Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 06:27 AM EDT

PDB ID	:	1O26
Title	:	Crystal structure of Thymidylate Synthase Complementing Protein (TM0449) from Thermotoga maritima with FAD and dUMP at 1.6 A 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	:	1.60 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 (i) 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 (i)) were used in the production of this report:

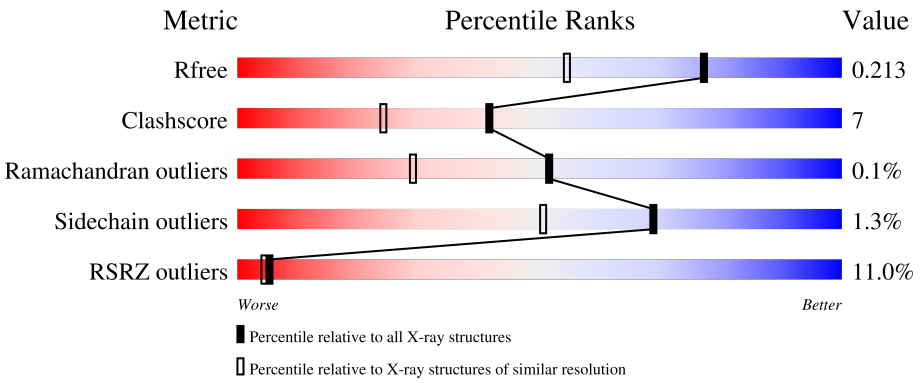
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	10% 76% 17% • 6%
1	B	232	12% 80% 15% 5%
1	C	232	9% 80% 14% 6%
1	D	232	11% 81% 12% 6%

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 criteria:

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 (i)

There are 5 unique types of molecules in this entry. The entry contains 7940 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
			Total	C	N	O	S			
1	A	219	1831	1190	314	321	6	0	0	0
1	B	221	1851	1203	317	325	6	0	0	0
1	C	218	1824	1187	311	320	6	0	0	0
1	D	218	1824	1187	311	320	6	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

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

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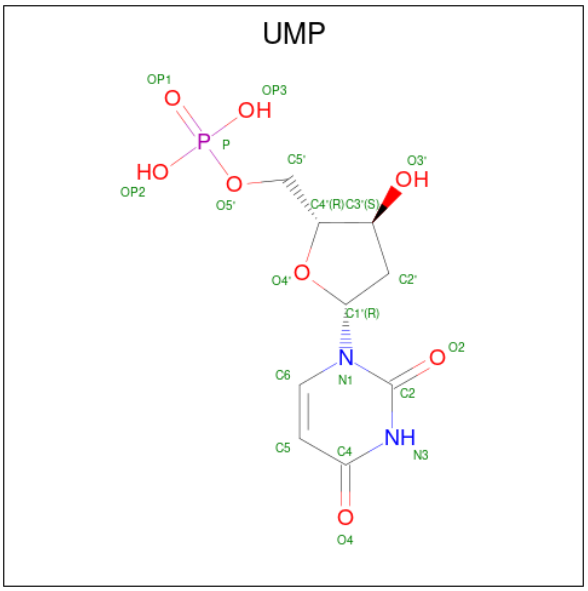
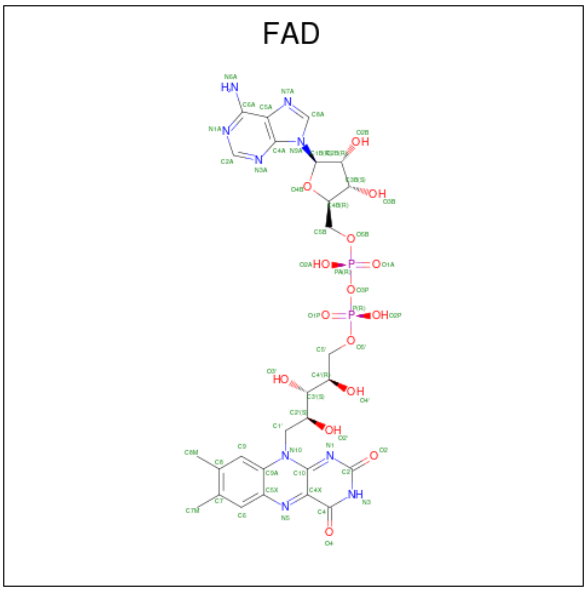
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q9WYT0
B	-1	HIS	-	expression tag	UNP Q9WYT0
B	0	HIS	-	expression tag	UNP Q9WYT0
C	-11	MET	-	expression tag	UNP Q9WYT0
C	-10	GLY	-	expression tag	UNP Q9WYT0
C	-9	SER	-	expression tag	UNP Q9WYT0
C	-8	ASP	-	expression tag	UNP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

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



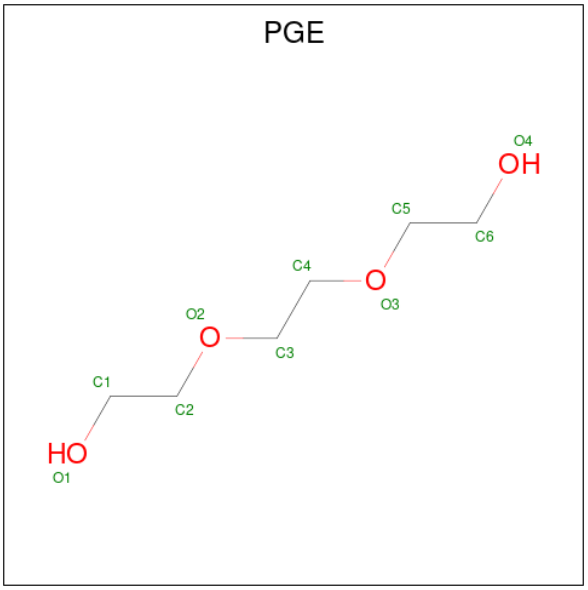
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	20	9	2	8	1	0	0
			Total	C	N	O	P		
2	B	1	20	9	2	8	1	0	0
			Total	C	N	O	P		
2	C	1	20	9	2	8	1	0	0
			Total	C	N	O	P		
2	D	1	20	9	2	8	1	0	0

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



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

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	6	4	0	0
4	B	1	10	6	4	0	0
4	B	1	10	6	4	0	0
4	D	1	10	6	4	0	0
4	D	1	10	6	4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	68	68	68	0	0

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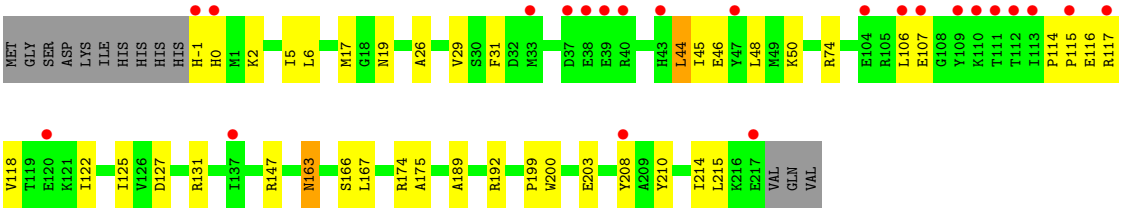
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	52	52	52	0	0
			Total	O		
5	C	82	82	82	0	0
			Total	O		
5	D	66	66	66	0	0

3 Residue-property plots (i)

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

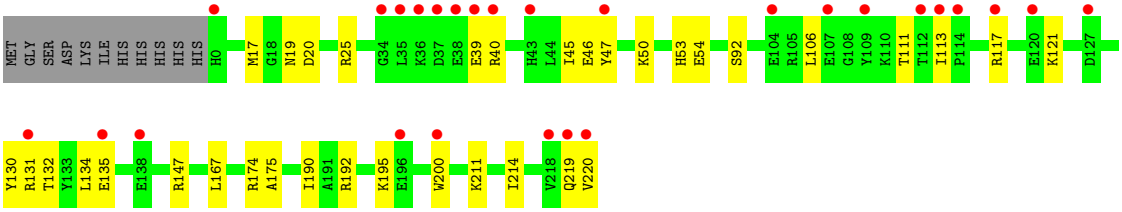
• Molecule 1: Thymidylate synthase thyX

Chain A:



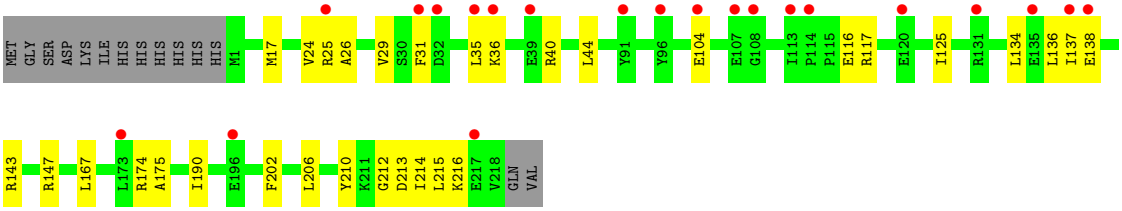
• Molecule 1: Thymidylate synthase thyX

Chain B:



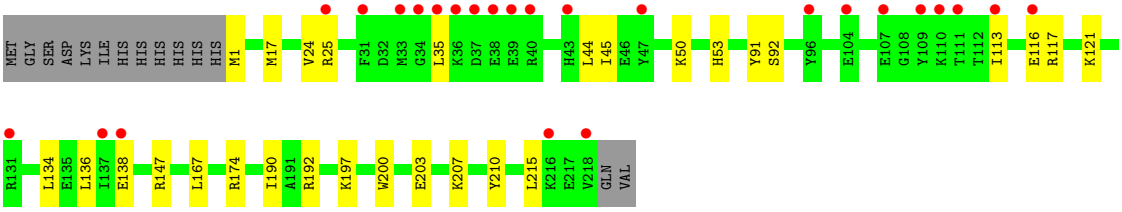
• Molecule 1: Thymidylate synthase thyX

Chain C:



• Molecule 1: Thymidylate synthase thyX

Chain D:


MET
GLY
SER
ASP
LYS
ILE
HIS
HIS
HIS
HIS
HIS
HIS
M1
M17
V24
R25
F31
D32
M33
G34
L35
K36
D37
E38
E39
R40
H43
L44
I45
E46
Y47
K50
H53
Y91
S92
Y96
E104
E107
G108
Y109
K110
T111
T112
I113
E116
R117
K121

