



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:03 PM UTC

PDB ID : 3N3Y / pdb_00003n3y
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 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)	:	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

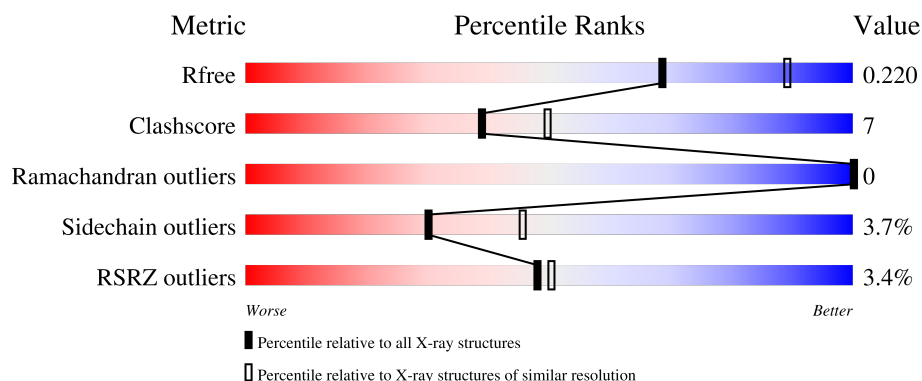
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. 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	4% 82% 13% ..
1	B	216	4% 76% 19% ..
1	C	216	5% 82% 13% ..
1	D	216	79% 16% ..

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:

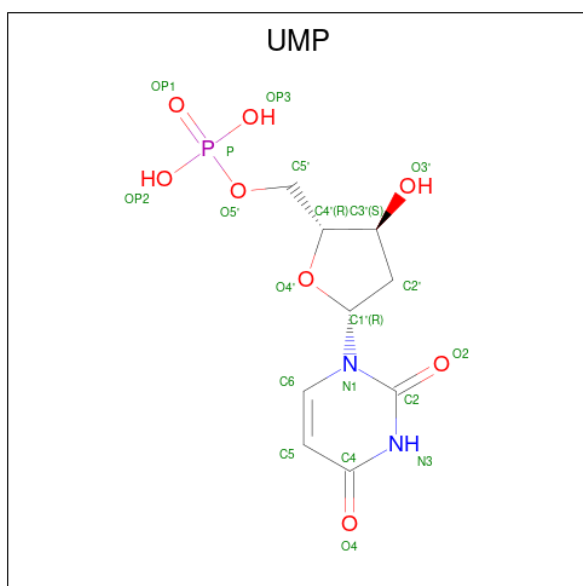
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP Q5UVJ4
A	-6	PRO	-	expression tag	UNP Q5UVJ4
A	-5	LEU	-	expression tag	UNP Q5UVJ4
A	-4	GLY	-	expression tag	UNP Q5UVJ4
A	-3	SER	-	expression tag	UNP Q5UVJ4
A	-2	PRO	-	expression tag	UNP Q5UVJ4
A	-1	GLU	-	expression tag	UNP Q5UVJ4
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 (CCD ID: 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 (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

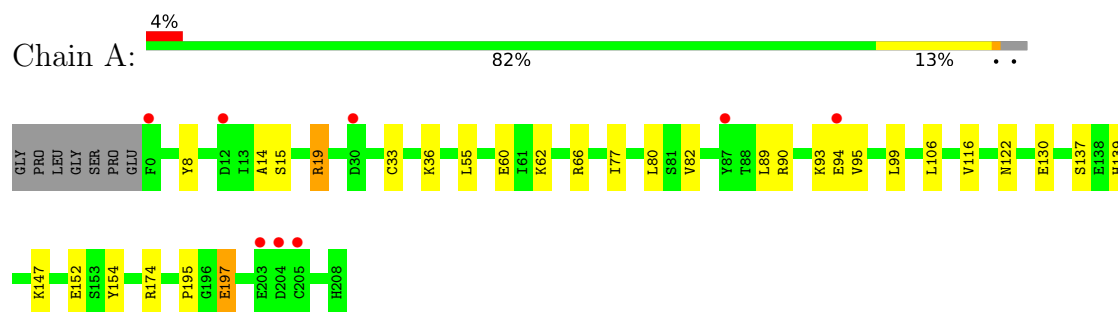
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	41	Total O 41 41	0	0
4	B	41	Total O 41 41	0	0
4	C	24	Total O 24 24	0	0
4	D	41	Total O 41 41	0	0

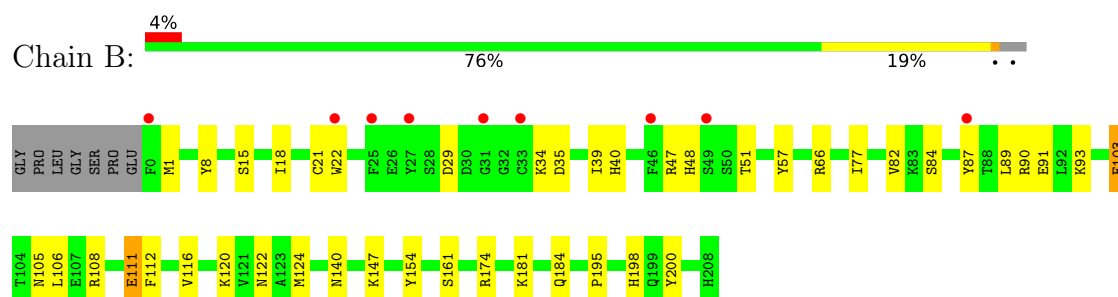
3 Residue-property plots [i](#)

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.

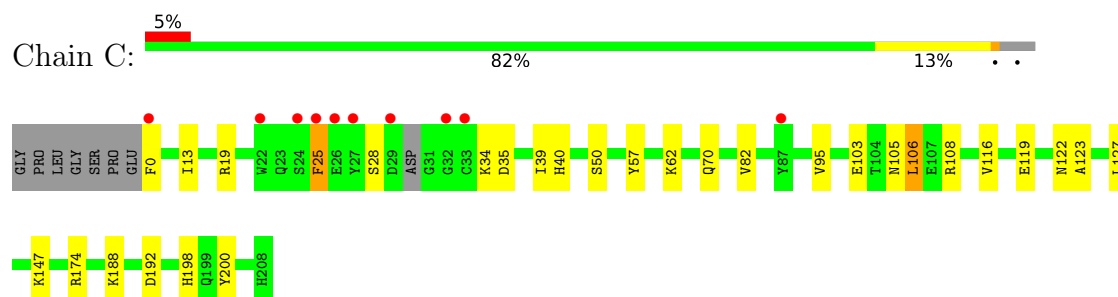
• Molecule 1: Thymidylate synthase thyX



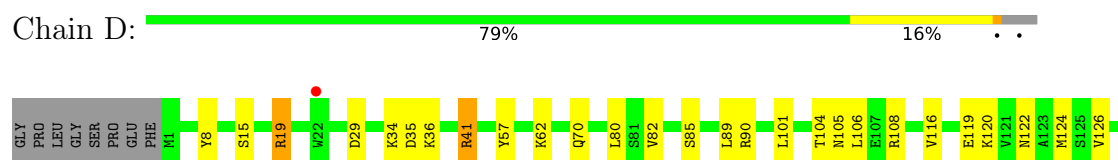
• Molecule 1: Thymidylate synthase thyX



• Molecule 1: Thymidylate synthase thyX



• Molecule 1: Thymidylate synthase thyX



S137	
K147	
H157	
Q168	
R174	
P195	
H198	
C205	
L206	
K207	
H208	

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 0.171 , 0.220	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 , 40.3	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	0.56	0/1735	0.76	0/2335
1	B	0.51	0/1735	0.76	1/2335 (0.0%)
1	C	0.51	0/1726	0.73	0/2321
1	D	0.52	0/1729	0.76	0/2327
All	All	0.52	0/6925	0.76	1/9318 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ILE	N-CA-C	5.53	112.13	106.21

