



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:43 am BST

PDB ID : 3N3Y
Title : Crystal structure of Thymidylate Synthase X (ThyX) from *Helicobacter pylori* with FAD and dUMP at 2.31Å resolution
Authors : Wang, K.; Wang, Q.; Chen, J.; Chen, L.; Jiang, H.; Shen, X.
Deposited on : 2010-05-21
Resolution : 2.31 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)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

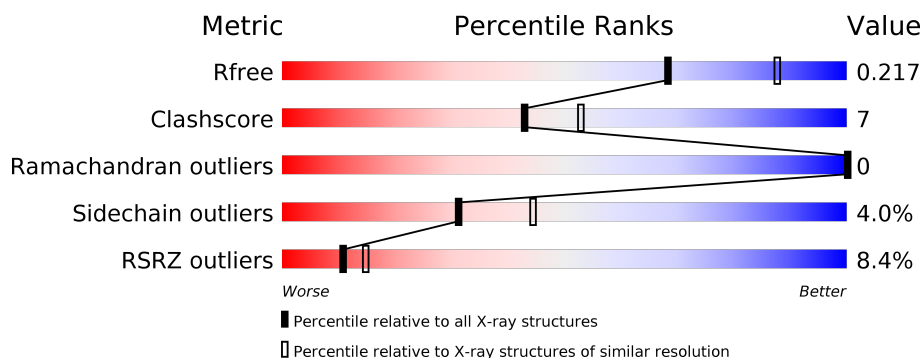
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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 $\leq 5\%$. 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	216	<div> <div>3%</div> <div>82%</div> <div>13%</div> <div>• •</div> </div>
1	B	216	<div> <div>11%</div> <div>77%</div> <div>19%</div> <div>• •</div> </div>
1	C	216	<div> <div>12%</div> <div>82%</div> <div>13%</div> <div>• •</div> </div>
1	D	216	<div> <div>7%</div> <div>79%</div> <div>17%</div> <div>• •</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7255 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 Thymidylate synthase thyX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1703	1077	299	319	8			
1	B	209	Total	C	N	O	S	0	0	0
			1703	1077	299	319	8			
1	C	208	Total	C	N	O	S	0	0	0
			1695	1073	298	316	8			
1	D	208	Total	C	N	O	S	0	1	0
			1695	1070	298	319	8			

There are 32 discrepancies between the modelled and reference sequences:

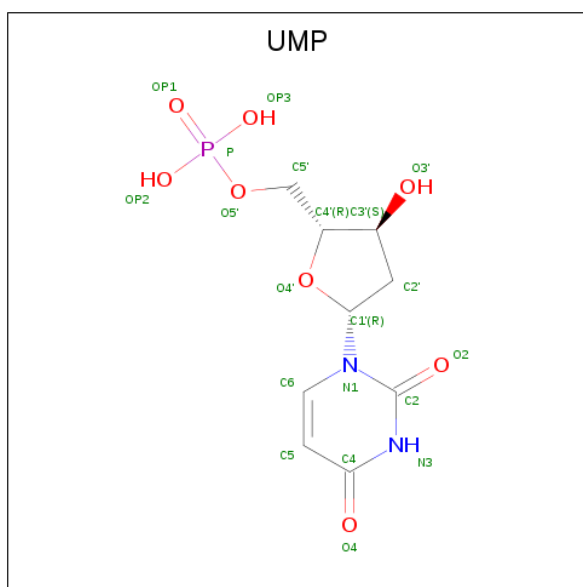
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP Q5UVJ4
A	-6	PRO	-	EXPRESSION TAG	UNP Q5UVJ4
A	-5	LEU	-	EXPRESSION TAG	UNP Q5UVJ4
A	-4	GLY	-	EXPRESSION TAG	UNP Q5UVJ4
A	-3	SER	-	EXPRESSION TAG	UNP Q5UVJ4
A	-2	PRO	-	EXPRESSION TAG	UNP Q5UVJ4
A	-1	GLU	-	EXPRESSION TAG	UNP Q5UVJ4
A	0	PHE	-	EXPRESSION TAG	UNP Q5UVJ4
B	-7	GLY	-	EXPRESSION TAG	UNP Q5UVJ4
B	-6	PRO	-	EXPRESSION TAG	UNP Q5UVJ4
B	-5	LEU	-	EXPRESSION TAG	UNP Q5UVJ4
B	-4	GLY	-	EXPRESSION TAG	UNP Q5UVJ4
B	-3	SER	-	EXPRESSION TAG	UNP Q5UVJ4
B	-2	PRO	-	EXPRESSION TAG	UNP Q5UVJ4
B	-1	GLU	-	EXPRESSION TAG	UNP Q5UVJ4
B	0	PHE	-	EXPRESSION TAG	UNP Q5UVJ4
C	-7	GLY	-	EXPRESSION TAG	UNP Q5UVJ4
C	-6	PRO	-	EXPRESSION TAG	UNP Q5UVJ4
C	-5	LEU	-	EXPRESSION TAG	UNP Q5UVJ4
C	-4	GLY	-	EXPRESSION TAG	UNP Q5UVJ4
C	-3	SER	-	EXPRESSION TAG	UNP Q5UVJ4

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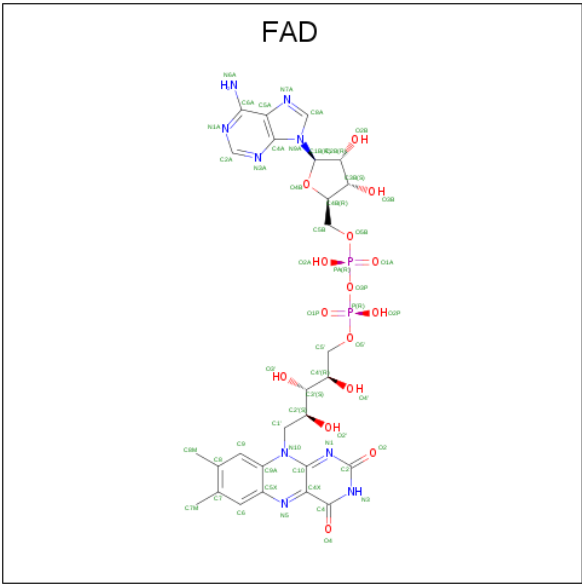
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PRO	-	EXPRESSION TAG	UNP Q5UVJ4
C	-1	GLU	-	EXPRESSION TAG	UNP Q5UVJ4
C	0	PHE	-	EXPRESSION TAG	UNP Q5UVJ4
D	-7	GLY	-	EXPRESSION TAG	UNP Q5UVJ4
D	-6	PRO	-	EXPRESSION TAG	UNP Q5UVJ4
D	-5	LEU	-	EXPRESSION TAG	UNP Q5UVJ4
D	-4	GLY	-	EXPRESSION TAG	UNP Q5UVJ4
D	-3	SER	-	EXPRESSION TAG	UNP Q5UVJ4
D	-2	PRO	-	EXPRESSION TAG	UNP Q5UVJ4
D	-1	GLU	-	EXPRESSION TAG	UNP Q5UVJ4
D	0	PHE	-	EXPRESSION TAG	UNP Q5UVJ4

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

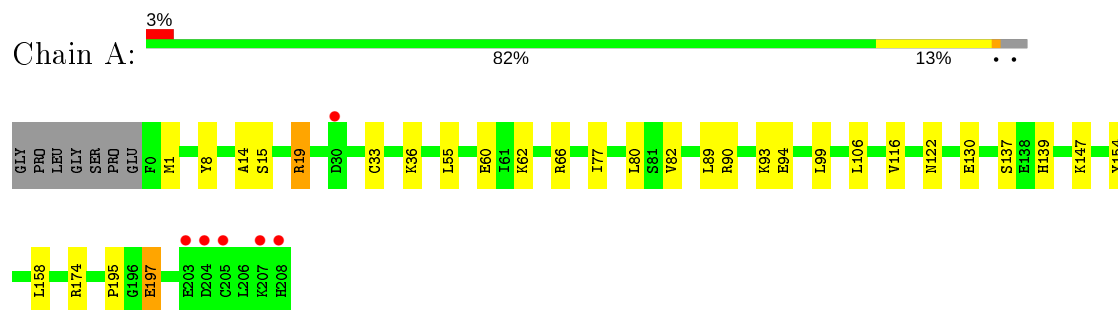
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



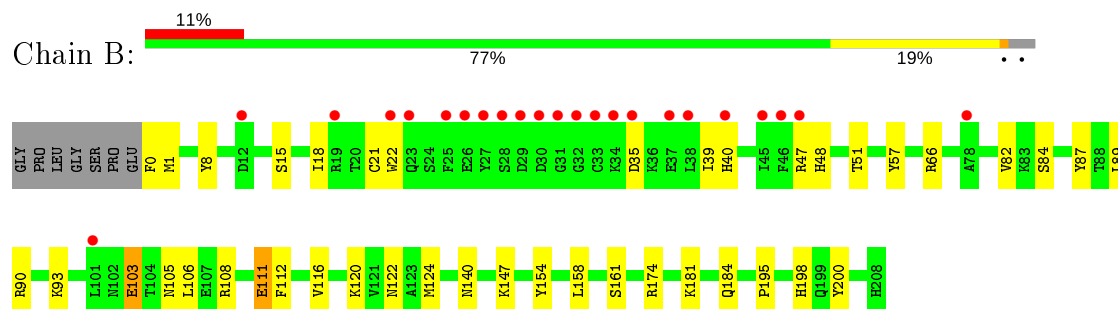
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

