3/7/7/7	-
3	PGE	B	301	-	-	3/7/7/7	-
5	PEG	D	304	-	-	1/4/4/4	-
4	FAD	C	302	-	-	2/34/50/50	0/6/6/6
2	PG4	A	302	-	-	5/10/10/10	-
4	FAD	D	305	-	-	3/34/50/50	0/6/6/6
5	PEG	D	306	-	-	3/4/4/4	-
5	PEG	D	302	-	-	0/4/4/4	-
3	PGE	D	303	-	-	2/7/7/7	-
2	PG4	A	301	-	-	7/10/10/10	-
4	FAD	B	302	-	-	3/34/50/50	0/6/6/6
2	PG4	C	301	-	-	7/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	302	FAD	P-O3P	2.23	1.61	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	304	FAD	C4-N3-C2	-2.37	121.44	125.64
4	A	304	FAD	C2B-C1B-N9A	2.31	119.05	113.30
4	D	305	FAD	C4'-C3'-C2'	2.31	117.41	113.57
4	B	302	FAD	C2B-C1B-N9A	2.23	118.84	113.30
4	C	302	FAD	C4-N3-C2	-2.17	121.78	125.64
4	D	305	FAD	O5'-C5'-C4'	-2.17	103.57	109.36
4	D	305	FAD	C2B-C1B-N9A	2.13	118.60	113.30
4	D	305	FAD	C4-N3-C2	-2.12	121.88	125.64
4	B	302	FAD	C4-N3-C2	-2.10	121.92	125.64

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	FAD	C3'-C4'-C5'-O5'
4	B	302	FAD	O4'-C4'-C5'-O5'
4	C	302	FAD	P-O3P-PA-O5B
3	B	301	PGE	O2-C3-C4-O3
2	A	302	PG4	O3-C5-C6-O4
2	A	301	PG4	O3-C5-C6-O4