R131
L134
E135
L136
I137
E138
R147
L167
R174
I190
A191
R192
K197
W200
E203
K207
Y210
L215
K216
E217
V218
GLN
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.56Å 117.73Å 141.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 50.25 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-1.60) 98.8 (50.25-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.218 0.197 , 0.213	Depositor DCC
R_{free} test set	6155 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 61.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7940	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.38	0/1881	0.61	0/2542
1	B	0.36	0/1901	0.60	0/2569
1	C	0.38	0/1873	0.62	0/2532
1	D	0.38	0/1873	0.61	0/2532
All	All	0.38	0/7528	0.61	0/10175

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	1831	0	1821	33	0
1	B	1851	0	1846	31	0
1	C	1824	0	1822	30	0
1	D	1824	0	1822	23	0
2	A	20	0	11	1	0
2	B	20	0	11	1	0
2	C	20	0	11	1	0
2	D	20	0	11	1	0
3	A	53	0	30	0	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	10	0	14	1	0
4	B	20	0	28	2	0
4	D	20	0	28	1	0
5	A	68	0	0	1	0
5	B	52	0	0	1	0
5	C	82	0	0	0	0
5	D	66	0	0	1	0
All	All	7940	0	7545	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (107) 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:132:THR:HG21	1:C:125:ILE:HD11	1.42	1.01
2:A:603:UMP:HN3	1:D:174:ARG:HH12	1.10	0.99
1:B:174:ARG:HH12	2:C:613:UMP:HN3	1.16	0.93
2:B:608:UMP:HN3	1:C:174:ARG:HH12	1.14	0.93
1:A:174:ARG:HH12	2:D:618:UMP:HN3	1.14	0.91
1:B:132:THR:CG2	1:C:125:ILE:HD11	2.07	0.85
1:C:17:MET:HB2	1:D:17:MET:HB2	1.64	0.79
1:B:53:HIS:HA	4:B:630:PGE:H3	1.66	0.78
1:A:17:MET:HB2	1:B:17:MET:HB2	1.65	0.77
1:B:111:THR:HG22	1:B:113:ILE:H	1.54	0.72
1:D:117:ARG:HG3	1:D:121:LYS:HE2	1.71	0.72
1:C:25:ARG:HG2	1:C:35:LEU:HD21	1.71	0.72
1:B:132:THR:CB	1:C:125:ILE:HD11	2.21	0.70
1:D:203:GLU:HG2	1:D:207:LYS:HE2	1.76	0.67
1:D:167:LEU:HD11	1:D:190:ILE:HG21	1.80	0.62
1:B:132:THR:HG21	1:C:125:ILE:CD1	2.25	0.62
1:C:25:ARG:HG3	1:C:35:LEU:HD11	1.81	0.62
1:A:116:GLU:H	1:A:116:GLU:CD	2.04	0.60
1:C:167:LEU:HD11	1:C:190:ILE:HG21	1.82	0.60
1:C:117:ARG:HH11	1:C:117:ARG:HG3	1.67	0.59
1:B:167:LEU:HD11	1:B:190:ILE:HG21	1.84	0.59
1:B:47:TYR:HA	1:B:50:LYS:HE2	1.84	0.59
1:A:50:LYS:HE3	1:A:208:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ILE:HD13	1:D:121:LYS:HE3	1.86	0.57
1:A:192:ARG:HG2	1:A:192:ARG:HH11	1.71	0.56
1:A:210:TYR:CE2	1:A:215:LEU:HB2	2.40	0.56
1:D:192:ARG:HH11	1:D:192:ARG:HG3	1.69	0.56
1:C:31:PHE:HA	1:D:92:SER:OG	2.06	0.56
1:A:127:ASP:O	1:A:131:ARG:HG3	2.06	0.55
1:A:45:ILE:HD12	1:A:200:TRP:HE3	1.72	0.55
1:A:175:ALA:HA	1:A:214:ILE:HD11	1.89	0.55
1:B:175:ALA:HA	1:B:214:ILE:HD11	1.89	0.55
1:C:104:GLU:HG2	1:C:104:GLU:O	2.06	0.54
1:D:167:LEU:HD11	1:D:190:ILE:CG2	2.37	0.54
1:B:25:ARG:HH11	1:B:25:ARG:HG3	1.73	0.53
1:B:131:ARG:O	1:B:135:GLU:HG3	2.07	0.53
1:A:31:PHE:HA	1:B:92:SER:OG	2.08	0.53
1:B:113:ILE:HB	1:B:117:ARG:HD3	1.91	0.53
1:C:167:LEU:HD11	1:C:190:ILE:CG2	2.38	0.53
1:D:203:GLU:CG	1:D:207:LYS:HE2	2.39	0.53
1:B:106:LEU:HD12	1:B:106:LEU:N	2.24	0.52
1:C:202:PHE:CE2	1:C:206:LEU:HD11	2.44	0.52
4:A:635:PGE:H22	3:C:605:FAD:H2'	1.92	0.52
1:B:167:LEU:HD11	1:B:190:ILE:CG2	2.40	0.52
1:A:114:PRO:HD2	1:A:117:ARG:HG3	1.92	0.52
1:D:50:LYS:HE3	5:D:314:HOH:O	2.10	0.51
1:C:35:LEU:N	1:C:35:LEU:HD22	2.25	0.51
1:B:46:GLU:O	1:B:50:LYS:HG2	2.10	0.51
1:D:134:LEU:O	1:D:138:GLU:HG3	2.11	0.51
1:C:137:ILE:HD11	1:C:143:ARG:HA	1.92	0.51
1:B:121:LYS:HD2	1:C:136:LEU:HD21	1.94	0.50
1:A:163:ASN:C	1:A:163:ASN:HD22	2.15	0.50
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.94	0.49
1:B:20:ASP:HB3	1:B:45:ILE:HD11	1.93	0.49
1:D:24:VAL:HG13	1:D:44:LEU:HD23	1.95	0.49
1:C:24:VAL:HG13	1:C:44:LEU:HD23	1.94	0.49
1:D:117:ARG:O	1:D:121:LYS:HG3	2.12	0.49
1:A:26:ALA:O	1:A:29:VAL:HG12	2.13	0.49
1:A:106:LEU:HD12	1:A:106:LEU:N	2.28	0.48
1:D:210:TYR:CE2	1:D:215:LEU:HB2	2.48	0.48
1:C:212:GLY:O	1:C:216:LYS:NZ	2.47	0.48
1:C:213:ASP:HA	1:C:216:LYS:NZ	2.28	0.48
1:C:134:LEU:O	1:C:138:GLU:HG3	2.14	0.48
1:A:199:PRO:O	1:A:203:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:HIS:O	1:A:0:HIS:ND1	2.46	0.47
1:D:116:GLU:H	1:D:116:GLU:CD	2.17	0.47
1:C:116:GLU:CD	1:C:116:GLU:H	2.16	0.47
1:B:195:LYS:HD3	1:B:220:VAL:HG12	1.97	0.47
1:A:46:GLU:HB3	1:A:50:LYS:NZ	2.31	0.46
1:B:20:ASP:HB3	1:B:45:ILE:CD1	2.44	0.46
1:A:114:PRO:HB3	1:A:116:GLU:OE1	2.16	0.46
1:A:44:LEU:O	1:A:48:LEU:HG	2.16	0.45
1:D:45:ILE:HD12	1:D:200:TRP:HE3	1.80	0.45
1:B:220:VAL:OXT	1:B:220:VAL:HG23	2.17	0.45
1:D:25:ARG:HG3	1:D:35:LEU:HD21	1.99	0.45
1:A:167:LEU:C	1:A:167:LEU:HD23	2.37	0.45
1:B:19:ASN:HB2	5:B:492:HOH:O	2.18	0.44
1:A:122:ILE:O	1:A:125:ILE:HG22	2.18	0.44
1:A:19:ASN:HB2	5:A:433:HOH:O	2.17	0.43
1:C:25:ARG:HG2	1:C:35:LEU:CD2	2.44	0.43
1:B:45:ILE:HD12	1:B:200:TRP:HE3	1.84	0.43
1:D:1:MET:HE2	1:D:197:LYS:HE2	2.01	0.43
1:C:36:LYS:HD3	1:C:40:ARG:HH11	1.84	0.43
1:A:74:ARG:HG2	4:D:620:PGE:H2	2.01	0.43
1:C:31:PHE:CE2	1:D:91:TYR:HB3	2.53	0.43
1:C:175:ALA:HA	1:C:214:ILE:HD11	2.01	0.43
1:B:39:GLU:HG3	1:B:40:ARG:N	2.33	0.43
1:B:54:GLU:H	4:B:630:PGE:H22	1.84	0.42
1:B:130:TYR:CE2	1:B:134:LEU:HD11	2.54	0.42
1:A:114:PRO:O	1:A:117:ARG:HB2	2.20	0.42
1:B:117:ARG:HH11	1:B:117:ARG:HG3	1.83	0.42
1:C:117:ARG:HG3	1:C:117:ARG:NH1	2.34	0.42
1:C:26:ALA:O	1:C:29:VAL:HG12	2.19	0.42
1:A:50:LYS:HE3	1:A:208:TYR:CZ	2.55	0.42
1:A:5:ILE:HG22	1:A:6:LEU:HG	2.02	0.42
1:B:219:GLN:O	1:B:220:VAL:OXT	2.37	0.42
1:C:25:ARG:CG	1:C:35:LEU:HD21	2.47	0.42
1:D:1:MET:CE	1:D:197:LYS:HE2	2.50	0.41
1:A:163:ASN:ND2	1:A:166:SER:H	2.18	0.41
1:A:210:TYR:CZ	1:A:215:LEU:HB2	2.55	0.41
1:A:114:PRO:HA	1:A:115:PRO:HD3	1.96	0.41
1:A:118:VAL:HG13	1:D:136:LEU:HD22	2.02	0.41
1:A:192:ARG:HH11	1:A:192:ARG:CG	2.32	0.41
1:D:113:ILE:CG2	1:D:117:ARG:HB3	2.51	0.40
1:A:50:LYS:HG2	1:A:208:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ILE:HD12	1:B:117:ARG:HD3	2.03	0.40
1:C:210:TYR:CE2	1:C:215:LEU:HB2	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	217/232 (94%)	212 (98%)	4 (2%)	1 (0%)	29	11
1	B	219/232 (94%)	215 (98%)	4 (2%)	0	100	100
1	C	216/232 (93%)	213 (99%)	3 (1%)	0	100	100
1	D	216/232 (93%)	212 (98%)	4 (2%)	0	100	100
All	All	868/928 (94%)	852 (98%)	15 (2%)	1 (0%)	51	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	GLU

