Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 09:45 am GMT

PDB ID	:	5OL2
Title	:	The electron transferring flavoprotein/butyryl-CoA dehydrogenase complex from Clostridium difficile
Authors	:	Demmer, J.K.; Chowdhury, N.P.; Selmer, T.; Ermler, U.; Buckel, W.
Deposited on	:	2017-07-26
Resolution	:	3.10 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:

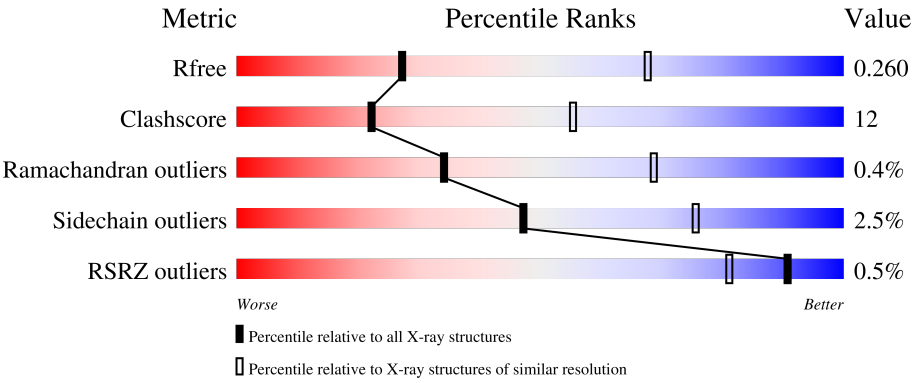
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	331	% 75% 24% .
1	D	331	% 73% 25% .
2	B	260	68% 28% .
2	E	260	71% 28% .
3	C	378	72% 26% ..

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Mol	Chain	Length	Quality of chain
3	F	378	73% 24%

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
5	CA	E	302	-	-	-	X
6	COS	C	402	-	-	-	X
6	COS	F	402	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15165 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 Electron transfer flavoprotein large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2494	1580	421	483	10			
1	D	331	Total	C	N	O	S	0	0	0
			2494	1580	421	483	10			

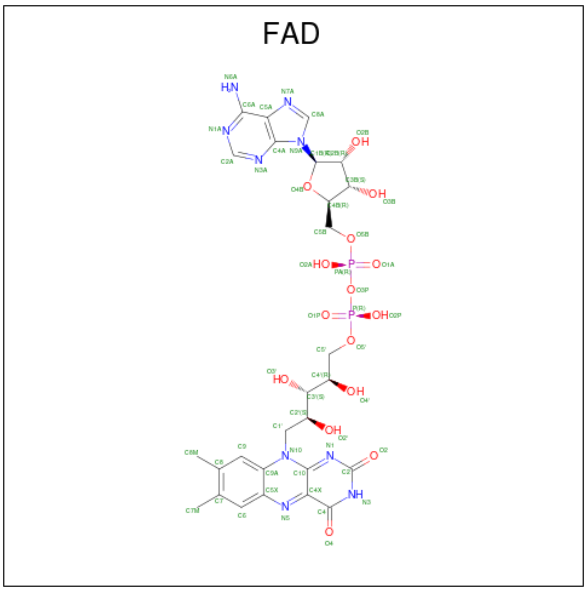
- Molecule 2 is a protein called Electron transfer flavoprotein small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	0	0	0
			1982	1254	326	390	12			
2	E	260	Total	C	N	O	S	0	0	0
			1982	1254	326	390	12			

- Molecule 3 is a protein called Acyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	0	0
			2896	1834	483	561	18			
3	F	378	Total	C	N	O	S	0	0	0
			2896	1834	483	561	18			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

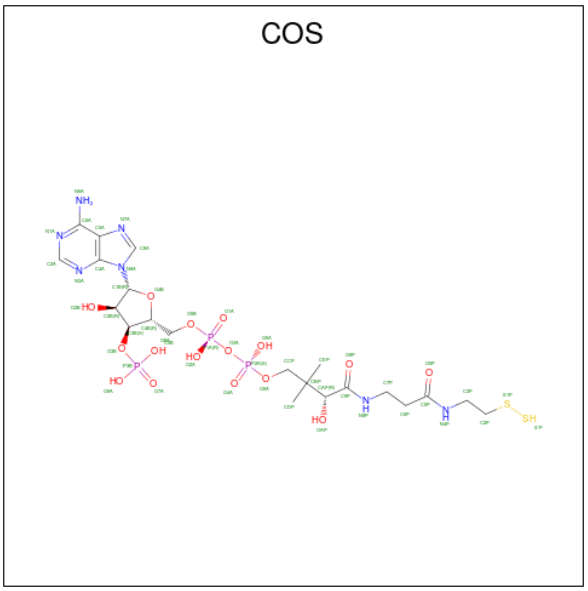


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		

- Molecule 6 is COENZYME A PERSULFIDE (three-letter code: COS) (formula: $C_{21}H_{36}N_7O_{16}P_3S_2$).



