



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:37 PM UTC

PDB ID : 4P5B / pdb_00004p5b
Title : Crystal structure of a UMP/dUMP methylase PolB from *Streptomyces cacaoi* bound with 5-Br dUMP
Authors : Li, Y.; Chen, W.; Li, J.; Xia, Z.; Deng, Z.; Zhou, J.
Deposited on : 2014-03-15
Resolution : 2.27 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

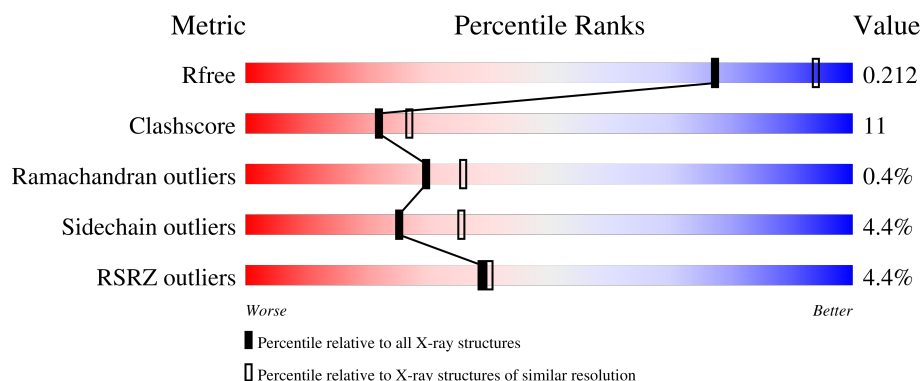
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	6% 74% 19% • •
1	B	239	5% 74% 21% • • •
1	C	239	5% 72% 22% • • •
1	D	239	2% 79% 19% •

2 Entry composition [i](#)

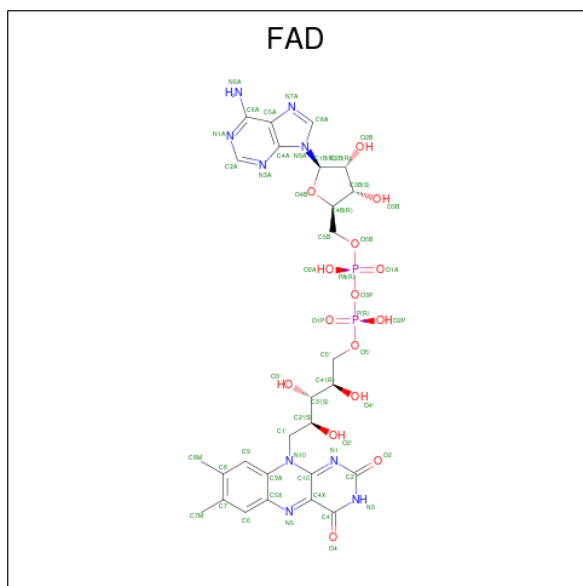
There are 5 unique types of molecules in this entry. The entry contains 8125 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	229	Total	C	N	O	S	0	1	0
			1813	1132	336	337	8			
1	B	235	Total	C	N	O	S	0	1	0
			1874	1169	346	351	8			
1	C	234	Total	C	N	O	S	0	1	0
			1854	1157	339	350	8			
1	D	235	Total	C	N	O	S	0	1	0
			1881	1175	346	352	8			

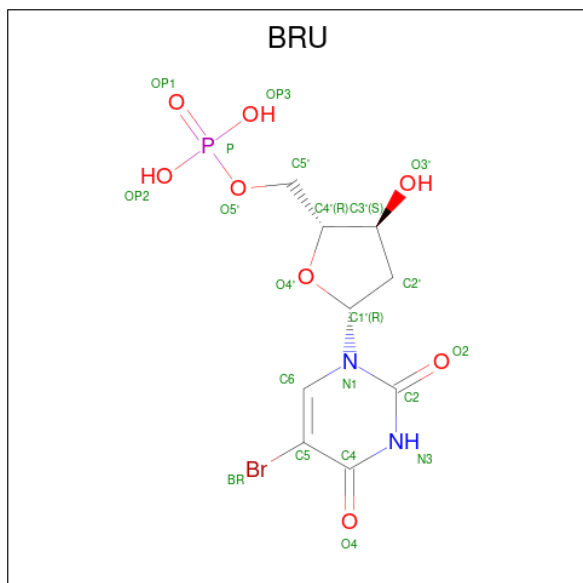
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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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-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (CCD ID: BRU) (formula: $C_9H_{12}BrN_2O_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	Br 1	C 9	N 2	O 8	P 1	0	0
3	B	1	Total 21	Br 1	C 9	N 2	O 8	P 1	0	0
3	C	1	Total 21	Br 1	C 9	N 2	O 8	P 1	0	0
3	D	1	Total 21	Br 1	C 9	N 2	O 8	P 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

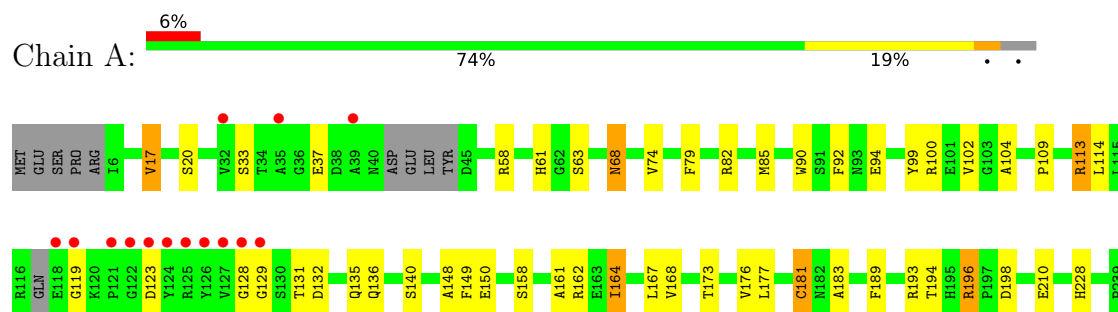
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		
5	B	97	Total	O	0	0
			97	97		
5	C	93	Total	O	0	0
			93	93		
5	D	108	Total	O	0	0
			108	108		

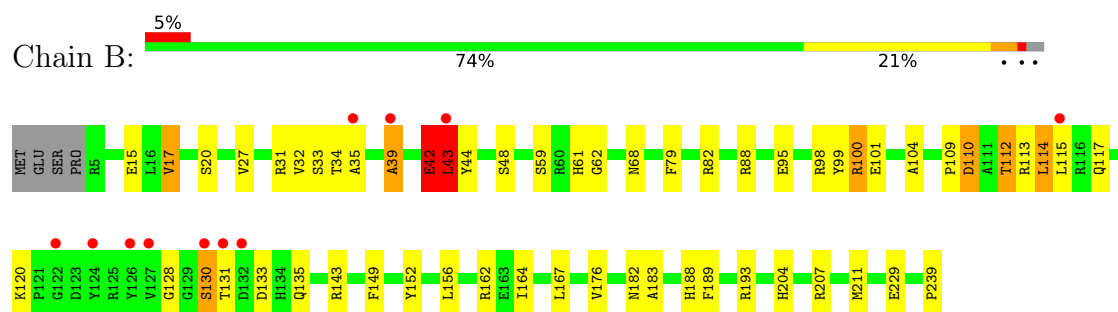
3 Residue-property plots [i](#)

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.

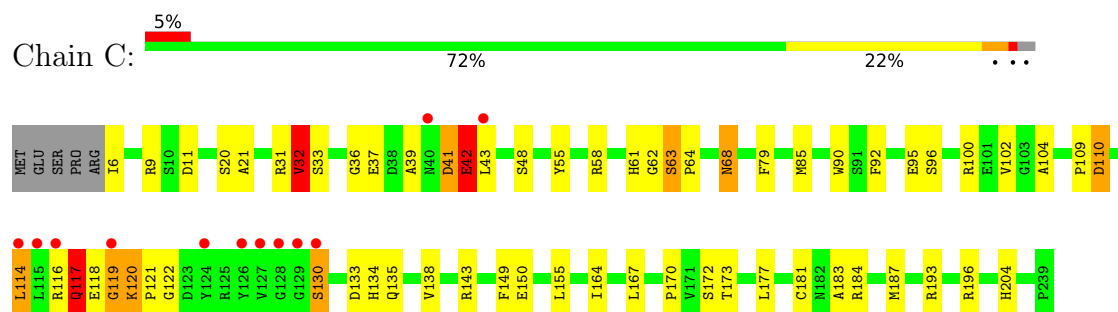
• Molecule 1: Thymidylate synthase ThyX



• Molecule 1: Thymidylate synthase ThyX

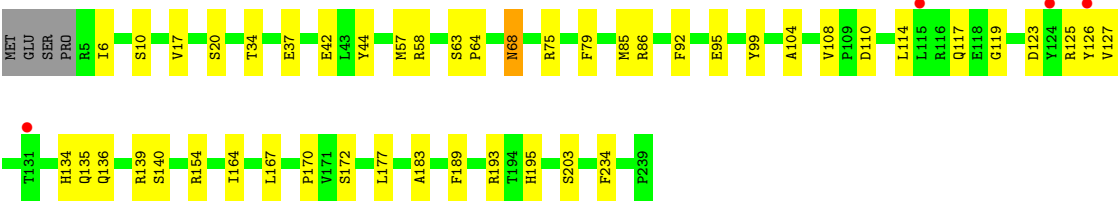


• Molecule 1: Thymidylate synthase ThyX



• Molecule 1: Thymidylate synthase ThyX





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.79Å 59.50Å 118.98Å 90.00° 120.31° 90.00°	Depositor
Resolution (Å)	50.00 – 2.27 50.00 – 2.27	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.27) 97.6 (50.00-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.164 , 0.216 0.163 , 0.212	Depositor DCC
R_{free} test set	2332 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8125	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BRU, SO4, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.26	2/1851 (0.1%)	1.18	5/2505 (0.2%)
1	B	1.25	5/1915 (0.3%)	1.15	6/2594 (0.2%)
1	C	1.29	4/1895 (0.2%)	1.18	13/2569 (0.5%)
1	D	1.20	0/1923	1.16	2/2605 (0.1%)
All	All	1.25	11/7584 (0.1%)	1.17	26/10273 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	SER	C-O	-6.29	1.18	1.24
1	C	32	VAL	CA-C	6.21	1.60	1.52
1	B	27	VAL	CA-CB	6.17	1.60	1.54
1	B	176	VAL	C-O	6.11	1.30	1.24
1	C	117	GLN	N-CA	5.40	1.53	1.46
1	B	188	HIS	CA-C	5.30	1.59	1.52
1	A	181	CYS	CA-C	5.29	1.59	1.52
1	B	15	GLU	CA-C	5.23	1.58	1.52
1	C	55	TYR	N-CA	-5.19	1.40	1.46
1	C	21	ALA	CA-C	-5.14	1.46	1.52
1	B	17	VAL	N-CA	-5.06	1.40	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	ASP	N-CA-C	8.34	120.45	110.44
1	C	118	GLU	N-CA-C	7.17	120.79	108.02
1	A	129	GLY	N-CA-C	6.49	118.68	110.96
1	A	196	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	A	17	VAL	CB-CA-C	6.04	116.56	110.65
1	B	120	LYS	CA-C-N	6.01	126.36	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	LYS	C-N-CA	6.01	126.36	119.93
1	A	17	VAL	N-CA-CB	-5.95	104.09	112.12
1	D	57	MET	N-CA-C	-5.91	104.76	111.14
1	B	43	LEU	N-CA-C	5.88	119.97	113.21
1	C	120	LYS	CA-C-N	5.80	126.09	119.83
1	C	120	LYS	C-N-CA	5.80	126.09	119.83
1	B	42	GLU	N-CA-C	5.63	122.79	110.80
1	C	196	ARG	CA-C-N	5.61	126.85	119.84
1	C	196	ARG	C-N-CA	5.61	126.85	119.84
1	C	62	GLY	N-CA-C	5.55	121.06	113.62
1	C	119	GLY	N-CA-C	5.50	126.23	113.18
1	D	234	PHE	N-CA-C	5.44	118.92	112.72
1	C	36	GLY	N-CA-C	5.40	121.07	111.73
1	C	187	MET	N-CA-C	5.25	117.01	111.28
1	A	164	ILE	N-CA-C	-5.24	107.31	111.81
1	C	63	SER	CA-C-N	-5.12	114.54	119.87
1	C	63	SER	C-N-CA	-5.12	114.54	119.87
1	B	128	GLY	N-CA-C	5.07	117.43	110.58
1	C	120	LYS	N-CA-C	5.04	125.10	111.00
1	B	44	TYR	N-CA-C	5.01	117.42	109.96