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	194/207 (94%)	190 (98%)	4 (2%)	53	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	197/207 (95%)	194 (98%)	3 (2%)	65	44
1	C	194/207 (94%)	193 (100%)	1 (0%)	88	80
1	D	194/207 (94%)	192 (99%)	2 (1%)	76	61
All	All	779/828 (94%)	769 (99%)	10 (1%)	69	50

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	44	LEU
1	A	147	ARG
1	A	163	ASN
1	B	147	ARG
1	B	192	ARG
1	B	211	LYS
1	C	147	ARG
1	D	53	HIS
1	D	147	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
4	PGE	A	635	-	9,9,9	0.76	0	8,8,8	0.68	0
4	PGE	B	625	-	9,9,9	0.47	0	8,8,8	1.00	0
2	UMP	B	608	-	21,21,21	1.71	6 (28%)	31,31,31	1.98	4 (12%)
2	UMP	A	603	-	21,21,21	1.83	8 (38%)	31,31,31	2.07	5 (16%)
4	PGE	B	630	-	9,9,9	0.72	0	8,8,8	0.79	0
3	FAD	B	610	-	53,58,58	2.65	21 (39%)	68,89,89	1.80	13 (19%)
4	PGE	D	620	-	9,9,9	0.61	0	8,8,8	0.88	0
3	FAD	A	615	-	53,58,58	2.57	21 (39%)	68,89,89	1.77	13 (19%)
3	FAD	C	605	-	53,58,58	2.53	21 (39%)	68,89,89	1.75	11 (16%)
3	FAD	D	600	-	53,58,58	2.62	23 (43%)	68,89,89	1.79	14 (20%)
2	UMP	C	613	-	21,21,21	1.72	7 (33%)	31,31,31	2.01	4 (12%)
4	PGE	D	640	-	9,9,9	0.74	0	8,8,8	0.79	0
2	UMP	D	618	-	21,21,21	1.68	5 (23%)	31,31,31	2.00	6 (19%)

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
4	PGE	A	635	-	-	2/7/7/7	-
2	UMP	C	613	-	-	0/10/22/22	0/2/2/2
4	PGE	B	625	-	-	2/7/7/7	-
2	UMP	A	603	-	-	0/10/22/22	0/2/2/2
2	UMP	B	608	-	-	0/10/22/22	0/2/2/2
4	PGE	B	630	-	-	4/7/7/7	-
4	PGE	D	620	-	-	4/7/7/7	-
2	UMP	D	618	-	-	0/10/22/22	0/2/2/2
3	FAD	A	615	-	1/1/9/9	2/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	D	600	-	1/1/9/9	2/30/50/50	0/6/6/6
3	FAD	B	610	-	1/1/9/9	3/30/50/50	0/6/6/6
4	PGE	D	640	-	-	3/7/7/7	-
3	FAD	C	605	-	1/1/9/9	2/30/50/50	0/6/6/6

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	605	FAD	C9A-C5X	6.31	1.51	1.41
3	B	610	FAD	C4A-N3A	6.19	1.44	1.35
3	D	600	FAD	C9A-C5X	6.19	1.51	1.41
3	B	610	FAD	C9A-C5X	6.17	1.51	1.41
3	C	605	FAD	C4A-N3A	6.12	1.44	1.35
3	A	615	FAD	C9A-C5X	6.02	1.51	1.41
3	D	600	FAD	C4A-N3A	5.87	1.43	1.35
3	B	610	FAD	C6-C7	5.76	1.48	1.39
3	A	615	FAD	C4A-N3A	5.56	1.43	1.35
3	D	600	FAD	C8A-N7A	-5.49	1.24	1.34
3	B	610	FAD	C4X-N5	5.42	1.41	1.30
3	B	610	FAD	C8A-N7A	-5.35	1.25	1.34
3	D	600	FAD	C6-C7	5.34	1.47	1.39
3	A	615	FAD	C8A-N7A	-5.31	1.25	1.34
3	D	600	FAD	C4X-N5	5.28	1.41	1.30
3	C	605	FAD	C4X-N5	5.22	1.40	1.30
3	A	615	FAD	C4X-N5	5.03	1.40	1.30
3	A	615	FAD	C6-C7	4.86	1.46	1.39
3	D	600	FAD	C9-C9A	4.84	1.47	1.39
3	D	600	FAD	C2B-C1B	4.80	1.61	1.53
3	C	605	FAD	C6-C7	4.79	1.46	1.39
3	C	605	FAD	C2B-C1B	4.78	1.61	1.53
3	A	615	FAD	C9-C9A	4.73	1.47	1.39
3	C	605	FAD	C8A-N7A	-4.61	1.26	1.34
3	B	610	FAD	C2B-C1B	4.54	1.60	1.53
3	A	615	FAD	C2B-C1B	4.51	1.60	1.53
3	B	610	FAD	C9-C9A	4.43	1.46	1.39
2	A	603	UMP	C2-N1	4.24	1.45	1.38
3	C	605	FAD	C6-C5X	4.24	1.46	1.40
3	D	600	FAD	C6-C5X	4.21	1.46	1.40
3	B	610	FAD	C6-C5X	4.21	1.46	1.40
3	A	615	FAD	C8-C7	4.15	1.51	1.40
3	C	605	FAD	C8-C7	4.09	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	600	FAD	C8-C7	4.09	1.51	1.40
3	A	615	FAD	C6-C5X	3.96	1.46	1.40
3	B	610	FAD	C2A-N3A	3.92	1.38	1.32
3	B	610	FAD	C10-N1	3.88	1.41	1.33
3	B	610	FAD	C8-C7	3.87	1.50	1.40
3	C	605	FAD	C9-C9A	3.83	1.45	1.39
3	D	600	FAD	C2A-N3A	3.81	1.38	1.32
3	D	600	FAD	C10-N1	3.76	1.40	1.33
2	C	613	UMP	C2-N1	3.63	1.44	1.38
3	A	615	FAD	C2A-N3A	3.59	1.37	1.32
3	C	605	FAD	C10-N1	3.54	1.40	1.33
3	A	615	FAD	C10-N1	3.41	1.40	1.33
3	B	610	FAD	C2A-N1A	3.41	1.40	1.33
3	C	605	FAD	C2A-N3A	3.41	1.37	1.32
3	A	615	FAD	O4B-C1B	3.36	1.45	1.41
3	A	615	FAD	C9-C8	3.35	1.44	1.39
2	A	603	UMP	O4'-C1'	3.21	1.49	1.42
2	B	608	UMP	C2-N1	3.15	1.43	1.38
3	D	600	FAD	C9-C8	3.14	1.44	1.39
3	A	615	FAD	C2A-N1A	3.05	1.39	1.33
2	D	618	UMP	C2-N1	3.03	1.43	1.38
3	D	600	FAD	C2A-N1A	3.02	1.39	1.33
2	D	618	UMP	C2'-C3'	3.01	1.60	1.52
2	B	608	UMP	C2'-C3'	3.00	1.60	1.52
2	A	603	UMP	C2'-C3'	2.98	1.60	1.52
3	C	605	FAD	C9-C8	2.97	1.43	1.39
3	B	610	FAD	C9-C8	2.93	1.43	1.39
3	C	605	FAD	O4B-C1B	2.85	1.45	1.41
3	D	600	FAD	O4B-C1B	2.81	1.45	1.41
3	B	610	FAD	O4B-C1B	2.78	1.45	1.41
2	B	608	UMP	C6-N1	2.75	1.44	1.38
2	C	613	UMP	C2'-C3'	2.74	1.60	1.52
2	D	618	UMP	C4-N3	2.74	1.43	1.38
3	A	615	FAD	C4-N3	2.74	1.43	1.38
3	B	610	FAD	C4-N3	2.72	1.43	1.38
3	B	610	FAD	C10-N10	2.71	1.43	1.37
3	C	605	FAD	C2A-N1A	2.68	1.38	1.33
3	C	605	FAD	C10-N10	2.67	1.43	1.37
3	A	615	FAD	C10-N10	2.64	1.43	1.37
2	C	613	UMP	C6-N1	2.62	1.44	1.38
2	A	603	UMP	C6-N1	2.61	1.44	1.38
2	C	613	UMP	O4'-C1'	2.59	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	608	UMP	C4-N3	2.58	1.43	1.38
2	C	613	UMP	C4-N3	2.51	1.43	1.38
2	D	618	UMP	C6-N1	2.50	1.44	1.38
3	D	600	FAD	C10-N10	2.46	1.42	1.37
3	B	610	FAD	PA-O5B	-2.41	1.49	1.59
2	A	603	UMP	C4-N3	2.41	1.42	1.38
3	D	600	FAD	C4-N3	2.36	1.43	1.38
2	D	618	UMP	O4'-C1'	2.35	1.47	1.42
3	A	615	FAD	C2-N3	2.33	1.44	1.39
3	C	605	FAD	C4-N3	2.31	1.43	1.38
2	A	603	UMP	P-OP2	-2.30	1.46	1.54
2	C	613	UMP	C2-N3	2.29	1.42	1.38
3	A	615	FAD	PA-O5B	-2.28	1.50	1.59
3	C	605	FAD	P-O5'	-2.27	1.50	1.59
3	B	610	FAD	P-O5'	-2.27	1.50	1.59
3	B	610	FAD	O5B-C5B	2.26	1.53	1.44
2	B	608	UMP	C2-N3	2.26	1.42	1.38
3	A	615	FAD	P-O5'	-2.26	1.50	1.59
3	B	610	FAD	C5A-C4A	2.24	1.46	1.40
2	B	608	UMP	P-OP3	-2.22	1.46	1.54
3	D	600	FAD	C5A-C4A	2.21	1.46	1.40
3	C	605	FAD	C5A-C4A	2.20	1.46	1.40
3	C	605	FAD	PA-O5B	-2.20	1.50	1.59
3	C	605	FAD	O5B-C5B	2.15	1.53	1.44
3	D	600	FAD	O5B-C5B	2.14	1.53	1.44
2	A	603	UMP	P-OP3	-2.14	1.46	1.54
3	D	600	FAD	C2-N3	2.10	1.43	1.39
3	D	600	FAD	PA-O5B	-2.09	1.50	1.59
3	B	610	FAD	C2-N3	2.09	1.43	1.39
3	A	615	FAD	C5B-C4B	2.08	1.58	1.51
3	C	605	FAD	C4'-C3'	2.06	1.57	1.53
2	C	613	UMP	P-OP3	-2.06	1.46	1.54
3	D	600	FAD	P-O5'	-2.03	1.51	1.59
3	D	600	FAD	C5B-C4B	2.03	1.57	1.51
3	D	600	FAD	C2'-C3'	2.03	1.57	1.53
3	A	615	FAD	C5A-C4A	2.02	1.46	1.40
2	A	603	UMP	C2-N3	2.01	1.41	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	610	FAD	C3B-C2B-C1B	-8.45	88.25	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	600	FAD	C3B-C2B-C1B	-8.43	88.28	100.98
2	C	613	UMP	C2'-C1'-N1	-8.20	94.89	113.77
3	A	615	FAD	C3B-C2B-C1B	-8.14	88.72	100.98
2	A	603	UMP	C2'-C1'-N1	-8.14	95.03	113.77
3	C	605	FAD	C3B-C2B-C1B	-7.95	89.02	100.98
2	B	608	UMP	C2'-C1'-N1	-7.89	95.60	113.77
2	D	618	UMP	C2'-C1'-N1	-7.71	96.02	113.77
2	A	603	UMP	O4'-C1'-N1	5.31	117.35	107.86
3	B	610	FAD	O2B-C2B-C1B	4.89	128.90	110.85
2	B	608	UMP	O4'-C1'-N1	4.86	116.55	107.86
3	C	605	FAD	O2B-C2B-C1B	4.78	128.50	110.85
2	C	613	UMP	O4'-C1'-N1	4.76	116.38	107.86
3	D	600	FAD	O2B-C2B-C1B	4.76	128.42	110.85
2	D	618	UMP	O4'-C1'-N1	4.73	116.32	107.86
3	A	615	FAD	O2B-C2B-C1B	4.68	128.15	110.85
3	B	610	FAD	N3A-C2A-N1A	-3.40	123.36	128.68
3	A	615	FAD	N3A-C2A-N1A	-3.32	123.48	128.68
3	D	600	FAD	N3A-C2A-N1A	-3.28	123.56	128.68
2	D	618	UMP	C4'-O4'-C1'	3.26	117.34	109.45
3	C	605	FAD	N3A-C2A-N1A	-3.25	123.60	128.68
2	A	603	UMP	C4'-O4'-C1'	3.11	116.96	109.45
2	B	608	UMP	C4'-O4'-C1'	3.10	116.94	109.45
3	B	610	FAD	C4A-C5A-N7A	-3.03	106.24	109.40
3	A	615	FAD	C4A-C5A-N7A	-3.03	106.24	109.40
3	D	600	FAD	C4-C4X-N5	2.99	122.48	118.23
3	B	610	FAD	C4-C4X-N5	2.89	122.34	118.23
3	C	605	FAD	C4A-C5A-N7A	-2.88	106.39	109.40
2	C	613	UMP	C4'-O4'-C1'	2.87	116.40	109.45
3	D	600	FAD	C4A-C5A-N7A	-2.87	106.41	109.40
3	A	615	FAD	O3B-C3B-C4B	2.78	119.09	111.05
3	C	605	FAD	O3B-C3B-C4B	2.78	119.07	111.05
3	D	600	FAD	O3B-C3B-C4B	2.68	118.79	111.05
3	C	605	FAD	O4B-C4B-C3B	2.66	110.38	105.11
3	B	610	FAD	O3B-C3B-C4B	2.65	118.70	111.05
3	B	610	FAD	C5B-C4B-C3B	-2.64	105.29	115.18
3	C	605	FAD	C5B-C4B-C3B	-2.63	105.32	115.18
3	A	615	FAD	C4-C4X-N5	2.59	121.92	118.23
3	D	600	FAD	C5B-C4B-C3B	-2.59	105.48	115.18
3	C	605	FAD	C2A-N1A-C6A	2.58	123.17	118.75
3	C	605	FAD	P-O5'-C5'	2.57	136.75	121.68
3	A	615	FAD	P-O5'-C5'	2.57	136.73	121.68
3	A	615	FAD	O4B-C4B-C3B	2.56	110.19	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	615	FAD	C2A-N1A-C6A	2.53	123.08	118.75
3	A	615	FAD	C5B-C4B-C3B	-2.53	105.72	115.18
3	B	610	FAD	O4B-C4B-C3B	2.52	110.10	105.11
3	D	600	FAD	O4B-C4B-C3B	2.50	110.07	105.11
3	B	610	FAD	P-O5'-C5'	2.47	136.14	121.68
3	C	605	FAD	C4-C4X-N5	2.46	121.74	118.23
2	D	618	UMP	O4'-C4'-C3'	-2.46	99.93	105.67
3	D	600	FAD	P-O5'-C5'	2.42	135.89	121.68
3	B	610	FAD	C2A-N1A-C6A	2.33	122.73	118.75
3	D	600	FAD	C2A-N1A-C6A	2.32	122.72	118.75
3	A	615	FAD	C9-C9A-N10	2.32	124.97	121.84
3	D	600	FAD	C10-N1-C2	2.28	121.45	116.90
2	A	603	UMP	O4'-C4'-C3'	-2.24	100.45	105.67
2	B	608	UMP	O4'-C4'-C3'	-2.20	100.53	105.67
3	C	605	FAD	C10-N1-C2	2.16	121.22	116.90
3	B	610	FAD	C10-N1-C2	2.16	121.21	116.90
3	A	615	FAD	C10-N1-C2	2.15	121.20	116.90
3	D	600	FAD	P-O3P-PA	2.14	140.17	132.83
3	D	600	FAD	C9-C9A-N10	2.13	124.72	121.84
2	C	613	UMP	O4'-C4'-C3'	-2.13	100.71	105.67
2	D	618	UMP	C5-C6-N1	2.12	125.36	121.81
3	B	610	FAD	C9-C9A-N10	2.12	124.71	121.84
3	B	610	FAD	C10-C4X-N5	-2.12	120.36	124.86
3	D	600	FAD	C10-C4X-N5	-2.11	120.37	124.86
3	A	615	FAD	C10-C4X-N5	-2.04	120.53	124.86
2	D	618	UMP	O4'-C1'-C2'	-2.04	102.40	106.25
2	A	603	UMP	C6-N1-C2	-2.01	118.43	120.99