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	33	0
1	C	1695	0	1695	24	0
1	D	1695	0	1696	23	0
2	A	20	0	11	0	0
2	B	40	0	22	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	20	0	11	3	0
2	D	20	0	11	2	0
3	A	53	0	31	1	0
3	B	53	0	31	0	0
3	C	53	0	31	0	0
3	D	53	0	31	0	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:HH11	1:D:41:ARG:HG3	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:103:GLU:CD	1:B:103:GLU:H	1.93	0.77
1:B:116:VAL:H	1:B:122:ASN:HD21	1.31	0.76
1:A:197:GLU:HB3	4:A:220:HOH:O	1.92	0.69
1:D:41:ARG:HH11	1:D:41:ARG:CG	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:CD1	1:C:0:PHE:O	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:C:40:HIS:HB2	1:C:200:TYR:HE2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:90:ARG:HH12	1:B:93:LYS:HZ2	1.51	0.55
1:A:139:HIS:ND1	1:B:120:LYS:HE3	2.21	0.55
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
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
1:C:19:ARG:HD2	1:C:28:SER:HB2	1.95	0.48
1:C:123:ALA:O	1:C:127:LEU:HG	2.13	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:HD12	1:C:106:LEU:HA	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:B:29:ASP:CG	1:B:34:LYS:HB2	2.43	0.44
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:HB2	1:C:62:LYS:HE2	1.73	0.44
1:A:99:LEU:HG	1:A:130:GLU:HG2	1.99	0.43
1:B:89:LEU:C	1:B:91:GLU:H	2.25	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:HD23	1:D:89:LEU:HA	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:B:89:LEU:C	1:B:91:GLU:N	2.78	0.41
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:A:15:SER:O	1:A:19:ARG:HG3	2.20	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:B:111:GLU:HG2	1:B:112:PHE:CD2	2.55	0.41
1:D:206:LEU:O	1:D:208:HIS:CD2	2.74	0.41
1:A:8:TYR:CE2	1:A:195:PRO:HG3	2.56	0.40
1:A:80:LEU:HD12	1:A:80:LEU:N	2.36	0.40
1:B:174:ARG:O	1:B:184:GLN:HA	2.21	0.40
1:B:181:LYS:HA	1:B:181:LYS:HD2	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%)	26	39
1	B	188/193 (97%)	183 (97%)	5 (3%)	39	58
1	C	187/193 (97%)	180 (96%)	7 (4%)	30	45
1	D	188/193 (97%)	180 (96%)	8 (4%)	26	39
All	All	751/772 (97%)	723 (96%)	28 (4%)	30	45

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	90	ARG
1	A	94	GLU
1	A	95	VAL
1	A	106	LEU
1	A	147	LYS
1	A	152	GLU
1	A	197	GLU

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Mol	Chain	Res	Type
1	B	1	MET
1	B	103	GLU
1	B	106	LEU
1	B	111	GLU
1	B	147	LYS
1	C	13	ILE
1	C	25	PHE
1	C	95	VAL
1	C	103	GLU
1	C	106	LEU
1	C	119	GLU
1	C	147	LYS
1	D	19	ARG
1	D	36	LYS
1	D	41	ARG
1	D	80	LEU
1	D	101	LEU
1	D	106	LEU
1	D	119	GLU
1	D	137	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	105	ASN
1	A	122	ASN
1	A	131	ASN
1	A	140	ASN
1	A	168	GLN
1	A	198	HIS
1	B	40	HIS
1	B	70	GLN
1	B	105	ASN
1	B	122	ASN
1	B	131	ASN
1	B	140	ASN
1	B	198	HIS
1	B	199	GLN
1	C	105	ASN
1	C	122	ASN
1	C	131	ASN

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Mol	Chain	Res	Type
1	C	139	HIS
1	C	168	GLN
1	C	198	HIS
1	D	44	ASN
1	D	48	HIS
1	D	70	GLN
1	D	105	ASN
1	D	122	ASN
1	D	131	ASN
1	D	140	ASN
1	D	168	GLN
1	D	198	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](#)

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	A	305	-	21,21,21	0.90	1 (4%)	30,31,31	1.80	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	C	302	-	58,58,58	1.12	7 (12%)	85,89,89	1.53	17 (20%)
2	UMP	C	303	-	21,21,21	0.88	1 (4%)	30,31,31	1.60	7 (23%)
2	UMP	D	302	-	21,21,21	0.95	1 (4%)	30,31,31	1.81	7 (23%)
3	FAD	D	303	-	58,58,58	1.12	7 (12%)	85,89,89	1.50	15 (17%)
2	UMP	B	301	-	21,21,21	0.83	0	30,31,31	1.71	6 (20%)
3	FAD	B	209	-	58,58,58	1.06	5 (8%)	85,89,89	1.58	19 (22%)
2	UMP	B	304	-	21,21,21	0.81	0	30,31,31	1.68	6 (20%)
3	FAD	A	304	-	58,58,58	1.04	4 (6%)	85,89,89	1.58	16 (18%)

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	A	305	-	-	0/10/22/22	0/2/2/2
3	FAD	C	302	-	-	2/34/50/50	0/6/6/6
2	UMP	C	303	-	-	4/10/22/22	0/2/2/2
2	UMP	D	302	-	-	0/10/22/22	0/2/2/2
3	FAD	D	303	-	-	2/34/50/50	0/6/6/6
2	UMP	B	301	-	-	0/10/22/22	0/2/2/2
3	FAD	B	209	-	-	2/34/50/50	0/6/6/6
2	UMP	B	304	-	-	0/10/22/22	0/2/2/2
3	FAD	A	304	-	-	1/34/50/50	0/6/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	FAD	C4X-N5	3.81	1.39	1.30
3	D	303	FAD	C4X-N5	3.54	1.38	1.30
3	B	209	FAD	C4X-N5	3.25	1.37	1.30
3	A	304	FAD	C4X-N5	3.14	1.37	1.30
3	C	302	FAD	C10-N1	2.91	1.39	1.33
3	D	303	FAD	PA-O3P	2.89	1.62	1.59
3	D	303	FAD	C2A-N1A	2.66	1.38	1.33
3	C	302	FAD	PA-O3P	2.64	1.62	1.59
3	A	304	FAD	C10-N1	2.60	1.38	1.33
3	D	303	FAD	P-O3P	2.59	1.62	1.59
3	A	304	FAD	C2A-N1A	2.53	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	209	FAD	C2A-N3A	2.52	1.38	1.33
3	B	209	FAD	C2A-N1A	2.40	1.38	1.33
3	C	302	FAD	C2A-N1A	2.33	1.38	1.33
3	B	209	FAD	C10-N1	2.28	1.37	1.33
2	D	302	UMP	C5-C4	-2.28	1.38	1.43
3	D	303	FAD	C2A-N3A	2.20	1.37	1.33
3	C	302	FAD	P-O3P	2.15	1.61	1.59
3	D	303	FAD	C10-N1	2.15	1.37	1.33
3	C	302	FAD	C2A-N3A	2.13	1.37	1.33
3	D	303	FAD	C8A-N7A	2.13	1.35	1.31
3	B	209	FAD	C8A-N7A	2.11	1.35	1.31
3	C	302	FAD	C8A-N7A	2.04	1.35	1.31
3	A	304	FAD	C2A-N3A	2.04	1.37	1.33
2	C	303	UMP	C6-C5	2.02	1.39	1.35
2	A	305	UMP	C5-C4	-2.01	1.39	1.43