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	1813	0	1761	44	0
1	B	1874	0	1818	55	0
1	C	1854	0	1785	42	0
1	D	1881	0	1825	40	0
2	A	53	0	31	3	0
2	B	53	0	31	4	0
2	C	53	0	31	2	0
2	D	53	0	31	3	0
3	A	21	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	10	4	0
3	C	21	0	10	2	0
3	D	21	0	10	1	0
4	A	5	0	0	0	0
5	A	104	0	0	6	0
5	B	97	0	0	5	0
5	C	93	0	0	3	1
5	D	108	0	0	3	0
All	All	8125	0	7353	162	1

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 11.

All (162) 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)
2:B:302:FAD:O1A	5:B:463:HOH:O	1.70	1.09
2:A:301:FAD:O1A	5:A:475:HOH:O	1.72	1.06
2:D:302:FAD:O1A	5:D:449:HOH:O	1.77	1.01
1:D:68:ASN:HD21	1:D:183:ALA:H	1.07	1.00
1:D:10:SER:HB3	1:D:108:VAL:O	1.61	0.99
1:A:193:ARG:HH12	3:B:301:BRU:HN3	1.15	0.93
1:A:119:GLY:HA2	5:A:477:HOH:O	1.66	0.93
1:B:68:ASN:HD21	1:B:183:ALA:H	1.08	0.93
1:A:68:ASN:HD21	1:A:183:ALA:H	1.11	0.90
3:A:302:BRU:HN3	1:B:193:ARG:HH12	1.17	0.90
1:C:68:ASN:HD21	1:C:183:ALA:H	1.19	0.90
2:C:301:FAD:HM72	5:C:461:HOH:O	1.75	0.86
1:C:193:ARG:HH12	3:D:301:BRU:HN3	1.22	0.84
3:C:302:BRU:HN3	1:D:193:ARG:HH12	1.26	0.82
1:B:207:ARG:HG3	1:B:211:MET:HE3	1.61	0.82
1:A:119:GLY:CA	5:A:477:HOH:O	2.30	0.77
1:A:68:ASN:HD21	1:A:183:ALA:N	1.83	0.76
1:A:228:HIS:CD2	5:A:464:HOH:O	2.38	0.76
1:B:229:GLU:HG2	5:B:402:HOH:O	1.88	0.74
1:B:110:ASP:OD2	1:B:112:THR:HG23	1.88	0.73
1:D:85:MET:HE3	1:D:177:LEU:HD13	1.70	0.72
1:A:79:PHE:CE1	1:B:167:LEU:HD22	2.24	0.72
1:B:68:ASN:HD21	1:B:183:ALA:N	1.86	0.72
1:D:58:ARG:HD3	5:D:499:HOH:O	1.90	0.71
1:B:115:LEU:HD23	1:B:130:SER:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASN:HD21	1:C:183:ALA:N	1.88	0.70
1:A:161:ALA:H	1:B:117:GLN:HE21	1.40	0.69
1:D:68:ASN:HD21	1:D:183:ALA:N	1.87	0.68
1:B:114:LEU:HD13	1:B:117:GLN:OE1	1.94	0.68
1:C:114:LEU:O	1:C:117:GLN:HG3	1.96	0.66
2:B:302:FAD:HM73	5:D:508:HOH:O	1.95	0.66
1:A:100:ARG:HD2	1:D:34:THR:O	1.96	0.66
1:C:63:SER:HB2	5:C:493:HOH:O	1.94	0.66
1:C:85:MET:HE2	1:C:92:PHE:HB3	1.77	0.65
1:A:100:ARG:HD2	1:D:34:THR:C	2.22	0.65
1:B:20:SER:HB2	1:C:20:SER:HB2	1.79	0.64
1:A:104:ALA:HB2	1:A:149:PHE:CZ	2.32	0.64
1:B:59:SER:HB2	1:B:61[B]:HIS:CD2	2.33	0.63
1:A:85:MET:HE2	1:A:92:PHE:HB3	1.80	0.63
1:C:85:MET:HE2	1:C:92:PHE:CB	2.29	0.62
1:A:85:MET:HE3	1:A:177:LEU:CD2	2.29	0.62
1:B:33:SER:HA	1:C:95:GLU:HA	1.80	0.62
1:A:20:SER:HB2	1:D:20:SER:HB2	1.82	0.61
1:B:99:TYR:CE2	3:B:301:BRU:BR	3.10	0.60
1:D:85:MET:HE2	1:D:92:PHE:HB3	1.84	0.59
1:B:100:ARG:HA	1:B:162:ARG:HH11	1.68	0.59
5:A:482:HOH:O	1:D:37:GLU:HG3	2.02	0.58
1:B:42:GLU:HG2	1:B:43:LEU:H	1.69	0.58
1:B:62:GLY:HA2	1:B:239:PRO:HB2	1.85	0.58
1:A:196:ARG:NH1	5:A:458:HOH:O	2.36	0.57
1:B:68:ASN:ND2	1:B:183:ALA:H	1.92	0.57
1:A:161:ALA:HB2	1:B:117:GLN:HB3	1.87	0.57
1:D:119:GLY:HA3	1:D:126:TYR:HB3	1.87	0.56
1:B:104:ALA:HB2	1:B:149:PHE:CZ	2.40	0.56
1:A:161:ALA:H	1:B:117:GLN:NE2	2.03	0.56
1:B:131:THR:O	1:B:131:THR:HG22	2.06	0.56
1:C:104:ALA:HB2	1:C:149:PHE:CE2	2.41	0.56
1:C:114:LEU:HD13	1:C:134:HIS:HA	1.87	0.56
1:B:95:GLU:HA	1:C:33:SER:HA	1.87	0.55
1:A:85:MET:HE3	1:A:177:LEU:HD23	1.89	0.55
1:B:32:VAL:HA	1:B:39:ALA:HB2	1.87	0.55
1:B:114:LEU:HD12	1:B:133:ASP:CB	2.36	0.55
1:A:177:LEU:C	1:A:177:LEU:HD12	2.31	0.55
1:C:167:LEU:HD22	1:D:79:PHE:CE1	2.42	0.55
1:C:143:ARG:HH21	1:D:154:ARG:HH11	1.52	0.54
1:A:99:TYR:O	1:A:162:ARG:NH1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ILE:O	1:C:167:LEU:HG	2.08	0.54
1:B:34:THR:C	1:C:100:ARG:HD2	2.33	0.53
1:C:61[B]:HIS:O	1:C:64:PRO:HD2	2.09	0.53
1:C:122:GLY:HA2	1:C:204:HIS:CD2	2.43	0.53
1:A:164:ILE:O	1:A:167:LEU:HG	2.08	0.53
1:B:99:TYR:HE2	3:B:301:BRU:BR	2.47	0.52
1:A:161:ALA:CB	1:B:117:GLN:HB3	2.39	0.52
2:A:301:FAD:O4'	2:A:301:FAD:H9	2.09	0.52
1:B:114:LEU:O	1:B:117:GLN:OE1	2.28	0.52
1:B:101:GLU:H	1:B:162:ARG:NH1	2.08	0.52
1:C:172:SER:HB3	1:D:167:LEU:HB3	1.92	0.51
1:A:167:LEU:HD22	1:B:79:PHE:CE1	2.46	0.51
1:A:90:TRP:CD2	1:A:181:CYS:HB3	2.46	0.51
1:B:59:SER:CB	1:B:61[B]:HIS:CD2	2.94	0.51
1:C:110:ASP:OD1	1:C:110:ASP:C	2.53	0.51
1:D:68:ASN:ND2	1:D:183:ALA:H	1.91	0.50
1:B:189:PHE:CE2	1:B:193:ARG:HG3	2.47	0.50
1:B:95:GLU:OE1	1:B:100:ARG:HD3	2.12	0.50
1:D:85:MET:CE	1:D:177:LEU:HD13	2.39	0.50
1:B:88:ARG:NE	2:B:302:FAD:O2A	2.34	0.50
1:B:164:ILE:O	1:B:167:LEU:HG	2.12	0.50
1:C:121:PRO:HD2	1:D:99:TYR:CE2	2.47	0.50
1:C:130:SER:O	1:C:133:ASP:HB2	2.12	0.50
1:A:85:MET:HE3	1:A:177:LEU:HD22	1.93	0.49
1:A:104:ALA:HB2	1:A:149:PHE:CE1	2.47	0.49
1:A:109:PRO:HB3	1:A:113:ARG:HG3	1.94	0.49
1:B:114:LEU:HD12	1:B:133:ASP:HB3	1.95	0.49
1:D:189:PHE:CE2	1:D:193:ARG:HG3	2.46	0.49
1:A:37:GLU:CB	1:D:75:ARG:HH12	2.25	0.49
1:B:182:ASN:ND2	2:D:302:FAD:N1A	2.59	0.49
3:C:302:BRU:HN3	1:D:193:ARG:NH1	2.04	0.48
1:B:95:GLU:OE1	1:B:100:ARG:NH2	2.44	0.48
1:C:102:VAL:HG11	1:C:173:THR:HG21	1.94	0.48
2:B:302:FAD:N3A	5:B:452:HOH:O	2.35	0.48
1:C:42:GLU:HB3	1:C:43:LEU:H	1.53	0.48
1:D:10:SER:CB	1:D:108:VAL:O	2.49	0.48
1:B:115:LEU:CD2	1:B:130:SER:HA	2.44	0.47
1:B:182:ASN:HD21	2:D:302:FAD:C2A	2.28	0.47
1:C:61[B]:HIS:HD2	5:C:469:HOH:O	1.98	0.47
1:D:135:GLN:HG2	1:D:139:ARG:HD3	1.97	0.47
1:D:195:HIS:HD2	1:D:203:SER:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PHE:CE2	1:A:193:ARG:HG3	2.50	0.46
1:A:90:TRP:CE3	1:A:181:CYS:HB3	2.52	0.45
1:B:114:LEU:HD12	1:B:133:ASP:HB2	1.98	0.45
1:D:123:ASP:OD1	1:D:125:ARG:HG2	2.15	0.45
1:C:116:ARG:O	1:C:117:GLN:O	2.33	0.45
1:C:31:ARG:CB	1:C:39:ALA:HB1	2.47	0.45
1:A:194:THR:HA	1:A:210:GLU:HG3	1.99	0.45
1:C:9:ARG:HB3	1:C:11:ASP:OD1	2.16	0.45
1:A:177:LEU:HD12	1:A:177:LEU:O	2.16	0.44
1:C:79:PHE:CE1	1:D:167:LEU:HD22	2.52	0.44
2:A:301:FAD:O3B	1:C:184:ARG:NH1	2.50	0.44
1:B:104:ALA:HB2	1:B:149:PHE:CE2	2.53	0.44
1:A:102:VAL:HG11	1:A:173:THR:HG21	1.99	0.44
1:B:59:SER:HB2	1:B:61[B]:HIS:HD2	1.79	0.44
1:B:204:HIS:ND1	5:B:469:HOH:O	2.37	0.44
1:D:114:LEU:CD1	1:D:134:HIS:HA	2.48	0.44
1:C:134:HIS:O	1:C:138:VAL:HG23	2.17	0.44
1:C:155:LEU:HD21	1:D:140:SER:CB	2.47	0.44
1:D:63:SER:OG	1:D:64:PRO:HD3	2.17	0.44
1:B:31:ARG:NH2	1:B:35:ALA:HB2	2.32	0.43
1:A:33:SER:HA	1:D:95:GLU:HA	2.00	0.43
1:C:31:ARG:HB3	1:C:39:ALA:HB1	2.00	0.43
1:C:90:TRP:CD2	1:C:181:CYS:HB3	2.53	0.43
1:D:136:GLN:O	1:D:140:SER:HB2	2.17	0.43
1:C:63:SER:N	1:C:64:PRO:CD	2.82	0.43
1:A:85:MET:HE1	1:A:94:GLU:HB2	2.01	0.43
1:A:82:ARG:HD3	1:B:82:ARG:HD3	2.01	0.42
1:A:196:ARG:HD2	1:A:198:ASP:OD1	2.19	0.42
1:B:109:PRO:HB3	1:B:113:ARG:HD2	2.02	0.42
1:D:114:LEU:O	1:D:117:GLN:HG3	2.20	0.42
1:C:11:ASP:OD1	1:C:11:ASP:N	2.53	0.42
1:C:109:PRO:HG2	1:C:114:LEU:HD11	2.02	0.42
1:C:31:ARG:O	1:C:32:VAL:C	2.62	0.42
1:C:167:LEU:HB3	1:D:172:SER:HB3	2.02	0.42
1:D:86:ARG:HD2	1:D:86:ARG:HA	1.85	0.42
1:A:61[A]:HIS:HE1	2:C:301:FAD:O2'	2.03	0.41
1:D:42:GLU:HB2	1:D:44:TYR:CZ	2.56	0.41
1:B:62:GLY:CA	1:B:239:PRO:HB2	2.48	0.41
1:D:6:ILE:HA	1:D:104:ALA:HB1	2.03	0.41
1:A:148:ALA:HB1	1:A:168:VAL:O	2.21	0.41
1:C:119:GLY:HA3	1:C:120:LYS:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PHE:CD1	1:B:167:LEU:HD22	2.56	0.41
1:B:114:LEU:HD22	1:B:114:LEU:HA	1.80	0.41
1:C:96:SER:O	1:C:100:ARG:HB2	2.20	0.41
1:D:110:ASP:OD1	1:D:110:ASP:C	2.64	0.41
1:D:164:ILE:O	1:D:167:LEU:HG	2.21	0.41
1:A:74:VAL:O	1:A:176:VAL:HA	2.21	0.41
1:C:170:PRO:HA	1:D:170:PRO:HA	2.03	0.41
1:D:117:GLN:O	1:D:127:VAL:HA	2.21	0.41
1:A:114:LEU:HB3	1:A:128:GLY:O	2.21	0.40
1:B:162:ARG:NH1	5:B:465:HOH:O	2.54	0.40
1:A:150:GLU:OE1	1:B:143:ARG:NH1	2.46	0.40
1:B:152:TYR:CZ	1:B:156:LEU:HD11	2.57	0.40
1:B:98:ARG:HD3	3:B:301:BRU:BR	2.76	0.40
1:A:136:GLN:O	1:A:140:SER:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:401:HOH:O	5:C:409:HOH:O[2_556]	2.04	0.16