All (4) chirality outliers are listed below:

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

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	625	PGE	O1-C1-C2-O2
4	B	625	PGE	O3-C5-C6-O4
4	D	620	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
4	B	630	PGE	O3-C5-C6-O4
4	D	620	PGE	O1-C1-C2-O2
4	D	620	PGE	O2-C3-C4-O3
4	D	640	PGE	C4-C3-O2-C2
4	D	640	PGE	C6-C5-O3-C4
3	B	610	FAD	PA-O3P-P-O1P
3	D	600	FAD	PA-O3P-P-O1P
4	D	620	PGE	C4-C3-O2-C2
3	A	615	FAD	PA-O3P-P-O1P
3	C	605	FAD	PA-O3P-P-O1P
4	B	630	PGE	C1-C2-O2-C3
4	B	630	PGE	C4-C3-O2-C2
3	D	600	FAD	O4'-C4'-C5'-O5'
4	A	635	PGE	O2-C3-C4-O3
4	A	635	PGE	C6-C5-O3-C4
3	B	610	FAD	PA-O3P-P-O2P
3	C	605	FAD	PA-O3P-P-O2P
4	D	640	PGE	O2-C3-C4-O3
4	B	630	PGE	O2-C3-C4-O3
3	A	615	FAD	O4'-C4'-C5'-O5'
3	B	610	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

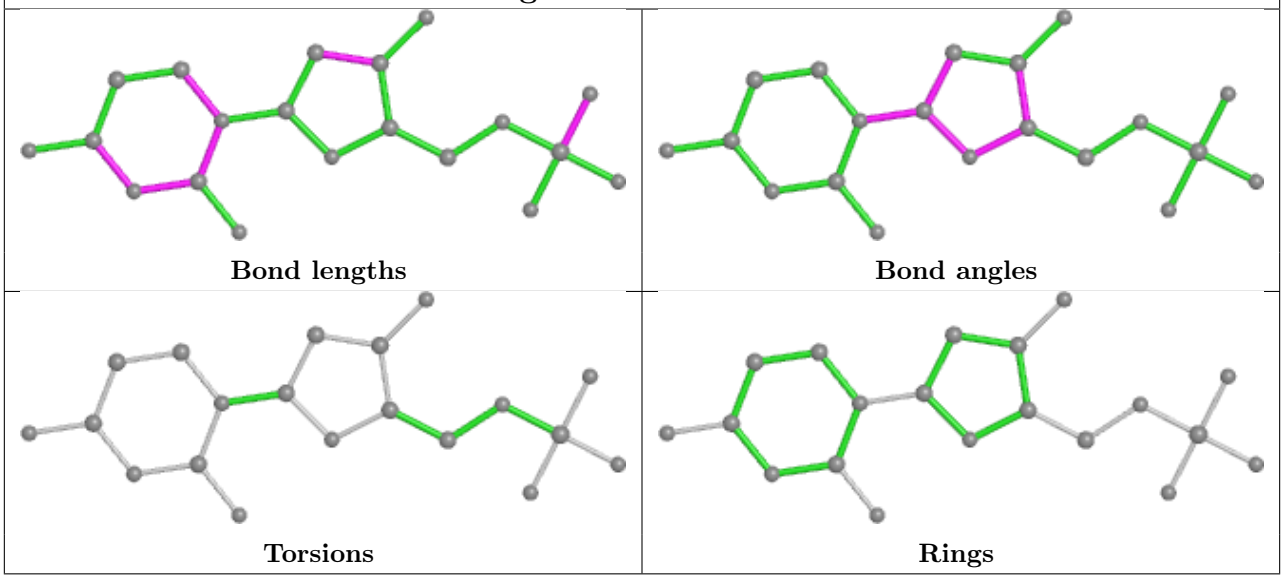
8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	635	PGE	1	0
2	B	608	UMP	1	0
2	A	603	UMP	1	0
4	B	630	PGE	2	0
4	D	620	PGE	1	0
3	C	605	FAD	1	0
2	C	613	UMP	1	0
2	D	618	UMP	1	0

