



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:07 AM UTC

PDB ID : 4P5A / pdb_00004p5a
Title : Crystal structure of a UMP/dUMP methylase PolB from *Streptomyces cacaoi* bound with 5-Br UMP
Authors : Li, Y.; Chen, W.; Li, J.; Xia, Z.; Deng, Z.; Zhou, J.
Deposited on : 2014-03-15
Resolution : 1.76 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

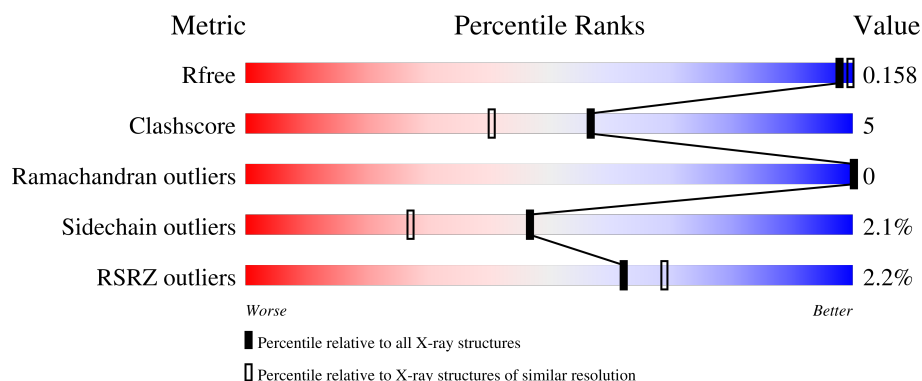
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	239	
1	B	239	
1	C	239	
1	D	239	

2 Entry composition [i](#)

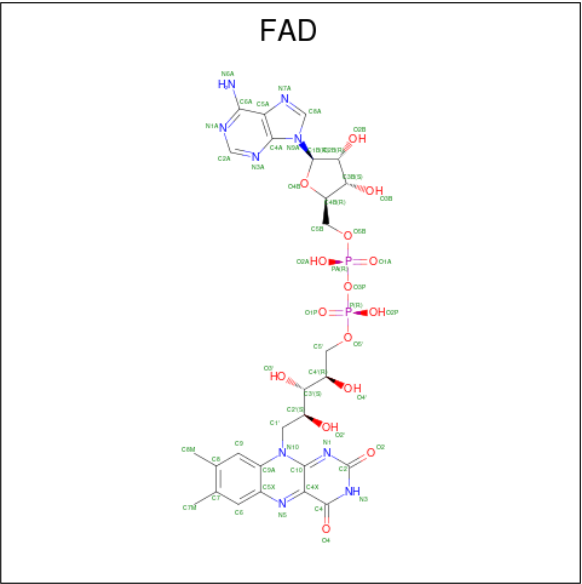
There are 4 unique types of molecules in this entry. The entry contains 8303 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	226	Total	C	N	O	S	0	1	0
			1816	1137	340	331	8			
1	B	227	Total	C	N	O	S	0	4	0
			1852	1160	347	337	8			
1	C	223	Total	C	N	O	S	0	2	0
			1798	1128	333	329	8			
1	D	225	Total	C	N	O	S	0	1	0
			1804	1129	335	332	8			

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



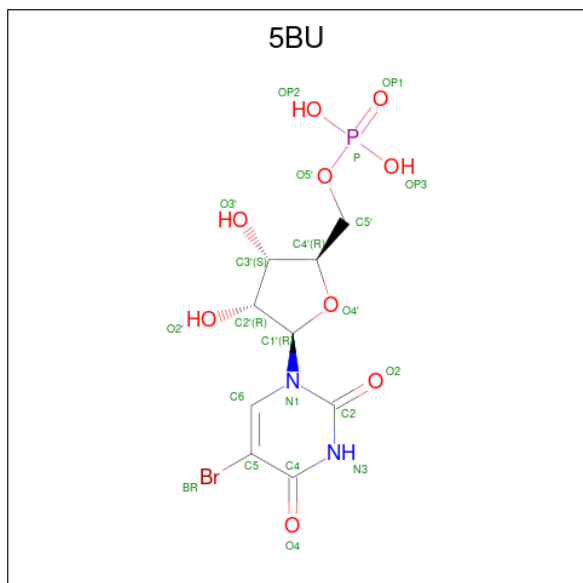
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 5-BROMO-URIDINE-5'-MONOPHOSPHATE (CCD ID: 5BU) (formula: $C_9H_{12}BrN_2O_9P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 22	Br 1	C 9	N 2	O 9	P 1	0	0
3	B	1	Total 22	Br 1	C 9	N 2	O 9	P 1	0	0
3	C	1	Total 22	Br 1	C 9	N 2	O 9	P 1	0	0
3	D	1	Total 22	Br 1	C 9	N 2	O 9	P 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total	O	0	0
			187	187		
4	B	173	Total	O	0	0
			173	173		
4	C	185	Total	O	0	0
			185	185		

Continued on next page...

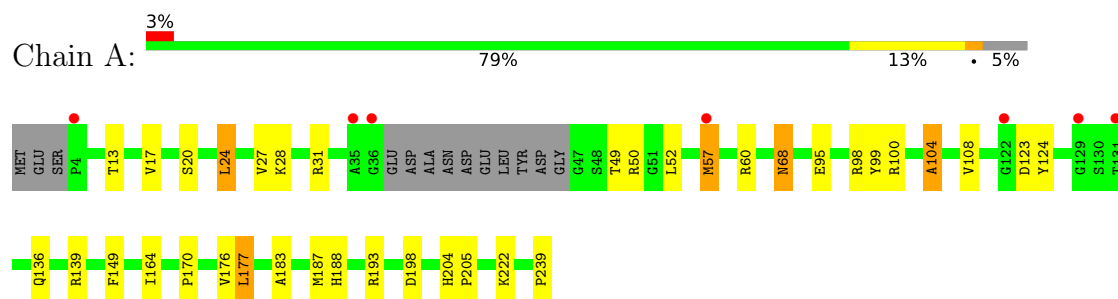
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	188	Total 188	O 188	0	0

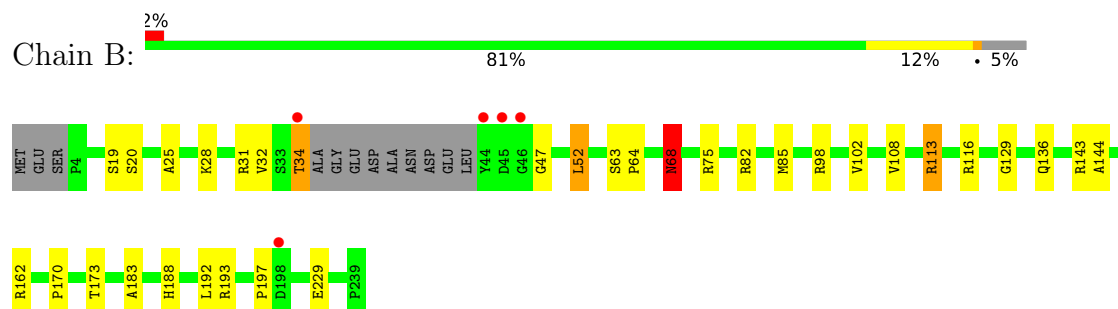
3 Residue-property plots [i](#)

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.