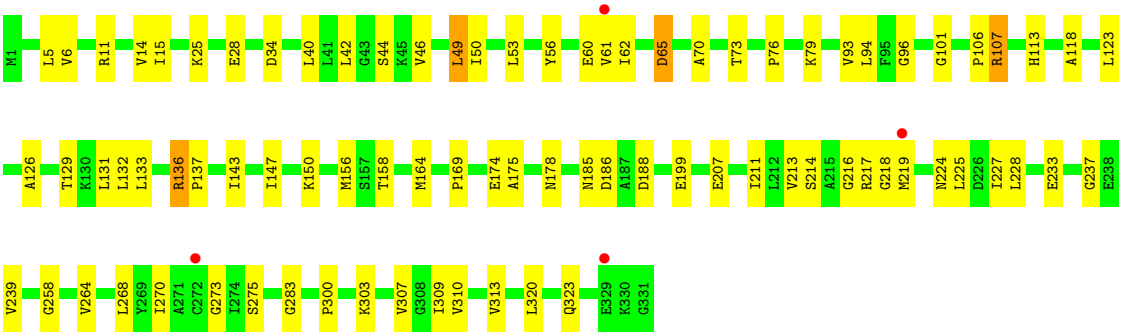
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	S	0	0
			49	21	7	16	3	2		
6	F	1	Total	C	N	O	P	S	0	0
			49	21	7	16	3	2		

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.

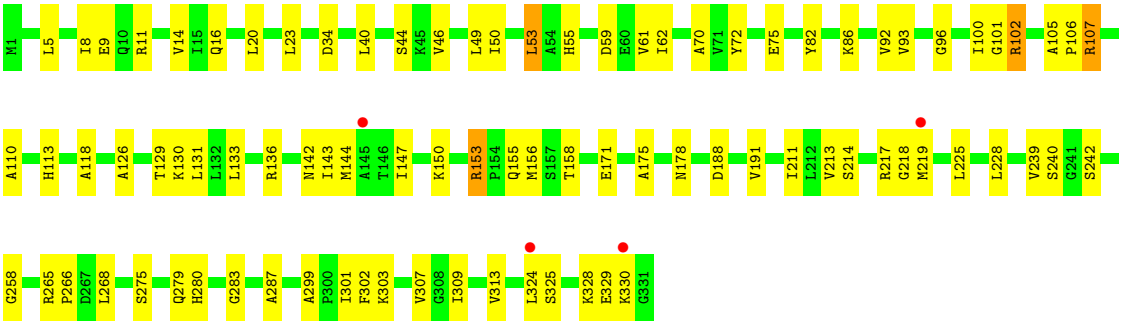
• Molecule 1: Electron transfer flavoprotein large subunit

Chain A:



• Molecule 1: Electron transfer flavoprotein large subunit

Chain D:

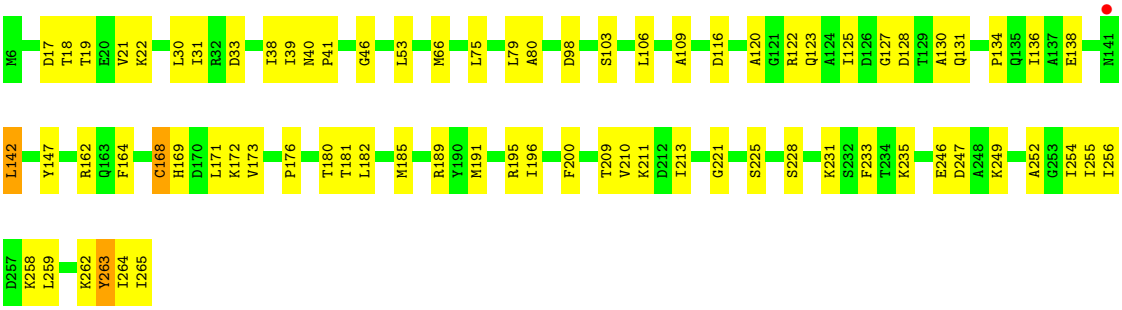


• Molecule 2: Electron transfer flavoprotein small subunit

Chain B:

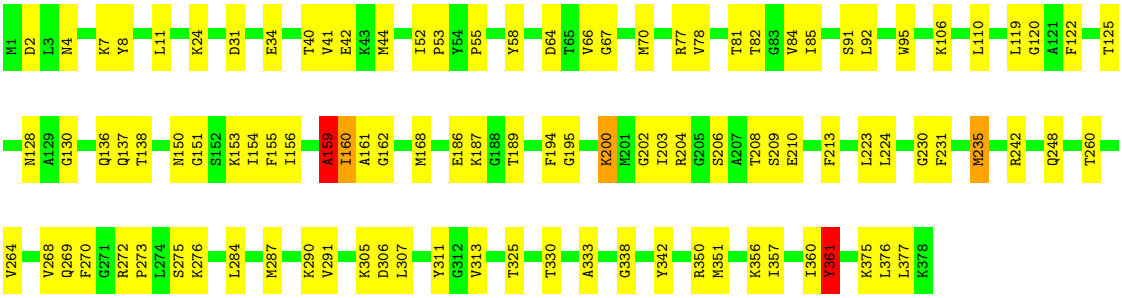
• Molecule 2: Electron transfer flavoprotein small subunit

Chain E:



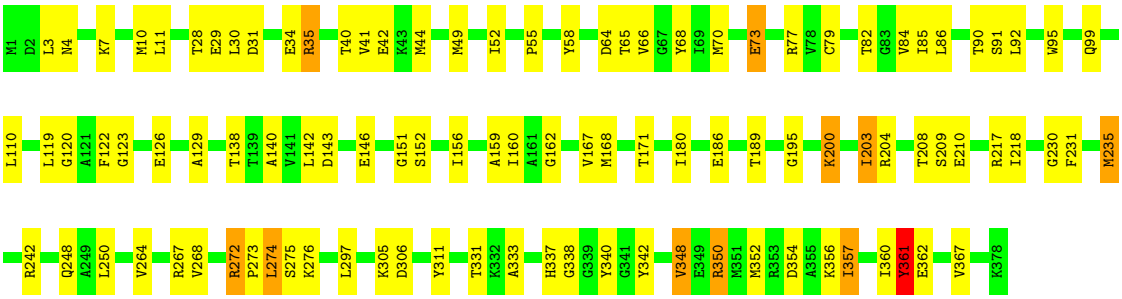
• Molecule 3: Acyl-CoA dehydrogenase

Chain C:



• Molecule 3: Acyl-CoA dehydrogenase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	177.06Å 177.06Å 493.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.87 – 3.10 48.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.87-3.10) 98.9 (48.87-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.209 , 0.260 0.209 , 0.260	Depositor DCC
R_{free} test set	3516 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	104.6	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 103.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15165	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7999e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CA, FAD, COS

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	0.69	0/2525	0.90	4/3417 (0.1%)
1	D	0.72	1/2525 (0.0%)	0.93	4/3417 (0.1%)
2	B	0.85	3/2013 (0.1%)	1.03	8/2729 (0.3%)
2	E	0.82	1/2013 (0.0%)	1.02	10/2729 (0.4%)
3	C	0.87	2/2943 (0.1%)	1.02	8/3955 (0.2%)
3	F	0.93	7/2943 (0.2%)	1.02	10/3955 (0.3%)
All	All	0.82	14/14962 (0.1%)	0.99	44/20202 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	3
3	F	0	2
All	All	0	5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	42	GLU	CG-CD	8.56	1.64	1.51
3	C	42	GLU	CG-CD	7.95	1.63	1.51
2	B	11	CYS	CB-SG	-7.30	1.69	1.82
3	F	42	GLU	CB-CG	7.21	1.65	1.52
3	C	42	GLU	CB-CG	7.01	1.65	1.52
3	F	367	VAL	CB-CG1	-6.77	1.38	1.52
2	B	208	TRP	CB-CG	-6.55	1.38	1.50
2	E	173	VAL	CB-CG2	-6.51	1.39	1.52
2	B	173	VAL	CB-CG2	-6.06	1.40	1.52
1	D	153	ARG	CB-CG	5.89	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	73	GLU	CD-OE1	5.33	1.31	1.25
3	F	357	ILE	CB-CG2	-5.08	1.37	1.52
3	F	167	VAL	CB-CG2	-5.07	1.42	1.52
3	F	348	VAL	CB-CG1	-5.01	1.42	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	361	TYR	CB-CG-CD2	-11.50	114.10	121.00
1	D	102	ARG	NE-CZ-NH1	7.84	124.22	120.30
2	E	189	ARG	NE-CZ-NH1	-7.82	116.39	120.30
3	F	35	ARG	NE-CZ-NH1	-7.77	116.42	120.30
3	C	361	TYR	CB-CG-CD2	-7.76	116.34	121.00
3	C	41	VAL	CG1-CB-CG2	-7.59	98.76	110.90
3	F	274	LEU	CB-CG-CD2	-7.41	98.40	111.00
1	A	49	LEU	CA-CB-CG	7.23	131.93	115.30
3	C	376	LEU	CB-CG-CD2	-7.01	99.07	111.00
3	F	242	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	D	102	ARG	NE-CZ-NH2	-6.43	117.08	120.30
2	B	189	ARG	CG-CD-NE	6.41	125.27	111.80
3	C	376	LEU	CA-CB-CG	6.26	129.70	115.30
2	B	222	LEU	CA-CB-CG	6.06	129.23	115.30
2	E	142	LEU	CB-CG-CD2	-6.04	100.73	111.00
3	F	203	ILE	CG1-CB-CG2	-5.99	98.23	111.40
2	E	75	LEU	CB-CG-CD1	-5.99	100.83	111.00
3	F	86	LEU	CB-CG-CD1	-5.98	100.83	111.00
3	F	350	ARG	NE-CZ-NH2	-5.93	117.33	120.30
2	B	47	LEU	CB-CG-CD2	-5.80	101.14	111.00
2	E	172	LYS	CD-CE-NZ	5.78	125.00	111.70
2	B	106	LEU	CA-CB-CG	5.78	128.59	115.30
2	E	189	ARG	NE-CZ-NH2	5.77	123.19	120.30
2	B	85	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	D	191	VAL	CG1-CB-CG2	-5.54	102.03	110.90
3	F	41	VAL	CG1-CB-CG2	-5.45	102.18	110.90
3	C	242	ARG	NE-CZ-NH1	-5.42	117.59	120.30
2	B	30	LEU	CA-CB-CG	5.36	127.63	115.30
2	E	106	LEU	CA-CB-CG	5.36	127.63	115.30
3	F	142	LEU	CA-CB-CG	5.33	127.56	115.30
3	F	242	ARG	NE-CZ-NH2	5.30	122.95	120.30
2	E	182	LEU	CB-CG-CD1	-5.25	102.08	111.00
2	E	66	MET	CG-SD-CE	5.22	108.55	100.20
3	C	242	ARG	CB-CG-CD	5.18	125.07	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	D	53	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	A	107	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	B	259	LEU	CB-CG-CD1	5.13	119.72	111.00
1	A	53	LEU	CB-CG-CD2	-5.09	102.34	111.00
2	E	75	LEU	CA-CB-CG	5.07	126.96	115.30
2	B	89	LEU	CB-CG-CD2	5.04	119.57	111.00
3	C	351	MET	CG-SD-CE	-5.03	92.16	100.20
3	C	307	LEU	CB-CG-CD2	-5.02	102.46	111.00
2	E	263	TYR	CB-CG-CD2	-5.02	117.99	121.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	159	ALA	Peptide
3	C	361	TYR	Sidechain
3	C	377	LEU	Peptide
3	F	159	ALA	Peptide
3	F	361	TYR	Sidechain