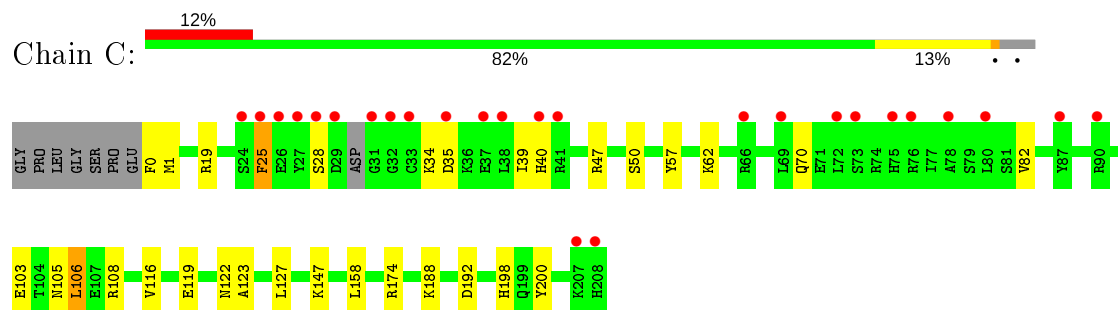
- Molecule 1: Thymidylate synthase thyX



- Molecule 1: Thymidylate synthase thyX

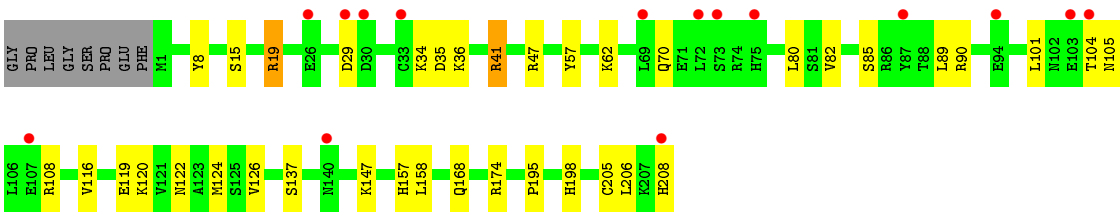


- Molecule 1: Thymidylate synthase thyX



- Molecule 1: Thymidylate synthase thyX





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.53Å 79.96Å 96.41Å 90.00° 103.14° 90.00°	Depositor
Resolution (Å)	37.69 – 2.31 37.69 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.3 (37.69-2.31) 99.3 (37.69-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.174 , 0.223 0.170 , 0.217	Depositor DCC
R_{free} test set	2144 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7255	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: UMP, 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	0.45	0/1735	0.54	0/2335
1	B	0.42	0/1735	0.52	0/2335
1	C	0.40	0/1726	0.51	0/2321
1	D	0.41	0/1729	0.52	0/2327
All	All	0.42	0/6925	0.52	0/9318

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 [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	1703	0	1700	19	0
1	B	1703	0	1700	31	0
1	C	1695	0	1695	25	0
1	D	1695	0	1696	24	0
2	A	20	0	11	0	0
2	B	40	0	22	4	0
2	C	20	0	11	3	0
2	D	20	0	11	2	0
3	A	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	53	0	31	1	0
3	C	53	0	31	0	0
3	D	53	0	31	1	0
4	A	41	0	0	2	0
4	B	41	0	0	0	0
4	C	24	0	0	1	0
4	D	41	0	0	0	0
All	All	7255	0	6970	96	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 7.

All (96) 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:174:ARG:HH12	2:B:301:UMP:HN3	1.10	0.97
1:A:174:ARG:HH12	2:B:304:UMP:HN3	1.04	0.96
1:D:116:VAL:H	1:D:122:ASN:HD21	1.15	0.95
2:C:303:UMP:HN3	1:D:174:ARG:HH12	1.14	0.93
1:C:174:ARG:HH12	2:D:302:UMP:HN3	1.16	0.92
1:A:116:VAL:H	1:A:122:ASN:HD21	1.23	0.87
1:D:41:ARG:HG3	1:D:41:ARG:HH11	1.38	0.87
1:C:116:VAL:H	1:C:122:ASN:HD21	1.26	0.82
1:C:19:ARG:HD3	1:C:25:PHE:HA	1.62	0.80
1:B:116:VAL:H	1:B:122:ASN:HD21	1.31	0.76
1:B:103:GLU:H	1:B:103:GLU:CD	1.93	0.72
1:A:197:GLU:HB3	4:A:220:HOH:O	1.92	0.69
1:D:41:ARG:CG	1:D:41:ARG:HH11	2.07	0.67
1:C:70:GLN:NE2	1:D:70:GLN:HG2	2.14	0.63
1:C:57:TYR:OH	1:C:198:HIS:HD2	1.83	0.62
1:C:19:ARG:HH22	1:C:34:LYS:CG	2.12	0.62
1:B:8:TYR:CE2	1:B:195:PRO:HG3	2.36	0.61
1:C:0:PHE:O	1:C:0:PHE:CD1	2.54	0.60
1:C:19:ARG:HH22	1:C:34:LYS:HG3	1.68	0.59
1:A:93:LYS:HD2	1:A:137:SER:HA	1.84	0.59
1:B:40:HIS:HB2	1:B:200:TYR:HE2	1.67	0.58
1:D:15:SER:O	1:D:19:ARG:HG3	2.03	0.58
1:B:90:ARG:HH12	1:B:93:LYS:HZ2	1.50	0.58
1:C:40:HIS:HB2	1:C:200:TYR:HE2	1.70	0.57
1:B:18:ILE:HG12	1:B:51:THR:HG21	1.87	0.56
1:D:168:GLN:HG2	1:D:205:CYS:SG	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:HIS:ND1	1:B:120:LYS:HE3	2.21	0.55
1:B:47:ARG:HD3	3:D:303:FAD:HM73	1.88	0.54
1:C:19:ARG:CD	1:C:28:SER:HB2	2.38	0.54
1:A:82:VAL:HB	2:B:301:UMP:H4'	1.90	0.54
1:B:15:SER:CA	1:B:39:ILE:HD11	2.37	0.54
1:B:105:ASN:ND2	1:B:108:ARG:HH11	2.06	0.53
1:D:19:ARG:NH1	1:D:35:ASP:OD1	2.40	0.53
1:A:77:ILE:HD12	3:A:304:FAD:H51A	1.91	0.52
2:C:303:UMP:HN3	1:D:174:ARG:NH1	1.95	0.51
1:C:105:ASN:ND2	1:C:108:ARG:HH11	2.08	0.51
1:D:57:TYR:OH	1:D:198:HIS:HD2	1.93	0.51
1:C:19:ARG:NH1	1:C:35:ASP:OD1	2.44	0.51
1:B:35:ASP:O	1:B:39:ILE:HG12	2.11	0.50
1:B:15:SER:N	1:B:39:ILE:HD11	2.26	0.50
1:C:188:LYS:HE3	1:C:192:ASP:OD2	2.11	0.50
1:B:57:TYR:OH	1:B:198:HIS:HD2	1.95	0.50
1:C:50:SER:HB2	4:C:231:HOH:O	2.12	0.50
1:D:41:ARG:CG	1:D:41:ARG:NH1	2.71	0.50
3:A:304:FAD:HM73	1:C:47:ARG:HD3	1.94	0.49
1:B:18:ILE:HD12	1:B:39:ILE:HD13	1.95	0.49
1:B:8:TYR:CD2	1:B:195:PRO:HG3	2.48	0.49
1:A:8:TYR:CD2	1:A:195:PRO:HG3	2.48	0.48
1:B:40:HIS:HB2	1:B:200:TYR:CE2	2.47	0.48
1:A:139:HIS:CE1	1:B:120:LYS:HE3	2.49	0.48
1:D:8:TYR:CE2	1:D:195:PRO:HG3	2.49	0.48
3:B:209:FAD:HM73	1:D:47:ARG:HD3	1.96	0.48
1:C:123:ALA:O	1:C:127:LEU:HG	2.13	0.48
1:C:19:ARG:HD2	1:C:28:SER:HB2	1.95	0.48
1:D:104:THR:O	1:D:108:ARG:HG3	2.14	0.47
1:D:82:VAL:HB	2:D:302:UMP:H4'	1.96	0.47
1:D:85:SER:OG	1:D:147:LYS:HE2	2.15	0.47
1:C:19:ARG:HH22	1:C:34:LYS:HG2	1.78	0.47
1:D:120:LYS:O	1:D:124:MET:HG2	2.15	0.47
1:A:33:CYS:HA	1:A:36:LYS:HE2	1.97	0.46
1:B:21:CYS:HB2	1:B:22:TRP:CE3	2.49	0.46
1:B:93:LYS:NZ	1:B:140:ASN:ND2	2.64	0.46
1:C:106:LEU:HA	1:C:106:LEU:HD12	1.83	0.46
1:D:62:LYS:HG2	1:D:157:HIS:CD2	2.51	0.46
1:D:122:ASN:O	1:D:126:VAL:HG23	2.15	0.46
1:C:40:HIS:HB2	1:C:200:TYR:CE2	2.51	0.45
1:D:105:ASN:ND2	1:D:108:ARG:HH11	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ARG:NH2	1:C:34:LYS:HG2	2.31	0.45
1:B:82:VAL:HB	2:B:304:UMP:H4'	1.98	0.45
1:C:105:ASN:HD22	1:C:108:ARG:HD3	1.82	0.45
1:D:90:ARG:HG2	1:D:90:ARG:HH11	1.82	0.44
1:B:66:ARG:HG2	1:B:154:TYR:O	2.17	0.44
1:C:62:LYS:HE2	1:C:62:LYS:HB2	1.73	0.44
1:A:99:LEU:HG	1:A:130:GLU:HG2	1.99	0.43
1:B:120:LYS:O	1:B:124:MET:HG2	2.19	0.43
1:C:35:ASP:O	1:C:39:ILE:HG13	2.19	0.43
1:B:111:GLU:O	1:B:111:GLU:HG3	2.18	0.43
1:D:89:LEU:HA	1:D:89:LEU:HD23	1.88	0.43
1:A:93:LYS:NZ	4:A:219:HOH:O	2.52	0.42
1:B:84:SER:HB3	1:B:87:TYR:CD2	2.54	0.42
1:D:29:ASP:OD2	1:D:34:LYS:HB2	2.19	0.42
1:A:14:ALA:HB2	1:A:55:LEU:HD21	2.02	0.42
1:A:60:GLU:OE2	1:A:62:LYS:HD3	2.20	0.42
1:C:82:VAL:HB	2:C:303:UMP:H4'	2.02	0.41
1:B:47:ARG:HG3	1:B:48:HIS:CE1	2.54	0.41
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.84	0.41
1:A:66:ARG:HG2	1:A:154:TYR:O	2.21	0.41
1:B:111:GLU:HG2	1:B:112:PHE:CD2	2.55	0.41
1:B:57:TYR:O	1:B:161:SER:HA	2.21	0.41
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.85	0.41
1:A:15:SER:O	1:A:19:ARG:HG3	2.20	0.41
1:D:206:LEU:O	1:D:208:HIS:CD2	2.74	0.41
1:A:80:LEU:N	1:A:80:LEU:HD12	2.36	0.40
1:A:8:TYR:CE2	1:A:195:PRO:HG3	2.56	0.40
1:B:174:ARG:O	1:B:184:GLN:HA	2.21	0.40
1:B:181:LYS:HD2	1:B:181:LYS:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	207/216 (96%)	204 (99%)	3 (1%)	0	100	100
1	B	207/216 (96%)	197 (95%)	10 (5%)	0	100	100
1	C	204/216 (94%)	202 (99%)	2 (1%)	0	100	100
1	D	207/216 (96%)	199 (96%)	8 (4%)	0	100	100
All	All	825/864 (96%)	802 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	188/193 (97%)	180 (96%)	8 (4%)	29	40
1	B	188/193 (97%)	181 (96%)	7 (4%)	34	48
1	C	187/193 (97%)	180 (96%)	7 (4%)	34	48
1	D	188/193 (97%)	180 (96%)	8 (4%)	29	40
All	All	751/772 (97%)	721 (96%)	30 (4%)	31	44