2	A	301	PG4	O2-C3-C4-O3
3	B	301	PGE	O3-C5-C6-O4
3	D	301	PGE	O2-C3-C4-O3
2	C	301	PG4	O4-C7-C8-O5
3	D	301	PGE	O3-C5-C6-O4
2	C	301	PG4	O2-C3-C4-O3
3	D	303	PGE	O1-C1-C2-O2
5	D	306	PEG	O1-C1-C2-O2
2	A	301	PG4	O4-C7-C8-O5
2	C	301	PG4	O1-C1-C2-O2
3	A	303	PGE	O2-C3-C4-O3
2	A	302	PG4	O4-C7-C8-O5
5	D	306	PEG	O2-C3-C4-O4
3	A	303	PGE	C3-C4-O3-C5
4	A	304	FAD	P-O3P-PA-O5B
4	B	302	FAD	P-O3P-PA-O5B
4	D	305	FAD	P-O3P-PA-O5B
2	C	301	PG4	C4-C3-O2-C2
5	D	306	PEG	C1-C2-O2-C3
2	A	301	PG4	C5-C6-O4-C7
2	A	302	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
2	C	301	PG4	C3-C4-O3-C5
3	D	303	PGE	C4-C3-O2-C2
3	D	301	PGE	O1-C1-C2-O2
3	B	301	PGE	C3-C4-O3-C5
2	C	301	PG4	C8-C7-O4-C6
3	A	303	PGE	C4-C3-O2-C2
2	A	301	PG4	C8-C7-O4-C6
4	C	302	FAD	C5'-O5'-P-O1P
4	D	305	FAD	C5'-O5'-P-O1P
2	A	302	PG4	O1-C1-C2-O2
3	A	303	PGE	C1-C2-O2-C3
2	A	301	PG4	C3-C4-O3-C5
2	A	301	PG4	C6-C5-O3-C4
3	A	303	PGE	C6-C5-O3-C4
2	A	302	PG4	O2-C3-C4-O3
5	D	304	PEG	O1-C1-C2-O2
2	C	301	PG4	O3-C5-C6-O4
4	D	305	FAD	PA-O3P-P-O2P

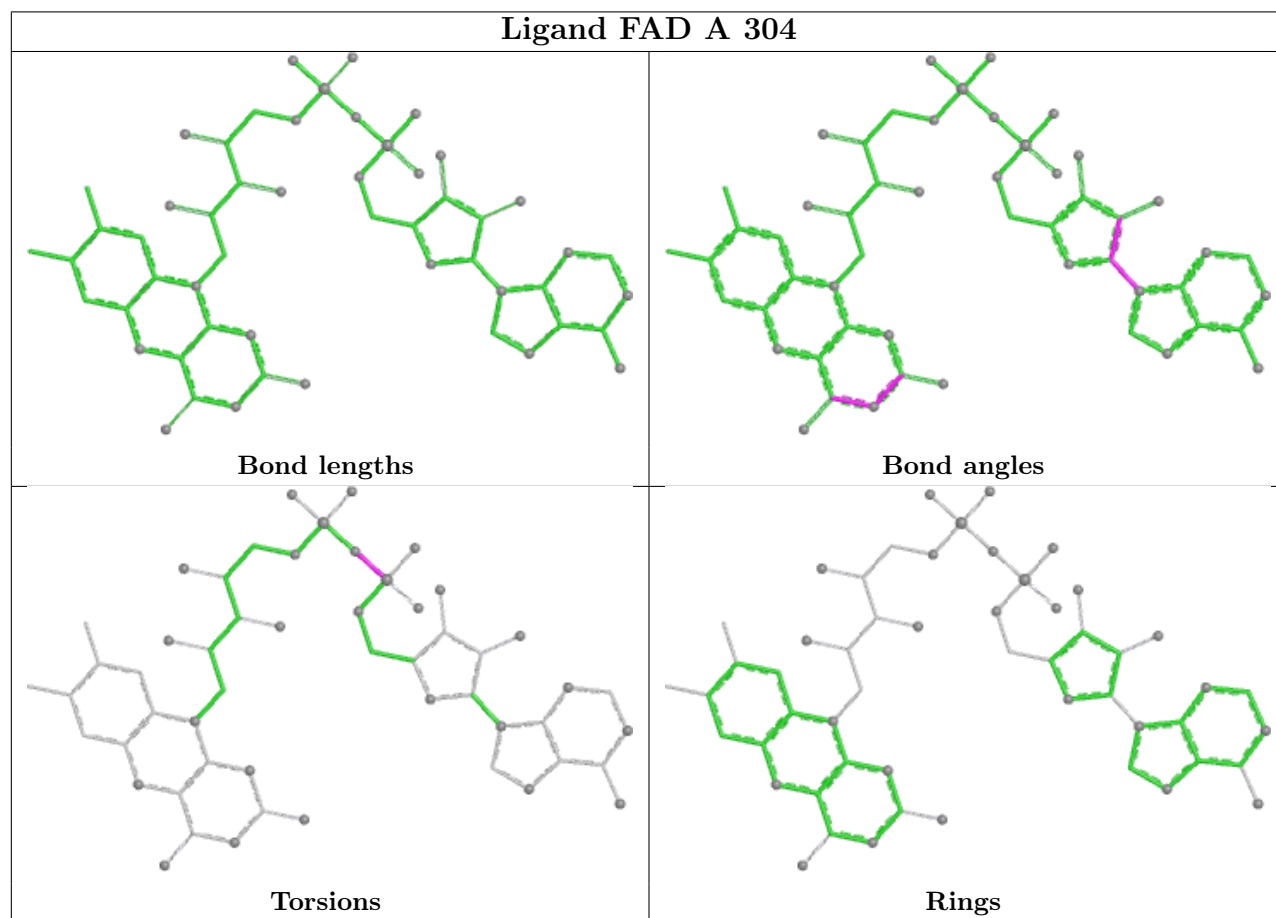
There are no ring outliers.