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	224/239 (94%)	220 (98%)	4 (2%)	0	100	100
1	B	234/239 (98%)	225 (96%)	7 (3%)	2 (1%)	14	15
1	C	233/239 (98%)	222 (95%)	9 (4%)	2 (1%)	14	15
1	D	234/239 (98%)	228 (97%)	6 (3%)	0	100	100
All	All	925/956 (97%)	895 (97%)	26 (3%)	4 (0%)	30	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	42	GLU
1	C	117	GLN
1	B	39	ALA
1	C	42	GLU

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	189/201 (94%)	180 (95%)	9 (5%)	23	32
1	B	196/201 (98%)	187 (95%)	9 (5%)	24	34
1	C	193/201 (96%)	179 (93%)	14 (7%)	13	16
1	D	197/201 (98%)	195 (99%)	2 (1%)	68	81
All	All	775/804 (96%)	741 (96%)	34 (4%)	25	35

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	58	ARG
1	A	68	ASN
1	A	113	ARG
1	A	123	ASP
1	A	131	THR
1	A	132	ASP
1	A	135	GLN
1	A	158	SER
1	B	17	VAL
1	B	43	LEU
1	B	48	SER
1	B	100	ARG
1	B	110	ASP
1	B	112	THR
1	B	114	LEU

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Mol	Chain	Res	Type
1	B	130	SER
1	B	135	GLN
1	C	6	ILE
1	C	32	VAL
1	C	37	GLU
1	C	41	ASP
1	C	42	GLU
1	C	48	SER
1	C	58	ARG
1	C	68	ASN
1	C	110	ASP
1	C	114	LEU
1	C	130	SER
1	C	135	GLN
1	C	150	GLU
1	C	177	LEU
1	D	17	VAL
1	D	68	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	93	ASN
1	A	188	HIS
1	A	195	HIS
1	B	40	ASN
1	B	68	ASN
1	B	93	ASN
1	B	117	GLN
1	B	136	GLN
1	B	195	HIS
1	B	204	HIS
1	C	68	ASN
1	C	93	ASN
1	C	195	HIS
1	C	204	HIS
1	C	215	GLN
1	D	40	ASN
1	D	68	ASN
1	D	93	ASN
1	D	195	HIS

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Mol	Chain	Res	Type
1	D	204	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 oligosaccharides 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	FAD	C	301	-	58,58,58	2.45	12 (20%)	85,89,89	1.90	24 (28%)
3	BRU	D	301	-	22,22,22	1.65	6 (27%)	32,33,33	3.00	13 (40%)
4	SO4	A	303	-	4,4,4	0.18	0	6,6,6	0.51	0
3	BRU	C	302	-	22,22,22	1.41	3 (13%)	32,33,33	3.01	10 (31%)
2	FAD	B	302	-	58,58,58	2.35	12 (20%)	85,89,89	2.02	30 (35%)
3	BRU	B	301	-	22,22,22	1.62	3 (13%)	32,33,33	2.16	10 (31%)
2	FAD	A	301	-	58,58,58	2.15	12 (20%)	85,89,89	2.24	32 (37%)
3	BRU	A	302	-	22,22,22	1.60	3 (13%)	32,33,33	2.52	11 (34%)
2	FAD	D	302	-	58,58,58	2.01	13 (22%)	85,89,89	1.87	25 (29%)

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	C	301	-	-	3/34/50/50	0/6/6/6
3	BRU	D	301	-	-	2/10/22/22	0/2/2/2
3	BRU	C	302	-	-	1/10/22/22	0/2/2/2
2	FAD	B	302	-	-	5/34/50/50	0/6/6/6
3	BRU	B	301	-	-	0/10/22/22	0/2/2/2
2	FAD	A	301	-	-	10/34/50/50	0/6/6/6
3	BRU	A	302	-	-	0/10/22/22	0/2/2/2
2	FAD	D	302	-	-	7/34/50/50	0/6/6/6

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	FAD	PA-O3P	13.20	1.73	1.59
2	A	301	FAD	PA-O3P	11.64	1.72	1.59
2	C	301	FAD	PA-O3P	11.23	1.71	1.59
2	C	301	FAD	P-O3P	7.49	1.67	1.59
2	D	302	FAD	PA-O3P	6.64	1.66	1.59
2	D	302	FAD	C10-N1	5.57	1.44	1.33
2	D	302	FAD	C4X-N5	5.53	1.42	1.30
2	C	301	FAD	C4X-N5	5.47	1.42	1.30
2	A	301	FAD	C4X-N5	4.49	1.40	1.30
2	B	302	FAD	C10-N1	4.30	1.41	1.33
2	C	301	FAD	PA-O5B	4.21	1.75	1.59
3	A	302	BRU	P-O5'	4.14	1.73	1.60
2	D	302	FAD	P-O3P	-4.04	1.55	1.59
2	C	301	FAD	C10-N1	3.99	1.41	1.33
2	D	302	FAD	C2-N1	3.83	1.45	1.36
2	C	301	FAD	PA-O1A	3.82	1.64	1.50
3	B	301	BRU	O4'-C4'	3.77	1.53	1.45
2	B	302	FAD	C4X-N5	3.76	1.38	1.30
3	C	302	BRU	P-O5'	3.74	1.72	1.60
2	B	302	FAD	PA-O5B	3.74	1.74	1.59
2	D	302	FAD	C4-N3	3.54	1.45	1.38
3	D	301	BRU	P-O5'	3.53	1.71	1.60
2	D	302	FAD	PA-O5B	3.46	1.72	1.59
3	B	301	BRU	C4-C5	-3.30	1.38	1.45
2	B	302	FAD	C2-N1	3.26	1.44	1.36
3	B	301	BRU	C4-N3	-3.01	1.33	1.38
2	A	301	FAD	PA-O5B	2.97	1.71	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	BRU	C6-C5	2.95	1.40	1.34
2	A	301	FAD	C10-N1	2.89	1.39	1.33
2	A	301	FAD	O3B-C3B	2.83	1.50	1.43
2	D	302	FAD	C10-N10	2.77	1.43	1.37
2	B	302	FAD	C4-N3	2.76	1.44	1.38
2	C	301	FAD	C8M-C8	2.75	1.56	1.51
3	C	302	BRU	C4-C5	-2.71	1.39	1.45
2	B	302	FAD	C7M-C7	2.68	1.56	1.51
3	D	301	BRU	C2'-C1'	2.68	1.59	1.52
3	D	301	BRU	C4-C5	-2.65	1.39	1.45
3	D	301	BRU	P-OP3	-2.63	1.45	1.54
2	B	302	FAD	C9-C9A	2.58	1.43	1.39
2	A	301	FAD	C9-C8	2.57	1.43	1.39
2	C	301	FAD	C8A-N7A	2.54	1.36	1.31
2	B	302	FAD	C8M-C8	2.54	1.55	1.51
2	C	301	FAD	C5'-C4'	2.50	1.55	1.51
3	A	302	BRU	C6-C5	2.47	1.39	1.34
3	C	302	BRU	C6-C5	2.46	1.39	1.34
2	A	301	FAD	C7M-C7	2.44	1.55	1.51
2	C	301	FAD	C5X-N5	2.42	1.43	1.39
2	C	301	FAD	C4-N3	2.32	1.43	1.38
2	B	302	FAD	C9-C8	2.28	1.42	1.39
2	B	302	FAD	C9A-N10	2.24	1.45	1.41
2	A	301	FAD	C8M-C8	2.22	1.55	1.51
2	C	301	FAD	O5B-C5B	2.21	1.53	1.44
3	D	301	BRU	O4'-C1'	-2.21	1.37	1.42
2	D	302	FAD	PA-O2A	2.21	1.65	1.55
2	A	301	FAD	C4A-N3A	2.17	1.38	1.34
2	D	302	FAD	C5A-N7A	-2.16	1.35	1.39
2	D	302	FAD	C9-C8	2.16	1.42	1.39
2	A	301	FAD	C10-N10	2.15	1.42	1.37
2	A	301	FAD	O2-C2	-2.13	1.20	1.24
2	A	301	FAD	C6A-N6A	2.05	1.39	1.34
3	A	302	BRU	O4'-C4'	-2.04	1.40	1.45
2	D	302	FAD	C8M-C8	2.04	1.54	1.51
2	D	302	FAD	C2-N3	2.03	1.43	1.39
2	B	302	FAD	C10-N10	2.01	1.41	1.37

