Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 10:34 AM EDT

PDB ID	:	1O29
Title	:	Crystal structure of Thymidylate Synthase Complementing Protein (TM0449) from Thermotoga maritima with FAD and FdUMP at 2.0 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	:	2.00 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:

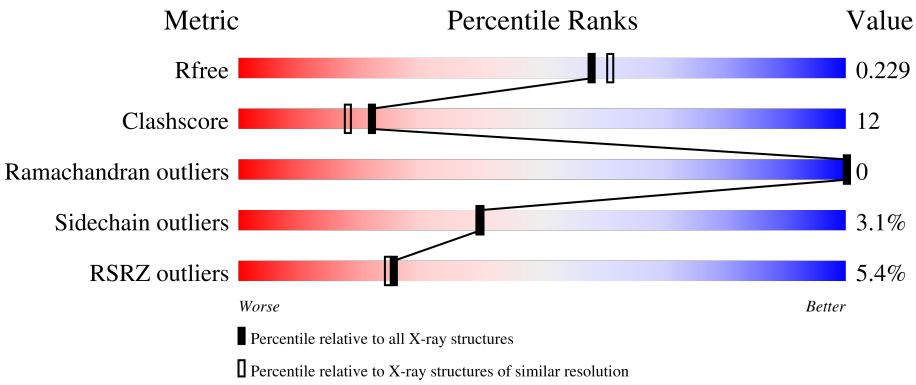
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	4% 65% 26% • 7%
1	B	232	6% 71% 22% • 5%
1	C	232	3% 76% 16% • 7%
1	D	232	7% 66% 25% • 7%

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	815	X	-	-	-
3	FAD	B	810	X	-	-	-
3	FAD	C	805	X	-	-	-
3	FAD	D	800	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7990 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	216	1809	1177	310	316	6	0	0	0
			Total	C	N	O	S			
1	B	220	1841	1197	314	324	6	0	0	0
			Total	C	N	O	S			
1	C	216	1813	1180	310	318	5	0	0	0
			Total	C	N	O	S			
1	D	215	1803	1173	307	317	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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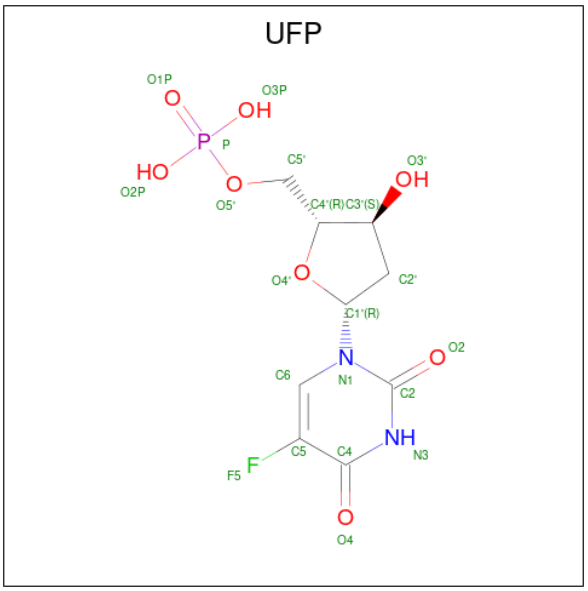
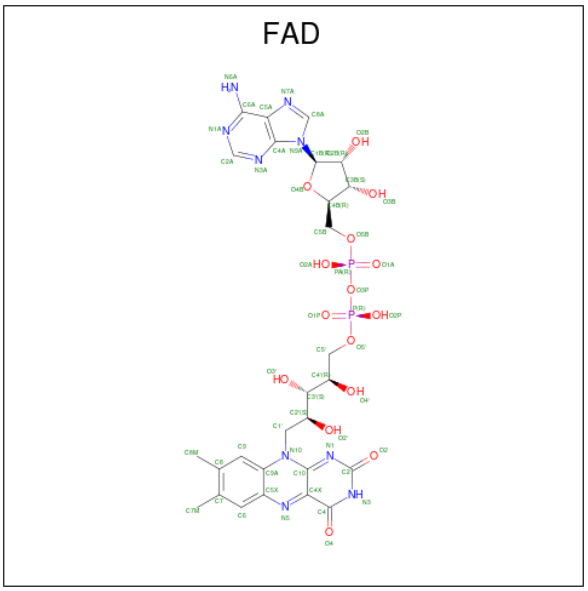
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q9WYT0
B	-1	HIS	-	expression tag	UNP Q9WYT0
B	0	HIS	-	expression tag	UNP Q9WYT0
C	-11	MET	-	expression tag	UNP Q9WYT0
C	-10	GLY	-	expression tag	UNP Q9WYT0
C	-9	SER	-	expression tag	UNP Q9WYT0
C	-8	ASP	-	expression tag	UNP 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 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: $C_9H_{12}FN_2O_8P$).



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

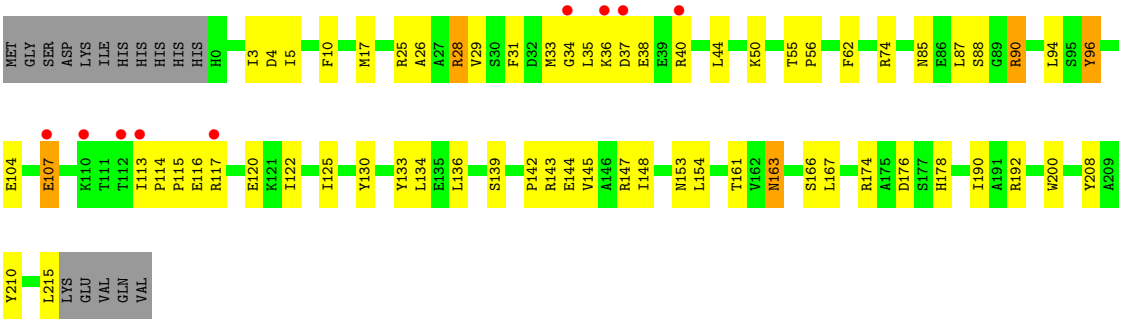
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	111	111	111	0	0
4	B	97	97	97	0	0
4	C	116	116	116	0	0
4	D	104	104	104	0	0

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.

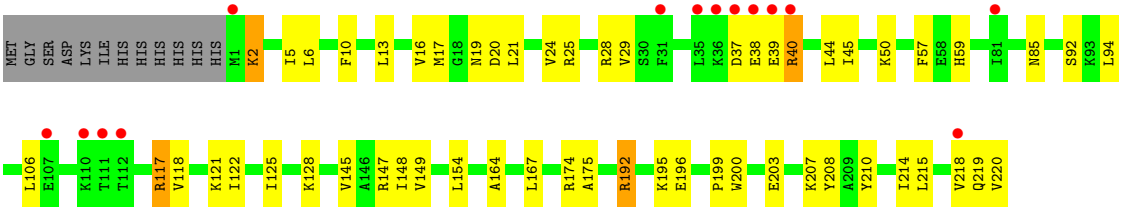
• Molecule 1: Thymidylate synthase thyX

Chain A:



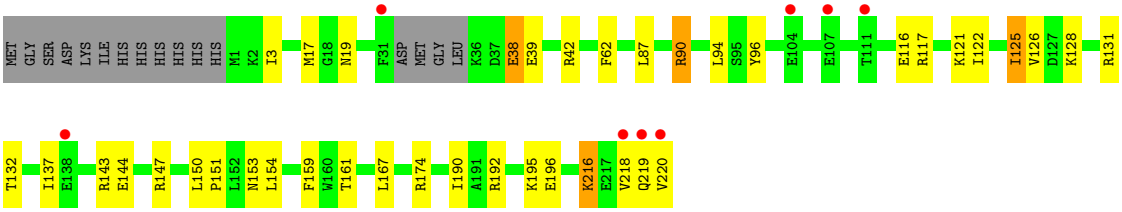
• Molecule 1: Thymidylate synthase thyX

Chain B:



• Molecule 1: Thymidylate synthase thyX

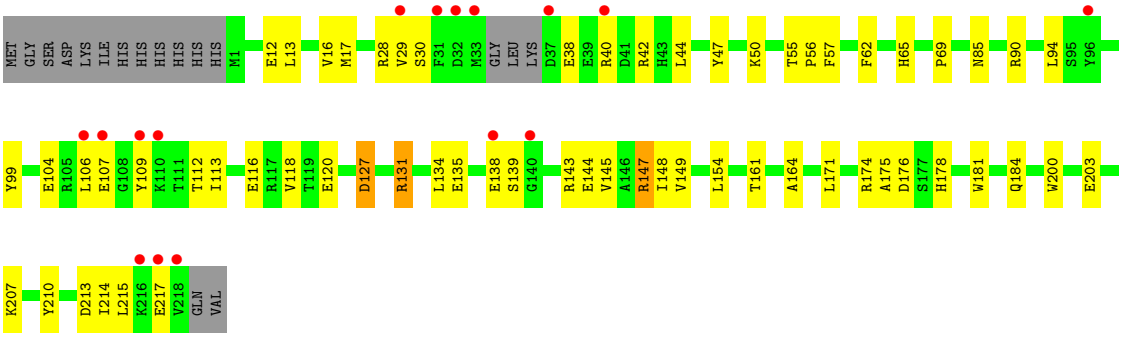
Chain C:



• Molecule 1: Thymidylate synthase thyX

Chain D:

7%
66%
25%
7%


MET GLY SER ASP LYS ILE HIS HIS HIS HIS HIS HIS HIS M1 E12 L13 V16 M17 R28 V29 S30 F31 D32 M33 GLY LEU LYS D37 E38 E39 R40 D41 R42 H43 L44 Y47 K50 T55 P56 F57 F62 H65 P69 N85 R90 L94 S95 Y96
Y99 E104 R105 L106 E107 G108 Y109 K110 T111 T112 I113 E116 R117 V118 T119 E120 D127 R131 L134 E135 E138 S139 G140 R143 E144 V145 A146 R147 I148 V149 L154 T161 A164 L171 R174 A175 D176 S177 H178 W181 Q184 W200 E203
K207 Y210 D213 I214 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	54.64Å 116.95Å 141.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 45.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.00) 99.2 (45.13-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.232 0.190 , 0.229	Depositor DCC
R_{free} test set	3649 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.9	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	0.95	EDS
Total number of atoms	7990	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: UFP, 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	0.34	0/1859	0.57	0/2514
1	B	0.33	0/1890	0.57	0/2554
1	C	0.34	0/1861	0.57	0/2514
1	D	0.33	0/1851	0.56	0/2502
All	All	0.34	0/7461	0.57	0/10084

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	1809	0	1801	52	0
1	B	1841	0	1839	47	0
1	C	1813	0	1811	39	0
1	D	1803	0	1794	51	0
2	A	21	0	10	1	0
2	B	21	0	10	2	0
2	C	21	0	10	2	0
2	D	21	0	10	1	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	1	0
3	C	53	0	30	2	0
3	D	53	0	30	1	0
4	A	111	0	0	1	0
4	B	97	0	0	4	0
4	C	116	0	0	2	0
4	D	104	0	0	3	0
All	All	7990	0	7405	177	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 12.