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	19	ARG
1	A	90	ARG
1	A	94	GLU
1	A	106	LEU
1	A	147	LYS
1	A	158	LEU
1	A	197	GLU
1	B	0	PHE
1	B	1	MET
1	B	103	GLU
1	B	106	LEU
1	B	111	GLU

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Mol	Chain	Res	Type
1	B	147	LYS
1	B	158	LEU
1	C	1	MET
1	C	25	PHE
1	C	103	GLU
1	C	106	LEU
1	C	119	GLU
1	C	147	LYS
1	C	158	LEU
1	D	19	ARG
1	D	36	LYS
1	D	41	ARG
1	D	80	LEU
1	D	101	LEU
1	D	119	GLU
1	D	137	SER
1	D	158	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	105	ASN
1	A	122	ASN
1	A	131	ASN
1	A	140	ASN
1	A	168	GLN
1	B	105	ASN
1	B	122	ASN
1	B	131	ASN
1	B	140	ASN
1	B	168	GLN
1	B	198	HIS
1	B	199	GLN
1	C	105	ASN
1	C	122	ASN
1	C	131	ASN
1	C	168	GLN
1	C	169	ASN
1	C	198	HIS
1	D	105	ASN
1	D	122	ASN

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Mol	Chain	Res	Type
1	D	131	ASN
1	D	140	ASN
1	D	168	GLN
1	D	169	ASN
1	D	198	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 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	UMP	B	304	-	18,21,21	1.05	1 (5%)	21,31,31	0.94	1 (4%)
2	UMP	A	305	-	18,21,21	0.98	1 (5%)	21,31,31	0.78	0
2	UMP	C	303	-	18,21,21	1.17	1 (5%)	21,31,31	1.06	2 (9%)
3	FAD	D	303	-	51,58,58	1.28	6 (11%)	60,89,89	1.69	9 (15%)
2	UMP	D	302	-	18,21,21	1.10	1 (5%)	21,31,31	1.09	2 (9%)
3	FAD	B	209	-	51,58,58	1.34	7 (13%)	60,89,89	1.58	8 (13%)
3	FAD	C	302	-	51,58,58	1.39	7 (13%)	60,89,89	1.57	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UMP	B	301	-	18,21,21	1.16	1 (5%)	21,31,31	1.07	2 (9%)
3	FAD	A	304	-	51,58,58	1.29	6 (11%)	60,89,89	1.58	8 (13%)

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	UMP	B	304	-	-	0/7/22/22	0/2/2/2
2	UMP	A	305	-	-	0/7/22/22	0/2/2/2
2	UMP	C	303	-	-	4/7/22/22	0/2/2/2
3	FAD	D	303	-	-	2/30/50/50	0/6/6/6
2	UMP	D	302	-	-	0/7/22/22	0/2/2/2
3	FAD	B	209	-	-	2/30/50/50	0/6/6/6
3	FAD	C	302	-	-	2/30/50/50	0/6/6/6
2	UMP	B	301	-	-	0/7/22/22	0/2/2/2
3	FAD	A	304	-	-	1/30/50/50	0/6/6/6

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	FAD	C10-N1	4.55	1.39	1.33
3	A	304	FAD	C10-N1	4.06	1.38	1.33
3	C	302	FAD	C4X-N5	3.96	1.39	1.33
3	B	209	FAD	C2A-N3A	3.92	1.38	1.32
2	B	301	UMP	C4-N3	3.57	1.39	1.33
3	D	303	FAD	C2A-N3A	3.56	1.37	1.32
3	B	209	FAD	C10-N1	3.56	1.37	1.33
3	D	303	FAD	C4X-N5	3.55	1.38	1.33
3	C	302	FAD	C2A-N3A	3.49	1.37	1.32
3	B	209	FAD	C4-N3	3.45	1.39	1.33
3	A	304	FAD	C2A-N3A	3.39	1.37	1.32
2	C	303	UMP	C4-N3	3.37	1.38	1.33
3	D	303	FAD	C10-N1	3.34	1.37	1.33
2	D	302	UMP	C4-N3	3.28	1.38	1.33
2	B	304	UMP	C4-N3	3.20	1.38	1.33
3	D	303	FAD	C4-N3	3.19	1.38	1.33
3	C	302	FAD	C1'-N10	3.12	1.51	1.48
3	A	304	FAD	C4-N3	3.11	1.38	1.33
3	B	209	FAD	C4X-N5	3.10	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	304	FAD	C1'-N10	3.07	1.51	1.48
3	A	304	FAD	C4X-N5	2.94	1.37	1.33
3	C	302	FAD	C4-N3	2.81	1.37	1.33
3	B	209	FAD	C1'-N10	2.76	1.51	1.48
2	A	305	UMP	C4-N3	2.69	1.37	1.33
3	D	303	FAD	C2A-N1A	2.55	1.38	1.33
3	A	304	FAD	C2A-N1A	2.43	1.38	1.33
3	D	303	FAD	C1'-N10	2.34	1.50	1.48
3	B	209	FAD	C2A-N1A	2.31	1.38	1.33
3	C	302	FAD	C2A-N1A	2.24	1.38	1.33
3	C	302	FAD	C5X-N5	2.08	1.38	1.35
3	B	209	FAD	C6-C5X	-2.03	1.38	1.41

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	FAD	C4-N3-C2	6.29	120.45	115.14
3	D	303	FAD	C4-N3-C2	6.21	120.38	115.14
3	C	302	FAD	N3A-C2A-N1A	-5.58	119.95	128.68
3	B	209	FAD	N3A-C2A-N1A	-5.49	120.09	128.68
3	D	303	FAD	N3A-C2A-N1A	-5.44	120.17	128.68
3	A	304	FAD	N3A-C2A-N1A	-5.25	120.47	128.68
3	A	304	FAD	C4-N3-C2	5.16	119.50	115.14
3	D	303	FAD	C1'-N10-C9A	5.11	122.31	118.29
3	B	209	FAD	C4-N3-C2	4.64	119.06	115.14
3	B	209	FAD	C4X-N5-C5X	4.64	121.41	116.77
3	B	209	FAD	C10-C4X-N5	-4.31	118.28	121.26
3	C	302	FAD	C1'-N10-C9A	4.12	121.53	118.29
3	A	304	FAD	C1'-N10-C9A	4.06	121.49	118.29
3	A	304	FAD	C4X-N5-C5X	4.03	120.80	116.77
3	D	303	FAD	C4X-N5-C5X	3.52	120.28	116.77
2	D	302	UMP	C2'-C1'-N1	-3.29	106.68	114.27
3	C	302	FAD	C5X-C9A-N10	3.27	120.08	117.72
3	A	304	FAD	P-O3P-PA	-3.23	121.74	132.83
2	B	301	UMP	C2'-C1'-N1	-3.11	107.11	114.27
3	D	303	FAD	C4X-C4-N3	-3.01	119.31	123.43
3	D	303	FAD	C10-C4X-N5	-2.97	119.20	121.26
2	B	304	UMP	C2'-C1'-N1	-2.79	107.84	114.27
3	B	209	FAD	C1'-N10-C9A	2.77	120.47	118.29
2	B	301	UMP	P-O5'-C5'	2.53	125.26	118.30
3	A	304	FAD	C5X-C9A-N10	2.52	119.54	117.72
3	D	303	FAD	P-O3P-PA	-2.49	124.29	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	FAD	C4X-C4-N3	-2.48	120.04	123.43
3	B	209	FAD	C4-C4X-N5	2.46	121.41	118.60
2	C	303	UMP	C2'-C1'-N1	-2.45	108.63	114.27
3	D	303	FAD	C5X-C9A-N10	2.42	119.47	117.72
2	C	303	UMP	OP2-P-O5'	2.41	113.13	106.73
3	B	209	FAD	C4X-C4-N3	-2.36	120.20	123.43
3	A	304	FAD	C4X-C4-N3	-2.34	120.23	123.43
3	D	303	FAD	C4-C4X-N5	2.30	121.22	118.60
3	A	304	FAD	C10-C4X-N5	-2.26	119.69	121.26
3	C	302	FAD	O4'-C4'-C5'	-2.26	104.85	109.92
3	C	302	FAD	C9A-N10-C10	-2.08	119.18	121.91
3	B	209	FAD	O2B-C2B-C1B	-2.08	103.18	110.85
2	D	302	UMP	OP2-P-O5'	2.07	112.25	106.73
3	C	302	FAD	P-O3P-PA	-2.06	125.76	132.83
3	C	302	FAD	C4X-N5-C5X	2.03	118.80	116.77