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	BRU	C4-N3-C2	-6.93	118.25	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	BRU	N3-C2-N1	6.85	123.81	114.89
3	C	302	BRU	C4-N3-C2	-6.78	118.45	127.34
3	D	301	BRU	OP2-P-O5'	-6.39	90.00	106.67
2	B	302	FAD	O5B-PA-O1A	-6.25	84.15	108.94
2	D	302	FAD	O5B-PA-O1A	-6.22	84.27	108.94
3	C	302	BRU	OP2-P-O5'	-6.21	90.49	106.67
3	A	302	BRU	N3-C2-N1	6.18	122.93	114.89
3	C	302	BRU	N3-C2-N1	6.06	122.78	114.89
3	C	302	BRU	C5-C4-N3	5.72	119.92	113.34
2	A	301	FAD	C4A-N9A-C8A	5.68	111.70	105.74
3	D	301	BRU	O5'-P-OP1	-5.61	91.27	106.44
3	A	302	BRU	C4-N3-C2	-5.55	120.07	127.34
3	C	302	BRU	OP3-P-O5'	-5.50	92.32	106.67
3	A	302	BRU	OP2-P-O5'	-5.42	92.55	106.67
2	C	301	FAD	O2A-PA-O5B	-5.23	83.86	107.57
2	A	301	FAD	O2-C2-N1	-5.20	113.17	121.80
3	D	301	BRU	OP3-P-OP2	5.16	127.14	107.80
2	A	301	FAD	N9A-C8A-N7A	-4.99	106.86	113.94
3	B	301	BRU	C4-N3-C2	-4.93	120.88	127.34
3	C	302	BRU	OP2-P-OP1	4.91	129.98	110.83
3	B	301	BRU	N3-C2-N1	4.86	121.22	114.89
2	A	301	FAD	O4B-C4B-C5B	-4.78	94.03	109.33
2	D	302	FAD	C5A-C4A-N3A	-4.54	120.47	126.72
2	A	301	FAD	O2A-PA-O5B	-4.52	87.07	107.57
2	A	301	FAD	C4X-C10-N10	4.52	122.95	116.48
3	C	302	BRU	O4-C4-C5	-4.51	120.05	125.80
2	A	301	FAD	C10-C4X-N5	-4.34	115.95	124.81
2	D	302	FAD	O2A-PA-O5B	-4.32	87.96	107.57
3	B	301	BRU	C5-C4-N3	4.32	118.31	113.34
3	D	301	BRU	C5-C4-N3	4.29	118.28	113.34
3	B	301	BRU	OP3-P-O5'	-4.26	95.55	106.67
2	A	301	FAD	C4-N3-C2	-4.26	118.08	125.64
2	C	301	FAD	N9A-C8A-N7A	-4.25	107.91	113.94
2	C	301	FAD	C5A-C4A-N3A	-4.24	120.87	126.72
2	B	302	FAD	N9A-C8A-N7A	-4.20	107.97	113.94
3	A	302	BRU	OP3-P-OP2	4.14	123.32	107.80
2	B	302	FAD	C4A-N9A-C8A	4.09	110.03	105.74
2	A	301	FAD	N3A-C2A-N1A	-4.09	122.39	128.58
2	C	301	FAD	O3P-PA-O1A	4.07	122.94	110.70
2	A	301	FAD	O5B-PA-O1A	-4.06	92.86	108.94
3	A	302	BRU	OP3-P-O5'	-4.03	96.15	106.67
3	A	302	BRU	O2-C2-N1	-3.91	117.71	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	FAD	O2A-PA-O3P	3.91	117.84	107.27
2	B	302	FAD	N3A-C2A-N1A	-3.90	122.68	128.58
3	C	302	BRU	O5'-P-OP1	-3.81	96.16	106.44
3	D	301	BRU	O2-C2-N1	-3.77	117.89	122.80
2	B	302	FAD	C4-N3-C2	-3.72	119.04	125.64
2	C	301	FAD	C4A-C5A-N7A	-3.69	106.36	110.58
2	B	302	FAD	O4B-C4B-C5B	-3.68	97.55	109.33
3	C	302	BRU	O2-C2-N1	-3.63	118.07	122.80
3	A	302	BRU	C5-C4-N3	3.58	117.46	113.34
2	A	301	FAD	N3A-C4A-N9A	3.52	133.15	127.17
2	A	301	FAD	C5A-C4A-N3A	-3.52	121.88	126.72
2	C	301	FAD	C4A-N9A-C8A	3.50	109.42	105.74
2	D	302	FAD	O3P-PA-O1A	3.50	121.24	110.70
2	B	302	FAD	O4-C4-C4X	-3.43	117.47	126.53
3	D	301	BRU	C6-N1-C2	-3.43	117.88	121.30
2	C	301	FAD	O5B-PA-O1A	-3.40	95.47	108.94
2	C	301	FAD	C5A-N7A-C8A	3.38	108.77	103.45
2	A	301	FAD	O2A-PA-O3P	3.37	116.39	107.27
2	A	301	FAD	C5A-N7A-C8A	3.31	108.66	103.45
2	D	302	FAD	N3A-C4A-N9A	3.29	132.76	127.17
2	B	302	FAD	C5A-C4A-N3A	-3.24	122.25	126.72
2	D	302	FAD	N9A-C8A-N7A	-3.24	109.34	113.94
2	B	302	FAD	O2A-PA-O5B	-3.24	92.90	107.57
2	B	302	FAD	N3A-C4A-N9A	3.19	132.60	127.17
2	A	301	FAD	C4-C4X-N5	3.13	122.53	118.21
2	D	302	FAD	C4-N3-C2	-3.10	120.13	125.64
3	B	301	BRU	O2-C2-N1	-3.10	118.76	122.80
2	A	301	FAD	O2-C2-N3	3.08	124.49	118.58
2	B	302	FAD	C5A-N7A-C8A	3.06	108.26	103.45
2	D	302	FAD	C10-C4X-N5	-3.06	118.57	124.81
2	A	301	FAD	O2A-PA-O1A	3.04	126.57	112.44
2	A	301	FAD	C7M-C7-C6	-3.03	114.23	119.57
2	C	301	FAD	C4-N3-C2	-2.99	120.32	125.64
2	D	302	FAD	O5'-C5'-C4'	2.97	117.30	109.36
2	B	302	FAD	C4X-C4-N3	2.95	120.75	113.25
2	C	301	FAD	N3A-C2A-N1A	-2.94	124.13	128.58
2	C	301	FAD	O2A-PA-O1A	2.94	126.12	112.44
3	B	301	BRU	OP2-P-O5'	-2.90	99.11	106.67
2	B	302	FAD	O3P-PA-O1A	2.89	119.40	110.70
2	D	302	FAD	C4X-C4-N3	2.88	120.59	113.25
2	C	301	FAD	C4X-C10-N10	2.85	120.56	116.48
2	B	302	FAD	O3'-C3'-C2'	2.82	115.34	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	BRU	C6-C5-C4	2.82	123.54	120.67
2	D	302	FAD	N3A-C2A-N1A	-2.80	124.34	128.58
2	D	302	FAD	C5A-N7A-C8A	2.79	107.84	103.45
2	A	301	FAD	C5X-C9A-N10	-2.78	115.45	117.97
2	D	302	FAD	C4X-C10-N10	2.75	120.42	116.48
2	C	301	FAD	C10-C4X-N5	-2.72	119.26	124.81
3	D	301	BRU	C1'-N1-C6	2.68	125.24	120.74
2	A	301	FAD	C7M-C7-C8	2.66	126.20	120.76
2	A	301	FAD	C4-C4X-C10	2.64	121.46	116.93
2	C	301	FAD	O4B-C4B-C5B	-2.64	100.89	109.33
2	C	301	FAD	C4-C4X-N5	2.61	121.81	118.21
2	C	301	FAD	N3A-C4A-N9A	2.61	131.60	127.17
2	B	302	FAD	C9-C9A-N10	2.60	125.36	121.85
2	C	301	FAD	C2A-N3A-C4A	2.60	118.18	111.83
2	B	302	FAD	O5B-C5B-C4B	2.59	117.82	108.99
2	D	302	FAD	O2A-PA-O3P	2.59	114.27	107.27
2	A	301	FAD	C2A-N1A-C6A	2.59	122.98	118.73
2	C	301	FAD	C4X-C4-N3	2.59	119.83	113.25
3	B	301	BRU	O4-C4-C5	-2.56	122.54	125.80
2	D	302	FAD	C2B-C1B-N9A	2.51	119.54	113.30
2	D	302	FAD	C4A-C5A-N7A	-2.51	107.71	110.58
3	B	301	BRU	OP2-P-OP1	2.50	120.59	110.83
2	B	302	FAD	C4X-C10-N10	2.50	120.06	116.48
2	C	301	FAD	C9A-C5X-N5	-2.48	119.82	122.45
2	D	302	FAD	C4A-N9A-C8A	2.48	108.34	105.74
2	B	302	FAD	C7M-C7-C6	-2.48	115.20	119.57
2	B	302	FAD	C10-C4X-N5	-2.48	119.75	124.81
2	B	302	FAD	C4-C4X-C10	2.47	121.17	116.93
2	A	301	FAD	O4B-C1B-N9A	-2.47	103.34	108.09
2	D	302	FAD	O4-C4-C4X	-2.47	120.01	126.53
2	B	302	FAD	C2A-N3A-C4A	2.46	117.84	111.83
3	A	302	BRU	O4'-C1'-N1	-2.42	103.56	107.86
2	A	301	FAD	C4A-C5A-N7A	-2.41	107.83	110.58
3	A	302	BRU	O5'-P-OP1	-2.41	99.93	106.44
2	A	301	FAD	C4X-C10-N1	-2.40	118.71	124.59
3	A	302	BRU	C6-C5-C4	2.40	123.11	120.67
3	D	301	BRU	BR-C5-C6	-2.39	117.31	120.64
2	B	302	FAD	C4X-C10-N1	-2.35	118.84	124.59
3	D	301	BRU	OP2-P-OP1	2.33	119.92	110.83
2	B	302	FAD	C10-N1-C2	2.33	121.89	116.85
2	D	302	FAD	C10-N1-C2	2.30	121.83	116.85
2	A	301	FAD	C2A-N3A-C4A	2.30	117.45	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	FAD	C2B-C1B-N9A	2.27	118.94	113.30
2	C	301	FAD	O4-C4-C4X	-2.27	120.55	126.53
2	C	301	FAD	C4'-C3'-C2'	-2.24	109.84	113.57
2	A	301	FAD	O5B-C5B-C4B	2.24	116.61	108.99
2	B	302	FAD	C2A-N1A-C6A	2.23	122.39	118.73
3	B	301	BRU	C6-C5-C4	2.20	122.91	120.67
2	B	302	FAD	C6-C5X-C9A	2.19	122.06	119.05
3	B	301	BRU	C1'-N1-C6	2.17	124.38	120.74
2	B	302	FAD	C4'-C3'-C2'	-2.17	109.97	113.57
2	D	302	FAD	C4X-C10-N1	-2.15	119.31	124.59
2	D	302	FAD	C2A-N3A-C4A	2.15	117.07	111.83
2	D	302	FAD	C4-C4X-N5	2.14	121.16	118.21
2	B	302	FAD	C7M-C7-C8	2.13	125.12	120.76
2	A	301	FAD	C4X-C4-N3	2.13	118.67	113.25
3	C	302	BRU	BR-C5-C4	2.11	120.45	118.02
2	B	302	FAD	C5X-C9A-N10	-2.11	116.06	117.97
3	A	302	BRU	C1'-N1-C6	2.11	124.28	120.74
2	C	301	FAD	O5B-C5B-C4B	2.10	116.16	108.99
2	A	301	FAD	O3B-C3B-C4B	2.08	117.06	111.08
2	A	301	FAD	O3P-PA-O1A	2.08	116.95	110.70
2	A	301	FAD	O4-C4-C4X	-2.07	121.07	126.53
2	D	302	FAD	O3'-C3'-C2'	2.06	113.62	108.93
2	D	302	FAD	O5'-P-O1P	2.06	117.10	108.94
3	D	301	BRU	O4-C4-C5	-2.05	123.19	125.80
2	C	301	FAD	O4B-C1B-C2B	2.05	111.00	106.62
2	C	301	FAD	O5'-P-O1P	2.03	116.97	108.94
2	A	301	FAD	C9-C9A-N10	2.02	124.57	121.85
2	D	302	FAD	C6A-C5A-C4A	2.00	119.91	117.18