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	305	UMP	C4-N3-C2	-5.78	119.43	126.61
3	C	302	FAD	N3A-C2A-N1A	-5.70	119.95	128.58
3	B	209	FAD	N3A-C2A-N1A	-5.61	120.09	128.58
3	D	303	FAD	N3A-C2A-N1A	-5.56	120.17	128.58
2	D	302	UMP	C4-N3-C2	-5.52	119.76	126.61
3	A	304	FAD	N3A-C2A-N1A	-5.36	120.47	128.58
2	B	304	UMP	C4-N3-C2	-5.31	120.02	126.61
2	B	301	UMP	C4-N3-C2	-5.28	120.06	126.61
3	A	304	FAD	N9A-C8A-N7A	-4.59	107.42	113.94
2	C	303	UMP	C4-N3-C2	-4.58	120.92	126.61
2	A	305	UMP	C5-C4-N3	4.21	120.70	114.80
2	B	301	UMP	C5-C4-N3	4.19	120.67	114.80
3	C	302	FAD	N9A-C8A-N7A	-4.18	108.00	113.94
3	D	303	FAD	N9A-C8A-N7A	-4.15	108.05	113.94
2	A	305	UMP	N3-C2-N1	3.99	120.09	114.89
3	B	209	FAD	N9A-C8A-N7A	-3.94	108.34	113.94
2	D	302	UMP	N3-C2-N1	3.90	119.97	114.89
2	B	304	UMP	N3-C2-N1	3.84	119.89	114.89
3	B	209	FAD	C5A-C4A-N3A	-3.80	121.48	126.72
3	A	304	FAD	C5A-C4A-N3A	-3.77	121.53	126.72
3	A	304	FAD	C5A-N7A-C8A	3.76	109.36	103.45
3	B	209	FAD	C4-N3-C2	-3.70	119.06	125.64
2	D	302	UMP	C5-C4-N3	3.68	119.95	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	FAD	C5A-C4A-N3A	-3.67	121.66	126.72
2	B	304	UMP	C5-C4-N3	3.60	119.85	114.80
2	C	303	UMP	C5-C4-N3	3.58	119.82	114.80
3	A	304	FAD	C4-N3-C2	-3.46	119.50	125.64
3	D	303	FAD	C5A-N7A-C8A	3.40	108.80	103.45
3	D	303	FAD	C5A-C4A-N3A	-3.40	122.04	126.72
3	C	302	FAD	C5A-N7A-C8A	3.29	108.62	103.45
3	B	209	FAD	C4X-C10-N10	3.29	121.19	116.48
3	D	303	FAD	C4X-C10-N10	3.27	121.16	116.48
3	C	302	FAD	C2A-N3A-C4A	3.26	119.80	111.83
2	B	301	UMP	N3-C2-N1	3.25	119.13	114.89
2	C	303	UMP	N3-C2-N1	3.25	119.12	114.89
3	B	209	FAD	C10-C4X-N5	-3.20	118.28	124.81
2	D	302	UMP	O2-C2-N1	-3.13	118.73	122.80
2	D	302	UMP	O4-C4-C5	-3.12	119.78	125.16
3	B	209	FAD	C5A-N7A-C8A	3.11	108.34	103.45
3	B	209	FAD	C2A-N3A-C4A	3.04	119.25	111.83
3	A	304	FAD	C2A-N3A-C4A	2.97	119.08	111.83
3	D	303	FAD	C4-N3-C2	-2.96	120.38	125.64
2	B	301	UMP	O4-C4-C5	-2.96	120.06	125.16
3	C	302	FAD	C4-N3-C2	-2.92	120.45	125.64
3	C	302	FAD	C4X-C10-N10	2.88	120.60	116.48
2	D	302	UMP	C2'-C1'-N1	-2.85	106.68	113.81
3	A	304	FAD	C4X-C10-N10	2.83	120.53	116.48
3	D	303	FAD	C2A-N3A-C4A	2.80	118.68	111.83
3	D	303	FAD	C10-C4X-N5	-2.75	119.20	124.81
3	A	304	FAD	C4A-N9A-C8A	2.74	108.62	105.74
3	A	304	FAD	C4X-C4-N3	2.74	120.23	113.25
3	B	209	FAD	C4X-C4-N3	2.73	120.20	113.25
2	C	303	UMP	O2-C2-N1	-2.72	119.26	122.80
2	B	301	UMP	C2'-C1'-N1	-2.68	107.11	113.81
3	A	304	FAD	N3A-C4A-N9A	2.68	131.72	127.17
3	C	302	FAD	C4X-C4-N3	2.67	120.04	113.25
3	B	209	FAD	C4X-C10-N1	-2.62	118.17	124.59
2	A	305	UMP	O4-C4-C5	-2.61	120.67	125.16
2	B	304	UMP	O2-C2-N1	-2.60	119.41	122.80
2	B	304	UMP	O4-C4-C5	-2.56	120.74	125.16
2	A	305	UMP	O4'-C1'-N1	2.53	112.36	107.86
3	C	302	FAD	O2A-PA-O3P	2.52	114.08	107.27
3	B	209	FAD	N3A-C4A-N9A	2.51	131.43	127.17
3	A	304	FAD	C10-C4X-N5	-2.51	119.69	124.81
2	C	303	UMP	OP2-P-O5'	2.48	113.13	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	FAD	N3A-C4A-N9A	2.46	131.36	127.17
3	D	303	FAD	C4A-C5A-N7A	-2.43	107.81	110.58
3	C	302	FAD	C4A-N9A-C8A	2.41	108.27	105.74
3	C	302	FAD	O2P-P-O3P	2.41	113.78	107.27
3	A	304	FAD	C4X-C10-N1	-2.39	118.72	124.59
2	B	304	UMP	C2'-C1'-N1	-2.39	107.84	113.81
3	A	304	FAD	C4A-C5A-N7A	-2.38	107.86	110.58
3	D	303	FAD	C4X-C4-N3	2.38	119.31	113.25
3	A	304	FAD	C9A-C5X-N5	-2.35	119.96	122.45
3	B	209	FAD	C4A-N9A-C8A	2.34	108.20	105.74
3	C	302	FAD	C5X-C9A-N10	2.34	120.08	117.97
2	C	303	UMP	O4-C4-C5	-2.33	121.14	125.16
3	C	302	FAD	O4'-C4'-C5'	-2.33	104.85	109.99
3	B	209	FAD	C4-C4X-N5	2.32	121.41	118.21
3	B	209	FAD	C10-N1-C2	2.31	121.84	116.85
2	A	305	UMP	O2-C2-N1	-2.28	119.83	122.80
2	B	301	UMP	O2-C2-N1	-2.24	119.88	122.80
3	B	209	FAD	C4A-C5A-N7A	-2.23	108.03	110.58
3	D	303	FAD	C4A-N9A-C8A	2.21	108.06	105.74
3	D	303	FAD	O4-C4-C4X	-2.18	120.77	126.53
3	D	303	FAD	C4-C4X-N5	2.18	121.22	118.21
3	B	209	FAD	O3'-C3'-C4'	-2.18	103.99	108.93
3	C	302	FAD	C4A-C5A-N7A	-2.14	108.13	110.58
3	A	304	FAD	O4-C4-C4X	-2.14	120.87	126.53
2	D	302	UMP	OP2-P-O5'	2.14	112.25	106.67
3	B	209	FAD	O4-C4-C4X	-2.14	120.89	126.53
3	D	303	FAD	C9A-C5X-N5	-2.10	120.23	122.45
2	C	303	UMP	C2'-C1'-N1	-2.07	108.63	113.81
3	C	302	FAD	C10-C4X-N5	-2.07	120.58	124.81
3	D	303	FAD	N3A-C4A-N9A	2.06	130.67	127.17
3	B	209	FAD	C5X-N5-C4X	2.05	121.41	118.09
3	A	304	FAD	O2P-P-O3P	2.03	112.75	107.27
3	C	302	FAD	O4-C4-C4X	-2.02	121.20	126.53
3	B	209	FAD	O2B-C2B-C1B	-2.01	103.18	110.10

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'

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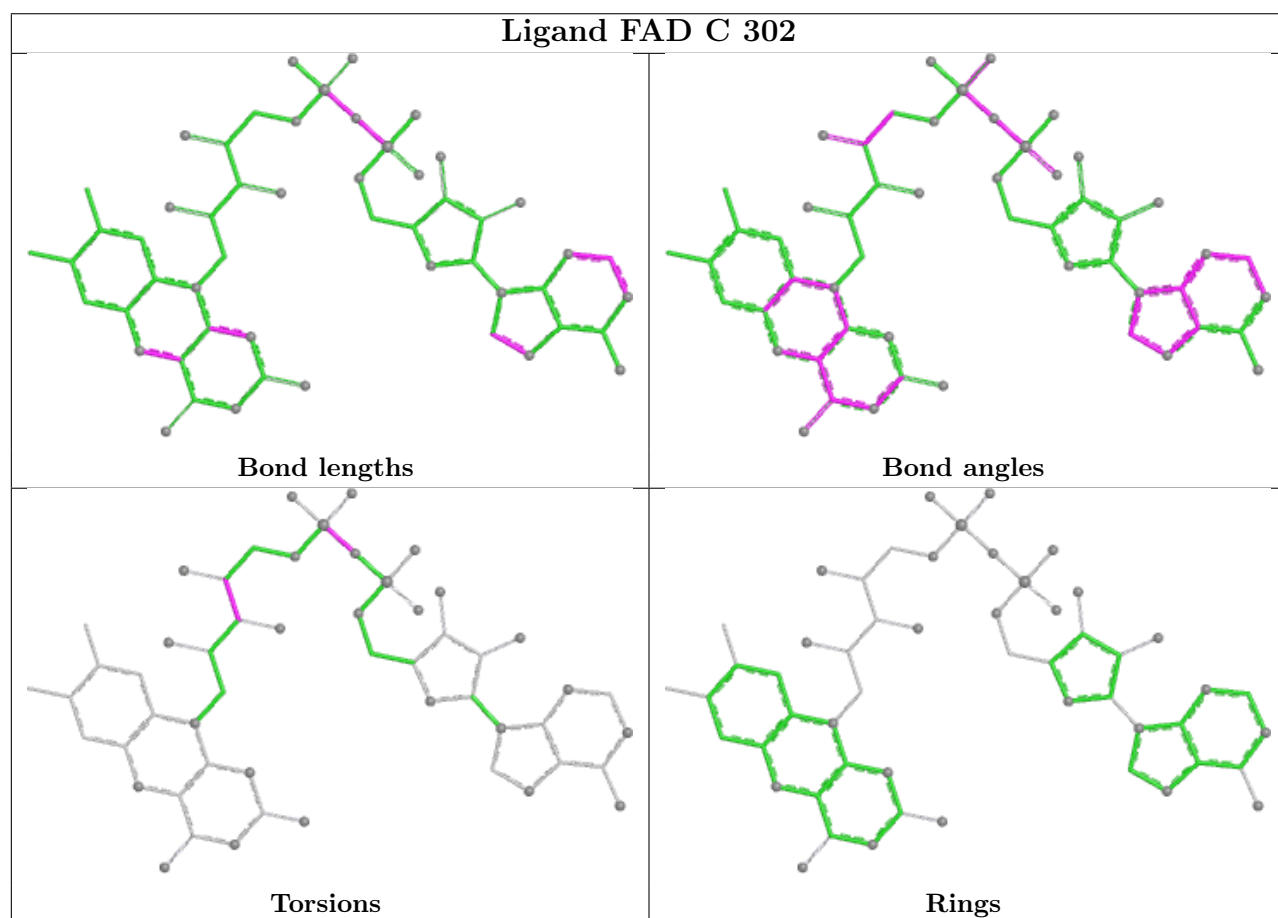
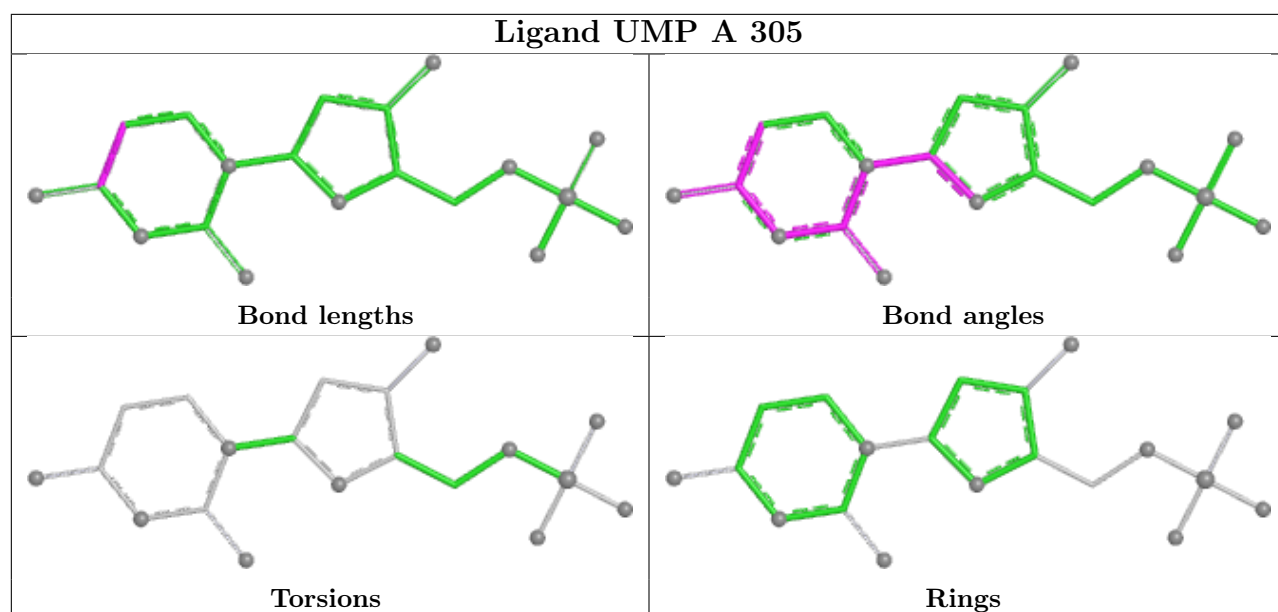
Mol	Chain	Res	Type	Atoms
3	B	209	FAD	C5'-O5'-P-O1P
3	D	303	FAD	C5'-O5'-P-O1P
3	A	304	FAD	PA-O3P-P-O2P
3	C	302	FAD	PA-O3P-P-O2P
3	C	302	FAD	C2'-C3'-C4'-C5'
3	D	303	FAD	C2'-C3'-C4'-O4'
3	B	209	FAD	PA-O3P-P-O1P
2	C	303	UMP	C5'-O5'-P-OP3