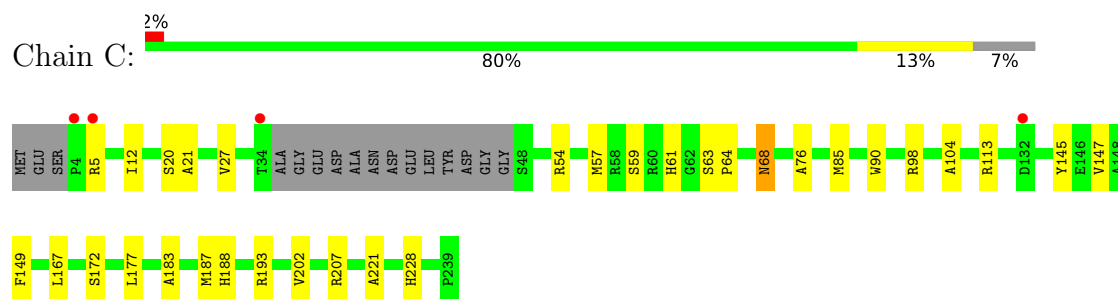
• Molecule 1: Thymidylate synthase ThyX



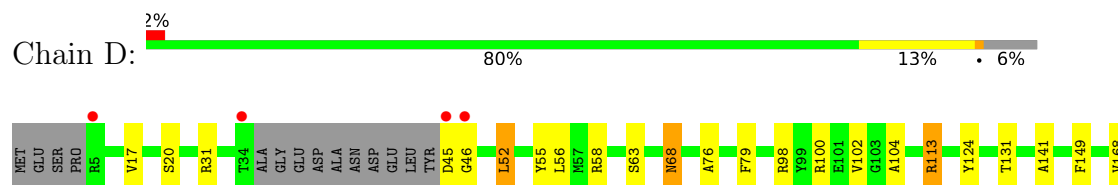
• Molecule 1: Thymidylate synthase ThyX

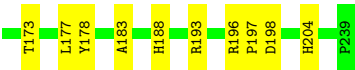


• Molecule 1: Thymidylate synthase ThyX



• Molecule 1: Thymidylate synthase ThyX





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.90Å 94.16Å 91.95Å 90.00° 98.30° 90.00°	Depositor
Resolution (Å)	50.00 – 1.76 50.00 – 1.76	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-1.76) 98.7 (50.00-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.154 , 0.193 0.157 , 0.158	Depositor DCC
R_{free} test set	5188 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8303	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: FAD, 5BU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.60	10/1856 (0.5%)	1.29	0/2511
1	B	1.63	11/1900 (0.6%)	1.32	7/2570 (0.3%)
1	C	1.65	12/1844 (0.7%)	1.34	2/2495 (0.1%)
1	D	1.59	7/1846 (0.4%)	1.33	7/2497 (0.3%)
All	All	1.62	40/7446 (0.5%)	1.32	16/10073 (0.2%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	76	ALA	CA-CB	10.87	1.70	1.54
1	D	76	ALA	CA-CB	9.84	1.67	1.53
1	A	17	VAL	CA-CB	8.98	1.67	1.54
1	C	202	VAL	CA-CB	7.19	1.61	1.53
1	B	162	ARG	CB-CG	-6.78	1.32	1.52
1	D	17	VAL	CA-CB	6.56	1.64	1.54
1	D	100	ARG	N-CA	6.53	1.54	1.46
1	A	57	MET	C-O	6.35	1.31	1.24
1	B	144	ALA	CA-CB	-6.28	1.43	1.53
1	B	28	LYS	N-CA	6.13	1.53	1.46
1	A	108	VAL	CA-CB	6.01	1.61	1.54
1	B	108	VAL	CA-CB	5.99	1.64	1.54
1	A	104	ALA	CA-CB	5.82	1.60	1.52
1	A	49	THR	N-CA	5.78	1.53	1.46
1	D	79	PHE	CA-C	5.77	1.60	1.52
1	B	19	SER	C-O	5.70	1.30	1.23
1	C	61	HIS	CA-CB	5.68	1.60	1.52
1	C	27	VAL	CA-CB	5.62	1.60	1.54
1	A	27	VAL	CA-CB	5.55	1.61	1.54
1	C	21	ALA	CA-CB	-5.46	1.44	1.53
1	C	85	MET	SD-CE	-5.43	1.66	1.79
1	C	177	LEU	N-CA	5.37	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ASP	CA-C	5.29	1.60	1.52
1	C	145	TYR	N-CA	5.28	1.52	1.46
1	A	60	ARG	CA-CB	5.26	1.61	1.53
1	C	59	SER	N-CA	-5.26	1.39	1.46
1	D	63	SER	CA-C	5.22	1.59	1.52
1	D	178	TYR	C-O	5.22	1.30	1.23
1	B	25	ALA	CA-CB	5.20	1.61	1.53
1	A	205	PRO	C-O	5.18	1.29	1.23
1	C	207	ARG	CA-C	5.16	1.59	1.52
1	A	50	ARG	C-O	5.13	1.30	1.24
1	C	90	TRP	C-O	5.13	1.30	1.23
1	B	85	MET	SD-CE	-5.13	1.66	1.79
1	B	68	ASN	CG-ND2	-5.13	1.22	1.33
1	B	129	GLY	N-CA	5.11	1.50	1.44
1	C	147	VAL	N-CA	-5.05	1.40	1.46
1	D	168	VAL	N-CA	5.03	1.52	1.46
1	B	82	ARG	CD-NE	-5.01	1.39	1.46
1	B	192	LEU	N-CA	5.00	1.52	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	ARG	CG-CD-NE	-6.97	96.66	112.00
1	B	82	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	C	172	SER	N-CA-C	5.98	120.42	113.18
1	D	141	ALA	N-CA-C	-5.78	105.06	111.36
1	D	46	GLY	CA-C-N	5.76	132.70	121.41
1	D	46	GLY	C-N-CA	5.76	132.70	121.41
1	D	196	ARG	CA-C-N	5.59	125.95	119.47
1	D	196	ARG	C-N-CA	5.59	125.95	119.47
1	C	12	ILE	N-CA-C	-5.53	99.58	107.77
1	D	177	LEU	CD1-CG-CD2	-5.26	99.23	110.80
1	B	47	GLY	N-CA-C	-5.25	105.22	111.36
1	B	197	PRO	CA-C-N	5.25	129.48	120.72
1	B	197	PRO	C-N-CA	5.25	129.48	120.72
1	B	52	LEU	CD1-CG-CD2	5.10	122.02	110.80
1	B	82	ARG	CA-C-O	-5.07	115.50	120.82
1	D	55	TYR	N-CA-C	-5.02	105.89	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1816	0	1792	22	0
1	B	1852	0	1824	16	0
1	C	1798	0	1778	19	0
1	D	1804	0	1775	16	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	22	0	10	2	0
3	B	22	0	10	2	0
3	C	22	0	10	2	0
3	D	22	0	10	2	0
4	A	187	0	0	4	0
4	B	173	0	0	6	0
4	C	185	0	0	6	0
4	D	188	0	0	5	0
All	All	8303	0	7333	69	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 5.

All (69) 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:D:198:ASP:HB3	4:D:413:HOH:O	1.50	1.10
1:B:68:ASN:HD21	1:B:183:ALA:H	1.19	0.90
1:C:193:ARG:HH12	3:D:301:5BU:H3	1.19	0.90
3:C:302:5BU:H3	1:D:193:ARG:HH12	1.17	0.89
1:A:193:ARG:HH12	3:B:301:5BU:H3	1.21	0.89
3:A:302:5BU:H3	1:B:193:ARG:HH12	1.20	0.88
1:A:68:ASN:HD21	1:A:183:ALA:H	1.19	0.86
1:C:54:ARG:HH21	1:C:54:ARG:HG3	1.38	0.86
1:C:68:ASN:HD21	1:C:183:ALA:H	1.23	0.85
1:D:68:ASN:HD21	1:D:183:ALA:H	1.22	0.84
1:C:54:ARG:HH21	1:C:54:ARG:CG	2.02	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:MET:HE1	1:A:187:MET:SD	2.31	0.70
1:A:20:SER:HB2	1:D:20:SER:HB2	1.75	0.69
1:C:5:ARG:HD3	4:C:483:HOH:O	1.93	0.66
1:C:54:ARG:CG	1:C:54:ARG:NH2	2.58	0.64
1:C:54:ARG:HG3	1:C:54:ARG:NH2	2.13	0.63
1:A:68:ASN:HD21	1:A:183:ALA:N	1.96	0.62
1:D:113:ARG:HG2	4:D:561:HOH:O	2.02	0.60
1:A:136:GLN:NE2	1:A:139:ARG:HH21	1.99	0.59
1:B:68:ASN:HD21	1:B:183:ALA:N	1.96	0.59
1:A:99:TYR:HD2	1:A:100:ARG:HG3	1.68	0.59
1:B:20:SER:HB2	1:C:20:SER:HB2	1.84	0.59
1:C:68:ASN:HD21	1:C:183:ALA:N	1.98	0.57
1:D:68:ASN:HD21	1:D:183:ALA:N	2.00	0.57
1:B:188:HIS:HD2	4:B:559:HOH:O	1.88	0.56
1:D:31:ARG:NH2	4:D:401:HOH:O	2.20	0.56
1:D:104:ALA:HB2	1:D:149:PHE:CZ	2.42	0.54
1:A:222:LYS:NZ	4:A:570:HOH:O	2.40	0.53
1:A:104:ALA:HB2	1:A:149:PHE:CZ	2.44	0.53
1:C:104:ALA:HB2	1:C:149:PHE:CZ	2.44	0.53
1:C:188:HIS:HD2	4:C:548:HOH:O	1.91	0.53
1:A:24:LEU:HD22	1:A:28:LYS:HG3	1.90	0.52
1:D:124:TYR:HB2	1:D:204:HIS:HB3	1.91	0.52
1:A:98:ARG:HD3	3:A:302:5BU:BR	2.64	0.52
1:D:52:LEU:C	1:D:52:LEU:HD23	2.35	0.52
1:B:98:ARG:HD3	3:B:301:5BU:BR	2.65	0.52
1:B:75:ARG:NH2	4:B:539:HOH:O	2.42	0.52
1:C:188:HIS:HE1	4:C:544:HOH:O	1.95	0.50
1:D:58:ARG:HD2	4:D:497:HOH:O	2.12	0.49
1:A:188:HIS:HD2	4:A:422:HOH:O	1.97	0.48
1:C:54:ARG:NH2	4:C:401:HOH:O	1.98	0.47
1:D:52:LEU:HD21	1:D:56:LEU:HD11	1.95	0.47
1:C:63:SER:HB3	1:C:64:PRO:HD3	1.95	0.47
1:D:102:VAL:HG11	1:D:173:THR:HG21	1.97	0.47
1:A:57:MET:SD	1:A:239:PRO:HG3	2.56	0.46
1:D:98:ARG:HD3	3:D:301:5BU:BR	2.71	0.45
1:B:31:ARG:O	1:B:32:VAL:C	2.59	0.45
1:B:229:GLU:HG2	4:B:409:HOH:O	2.16	0.45
1:D:188:HIS:HD2	4:D:444:HOH:O	1.99	0.45
1:A:123:ASP:O	1:A:124:TYR:C	2.59	0.44
1:A:124:TYR:HB2	1:A:204:HIS:HB3	1.99	0.44
1:B:116:ARG:NH1	4:B:508:HOH:O	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:PRO:HA	1:B:170:PRO:HA	2.00	0.44
1:B:34:THR:HG23	4:B:513:HOH:O	2.18	0.43
1:A:95:GLU:CD	1:A:176:VAL:HG12	2.44	0.43
1:C:98:ARG:HD3	3:C:302:5BU:BR	2.74	0.43
1:B:136:GLN:NE2	4:B:401:HOH:O	2.22	0.42
1:C:5:ARG:CD	4:C:483:HOH:O	2.60	0.42
1:A:31:ARG:CZ	1:A:52:LEU:HD22	2.50	0.42
1:C:188:HIS:CD2	4:C:548:HOH:O	2.69	0.42
1:A:177:LEU:HD22	1:A:177:LEU:O	2.19	0.42
1:B:63:SER:HB3	1:B:64:PRO:HD3	2.02	0.42
1:A:164:ILE:HD11	1:B:113:ARG:CZ	2.50	0.41
1:C:221:ALA:HB2	1:C:228:HIS:CD2	2.54	0.41
1:B:102:VAL:HG11	1:B:173:THR:HG21	2.03	0.41
1:A:13:THR:HG23	4:A:488:HOH:O	2.20	0.41
1:A:188:HIS:CD2	4:A:422:HOH:O	2.72	0.40
1:D:31:ARG:HH22	1:D:45:ASP:HB2	1.85	0.40
1:C:57:MET:HE1	1:C:187:MET:SD	2.61	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	223/239 (93%)	221 (99%)	2 (1%)	0	100	100
1	B	227/239 (95%)	224 (99%)	3 (1%)	0	100	100
1	C	221/239 (92%)	218 (99%)	3 (1%)	0	100	100
1	D	222/239 (93%)	220 (99%)	2 (1%)	0	100	100
All	All	893/956 (93%)	883 (99%)	10 (1%)	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	191/201 (95%)	188 (98%)	3 (2%)	55	38
1	B	196/201 (98%)	191 (97%)	5 (3%)	40	20
1	C	192/201 (96%)	189 (98%)	3 (2%)	55	38
1	D	191/201 (95%)	186 (97%)	5 (3%)	40	20
All	All	770/804 (96%)	754 (98%)	16 (2%)	47	27