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	FAD	C5'-O5'-P-O2P
2	B	302	FAD	C1'-C2'-C3'-O3'
2	B	302	FAD	C1'-C2'-C3'-C4'
2	D	302	FAD	C3'-C4'-C5'-O5'
2	D	302	FAD	O4'-C4'-C5'-O5'
2	D	302	FAD	C5'-O5'-P-O1P
2	D	302	FAD	C5'-O5'-P-O3P
2	D	302	FAD	PA-O3P-P-O5'
2	A	301	FAD	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
2	A	301	FAD	O3'-C3'-C4'-C5'
2	A	301	FAD	O3'-C3'-C4'-O4'
2	A	301	FAD	C2'-C3'-C4'-C5'
3	D	301	BRU	C3'-C4'-C5'-O5'
3	D	301	BRU	O4'-C4'-C5'-O5'
2	A	301	FAD	C3'-C4'-C5'-O5'
2	A	301	FAD	P-O3P-PA-O2A
2	A	301	FAD	O4'-C4'-C5'-O5'
2	A	301	FAD	C5'-O5'-P-O1P
2	A	301	FAD	C5'-O5'-P-O3P
2	B	302	FAD	C5'-O5'-P-O1P
2	D	302	FAD	C5'-O5'-P-O2P
2	D	302	FAD	C4'-C5'-O5'-P
2	B	302	FAD	P-O3P-PA-O2A
2	C	301	FAD	P-O3P-PA-O2A
2	C	301	FAD	C2'-C3'-C4'-O4'
3	C	302	BRU	C2'-C1'-N1-C2
2	B	302	FAD	PA-O3P-P-O2P
2	C	301	FAD	PA-O3P-P-O2P

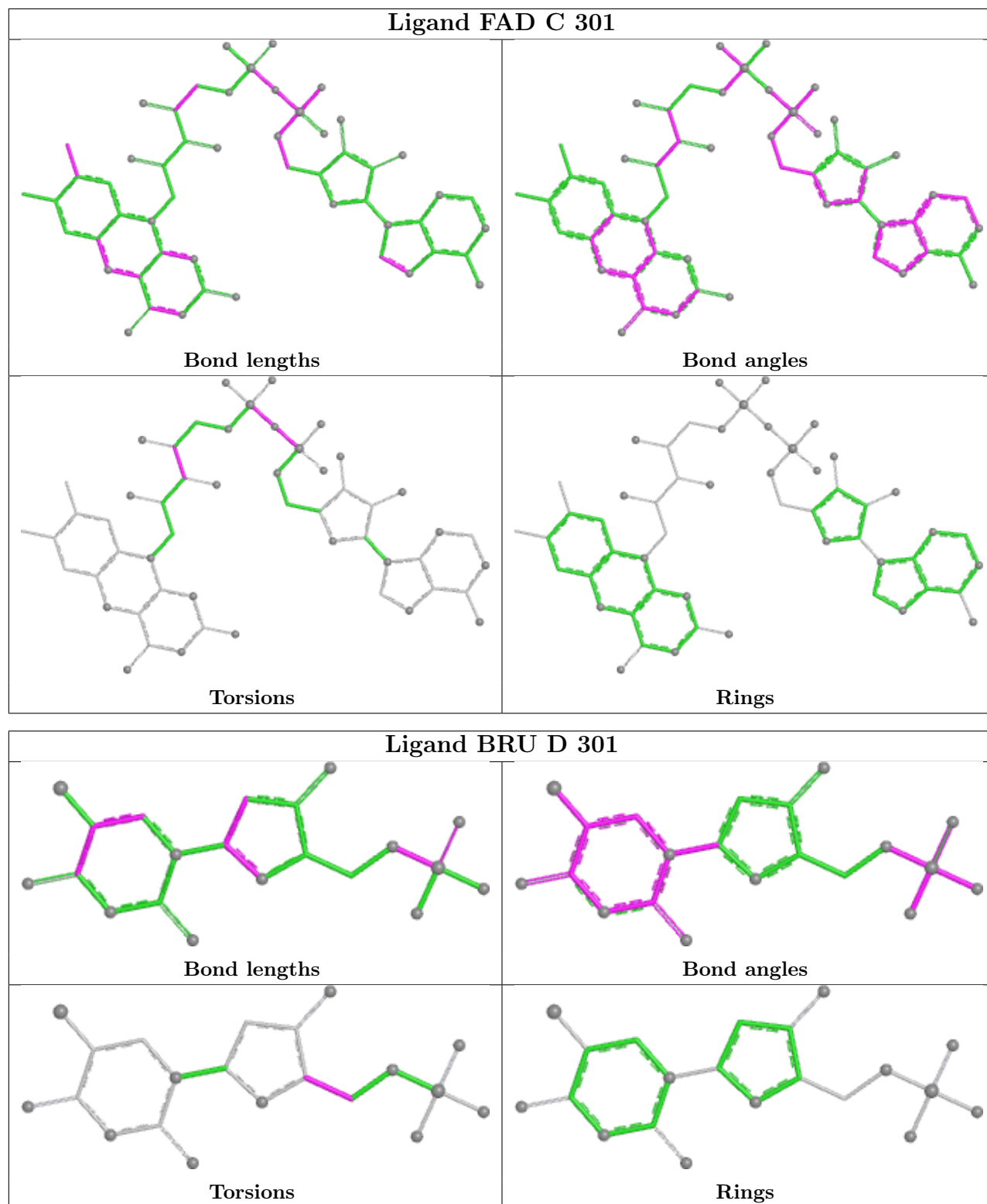
There are no ring outliers.