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	2494	0	2578	62	0
1	D	2494	0	2577	62	0
2	B	1982	0	2017	60	1
2	E	1982	0	2017	57	0
3	C	2896	0	2911	67	0
3	F	2896	0	2912	68	0
4	A	53	0	31	4	0
4	B	53	0	31	4	0
4	C	53	0	31	3	0
4	D	53	0	30	7	0
4	E	53	0	31	1	0
4	F	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	C	49	0	32	3	1
6	F	49	0	32	2	0
All	All	15165	0	15261	355	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (355) 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)
6:F:402:COS:C1B	6:F:402:COS:O4B	1.66	1.23
2:B:259:LEU:HD21	2:B:264:ILE:HD13	1.28	1.10
6:C:402:COS:O4B	6:C:402:COS:C1B	1.67	1.10
2:B:248:ALA:H	2:B:250:THR:HG22	1.09	1.08
2:B:248:ALA:N	2:B:250:THR:HG22	1.69	1.07
2:E:231:LYS:HE2	2:E:233:PHE:HE2	1.41	0.85
1:A:73:THR:HG23	1:A:76:PRO:HD2	1.58	0.84
3:F:34:GLU:HG2	3:F:204:ARG:HB3	1.59	0.83
2:B:259:LEU:CD2	2:B:264:ILE:HD13	2.07	0.83
2:B:248:ALA:H	2:B:250:THR:CG2	1.92	0.82
2:B:209:THR:HG23	2:B:211:LYS:HG2	1.60	0.82
1:D:5:LEU:HD21	1:D:40:LEU:HB2	1.61	0.81
2:B:122:ARG:NH1	2:B:123:GLN:OE1	2.14	0.80
1:D:275:SER:OG	4:D:401:FAD:O1A	1.99	0.80
3:C:34:GLU:HG2	3:C:204:ARG:HB3	1.62	0.80
2:B:62:THR:HG23	2:B:85:ARG:HB3	1.65	0.76
1:A:44:SER:HB2	1:A:70:ALA:HA	1.69	0.73
2:E:231:LYS:HE2	2:E:233:PHE:CE2	2.22	0.73
1:D:126:ALA:HB2	1:D:133:LEU:HD11	1.69	0.73
1:D:102:ARG:HH21	2:E:130:ALA:HB3	1.54	0.73
3:C:138:THR:HG23	3:C:151:GLY:HA3	1.72	0.71
2:E:122:ARG:NH1	2:E:123:GLN:OE1	2.23	0.71
1:D:258:GLY:HA2	1:D:283:GLY:HA3	1.73	0.70
1:A:79:LYS:NZ	1:A:188:ASP:OD2	2.19	0.69
3:F:235:MET:HE3	3:F:235:MET:HA	1.75	0.68
1:A:275:SER:OG	4:A:401:FAD:O1A	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:THR:O	3:C:44:MET:HB2	1.94	0.66
1:D:131:LEU:HD21	1:D:150:LYS:HA	1.77	0.66
1:D:211:ILE:HG23	1:D:268:LEU:HB3	1.78	0.65
1:A:62:ILE:HA	1:A:178:ASN:HB3	1.77	0.65
2:E:252:ALA:O	2:E:256:ILE:HG12	1.97	0.65
1:A:50:ILE:HG23	1:A:61:VAL:HG11	1.79	0.65
3:C:95:TRP:HE1	3:C:305:LYS:HZ3	1.44	0.65
2:E:259:LEU:HD23	2:E:264:ILE:HG12	1.78	0.64
4:C:401:FAD:O2'	6:C:402:COS:S1P	2.54	0.64
1:A:5:LEU:HD21	1:A:40:LEU:HB2	1.79	0.64
3:C:186:GLU:O	3:C:189:THR:HG23	1.96	0.64
1:A:40:LEU:HD22	1:A:42:LEU:HG	1.77	0.64
2:E:38:ILE:HD12	2:E:38:ILE:C	2.18	0.64
1:A:93:VAL:HB	1:A:156:MET:HG2	1.80	0.64
2:B:49:GLU:HG2	2:B:186:ASN:HD22	1.64	0.63
2:B:159:LEU:HD23	2:B:172:LYS:HG3	1.81	0.63
3:F:40:THR:O	3:F:44:MET:HB2	1.98	0.63
3:C:95:TRP:HE1	3:C:305:LYS:NZ	1.97	0.63
3:C:160:ILE:H	3:C:160:ILE:HD12	1.64	0.63
3:F:95:TRP:HE1	3:F:305:LYS:HZ3	1.47	0.62