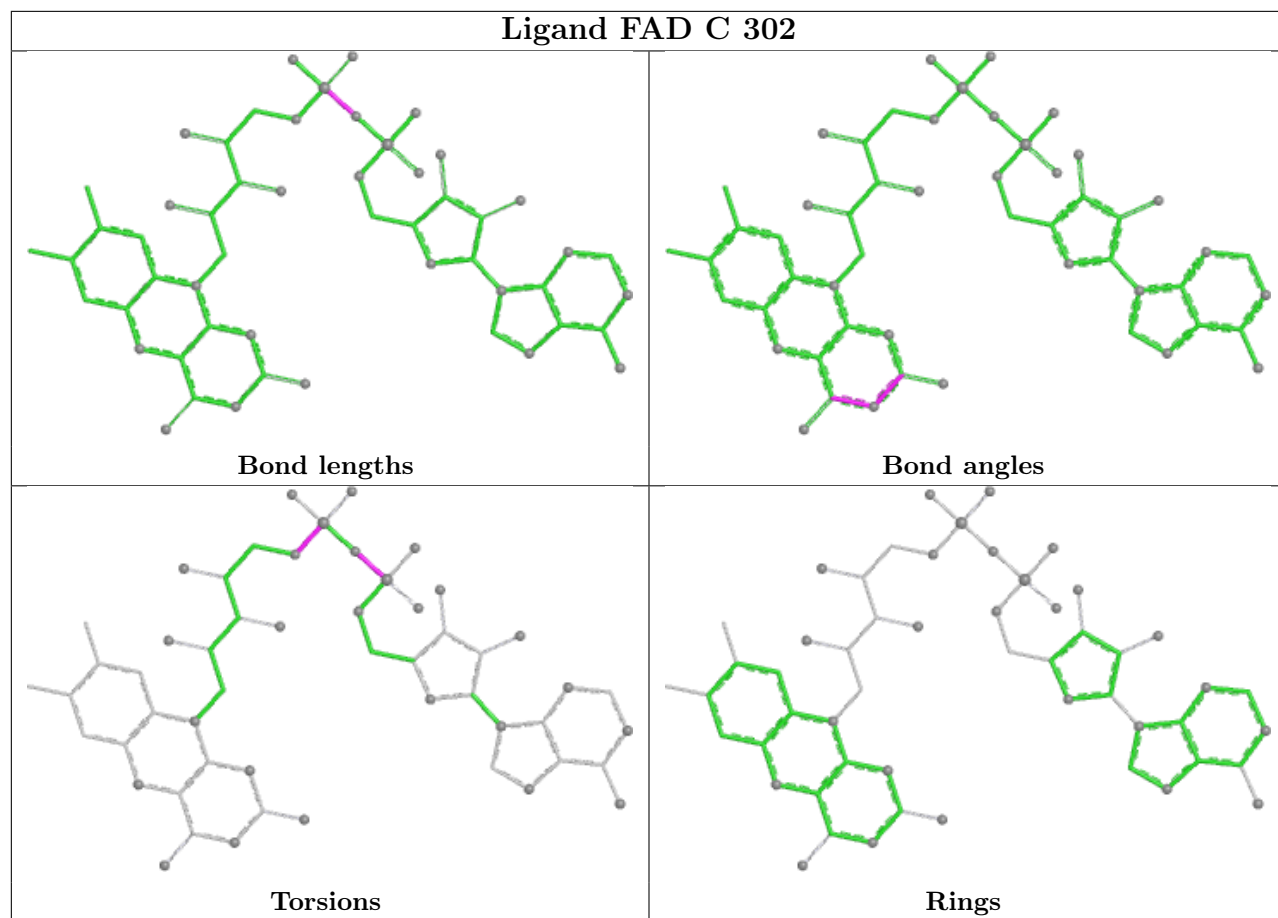
10 monomers are involved in 21 short contacts:

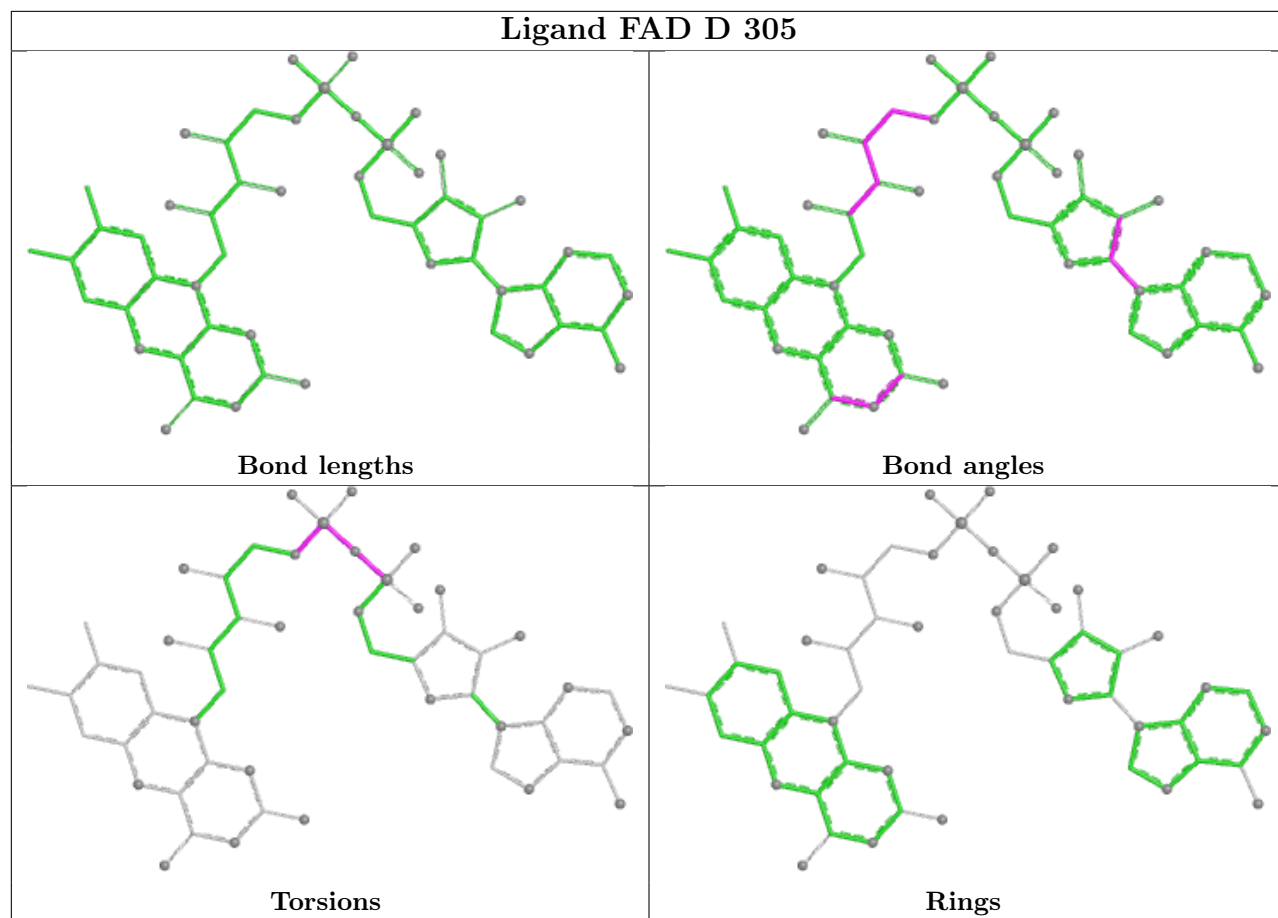
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	FAD	1	0
3	D	301	PGE	3	0
3	B	301	PGE	1	0
4	C	302	FAD	1	0
2	A	302	PG4	4	0
4	D	305	FAD	1	0
5	D	306	PEG	1	0
3	D	303	PGE	3	0
2	A	301	PG4	5	0
4	B	302	FAD	1	0

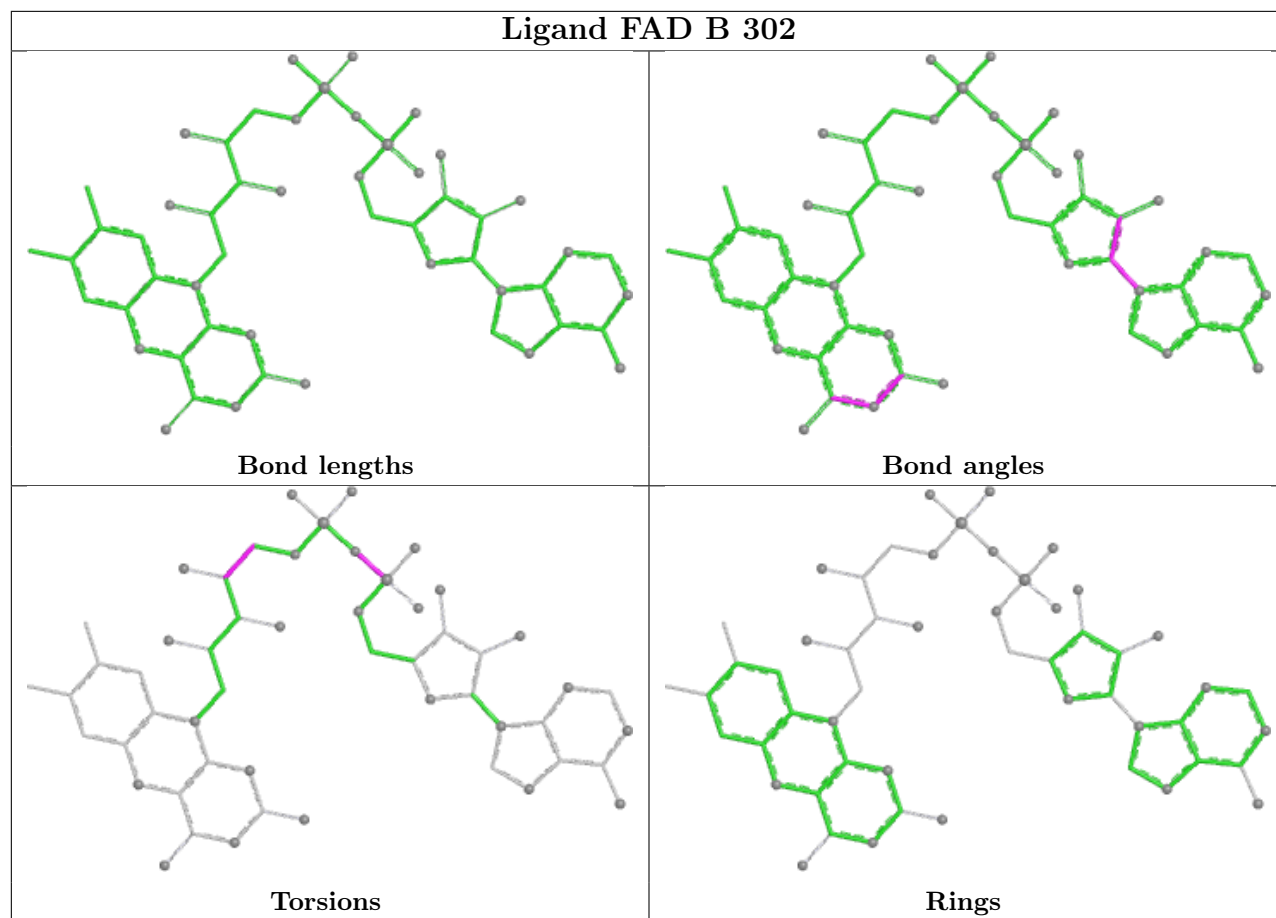
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	215/232 (92%)	0.29	8 (3%) 45 42	30, 41, 66, 80	0
1	B	215/232 (92%)	0.13	2 (0%) 81 79	27, 39, 56, 64	0