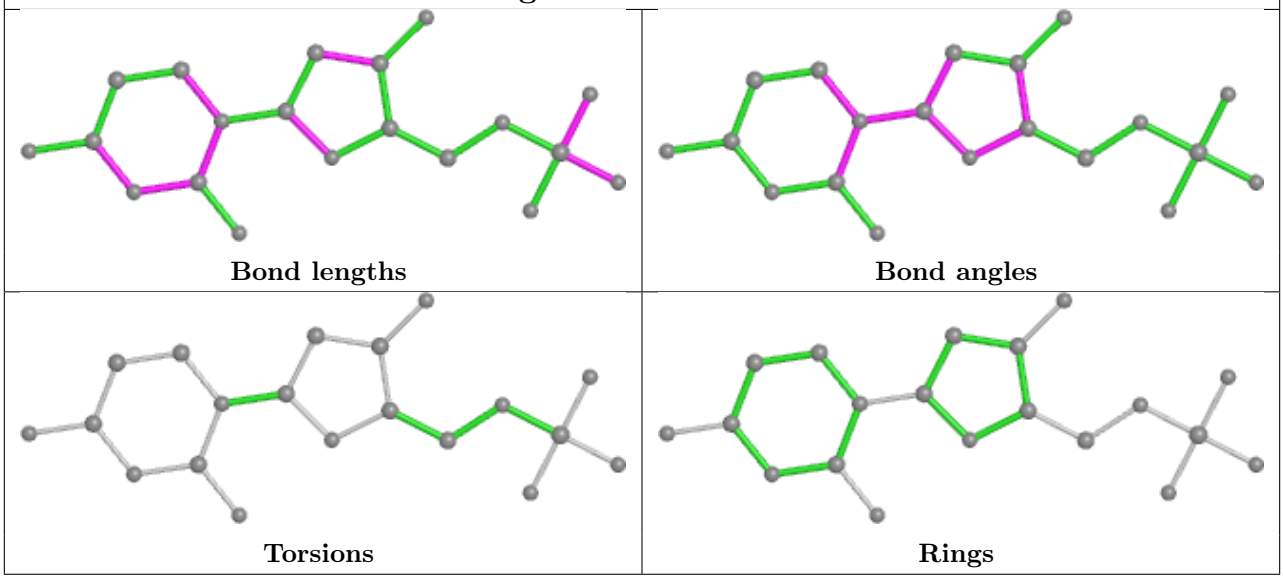
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