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	68	ASN
1	A	177	LEU
1	B	34	THR
1	B	52	LEU
1	B	68	ASN
1	B	113	ARG
1	B	143	ARG
1	C	68	ASN
1	C	113	ARG
1	C	167	LEU
1	D	52	LEU
1	D	68	ASN
1	D	113	ARG
1	D	131	THR
1	D	197	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	136	GLN
1	A	188	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	HIS
1	A	204	HIS
1	B	68	ASN
1	B	93	ASN
1	B	117	GLN
1	B	135	GLN
1	B	188	HIS
1	B	195	HIS
1	B	215	GLN
1	C	68	ASN
1	C	135	GLN
1	C	188	HIS
1	C	195	HIS
1	D	68	ASN
1	D	117	GLN
1	D	188	HIS
1	D	195	HIS
1	D	204	HIS
1	D	215	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	A	301	-	58,58,58	1.81	12 (20%)	85,89,89	1.66	18 (21%)
2	FAD	B	302	-	58,58,58	1.88	13 (22%)	85,89,89	1.71	21 (24%)
3	5BU	D	301	-	23,23,23	1.70	6 (26%)	34,35,35	2.34	13 (38%)
3	5BU	A	302	-	23,23,23	1.48	4 (17%)	34,35,35	2.39	8 (23%)
2	FAD	D	302	-	58,58,58	1.79	13 (22%)	85,89,89	1.93	25 (29%)
3	5BU	C	302	-	23,23,23	1.76	8 (34%)	34,35,35	2.21	11 (32%)
3	5BU	B	301	-	23,23,23	1.66	5 (21%)	34,35,35	1.91	11 (32%)
2	FAD	C	301	-	58,58,58	2.00	11 (18%)	85,89,89	1.80	23 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	301	-	-	1/34/50/50	0/6/6/6
2	FAD	B	302	-	-	0/34/50/50	0/6/6/6
3	5BU	D	301	-	-	2/10/26/26	0/2/2/2
3	5BU	A	302	-	-	1/10/26/26	0/2/2/2
2	FAD	D	302	-	-	1/34/50/50	0/6/6/6
3	5BU	C	302	-	-	0/10/26/26	0/2/2/2
3	5BU	B	301	-	-	0/10/26/26	0/2/2/2
2	FAD	C	301	-	-	1/34/50/50	0/6/6/6

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	FAD	C7M-C7	6.81	1.63	1.51
2	C	301	FAD	C5'-C4'	6.61	1.60	1.51
2	C	301	FAD	C1'-C2'	5.54	1.60	1.52
2	A	301	FAD	C4X-N5	5.24	1.42	1.30
2	B	302	FAD	C4'-C3'	5.16	1.62	1.53
2	B	302	FAD	C4X-N5	5.13	1.41	1.30
2	B	302	FAD	C1'-C2'	5.11	1.59	1.52
2	A	301	FAD	C1'-C2'	5.08	1.59	1.52
2	D	302	FAD	C1'-C2'	5.06	1.59	1.52
2	D	302	FAD	C10-N1	5.02	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	FAD	C5X-N5	4.57	1.47	1.39
2	D	302	FAD	O4B-C1B	4.14	1.51	1.42
3	D	301	5BU	C4-C5	-4.12	1.36	1.45
3	C	302	5BU	C5'-C4'	3.89	1.63	1.51
2	A	301	FAD	C5X-N5	3.89	1.46	1.39
2	D	302	FAD	C7M-C7	3.79	1.58	1.51
3	A	302	5BU	C5'-C4'	3.71	1.62	1.51
3	B	301	5BU	C4-C5	-3.70	1.37	1.45
2	A	301	FAD	C4'-C3'	3.39	1.59	1.53
3	D	301	5BU	BR-C5	3.28	1.96	1.88
3	B	301	5BU	O4'-C4'	3.28	1.52	1.45
2	B	302	FAD	C9-C9A	3.24	1.44	1.39
2	D	302	FAD	C8A-N7A	3.22	1.37	1.31
2	D	302	FAD	C6-C5X	3.17	1.44	1.40
2	D	302	FAD	PA-O1A	-3.15	1.39	1.50
2	C	301	FAD	PA-O3P	-3.08	1.56	1.59
3	C	302	5BU	C2-N1	-3.07	1.33	1.38
2	C	301	FAD	C4X-N5	3.02	1.37	1.30
2	B	302	FAD	C4A-N9A	-3.00	1.31	1.37
3	C	302	5BU	C6-N1	3.00	1.43	1.38
2	A	301	FAD	C9-C9A	2.99	1.44	1.39
2	B	302	FAD	C8M-C8	2.96	1.56	1.51
2	B	302	FAD	PA-O3P	-2.92	1.56	1.59
2	D	302	FAD	C4X-N5	2.88	1.37	1.30
2	B	302	FAD	O4B-C1B	2.87	1.48	1.42
3	B	301	5BU	O3'-C3'	2.84	1.50	1.43
2	B	302	FAD	C5'-C4'	2.74	1.55	1.51
2	A	301	FAD	C2A-N3A	2.67	1.38	1.33
3	C	302	5BU	C4-C5	-2.66	1.39	1.45
2	D	302	FAD	C5B-C4B	2.65	1.59	1.51
2	D	302	FAD	C8M-C8	2.64	1.56	1.51
2	D	302	FAD	O5B-C5B	-2.63	1.34	1.44
3	D	301	5BU	C5'-C4'	2.59	1.59	1.51
2	B	302	FAD	C10-N1	2.57	1.38	1.33
3	A	302	5BU	C6-N1	2.54	1.42	1.38
2	A	301	FAD	P-O3P	-2.53	1.56	1.59
3	A	302	5BU	BR-C5	2.51	1.94	1.88
2	A	301	FAD	C2'-C3'	2.51	1.57	1.53
3	D	301	5BU	P-OP2	-2.45	1.45	1.54
2	B	302	FAD	PA-O2A	-2.44	1.44	1.55
2	C	301	FAD	C9A-C5X	2.37	1.45	1.41
3	D	301	5BU	O4'-C4'	2.35	1.50	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302	FAD	C2A-N3A	2.33	1.38	1.33
3	A	302	5BU	O5'-C5'	-2.32	1.35	1.44
3	C	302	5BU	C1'-N1	2.31	1.54	1.47
2	A	301	FAD	C9-C8	2.29	1.42	1.39
3	D	301	5BU	C1'-N1	2.25	1.53	1.47
3	B	301	5BU	P-OP3	-2.24	1.46	1.54
2	C	301	FAD	PA-O2A	-2.15	1.45	1.55
2	C	301	FAD	C4'-C3'	2.14	1.57	1.53
3	C	302	5BU	O2'-C2'	2.13	1.48	1.43
2	B	302	FAD	C4X-C10	-2.12	1.37	1.44
2	A	301	FAD	C10-N1	2.12	1.37	1.33
2	A	301	FAD	C9A-N10	2.10	1.44	1.41
2	C	301	FAD	O2B-C2B	2.08	1.48	1.43
3	B	301	5BU	P-OP2	-2.05	1.47	1.54
2	A	301	FAD	O2'-C2'	2.04	1.47	1.43
2	D	302	FAD	C2-N1	-2.04	1.32	1.36
3	C	302	5BU	BR-C5	2.03	1.93	1.88
3	C	302	5BU	C3'-C4'	-2.01	1.47	1.53
2	B	302	FAD	O2B-C2B	2.00	1.47	1.43
2	C	301	FAD	C2B-C3B	2.00	1.58	1.53