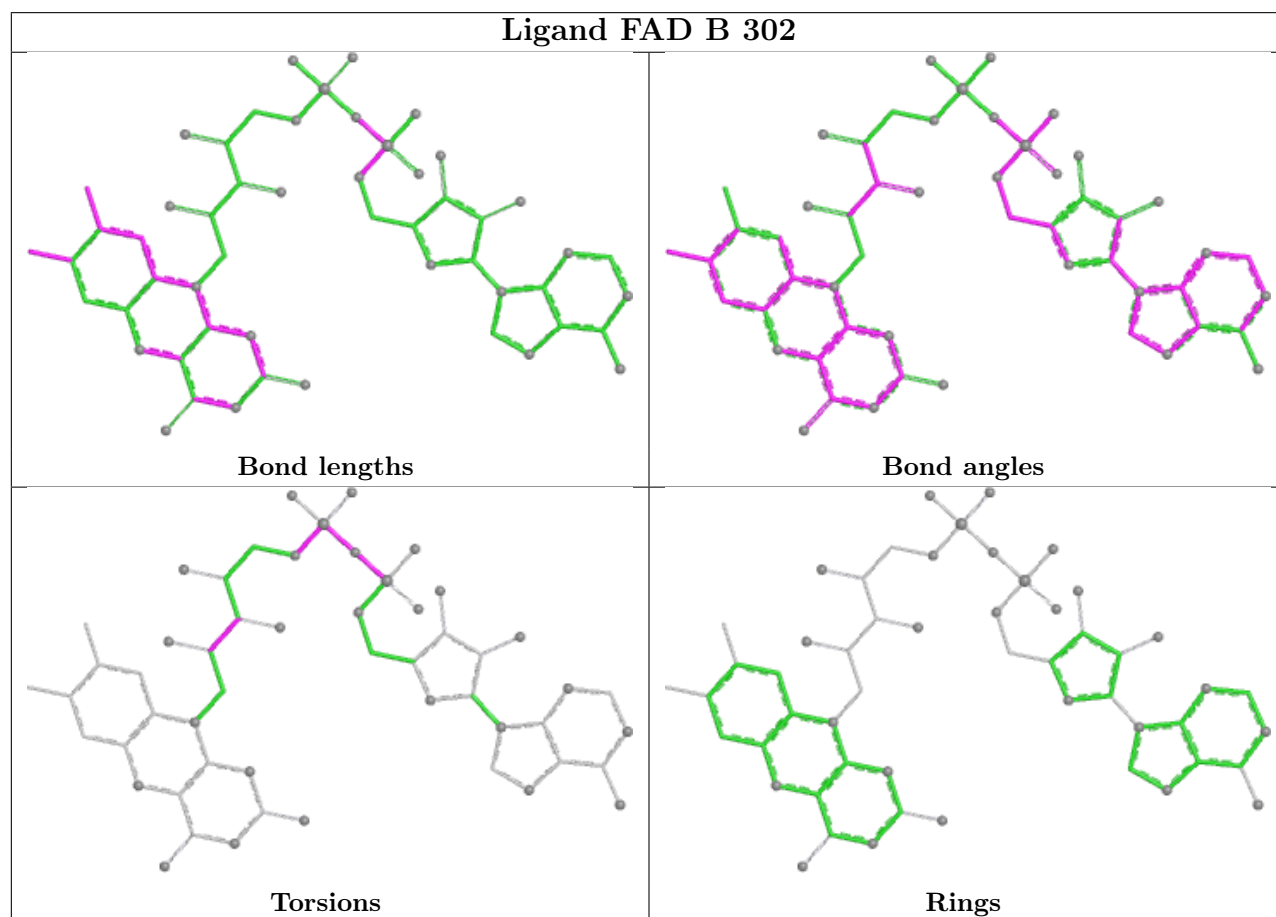
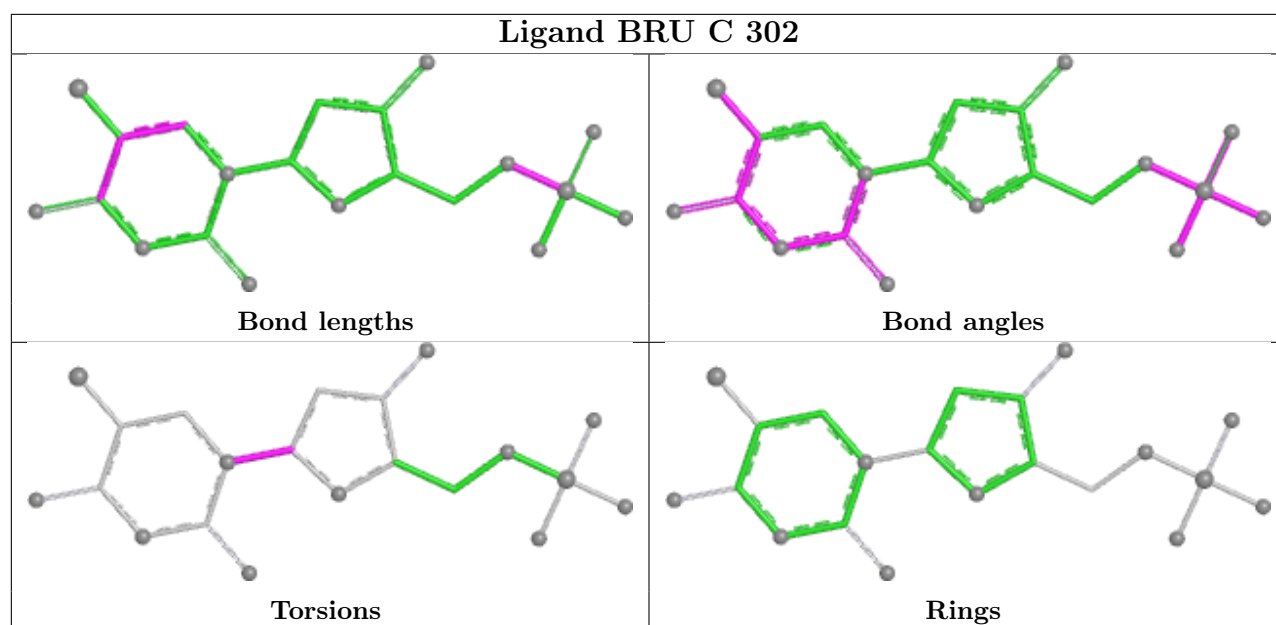
8 monomers are involved in 20 short contacts:

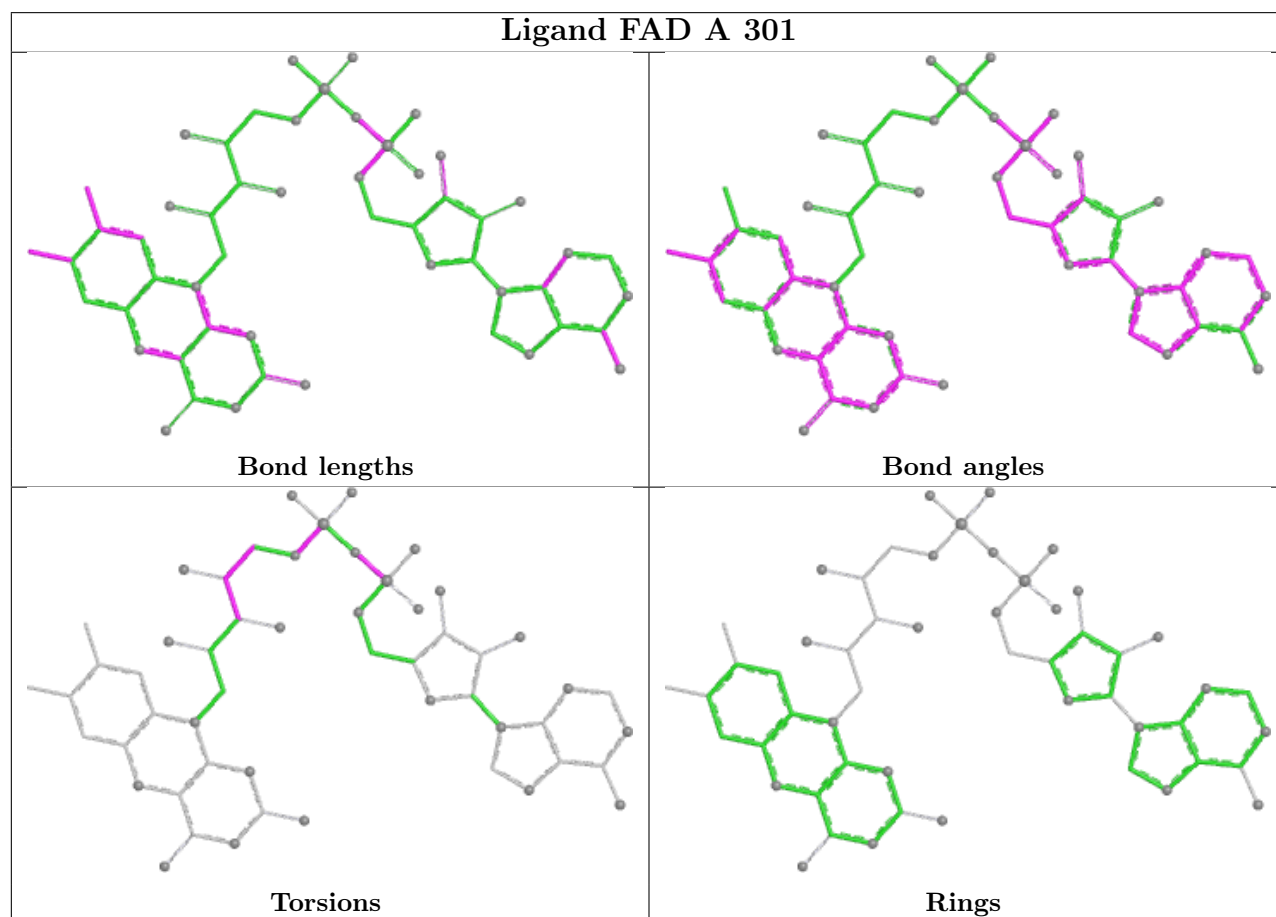
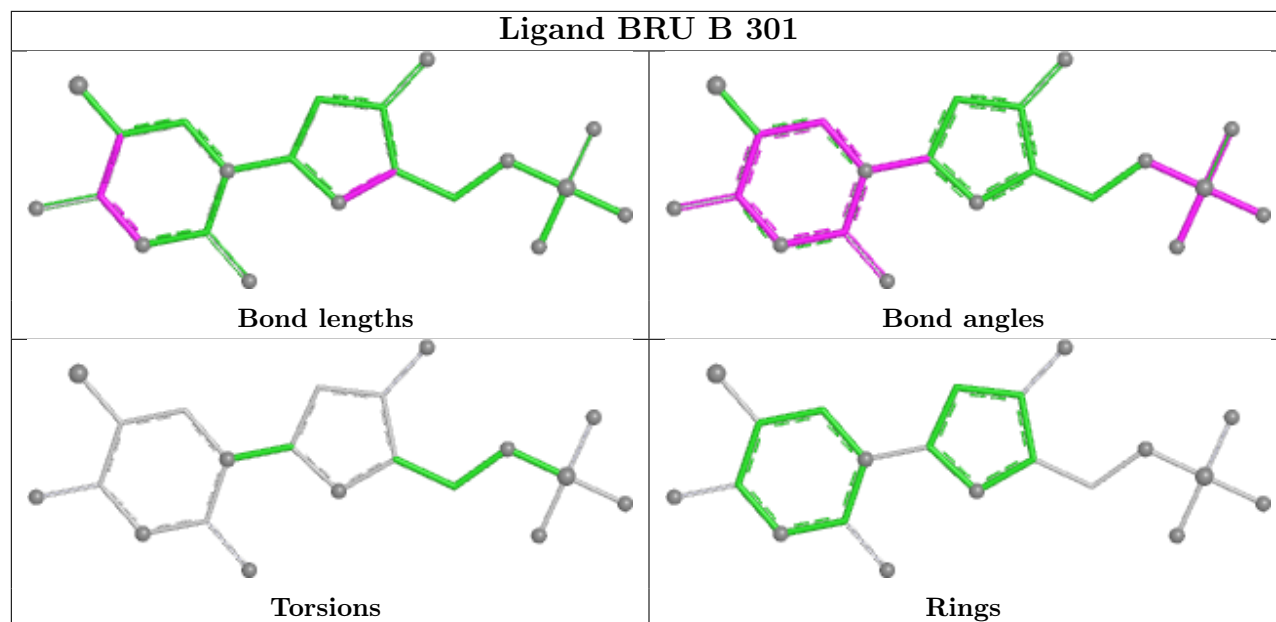
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	FAD	2	0
3	D	301	BRU	1	0
3	C	302	BRU	2	0
2	B	302	FAD	4	0
3	B	301	BRU	4	0
2	A	301	FAD	3	0
3	A	302	BRU	1	0
2	D	302	FAD	3	0

