



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:06 am BST

PDB ID : 1O27
Title : Crystal structure of Thymidylate Synthase Complementing Protein (TM0449) from *Thermotoga maritima* with FAD and BrdUMP at 2.3 Å resolution
Authors : Mathews, I.I.; Deacon, A.M.; Canaves, J.M.; McMullan, D.; Lesley, S.A.; Agarwalla, S.; Kuhn, P.; Joint Center for Structural Genomics (JCSG)
Deposited on : 2003-02-18
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

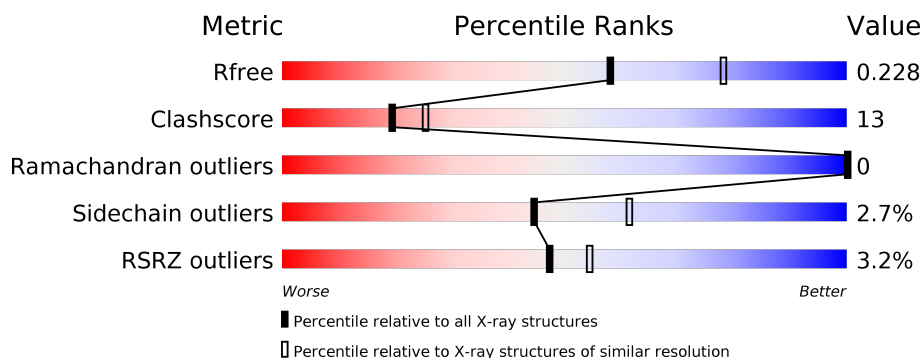
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>31%</div> <div>7%</div> </div> </div>
1	B	232	<div> <div></div> <div> <div>66%</div> <div>26%</div> <div>6%</div> </div> </div>
1	C	232	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>7%</div> </div> </div>
1	D	232	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>24%</div> <div>7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FAD	A	615	X	-	-	-
3	FAD	B	610	X	-	-	-
3	FAD	C	605	X	-	-	-
3	FAD	D	600	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7718 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	216	Total	C	N	O	S	0	0	0
			1793	1167	308	312	6			
1	B	217	Total	C	N	O	S	0	0	0
			1812	1179	310	317	6			
1	C	216	Total	C	N	O	S	0	0	0
			1813	1180	310	318	5			
1	D	215	Total	C	N	O	S	0	0	0
			1803	1173	307	317	6			

There are 48 discrepancies between the modelled and reference sequences:

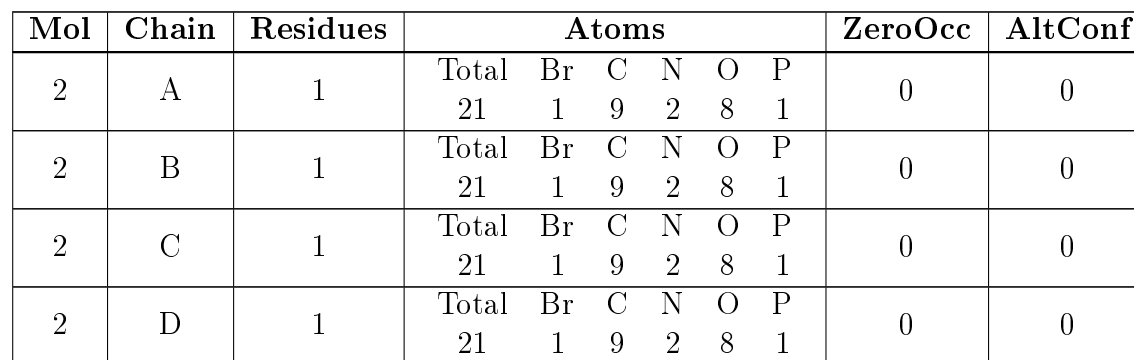
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
A	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
A	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
B	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYT0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
B	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
C	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
C	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
C	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
C	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
C	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-11	MET	-	LEADER SEQUENCE	UNP Q9WYT0
D	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYT0
D	-9	SER	-	LEADER SEQUENCE	UNP Q9WYT0
D	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYT0
D	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYT0
D	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYT0
D	0	HIS	-	LEADER SEQUENCE	UNP Q9WYT0

- Molecule 2 is 5-BROMO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: BRU) (formula: C₉H₁₂BrN₂O₈P).



- # FAD

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

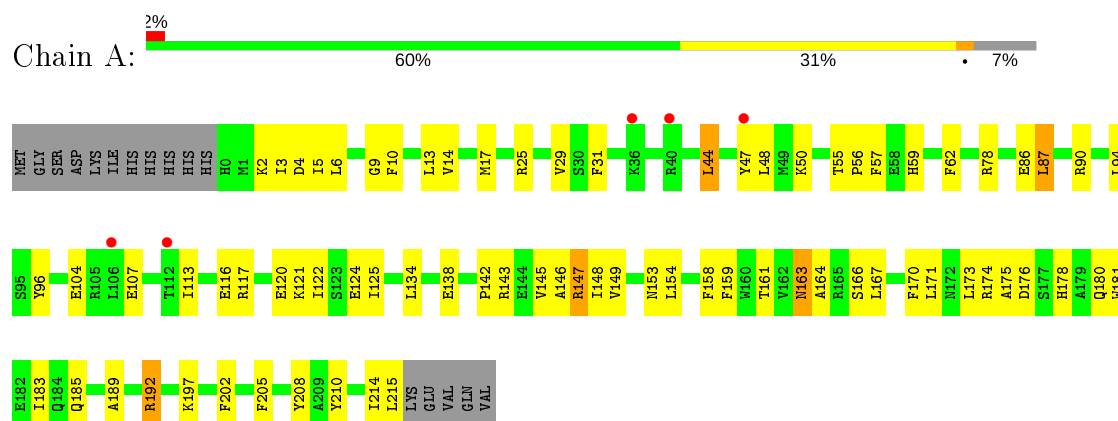
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	52	Total	O	0	0
			52	52		
4	C	53	Total	O	0	0
			53	53		
4	D	41	Total	O	0	0
			41	41		

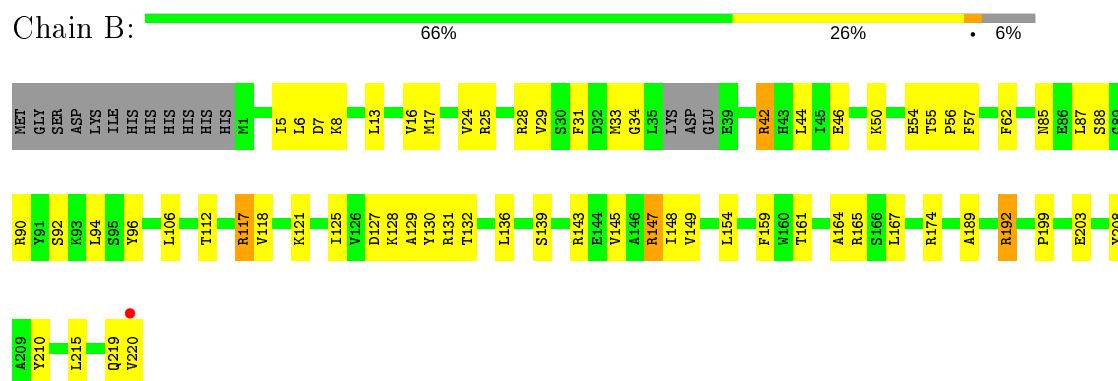
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

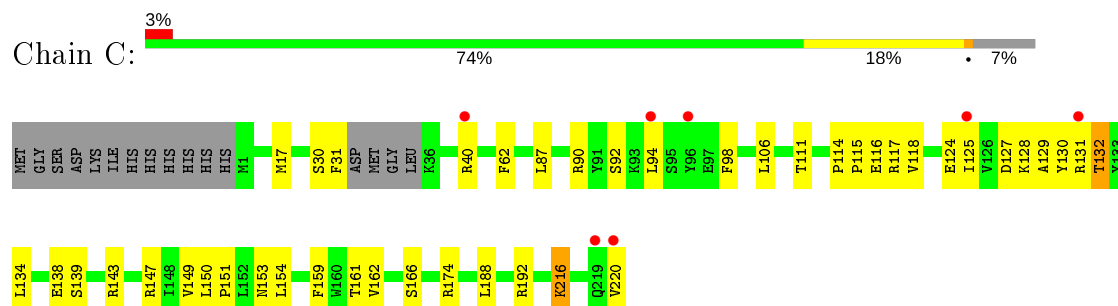
• Molecule 1: Thymidylate synthase thyX



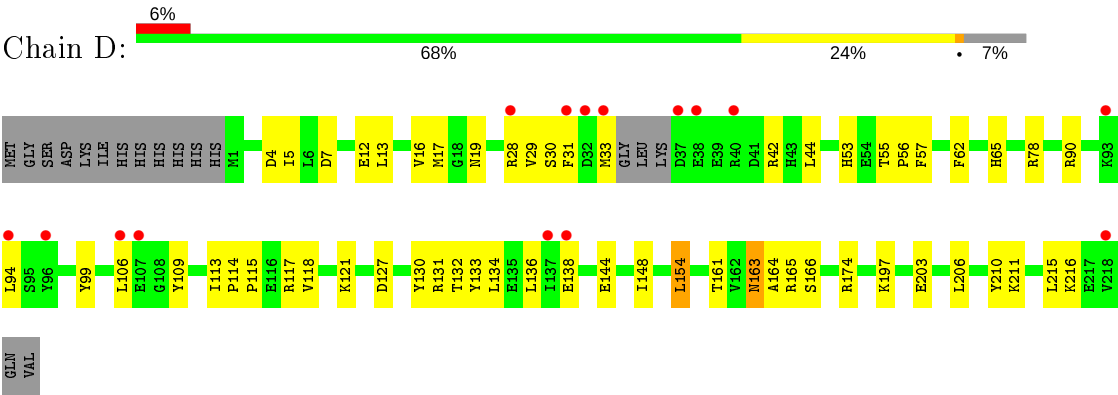
• Molecule 1: Thymidylate synthase thyX



• Molecule 1: Thymidylate synthase thyX



● Molecule 1: Thymidylate synthase thyX



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.35Å 116.43Å 140.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 46.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-2.30) 97.8 (46.48-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.188 , 0.230 0.184 , 0.228	Depositor DCC
R_{free} test set	1986 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.0	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	0.95	EDS
Total number of atoms	7718	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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: BRU, 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	0.35	0/1842	0.58	0/2490
1	B	0.35	0/1860	0.59	0/2513
1	C	0.36	0/1861	0.59	0/2514
1	D	0.36	0/1851	0.58	0/2502
All	All	0.36	0/7414	0.58	0/10019

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1793	0	1785	59	0
1	B	1812	0	1806	64	0
1	C	1813	0	1811	44	0
1	D	1803	0	1794	50	0
2	A	21	0	10	3	0
2	B	21	0	10	2	0
2	C	21	0	10	3	0
2	D	21	0	10	2	0
3	A	53	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	53	0	30	0	0
3	C	53	0	30	1	0
3	D	53	0	30	0	0
4	A	55	0	0	0	0
4	B	52	0	0	0	0
4	C	53	0	0	0	0
4	D	41	0	0	3	0
All	All	7718	0	7356	191	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 13.