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	5BU	N3-C2-N1	6.37	123.18	114.89
3	A	302	5BU	C4-N3-C2	-6.32	119.06	127.34
2	D	302	FAD	C5A-C4A-N3A	-5.99	118.47	126.72
3	A	302	5BU	C6-C5-C4	5.85	126.62	120.67
3	C	302	5BU	C4-N3-C2	-5.41	120.24	127.34
3	D	301	5BU	C6-C5-C4	5.22	125.97	120.67
2	C	301	FAD	C5A-C4A-N3A	-5.18	119.58	126.72
3	B	301	5BU	O2-C2-N1	-5.13	116.12	122.80
2	A	301	FAD	C5A-C4A-N3A	-4.97	119.88	126.72
3	C	302	5BU	N3-C2-N1	4.86	121.21	114.89
3	D	301	5BU	N3-C2-N1	4.80	121.14	114.89
3	A	302	5BU	O2-C2-N1	-4.77	116.59	122.80
2	C	301	FAD	N3A-C2A-N1A	-4.75	121.39	128.58
2	C	301	FAD	C4X-C10-N10	4.72	123.24	116.48
3	D	301	5BU	O2-C2-N1	-4.66	116.73	122.80
3	D	301	5BU	C4-N3-C2	-4.63	121.27	127.34
2	D	302	FAD	N9A-C8A-N7A	-4.62	107.38	113.94
2	A	301	FAD	C4X-C10-N10	4.60	123.07	116.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	FAD	N3A-C2A-N1A	-4.52	121.74	128.58
2	A	301	FAD	N3A-C2A-N1A	-4.43	121.87	128.58
2	B	302	FAD	C4X-C10-N10	4.36	122.72	116.48
3	C	302	5BU	BR-C5-C6	-4.31	114.61	120.64
2	D	302	FAD	C4X-C10-N10	4.16	122.44	116.48
2	D	302	FAD	C4A-C5A-N7A	-3.99	106.02	110.58
3	D	301	5BU	C3'-C2'-C1'	3.96	108.95	101.46
2	B	302	FAD	C4A-C5A-N7A	-3.91	106.11	110.58
2	D	302	FAD	N3A-C2A-N1A	-3.86	122.75	128.58
2	C	301	FAD	O4-C4-C4X	-3.80	116.51	126.53
3	C	302	5BU	C6-C5-C4	3.76	124.50	120.67
3	B	301	5BU	N3-C2-N1	3.74	119.76	114.89
2	B	302	FAD	C4-C4X-N5	3.70	123.31	118.21
2	D	302	FAD	O2A-PA-O3P	3.68	117.23	107.27
3	C	302	5BU	C5-C4-N3	3.67	117.56	113.34
2	A	301	FAD	C3B-C2B-C1B	-3.60	94.66	101.46
2	D	302	FAD	C5A-N7A-C8A	3.54	109.02	103.45
3	A	302	5BU	BR-C5-C6	-3.37	115.93	120.64
3	C	302	5BU	O2-C2-N1	-3.31	118.48	122.80
2	B	302	FAD	C6-C5X-N5	3.31	123.93	118.44
3	B	301	5BU	C6-N1-C2	-3.30	118.02	121.30
2	B	302	FAD	C4A-N9A-C8A	3.29	109.20	105.74
2	D	302	FAD	N3A-C4A-N9A	3.29	132.76	127.17
2	C	301	FAD	C4-N3-C2	-3.28	119.82	125.64
2	D	302	FAD	C8M-C8-C7	3.24	127.38	120.76
2	B	302	FAD	C5A-C4A-N3A	-3.21	122.29	126.72
2	C	301	FAD	C8M-C8-C9	-3.20	113.93	119.57
3	D	301	5BU	O5'-P-OP1	-3.19	97.81	106.44
2	D	302	FAD	O4B-C4B-C5B	-3.14	99.26	109.33
3	B	301	5BU	C6-C5-C4	3.14	123.87	120.67
2	B	302	FAD	C10-C4X-N5	-3.14	118.41	124.81
2	D	302	FAD	C6A-C5A-C4A	3.13	121.45	117.18
2	D	302	FAD	C6-C7-C8	3.09	124.23	119.69
3	B	301	5BU	BR-C5-C6	-3.05	116.38	120.64
3	D	301	5BU	BR-C5-C6	-3.03	116.40	120.64
2	D	302	FAD	C2A-N3A-C4A	3.02	119.20	111.83
3	A	302	5BU	C3'-C2'-C1'	3.01	107.16	101.46
3	C	302	5BU	O4'-C1'-N1	-3.00	101.56	108.36
3	B	301	5BU	C4-N3-C2	-2.98	123.43	127.34
2	B	302	FAD	C6-C5X-C9A	-2.96	114.99	119.05
2	D	302	FAD	C4A-N9A-C8A	2.92	108.81	105.74
3	B	301	5BU	OP2-P-O5'	-2.91	99.07	106.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302	FAD	C7M-C7-C6	-2.91	114.45	119.57
2	D	302	FAD	O3B-C3B-C4B	-2.88	102.80	111.08
2	C	301	FAD	C2A-N3A-C4A	2.84	118.77	111.83
3	D	301	5BU	OP2-P-OP1	2.84	121.91	110.83
2	C	301	FAD	C4X-C4-N3	2.82	120.44	113.25
2	A	301	FAD	O2-C2-N3	2.78	123.91	118.58
2	C	301	FAD	C4A-C5A-N7A	-2.72	107.47	110.58
2	D	302	FAD	C5A-C4A-N9A	2.70	108.75	105.81
3	A	302	5BU	C5-C6-N1	-2.66	114.69	120.91
2	B	302	FAD	C4X-C4-N3	2.63	119.95	113.25
2	A	301	FAD	C5A-C4A-N9A	2.63	108.68	105.81
3	C	302	5BU	C5-C6-N1	-2.61	114.80	120.91
3	A	302	5BU	C5-C4-N3	2.59	116.33	113.34
2	C	301	FAD	C2A-N1A-C6A	2.58	122.97	118.73
3	D	301	5BU	OP3-P-OP2	2.58	117.46	107.80
2	B	302	FAD	C4-N3-C2	-2.58	121.07	125.64
2	B	302	FAD	C9-C8-C7	-2.56	115.93	119.69
2	A	301	FAD	C2A-N3A-C4A	2.56	118.08	111.83
2	C	301	FAD	C5'-C4'-C3'	-2.56	107.39	112.22
2	C	301	FAD	O2A-PA-O3P	2.56	114.18	107.27
2	B	302	FAD	C2A-N3A-C4A	2.50	117.94	111.83
2	A	301	FAD	O2A-PA-O3P	2.50	114.03	107.27
2	D	302	FAD	C9-C9A-N10	-2.50	118.49	121.85
2	B	302	FAD	O2'-C2'-C3'	-2.48	103.44	109.25
2	D	302	FAD	C4B-O4B-C1B	-2.48	103.99	109.47
2	C	301	FAD	N3A-C4A-N9A	2.46	131.36	127.17
2	C	301	FAD	C5A-C4A-N9A	2.46	108.49	105.81
2	D	302	FAD	C8M-C8-C9	-2.45	115.25	119.57
2	A	301	FAD	N3A-C4A-N9A	2.43	131.30	127.17
2	C	301	FAD	C10-N1-C2	2.43	122.11	116.85
3	C	302	5BU	OP3-P-OP2	2.38	116.72	107.80
2	B	302	FAD	C2A-N1A-C6A	2.37	122.62	118.73
2	A	301	FAD	N9A-C8A-N7A	-2.32	110.64	113.94
2	C	301	FAD	C6A-C5A-C4A	2.31	120.33	117.18
2	B	302	FAD	N9A-C8A-N7A	-2.30	110.67	113.94
2	C	301	FAD	C4X-C10-N1	-2.30	118.95	124.59
3	C	302	5BU	BR-C5-C4	2.30	120.67	118.02
2	A	301	FAD	O4B-C1B-C2B	2.29	111.52	106.62
2	D	302	FAD	C4-N3-C2	-2.27	121.61	125.64
2	C	301	FAD	O5'-C5'-C4'	-2.27	103.31	109.36
2	A	301	FAD	C5X-N5-C4X	-2.25	114.44	118.09
2	D	302	FAD	C4X-C10-N1	-2.24	119.09	124.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	FAD	C7M-C7-C6	-2.23	115.64	119.57
2	C	301	FAD	C1B-N9A-C8A	2.22	132.03	127.09
2	A	301	FAD	O3'-C3'-C2'	2.19	113.91	108.93
2	D	302	FAD	O2P-P-O3P	2.19	113.19	107.27
2	D	302	FAD	C10-C4X-N5	-2.18	120.35	124.81
2	A	301	FAD	C4A-C5A-N7A	-2.18	108.09	110.58
3	B	301	5BU	C2'-C1'-N1	-2.17	107.21	113.25
2	C	301	FAD	C6-C5X-N5	2.16	122.03	118.44
2	B	302	FAD	O2A-PA-O1A	2.16	122.48	112.44
2	A	301	FAD	O4'-C4'-C5'	2.14	114.70	109.99
3	B	301	5BU	OP3-P-OP2	2.13	115.80	107.80
3	D	301	5BU	OP2-P-O5'	-2.11	101.16	106.67
3	D	301	5BU	O3'-C3'-C4'	-2.11	105.03	111.08
2	D	302	FAD	C4X-C4-N3	2.10	118.61	113.25
2	B	302	FAD	C6A-C5A-N7A	2.10	136.14	132.09
2	B	302	FAD	C10-N1-C2	2.09	121.38	116.85
2	A	301	FAD	C9-C9A-N10	-2.08	119.06	121.85
3	D	301	5BU	O4-C4-C5	-2.08	123.16	125.80
2	C	301	FAD	C6-C5X-C9A	-2.07	116.21	119.05
2	B	302	FAD	C6-C7-C8	2.06	122.72	119.69
2	C	301	FAD	O4B-C1B-C2B	2.04	110.99	106.62
3	D	301	5BU	C2'-C3'-C4'	-2.04	98.66	102.61
2	A	301	FAD	O2'-C2'-C3'	-2.04	104.47	109.25
2	C	301	FAD	C2B-C3B-C4B	-2.03	98.68	102.61
3	B	301	5BU	C3'-C2'-C1'	2.03	105.30	101.46
3	C	302	5BU	C2'-C1'-N1	-2.01	107.64	113.25
2	A	301	FAD	C6A-C5A-C4A	2.01	119.92	117.18
3	B	301	5BU	OP3-P-O5'	-2.01	101.43	106.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

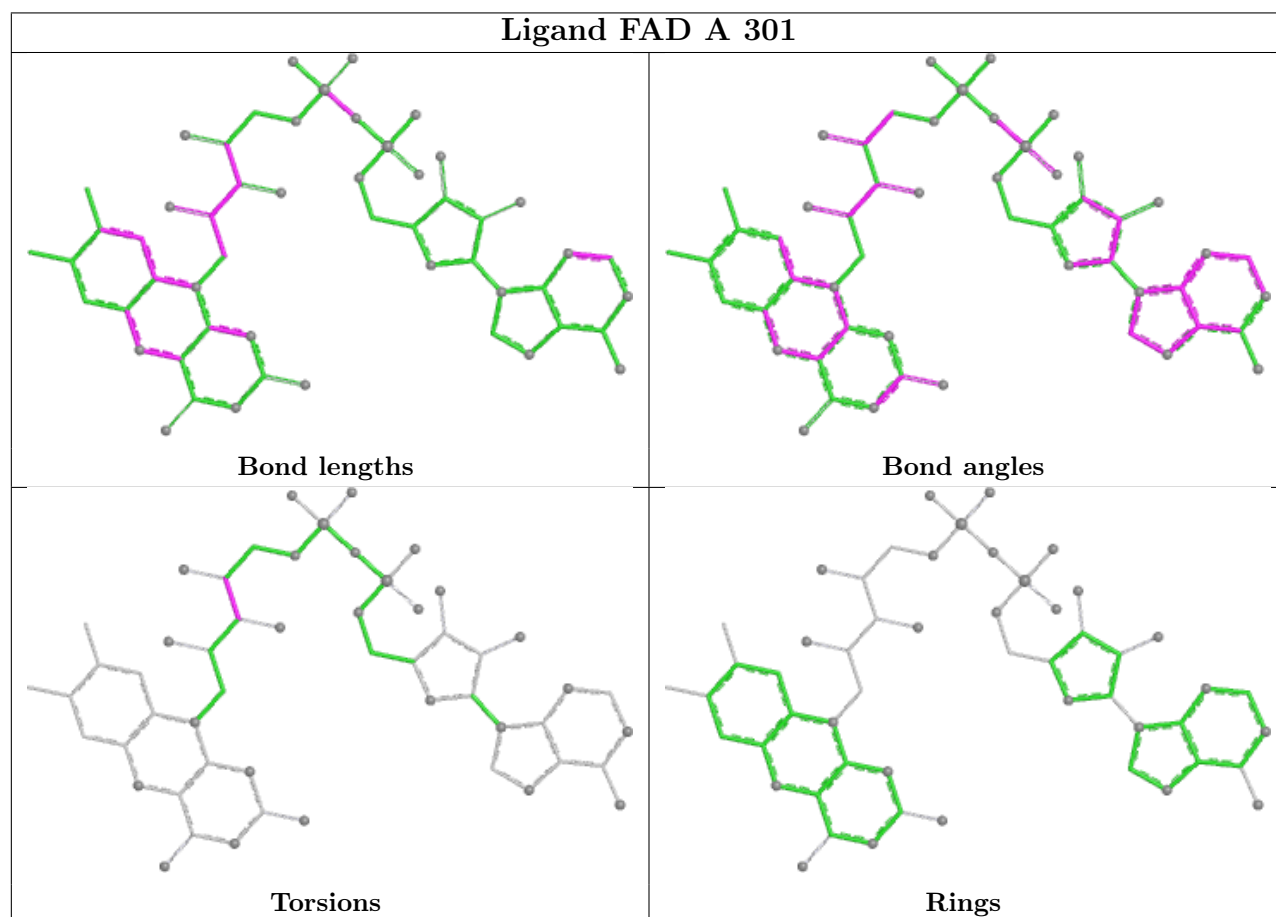
Mol	Chain	Res	Type	Atoms
2	A	301	FAD	C2'-C3'-C4'-O4'
3	D	301	5BU	C5'-O5'-P-OP1
3	A	302	5BU	C5'-O5'-P-OP3
3	D	301	5BU	C5'-O5'-P-OP2
2	C	301	FAD	PA-O3P-P-O2P
2	D	302	FAD	PA-O3P-P-O2P

There are no ring outliers.