2:B:165:GLU:OE1	2:B:165:GLU:N	2.31	0.62
1:D:275:SER:HB3	4:D:401:FAD:H51A	1.81	0.62
1:D:93:VAL:HB	1:D:156:MET:HG2	1.81	0.62
2:B:109:ALA:HA	2:B:213:ILE:HG22	1.82	0.61
3:F:200:LYS:NZ	3:F:208:THR:OG1	2.33	0.61
3:F:203:ILE:HD11	3:F:357:ILE:HG21	1.82	0.61
3:C:84:VAL:HG22	3:C:248:GLN:OE1	2.01	0.61
2:E:38:ILE:HD12	2:E:38:ILE:O	2.00	0.61
2:E:254:ILE:O	2:E:258:LYS:HG2	2.00	0.61
3:F:3:LEU:HD13	3:F:3:LEU:O	2.01	0.61
3:C:64:ASP:HB2	3:C:306:ASP:OD2	2.00	0.61
1:A:118:ALA:O	1:A:136:ARG:NH1	2.32	0.60
2:E:120:ALA:O	2:E:180:THR:HA	2.01	0.60
3:F:119:LEU:HD23	3:F:120:GLY:N	2.17	0.60
1:A:258:GLY:HA2	1:A:283:GLY:HA3	1.84	0.60
3:C:235:MET:HE3	3:C:235:MET:HA	1.82	0.60
2:E:181:THR:OG1	2:E:185:MET:SD	2.60	0.60
3:F:73:GLU:HG3	3:F:250:LEU:HD23	1.84	0.60
2:B:18:THR:HA	2:B:21:VAL:HG23	1.84	0.60
2:E:255:ILE:HD12	2:E:256:ILE:HG23	1.83	0.60
1:A:268:LEU:HD22	2:B:258:LYS:HE3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:196:ILE:HD12	3:F:11:LEU:HD23	1.84	0.60
1:D:325:SER:O	1:D:329:GLU:HB2	2.02	0.59
2:E:191:MET:HE1	3:F:10:MET:HG3	1.83	0.59
3:C:119:LEU:HD23	3:C:120:GLY:N	2.18	0.59
1:D:136:ARG:NH2	2:E:127:GLY:O	2.35	0.59
3:F:180:ILE:HD12	3:F:231:PHE:HB2	1.85	0.59
2:B:80:ALA:HA	2:B:195:ARG:HD3	1.85	0.59
2:E:79:LEU:O	2:E:195:ARG:NH2	2.35	0.59
3:F:337:HIS:NE2	3:F:348:VAL:HG11	2.18	0.59
1:D:217:ARG:HD2	4:D:401:FAD:O2A	2.03	0.59
2:B:209:THR:HG23	2:B:211:LYS:CG	2.32	0.58
1:A:213:VAL:O	1:A:239:VAL:HA	2.03	0.58
3:F:68:TYR:CE1	3:F:90:THR:OG1	2.53	0.58
1:A:15:ILE:HG13	1:A:49:LEU:HD12	1.84	0.58
1:D:118:ALA:O	1:D:136:ARG:NH1	2.36	0.58
2:B:46:GLY:CA	2:B:181:THR:HG21	2.33	0.58
2:B:132:VAL:HB	4:B:300:FAD:H51A	1.86	0.58
2:B:202:ASN:OD1	2:B:203:ASP:N	2.37	0.58
1:A:126:ALA:HB2	1:A:133:LEU:HD11	1.86	0.58
3:F:64:ASP:HB2	3:F:306:ASP:OD2	2.04	0.58
2:E:109:ALA:HA	2:E:213:ILE:HG22	1.86	0.57
3:C:138:THR:HG23	3:C:151:GLY:CA	2.34	0.57
2:B:23:LEU:HD23	2:B:23:LEU:H	1.69	0.57
1:A:323:GLN:OE1	2:B:251:SER:HB2	2.05	0.57
3:F:119:LEU:HD23	3:F:120:GLY:H	1.70	0.57
2:E:209:THR:HG23	2:E:211:LYS:HG2	1.86	0.57
1:A:118:ALA:HB2	2:B:131:GLN:OE1	2.04	0.57
1:A:219:MET:SD	1:A:313:VAL:HG11	2.45	0.57
1:A:147:ILE:HG23	2:B:228:SER:O	2.04	0.56
3:C:128:ASN:HB2	3:C:137:GLN:OE1	2.05	0.56
3:C:159:ALA:O	3:C:161:ALA:N	2.38	0.56
2:E:116:ASP:O	2:E:176:PRO:HA	2.05	0.56
1:D:225:LEU:HD22	1:D:228:LEU:HD12	1.88	0.56
3:F:331:THR:HG23	3:F:352:MET:HE3	1.88	0.56
1:D:46:VAL:HG22	1:D:49:LEU:HG	1.88	0.56
1:D:213:VAL:O	1:D:239:VAL:HA	2.06	0.55
1:A:300:PRO:O	1:A:303:LYS:HB3	2.05	0.55