1	C	214/232 (92%)	0.23	7 (3%) 49 46	29, 41, 62, 72	0
1	D	213/232 (91%)	0.15	4 (1%) 66 63	29, 40, 57, 71	0
All	All	857/928 (92%)	0.20	21 (2%) 58 55	27, 40, 60, 80	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	218	VAL	5.0
1	C	38	GLU	3.6
1	D	216	LYS	3.4
1	A	1	MET	3.0
1	D	30	SER	2.8
1	A	218	VAL	2.8
1	A	220	VAL	2.8
1	A	106	LEU	2.5
1	C	112	THR	2.5
1	C	50	LYS	2.5
1	C	108	GLY	2.5
1	C	130	TYR	2.4
1	D	137	ILE	2.3
1	A	37	ASP	2.3
1	C	107	GLU	2.2
1	C	114	PRO	2.2
1	A	216	LYS	2.2
1	B	218	VAL	2.2
1	A	95	SER	2.1
1	B	139	SER	2.1
1	A	107	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

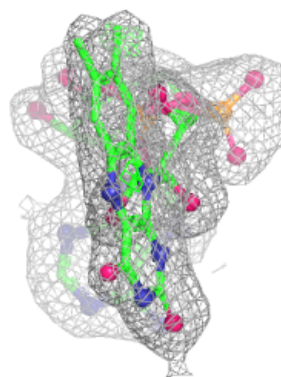
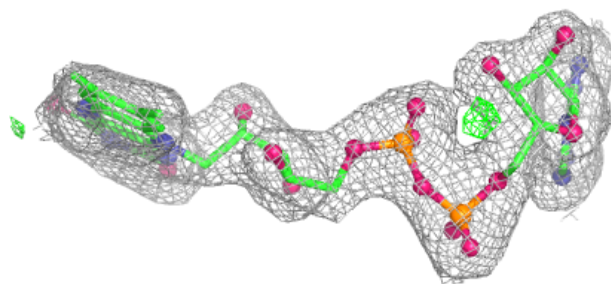
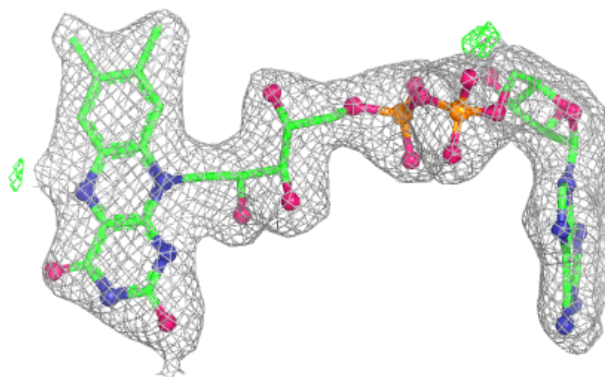
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PGE	A	303	10/10	0.80	0.17	65,66,67,68	0
3	PGE	B	301	10/10	0.84	0.18	58,59,60,60	0
5	PEG	D	304	7/7	0.85	0.14	58,58,58,58	0
2	PG4	A	301	13/13	0.87	0.14	56,57,58,58	0
5	PEG	D	306	7/7	0.87	0.16	68,68,69,69	0
2	PG4	A	302	13/13	0.88	0.14	51,52,53,53	0
3	PGE	D	303	10/10	0.88	0.12	58,59,60,60	0