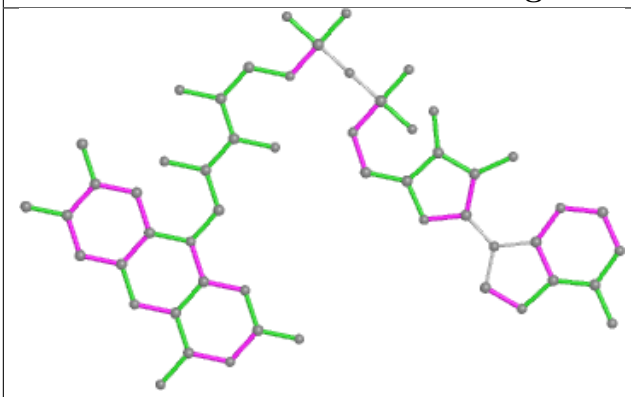
Ligand UMP B 608



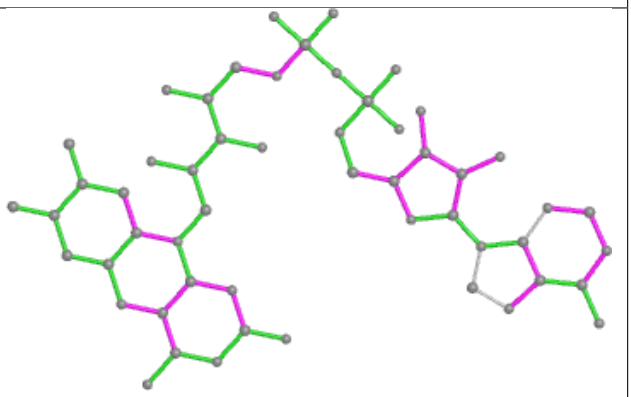
Ligand UMP A 603



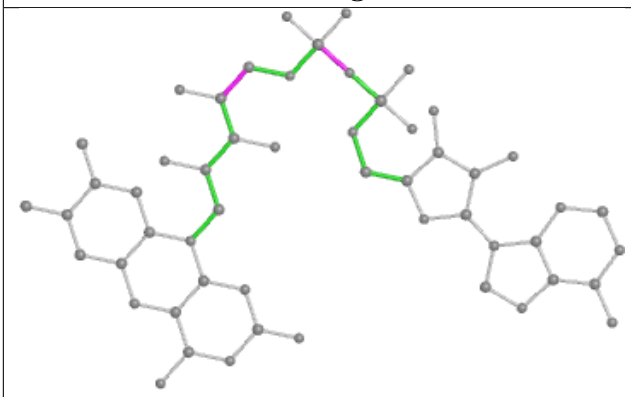
Ligand FAD B 610



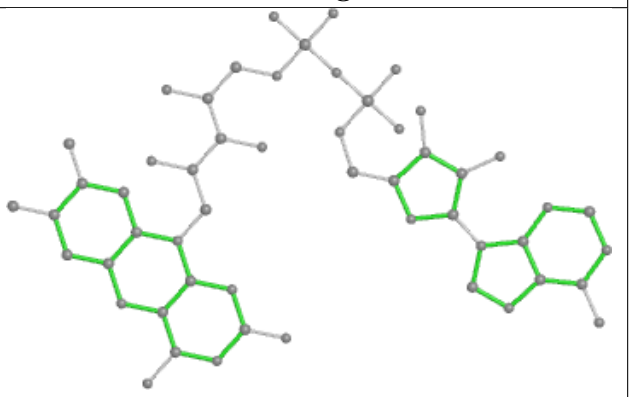
Bond lengths



Bond angles

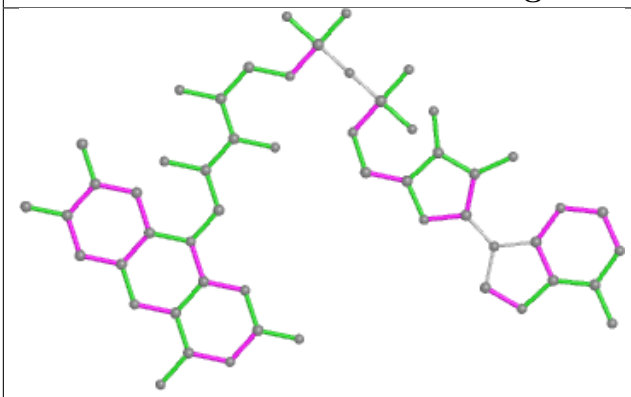


Torsions

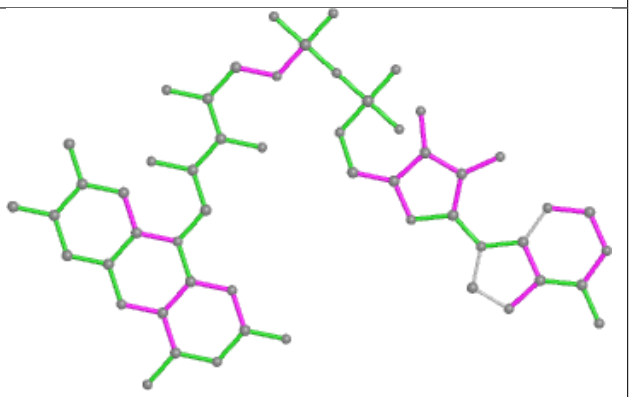


Rings

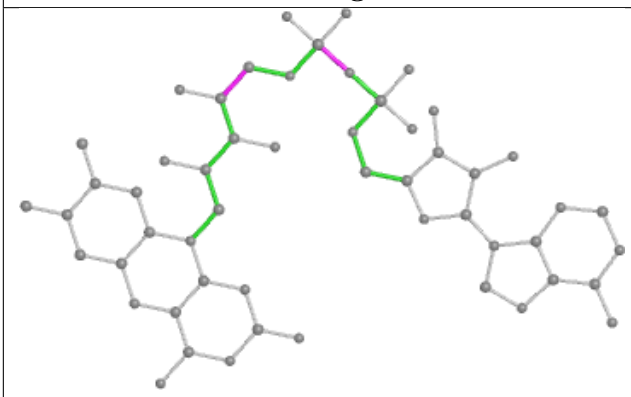
Ligand FAD A 615



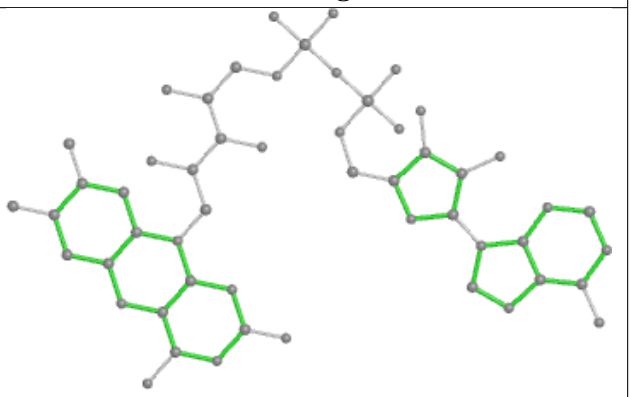
Bond lengths



Bond angles

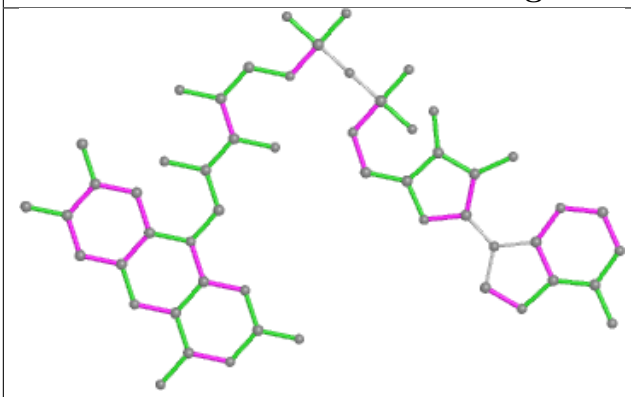


Torsions

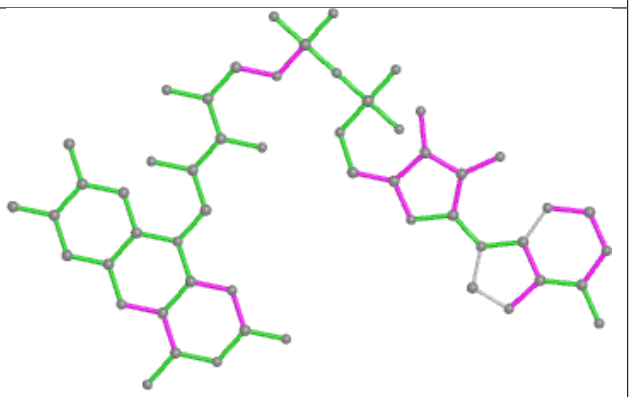


Rings

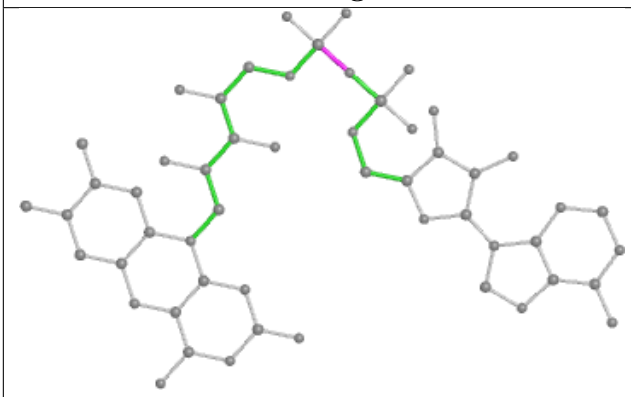
Ligand FAD C 605



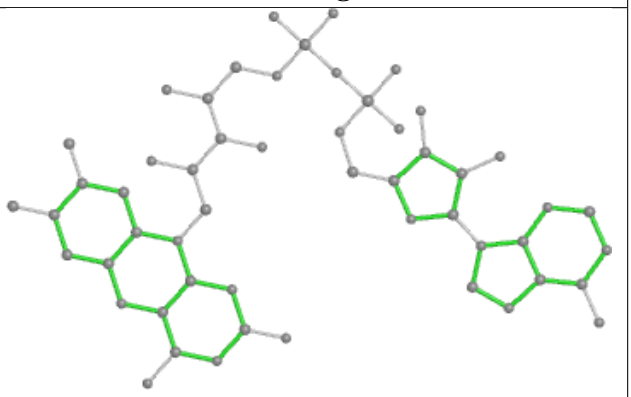
Bond lengths



Bond angles

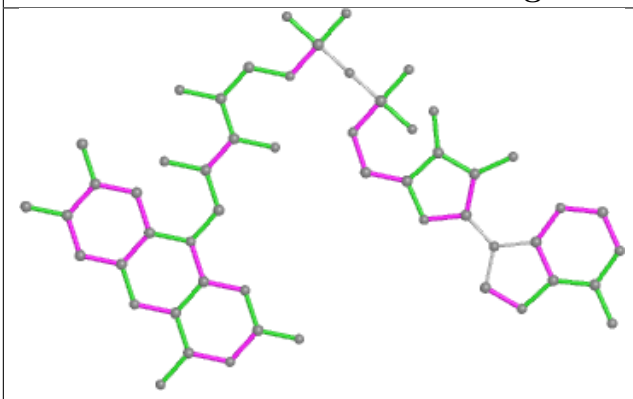


Torsions

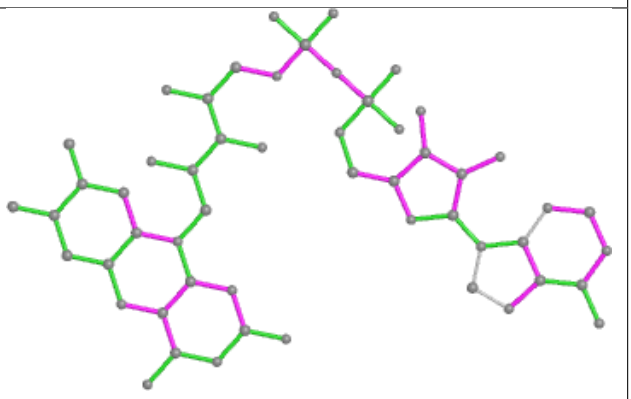


Rings

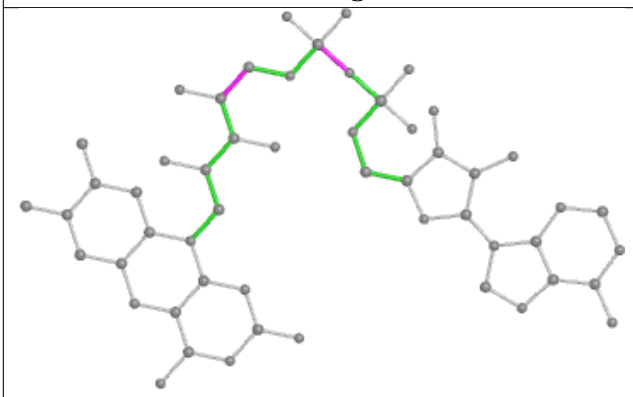
Ligand FAD D 600



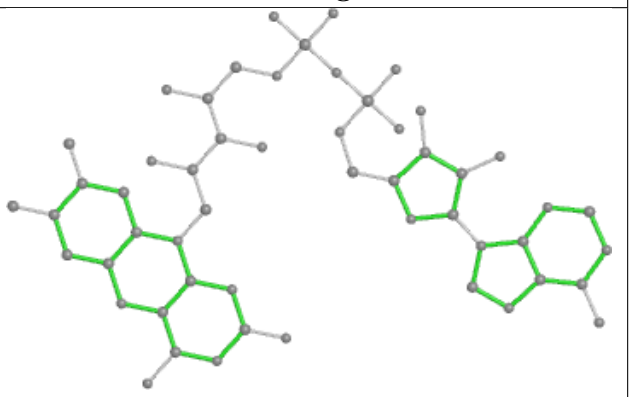
Bond lengths



Bond angles

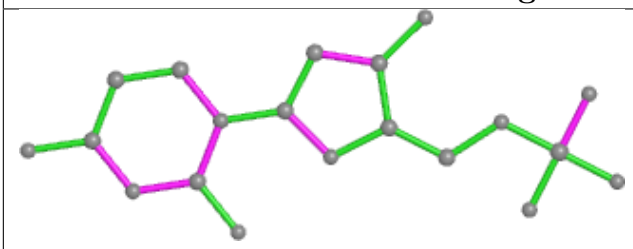


Torsions

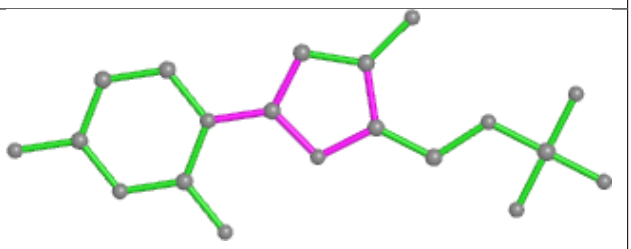


Rings

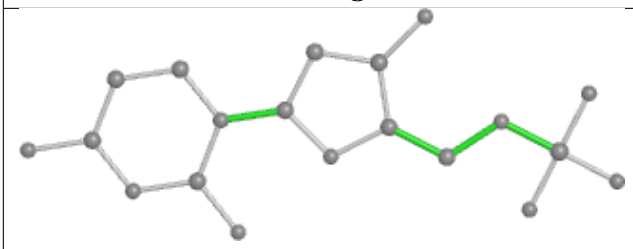
Ligand UMP C 613



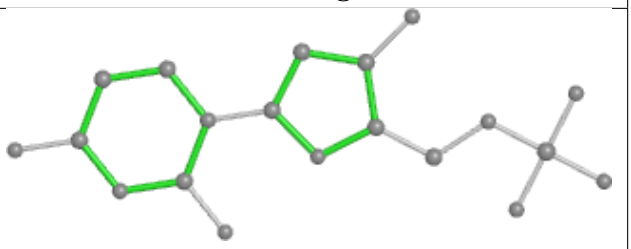
Bond lengths



Bond angles

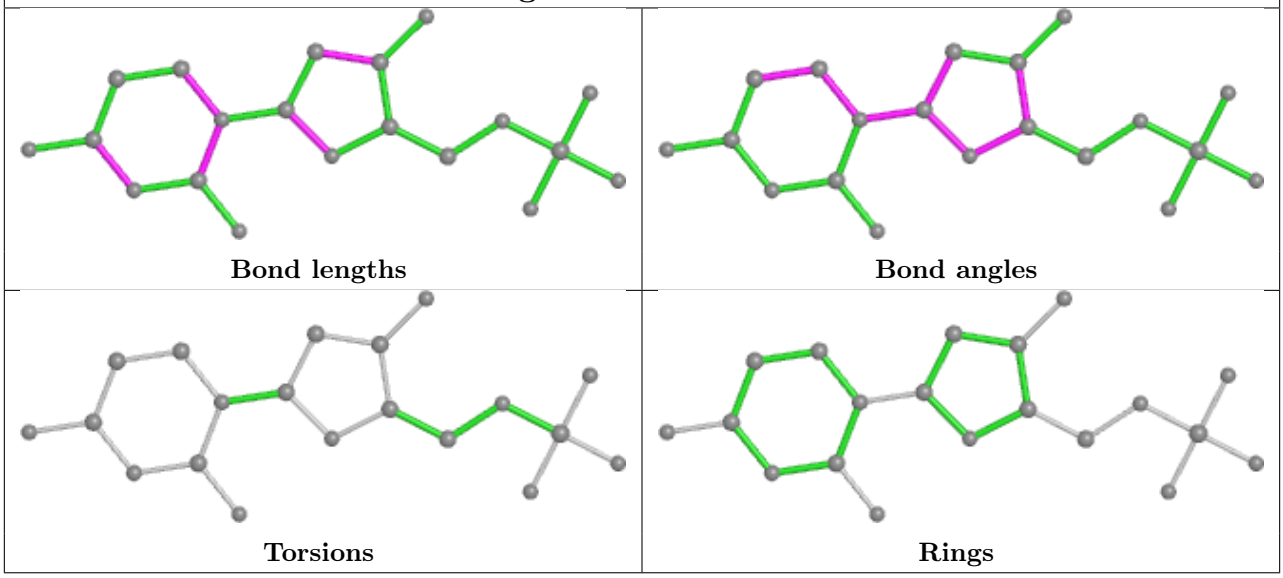


Torsions



Rings

Ligand UMP D 618



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	219/232 (94%)	0.62	23 (10%)	6	5	15, 29, 57, 64	0
1	B	221/232 (95%)	0.57	27 (12%)	4	3	17, 31, 57, 62	0
1	C	218/232 (93%)	0.53	21 (9%)	8	7	16, 28, 51, 58	0
1	D	218/232 (93%)	0.56	25 (11%)	4	4	16, 31, 56, 60	0
All	All	876/928 (94%)	0.57	96 (10%)	5	4	15, 30, 56, 64	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	VAL	10.0
1	D	35	LEU	6.2
1	D	40	ARG	5.8
1	B	219	GLN	5.3
1	D	37	ASP	5.3
1	A	113	ILE	5.2
1	A	112	THR	5.1
1	D	36	LYS	4.7
1	B	35	LEU	4.5
1	A	110	LYS	4.2
1	B	34	GLY	4.0
1	D	138	GLU	3.9
1	B	37	ASP	3.9
1	C	137	ILE	3.8
1	B	107	GLU	3.8
1	C	35	LEU	3.8
1	D	111	THR	3.7
1	C	96	TYR	3.7
1	A	117	ARG	3.7
1	B	38	GLU	3.6
1	C	39	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	104	GLU	3.6
1	A	107	GLU	3.6
1	D	107	GLU	3.6
1	D	110	LYS	3.5
1	B	47	TYR	3.5
1	B	120	GLU	3.4
1	B	138	GLU	3.4
1	D	218	VAL	3.4
1	D	33	MET	3.3
1	B	36	LYS	3.3