All (177) 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:A:174:ARG:HH12	2:D:818:UFP:HN3	1.09	0.99
1:A:17:MET:HB2	1:B:17:MET:HB2	1.46	0.97
2:A:803:UFP:HN3	1:D:174:ARG:HH12	1.11	0.94
1:B:174:ARG:HH12	2:C:813:UFP:HN3	1.09	0.90
2:B:808:UFP:HN3	1:C:174:ARG:HH12	1.12	0.89
1:C:17:MET:HB2	1:D:17:MET:HB2	1.58	0.85
1:A:116:GLU:O	1:A:120:GLU:HG2	1.78	0.84
1:D:112:THR:HG23	1:D:113:ILE:HG23	1.61	0.82
1:A:28:ARG:HG2	1:A:34:GLY:O	1.86	0.76
1:B:195:LYS:NZ	1:B:220:VAL:HG12	2.03	0.72
1:D:131:ARG:O	1:D:135:GLU:HG3	1.89	0.71
1:C:195:LYS:NZ	1:C:220:VAL:HG12	2.08	0.69
1:C:94:LEU:HD13	1:C:154:LEU:HD21	1.75	0.69
1:B:192:ARG:C	1:B:192:ARG:HD3	2.14	0.67
1:C:87:LEU:HA	1:D:30:SER:HA	1.75	0.66
1:D:94:LEU:HD13	1:D:154:LEU:HD21	1.77	0.66
1:C:167:LEU:HD21	1:C:190:ILE:HG21	1.78	0.66
1:C:122:ILE:O	1:C:125:ILE:HD13	1.96	0.65
1:C:19:ASN:HB2	4:C:425:HOH:O	1.98	0.64
1:C:167:LEU:HD21	1:C:190:ILE:CG2	2.29	0.63
1:B:19:ASN:HB2	4:B:493:HOH:O	1.98	0.62
1:A:167:LEU:HD11	1:A:190:ILE:CG2	2.30	0.62
1:B:117:ARG:HD2	1:B:121:LYS:HE2	1.82	0.62
1:A:25:ARG:HE	1:A:35:LEU:HD11	1.65	0.62
1:B:207:LYS:HE3	1:B:208:TYR:CE1	2.35	0.61
1:B:195:LYS:HZ2	1:B:220:VAL:HG12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LYS:HE3	1:B:10:PHE:CG	2.36	0.61
1:D:85:ASN:ND2	4:D:458:HOH:O	2.34	0.60
1:A:167:LEU:HD11	1:A:190:ILE:HG21	1.84	0.59
1:A:143:ARG:HG3	4:A:469:HOH:O	2.02	0.59
1:C:159:PHE:CE1	1:D:29:VAL:HG21	2.39	0.57
1:D:104:GLU:H	1:D:104:GLU:CD	2.07	0.57
1:A:163:ASN:C	1:A:163:ASN:HD22	2.07	0.57
1:C:117:ARG:NH2	1:C:121:LYS:HZ2	2.03	0.57
1:A:113:ILE:HG12	1:D:139:SER:OG	2.05	0.57
1:B:37:ASP:OD2	1:B:39:GLU:HB3	2.05	0.56
1:A:163:ASN:ND2	1:A:166:SER:H	2.03	0.56
1:A:142:PRO:HG3	1:D:109:TYR:CE2	2.40	0.56
1:D:12:GLU:CG	1:D:65:HIS:HB3	2.36	0.56
1:A:114:PRO:HD2	1:A:117:ARG:HG3	1.88	0.55
1:D:13:LEU:HD11	1:D:16:VAL:CG2	2.37	0.55
1:D:38:GLU:HG3	1:D:200:TRP:CH2	2.42	0.55
1:D:116:GLU:H	1:D:116:GLU:CD	2.11	0.55
1:C:137:ILE:HD11	1:C:143:ARG:HA	1.89	0.54
1:B:94:LEU:HD13	1:B:154:LEU:HD21	1.90	0.54
1:A:55:THR:OG1	1:A:56:PRO:HD3	2.07	0.54
1:B:175:ALA:HA	1:B:214:ILE:HD11	1.90	0.54
1:B:195:LYS:HZ3	1:B:220:VAL:HG12	1.71	0.54
1:A:136:LEU:O	1:A:139:SER:HB3	2.08	0.53
1:D:143:ARG:HG3	4:D:395:HOH:O	2.09	0.53
1:C:117:ARG:HH21	1:C:121:LYS:NZ	2.08	0.52
1:D:28:ARG:HH11	1:D:28:ARG:HG3	1.74	0.52
1:C:117:ARG:NH2	1:C:121:LYS:NZ	2.57	0.52
1:D:42:ARG:HH21	1:D:203:GLU:CD	2.12	0.52
1:C:195:LYS:HZ3	1:C:220:VAL:HG12	1.75	0.51
1:B:219:GLN:O	1:B:220:VAL:HG22	2.10	0.51
1:C:122:ILE:HA	1:C:125:ILE:CD1	2.41	0.51
1:D:134:LEU:O	1:D:138:GLU:HG3	2.11	0.51
1:B:37:ASP:OD1	1:B:40:ARG:HB2	2.10	0.51
1:A:104:GLU:O	1:A:107:GLU:HB2	2.11	0.51
1:B:38:GLU:HG3	1:B:200:TRP:CH2	2.46	0.50
1:B:28:ARG:HG3	1:B:28:ARG:HH11	1.75	0.50
1:C:216:LYS:HB2	1:C:216:LYS:NZ	2.27	0.50
1:D:47:TYR:HA	1:D:50:LYS:HZ3	1.76	0.50
1:C:38:GLU:HG3	1:C:39:GLU:N	2.26	0.50
1:A:38:GLU:HG3	1:A:200:TRP:CH2	2.47	0.49
1:B:50:LYS:HE2	1:B:208:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLU:HB2	4:B:444:HOH:O	2.11	0.49
1:A:94:LEU:HD13	1:A:154:LEU:HD21	1.95	0.49
1:B:13:LEU:HD11	1:B:16:VAL:HG22	1.95	0.49
1:A:31:PHE:O	1:A:33:MET:HG3	2.11	0.49
1:C:151:PRO:HB2	1:C:153:ASN:OD1	2.13	0.49
1:A:210:TYR:CE2	1:A:215:LEU:HB2	2.48	0.49
1:C:125:ILE:HD13	1:C:125:ILE:H	1.78	0.48
1:D:213:ASP:OD1	1:D:214:ILE:HG23	2.13	0.48
1:D:210:TYR:CE2	1:D:215:LEU:HB2	2.47	0.48
1:B:21:LEU:O	1:B:25:ARG:HG3	2.14	0.48
1:D:12:GLU:HG3	1:D:65:HIS:HB3	1.96	0.48
1:C:216:LYS:HB2	1:C:216:LYS:HZ2	1.79	0.48
1:A:125:ILE:HG21	1:D:149:VAL:HB	1.95	0.47
1:B:145:VAL:O	1:B:148:ILE:HG12	2.15	0.47
1:D:127:ASP:HB3	1:D:131:ARG:NH1	2.29	0.47
1:A:31:PHE:HA	1:B:92:SER:OG	2.14	0.47
1:B:125:ILE:HD11	1:C:132:THR:OG1	2.15	0.47
1:D:106:LEU:HD11	1:D:118:VAL:HG11	1.97	0.47
1:A:28:ARG:NH2	1:A:36:LYS:HD2	2.29	0.47
1:D:104:GLU:CD	1:D:104:GLU:N	2.67	0.47
1:A:90:ARG:CB	1:A:144:GLU:HB3	2.45	0.46
1:A:87:LEU:HA	1:B:29:VAL:O	2.16	0.46
1:B:20:ASP:HB3	1:B:45:ILE:CD1	2.45	0.46
1:B:149:VAL:HB	1:C:125:ILE:HG13	1.97	0.46
1:D:50:LYS:HZ3	1:D:50:LYS:HB3	1.80	0.46
1:D:203:GLU:HG2	1:D:207:LYS:HE2	1.96	0.46
1:B:207:LYS:HE3	1:B:208:TYR:CZ	2.50	0.46
1:D:50:LYS:HB3	1:D:50:LYS:NZ	2.31	0.46
1:C:125:ILE:HG12	1:C:126:VAL:N	2.31	0.46
1:A:145:VAL:O	1:A:148:ILE:HG12	2.15	0.46
1:A:104:GLU:OE1	1:A:104:GLU:N	2.44	0.46
1:C:116:GLU:CD	1:C:116:GLU:H	2.19	0.46
1:D:62:PHE:O	1:D:161:THR:HA	2.14	0.46
1:C:62:PHE:O	1:C:161:THR:HA	2.16	0.46
1:D:181:TRP:O	1:D:184:GLN:HB2	2.15	0.46
1:C:122:ILE:O	1:C:125:ILE:CD1	2.64	0.46
1:D:90:ARG:HB2	1:D:144:GLU:HB3	1.98	0.46
1:A:74:ARG:HA	4:D:622:HOH:O	2.16	0.45
1:B:210:TYR:CE2	1:B:215:LEU:HB2	2.51	0.45
1:D:47:TYR:HA	1:D:50:LYS:NZ	2.31	0.45
1:A:87:LEU:HD23	1:A:88:SER:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:TYR:C	1:A:96:TYR:CD2	2.90	0.45
1:C:218:VAL:HG12	1:C:219:GLN:N	2.31	0.45
1:D:147:ARG:HD2	1:D:148:ILE:N	2.32	0.45
1:B:57:PHE:O	1:B:164:ALA:HB3	2.16	0.45
1:D:29:VAL:HG12	1:D:29:VAL:O	2.16	0.45
1:A:96:TYR:C	1:A:96:TYR:HD2	2.21	0.45
1:B:25:ARG:NH2	4:B:643:HOH:O	2.49	0.45
1:B:13:LEU:HD21	1:B:16:VAL:CG2	2.47	0.45
1:C:94:LEU:HD13	1:C:154:LEU:CD2	2.43	0.45
1:C:117:ARG:CZ	1:C:121:LYS:HZ2	2.30	0.45
1:A:25:ARG:HG3	1:A:35:LEU:HD21	1.98	0.44
1:B:167:LEU:C	1:B:167:LEU:HD23	2.37	0.44
1:B:5:ILE:HG22	1:B:6:LEU:HG	1.99	0.44
1:B:24:VAL:HG13	1:B:44:LEU:HD23	1.99	0.44
1:B:192:ARG:HD3	1:B:192:ARG:O	2.17	0.44
1:A:62:PHE:O	1:A:161:THR:HA	2.17	0.44
1:A:122:ILE:O	1:A:125:ILE:HG22	2.18	0.44
1:D:176:ASP:OD2	1:D:178:HIS:HD2	2.01	0.44
1:C:131:ARG:NH1	4:C:590:HOH:O	2.50	0.44
1:D:217:GLU:HA	1:D:217:GLU:OE1	2.16	0.44
1:A:26:ALA:O	1:A:29:VAL:HG12	2.17	0.44
1:A:38:GLU:HG3	1:A:200:TRP:HH2	1.83	0.43
1:C:3:ILE:HD11	1:C:192:ARG:HD2	2.00	0.43
1:A:90:ARG:HB3	1:A:144:GLU:HB3	2.01	0.43
1:D:55:THR:N	1:D:56:PRO:CD	2.82	0.43
1:A:192:ARG:HH11	1:A:192:ARG:HG3	1.84	0.43
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.83	0.43
1:C:90:ARG:HB2	1:C:144:GLU:HB3	1.99	0.43
1:A:85:ASN:HD22	1:B:59:HIS:CD2	2.37	0.43
1:D:40:ARG:HH11	1:D:40:ARG:HG2	1.83	0.43
1:A:4:ASP:O	1:A:5:ILE:HD13	2.19	0.43
3:A:815:FAD:H4B	3:C:805:FAD:O2B	2.19	0.43
1:B:118:VAL:O	1:B:122:ILE:HG13	2.19	0.43
1:C:42:ARG:HH11	1:C:42:ARG:HG2	1.84	0.43
1:C:192:ARG:NH1	1:C:220:VAL:CG2	2.82	0.43
1:C:192:ARG:NH1	1:C:220:VAL:HG21	2.33	0.42
1:B:40:ARG:HH11	1:B:40:ARG:HG3	1.84	0.42
1:A:3:ILE:HD13	1:A:192:ARG:HD2	2.01	0.42
1:A:37:ASP:CG	1:A:40:ARG:HH11	2.23	0.42
1:A:50:LYS:HE2	1:A:208:TYR:CE2	2.55	0.42
1:C:94:LEU:HD12	1:C:150:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:THR:OG1	1:D:56:PRO:HD3	2.19	0.42
1:A:130:TYR:CE2	1:A:134:LEU:HD11	2.55	0.42
1:A:192:ARG:HG3	1:A:192:ARG:NH1	2.35	0.41
1:D:38:GLU:HG3	1:D:200:TRP:CZ2	2.55	0.41
1:A:176:ASP:OD2	1:A:178:HIS:HD2	2.03	0.41
1:B:85:ASN:ND2	4:B:452:HOH:O	2.52	0.41
3:B:810:FAD:O2B	3:D:800:FAD:H4B	2.20	0.41
1:D:116:GLU:O	1:D:120:GLU:HG3	2.21	0.41
1:A:153:ASN:HB3	1:D:148:ILE:HB	2.01	0.41
1:B:199:PRO:O	1:B:203:GLU:HG2	2.21	0.41
2:B:808:UFP:HN3	1:C:174:ARG:NH1	1.96	0.41
1:A:10:PHE:CD2	1:A:10:PHE:C	2.93	0.41
1:B:174:ARG:NH1	2:C:813:UFP:HN3	1.93	0.41
1:A:130:TYR:O	1:A:133:TYR:HB3	2.21	0.41
1:B:128:LYS:NZ	1:C:128:LYS:HD3	2.35	0.41
1:D:69:PRO:HG3	1:D:99:TYR:HB2	2.02	0.41
1:D:145:VAL:O	1:D:148:ILE:HG12	2.21	0.41
1:B:106:LEU:HD12	1:B:106:LEU:N	2.36	0.40
1:B:167:LEU:HD23	1:B:167:LEU:O	2.21	0.40
1:D:13:LEU:HD11	1:D:16:VAL:HG23	2.02	0.40
1:D:90:ARG:CB	1:D:144:GLU:HB3	2.51	0.40
1:D:104:GLU:O	1:D:107:GLU:HB2	2.21	0.40
1:A:163:ASN:HD21	3:C:805:FAD:H2A	1.85	0.40
1:D:57:PHE:O	1:D:164:ALA:HB3	2.21	0.40
1:B:175:ALA:CA	1:B:214:ILE:HD11	2.51	0.40
1:B:218:VAL:HG12	1:B:219:GLN:N	2.36	0.40
1:D:171:LEU:O	1:D:175:ALA:HB3	2.22	0.40
1:A:114:PRO:HA	1:A:115:PRO:HD3	2.00	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%)	209 (98%)	5 (2%)	0	100	100
1	B	218/232 (94%)	212 (97%)	6 (3%)	0	100	100
1	C	212/232 (91%)	204 (96%)	8 (4%)	0	100	100
1	D	211/232 (91%)	205 (97%)	6 (3%)	0	100	100
All	All	855/928 (92%)	830 (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	192/207 (93%)	185 (96%)	7 (4%)	35	34
1	B	196/207 (95%)	190 (97%)	6 (3%)	40	40
1	C	193/207 (93%)	186 (96%)	7 (4%)	35	34
1	D	192/207 (93%)	188 (98%)	4 (2%)	53	57
All	All	773/828 (93%)	749 (97%)	24 (3%)	40	40