2	PG4	C	301	13/13	0.90	0.12	48,49,51,51	0
3	PGE	D	301	10/10	0.92	0.12	56,57,57,57	0
5	PEG	D	302	7/7	0.93	0.09	45,45,46,47	0
4	FAD	C	302	53/53	0.95	0.08	31,35,38,40	0
4	FAD	B	302	53/53	0.96	0.07	27,33,40,41	0
4	FAD	A	304	53/53	0.96	0.07	28,35,39,39	0
4	FAD	D	305	53/53	0.96	0.07	29,34,41,42	0

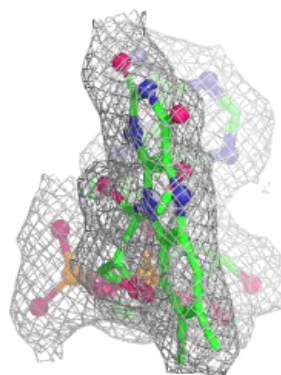
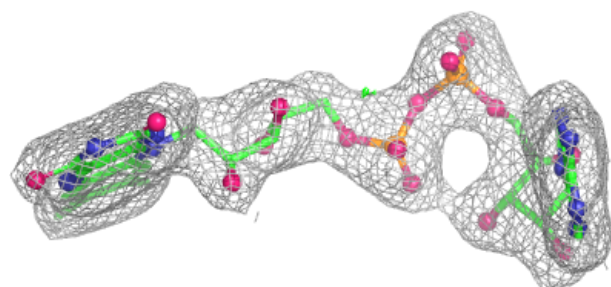
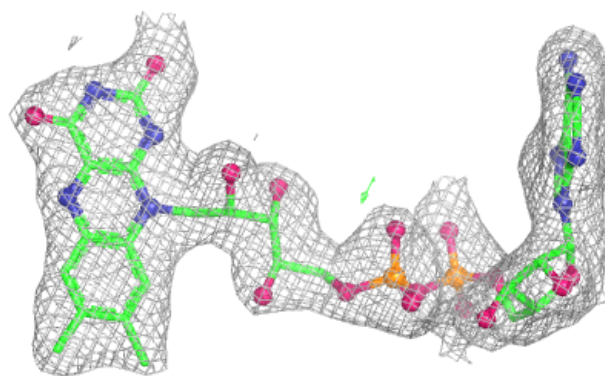
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around FAD C 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