2:E:122:ARG:HD2	2:E:147:TYR:CZ	2.42	0.55
3:C:313:VAL:HG21	3:C:375:LYS:HG3	1.89	0.55
1:A:207:GLU:HA	1:A:264:VAL:HG12	1.89	0.55
3:C:357:ILE:HD12	3:C:360:ILE:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:ILE:HA	1:D:178:ASN:HB3	1.88	0.55
2:E:200:PHE:HB2	3:F:7:LYS:HG3	1.89	0.55
3:F:84:VAL:HG22	3:F:248:GLN:OE1	2.06	0.55
2:B:184:ASP:O	2:B:186:ASN:N	2.39	0.55
1:A:211:ILE:HB	1:A:237:GLY:HA3	1.89	0.55
3:F:209:SER:OG	3:F:210:GLU:N	2.40	0.54
2:B:109:ALA:CA	2:B:213:ILE:HG22	2.36	0.54
3:C:338:GLY:HA3	4:F:401:FAD:H52A	1.90	0.54
1:D:118:ALA:HA	1:D:158:THR:OG1	2.06	0.54
3:F:203:ILE:CD1	3:F:357:ILE:HG21	2.37	0.54
2:B:120:ALA:O	2:B:180:THR:HA	2.08	0.54
2:B:259:LEU:HD23	2:B:264:ILE:HB	1.89	0.54
3:C:119:LEU:HD23	3:C:120:GLY:H	1.71	0.54
1:D:9:GLU:OE2	1:D:11:ARG:NH2	2.41	0.54
3:F:138:THR:HG23	3:F:151:GLY:HA3	1.89	0.54
3:C:82:THR:HA	3:C:85:ILE:HD12	1.90	0.53
1:D:242:SER:HA	1:D:280:HIS:CE1	2.42	0.53
2:B:146:THR:HG22	2:B:180:THR:OG1	2.09	0.53
3:C:209:SER:OG	3:C:210:GLU:N	2.42	0.53
3:F:119:LEU:HB3	3:F:162:GLY:HA2	1.90	0.53
3:F:186:GLU:O	3:F:189:THR:HG23	2.07	0.53
3:C:305:LYS:HD2	3:C:311:TYR:CZ	2.43	0.53
1:D:59:ASP:O	1:D:175:ALA:HB1	2.09	0.53
3:F:337:HIS:CD2	3:F:348:VAL:HG11	2.43	0.53
1:A:225:LEU:HD22	1:A:228:LEU:HD12	1.90	0.53
3:F:52:ILE:HD12	3:F:52:ILE:H	1.73	0.53
2:E:46:GLY:CA	2:E:181:THR:HG21	2.39	0.53
2:E:98:ASP:HA	4:E:301:FAD:H1'2	1.89	0.53
1:D:307:VAL:HG12	1:D:309:ILE:HD13	1.92	0.52
1:A:211:ILE:CG2	1:A:268:LEU:HD23	2.39	0.52
1:A:174:GLU:HG3	1:A:175:ALA:H	1.73	0.52
3:F:28:THR:HG22	3:F:350:ARG:HH21	1.73	0.52
2:B:231:LYS:HE2	2:B:233:PHE:HE2	1.74	0.52
3:F:305:LYS:HD2	3:F:311:TYR:CZ	2.45	0.52
3:F:354:ASP:O	3:F:357:ILE:HG22	2.10	0.52
1:A:174:GLU:HG3	1:A:175:ALA:N	2.25	0.52
1:D:299:ALA:HB1	1:D:301:ILE:HG22	1.91	0.52
2:E:164:PHE:HE2	2:E:169:HIS:CD2	2.28	0.52
2:E:256:ILE:HA	2:E:259:LEU:HD12	1.92	0.52
1:D:266:PRO:HD2	1:D:287:ALA:HB2	1.91	0.51
2:E:169:HIS:HB3	2:E:171:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HD2	4:A:401:FAD:O2A	2.10	0.51
2:B:210:VAL:O	2:B:213:ILE:HG12	2.11	0.51
1:D:44:SER:HB2	1:D:70:ALA:HA	1.91	0.51
1:D:20:LEU:HA	1:D:23:LEU:HD12	1.92	0.51
1:A:268:LEU:HD21	1:A:270:ILE:HD11	1.91	0.51
3:C:168:MET:HE1	3:C:230:GLY:O	2.11	0.51
1:D:129:THR:HB	1:D:131:LEU:CD1	2.40	0.51
1:A:275:SER:O	1:A:300:PRO:HD2	2.11	0.51
3:C:150:ASN:HA	3:C:213:PHE:O	2.10	0.51
2:B:231:LYS:HE2	2:B:233:PHE:CE2	2.45	0.51
3:C:55:PRO:HG2	3:C:58:TYR:HD2	1.75	0.51
3:F:110:LEU:HD13	3:F:110:LEU:O	2.11	0.51
3:C:330:THR:O	3:C:333:ALA:HB3	2.12	0.50