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	44	LEU
1	A	90	ARG
1	A	96	TYR
1	A	107	GLU
1	A	147	ARG
1	A	163	ASN
1	B	2	LYS
1	B	40	ARG
1	B	117	ARG
1	B	147	ARG
1	B	192	ARG
1	B	196	GLU

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Mol	Chain	Res	Type
1	C	38	GLU
1	C	90	ARG
1	C	96	TYR
1	C	125	ILE
1	C	147	ARG
1	C	196	GLU
1	C	216	LYS
1	D	44	LEU
1	D	127	ASP
1	D	131	ARG
1	D	147	ARG

Sometimes 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	B	85	ASN
1	B	185	GLN
1	C	185	GLN
1	C	219	GLN
1	D	178	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	UFP	B	808	-	22,22,22	2.62	10 (45%)	33,33,33	2.36	11 (33%)
3	FAD	C	805	-	53,58,58	2.85	23 (43%)	68,89,89	1.86	14 (20%)
2	UFP	A	803	-	22,22,22	2.68	10 (45%)	33,33,33	2.43	13 (39%)
3	FAD	B	810	-	53,58,58	2.93	23 (43%)	68,89,89	1.86	14 (20%)
2	UFP	D	818	-	22,22,22	2.58	10 (45%)	33,33,33	2.39	11 (33%)
3	FAD	A	815	-	53,58,58	2.92	21 (39%)	68,89,89	1.85	14 (20%)
2	UFP	C	813	-	22,22,22	2.58	11 (50%)	33,33,33	2.45	12 (36%)
3	FAD	D	800	-	53,58,58	2.93	23 (43%)	68,89,89	1.82	14 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UFP	B	808	-	-	0/10/22/22	0/2/2/2
3	FAD	C	805	-	1/1/9/9	2/30/50/50	0/6/6/6
2	UFP	A	803	-	-	3/10/22/22	0/2/2/2
3	FAD	B	810	-	1/1/9/9	1/30/50/50	0/6/6/6
2	UFP	D	818	-	-	1/10/22/22	0/2/2/2
3	FAD	A	815	-	1/1/9/9	1/30/50/50	0/6/6/6
2	UFP	C	813	-	-	1/10/22/22	0/2/2/2
3	FAD	D	800	-	1/1/9/9	1/30/50/50	0/6/6/6

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	803	UFP	C2-N1	7.30	1.50	1.38
3	B	810	FAD	C4A-N3A	7.28	1.45	1.35
2	D	818	UFP	C2-N1	6.89	1.49	1.38
3	A	815	FAD	C9A-C5X	6.84	1.52	1.41
2	C	813	UFP	C2-N1	6.83	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	800	FAD	C4A-N3A	6.81	1.45	1.35
2	B	808	UFP	C2-N1	6.80	1.49	1.38
3	C	805	FAD	C4A-N3A	6.77	1.45	1.35
3	C	805	FAD	C9A-C5X	6.70	1.52	1.41
3	D	800	FAD	C9A-C5X	6.69	1.52	1.41
3	B	810	FAD	C9A-C5X	6.63	1.52	1.41
3	A	815	FAD	C4A-N3A	6.58	1.44	1.35
3	B	810	FAD	C6-C7	6.28	1.48	1.39
3	D	800	FAD	C6-C7	6.04	1.48	1.39
3	A	815	FAD	C4X-N5	5.99	1.42	1.30
3	D	800	FAD	C4X-N5	5.96	1.42	1.30
3	B	810	FAD	C4X-N5	5.92	1.42	1.30
3	C	805	FAD	C4X-N5	5.84	1.42	1.30
3	A	815	FAD	C9-C9A	5.83	1.49	1.39
3	A	815	FAD	C6-C7	5.83	1.48	1.39
3	D	800	FAD	C9-C9A	5.80	1.49	1.39
3	C	805	FAD	C9-C9A	5.52	1.48	1.39
2	B	808	UFP	C6-N1	5.41	1.47	1.38
3	C	805	FAD	C6-C7	5.40	1.47	1.39
3	A	815	FAD	C2B-C1B	5.31	1.61	1.53
3	A	815	FAD	C8A-N7A	-5.23	1.25	1.34
3	B	810	FAD	C9-C9A	5.20	1.48	1.39
2	A	803	UFP	C6-N1	5.17	1.46	1.38
3	B	810	FAD	C8A-N7A	-5.11	1.25	1.34
2	D	818	UFP	C6-N1	5.04	1.46	1.38
3	D	800	FAD	C8A-N7A	-4.98	1.25	1.34
3	D	800	FAD	C2B-C1B	4.97	1.61	1.53
3	C	805	FAD	C2B-C1B	4.97	1.61	1.53
3	B	810	FAD	C2B-C1B	4.95	1.61	1.53
3	C	805	FAD	C8A-N7A	-4.92	1.25	1.34
2	C	813	UFP	C6-N1	4.81	1.46	1.38
3	B	810	FAD	C6-C5X	4.59	1.47	1.40
3	D	800	FAD	C6-C5X	4.48	1.47	1.40
3	A	815	FAD	C6-C5X	4.42	1.46	1.40
3	C	805	FAD	C8-C7	4.42	1.51	1.40
3	B	810	FAD	C10-N1	4.38	1.42	1.33
3	A	815	FAD	C8-C7	4.35	1.51	1.40
3	D	800	FAD	C8-C7	4.34	1.51	1.40
3	B	810	FAD	C8-C7	4.34	1.51	1.40
3	D	800	FAD	C2A-N3A	4.31	1.39	1.32
3	D	800	FAD	C10-N1	4.28	1.42	1.33
3	A	815	FAD	C10-N1	4.25	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	805	FAD	C6-C5X	4.21	1.46	1.40
3	C	805	FAD	C10-N1	4.19	1.41	1.33
3	B	810	FAD	C2A-N3A	4.15	1.38	1.32
3	A	815	FAD	C2A-N3A	3.99	1.38	1.32
3	A	815	FAD	C10-N10	3.95	1.46	1.37
3	D	800	FAD	C10-N10	3.94	1.45	1.37
3	C	805	FAD	C10-N10	3.91	1.45	1.37
3	C	805	FAD	C2A-N1A	3.73	1.40	1.33
3	B	810	FAD	C2A-N1A	3.71	1.40	1.33
3	A	815	FAD	C9-C8	3.70	1.45	1.39
3	C	805	FAD	C2A-N3A	3.69	1.38	1.32
3	D	800	FAD	O4B-C1B	3.67	1.46	1.41
3	B	810	FAD	C10-N10	3.65	1.45	1.37
2	A	803	UFP	O4'-C1'	3.60	1.50	1.42
3	A	815	FAD	C2A-N1A	3.51	1.40	1.33
3	D	800	FAD	C2A-N1A	3.48	1.40	1.33
3	A	815	FAD	O4B-C1B	3.47	1.45	1.41
3	B	810	FAD	C1'-C2'	3.47	1.57	1.52
3	D	800	FAD	C9-C8	3.45	1.44	1.39
2	C	813	UFP	O4'-C1'	3.44	1.50	1.42
3	C	805	FAD	C4-N3	3.41	1.45	1.38
2	D	818	UFP	O4'-C1'	3.38	1.49	1.42
3	B	810	FAD	C4-N3	3.37	1.45	1.38
3	D	800	FAD	C4-N3	3.37	1.45	1.38
3	C	805	FAD	C9-C8	3.35	1.44	1.39
2	C	813	UFP	C2-N3	3.34	1.43	1.38
3	B	810	FAD	C9-C8	3.34	1.44	1.39
2	D	818	UFP	C4-N3	3.28	1.44	1.38
2	C	813	UFP	C4-N3	3.25	1.44	1.38
2	B	808	UFP	O4'-C1'	3.21	1.49	1.42
2	B	808	UFP	C4-N3	3.18	1.44	1.38
2	A	803	UFP	C4-N3	3.08	1.44	1.38
3	A	815	FAD	C1'-C2'	3.07	1.57	1.52
3	B	810	FAD	O4B-C1B	3.04	1.45	1.41
3	A	815	FAD	C4-N3	3.00	1.44	1.38
2	B	808	UFP	C2-N3	2.98	1.43	1.38
3	C	805	FAD	O4B-C1B	2.93	1.45	1.41
3	C	805	FAD	C1'-C2'	2.91	1.56	1.52
3	D	800	FAD	C1'-C2'	2.85	1.56	1.52
2	C	813	UFP	C2'-C1'	2.81	1.60	1.52
2	A	803	UFP	O4'-C4'	2.75	1.51	1.45
2	D	818	UFP	C2-N3	2.74	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	803	UFP	C2-N3	2.72	1.42	1.38
2	B	808	UFP	C2'-C1'	2.69	1.59	1.52
2	B	808	UFP	P-O2P	-2.65	1.44	1.54
2	D	818	UFP	O4'-C4'	2.57	1.50	1.45
2	D	818	UFP	C2'-C1'	2.52	1.59	1.52
3	A	815	FAD	C5A-C4A	2.51	1.47	1.40
2	A	803	UFP	P-O2P	-2.51	1.45	1.54
2	A	803	UFP	C2'-C1'	2.50	1.59	1.52
2	A	803	UFP	C5'-C4'	2.47	1.59	1.51
3	C	805	FAD	C5A-C4A	2.45	1.47	1.40
2	C	813	UFP	O4'-C4'	2.43	1.50	1.45
2	B	808	UFP	O4'-C4'	2.42	1.50	1.45
2	D	818	UFP	P-O2P	-2.41	1.45	1.54
3	D	800	FAD	C5A-C4A	2.35	1.47	1.40
3	D	800	FAD	C2-N3	2.34	1.44	1.39
2	B	808	UFP	C2'-C3'	2.32	1.59	1.52
3	B	810	FAD	C5B-C4B	2.28	1.58	1.51
3	D	800	FAD	C5B-C4B	2.27	1.58	1.51
2	C	813	UFP	P-O2P	-2.25	1.46	1.54
3	D	800	FAD	O5B-C5B	2.24	1.53	1.44
3	A	815	FAD	PA-O5B	-2.23	1.50	1.59
3	B	810	FAD	P-O5'	-2.18	1.50	1.59
3	C	805	FAD	C2-N3	2.18	1.44	1.39
2	C	813	UFP	C5'-C4'	2.18	1.58	1.51
3	B	810	FAD	PA-O5B	-2.17	1.50	1.59
3	B	810	FAD	C5A-C4A	2.16	1.46	1.40
3	C	805	FAD	PA-O5B	-2.14	1.50	1.59
2	D	818	UFP	C5'-C4'	2.14	1.58	1.51
3	C	805	FAD	O5B-C5B	2.10	1.52	1.44
3	B	810	FAD	C2-N3	2.09	1.43	1.39
3	C	805	FAD	P-O5'	-2.09	1.50	1.59
2	C	813	UFP	C2'-C3'	2.08	1.58	1.52
3	A	815	FAD	O5B-C5B	2.07	1.52	1.44
2	C	813	UFP	P-O3P	-2.05	1.47	1.54
3	C	805	FAD	C5B-C4B	2.03	1.57	1.51
3	B	810	FAD	O5B-C5B	2.01	1.52	1.44
3	D	800	FAD	C2'-C3'	2.01	1.57	1.53
3	D	800	FAD	PA-O5B	-2.01	1.51	1.59
2	B	808	UFP	C5'-C4'	2.01	1.57	1.51
3	A	815	FAD	C2-N3	2.01	1.43	1.39
2	A	803	UFP	C2'-C3'	2.01	1.58	1.52
2	D	818	UFP	C4-C5	2.00	1.46	1.44