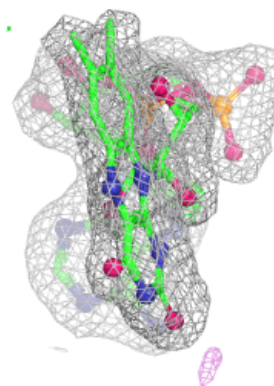
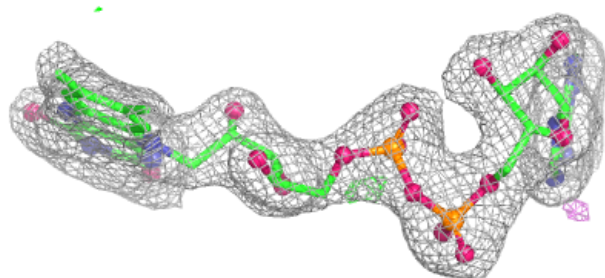
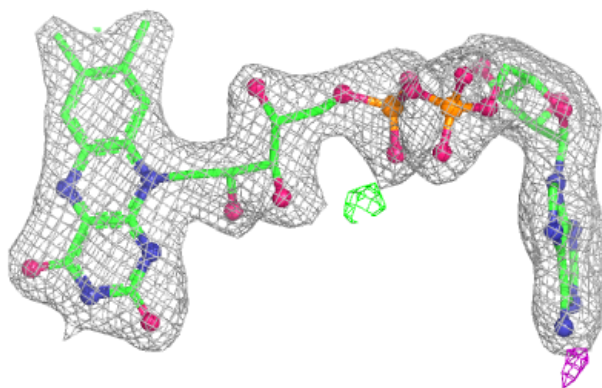
**Electron density around FAD B 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

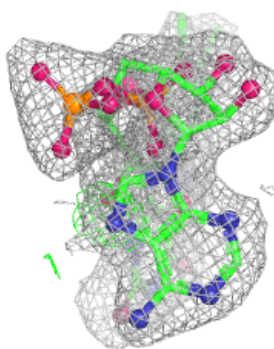
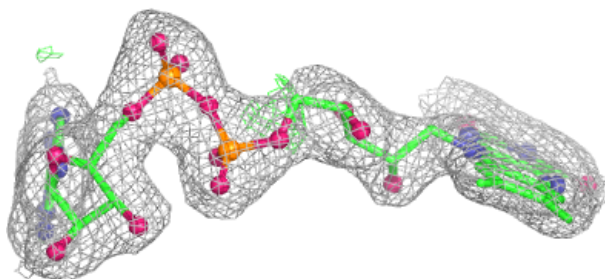
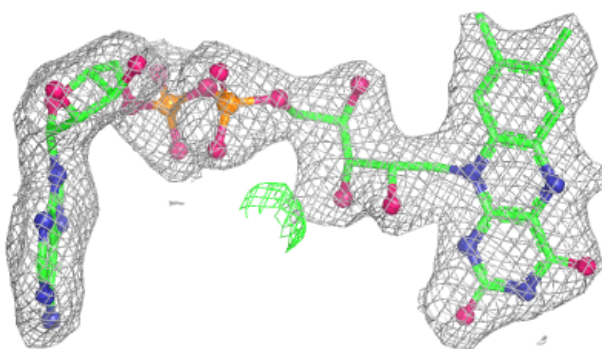


**Electron density around FAD A 304:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FAD D 305:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.