All (191) 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:125:ILE:HG13	1:C:132:THR:HG21	1.37	1.06
1:B:174:ARG:HH12	2:C:613:BRU:HN3	1.10	0.98
1:A:174:ARG:HH12	2:D:618:BRU:HN3	1.08	0.94
2:B:608:BRU:HN3	1:C:174:ARG:HH12	1.11	0.91
1:C:17:MET:HB2	1:D:17:MET:HB2	1.51	0.89
1:A:17:MET:HB2	1:B:17:MET:HB2	1.52	0.89
1:C:94:LEU:HD13	1:C:154:LEU:HD21	1.56	0.88
1:B:149:VAL:HB	1:C:125:ILE:HD13	1.54	0.87
1:A:116:GLU:O	1:A:120:GLU:HG2	1.77	0.84
1:B:125:ILE:CG1	1:C:132:THR:HG21	2.09	0.82
1:C:87:LEU:HA	1:D:30:SER:HA	1.61	0.81
2:A:603:BRU:HN3	1:D:174:ARG:HH12	1.25	0.80
1:D:113:ILE:HD13	1:D:121:LYS:HE3	1.67	0.76
1:D:106:LEU:HD22	1:D:115:PRO:HA	1.71	0.72
1:A:116:GLU:CD	1:A:116:GLU:H	1.94	0.71
1:A:55:THR:OG1	1:A:56:PRO:HD3	1.94	0.68
1:A:29:VAL:HG21	1:B:159:PHE:CE1	2.29	0.67
1:C:128:LYS:O	1:C:132:THR:HG22	1.95	0.67
1:B:54:GLU:HB3	1:B:165:ARG:HG3	1.78	0.66
1:D:94:LEU:HD13	1:D:154:LEU:HD11	1.78	0.65
1:C:129:ALA:O	1:C:132:THR:HG23	1.96	0.65
1:D:28:ARG:HD2	1:D:33:MET:HG3	1.79	0.63
1:B:125:ILE:HG21	1:C:149:VAL:HB	1.80	0.63
1:B:192:ARG:HH12	1:B:220:VAL:HG11	1.63	0.63
1:A:180:GLN:O	1:A:183:ILE:HG22	2.00	0.62
1:B:128:LYS:NZ	1:C:128:LYS:HD3	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:PRO:O	1:B:203:GLU:HG2	1.98	0.62
1:C:90:ARG:HD3	2:C:613:BRU:BR	2.54	0.62
1:D:113:ILE:HG22	1:D:117:ARG:HB3	1.81	0.61
1:B:5:ILE:HG22	1:B:6:LEU:HG	1.83	0.60
1:A:94:LEU:HD13	1:A:154:LEU:HD21	1.83	0.60
1:C:124:GLU:HG2	1:C:128:LYS:HE3	1.83	0.60
1:A:159:PHE:CD1	1:B:29:VAL:HG21	2.37	0.60
1:B:24:VAL:O	1:B:28:ARG:HG2	2.02	0.59
1:B:50:LYS:HB3	1:B:208:TYR:CD2	2.37	0.59
1:B:127:ASP:O	1:B:131:ARG:HG3	2.03	0.58
1:C:159:PHE:CE1	1:D:29:VAL:HG21	2.39	0.58
1:A:57:PHE:O	1:A:164:ALA:HB3	2.03	0.58
1:B:129:ALA:HA	1:C:125:ILE:HD12	1.87	0.57
1:C:151:PRO:HB2	1:C:153:ASN:OD1	2.05	0.57
1:C:87:LEU:HD23	1:D:29:VAL:C	2.25	0.57
1:A:2:LYS:HE3	1:A:4:ASP:OD1	2.03	0.57
1:B:174:ARG:NH1	2:C:613:BRU:HN3	1.93	0.57
1:B:42:ARG:HG3	1:B:42:ARG:HH11	1.69	0.56
1:C:116:GLU:CD	1:C:116:GLU:H	2.09	0.56
1:D:132:THR:O	1:D:136:LEU:HG	2.06	0.56
1:A:145:VAL:O	1:A:148:ILE:HG12	2.04	0.56
1:D:163:ASN:ND2	1:D:166:SER:H	2.03	0.56
1:B:129:ALA:HA	1:C:125:ILE:CD1	2.35	0.56
1:C:130:TYR:CE2	1:C:134:LEU:HD11	2.39	0.56
1:B:87:LEU:HD13	1:B:88:SER:N	2.21	0.55
1:B:127:ASP:HB3	1:B:131:ARG:NH1	2.22	0.55
1:A:163:ASN:HD22	1:A:163:ASN:C	2.11	0.55
1:B:57:PHE:O	1:B:164:ALA:HB3	2.07	0.54
1:D:117:ARG:HG3	1:D:117:ARG:HH11	1.72	0.54
1:D:57:PHE:O	1:D:164:ALA:HB3	2.08	0.54
1:D:12:GLU:HG3	1:D:65:HIS:HB3	1.89	0.54
1:C:30:SER:O	1:C:31:PHE:HB2	2.08	0.54
1:D:117:ARG:HH12	1:D:121:LYS:NZ	2.04	0.54
1:B:145:VAL:O	1:B:148:ILE:HG12	2.07	0.53
1:B:132:THR:O	1:B:136:LEU:HG	2.08	0.53
1:D:42:ARG:NH2	1:D:203:GLU:OE2	2.42	0.53
1:A:142:PRO:HG3	1:D:109:TYR:CE2	2.44	0.53
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.91	0.53
1:A:44:LEU:HD22	1:A:48:LEU:HG	1.89	0.53
1:A:134:LEU:O	1:A:138:GLU:HG3	2.08	0.53
1:A:171:LEU:O	1:A:175:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ASN:C	1:D:163:ASN:HD22	2.13	0.52
1:A:210:TYR:CE2	1:A:215:LEU:HB2	2.44	0.52
1:D:127:ASP:OD1	1:D:131:ARG:NH1	2.43	0.52
1:C:40:ARG:HG3	1:C:40:ARG:HH11	1.74	0.52
1:D:12:GLU:CG	1:D:65:HIS:HB3	2.40	0.51
1:A:2:LYS:C	1:A:2:LYS:HD2	2.31	0.51
1:C:62:PHE:O	1:C:161:THR:HA	2.11	0.51
1:D:29:VAL:O	1:D:29:VAL:HG12	2.11	0.50
1:B:128:LYS:HZ1	1:C:128:LYS:HD3	1.74	0.50
1:B:28:ARG:HG3	1:B:34:GLY:O	2.10	0.50
1:D:4:ASP:O	1:D:5:ILE:HD13	2.11	0.50
1:C:143:ARG:HG2	1:C:143:ARG:HH11	1.77	0.50
1:A:122:ILE:O	1:A:125:ILE:HG22	2.12	0.50
1:B:117:ARG:NH1	1:B:121:LYS:NZ	2.60	0.50
1:D:31:PHE:HB2	1:D:33:MET:HG2	1.93	0.50
1:C:94:LEU:HD13	1:C:154:LEU:CD2	2.36	0.49
1:D:206:LEU:O	1:D:216:LYS:HE3	2.12	0.49
1:D:55:THR:OG1	1:D:56:PRO:HD3	2.12	0.49
1:D:28:ARG:HB3	1:D:33:MET:HB2	1.94	0.49
1:A:174:ARG:HD2	1:A:183:ILE:HG12	1.95	0.49
1:A:62:PHE:O	1:A:161:THR:HA	2.13	0.49
1:B:13:LEU:HD11	1:B:16:VAL:HG22	1.94	0.49
1:C:94:LEU:HD12	1:C:150:LEU:HD12	1.95	0.49
1:B:106:LEU:HD11	1:B:118:VAL:HG11	1.94	0.48
1:D:106:LEU:HD21	1:D:118:VAL:HG21	1.95	0.48
1:B:127:ASP:HB3	1:B:131:ARG:HH12	1.78	0.48
1:B:117:ARG:NH1	1:B:121:LYS:HZ2	2.12	0.48
1:B:94:LEU:HD13	1:B:154:LEU:HD21	1.94	0.48
1:D:113:ILE:CG2	1:D:117:ARG:HB3	2.42	0.48
1:A:146:ALA:O	1:A:149:VAL:HG22	2.14	0.48
1:D:130:TYR:CE2	1:D:134:LEU:HD11	2.49	0.48
1:A:5:ILE:HG22	1:A:6:LEU:HG	1.96	0.47
1:B:128:LYS:HZ1	1:C:128:LYS:HB3	1.79	0.47
1:D:197:LYS:NZ	4:D:436:HOH:O	2.48	0.47
1:B:31:PHE:O	1:B:33:MET:HG3	2.15	0.47
1:B:42:ARG:HD3	1:B:42:ARG:O	2.16	0.46
1:A:86:GLU:HB2	1:A:158:PHE:HB3	1.97	0.46
1:B:13:LEU:HD21	1:B:16:VAL:HG21	1.96	0.46
1:A:2:LYS:HD2	1:A:3:ILE:N	2.31	0.46
1:B:167:LEU:O	1:B:167:LEU:HD23	2.16	0.46
1:A:29:VAL:HG21	1:B:159:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LEU:HD12	1:C:150:LEU:CD1	2.46	0.46
1:D:62:PHE:O	1:D:161:THR:HA	2.15	0.46
1:A:175:ALA:HA	1:A:214:ILE:HD11	1.97	0.46
1:D:7:ASP:OD1	1:D:99:TYR:HD2	1.99	0.46
1:B:7:ASP:CG	1:B:8:LYS:HD2	2.36	0.46
1:D:106:LEU:N	1:D:106:LEU:HD12	2.30	0.46
1:D:134:LEU:O	1:D:138:GLU:HG3	2.16	0.46
1:C:134:LEU:O	1:C:138:GLU:HG3	2.15	0.46
1:A:192:ARG:C	1:A:192:ARG:HD3	2.36	0.45
1:A:210:TYR:CZ	1:A:215:LEU:HB2	2.51	0.45
1:A:120:GLU:O	1:A:124:GLU:HG3	2.16	0.45
1:B:147:ARG:HD2	1:B:148:ILE:N	2.32	0.45
1:D:210:TYR:CZ	1:D:215:LEU:HB2	2.52	0.45
1:A:163:ASN:ND2	1:A:166:SER:H	2.15	0.45
1:A:13:LEU:CD2	1:A:197:LYS:HE3	2.47	0.45
1:B:13:LEU:HD21	1:B:16:VAL:CG2	2.47	0.45
1:B:139:SER:O	1:C:111:THR:HA	2.17	0.44
1:B:117:ARG:HH11	1:B:121:LYS:NZ	2.14	0.44
1:B:42:ARG:NH1	1:B:42:ARG:HG3	2.32	0.44
1:B:54:GLU:OE1	1:B:165:ARG:HD3	2.17	0.44
1:B:167:LEU:HD23	1:B:167:LEU:C	2.38	0.44
1:B:5:ILE:HD11	1:B:189:ALA:HB2	1.99	0.44
1:B:90:ARG:HD3	2:B:608:BRU:BR	2.72	0.44
1:A:176:ASP:OD2	1:A:178:HIS:HD2	2.01	0.44
1:B:143:ARG:O	1:B:147:ARG:HG3	2.17	0.44
1:D:130:TYR:O	1:D:133:TYR:HB3	2.18	0.44
1:B:46:GLU:O	1:B:50:LYS:HG2	2.18	0.44
1:B:62:PHE:O	1:B:161:THR:HA	2.18	0.43
2:A:603:BRU:H1'	1:D:78:ARG:NH1	2.32	0.43
1:A:31:PHE:HA	1:B:92:SER:OG	2.18	0.43
1:C:216:LYS:NZ	1:C:216:LYS:HB2	2.34	0.43
1:C:106:LEU:HD11	1:C:118:VAL:HG11	2.00	0.43
1:B:210:TYR:CE2	1:B:215:LEU:HB2	2.53	0.43
1:D:28:ARG:HG3	4:D:352:HOH:O	2.19	0.43
1:C:220:VAL:OXT	1:C:220:VAL:HG23	2.19	0.43
1:A:113:ILE:HD12	1:A:117:ARG:HB3	2.00	0.43
1:B:55:THR:OG1	1:B:56:PRO:HD3	2.19	0.43
1:D:19:ASN:HB2	4:D:498:HOH:O	2.17	0.43
1:A:59:HIS:CD2	1:B:85:ASN:HD22	2.37	0.43
1:D:117:ARG:HH12	1:D:121:LYS:HZ3	1.66	0.43
1:B:148:ILE:HB	1:C:153:ASN:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ASP:OD2	1:A:178:HIS:CD2	2.72	0.42
1:A:25:ARG:O	1:A:29:VAL:HG23	2.19	0.42
1:A:9:GLY:O	1:A:10:PHE:HB3	2.18	0.42
1:A:86:GLU:CG	1:A:87:LEU:N	2.83	0.42
1:A:104:GLU:HA	1:A:107:GLU:HG3	2.01	0.42
1:B:28:ARG:HB3	1:B:33:MET:O	2.20	0.42
1:C:87:LEU:HD23	1:D:30:SER:N	2.35	0.42
1:D:114:PRO:HA	1:D:115:PRO:HD3	1.97	0.42
1:A:117:ARG:O	1:A:121:LYS:HG3	2.20	0.42
1:B:220:VAL:HG23	1:B:220:VAL:OXT	2.20	0.42
1:B:96:TYR:HB2	1:B:130:TYR:CE2	2.55	0.42
1:A:44:LEU:O	1:A:47:TYR:HB3	2.20	0.41
1:D:211:LYS:HB3	1:D:211:LYS:HE2	1.87	0.41
1:A:167:LEU:HD23	1:A:167:LEU:C	2.40	0.41
1:D:210:TYR:CE2	1:D:215:LEU:HB2	2.55	0.41
1:A:147:ARG:HD2	1:A:148:ILE:N	2.35	0.41
1:A:90:ARG:HD3	2:A:603:BRU:BR	2.75	0.41
1:C:114:PRO:HA	1:C:115:PRO:HD3	1.98	0.41
1:C:150:LEU:HA	1:C:151:PRO:HD3	1.77	0.41
1:D:163:ASN:HD21	1:D:166:SER:H	1.65	0.41
1:A:173:LEU:HD13	3:A:615:FAD:O4'	2.20	0.41
1:A:181:TRP:O	1:A:185:GLN:HG2	2.21	0.41
1:C:127:ASP:OD2	1:C:131:ARG:NH1	2.48	0.41
1:A:153:ASN:HB3	1:D:148:ILE:HB	2.01	0.41
1:A:14:VAL:CG1	1:B:25:ARG:HH11	2.34	0.41
1:C:188:LEU:O	1:C:192:ARG:HG3	2.19	0.41
1:D:90:ARG:CB	1:D:144:GLU:HB3	2.51	0.41
1:A:202:PHE:O	1:A:205:PHE:HB3	2.20	0.41
1:A:163:ASN:HD21	3:C:605:FAD:H2A	1.86	0.41
1:A:78:ARG:NH1	2:D:618:BRU:H1'	2.35	0.41
1:A:143:ARG:O	1:A:147:ARG:HG3	2.20	0.41
1:B:112:THR:HB	1:C:139:SER:HB2	2.02	0.41
1:A:50:LYS:HE3	1:A:208:TYR:CE1	2.56	0.41
1:B:219:GLN:O	1:B:220:VAL:OXT	2.39	0.41
1:D:117:ARG:NH1	1:D:121:LYS:HE2	2.36	0.41
1:C:98:PHE:HE2	1:C:151:PRO:HD2	1.86	0.40
1:D:13:LEU:HD11	1:D:16:VAL:CG2	2.52	0.40
1:A:167:LEU:O	1:A:170:PHE:HB3	2.21	0.40
1:C:150:LEU:HA	1:C:150:LEU:HD23	1.91	0.40
1:C:162:VAL:CG2	1:C:166:SER:HB3	2.51	0.40
1:A:210:TYR:CE1	1:A:215:LEU:HD12	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LYS:HB3	1:B:208:TYR:CG	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/232 (92%)	208 (97%)	6 (3%)	0	100	100
1	B	213/232 (92%)	209 (98%)	4 (2%)	0	100	100
1	C	212/232 (91%)	205 (97%)	7 (3%)	0	100	100
1	D	211/232 (91%)	203 (96%)	8 (4%)	0	100	100
All	All	850/928 (92%)	825 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/207 (91%)	183 (97%)	6 (3%)	39	54
1	B	192/207 (93%)	187 (97%)	5 (3%)	46	63
1	C	193/207 (93%)	188 (97%)	5 (3%)	46	63
1	D	192/207 (93%)	187 (97%)	5 (3%)	46	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	766/828 (92%)	745 (97%)	21 (3%)	44 61