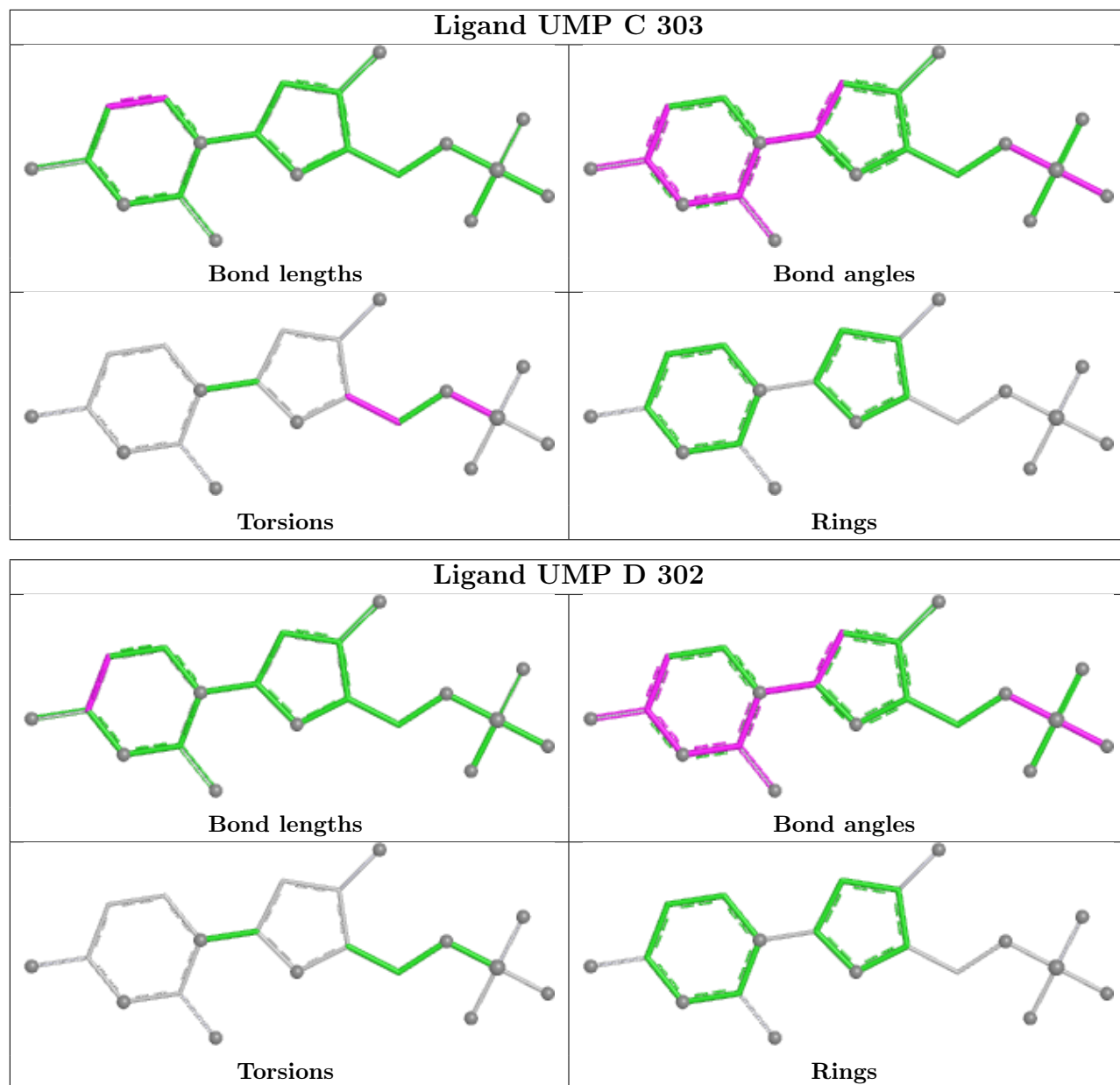
There are no ring outliers.

5 monomers are involved in 10 short contacts:

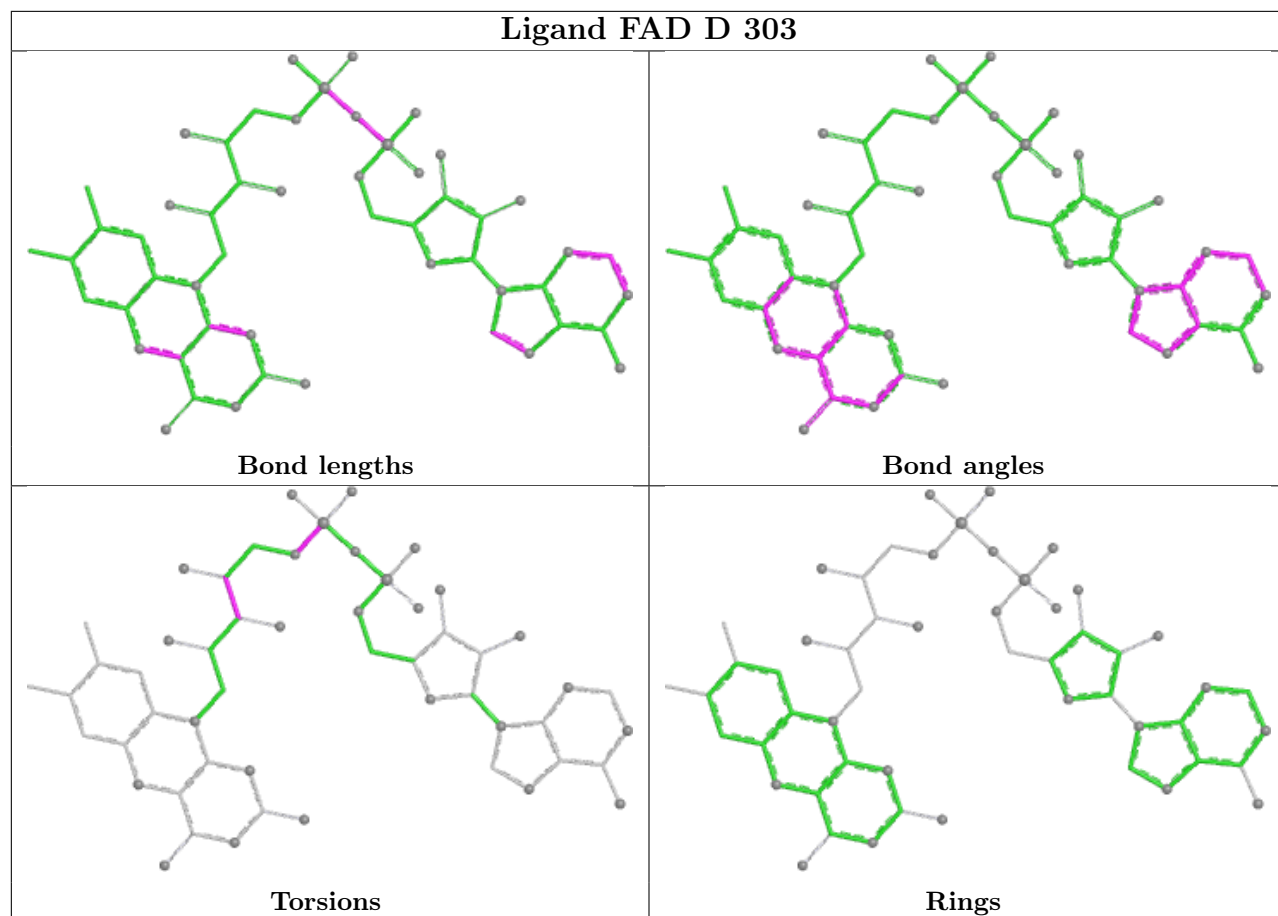
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	303	UMP	3	0
2	D	302	UMP	2	0
2	B	301	UMP	2	0
2	B	304	UMP	2	0
3	A	304	FAD	1	0