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	303	UMP	C5'-O5'-P-OP1
2	C	303	UMP	O4'-C4'-C5'-O5'
2	C	303	UMP	C3'-C4'-C5'-O5'
3	C	302	FAD	PA-O3P-P-O2P
3	A	304	FAD	PA-O3P-P-O2P
3	B	209	FAD	PA-O3P-P-O1P
2	C	303	UMP	C5'-O5'-P-OP3
3	C	302	FAD	C2'-C3'-C4'-C5'
3	D	303	FAD	C5'-O5'-P-O1P
3	B	209	FAD	C5'-O5'-P-O1P
3	D	303	FAD	C2'-C3'-C4'-O4'

There are no ring outliers.

7 monomers are involved in 13 short contacts:

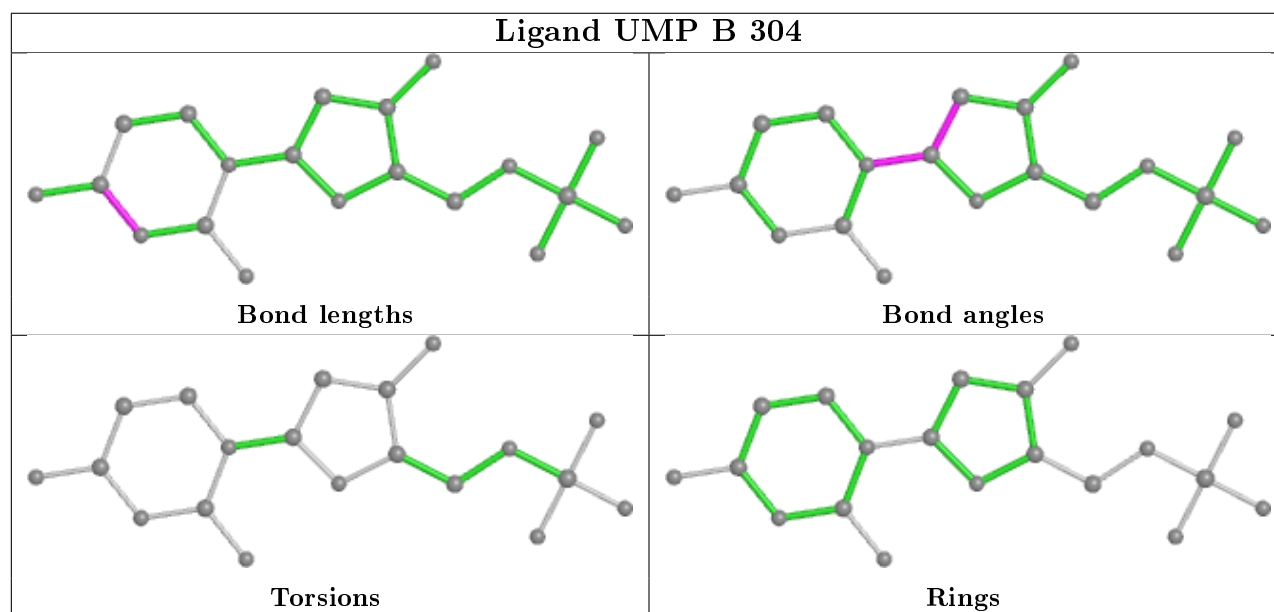
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	304	UMP	2	0
2	C	303	UMP	3	0
3	D	303	FAD	1	0
2	D	302	UMP	2	0
3	B	209	FAD	1	0

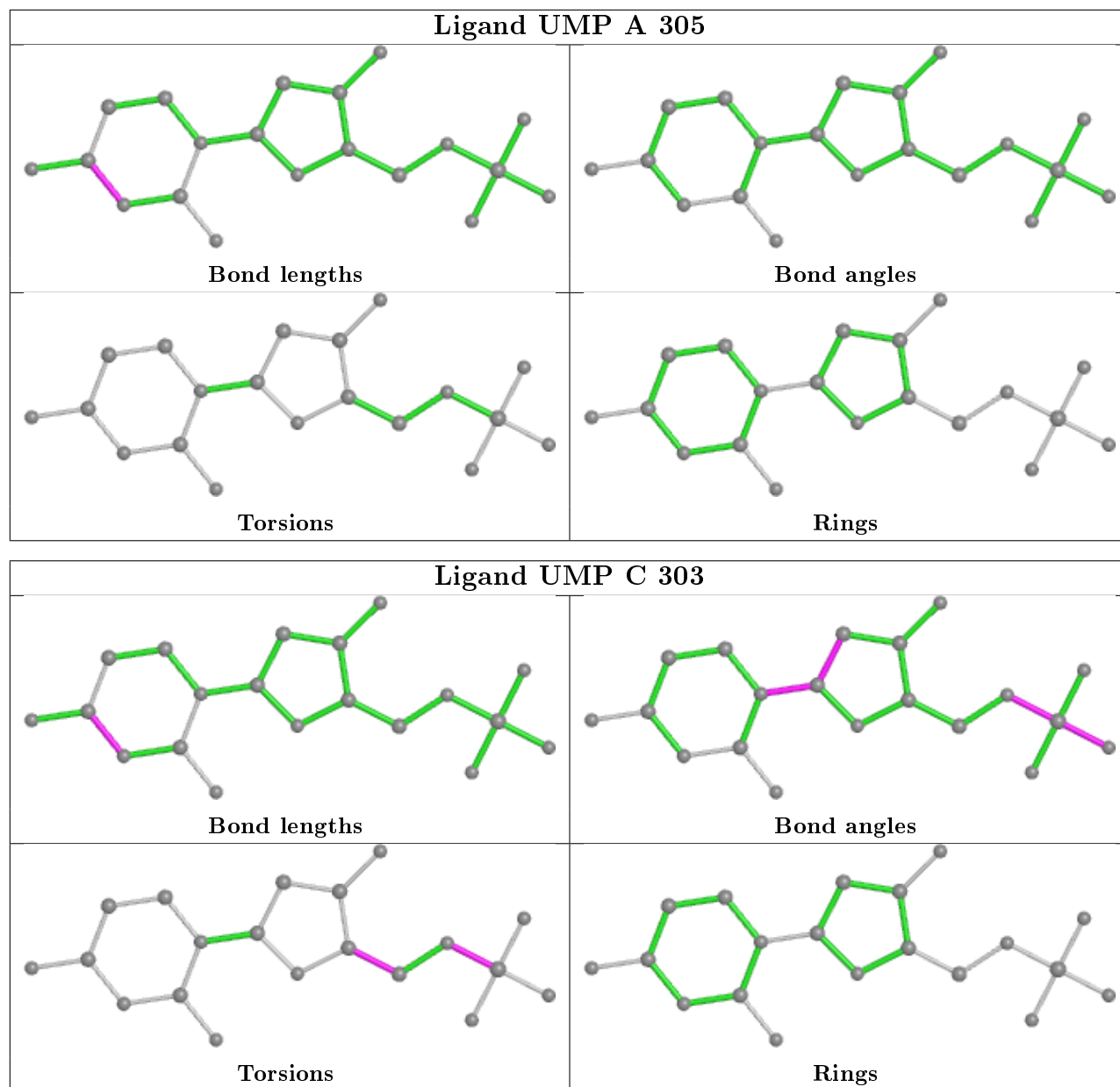
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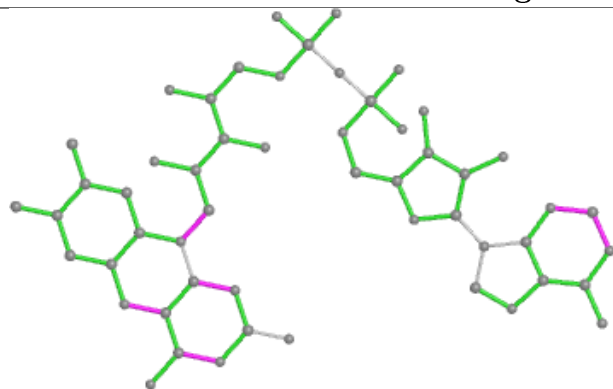
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	UMP	2	0
3	A	304	FAD	2	0

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.