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	87	LEU
1	A	96	TYR
1	A	147	ARG
1	A	163	ASN
1	A	192	ARG
1	B	42	ARG
1	B	44	LEU
1	B	117	ARG
1	B	147	ARG
1	B	192	ARG
1	C	92	SER
1	C	117	ARG
1	C	132	THR
1	C	147	ARG
1	C	216	LYS
1	D	44	LEU
1	D	53	HIS
1	D	154	LEU
1	D	163	ASN
1	D	165	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	178	HIS
1	A	185	GLN
1	B	85	ASN
1	C	51	HIS
1	D	163	ASN
1	D	178	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
3	FAD	A	615	-	51,58,58	3.53	24 (47%)	60,89,89	2.58	18 (30%)
3	FAD	C	605	-	51,58,58	3.27	24 (47%)	60,89,89	2.58	18 (30%)
2	BRU	D	618	-	19,22,22	2.61	8 (42%)	24,33,33	4.18	9 (37%)
3	FAD	D	600	-	51,58,58	3.31	22 (43%)	60,89,89	2.57	18 (30%)
3	FAD	B	610	-	51,58,58	3.32	24 (47%)	60,89,89	2.54	19 (31%)
2	BRU	C	613	-	19,22,22	2.68	8 (42%)	24,33,33	4.28	10 (41%)
2	BRU	A	603	-	19,22,22	2.55	7 (36%)	24,33,33	4.18	9 (37%)
2	BRU	B	608	-	19,22,22	2.46	8 (42%)	24,33,33	4.18	9 (37%)

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
3	FAD	A	615	-	1/1/9/9	1/30/50/50	0/6/6/6
2	BRU	D	618	-	-	0/7/22/22	0/2/2/2
3	FAD	D	600	-	1/1/9/9	1/30/50/50	0/6/6/6
2	BRU	A	603	-	-	0/7/22/22	0/2/2/2
3	FAD	B	610	-	1/1/9/9	1/30/50/50	0/6/6/6
2	BRU	C	613	-	-	0/7/22/22	0/2/2/2
3	FAD	C	605	-	1/1/9/9	1/30/50/50	0/6/6/6
2	BRU	B	608	-	-	0/7/22/22	0/2/2/2