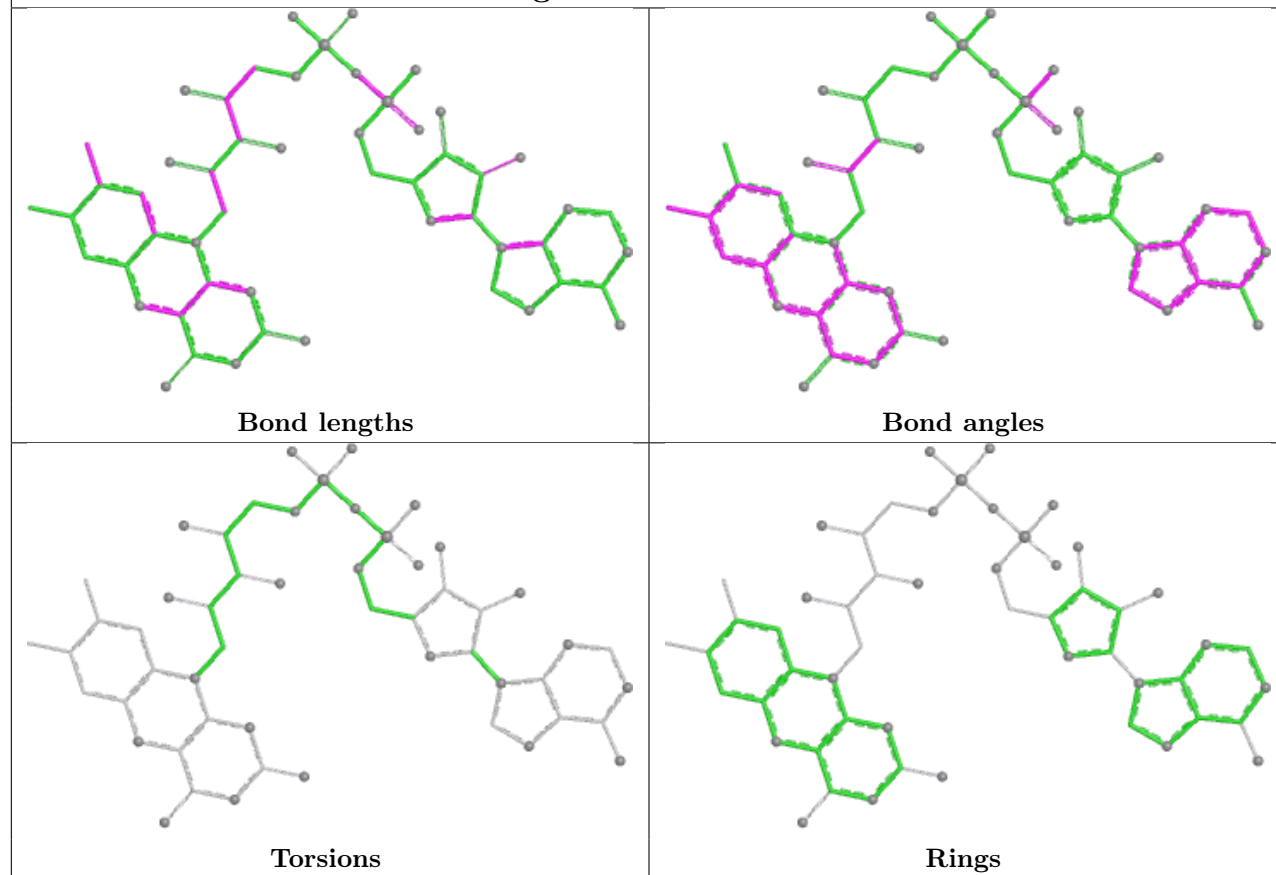
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	5BU	2	0
3	A	302	5BU	2	0
3	C	302	5BU	2	0
3	B	301	5BU	2	0

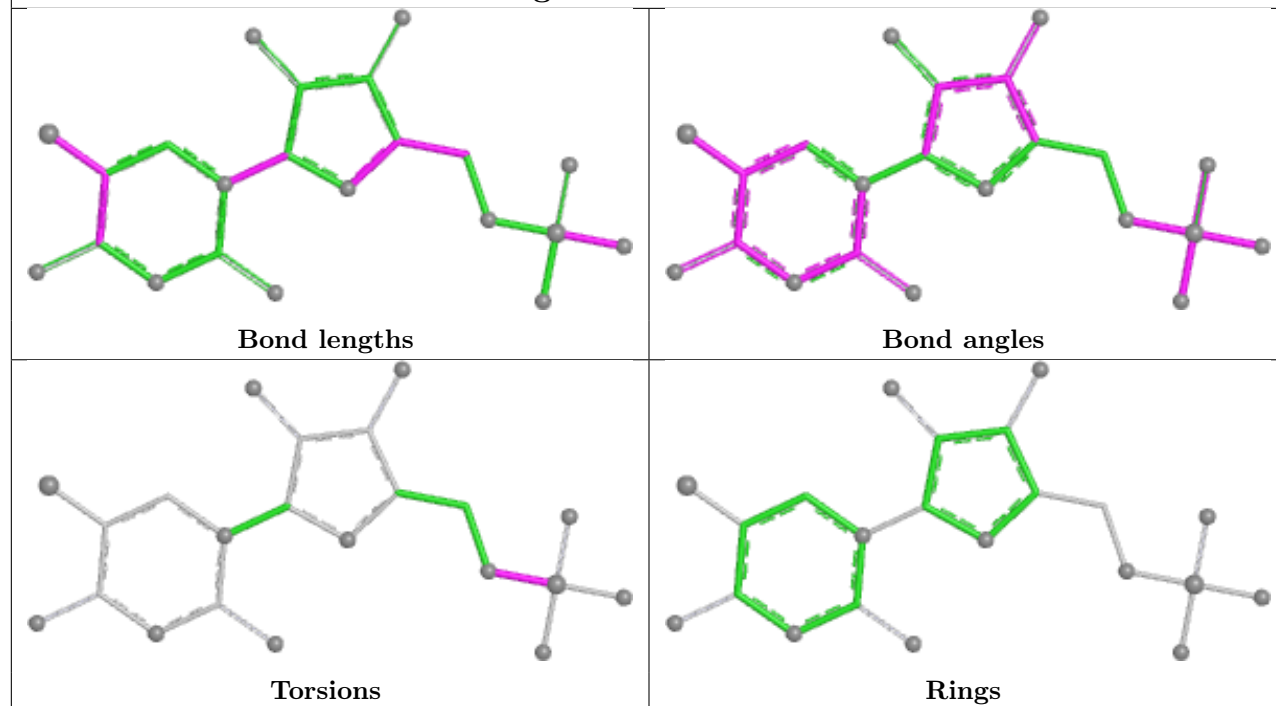
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