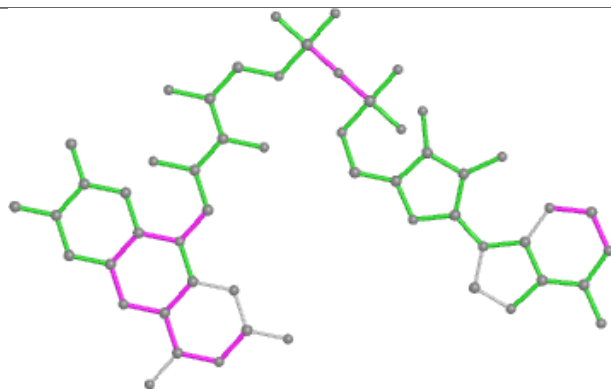




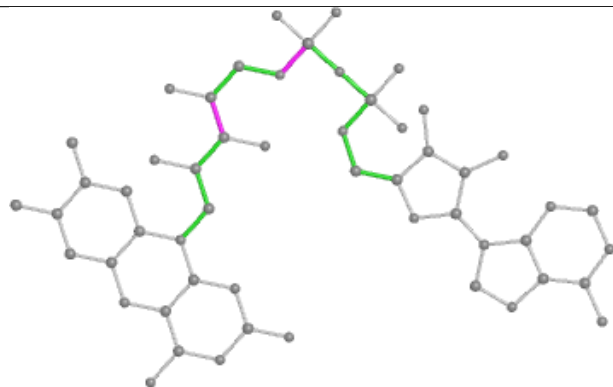
Ligand FAD D 303



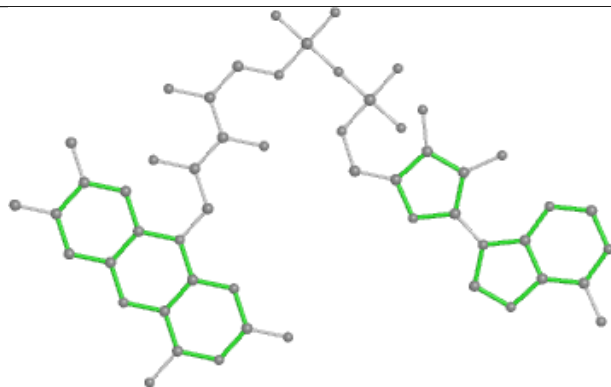
Bond lengths



Bond angles

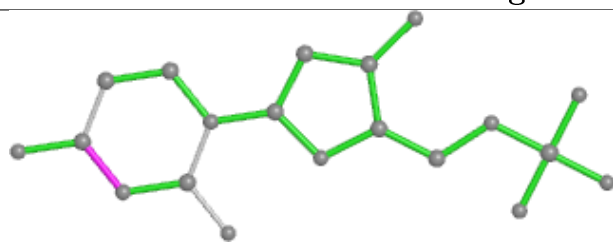


Torsions

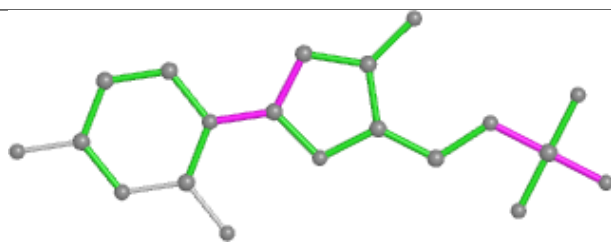


Rings

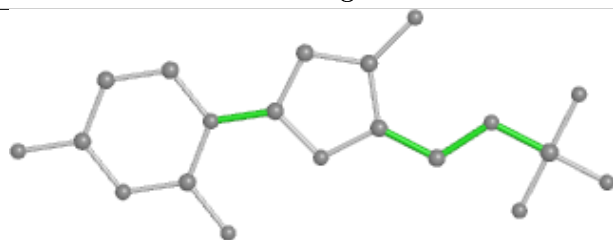
Ligand UMP D 302



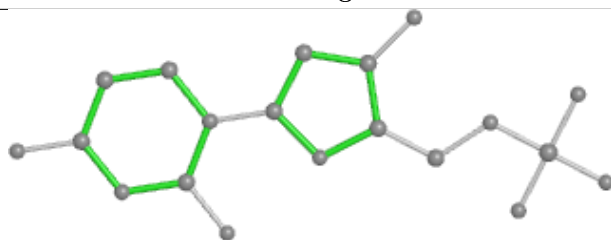
Bond lengths



Bond angles

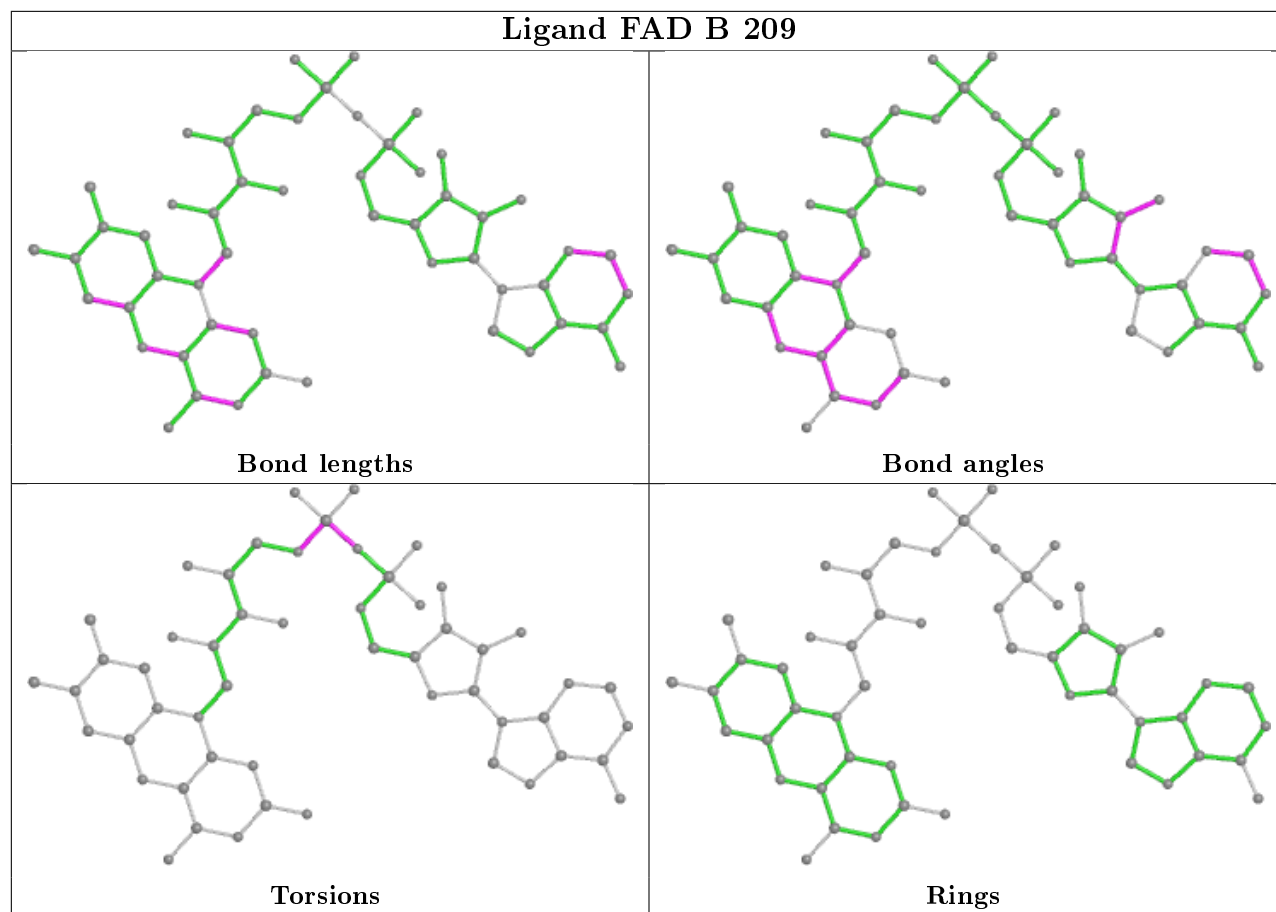


Torsions

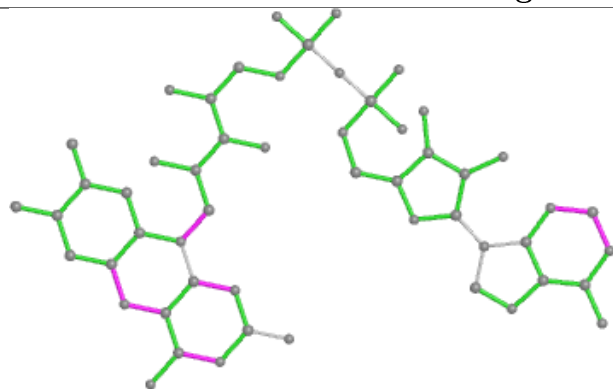


Rings

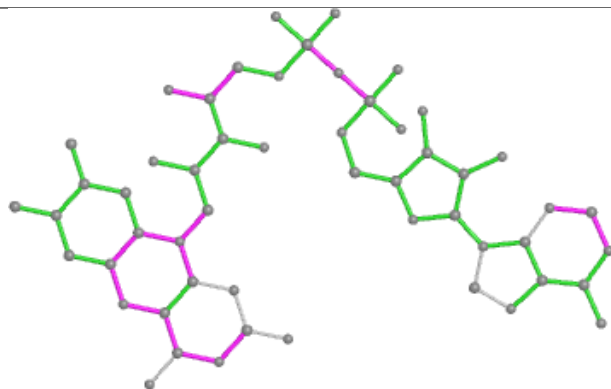
Ligand FAD B 209



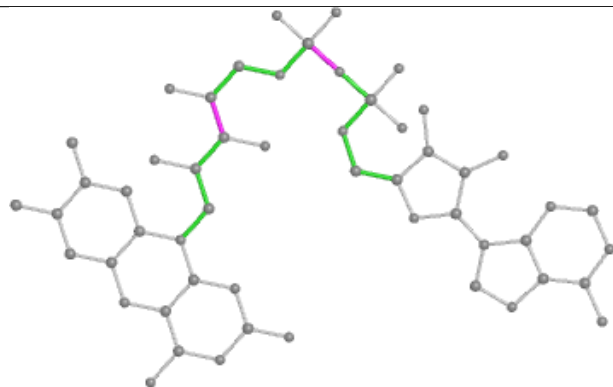
Ligand FAD C 302



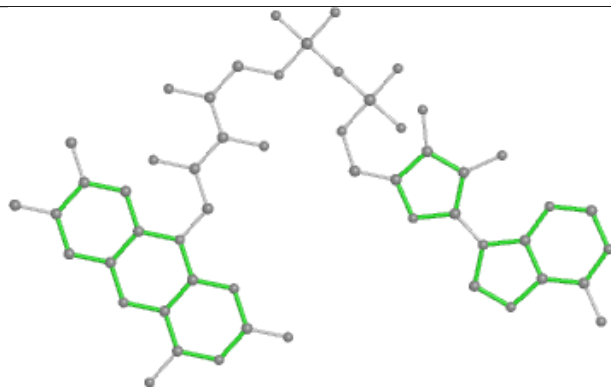
Bond lengths



Bond angles

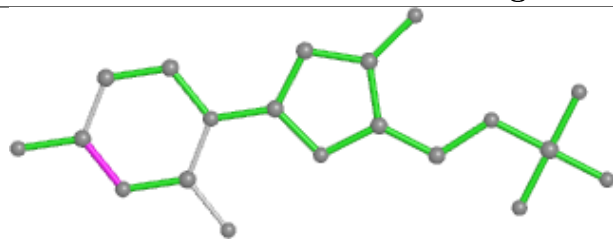


Torsions

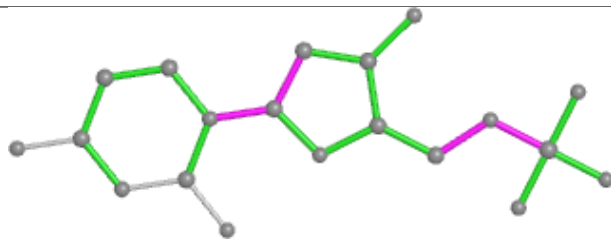


Rings

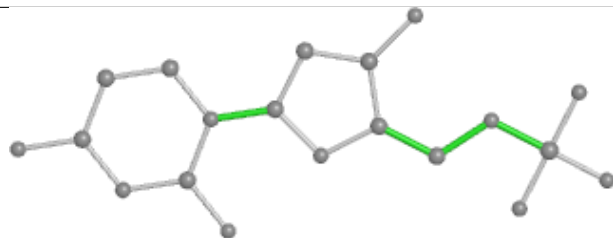
Ligand UMP B 301



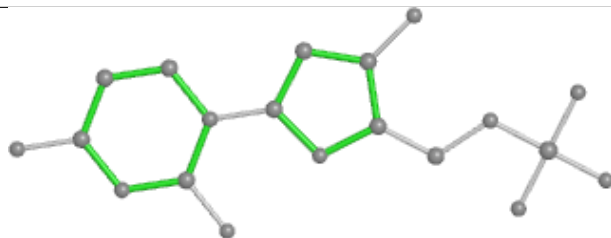
Bond lengths



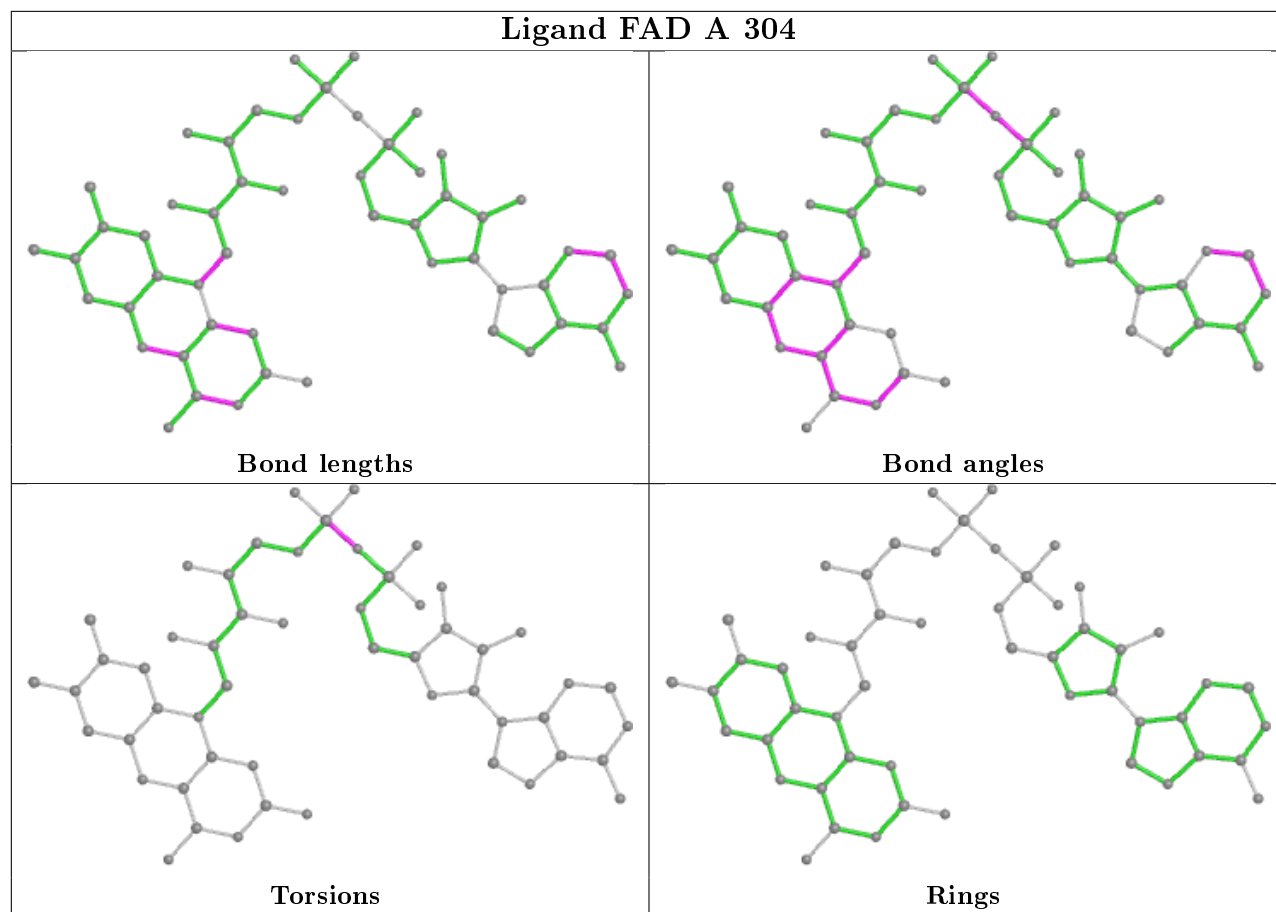
Bond angles



Torsions



Rings



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, 95th 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 ²)	Q<0.9
1	A	209/216 (96%)	0.08	6 (2%) 51 58	25, 38, 61, 79	0
1	B	209/216 (96%)	0.39	23 (11%) 5 7	22, 37, 80, 107	0
1	C	208/216 (96%)	0.66	26 (12%) 3 5	26, 42, 75, 106	0
1	D	208/216 (96%)	0.29	15 (7%) 15 20	27, 42, 69, 81	0