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	815	FAD	C3B-C2B-C1B	-8.52	88.14	100.98
3	B	810	FAD	C3B-C2B-C1B	-8.49	88.20	100.98
3	C	805	FAD	C3B-C2B-C1B	-8.47	88.22	100.98
3	D	800	FAD	C3B-C2B-C1B	-7.95	89.00	100.98
2	C	813	UFP	C2'-C1'-N1	-6.04	99.87	113.77
2	D	818	UFP	C2'-C1'-N1	-6.03	99.87	113.77
2	B	808	UFP	C2'-C1'-N1	-5.90	100.18	113.77
2	A	803	UFP	C2'-C1'-N1	-5.69	100.67	113.77
2	A	803	UFP	O4'-C1'-N1	5.62	117.92	107.86
2	B	808	UFP	O4'-C1'-N1	5.56	117.79	107.86
2	C	813	UFP	O4'-C1'-N1	5.52	117.73	107.86
2	D	818	UFP	O4'-C1'-N1	5.50	117.69	107.86
2	C	813	UFP	C5-C6-N1	4.95	126.51	120.62
3	B	810	FAD	O2B-C2B-C1B	4.79	128.53	110.85
3	C	805	FAD	O2B-C2B-C1B	4.76	128.44	110.85
2	C	813	UFP	F5-C5-C4	4.73	120.78	116.40
3	A	815	FAD	O2B-C2B-C1B	4.72	128.30	110.85
2	A	803	UFP	C5-C6-N1	4.70	126.22	120.62
2	D	818	UFP	C5-C6-N1	4.65	126.16	120.62
3	D	800	FAD	O2B-C2B-C1B	4.65	128.01	110.85
2	B	808	UFP	C5-C6-N1	4.61	126.11	120.62
2	A	803	UFP	C6-C5-C4	-4.50	118.41	122.60
2	A	803	UFP	F5-C5-C4	4.47	120.54	116.40
2	D	818	UFP	C6-C5-C4	-4.44	118.46	122.60
2	D	818	UFP	F5-C5-C4	4.36	120.43	116.40
2	B	808	UFP	C6-C5-C4	-4.26	118.62	122.60
2	C	813	UFP	C6-C5-C4	-4.19	118.69	122.60
2	B	808	UFP	F5-C5-C4	3.94	120.05	116.40
2	A	803	UFP	C5-C4-N3	3.77	116.27	112.56
3	B	810	FAD	N3A-C2A-N1A	-3.70	122.89	128.68
2	D	818	UFP	C5-C4-N3	3.63	116.14	112.56
2	B	808	UFP	C5-C4-N3	3.60	116.11	112.56
2	B	808	UFP	C6-N1-C2	-3.58	117.67	121.30
2	A	803	UFP	C6-N1-C2	-3.57	117.68	121.30
3	D	800	FAD	N3A-C2A-N1A	-3.52	123.18	128.68
2	C	813	UFP	C5-C4-N3	3.52	116.02	112.56
2	C	813	UFP	C6-N1-C2	-3.44	117.82	121.30
3	D	800	FAD	C4-C4X-N5	3.43	123.11	118.23
3	A	815	FAD	C4-C4X-N5	3.42	123.11	118.23
3	A	815	FAD	N3A-C2A-N1A	-3.40	123.36	128.68
3	B	810	FAD	C4-C4X-N5	3.40	123.07	118.23
3	C	805	FAD	N3A-C2A-N1A	-3.38	123.40	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	805	FAD	C4-C4X-N5	3.22	122.81	118.23
3	D	800	FAD	C4A-C5A-N7A	-3.18	106.08	109.40
2	D	818	UFP	C6-N1-C2	-3.17	118.08	121.30
3	A	815	FAD	C4A-C5A-N7A	-3.06	106.21	109.40
3	C	805	FAD	C4A-C5A-N7A	-3.05	106.22	109.40
3	B	810	FAD	C4A-C5A-N7A	-2.90	106.38	109.40
3	D	800	FAD	O3B-C3B-C4B	2.88	119.38	111.05
3	D	800	FAD	C5B-C4B-C3B	-2.83	104.57	115.18
3	D	800	FAD	P-O5'-C5'	2.83	138.26	121.68
3	A	815	FAD	P-O5'-C5'	2.81	138.18	121.68
3	B	810	FAD	O3B-C3B-C4B	2.75	119.00	111.05
3	C	805	FAD	C5B-C4B-C3B	-2.74	104.90	115.18
3	C	805	FAD	P-O5'-C5'	2.74	137.76	121.68
2	C	813	UFP	P-O5'-C5'	2.74	125.83	118.30
3	C	805	FAD	O4B-C4B-C3B	2.73	110.53	105.11
3	C	805	FAD	O3B-C3B-C4B	2.73	118.95	111.05
3	D	800	FAD	O4B-C4B-C3B	2.71	110.48	105.11
3	A	815	FAD	O4B-C4B-C3B	2.71	110.47	105.11
3	A	815	FAD	C5B-C4B-C3B	-2.70	105.04	115.18
2	A	803	UFP	P-O5'-C5'	2.69	125.70	118.30
3	B	810	FAD	P-O5'-C5'	2.68	137.40	121.68
3	A	815	FAD	O3B-C3B-C4B	2.67	118.78	111.05
3	B	810	FAD	O4B-C4B-C3B	2.66	110.38	105.11
3	B	810	FAD	C5B-C4B-C3B	-2.65	105.24	115.18
3	D	800	FAD	C10-N1-C2	2.57	122.05	116.90
3	A	815	FAD	C9-C9A-N10	2.57	125.31	121.84
3	C	805	FAD	P-O3P-PA	2.56	141.62	132.83
3	C	805	FAD	C9-C9A-N10	2.55	125.28	121.84
3	D	800	FAD	P-O3P-PA	2.54	141.53	132.83
3	B	810	FAD	P-O3P-PA	2.52	141.47	132.83
3	C	805	FAD	C10-N1-C2	2.52	121.94	116.90
3	A	815	FAD	C10-N1-C2	2.52	121.93	116.90
2	D	818	UFP	P-O5'-C5'	2.49	125.17	118.30
3	D	800	FAD	C9-C9A-N10	2.46	125.17	121.84
2	B	808	UFP	C4'-O4'-C1'	2.45	115.36	109.45
2	C	813	UFP	C4'-O4'-C1'	2.43	115.34	109.45
3	A	815	FAD	P-O3P-PA	2.43	141.17	132.83
3	B	810	FAD	C10-N1-C2	2.42	121.75	116.90
3	B	810	FAD	C9-C9A-N10	2.31	124.96	121.84
3	C	805	FAD	C2A-N1A-C6A	2.31	122.70	118.75
3	D	800	FAD	C10-C4X-N5	-2.30	119.97	124.86
3	A	815	FAD	C10-C4X-N5	-2.28	120.02	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	805	FAD	C10-C4X-N5	-2.26	120.06	124.86
2	A	803	UFP	C1'-N1-C2	2.24	122.06	117.64
3	B	810	FAD	C2A-N1A-C6A	2.24	122.58	118.75
2	A	803	UFP	C4'-O4'-C1'	2.24	114.86	109.45
3	A	815	FAD	C2A-N1A-C6A	2.24	122.58	118.75
3	B	810	FAD	C10-C4X-N5	-2.23	120.13	124.86
2	D	818	UFP	C4'-O4'-C1'	2.22	114.82	109.45
3	D	800	FAD	C2A-N1A-C6A	2.22	122.55	118.75
2	C	813	UFP	C2'-C3'-C4'	2.22	107.39	102.76
2	C	813	UFP	C1'-N1-C2	2.21	121.99	117.64
2	D	818	UFP	C2'-C3'-C4'	2.20	107.34	102.76
2	A	803	UFP	O4'-C4'-C3'	-2.15	100.65	105.67
2	B	808	UFP	P-O5'-C5'	2.14	124.20	118.30
2	A	803	UFP	C2'-C3'-C4'	2.12	107.17	102.76
2	B	808	UFP	O4'-C4'-C3'	-2.11	100.75	105.67
2	C	813	UFP	O4'-C4'-C3'	-2.06	100.87	105.67
2	A	803	UFP	O2-C2-N1	2.04	125.49	122.79
2	B	808	UFP	C2'-C3'-C4'	2.03	106.98	102.76
2	D	818	UFP	O4'-C4'-C3'	-2.02	100.96	105.67