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.

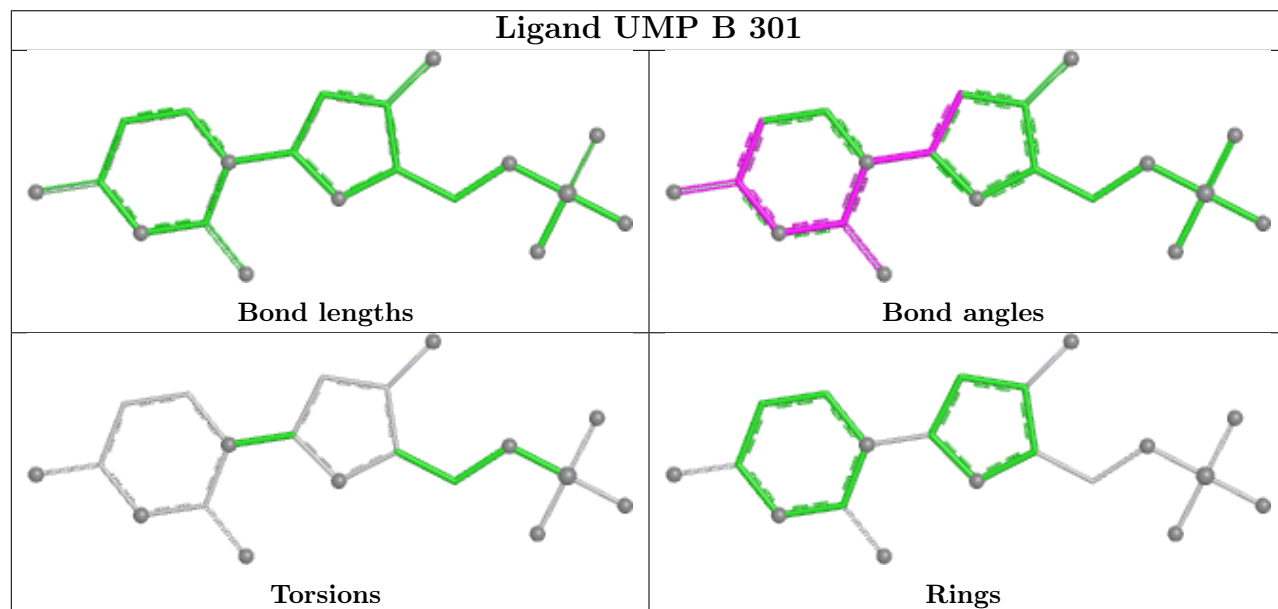




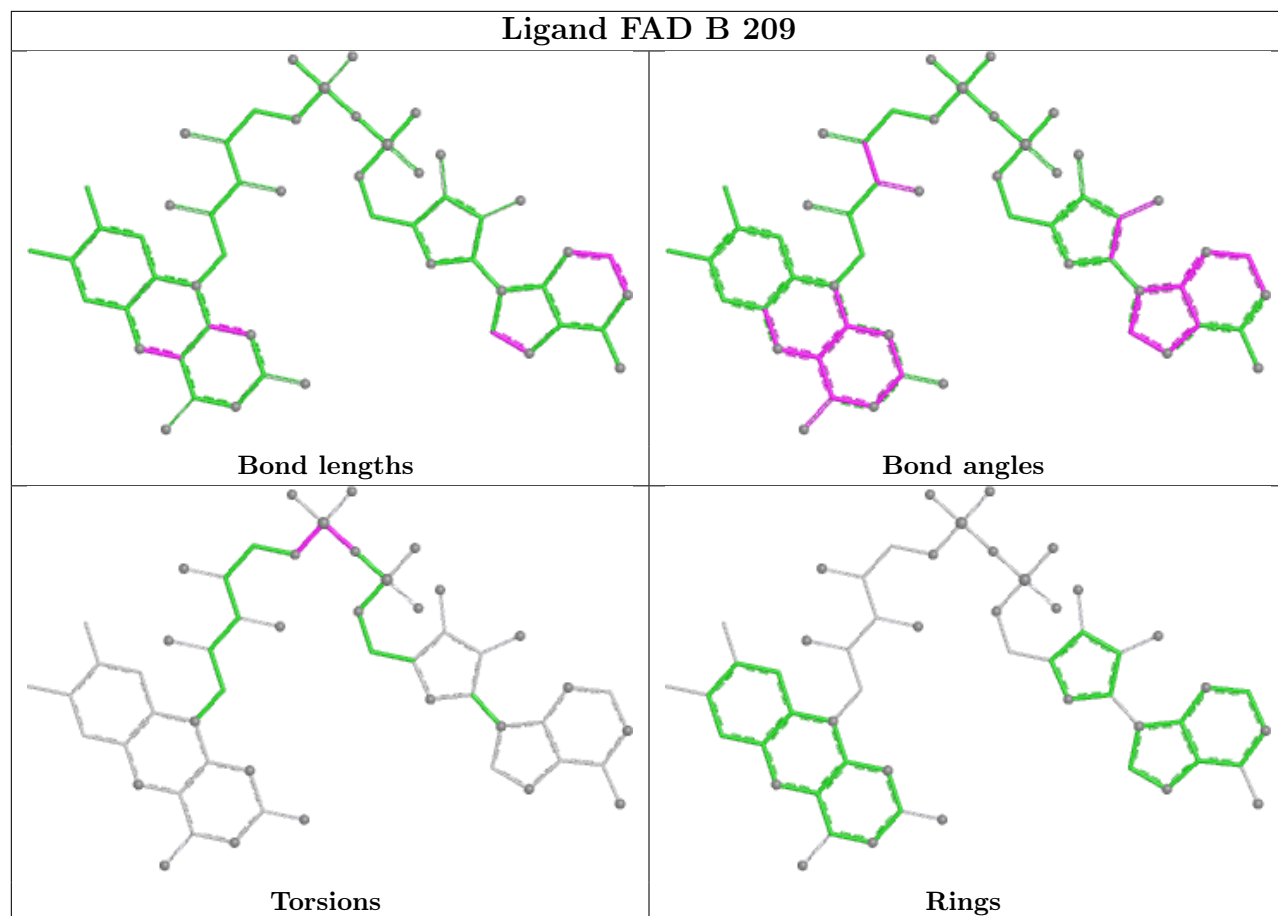
Ligand FAD D 303



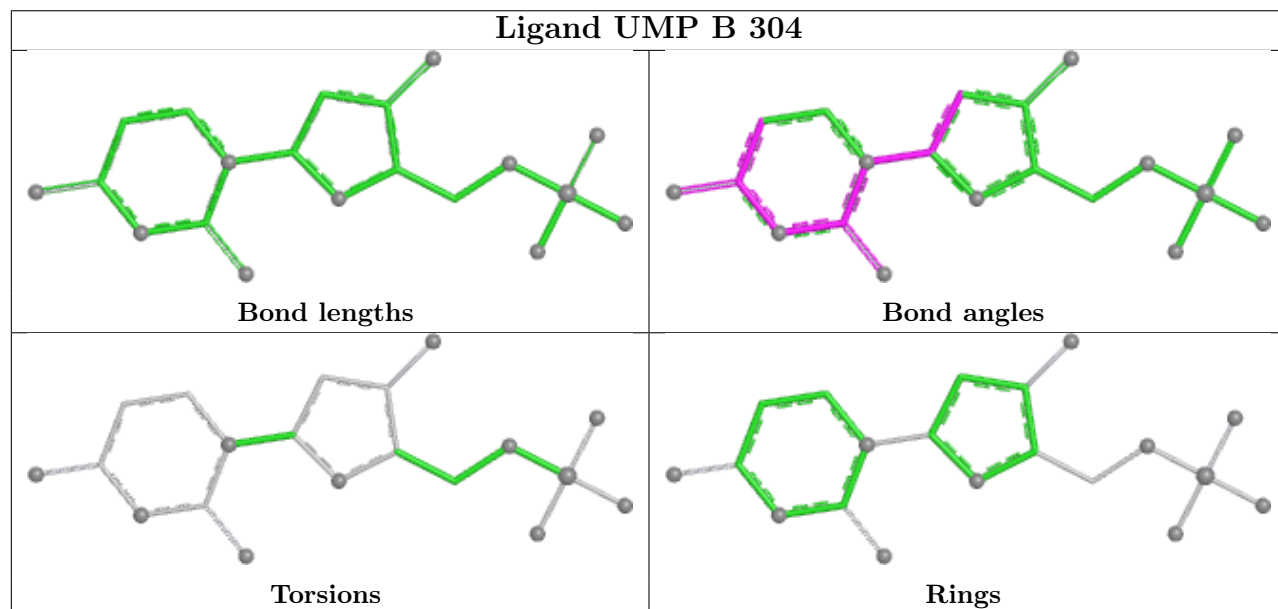
Ligand UMP B 301

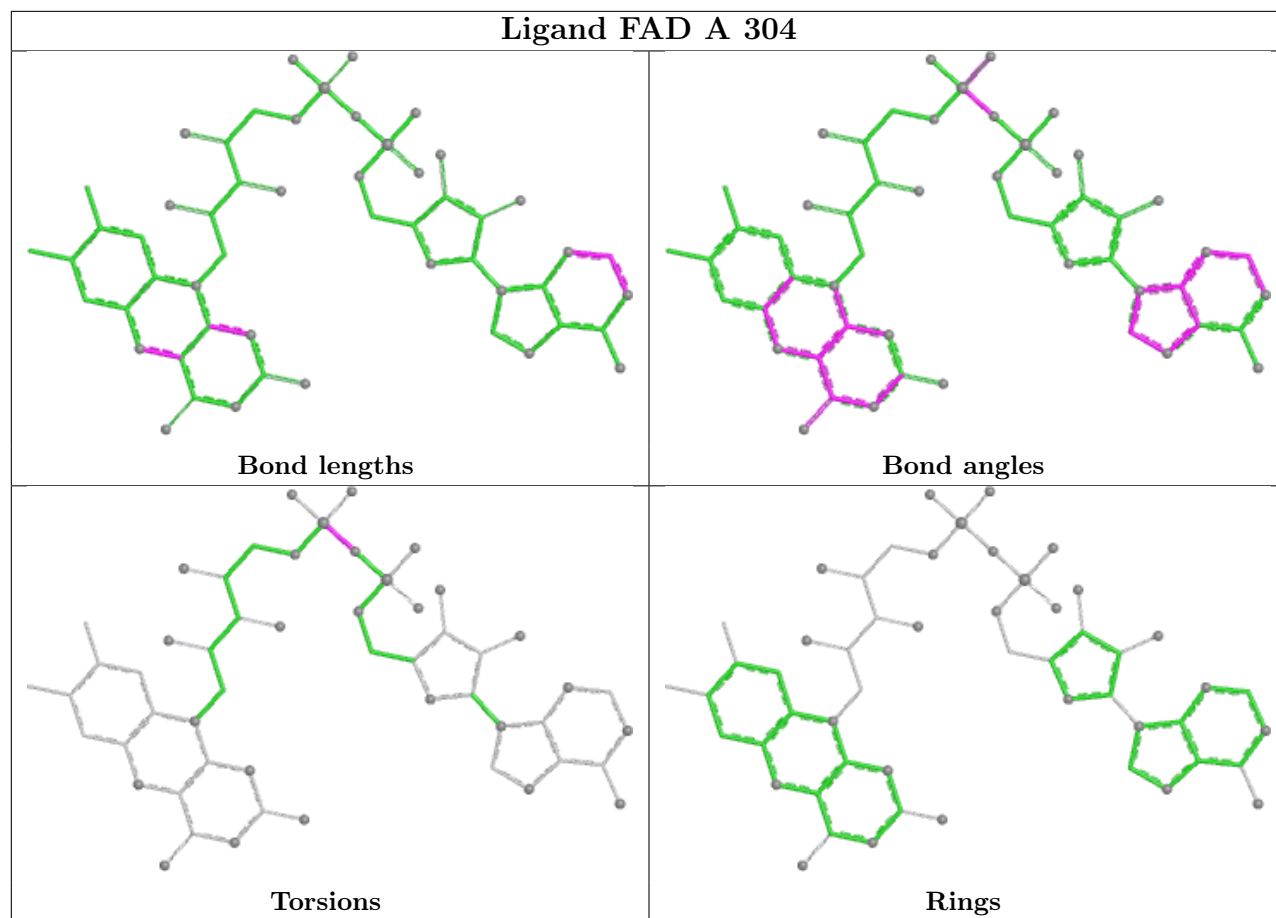


Ligand FAD B 209



Ligand UMP B 304





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%)	-0.07	8 (3%) 44 46	25, 38, 61, 79	0
1	B	209/216 (96%)	0.04	9 (4%) 40 41	22, 37, 80, 107	0
1	C	208/216 (96%)	0.16	10 (4%) 35 37	26, 42, 75, 106	0
1	D	208/216 (96%)	0.02	1 (0%) 87 87	19, 42, 69, 81	1 (0%)
All	All	834/864 (96%)	0.04	28 (3%) 48 50	19, 41, 73, 107	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	CYS	4.2
1	C	27	TYR	4.2
1	B	31	GLY	4.1
1	A	205	CYS	3.9
1	B	25	PHE	3.5
1	C	87	TYR	3.3
1	C	25	PHE	3.3
1	A	203	GLU	2.8
1	B	22	TRP	2.7
1	C	24	SER	2.7
1	B	49	SER	2.6
1	C	0	PHE	2.6
1	C	32	GLY	2.6
1	B	46	PHE	2.5
1	A	94	GLU	2.4