All	All	834/864 (96%)	0.35	70 (8%) 11 15	22, 41, 73, 107	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	CYS	9.9
1	C	27	TYR	9.3
1	B	31	GLY	8.5
1	C	32	GLY	7.1
1	B	25	PHE	6.7
1	C	29	ASP	6.6
1	C	31	GLY	5.8
1	B	33	CYS	5.8
1	B	27	TYR	5.7
1	C	25	PHE	5.3
1	C	87	TYR	5.0
1	B	30	ASP	4.7
1	B	46	PHE	4.7
1	C	28	SER	4.4
1	B	26	GLU	4.1
1	A	208	HIS	4.0
1	C	24	SER	4.0
1	D	26	GLU	4.0
1	B	22	TRP	3.6
1	B	29	ASP	3.5
1	A	205	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	208	HIS	3.5
1	C	69	LEU	3.5
1	B	38	LEU	3.4
1	B	28	SER	3.3
1	D	104	THR	3.3
1	D	69	LEU	3.3
1	C	38	LEU	3.2
1	B	23	GLN	3.2
1	D	33	CYS	3.2
1	B	19	ARG	3.2
1	D	29	ASP	3.2
1	D	107	GLU	3.1
1	D	73	SER	3.1
1	D	94	GLU	3.0
1	B	37	GLU	3.0
1	C	208	HIS	3.0
1	C	37	GLU	2.9
1	B	34	LYS	2.9
1	B	32	GLY	2.9
1	C	73	SER	2.9
1	A	203	GLU	2.8
1	B	35	ASP	2.8
1	C	90	ARG	2.8
1	C	35	ASP	2.7
1	B	12	ASP	2.6
1	C	26	GLU	2.6
1	A	207	LYS	2.5
1	C	80	LEU	2.5
1	D	72	LEU	2.5
1	C	66	ARG	2.5
1	B	45	ILE	2.4
1	A	204	ASP	2.4
1	C	41	ARG	2.4
1	C	72	LEU	2.4
1	C	75	HIS	2.4
1	C	40	HIS	2.3
1	D	30	ASP	2.2
1	C	78	ALA	2.2
1	B	101	LEU	2.2
1	A	30	ASP	2.2
1	B	47	ARG	2.2
1	D	140	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	75	HIS	2.1
1	C	207	LYS	2.1
1	B	40	HIS	2.0
1	B	78	ALA	2.0
1	D	87	TYR	2.0
1	D	103	GLU	2.0
1	C	76	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