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	815	FAD	C1B
3	B	810	FAD	C1B
3	C	805	FAD	C1B
3	D	800	FAD	C1B

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	803	UFP	C5'-O5'-P-O2P
2	A	803	UFP	C5'-O5'-P-O3P
3	A	815	FAD	PA-O3P-P-O1P
3	B	810	FAD	PA-O3P-P-O1P
3	C	805	FAD	PA-O3P-P-O1P
3	D	800	FAD	PA-O3P-P-O1P
2	A	803	UFP	C5'-O5'-P-O1P
3	C	805	FAD	O4'-C4'-C5'-O5'
2	C	813	UFP	C5'-O5'-P-O3P
2	D	818	UFP	C5'-O5'-P-O3P

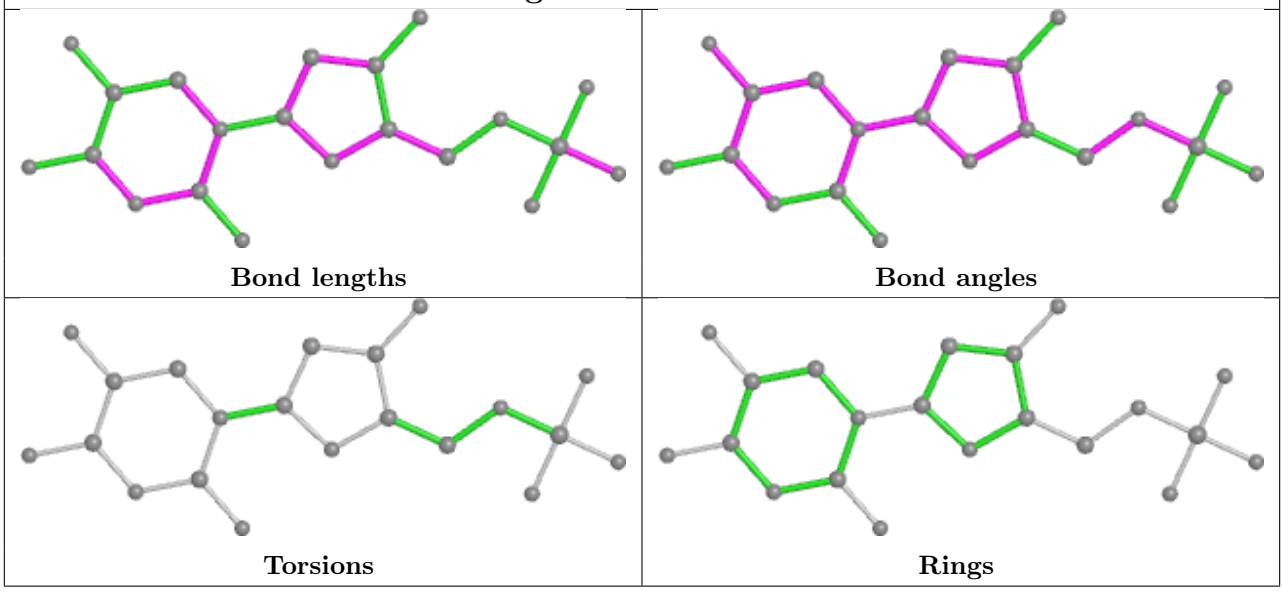
There are no ring outliers.

8 monomers are involved in 9 short contacts:

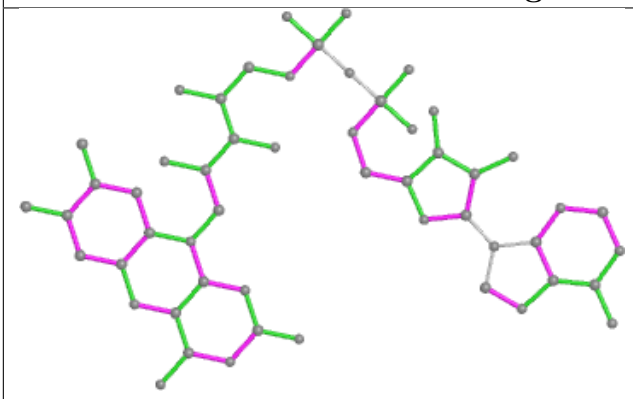
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	808	UFP	2	0
3	C	805	FAD	2	0
2	A	803	UFP	1	0
3	B	810	FAD	1	0
2	D	818	UFP	1	0
3	A	815	FAD	1	0
2	C	813	UFP	2	0
3	D	800	FAD	1	0

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

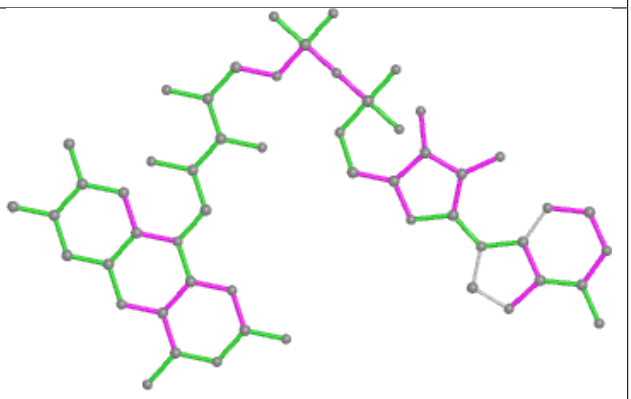
Ligand UFP B 808



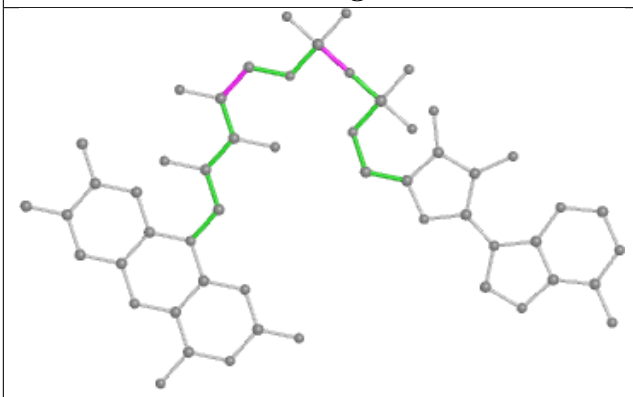
Ligand FAD C 805



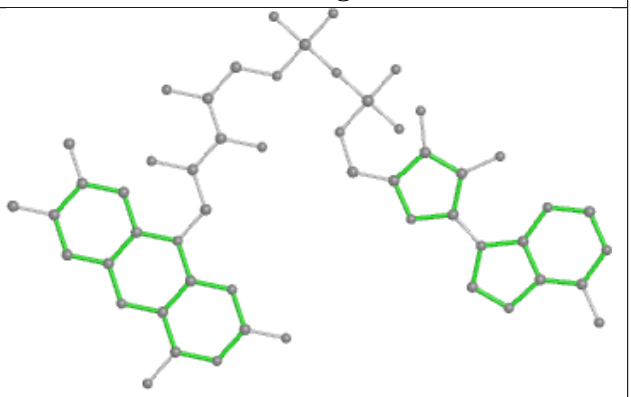
Bond lengths



Bond angles

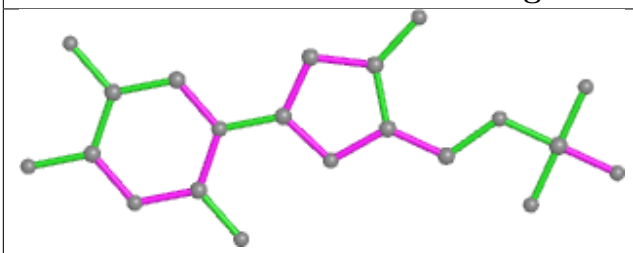


Torsions

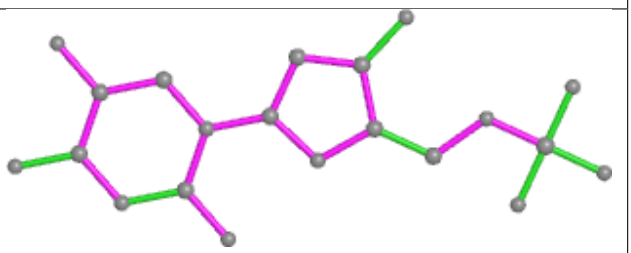


Rings

Ligand UFP A 803



Bond lengths



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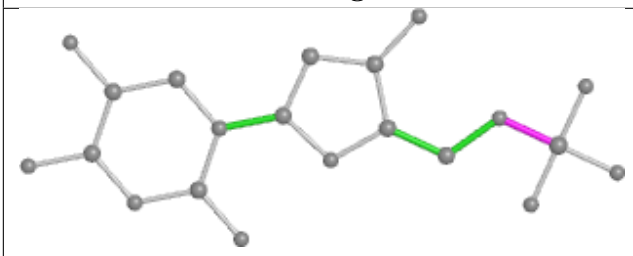

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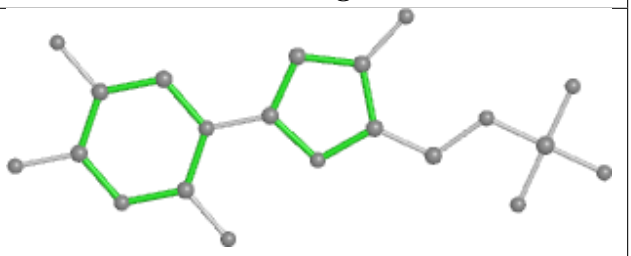
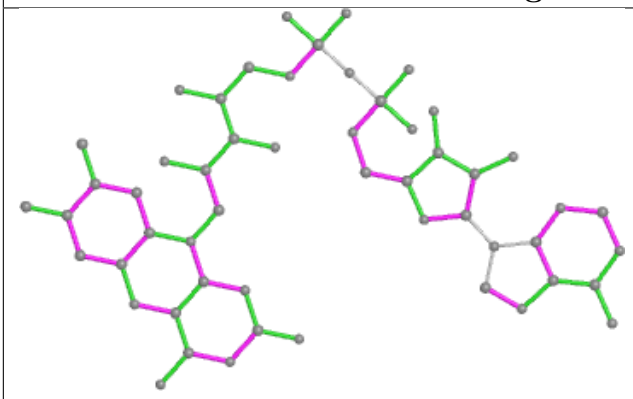
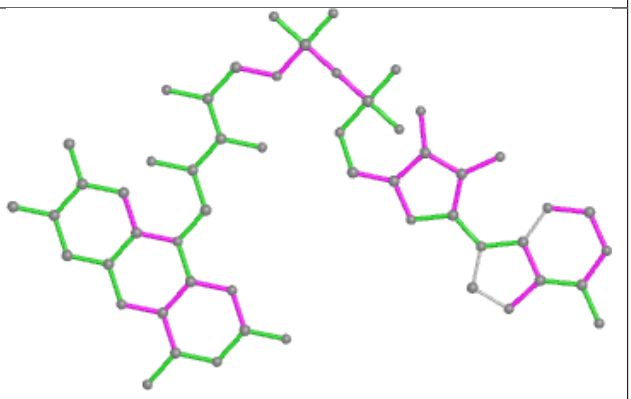