1:D:142:ASN:HB3	2:E:30:LEU:HD11	1.92	0.50
3:C:264:VAL:HG13	3:C:275:SER:HB3	1.94	0.50
3:C:203:ILE:HG22	3:C:206:SER:HB3	1.93	0.50
2:E:247:ASP:OD1	2:E:247:ASP:N	2.45	0.50
1:A:225:LEU:HD22	1:A:228:LEU:CD1	2.42	0.50
2:B:80:ALA:HA	2:B:195:ARG:HB3	1.93	0.50
2:B:80:ALA:HB3	2:B:191:MET:HE2	1.94	0.50
3:F:126:GLU:HB2	3:F:129:ALA:HB3	1.93	0.50
3:F:140:ALA:HB3	3:F:171:THR:HG22	1.93	0.50
2:E:131:GLN:O	2:E:134:PRO:HD2	2.12	0.49
3:F:55:PRO:HG2	3:F:58:TYR:HD2	1.77	0.49
3:F:362:GLU:HA	6:F:402:COS:S1P	2.51	0.49
1:A:320:LEU:HD12	2:B:255:ILE:HD11	1.94	0.49
3:C:125:THR:HG23	3:C:130:GLY:HA2	1.94	0.49
2:E:80:ALA:HA	2:E:195:ARG:HB3	1.94	0.49
3:C:52:ILE:HD12	3:C:52:ILE:H	1.77	0.49
1:D:11:ARG:NH1	1:D:16:GLN:OE1	2.46	0.49
2:E:17:ASP:HA	2:E:125:ILE:HD11	1.93	0.49
3:F:200:LYS:HZ3	3:F:208:THR:CB	2.26	0.48
1:D:107:ARG:NH2	2:E:142:LEU:O	2.47	0.48
1:D:126:ALA:O	1:D:130:LYS:HA	2.13	0.48
2:E:38:ILE:HD13	2:E:39:ILE:O	2.14	0.48
3:F:58:TYR:HB3	3:F:110:LEU:HD12	1.94	0.48
1:A:136:ARG:NH2	2:B:127:GLY:O	2.45	0.48
2:B:46:GLY:HA3	2:B:181:THR:HG21	1.94	0.48
1:D:218:GLY:HA2	4:D:401:FAD:C8A	2.43	0.48
1:A:25:LYS:NZ	1:A:28:GLU:OE2	2.47	0.48
2:B:98:ASP:HA	4:B:300:FAD:H1'2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:GLU:HG3	2:B:249:LYS:HB2	1.96	0.48
3:C:235:MET:HA	3:C:235:MET:CE	2.44	0.48
3:C:160:ILE:HA	3:C:194:PHE:CE2	2.48	0.48
1:A:11:ARG:O	1:A:14:VAL:HG22	2.14	0.48
3:C:273:PRO:HG2	3:C:276:LYS:HG2	1.96	0.48
1:D:75:GLU:HG2	1:D:188:ASP:HA	1.95	0.48
3:F:99:GLN:O	3:F:99:GLN:HG3	2.14	0.48
1:D:11:ARG:O	1:D:14:VAL:HG22	2.14	0.47
1:D:328:LYS:HB3	2:E:265:ILE:HG23	1.95	0.47
3:F:92:LEU:HB3	3:F:122:PHE:HB2	1.96	0.47
3:F:123:GLY:HA2	3:F:156:ILE:CD1	2.44	0.47
1:A:218:GLY:HA2	4:A:401:FAD:C8A	2.44	0.47
3:C:203:ILE:HD12	3:C:357:ILE:HG21	1.95	0.47
1:D:242:SER:HA	1:D:280:HIS:HE1	1.79	0.47
3:F:235:MET:HA	3:F:235:MET:CE	2.42	0.47
3:F:274:LEU:HA	3:F:274:LEU:HD23	1.64	0.47
1:A:217:ARG:HB3	4:A:401:FAD:H52A	1.96	0.47
2:B:45:ALA:O	2:B:48:GLU:HB3	2.15	0.47
4:C:401:FAD:H52A	3:F:338:GLY:HA3	1.97	0.47
1:A:96:GLY:O	1:A:101:GLY:HA3	2.15	0.47
3:C:92:LEU:HB3	3:C:122:PHE:CB	2.45	0.47
3:C:136:GLN:OE1	3:C:153:LYS:NZ	2.45	0.46
3:C:154:ILE:HD12	3:C:154:ILE:O	2.15	0.46
1:D:219:MET:SD	1:D:313:VAL:HG11	2.55	0.46
2:E:258:LYS:HB3	2:E:263:TYR:HD2	1.79	0.46
3:F:31:ASP:OD1	3:F:204:ARG:HD2	2.16	0.46
2:B:122:ARG:HD2	2:B:147:TYR:CZ	2.50	0.46
2:B:235:LYS:HA	2:B:235:LYS:HD2	1.40	0.46
3:C:287:MET:O	3:C:291:VAL:HG23	2.15	0.46
1:D:147:ILE:HG23	2:E:228:SER:O	2.14	0.46