1	C	107	GLU	3.2
1	D	96	TYR	3.2
1	A	33	MET	3.2
1	D	38	GLU	3.2
1	B	40	ARG	3.2
1	C	131	ARG	3.2
1	D	31	PHE	3.2
1	B	117	ARG	3.1
1	A	111	THR	3.1
1	B	43	HIS	3.0
1	B	109	TYR	3.0
1	A	0	HIS	3.0
1	A	120	GLU	3.0
1	D	43	HIS	3.0
1	C	113	ILE	3.0
1	D	131	ARG	2.9
1	A	43	HIS	2.9
1	D	34	GLY	2.9
1	C	91	TYR	2.9
1	D	47	TYR	2.9
1	A	-1	HIS	2.8
1	A	208	TYR	2.8
1	D	113	ILE	2.8
1	A	217	GLU	2.7
1	A	38	GLU	2.7
1	B	39	GLU	2.7
1	D	39	GLU	2.7
1	A	106	LEU	2.6
1	D	109	TYR	2.6
1	A	37	ASP	2.6
1	C	138	GLU	2.6
1	B	114	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	39	GLU	2.6
1	B	0	HIS	2.5
1	A	137	ILE	2.5
1	A	109	TYR	2.5
1	C	32	ASP	2.5
1	B	113	ILE	2.5
1	A	40	ARG	2.4
1	D	104	GLU	2.4
1	C	25	ARG	2.4
1	C	135	GLU	2.4
1	A	47	TYR	2.3
1	C	114	PRO	2.3
1	B	112	THR	2.3
1	C	36	LYS	2.3
1	D	25	ARG	2.2
1	D	137	ILE	2.2
1	B	104	GLU	2.2
1	B	200	TRP	2.2
1	A	115	PRO	2.1
1	C	217	GLU	2.1
1	A	104	GLU	2.1
1	C	173	LEU	2.1
1	D	116	GLU	2.1
1	D	216	LYS	2.1
1	C	31	PHE	2.1
1	B	135	GLU	2.1
1	B	218	VAL	2.1
1	B	196	GLU	2.1
1	B	131	ARG	2.0
1	C	120	GLU	2.0
1	C	108	GLY	2.0
1	C	196	GLU	2.0
1	B	127	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

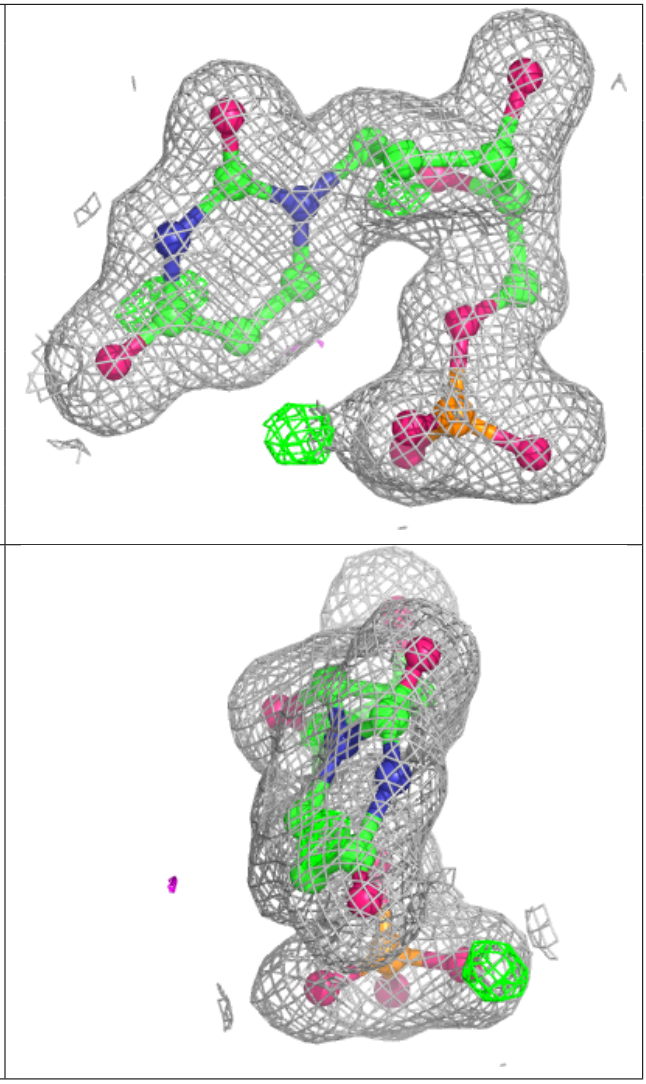
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

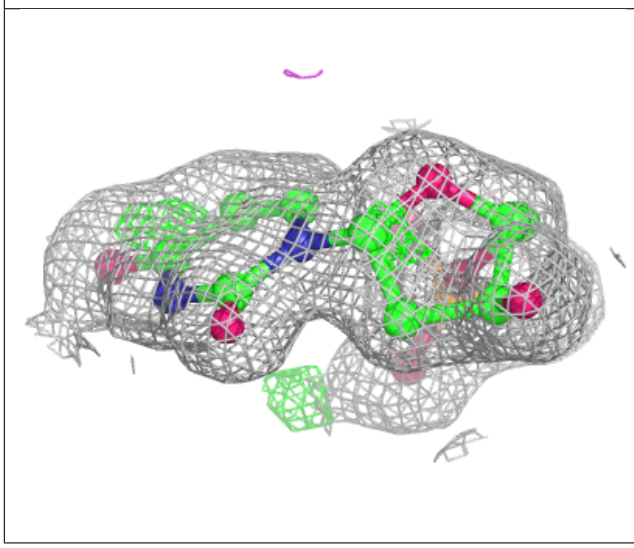
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PGE	A	635	10/10	0.70	0.25	48,50,53,54	0
4	PGE	B	630	10/10	0.79	0.18	52,53,54,54	0
4	PGE	D	640	10/10	0.79	0.19	54,55,56,56	0
4	PGE	D	620	10/10	0.85	0.12	37,38,40,43	0
4	PGE	B	625	10/10	0.91	0.13	36,37,40,42	0
2	UMP	C	613	20/20	0.94	0.09	21,22,24,25	0
2	UMP	A	603	20/20	0.96	0.09	20,21,25,25	0
3	FAD	B	610	53/53	0.96	0.10	17,22,25,26	0
3	FAD	D	600	53/53	0.96	0.10	17,22,25,26	0
2	UMP	B	608	20/20	0.96	0.12	17,20,22,22	0
3	FAD	A	615	53/53	0.97	0.12	16,20,23,24	0
2	UMP	D	618	20/20	0.97	0.09	18,21,24,24	0
3	FAD	C	605	53/53	0.97	0.13	16,19,22,23	0

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

Electron density around UMP C 613:

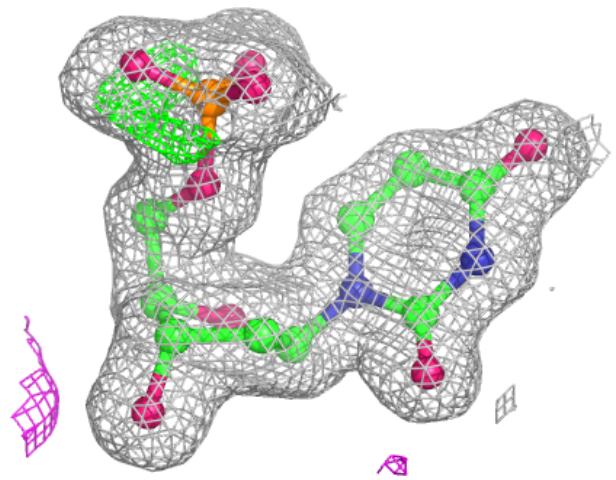
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

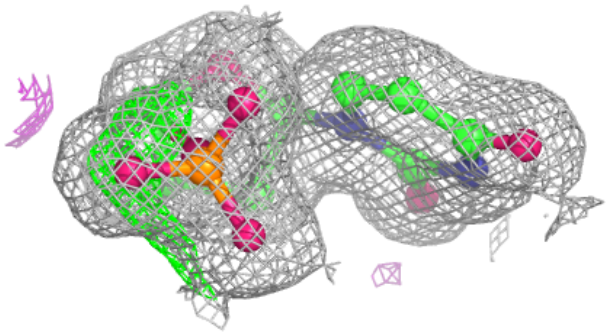


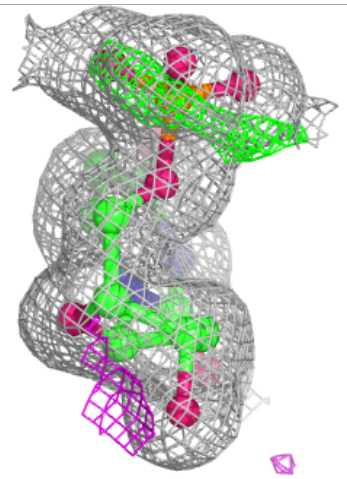


Electron density around UMP A 603:

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

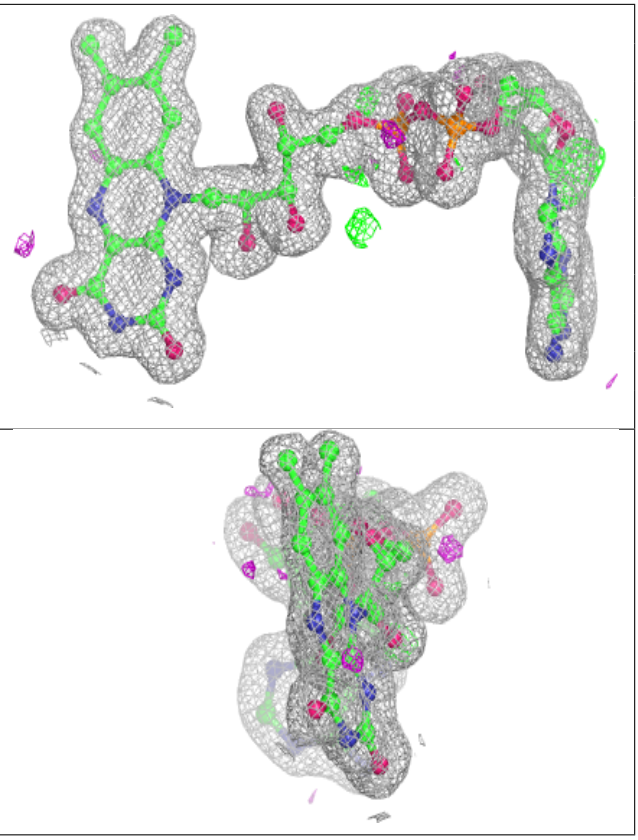






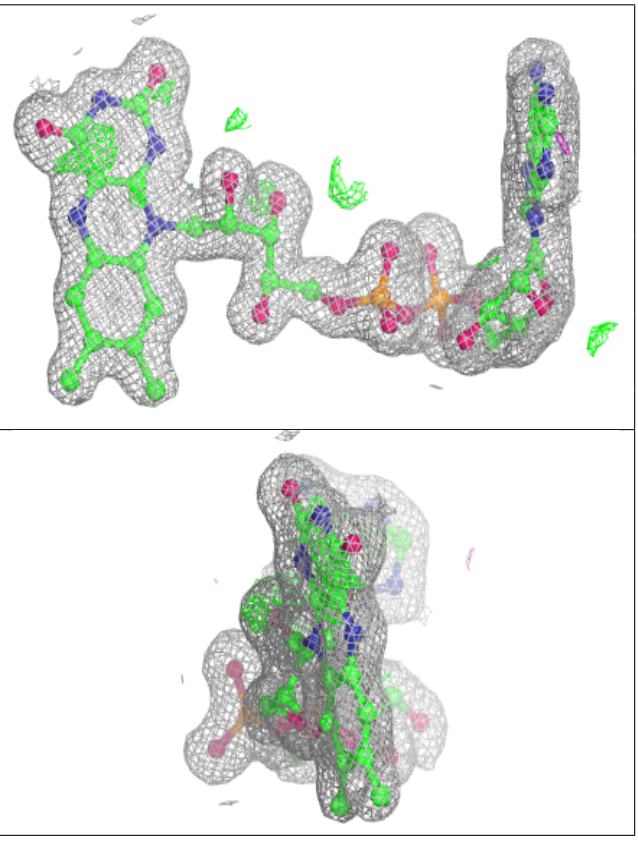
Electron density around FAD B 610:

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



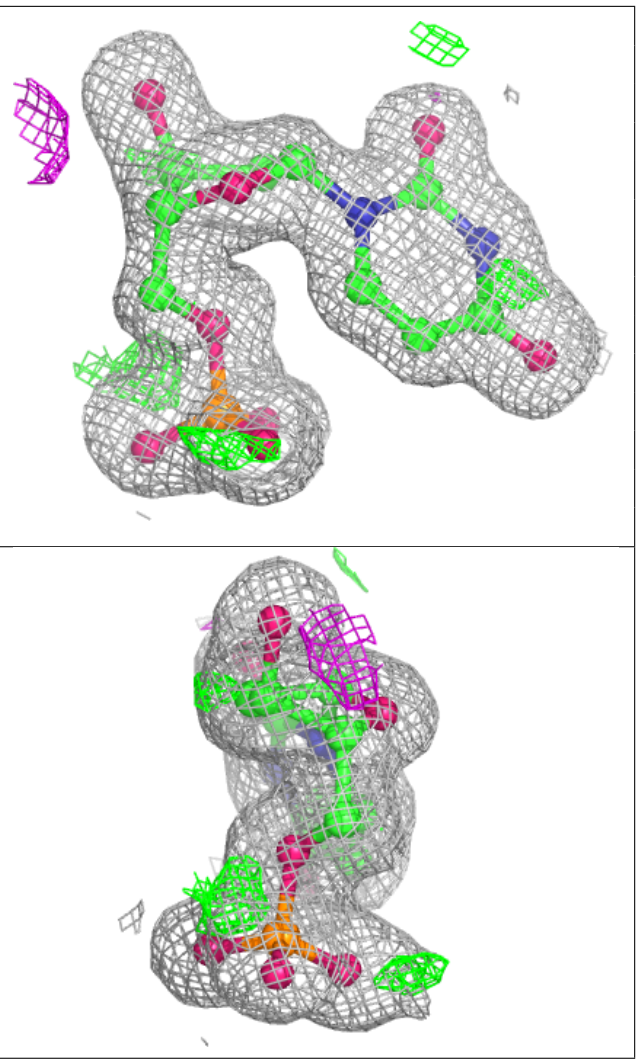
Electron density around FAD D 600:

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



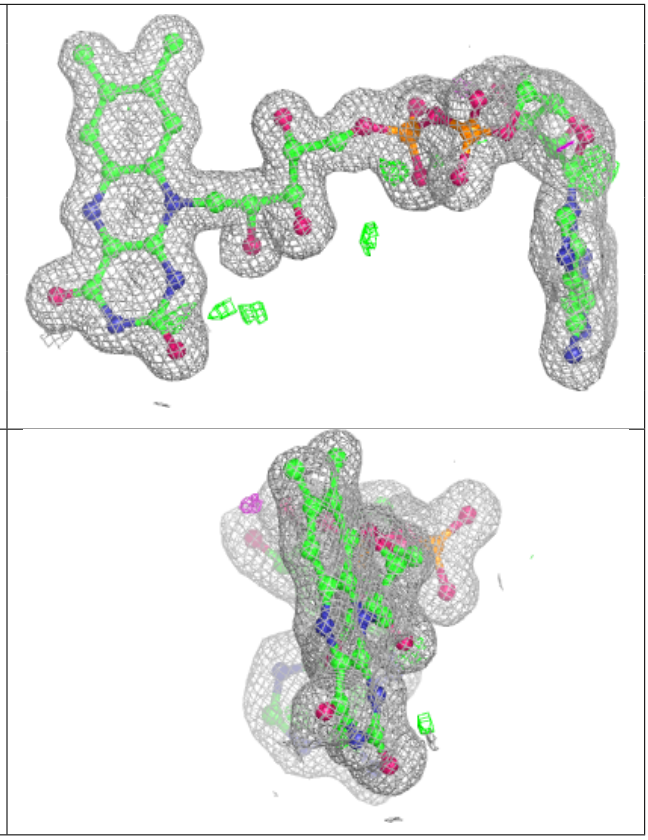
Electron density around UMP B 608:

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



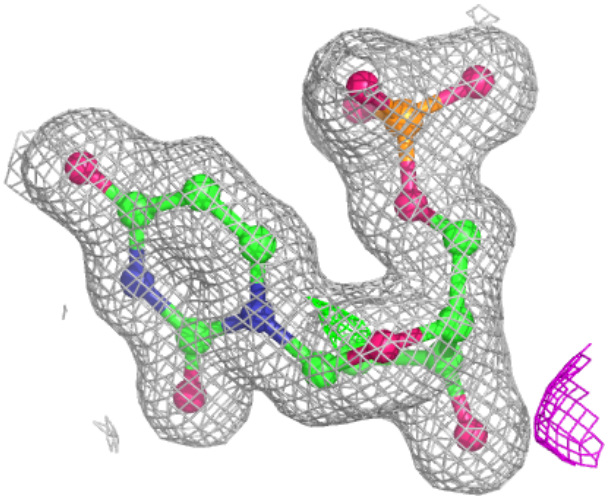
Electron density around FAD A 615:

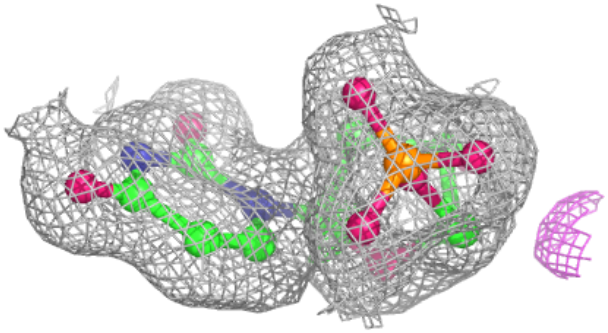
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

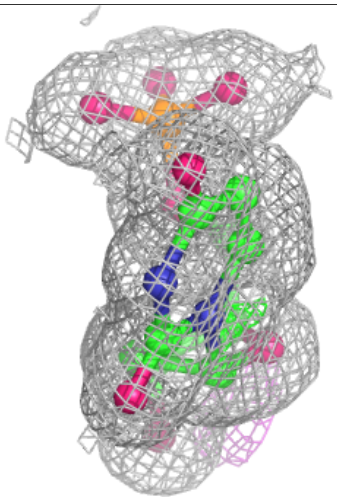


Electron density around UMP D 618:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

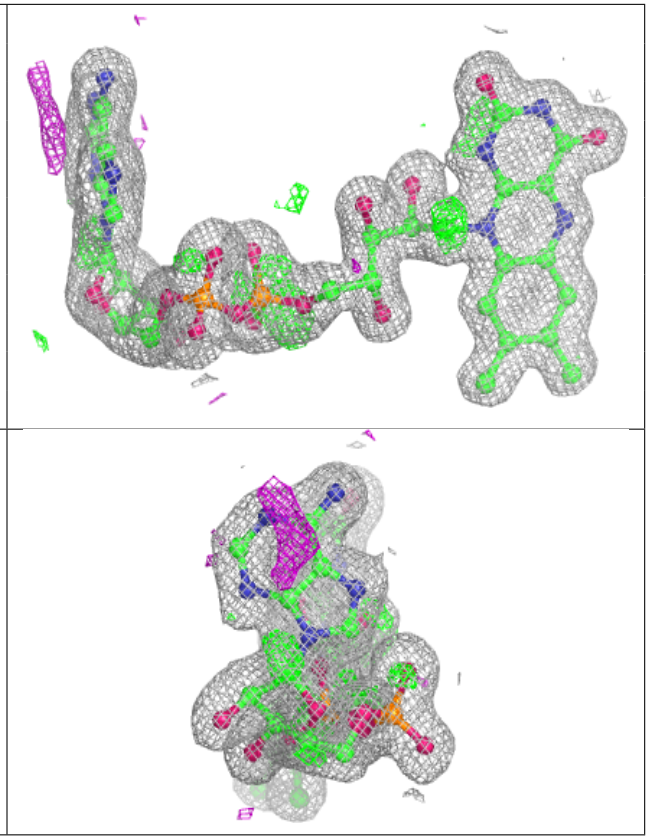






Electron density around FAD C 605:

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



6.5 Other polymers (i)

There are no such residues in this entry.