Rings

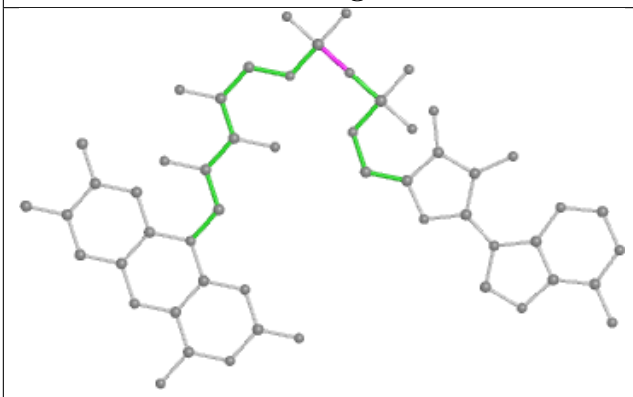
Ligand FAD B 810



Bond lengths



Bond angles



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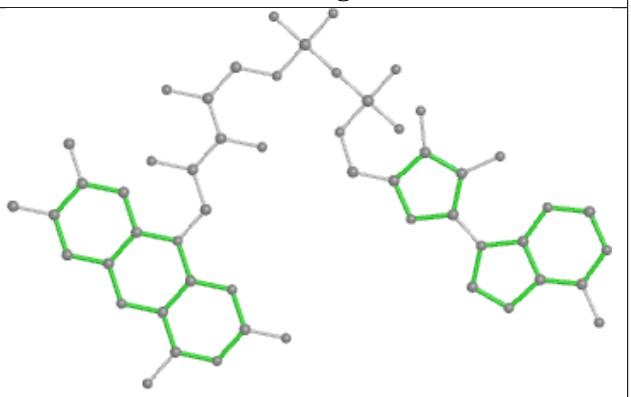
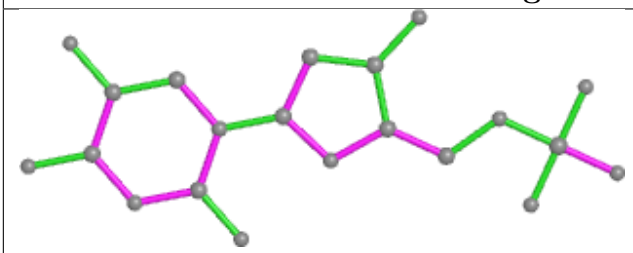
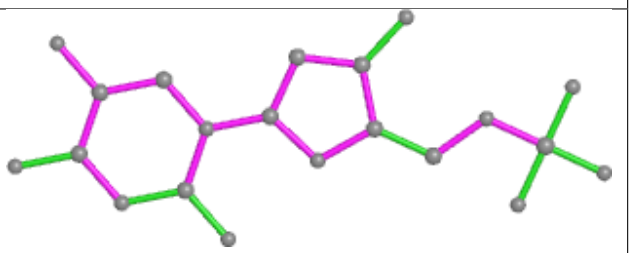


Rings

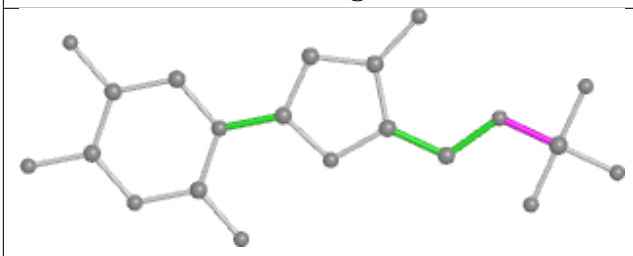
Ligand UFP D 818



Bond lengths



Bond angles



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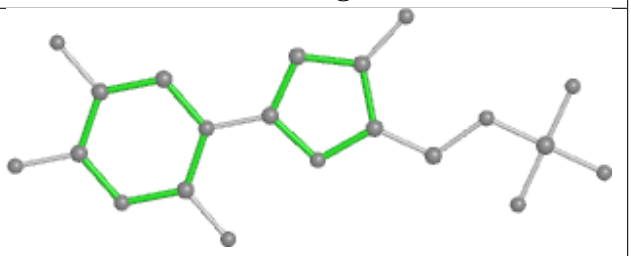
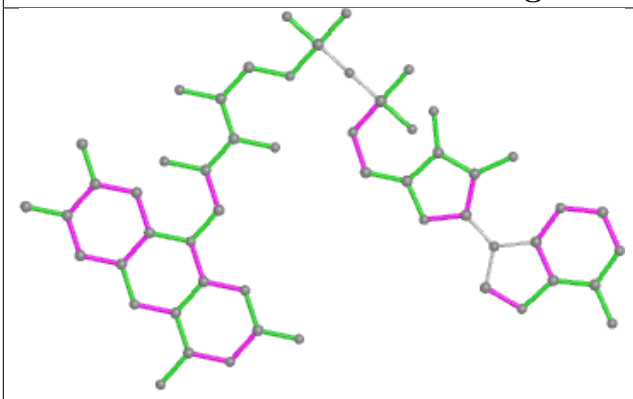
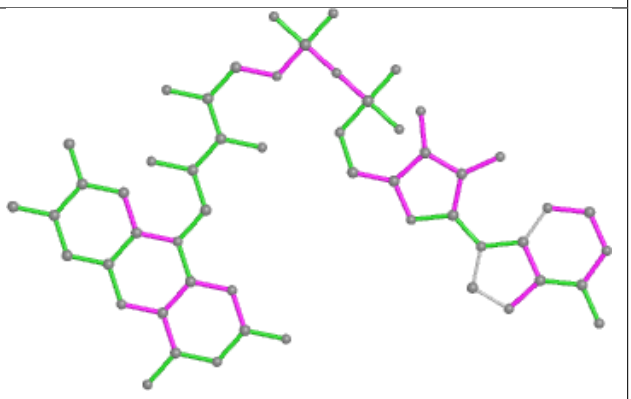