1	A	204	ASP	2.3
1	B	87	TYR	2.3
1	B	27	TYR	2.3
1	B	33	CYS	2.3
1	A	30	ASP	2.2
1	C	22	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	29	ASP	2.2
1	A	87	TYR	2.2
1	A	0	PHE	2.1
1	C	26	GLU	2.1
1	B	0	PHE	2.1
1	A	12	ASP	2.1
1	D	22	TRP	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](#)

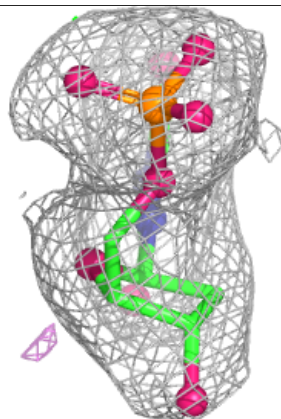
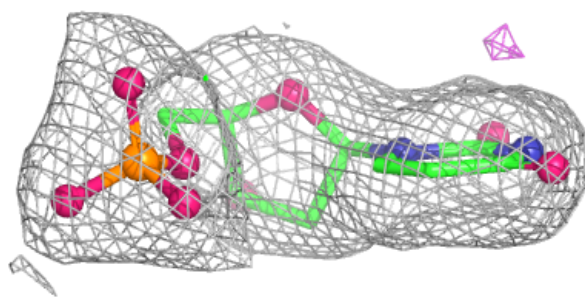
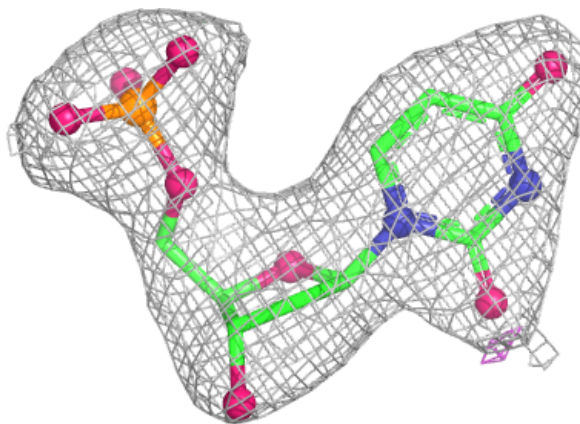
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UMP	A	305	20/20	0.92	0.08	38,49,59,60	0
2	UMP	B	304	20/20	0.96	0.07	28,35,38,39	0
3	FAD	A	304	53/53	0.96	0.07	28,34,40,42	0
2	UMP	C	303	20/20	0.97	0.05	33,42,49,50	0
2	UMP	D	302	20/20	0.97	0.06	32,36,39,41	0
2	UMP	B	301	20/20	0.97	0.06	25,30,35,37	0
3	FAD	B	209	53/53	0.97	0.06	24,28,34,35	0
3	FAD	C	302	53/53	0.97	0.06	26,32,38,38	0
3	FAD	D	303	53/53	0.97	0.07	28,37,43,46	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.