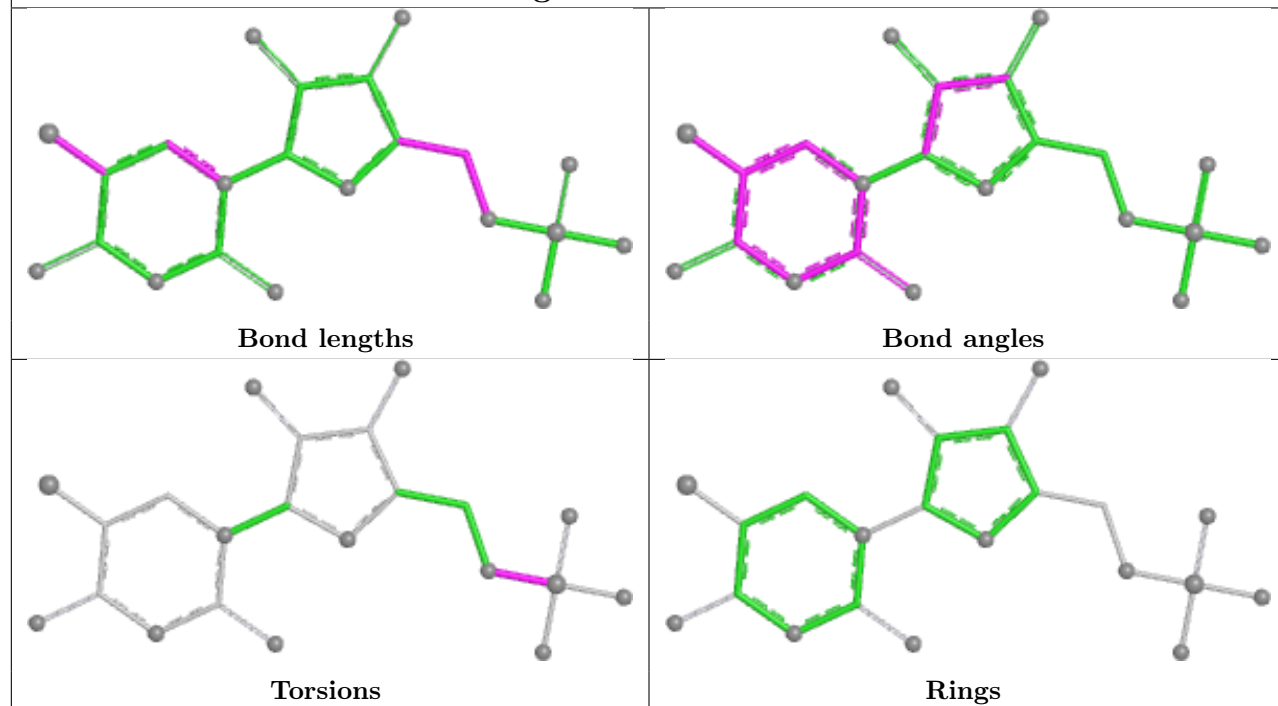
Ligand FAD B 302



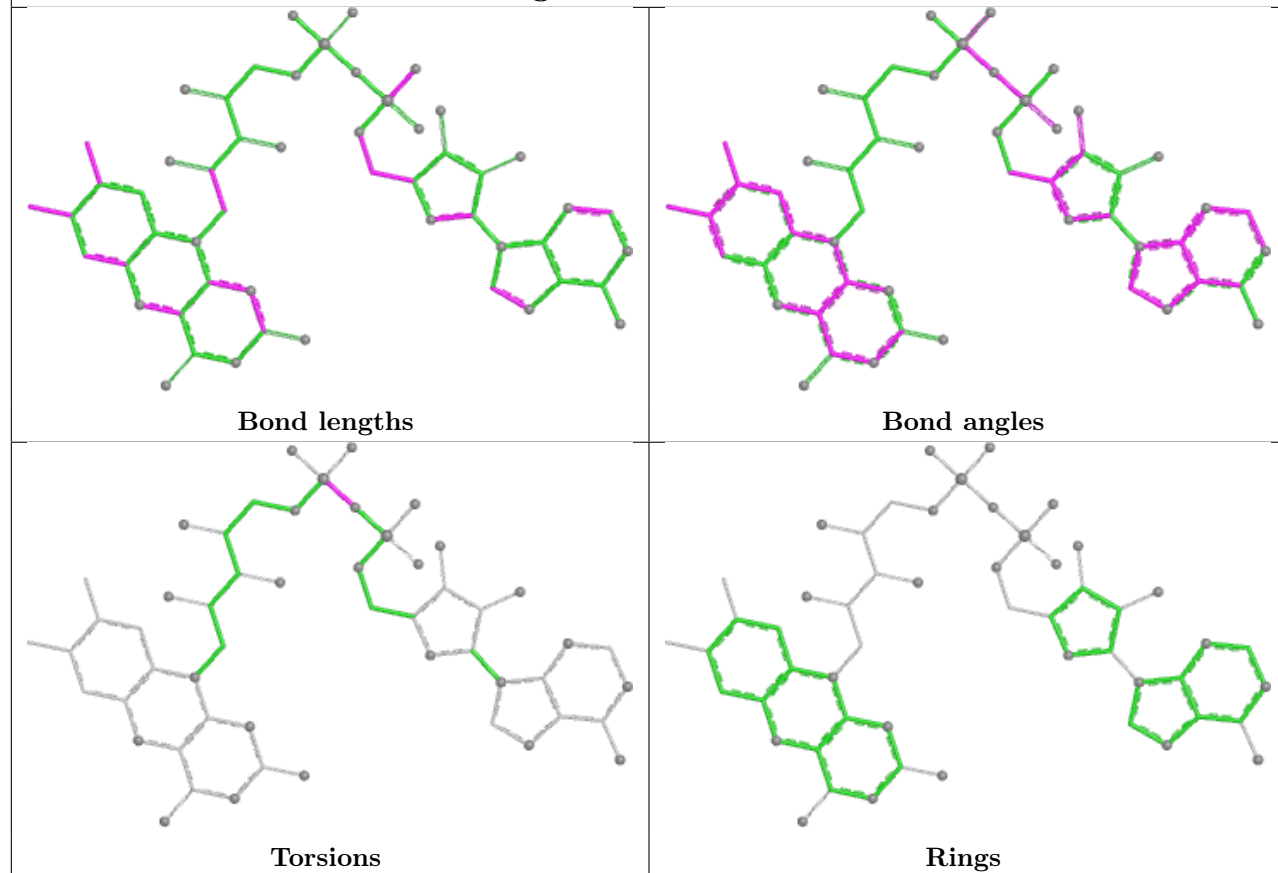
Ligand 5BU D 301



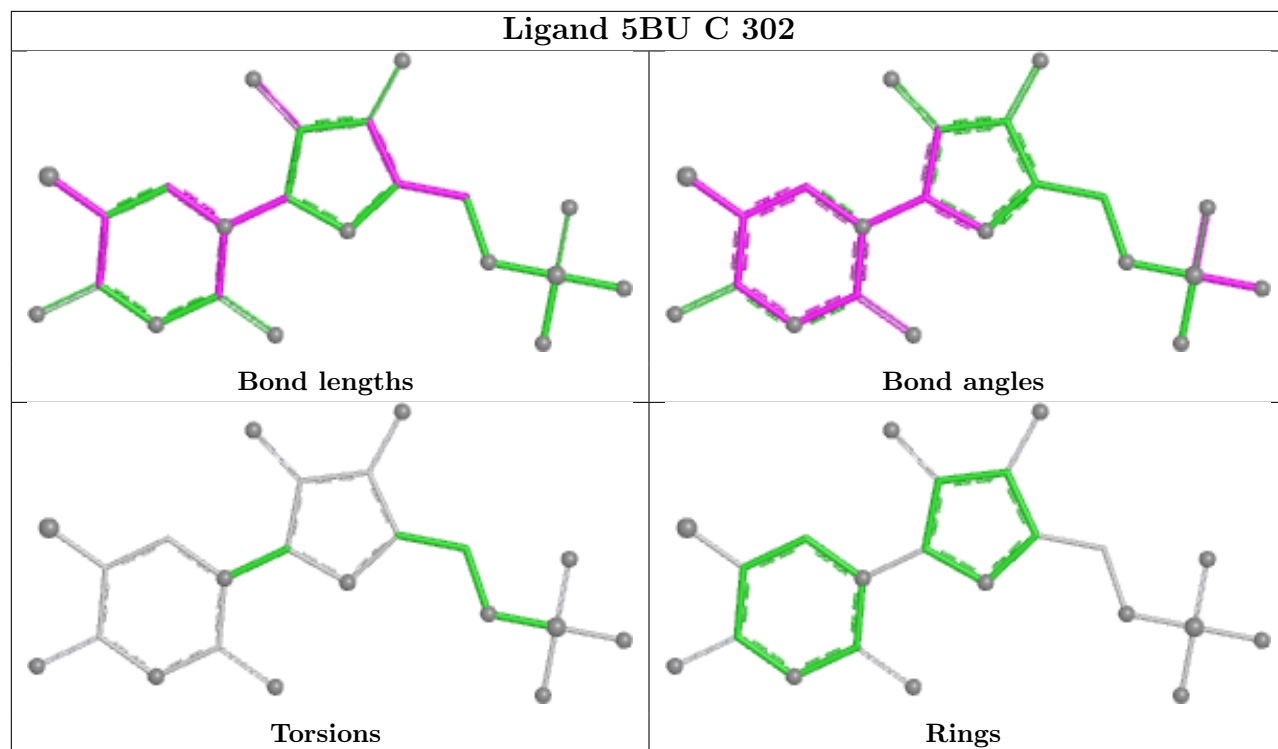
Ligand 5BU A 302



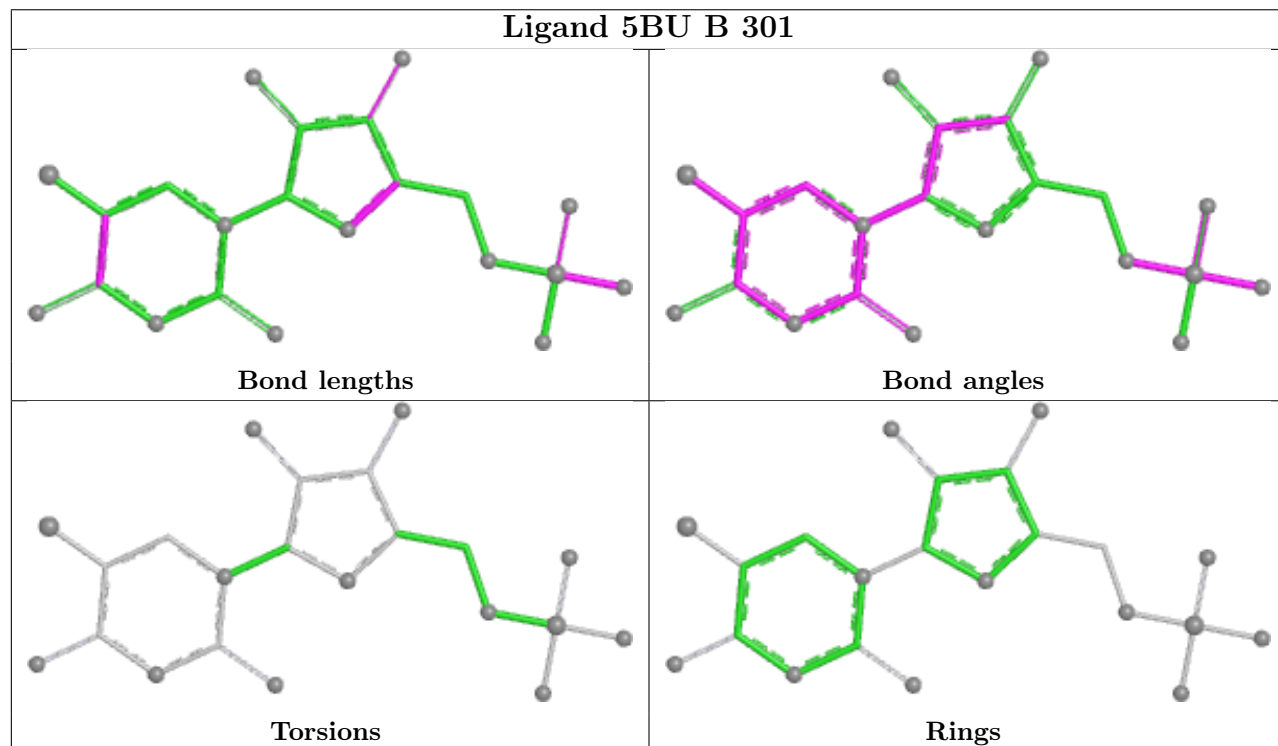
Ligand FAD D 302

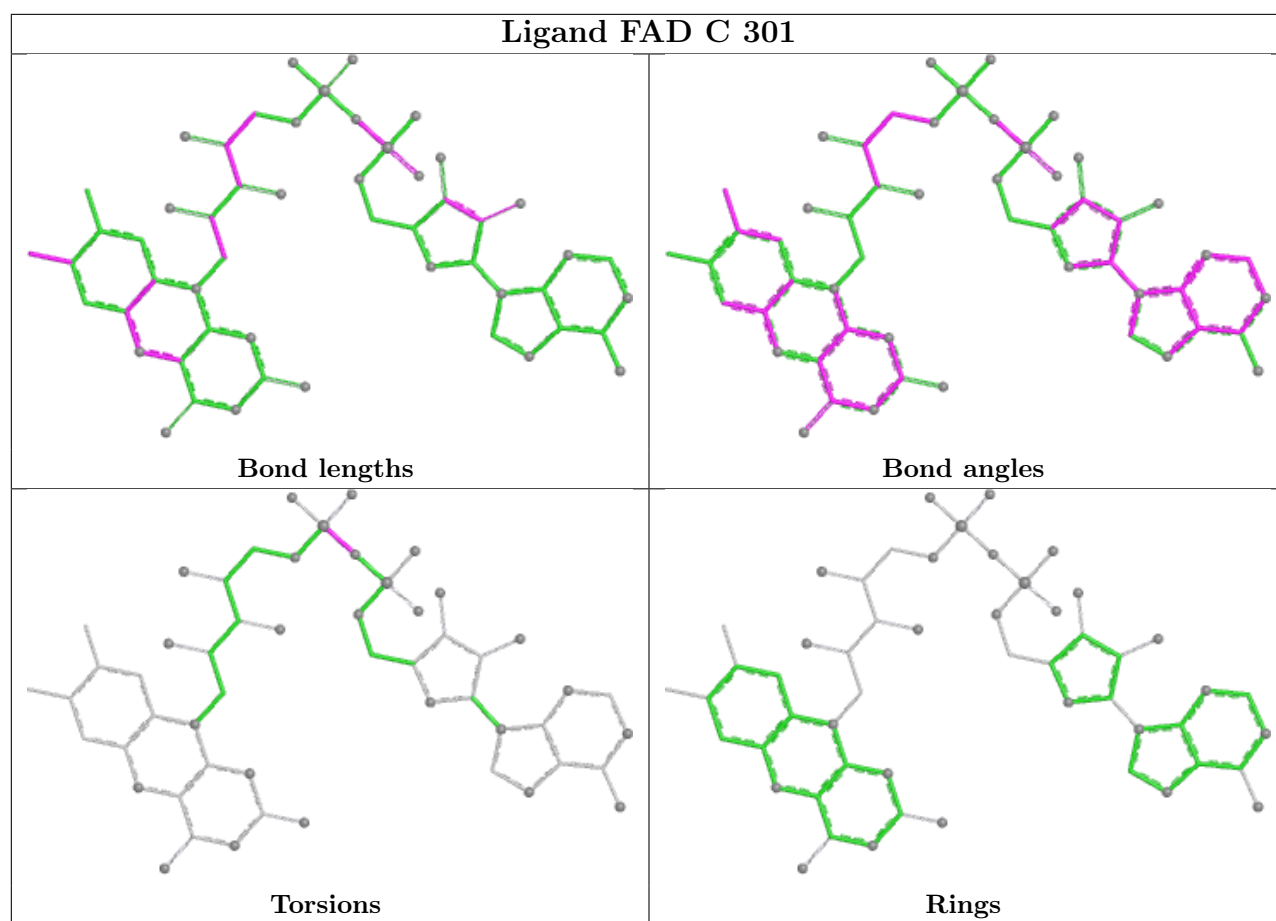


Ligand 5BU C 302



Ligand 5BU B 301





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	226/239 (94%)	-0.18	7 (3%) 51 58	7, 16, 43, 56	1 (0%)
1	B	227/239 (94%)	-0.24	5 (2%) 62 69	7, 16, 41, 50	4 (1%)
1	C	223/239 (93%)	-0.35	4 (1%) 67 74	6, 15, 34, 50	2 (0%)
1	D	225/239 (94%)	-0.20	4 (1%) 67 74	8, 16, 39, 59	1 (0%)
All	All	901/956 (94%)	-0.24	20 (2%) 62 69	6, 15, 40, 59	8 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	46	GLY	6.2
1	A	4	PRO	4.1
1	B	45	ASP	3.9
1	A	35	ALA	3.9
1	B	34	THR	3.8
1	D	45	ASP	3.7
1	A	57	MET	3.7
1	A	36	GLY	3.5
1	C	5	ARG	3.2
1	A	122	GLY	2.8
1	C	132	ASP	2.7
1	D	34	THR	2.7
1	B	46	GLY	2.6
1	C	34	THR	2.5
1	C	4	PRO	2.5
1	A	131	THR	2.2
1	B	44	TYR	2.1
1	A	129	GLY	2.1
1	D	5	ARG	2.0
1	B	198	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