Rings

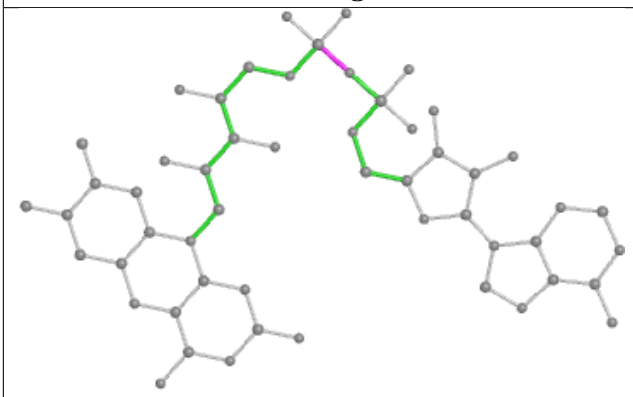
Ligand FAD A 815



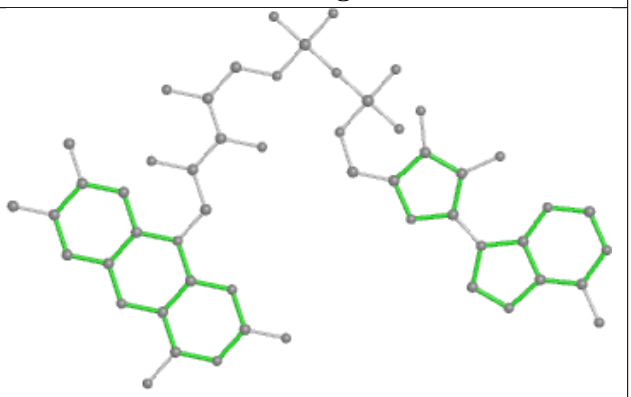
Bond lengths



Bond angles

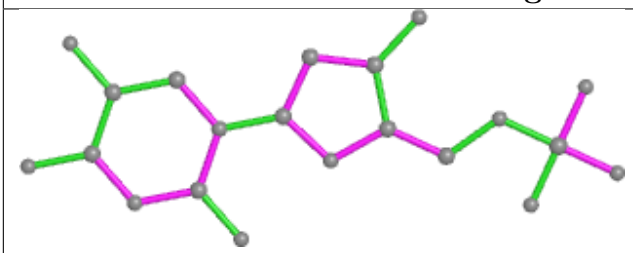


Torsions

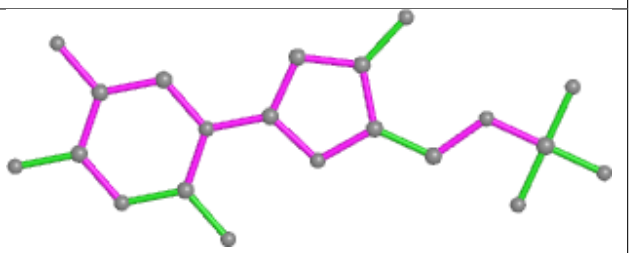


Rings

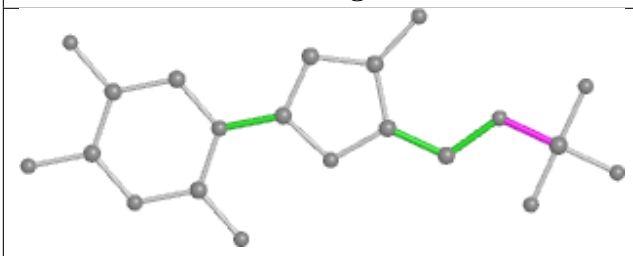
Ligand UFP C 813



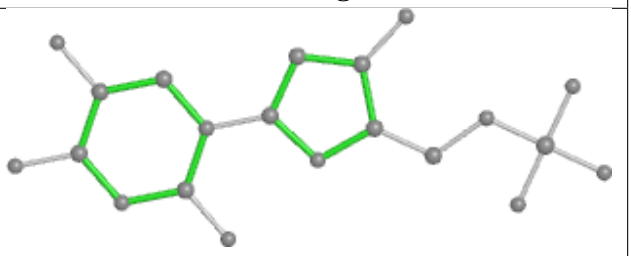
Bond lengths



Bond angles

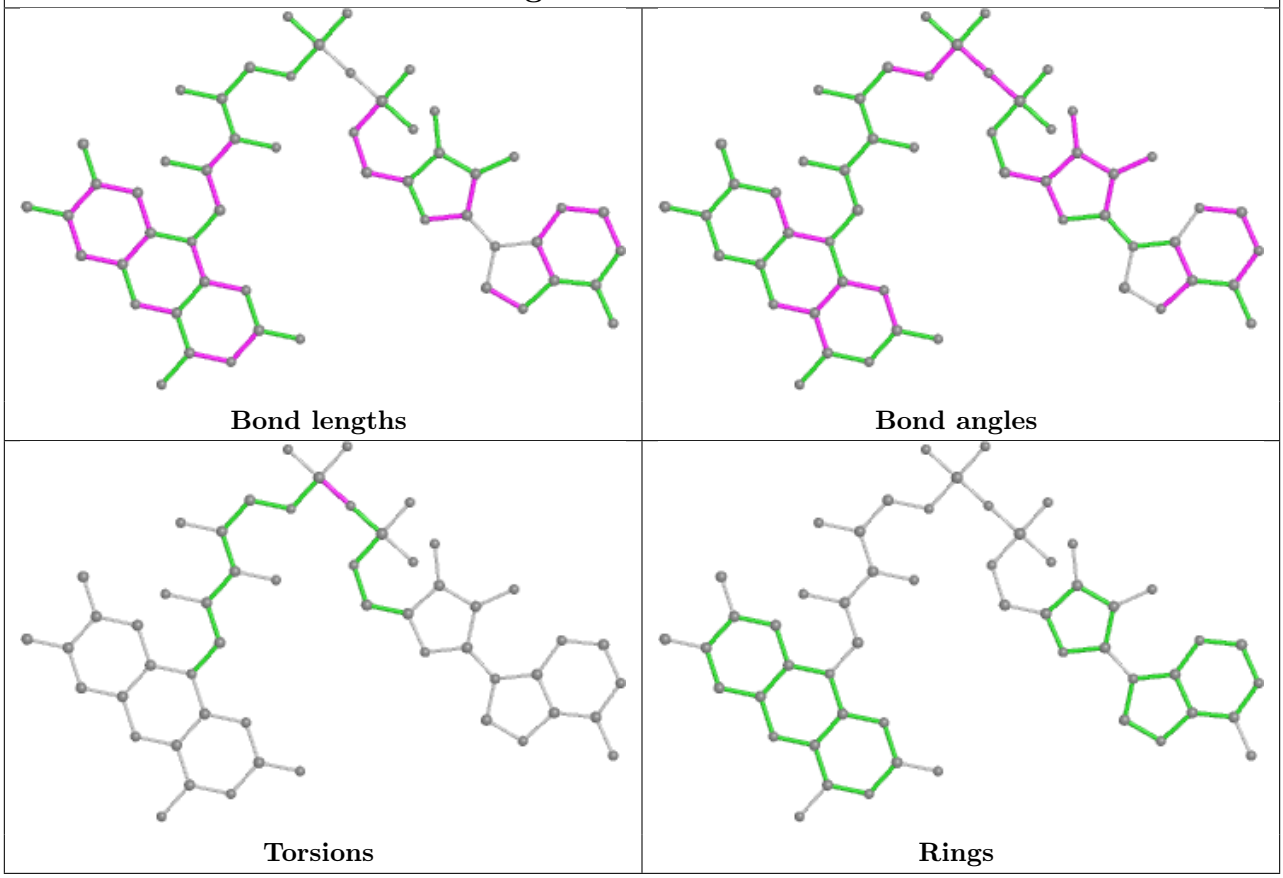


Torsions



Rings

Ligand FAD D 800



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	216/232 (93%)	0.10	9 (4%)	36	35	15, 27, 58, 66	0
1	B	220/232 (94%)	0.19	14 (6%)	19	18	15, 30, 64, 67	0
1	C	216/232 (93%)	-0.05	8 (3%)	41	41	16, 26, 55, 65	0
1	D	215/232 (92%)	0.18	16 (7%)	14	13	15, 28, 58, 66	0
All	All	867/928 (93%)	0.11	47 (5%)	25	24	15, 28, 59, 67	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	218	VAL	5.8
1	C	220	VAL	4.4
1	A	110	LYS	4.2
1	B	40	ARG	4.1
1	B	38	GLU	4.0
1	B	107	GLU	3.8
1	B	111	THR	3.5
1	D	31	PHE	3.5
1	D	32	ASP	3.4
1	A	117	ARG	3.2
1	D	40	ARG	3.2
1	C	104	GLU	3.2
1	B	35	LEU	3.1
1	C	219	GLN	3.1
1	D	217	GLU	3.1
1	B	112	THR	3.1
1	B	36	LYS	3.1
1	A	112	THR	3.0
1	D	216	LYS	3.0
1	D	33	MET	3.0
1	A	40	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	110	LYS	2.9
1	D	140	GLY	2.8
1	D	109	TYR	2.8
1	D	110	LYS	2.7
1	C	107	GLU	2.6
1	A	113	ILE	2.6
1	D	29	VAL	2.6
1	C	111	THR	2.6
1	D	106	LEU	2.6
1	B	37	ASP	2.5
1	C	138	GLU	2.5
1	D	96	TYR	2.5
1	A	34	GLY	2.5
1	D	138	GLU	2.4
1	A	37	ASP	2.4
1	A	107	GLU	2.3
1	D	37	ASP	2.3
1	C	218	VAL	2.3
1	C	31	PHE	2.3
1	B	1	MET	2.3
1	A	36	LYS	2.2
1	D	107	GLU	2.2
1	B	31	PHE	2.1
1	B	218	VAL	2.1
1	B	81	ILE	2.0
1	B	39	GLU	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)

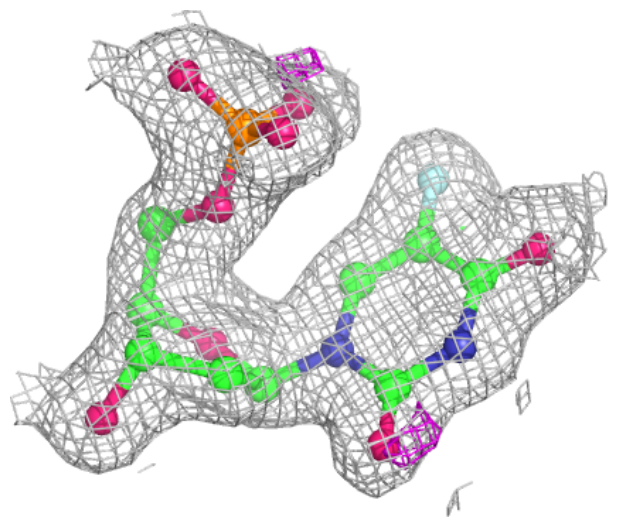
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

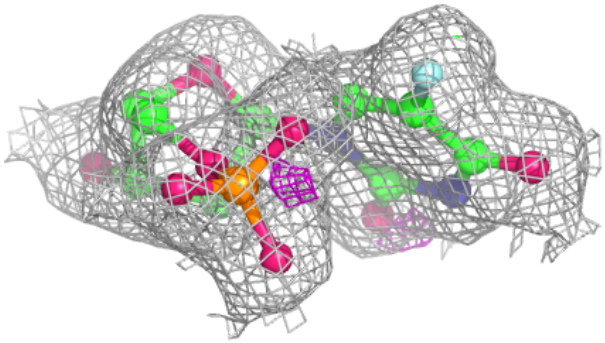
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UFP	C	813	21/21	0.95	0.11	20,23,28,29	0
3	FAD	B	810	53/53	0.95	0.14	17,23,27,30	0
3	FAD	D	800	53/53	0.95	0.13	18,23,28,29	0
3	FAD	A	815	53/53	0.96	0.12	17,21,24,25	0
2	UFP	B	808	21/21	0.96	0.12	18,20,22,24	0
2	UFP	D	818	21/21	0.96	0.10	19,23,25,27	0
3	FAD	C	805	53/53	0.97	0.12	16,21,25,26	0
2	UFP	A	803	21/21	0.97	0.10	21,23,25,29	0

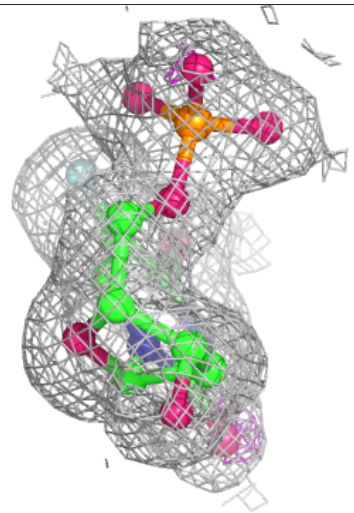
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UFP C 813:

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

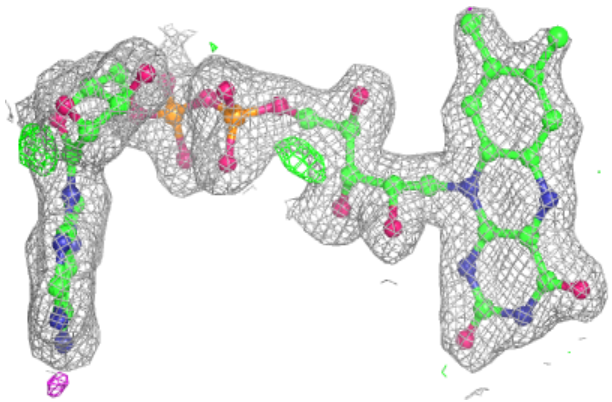


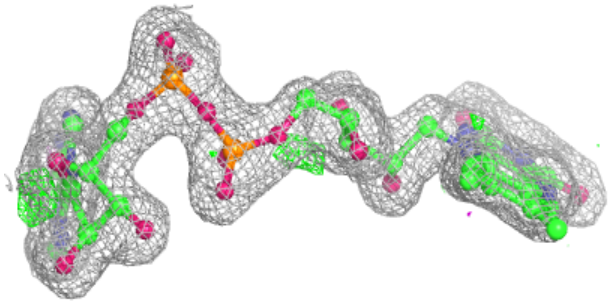


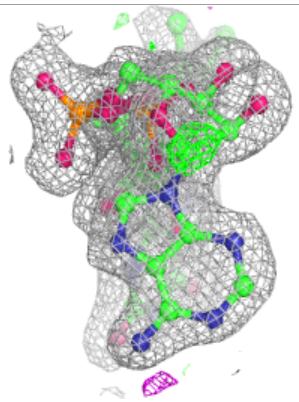


Electron density around FAD B 810:

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

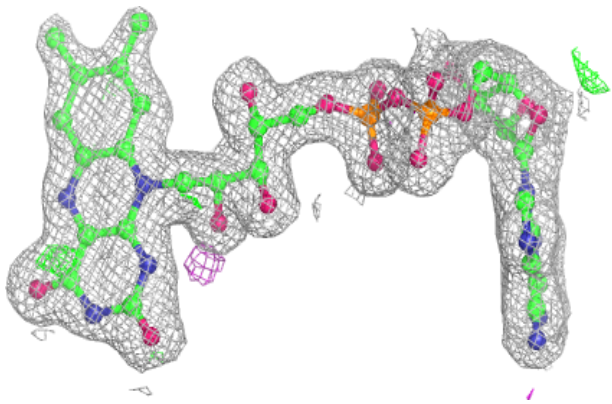


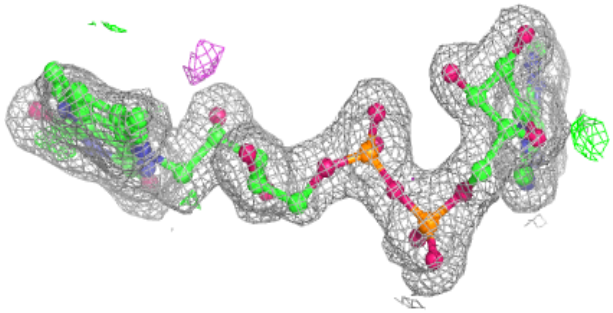


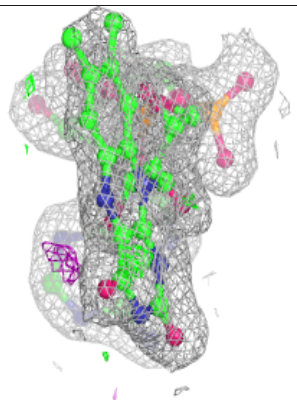


Electron density around FAD D 800:

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

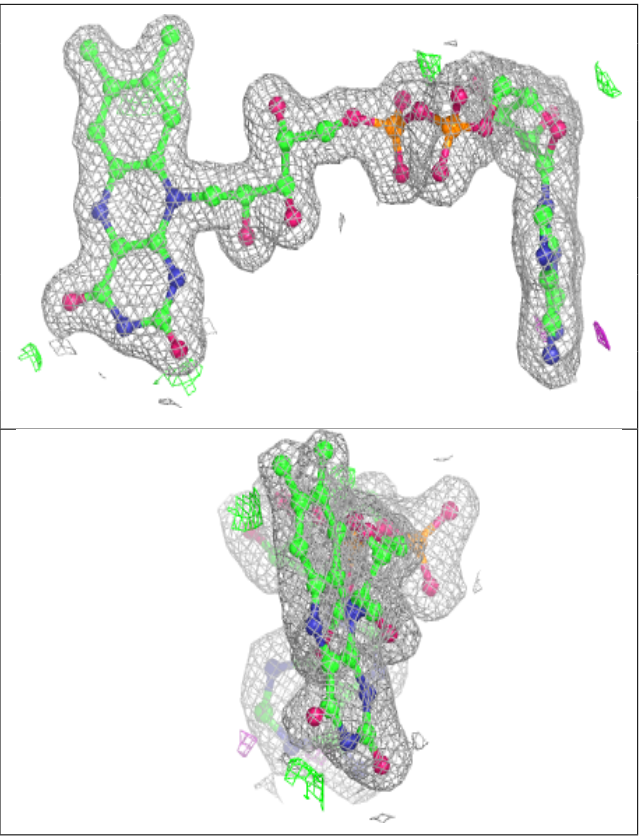


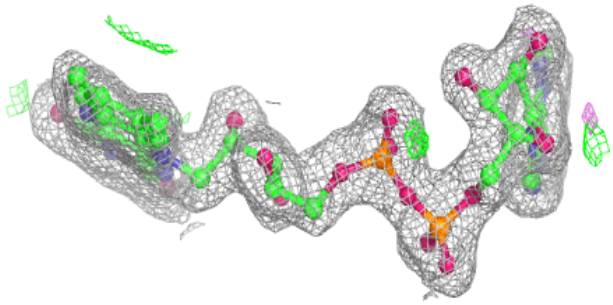




Electron density around FAD A 815:

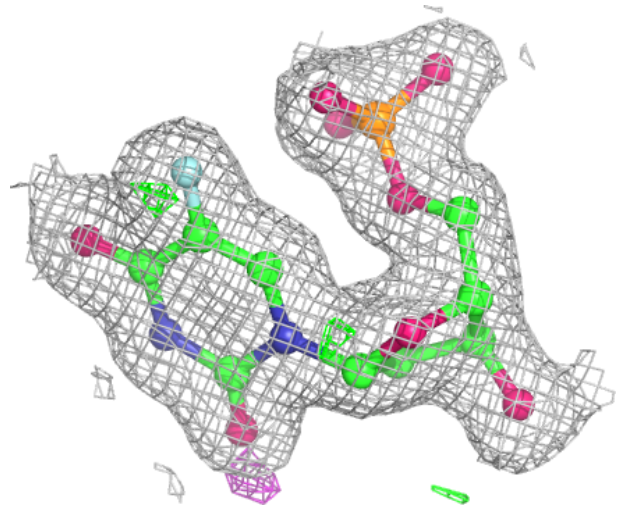
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

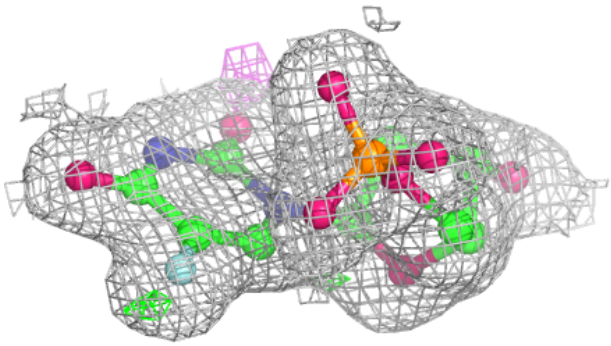


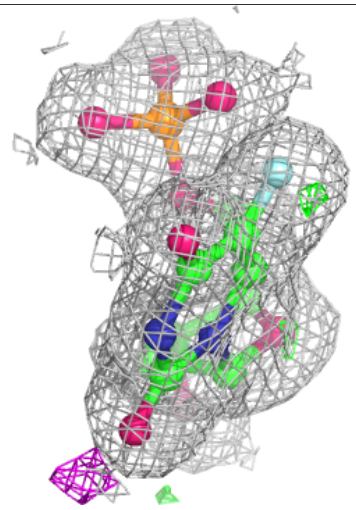


Electron density around UFP B 808:

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

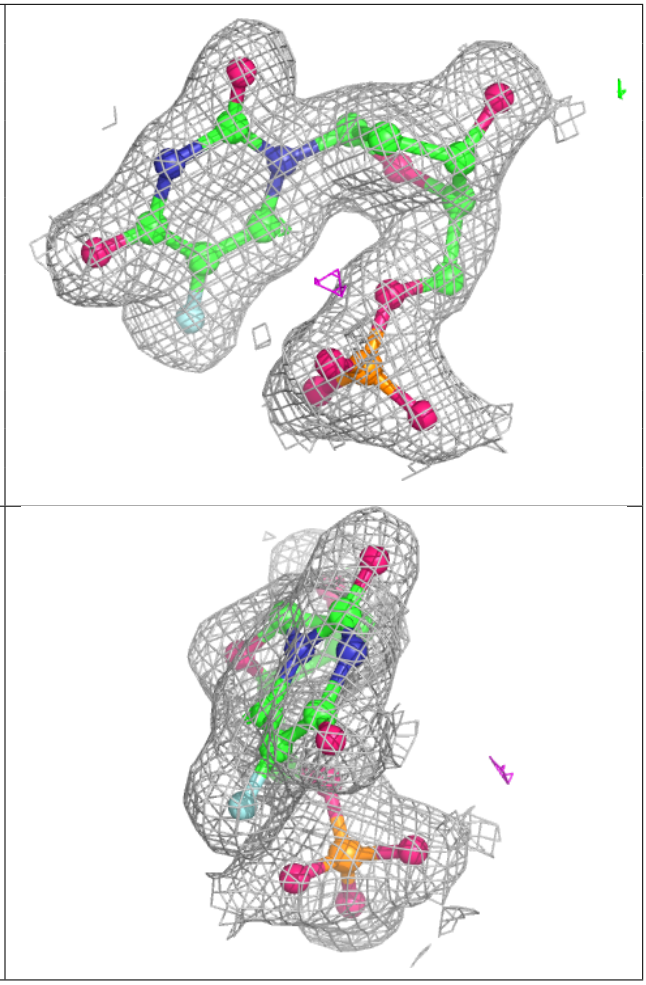






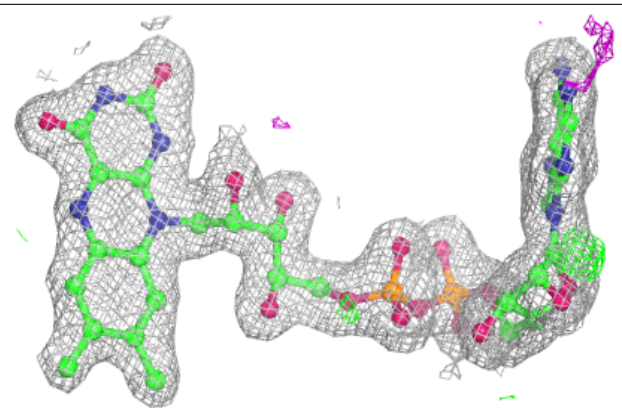
Electron density around UFP D 818:

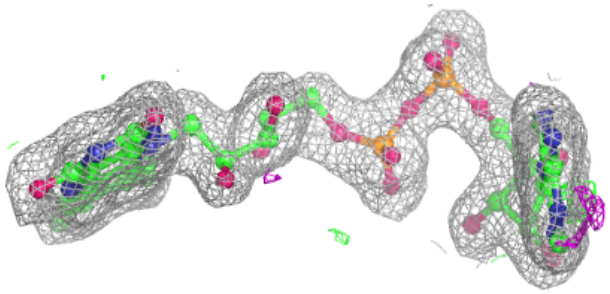
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

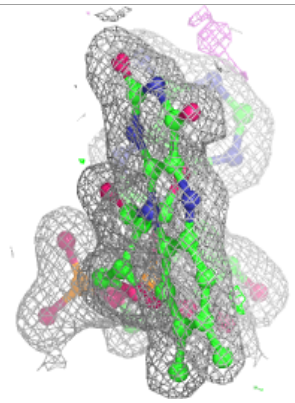


Electron density around FAD C 805:

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

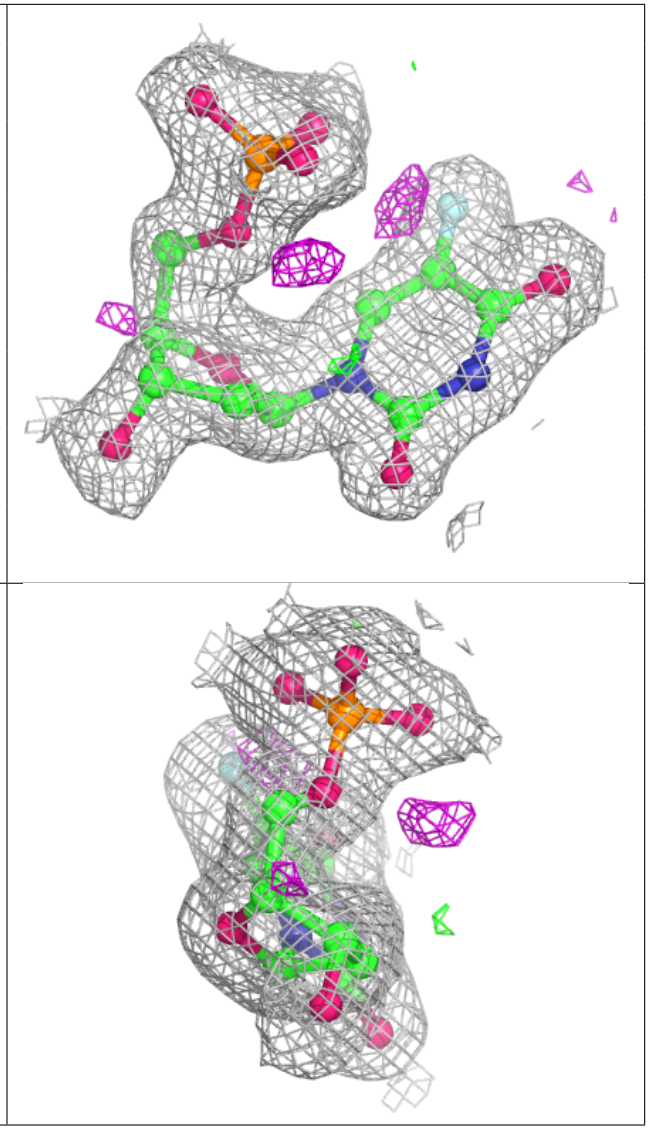






Electron density around UFP A 803:

$2mF_o$-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.