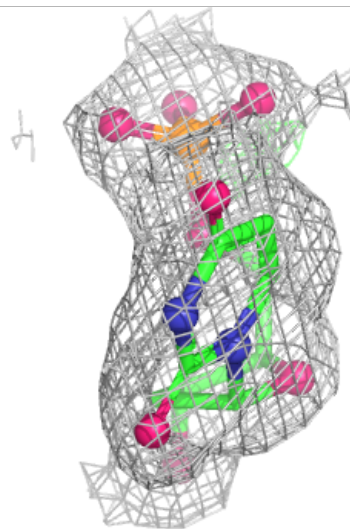
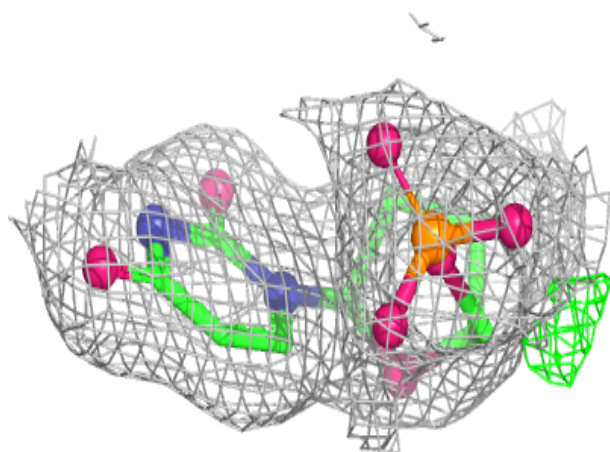
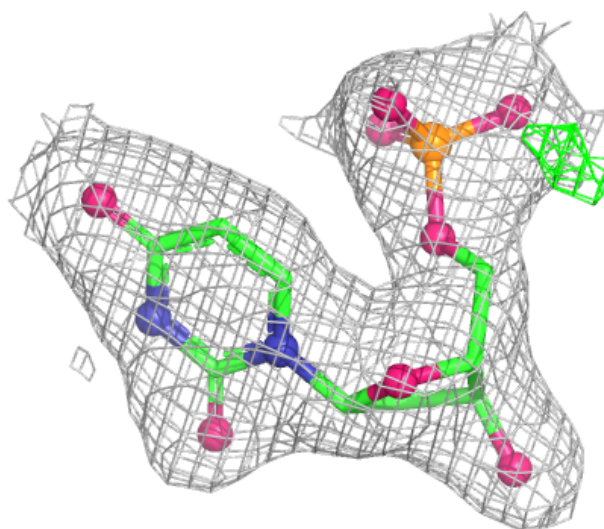
Electron density around UMP A 305:

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



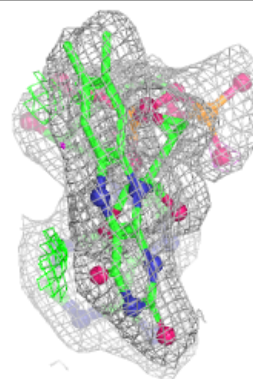
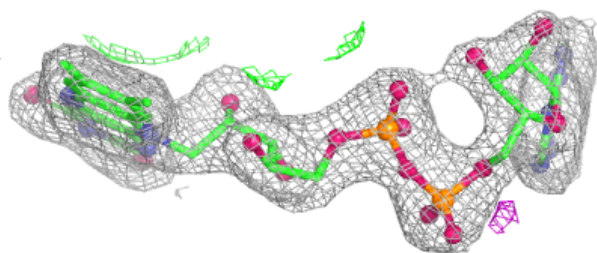
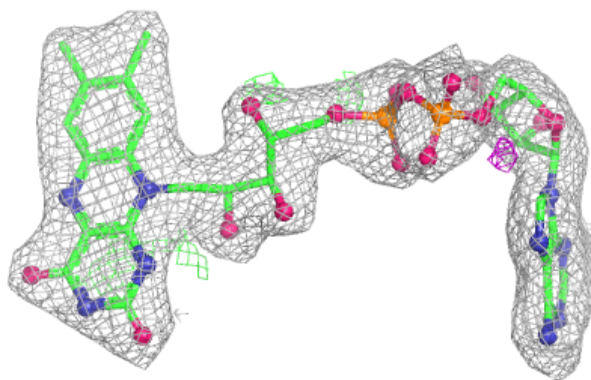
Electron density around UMP B 304:

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



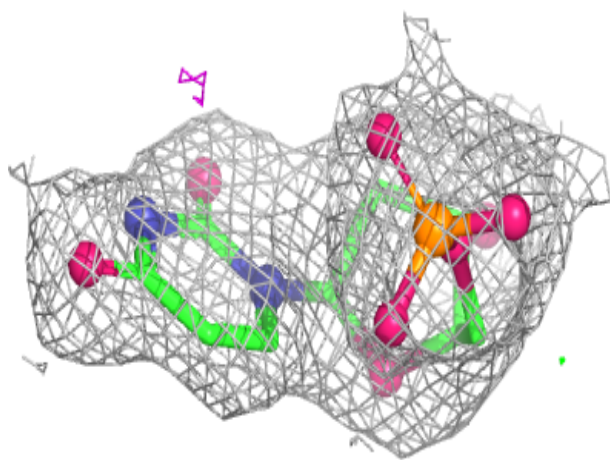
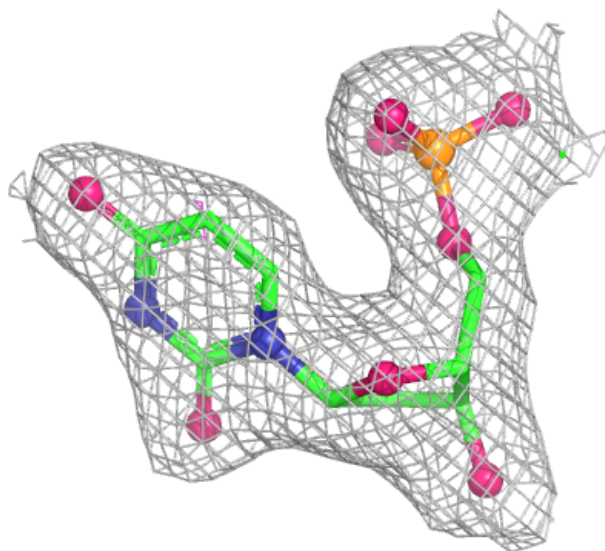
Electron density around FAD A 304:

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



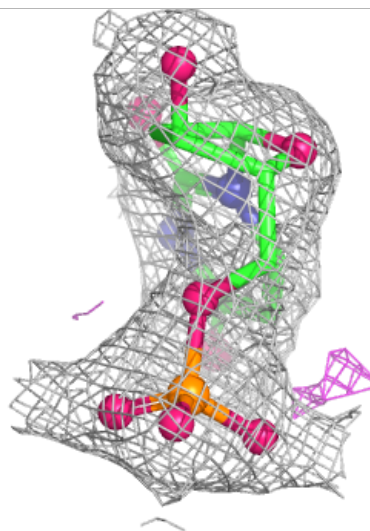
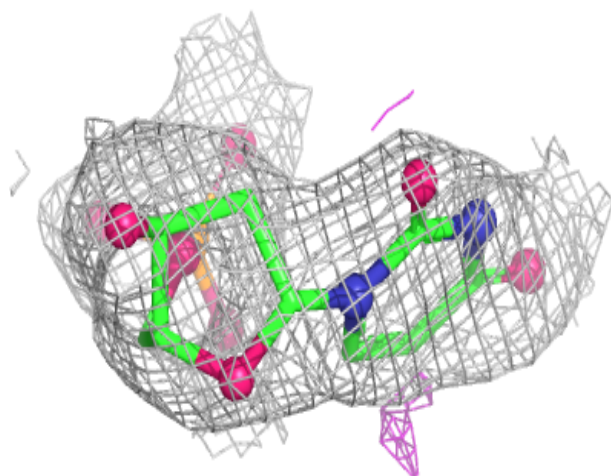
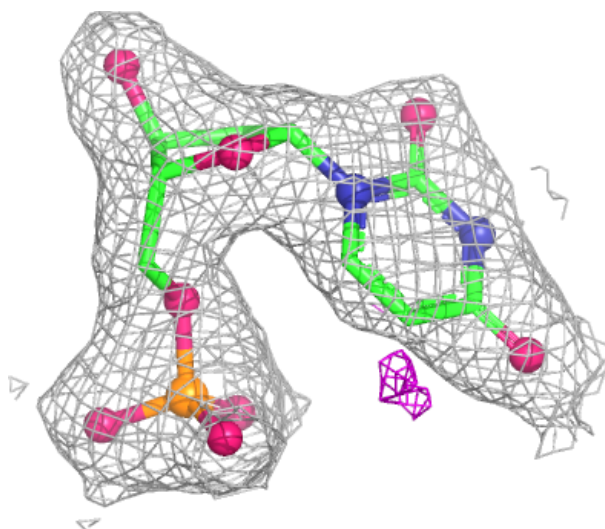
Electron density around UMP C 303:

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



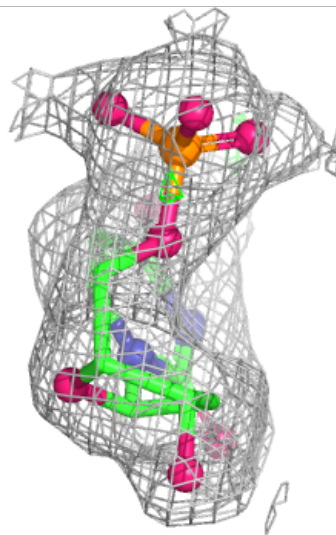
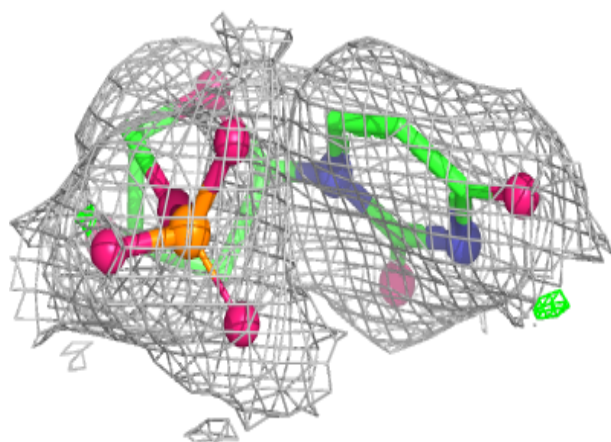
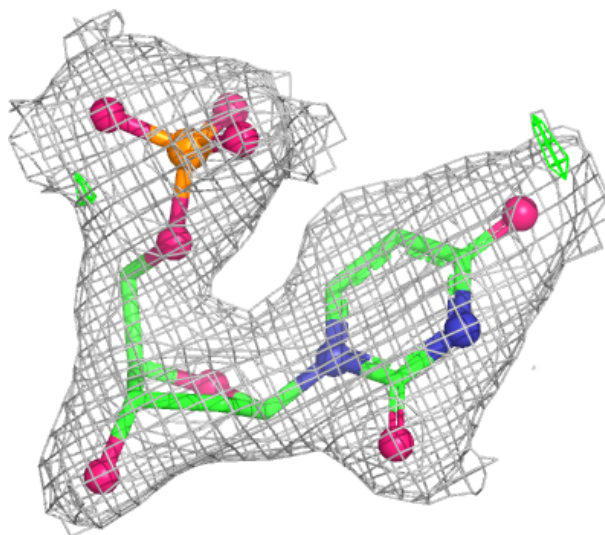
Electron density around UMP D 302:

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



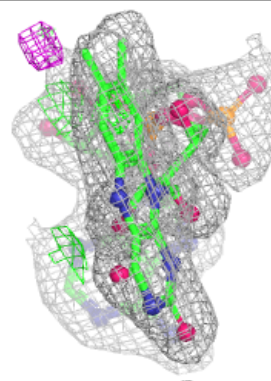
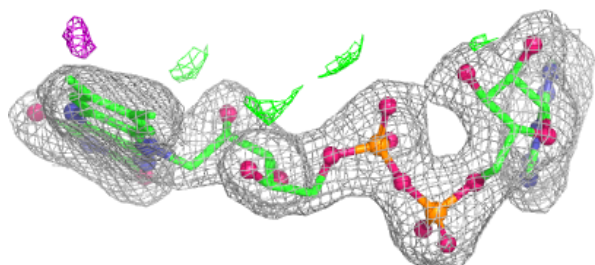
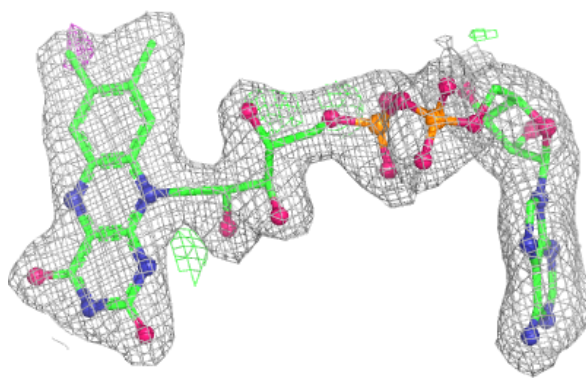
Electron density around UMP B 301:

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

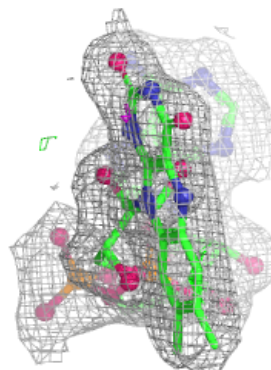
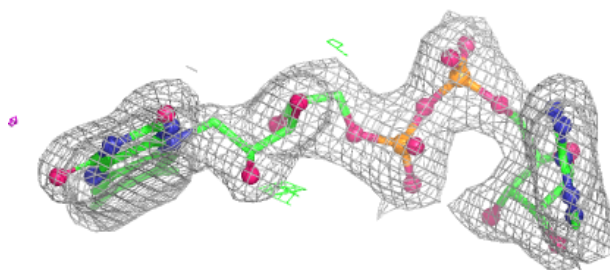
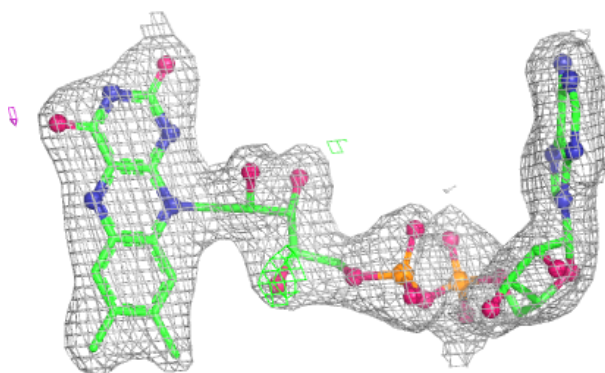


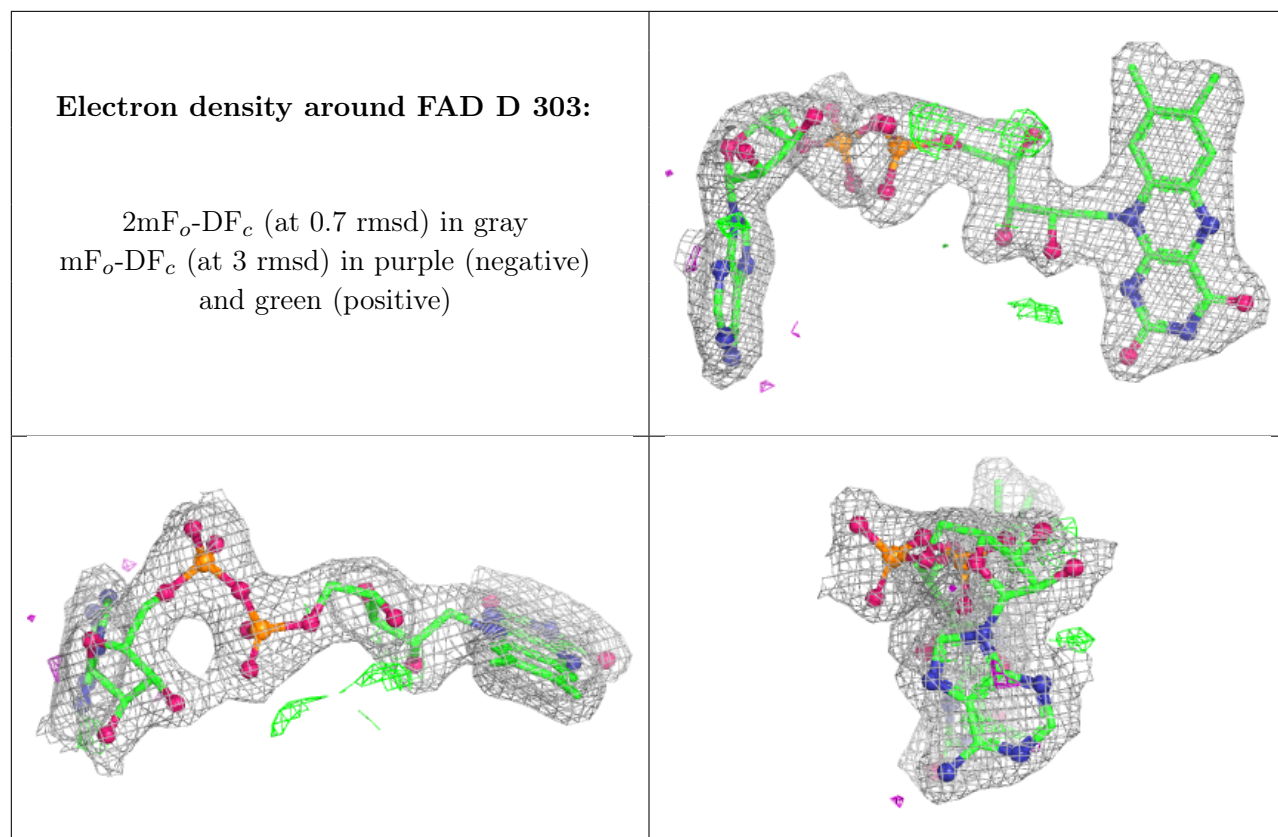
Electron density around FAD B 209:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.