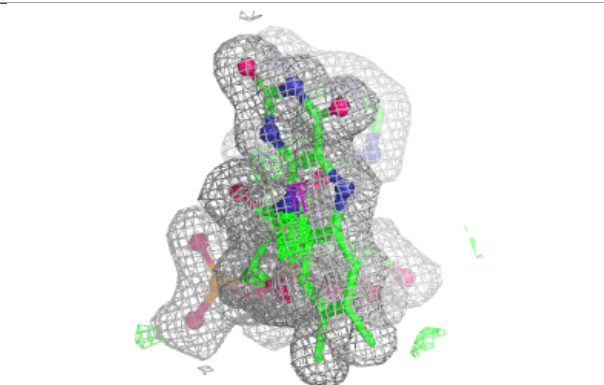
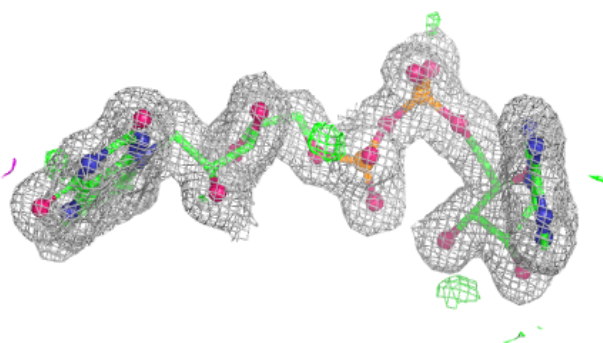
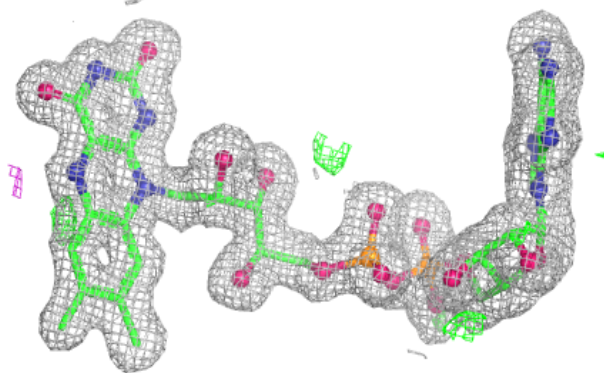
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FAD	A	301	53/53	0.98	0.04	6,11,15,17	0
2	FAD	B	302	53/53	0.99	0.04	7,11,16,20	0
2	FAD	C	301	53/53	0.99	0.04	7,10,14,14	0
2	FAD	D	302	53/53	0.99	0.03	7,9,15,20	0
3	5BU	A	302	22/22	0.99	0.04	9,11,16,17	0
3	5BU	B	301	22/22	0.99	0.04	8,12,17,17	0
3	5BU	C	302	22/22	0.99	0.03	8,11,15,17	0
3	5BU	D	301	22/22	0.99	0.05	7,12,15,17	0

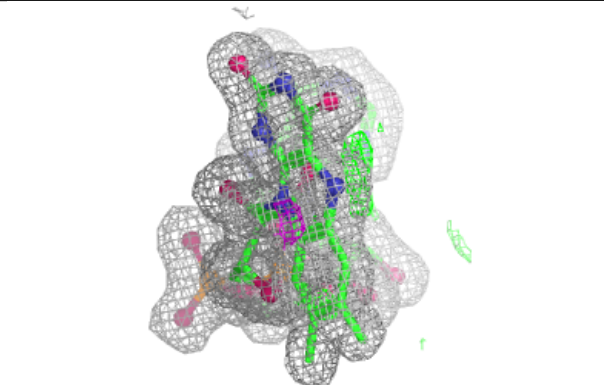
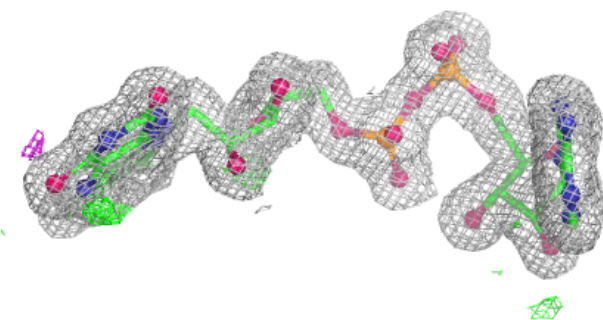
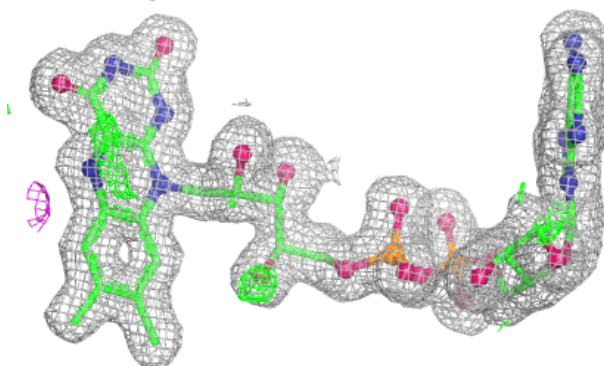
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 301:

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

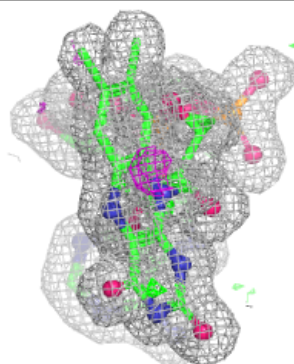
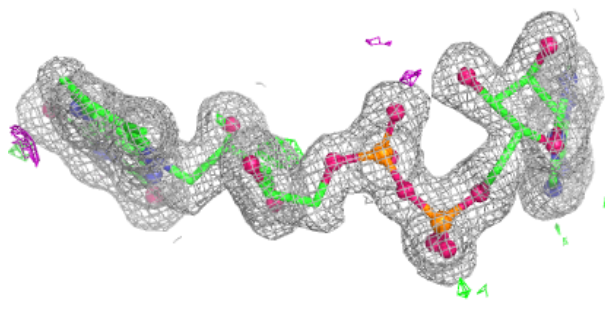
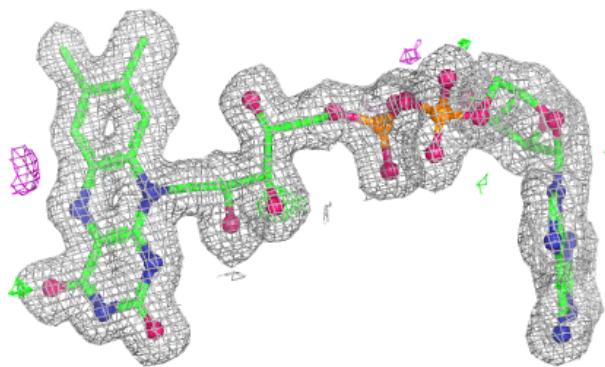
**Electron density around FAD B 302:**

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

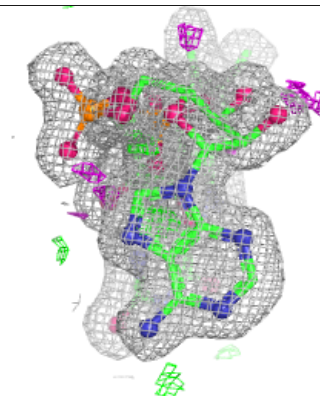
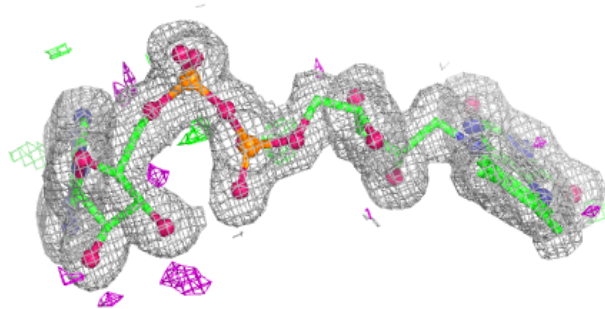
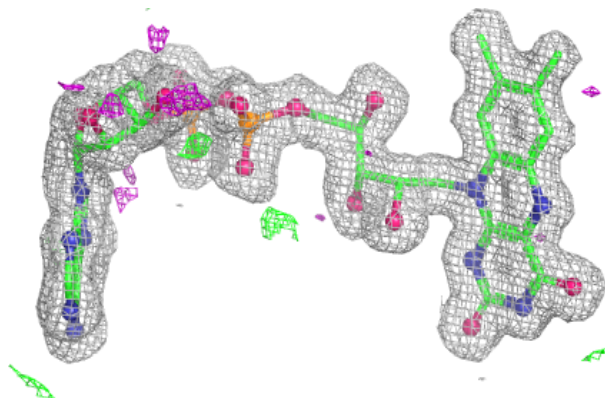