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	615	FAD	C4X-C10	11.39	1.50	1.38
3	B	610	FAD	C4X-C10	10.52	1.49	1.38
3	C	605	FAD	C4X-C10	10.07	1.48	1.38
3	D	600	FAD	C4X-C10	10.03	1.48	1.38
3	A	615	FAD	C10-N1	7.16	1.42	1.33
3	A	615	FAD	C4A-N3A	7.06	1.45	1.35
3	C	605	FAD	C10-N1	6.99	1.42	1.33
3	D	600	FAD	C10-N1	6.99	1.42	1.33
3	A	615	FAD	C4X-N5	6.76	1.43	1.33
3	D	600	FAD	C4A-N3A	6.72	1.44	1.35
3	B	610	FAD	C10-N1	6.68	1.41	1.33
3	A	615	FAD	C4-N3	6.67	1.44	1.33
3	B	610	FAD	C4-N3	6.66	1.44	1.33
3	D	600	FAD	C4-N3	6.59	1.44	1.33
3	C	605	FAD	C4-N3	6.55	1.44	1.33
3	B	610	FAD	C4A-N3A	6.50	1.44	1.35
2	C	613	BRU	C4-C5	6.46	1.46	1.38
2	D	618	BRU	C4-C5	6.43	1.46	1.38
3	C	605	FAD	C4A-N3A	6.28	1.44	1.35
2	C	613	BRU	C4-N3	6.08	1.43	1.33
2	D	618	BRU	C4-N3	6.03	1.43	1.33
2	B	608	BRU	C4-N3	6.00	1.43	1.33
2	A	603	BRU	C4-N3	5.97	1.43	1.33
3	C	605	FAD	C4X-N5	5.91	1.41	1.33
2	A	603	BRU	C4-C5	5.86	1.46	1.38
3	B	610	FAD	C4X-N5	5.81	1.41	1.33
3	A	615	FAD	C2B-C1B	5.75	1.62	1.53
3	B	610	FAD	C2B-C1B	5.74	1.62	1.53
3	D	600	FAD	C4X-N5	5.57	1.41	1.33
3	A	615	FAD	C4-C4X	5.40	1.50	1.41
3	B	610	FAD	C8A-N7A	-5.31	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	600	FAD	C8A-N7A	-5.30	1.25	1.34
3	A	615	FAD	C8A-N7A	-5.20	1.25	1.34
3	C	605	FAD	C8A-N7A	-5.10	1.25	1.34
3	C	605	FAD	C9A-C5X	5.06	1.52	1.42
3	A	615	FAD	C9A-C5X	5.03	1.52	1.42
2	B	608	BRU	C4-C5	4.98	1.44	1.38
3	D	600	FAD	C2B-C1B	4.94	1.61	1.53
3	C	605	FAD	C2B-C1B	4.85	1.61	1.53
3	B	610	FAD	C9A-C5X	4.79	1.52	1.42
3	B	610	FAD	C4-C4X	4.69	1.49	1.41
3	D	600	FAD	C9A-C5X	4.61	1.51	1.42
3	D	600	FAD	C8-C7	4.58	1.52	1.40
3	C	605	FAD	C8-C7	4.56	1.52	1.40
3	A	615	FAD	C8-C7	4.55	1.52	1.40
3	A	615	FAD	C9-C9A	4.53	1.49	1.40
3	D	600	FAD	C4-C4X	4.51	1.49	1.41
3	D	600	FAD	C2A-N3A	4.49	1.39	1.32
3	A	615	FAD	C5X-N5	4.48	1.42	1.35
3	B	610	FAD	C8-C7	4.48	1.52	1.40
3	A	615	FAD	C2A-N3A	4.43	1.39	1.32
3	C	605	FAD	C4-C4X	4.38	1.48	1.41
3	D	600	FAD	C9-C9A	4.32	1.49	1.40
3	A	615	FAD	C6-C7	4.24	1.48	1.37
3	C	605	FAD	C2A-N3A	4.21	1.38	1.32
3	B	610	FAD	C9-C9A	4.15	1.49	1.40
3	C	605	FAD	C9-C9A	4.15	1.49	1.40
2	C	613	BRU	O4'-C1'	4.12	1.51	1.42
3	D	600	FAD	O4B-C1B	4.10	1.46	1.41
3	B	610	FAD	C6-C7	4.08	1.48	1.37
3	B	610	FAD	C5X-N5	3.96	1.41	1.35
3	C	605	FAD	O4B-C1B	3.92	1.46	1.41
2	B	608	BRU	O4'-C1'	3.87	1.51	1.42
3	D	600	FAD	C6-C7	3.84	1.47	1.37
3	D	600	FAD	C6-C5X	3.80	1.47	1.41
2	A	603	BRU	O4'-C1'	3.79	1.50	1.42
3	D	600	FAD	C5X-N5	3.73	1.41	1.35
2	D	618	BRU	O4'-C1'	3.70	1.50	1.42
3	B	610	FAD	C2A-N3A	3.68	1.38	1.32
3	C	605	FAD	C6-C7	3.62	1.46	1.37
3	A	615	FAD	C2A-N1A	3.54	1.40	1.33
3	D	600	FAD	C2A-N1A	3.53	1.40	1.33
3	C	605	FAD	C5X-N5	3.49	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	605	FAD	C2A-N1A	3.43	1.40	1.33
3	A	615	FAD	C6-C5X	3.37	1.47	1.41
3	B	610	FAD	C6-C5X	3.37	1.47	1.41
3	A	615	FAD	O4B-C1B	3.36	1.45	1.41
3	B	610	FAD	C2A-N1A	3.31	1.40	1.33
3	C	605	FAD	C6-C5X	3.18	1.46	1.41
3	B	610	FAD	O4B-C1B	3.17	1.45	1.41
3	A	615	FAD	C2-N3	3.16	1.44	1.38
3	B	610	FAD	C2-N3	3.08	1.44	1.38
3	D	600	FAD	C9-C8	2.96	1.45	1.37
3	B	610	FAD	C9-C8	2.94	1.45	1.37
3	C	605	FAD	C9-C8	2.91	1.45	1.37
3	A	615	FAD	C9-C8	2.76	1.44	1.37
3	D	600	FAD	C2-N3	2.74	1.43	1.38
2	C	613	BRU	O4'-C4'	2.70	1.51	1.45
2	A	603	BRU	O4'-C4'	2.66	1.50	1.45
2	D	618	BRU	O4'-C4'	2.63	1.50	1.45
2	B	608	BRU	O4'-C4'	2.51	1.50	1.45
3	A	615	FAD	C5A-C4A	2.46	1.47	1.40
2	C	613	BRU	C2'-C1'	2.45	1.59	1.52
2	C	613	BRU	C2-N3	2.45	1.43	1.38
2	B	608	BRU	C2'-C3'	2.42	1.59	1.52
3	D	600	FAD	C5B-C4B	2.41	1.59	1.51
3	C	605	FAD	C5A-C4A	2.38	1.47	1.40
2	B	608	BRU	C2'-C1'	2.37	1.59	1.52
3	C	605	FAD	C2-N3	2.37	1.42	1.38
3	C	605	FAD	O5B-C5B	2.32	1.53	1.44
2	A	603	BRU	C2'-C1'	2.30	1.58	1.52
3	D	600	FAD	O5B-C5B	2.27	1.53	1.44
3	B	610	FAD	P-O5'	-2.26	1.50	1.59
2	A	603	BRU	C2'-C3'	2.25	1.58	1.52
3	D	600	FAD	C5A-C4A	2.25	1.46	1.40
2	D	618	BRU	C2'-C1'	2.25	1.58	1.52
2	C	613	BRU	C2'-C3'	2.22	1.58	1.52
3	A	615	FAD	C5B-C4B	2.19	1.58	1.51
2	A	603	BRU	P-OP2	-2.18	1.46	1.54
3	B	610	FAD	C5B-C4B	2.18	1.58	1.51
3	A	615	FAD	P-O5'	-2.18	1.50	1.59
3	B	610	FAD	PA-O5B	-2.18	1.50	1.59
2	C	613	BRU	P-OP2	-2.17	1.46	1.54
3	C	605	FAD	P-O5'	-2.16	1.50	1.59
2	B	608	BRU	C2-N3	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	610	FAD	C5A-C4A	2.13	1.46	1.40
2	D	618	BRU	P-OP2	-2.12	1.46	1.54
2	D	618	BRU	C2-N3	2.09	1.42	1.38
3	C	605	FAD	C5B-C4B	2.09	1.58	1.51
3	A	615	FAD	PA-O5B	-2.08	1.50	1.59
2	D	618	BRU	C2'-C3'	2.07	1.58	1.52
3	C	605	FAD	PA-O5B	-2.06	1.51	1.59
3	B	610	FAD	O5B-C5B	2.03	1.52	1.44
3	A	615	FAD	O5B-C5B	2.03	1.52	1.44
2	B	608	BRU	P-OP2	-2.00	1.47	1.54

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	613	BRU	C4-N3-C2	15.87	128.54	115.14
2	D	618	BRU	C4-N3-C2	15.64	128.34	115.14
2	B	608	BRU	C4-N3-C2	15.61	128.32	115.14
2	A	603	BRU	C4-N3-C2	15.52	128.25	115.14
3	C	605	FAD	C4-N3-C2	9.16	122.88	115.14
3	A	615	FAD	C4-N3-C2	9.15	122.87	115.14
3	D	600	FAD	C4-N3-C2	9.01	122.75	115.14
3	B	610	FAD	C4-N3-C2	8.63	122.43	115.14
3	D	600	FAD	C3B-C2B-C1B	-8.32	88.45	100.98
3	B	610	FAD	C3B-C2B-C1B	-8.29	88.50	100.98
3	A	615	FAD	C3B-C2B-C1B	-8.28	88.51	100.98
3	C	605	FAD	C3B-C2B-C1B	-8.20	88.64	100.98
2	A	603	BRU	C2'-C1'-N1	-7.31	97.41	114.27
2	C	613	BRU	C2'-C1'-N1	-7.29	97.45	114.27
2	C	613	BRU	C5-C4-N3	-7.23	114.98	123.64
2	B	608	BRU	C5-C4-N3	-7.11	115.13	123.64
2	D	618	BRU	C5-C4-N3	-7.05	115.20	123.64
2	D	618	BRU	C2'-C1'-N1	-7.05	98.01	114.27
2	A	603	BRU	C5-C4-N3	-6.82	115.47	123.64
2	B	608	BRU	C2'-C1'-N1	-6.69	98.85	114.27
3	C	605	FAD	C1'-N10-C9A	5.76	122.83	118.29
3	B	610	FAD	C1'-N10-C9A	5.49	122.61	118.29
3	D	600	FAD	C1'-N10-C9A	5.49	122.61	118.29
3	A	615	FAD	C1'-N10-C9A	5.26	122.44	118.29
2	C	613	BRU	C5-C6-N1	5.22	126.72	119.97
2	B	608	BRU	C5-C6-N1	5.07	126.53	119.97
3	A	615	FAD	O2B-C2B-C1B	4.89	128.91	110.85
3	B	610	FAD	O2B-C2B-C1B	4.88	128.86	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	BRU	C5-C6-N1	4.81	126.19	119.97
2	D	618	BRU	C5-C6-N1	4.77	126.14	119.97
3	D	600	FAD	O2B-C2B-C1B	4.70	128.21	110.85
3	A	615	FAD	C4-C4X-C10	-4.69	116.84	119.95
3	C	605	FAD	O2B-C2B-C1B	4.66	128.06	110.85
3	C	605	FAD	C1'-N10-C10	-4.60	114.29	118.41
3	A	615	FAD	C4X-C4-N3	-4.51	117.26	123.43
3	D	600	FAD	C1'-N10-C10	-4.48	114.40	118.41
3	D	600	FAD	C4X-C4-N3	-4.47	117.32	123.43
3	C	605	FAD	C4X-C4-N3	-4.43	117.38	123.43
3	B	610	FAD	C1'-N10-C10	-4.43	114.44	118.41
3	A	615	FAD	C1'-N10-C10	-4.38	114.49	118.41
3	C	605	FAD	C4-C4X-C10	-4.36	117.07	119.95
3	B	610	FAD	C4X-C4-N3	-4.33	117.51	123.43
3	D	600	FAD	C4-C4X-C10	-4.33	117.09	119.95
3	A	615	FAD	C4-C4X-N5	4.28	123.49	118.60
3	B	610	FAD	C4-C4X-C10	-4.08	117.25	119.95
3	D	600	FAD	C4X-N5-C5X	4.08	120.85	116.77
3	B	610	FAD	C4X-N5-C5X	4.07	120.84	116.77
3	C	605	FAD	C4X-N5-C5X	4.03	120.80	116.77
3	D	600	FAD	C4-C4X-N5	3.77	122.91	118.60
3	B	610	FAD	C4-C4X-N5	3.77	122.90	118.60
3	A	615	FAD	C4X-N5-C5X	3.67	120.44	116.77
3	C	605	FAD	C4-C4X-N5	3.63	122.75	118.60
3	B	610	FAD	N3A-C2A-N1A	-3.57	123.10	128.68
3	D	600	FAD	N3A-C2A-N1A	-3.54	123.14	128.68
3	A	615	FAD	N3A-C2A-N1A	-3.42	123.33	128.68
2	A	603	BRU	BR-C5-C4	-3.41	116.33	121.50
3	C	605	FAD	N3A-C2A-N1A	-3.39	123.37	128.68
2	A	603	BRU	BR-C5-C6	3.38	125.01	117.31
2	D	618	BRU	BR-C5-C4	-3.32	116.45	121.50
2	B	608	BRU	BR-C5-C4	-3.32	116.47	121.50
2	B	608	BRU	BR-C5-C6	3.25	124.72	117.31
2	D	618	BRU	BR-C5-C6	3.25	124.71	117.31
2	C	613	BRU	BR-C5-C6	3.20	124.59	117.31
3	C	605	FAD	C4A-C5A-N7A	-3.20	106.07	109.40
3	A	615	FAD	C4A-C5A-N7A	-3.15	106.11	109.40
2	C	613	BRU	P-O5'-C5'	3.08	126.78	118.30
3	B	610	FAD	C4A-C5A-N7A	-3.07	106.19	109.40
3	D	600	FAD	P-O5'-C5'	3.03	139.47	121.68
3	B	610	FAD	P-O3P-PA	3.01	143.17	132.83
2	C	613	BRU	BR-C5-C4	-3.00	116.94	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	600	FAD	C4A-C5A-N7A	-2.98	106.29	109.40
3	C	605	FAD	P-O5'-C5'	2.95	138.99	121.68
3	A	615	FAD	P-O5'-C5'	2.95	138.98	121.68
2	D	618	BRU	P-O5'-C5'	2.89	126.25	118.30
2	A	603	BRU	P-O5'-C5'	2.87	126.20	118.30
3	C	605	FAD	P-O3P-PA	2.86	142.64	132.83
3	D	600	FAD	P-O3P-PA	2.84	142.59	132.83
3	A	615	FAD	O3B-C3B-C4B	2.83	119.23	111.05
3	B	610	FAD	O3B-C3B-C4B	2.81	119.17	111.05
3	B	610	FAD	C5B-C4B-C3B	-2.81	104.66	115.18
3	B	610	FAD	O4B-C4B-C3B	2.80	110.66	105.11
2	B	608	BRU	P-O5'-C5'	2.80	126.00	118.30
3	A	615	FAD	P-O3P-PA	2.78	142.36	132.83
3	C	605	FAD	O3B-C3B-C4B	2.77	119.06	111.05
3	D	600	FAD	C5B-C4B-C3B	-2.75	104.88	115.18
3	C	605	FAD	C5B-C4B-C3B	-2.74	104.91	115.18
3	B	610	FAD	P-O5'-C5'	2.71	137.59	121.68
3	D	600	FAD	O3B-C3B-C4B	2.71	118.88	111.05
3	A	615	FAD	O4B-C4B-C3B	2.65	110.36	105.11
3	C	605	FAD	O4B-C4B-C3B	2.65	110.36	105.11
3	D	600	FAD	O4B-C4B-C3B	2.63	110.31	105.11
3	A	615	FAD	C5B-C4B-C3B	-2.61	105.40	115.18
2	B	608	BRU	O4'-C4'-C3'	-2.49	99.87	105.67
2	C	613	BRU	O4'-C4'-C3'	-2.44	99.97	105.67
2	A	603	BRU	C4'-O4'-C1'	2.36	115.15	109.45
2	A	603	BRU	O4'-C4'-C3'	-2.32	100.26	105.67
2	C	613	BRU	C4'-O4'-C1'	2.31	115.04	109.45
3	A	615	FAD	C10-C4X-N5	-2.30	119.67	121.26
3	B	610	FAD	C2A-N1A-C6A	2.27	122.64	118.75
2	D	618	BRU	O4'-C4'-C3'	-2.22	100.50	105.67
3	D	600	FAD	C4X-C10-N10	-2.20	118.04	120.30
2	D	618	BRU	C4'-O4'-C1'	2.17	114.70	109.45
3	C	605	FAD	C4X-C10-N10	-2.16	118.08	120.30
3	C	605	FAD	C2A-N1A-C6A	2.15	122.44	118.75
3	A	615	FAD	C2A-N1A-C6A	2.14	122.42	118.75
2	B	608	BRU	C4'-O4'-C1'	2.13	114.59	109.45
2	C	613	BRU	OP3-P-O5'	2.11	112.35	106.73
3	D	600	FAD	C2A-N1A-C6A	2.11	122.36	118.75
3	B	610	FAD	C4X-C10-N10	-2.08	118.16	120.30
3	B	610	FAD	C10-C4X-N5	-2.04	119.84	121.26