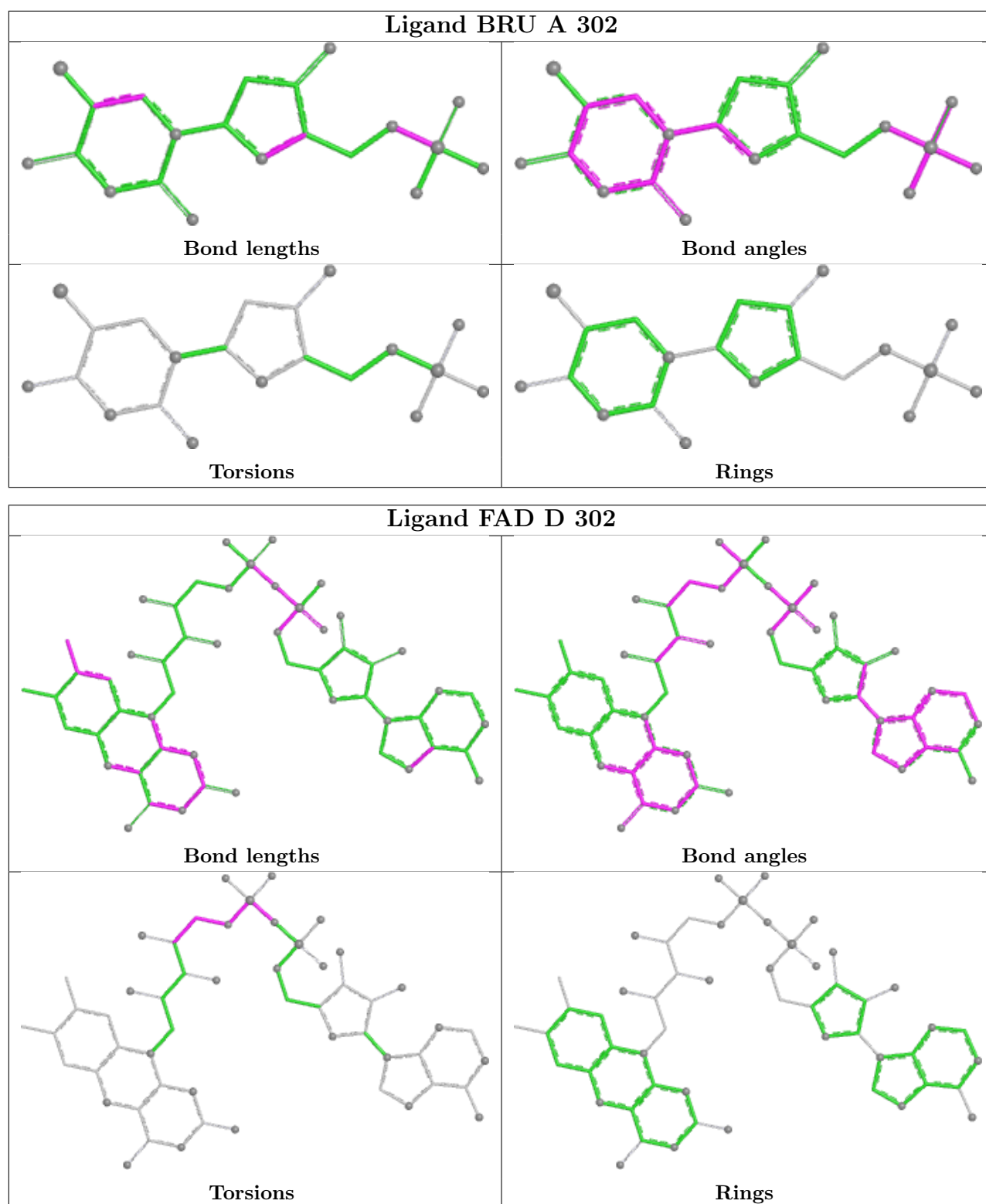
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	229/239 (95%)	-0.12	14 (6%) 27 28	12, 23, 74, 95	1 (0%)
1	B	235/239 (98%)	-0.09	11 (4%) 36 37	13, 26, 67, 77	1 (0%)
1	C	234/239 (97%)	-0.09	12 (5%) 33 34	13, 25, 72, 83	1 (0%)
1	D	235/239 (98%)	-0.17	4 (1%) 69 70	13, 26, 62, 76	1 (0%)
All	All	933/956 (97%)	-0.12	41 (4%) 39 40	12, 25, 69, 95	4 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	TYR	5.2
1	D	124	TYR	4.6
1	B	43	LEU	4.3
1	A	129	GLY	4.1
1	D	115	LEU	3.4
1	A	121	PRO	3.3
1	A	125	ARG	3.3
1	A	32	VAL	3.2
1	C	124	TYR	3.2
1	A	119	GLY	3.2
1	A	126	TYR	3.0
1	B	131	THR	3.0
1	C	127	VAL	2.9
1	B	39	ALA	2.9
1	B	124	TYR	2.8
1	C	119	GLY	2.8
1	B	126	TYR	2.7
1	D	126	TYR	2.7
1	C	129	GLY	2.7
1	A	127	VAL	2.7
1	A	122	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	2.6
1	C	116	ARG	2.6
1	A	35	ALA	2.6
1	C	114	LEU	2.6
1	C	43	LEU	2.4
1	A	123	ASP	2.4
1	B	130	SER	2.4
1	C	128	GLY	2.4
1	A	39	ALA	2.3
1	C	115	LEU	2.3
1	B	132	ASP	2.3
1	C	130	SER	2.3
1	A	118	GLU	2.3
1	B	35	ALA	2.2
1	B	127	VAL	2.2
1	A	128	GLY	2.2
1	B	122	GLY	2.2
1	C	126	TYR	2.1
1	C	40	ASN	2.0
1	D	131	THR	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	FAD	C	301	53/53	0.86	0.12	29,42,51,52	0
2	FAD	D	302	53/53	0.86	0.13	32,49,54,56	0
2	FAD	B	302	53/53	0.89	0.12	24,43,50,56	0

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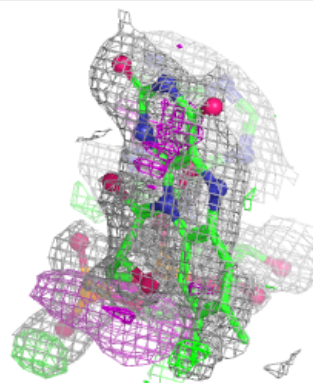
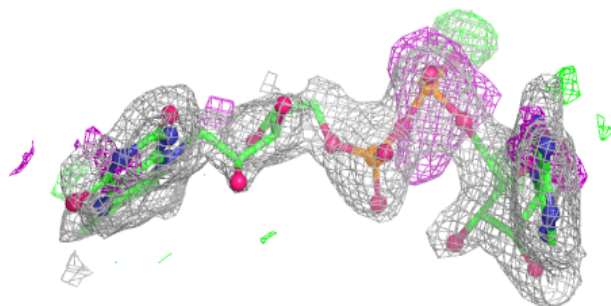
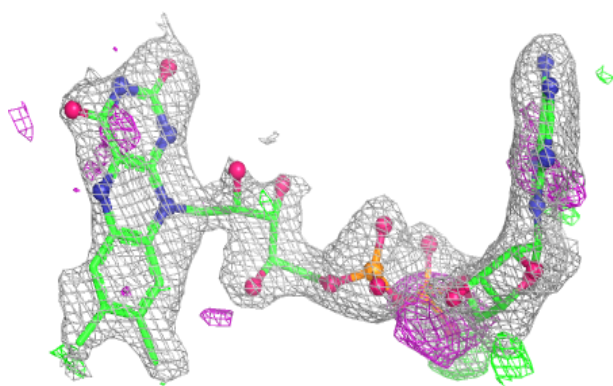
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	301	53/53	0.92	0.09	17,34,40,43	0
4	SO4	A	303	5/5	0.94	0.09	54,55,56,58	0
3	BRU	C	302	21/21	0.97	0.06	19,25,31,39	0
3	BRU	A	302	21/21	0.98	0.05	13,18,23,30	0
3	BRU	D	301	21/21	0.98	0.05	16,22,25,36	0
3	BRU	B	301	21/21	0.98	0.06	12,17,21,29	0

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

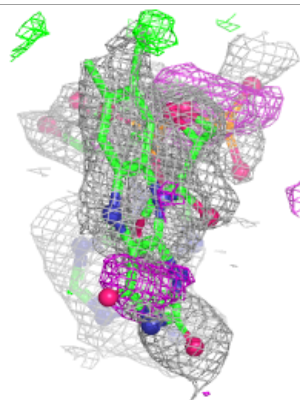
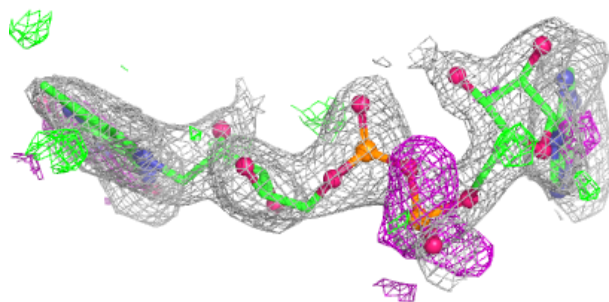
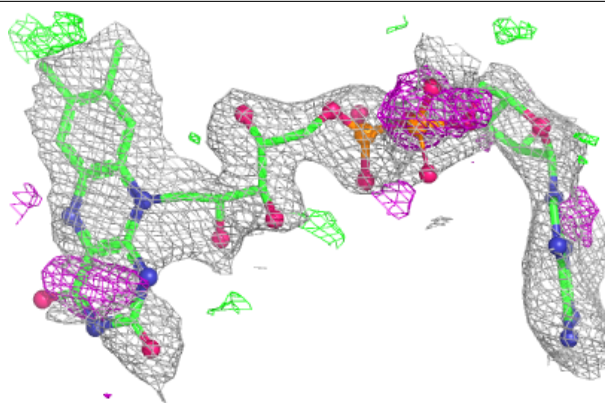
Electron density around FAD C 301:

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

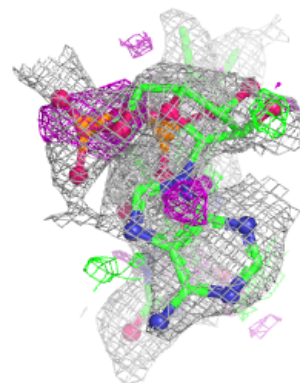
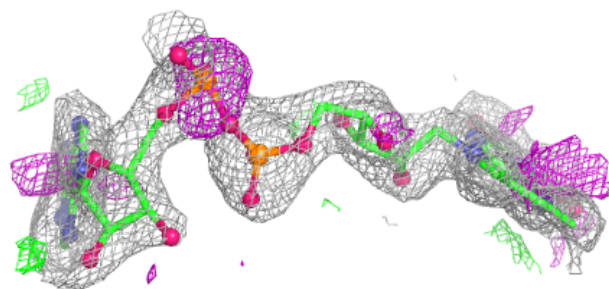
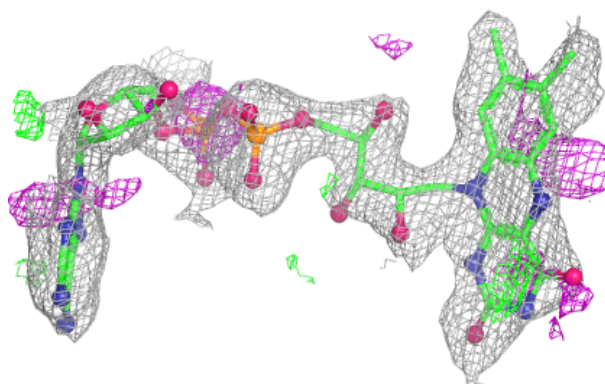


Electron density around FAD D 302:

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

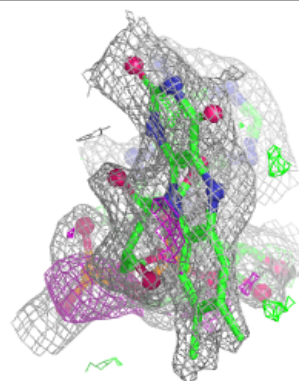
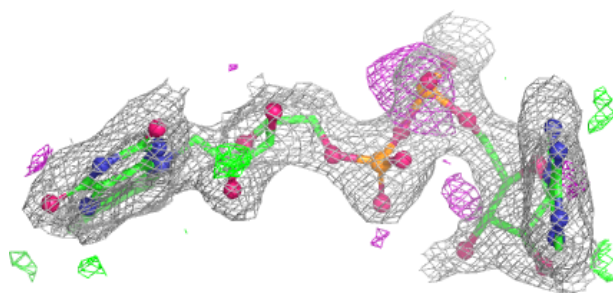
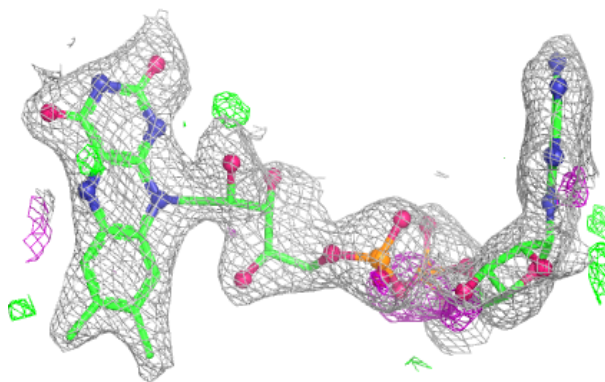
**Electron density around FAD B 302:**

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

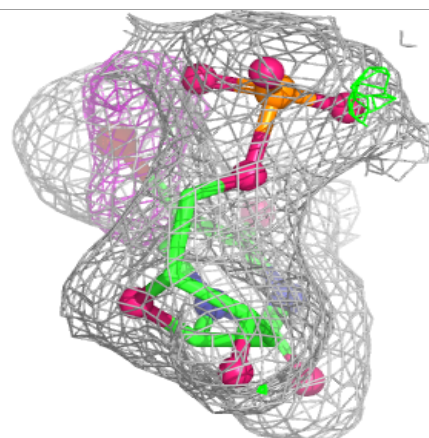
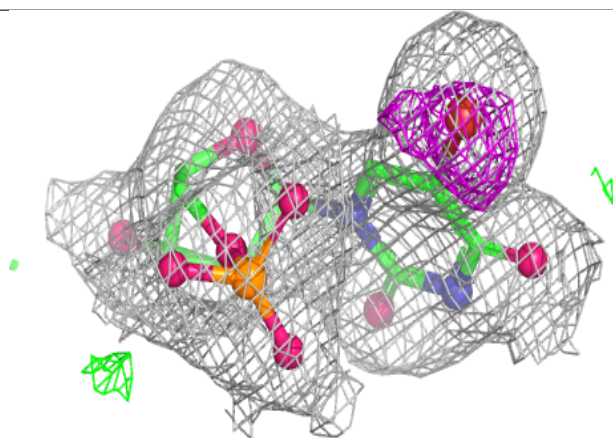
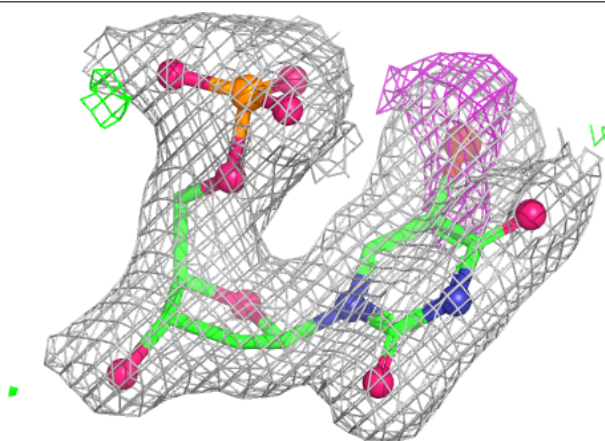


Electron density around FAD A 301:

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

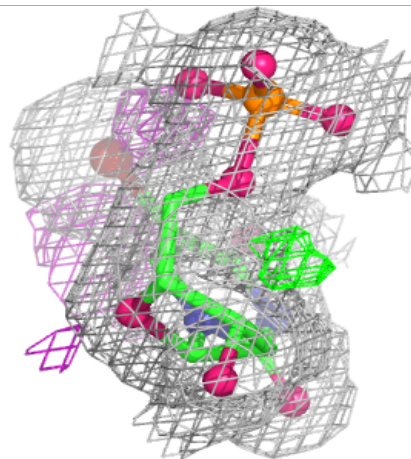
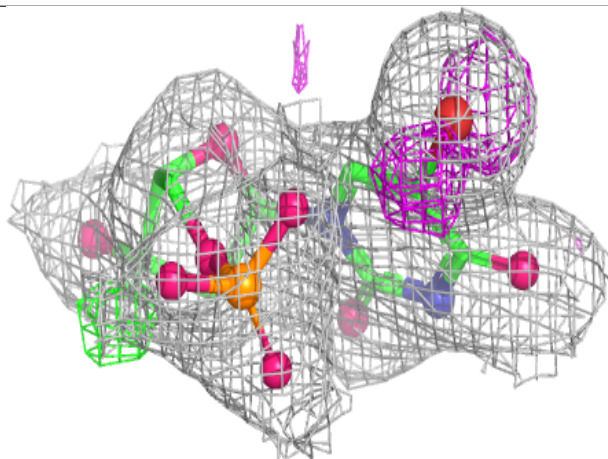
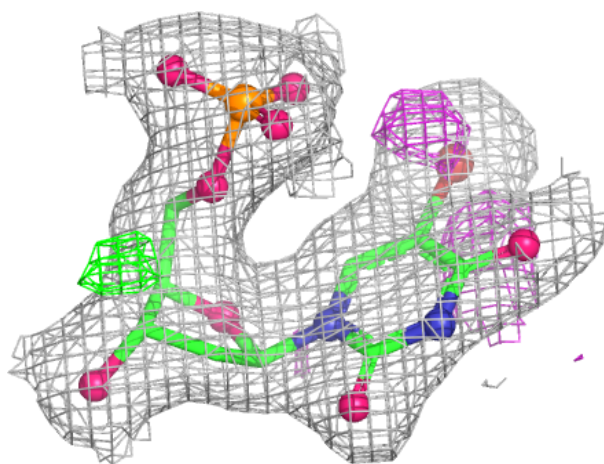
**Electron density around BRU C 302:**

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



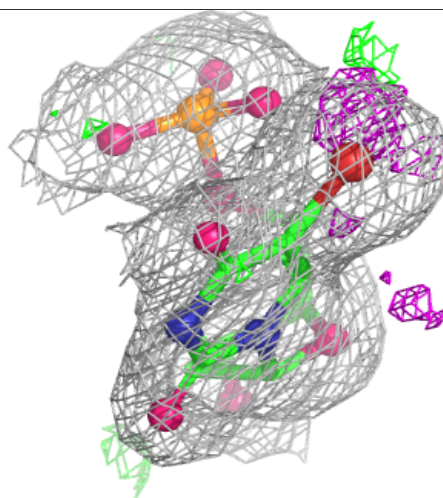
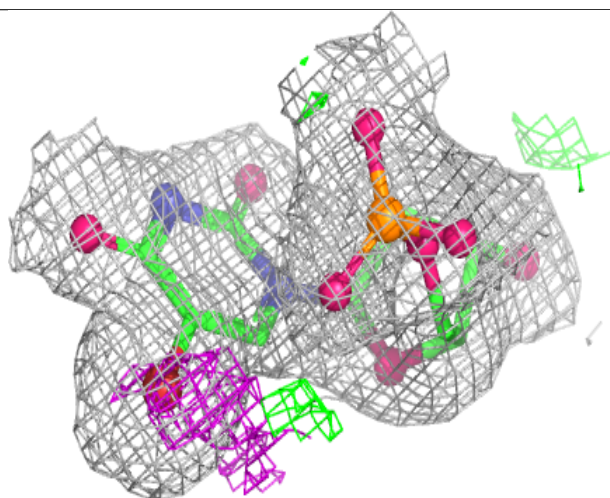
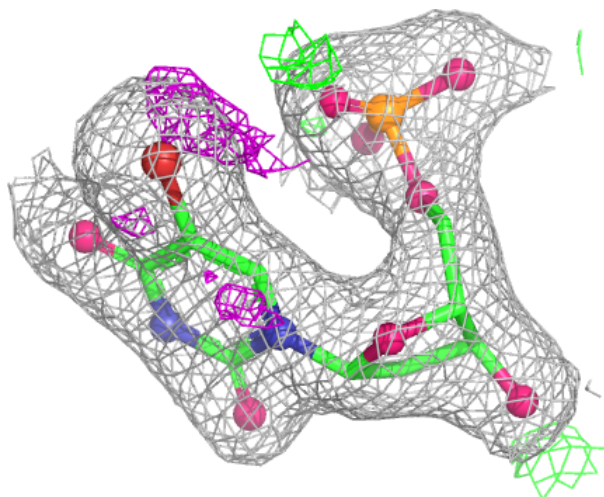
Electron density around BRU A 302:

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



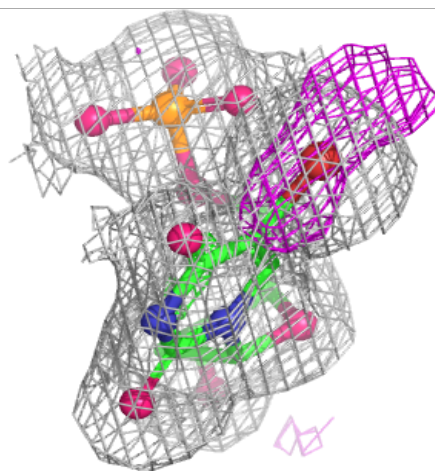
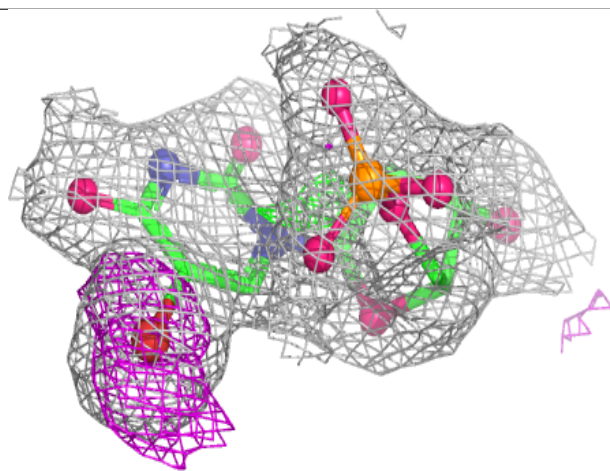
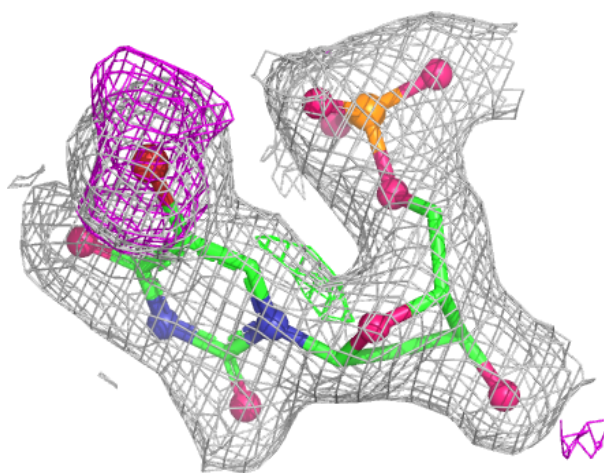
Electron density around BRU D 301:

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



Electron density around BRU 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.