Electron density around FAD C 301:

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

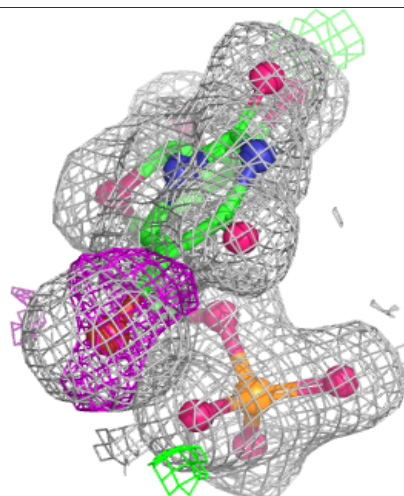
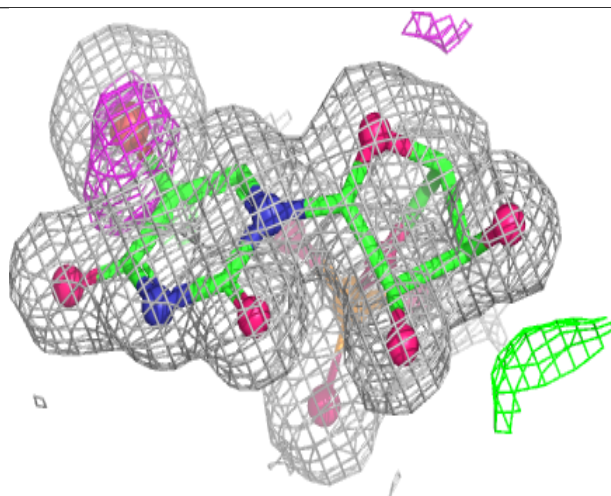
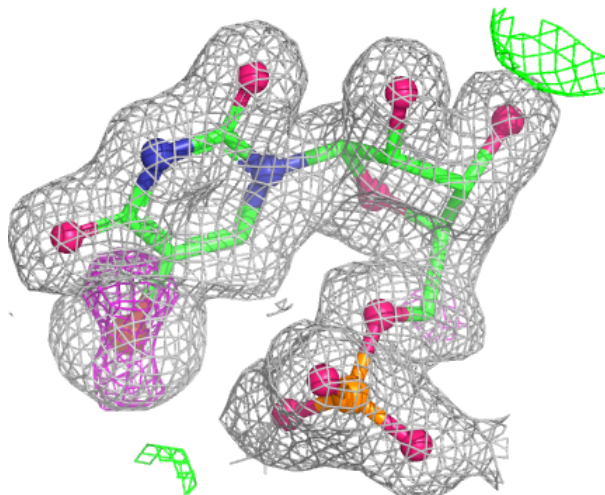
**Electron density around FAD D 302:**

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



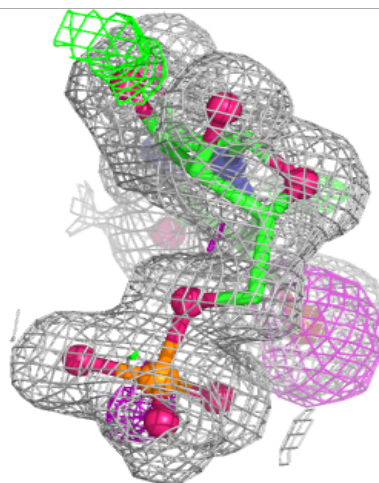
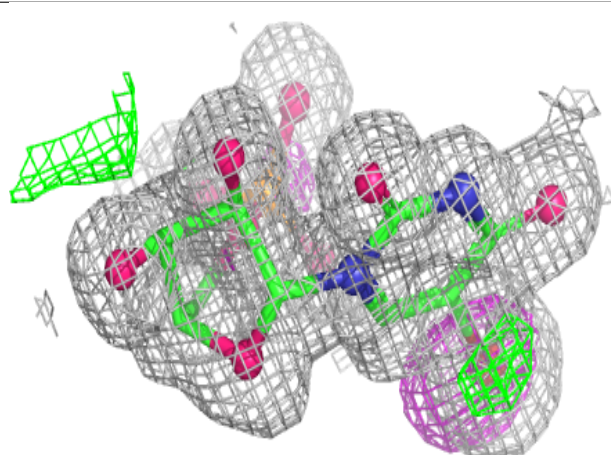
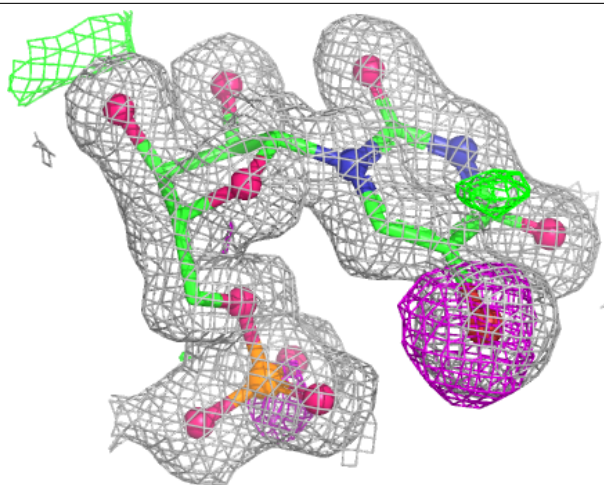
Electron density around 5BU A 302:

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



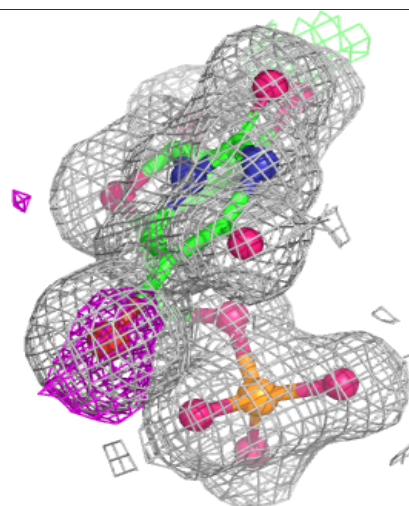
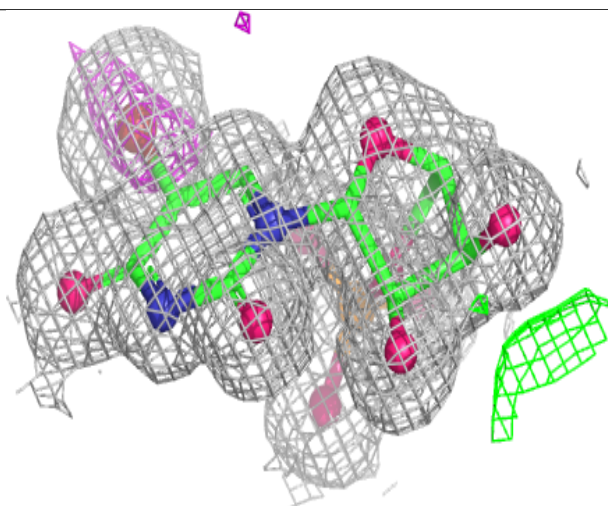
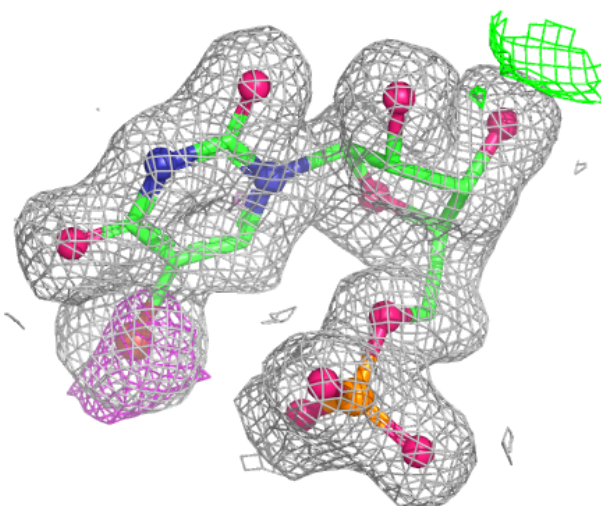
Electron density around 5BU B 301:

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



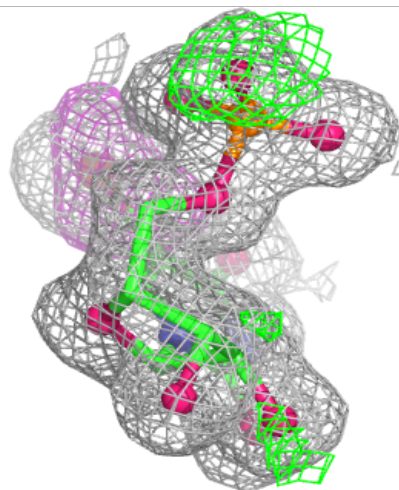
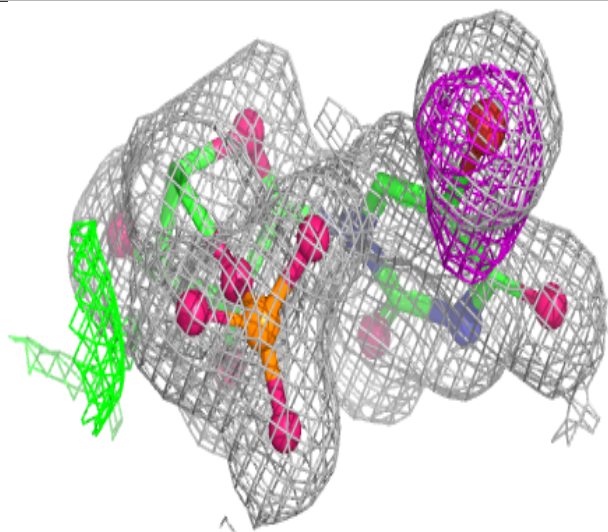
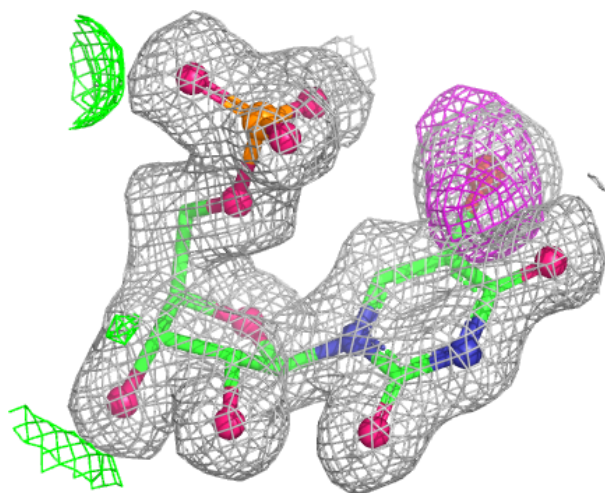
Electron density around 5BU C 302:

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



Electron density around 5BU D 301:

$2mF_o-DF_c$ (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.