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	615	FAD	C1B
3	C	605	FAD	C1B
3	D	600	FAD	C1B
3	B	610	FAD	C1B

All (4) torsion outliers are listed below:

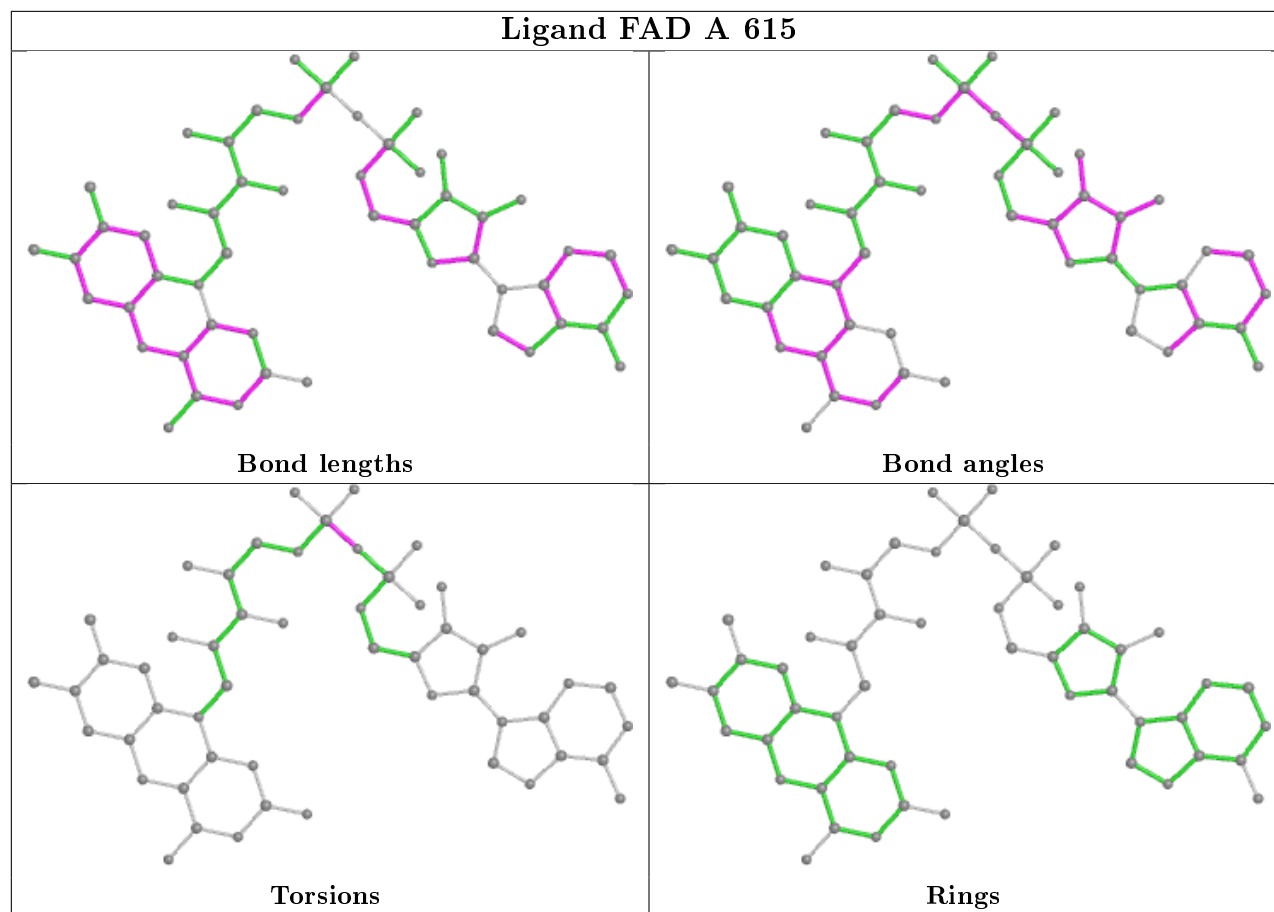
Mol	Chain	Res	Type	Atoms
3	A	615	FAD	PA-O3P-P-O1P
3	C	605	FAD	PA-O3P-P-O1P
3	D	600	FAD	PA-O3P-P-O1P
3	B	610	FAD	PA-O3P-P-O1P

There are no ring outliers.

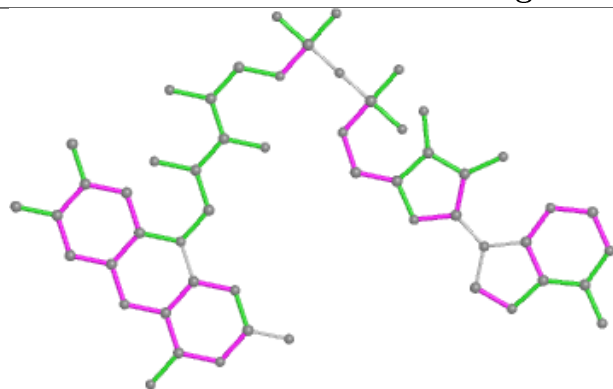
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	615	FAD	1	0
3	C	605	FAD	1	0
2	D	618	BRU	2	0
2	C	613	BRU	3	0
2	A	603	BRU	3	0
2	B	608	BRU	2	0

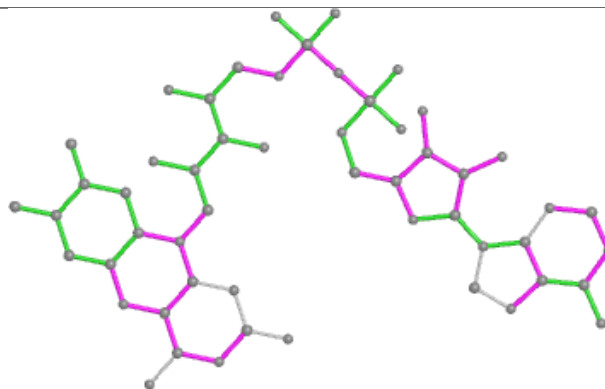
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