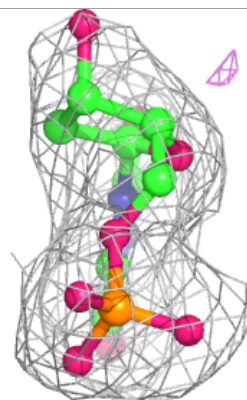
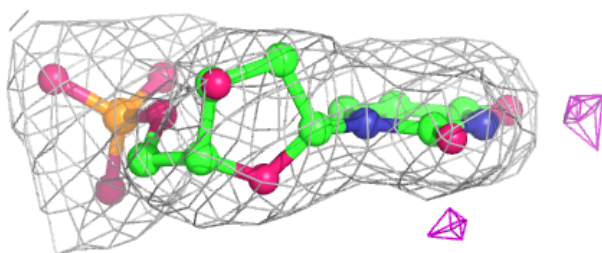
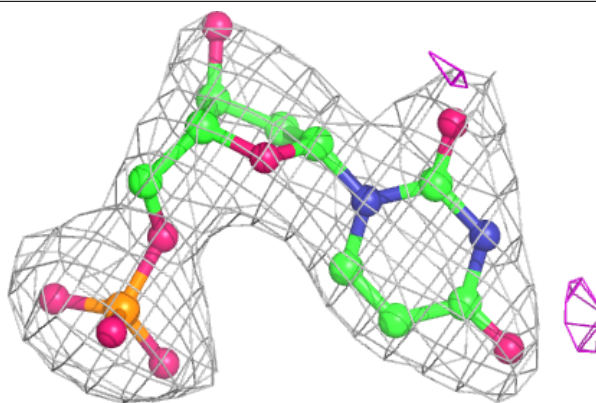
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	UMP	A	305	20/20	0.96	0.13	38,49,59,60	0
2	UMP	B	304	20/20	0.97	0.12	28,35,38,39	0
2	UMP	C	303	20/20	0.97	0.15	33,42,49,50	0
2	UMP	D	302	20/20	0.97	0.10	32,36,39,41	0
3	FAD	C	302	53/53	0.97	0.15	26,32,38,38	0
3	FAD	A	304	53/53	0.97	0.13	28,34,40,42	0
3	FAD	D	303	53/53	0.98	0.13	28,37,43,46	0
2	UMP	B	301	20/20	0.98	0.14	25,30,35,37	0
3	FAD	B	209	53/53	0.98	0.15	24,28,34,35	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.

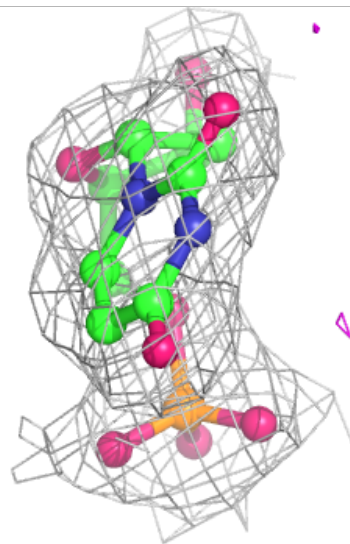
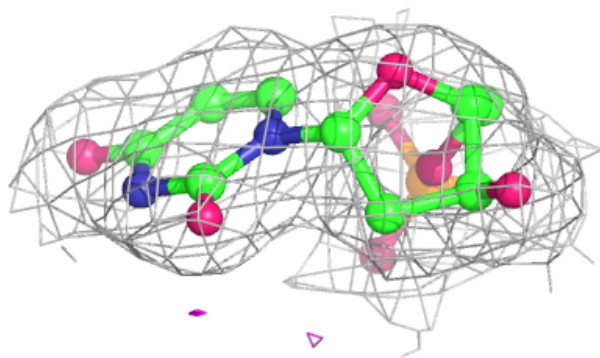
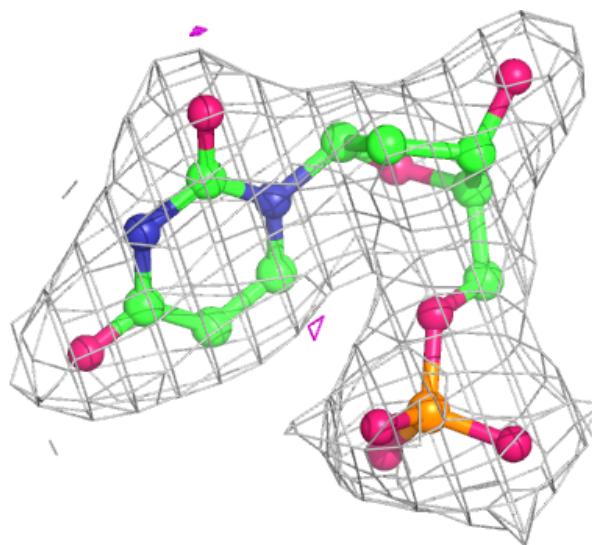
Electron density around UMP A 305:

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



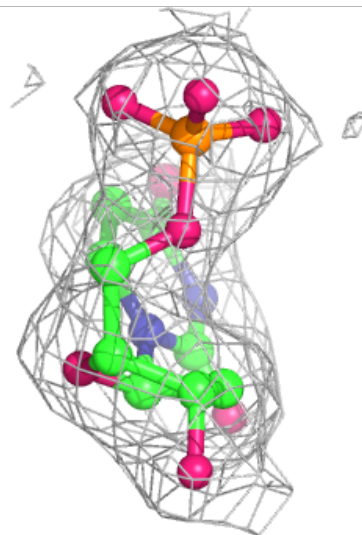
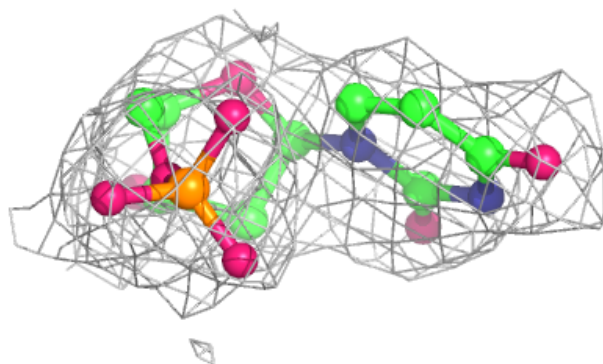
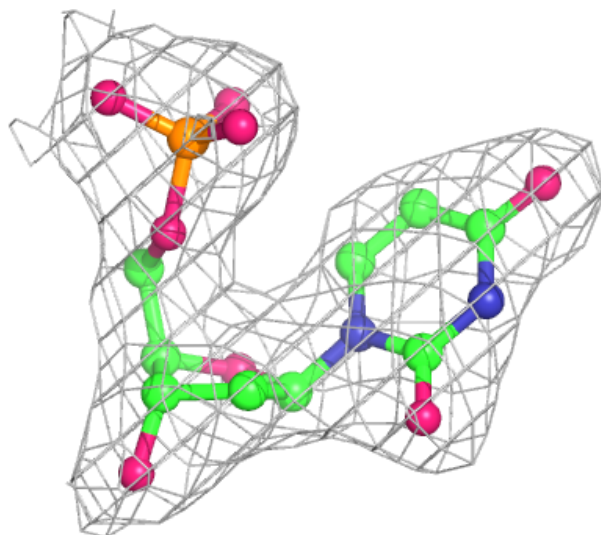
Electron density around UMP B 304:

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



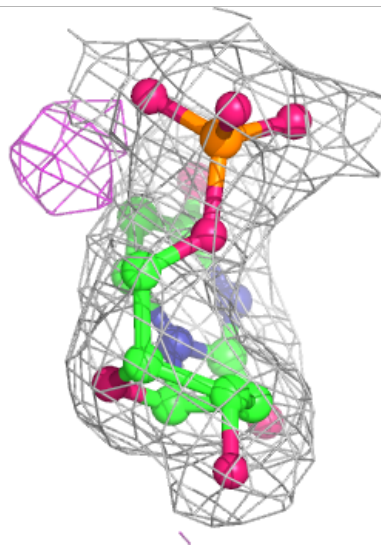
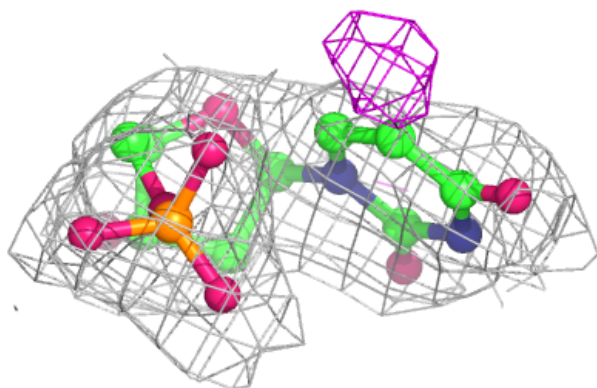
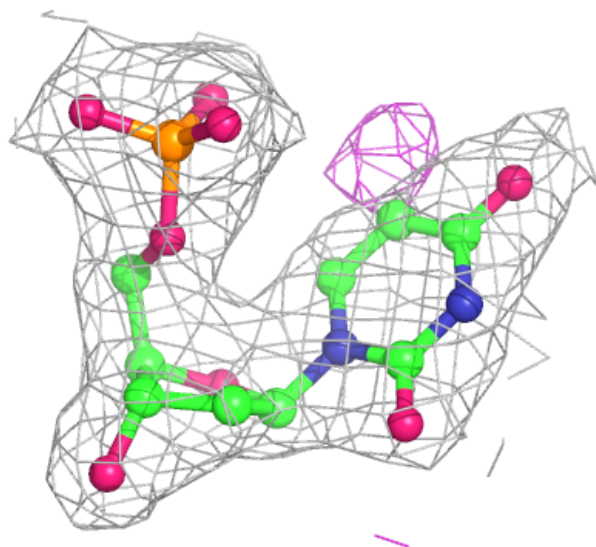
Electron density around UMP C 303:

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



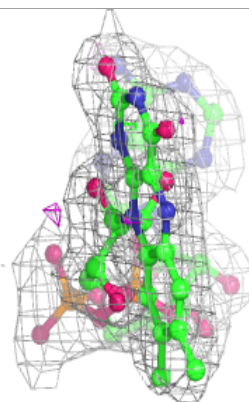
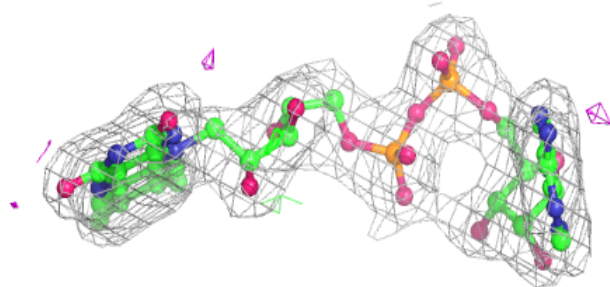
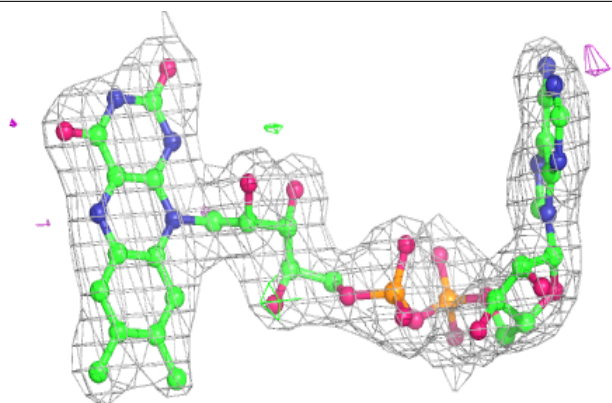
Electron density around UMP D 302:

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

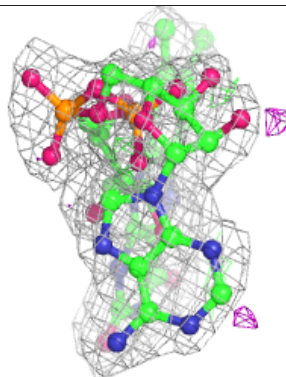
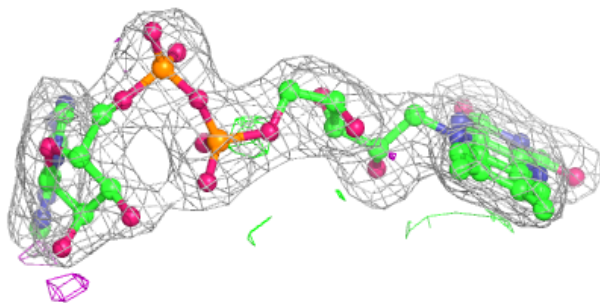
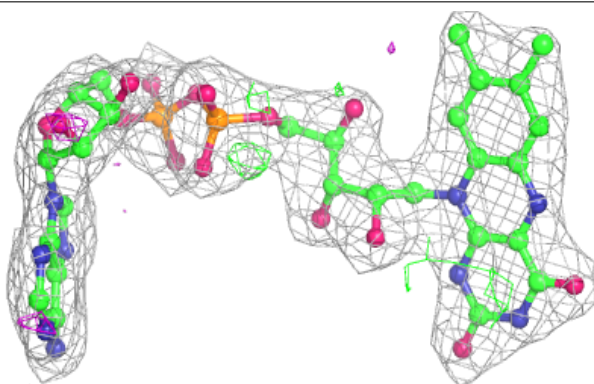


Electron density around FAD C 302:

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

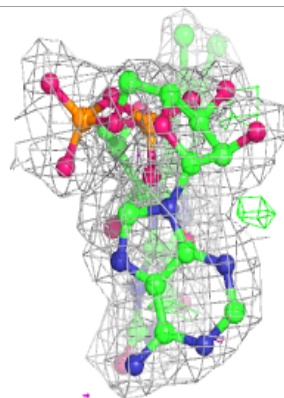
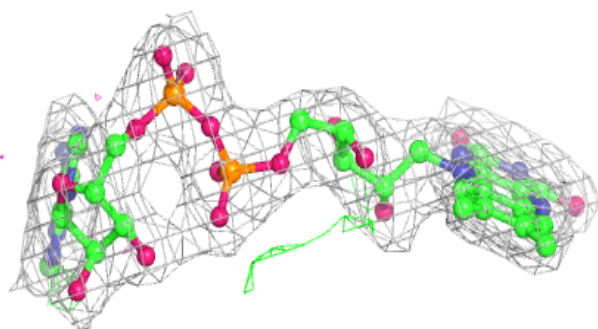
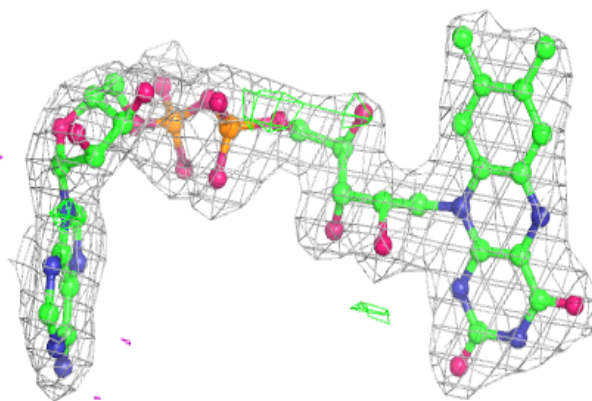
**Electron density around FAD A 304:**

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



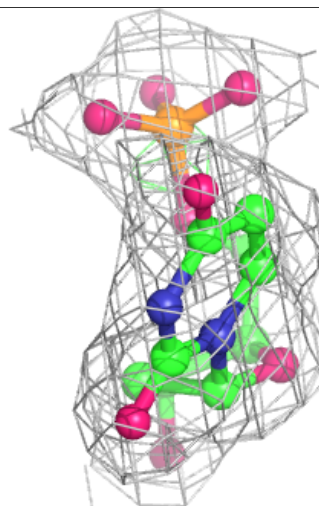
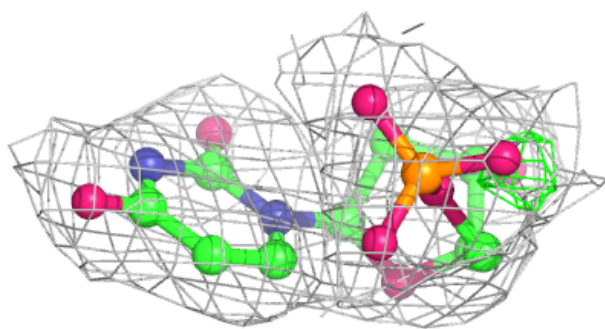
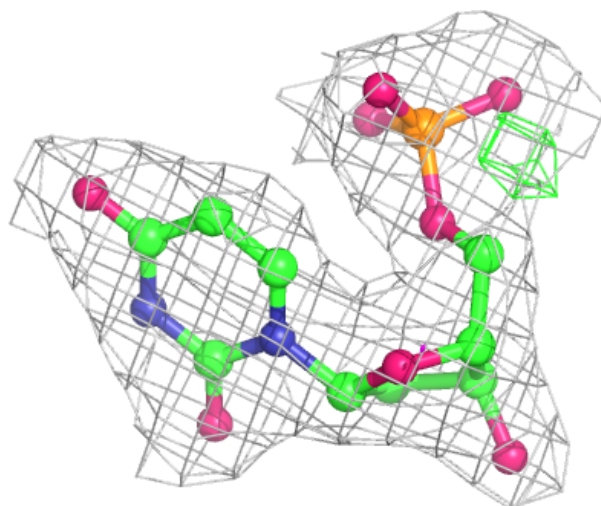
Electron density around FAD D 303:

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



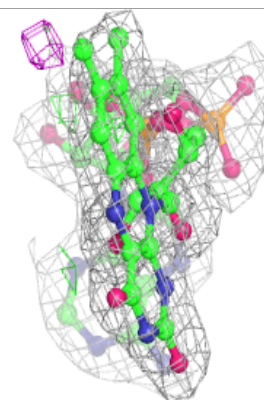
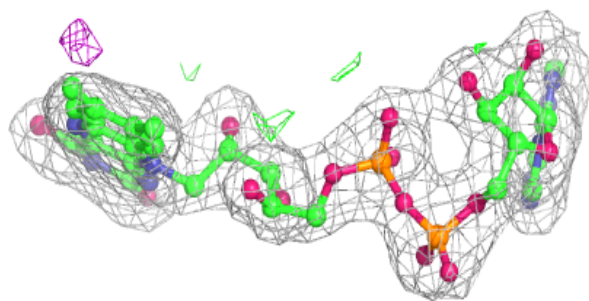
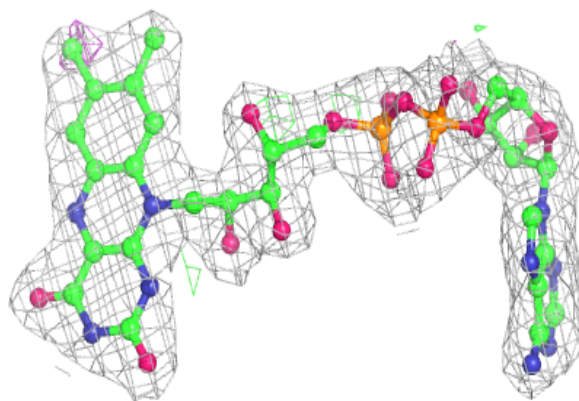
Electron density around UMP B 301:

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



Electron density around FAD B 209:

$2mF_o-DF_c$ (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.