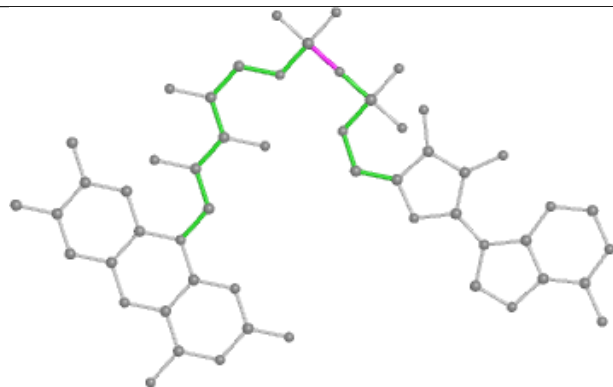
Ligand FAD C 605



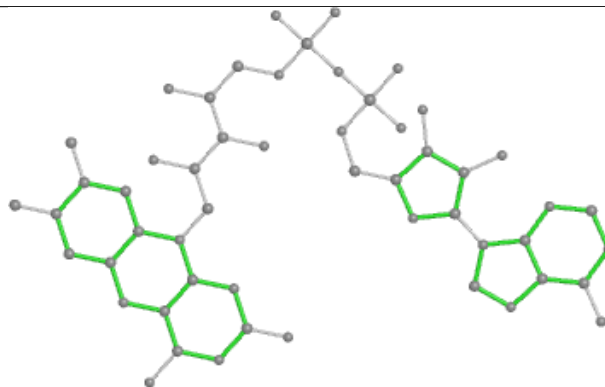
Bond lengths



Bond angles

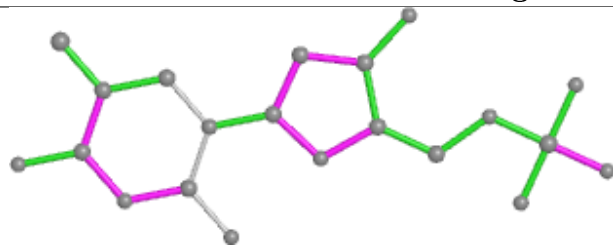


Torsions

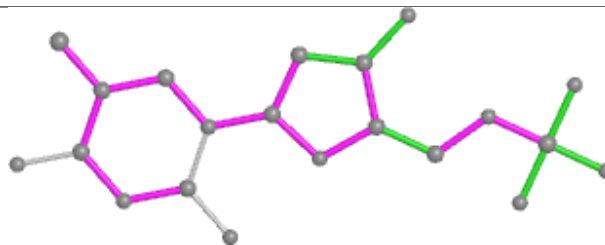


Rings

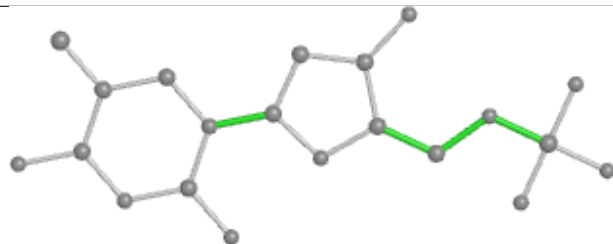
Ligand BRU D 618



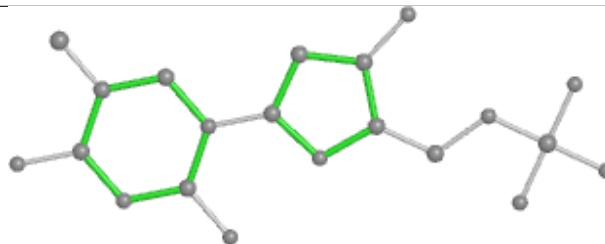
Bond lengths



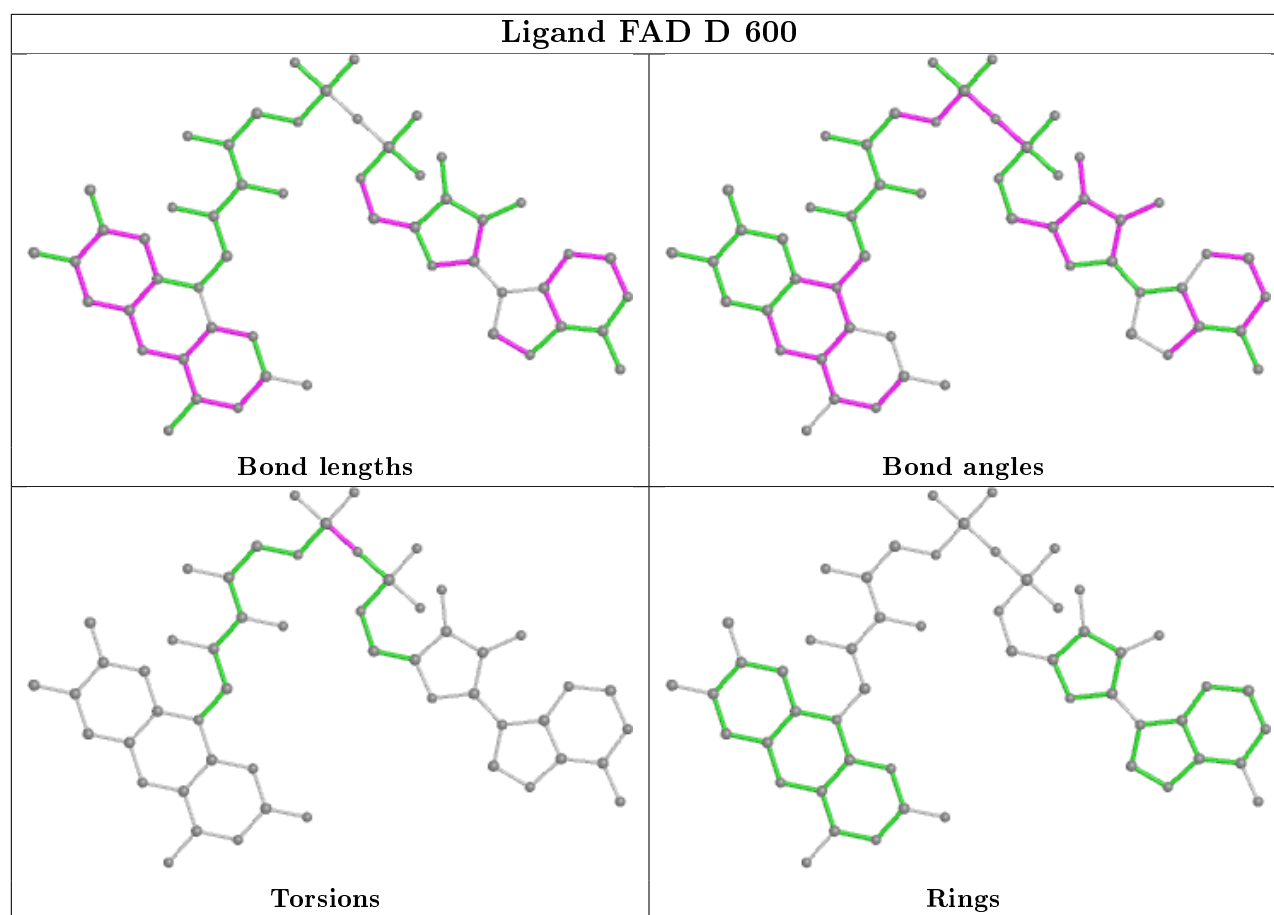
Bond angles



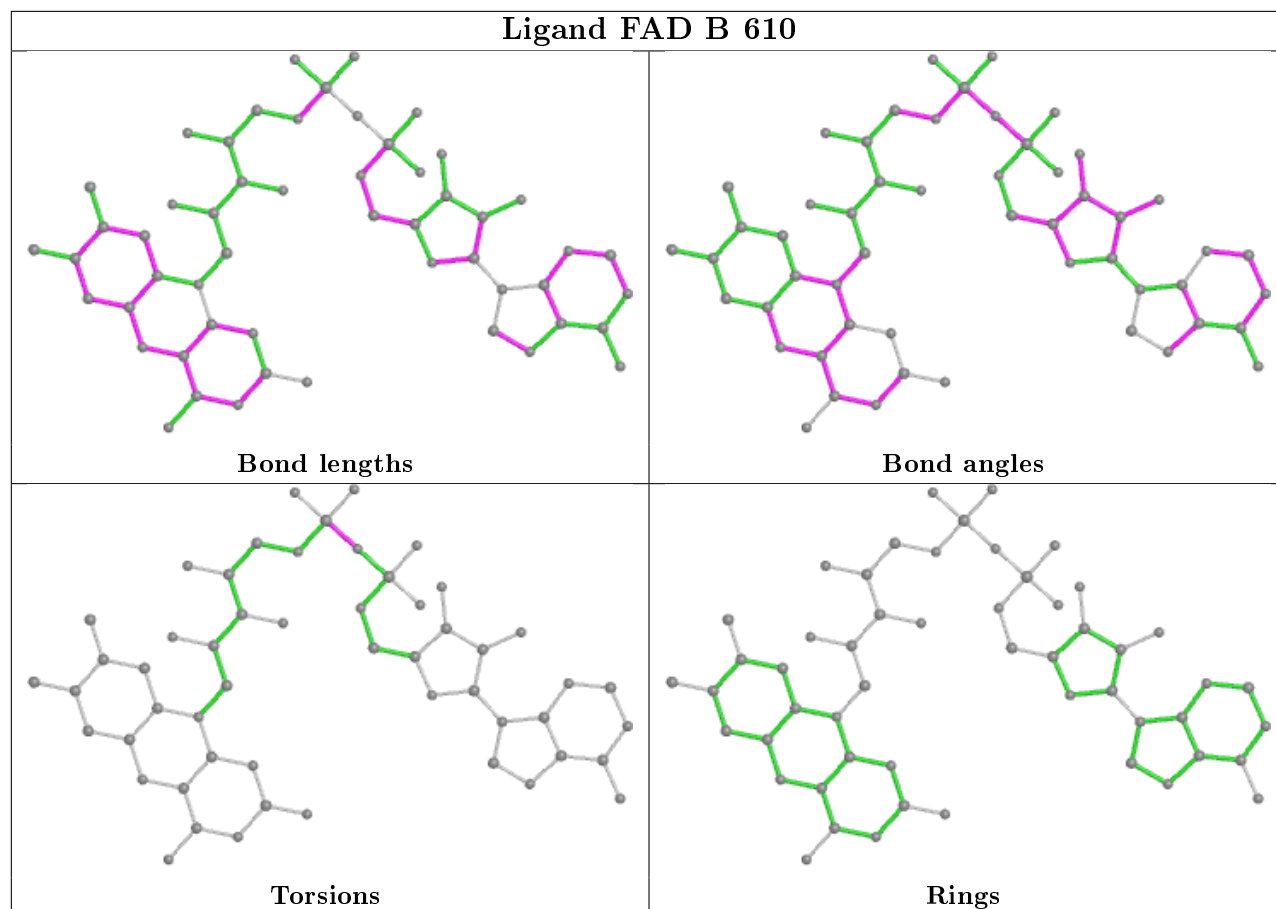
Torsions



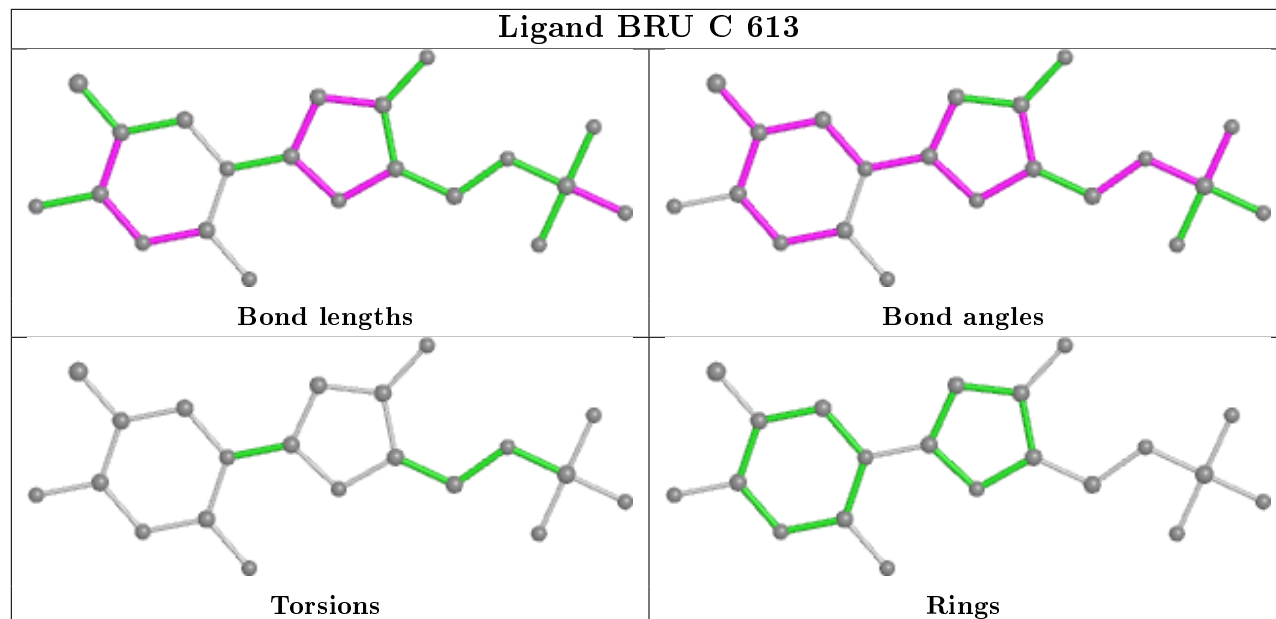
Rings

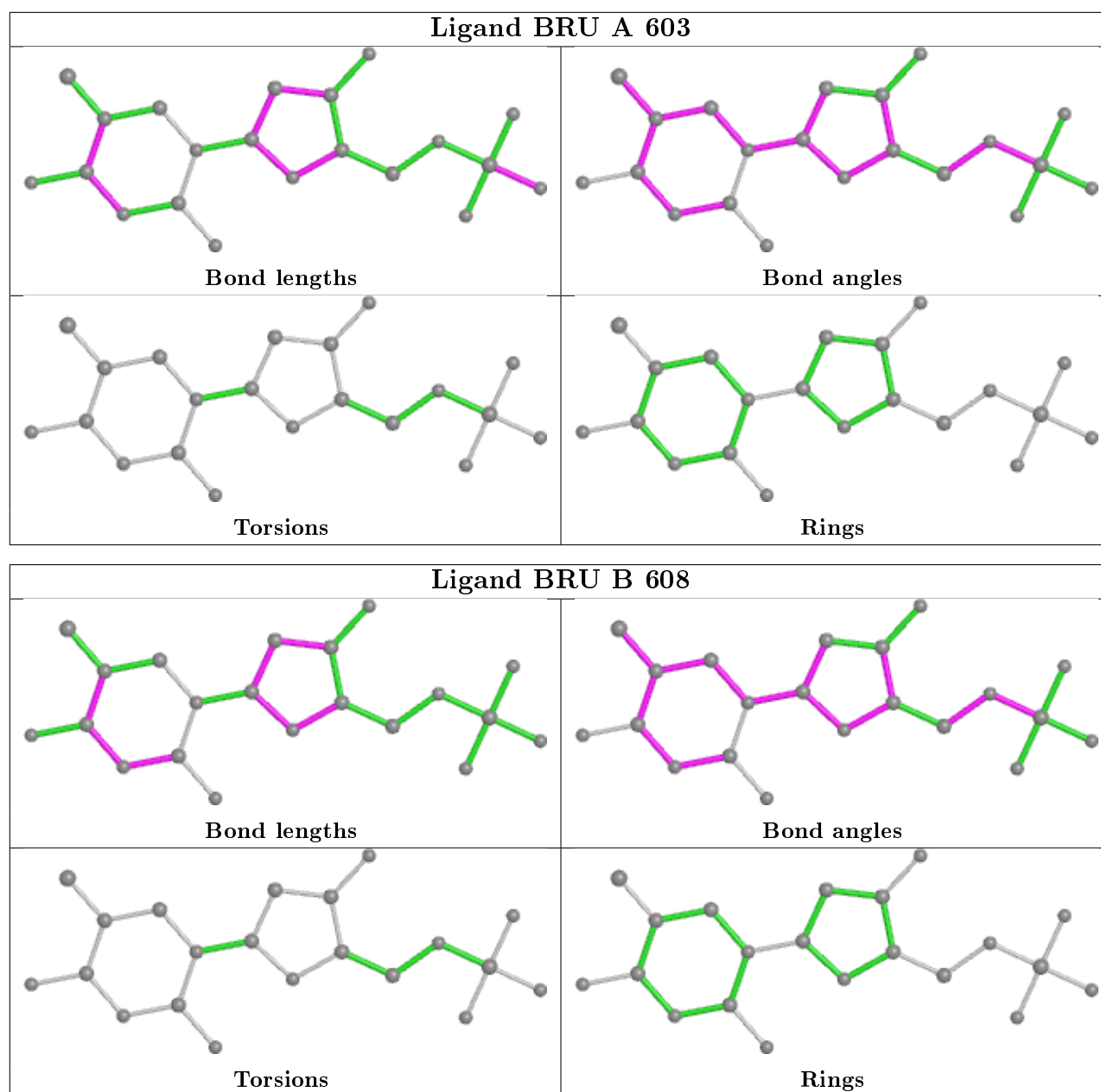


Ligand FAD B 610



Ligand BRU C 613





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	216/232 (93%)	-0.04	5 (2%) 60 67	18, 31, 50, 56	0
1	B	217/232 (93%)	-0.06	1 (0%) 91 94	19, 32, 52, 65	0
1	C	216/232 (93%)	-0.11	7 (3%) 47 54	19, 29, 50, 60	0
1	D	215/232 (92%)	0.15	15 (6%) 16 21	19, 31, 56, 65	0
All	All	864/928 (93%)	-0.02	28 (3%) 47 54	18, 30, 53, 65	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	33	MET	5.9
1	D	32	ASP	4.6
1	C	220	VAL	4.2
1	D	31	PHE	3.5
1	D	96	TYR	3.5
1	D	40	ARG	3.4
1	B	220	VAL	3.3
1	C	219	GLN	3.2
1	A	40	ARG	3.1
1	C	94	LEU	3.0
1	D	37	ASP	2.7
1	D	218	VAL	2.7
1	C	40	ARG	2.5
1	C	96	TYR	2.3
1	D	28	ARG	2.3
1	C	125	ILE	2.3
1	D	38	GLU	2.2
1	D	93	LYS	2.2
1	D	94	LEU	2.2
1	D	138	GLU	2.2
1	C	131	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	36	LYS	2.2
1	A	106	LEU	2.1
1	A	47	TYR	2.1
1	A	112	THR	2.1
1	D	106	LEU	2.0
1	D	107	GLU	2.0
1	D	137	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

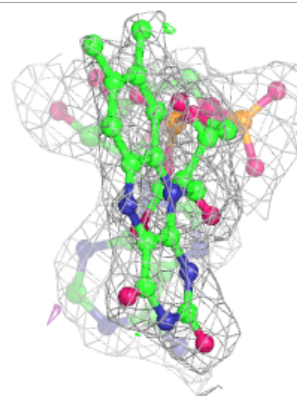
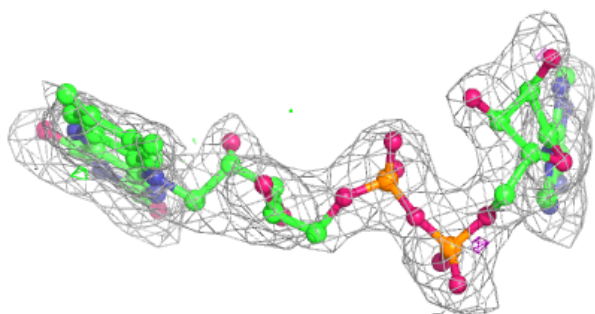
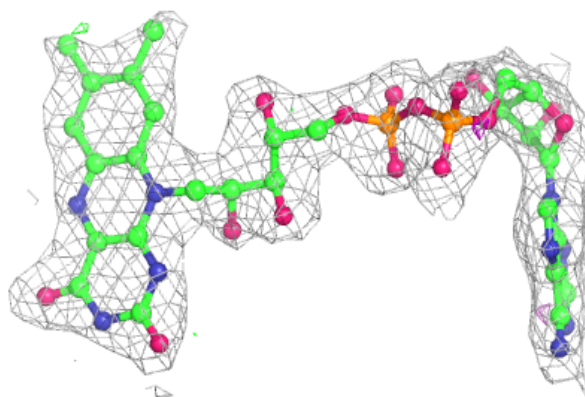
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FAD	A	615	53/53	0.94	0.15	24,34,40,41	0
3	FAD	B	610	53/53	0.95	0.14	20,29,32,34	0
2	BRU	D	618	21/21	0.96	0.12	29,33,38,43	0
3	FAD	C	605	53/53	0.96	0.17	22,26,28,33	0
3	FAD	D	600	53/53	0.97	0.14	20,27,30,31	0
2	BRU	C	613	21/21	0.97	0.11	24,28,31,35	0
2	BRU	A	603	21/21	0.97	0.11	25,28,30,33	0
2	BRU	B	608	21/21	0.97	0.12	23,24,26,29	0

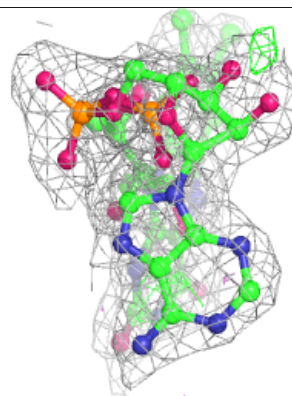
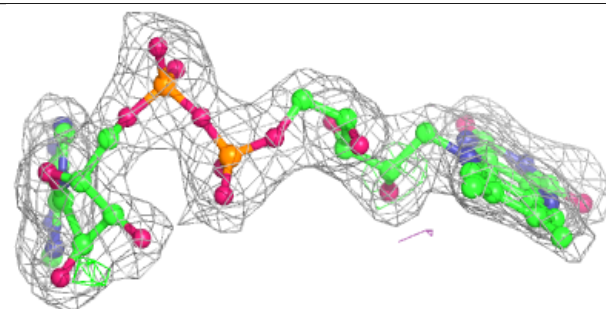
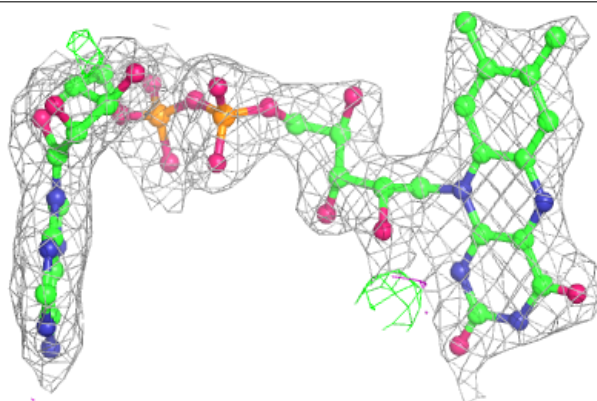
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 615:

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

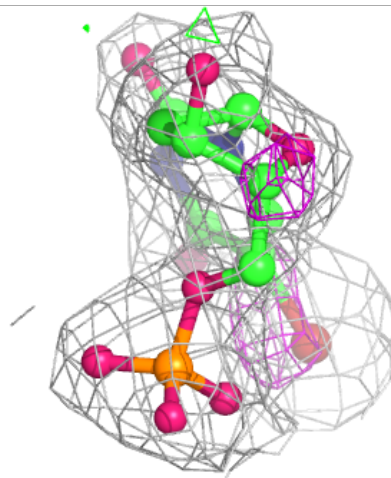
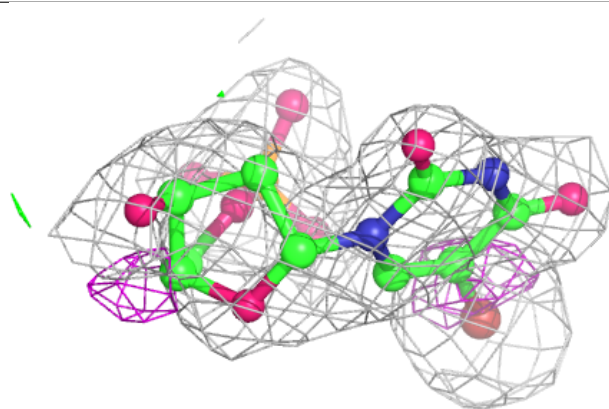
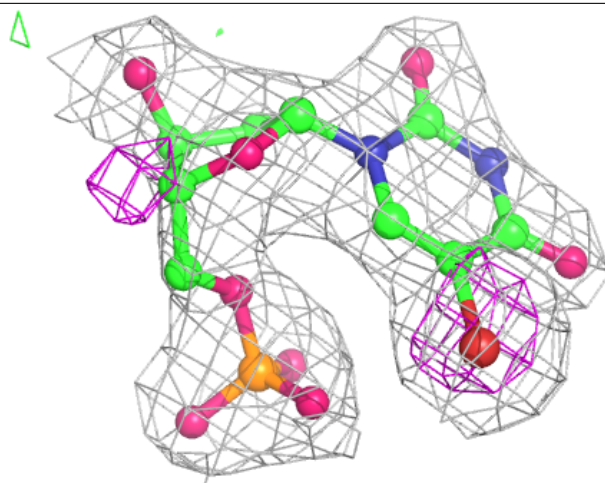
**Electron density around FAD B 610:**

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



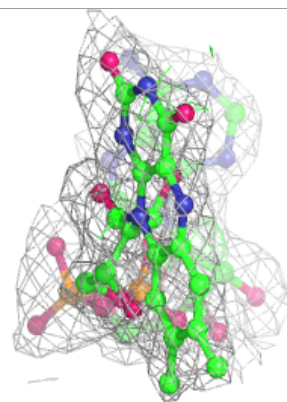
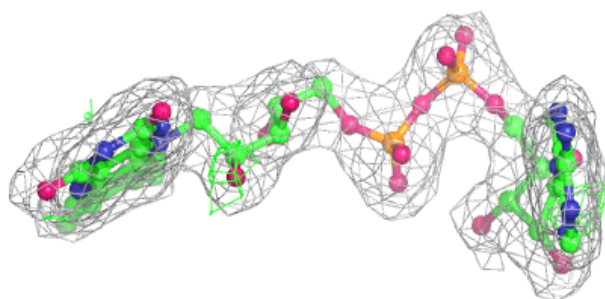
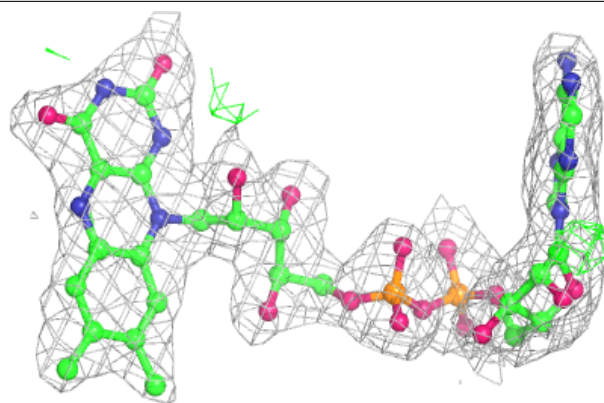
Electron density around BRU D 618:

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

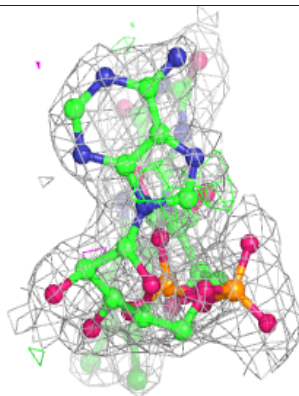
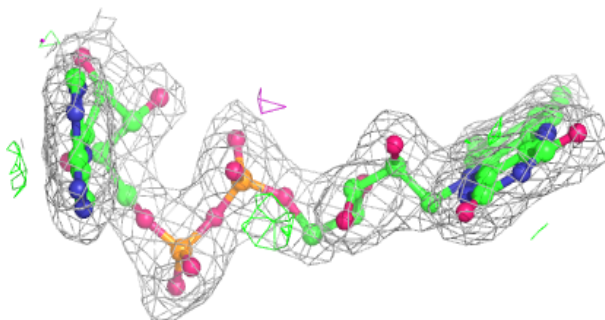
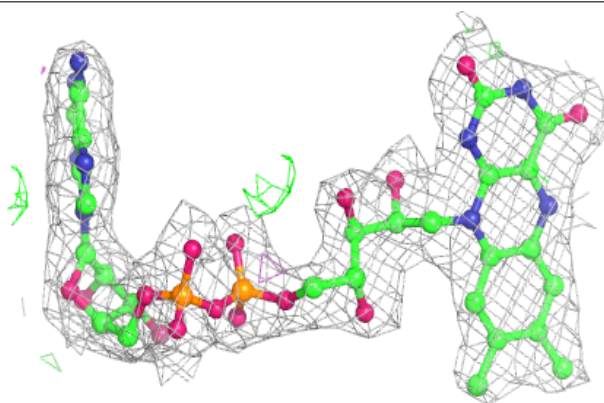


Electron density around FAD C 605:

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

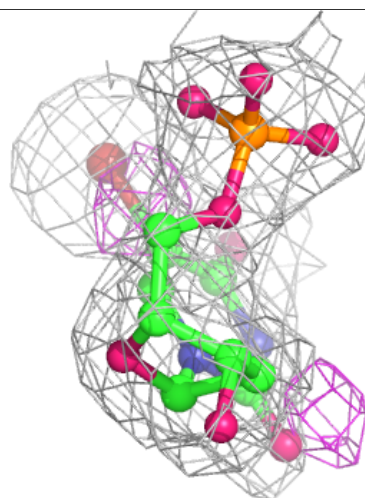
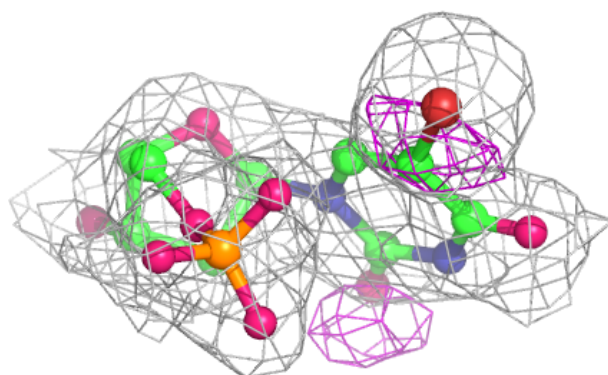
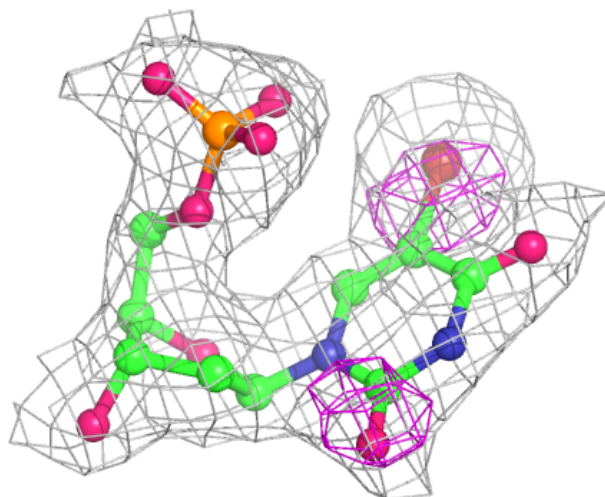
**Electron density around FAD D 600:**

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



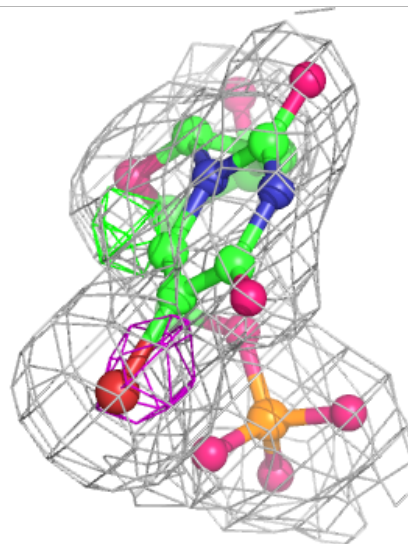
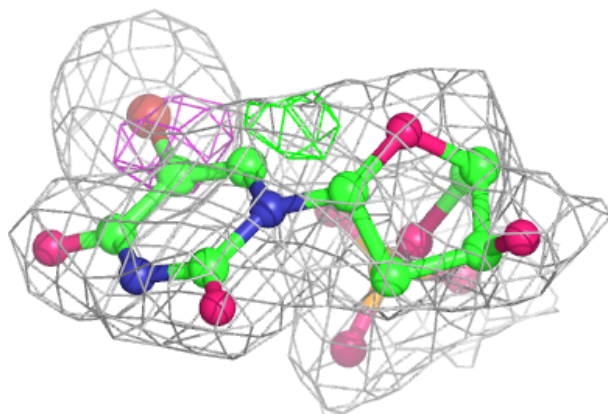
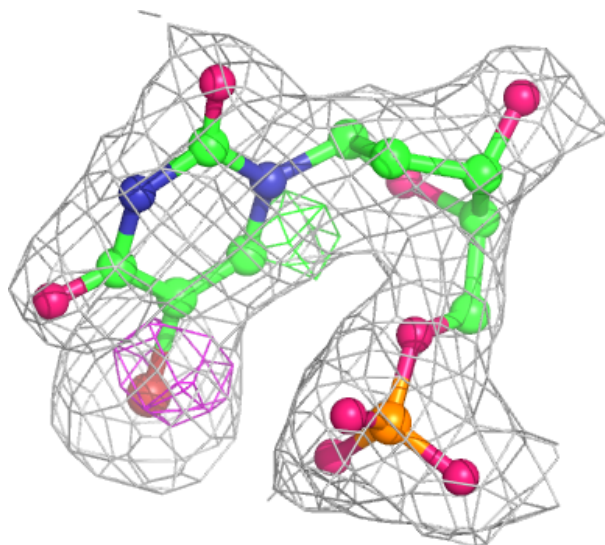
Electron density around BRU C 613:

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



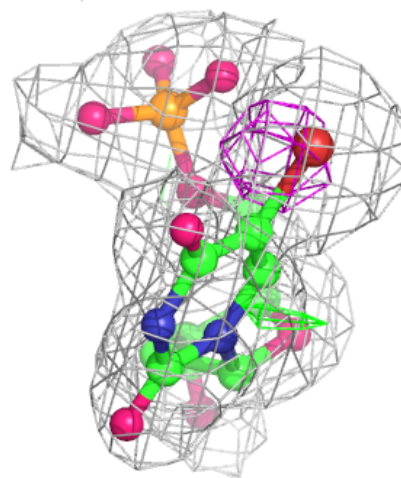
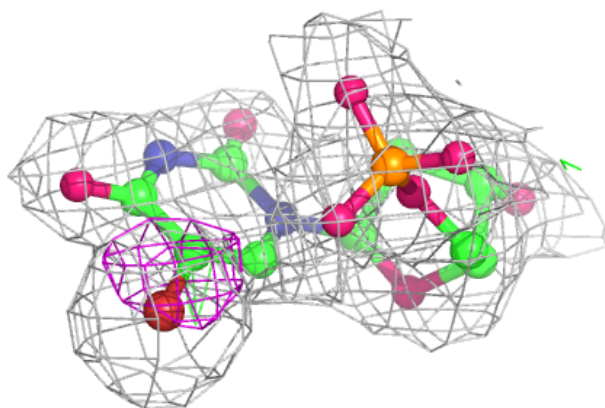
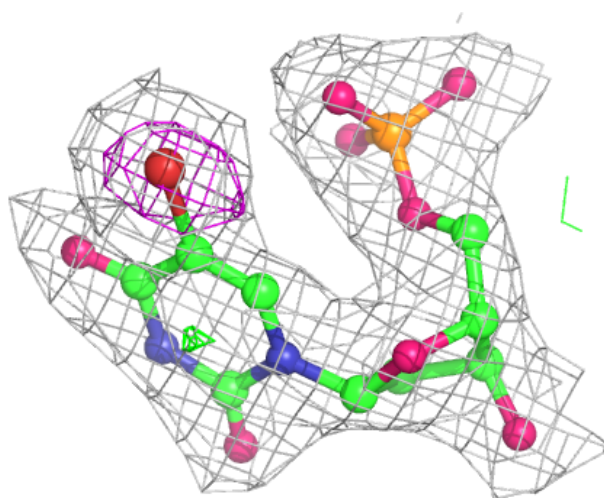
Electron density around BRU A 603:

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



Electron density around BRU B 608:

$2mF_o-DF_c$ (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.