3:C:200:LYS:HZ3	3:C:208:THR:CB	2.27	0.46
3:F:143:ASP:OD2	3:F:217:ARG:NH2	2.48	0.46
1:A:106:PRO:HB3	2:B:131:GLN:HG2	1.97	0.46
1:A:211:ILE:HG23	1:A:268:LEU:HB3	1.96	0.46
3:F:195:GLY:HA3	3:F:210:GLU:HB3	1.97	0.46
1:D:55:HIS:CE1	1:D:171:GLU:HA	2.51	0.46
2:E:235:LYS:HD2	2:E:235:LYS:HA	1.73	0.46
2:B:200:PHE:HB2	3:C:7:LYS:HG3	1.98	0.46
3:F:138:THR:HG23	3:F:151:GLY:CA	2.46	0.46
1:D:301:ILE:HG13	1:D:302:PHE:H	1.80	0.45
3:F:146:GLU:HA	3:F:218:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ILE:HG23	1:A:268:LEU:HD23	1.97	0.45
3:F:66:VAL:O	3:F:70:MET:HG3	2.17	0.45
2:B:40:ASN:HA	2:B:41:PRO:HD3	1.76	0.45
3:C:357:ILE:HD11	4:C:401:FAD:HM83	1.98	0.45
1:A:213:VAL:HG12	1:A:228:LEU:HD22	1.98	0.45
2:E:255:ILE:HD12	2:E:256:ILE:N	2.31	0.45
1:A:73:THR:HG23	1:A:76:PRO:CD	2.38	0.45
3:F:168:MET:HE1	3:F:230:GLY:O	2.17	0.45
3:F:92:LEU:HB3	3:F:122:PHE:CB	2.47	0.45
1:A:224:ASN:O	1:A:227:ILE:HG22	2.17	0.45
1:D:144:MET:HB2	2:E:233:PHE:CE1	2.52	0.45
2:E:40:ASN:HA	2:E:41:PRO:HD3	1.79	0.45
3:C:231:PHE:HZ	6:C:402:COS:H132	1.81	0.45
3:C:203:ILE:HG22	3:C:203:ILE:O	2.16	0.45
3:C:260:THR:HG21	3:C:333:ALA:HA	1.99	0.45
3:C:357:ILE:HB	3:F:342:TYR:CE1	2.52	0.45
1:A:131:LEU:HD21	1:A:150:LYS:HA	1.97	0.45
3:C:223:LEU:HD12	3:C:224:LEU:N	2.31	0.45
1:D:82:TYR:CZ	1:D:86:LYS:HD3	2.52	0.45
3:F:297:LEU:HD23	3:F:297:LEU:HA	1.74	0.44
1:A:129:THR:HB	1:A:131:LEU:HD12	1.98	0.44
3:C:8:TYR:HD1	3:C:11:LEU:HD12	1.82	0.44
3:F:156:ILE:HD13	3:F:156:ILE:HA	1.80	0.44
1:D:8:ILE:HG12	1:D:53:LEU:HD21	2.00	0.44
1:D:92:VAL:HG22	1:D:155:GLN:HB2	1.98	0.44
2:E:80:ALA:HB3	2:E:191:MET:HE2	2.00	0.44
1:D:301:ILE:O	1:D:302:PHE:HB2	2.18	0.44
1:D:275:SER:HB3	4:D:401:FAD:C5B	2.48	0.44
1:A:44:SER:HB2	1:A:70:ALA:CA	2.43	0.44
2:E:246:GLU:HB3	2:E:249:LYS:HG3	1.99	0.44
3:F:267:ARG:HG3	3:F:274:LEU:HG	1.99	0.44
3:C:268:VAL:HG13	3:C:272:ARG:C	2.38	0.44
1:D:96:GLY:O	1:D:101:GLY:HA3	2.17	0.44
2:B:40:ASN:HD22	2:B:43:ASP:CG	2.21	0.43
2:B:49:GLU:HG2	2:B:186:ASN:ND2	2.31	0.43
2:B:122:ARG:NH1	2:B:123:GLN:HB2	2.33	0.43
2:B:194:GLY:HA2	2:B:197:TYR:HB2	2.00	0.43
3:C:154:ILE:O	3:C:155:PHE:HB2	2.19	0.43
1:A:25:LYS:HG3	1:A:164:MET:SD	2.58	0.43
1:A:211:ILE:O	1:A:237:GLY:HA3	2.19	0.43
3:C:202:GLY:O	3:C:204:ARG:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:PRO:HB3	2:E:131:GLN:HG2	1.99	0.43
3:F:268:VAL:HG13	3:F:272:ARG:C	2.39	0.43
3:C:200:LYS:NZ	3:C:208:THR:OG1	2.41	0.43
4:D:401:FAD:H9	4:D:401:FAD:H1'1	1.74	0.43
3:C:81:THR:HG22	3:C:203:ILE:HG23	2.00	0.43
3:F:95:TRP:HE1	3:F:305:LYS:NZ	2.13	0.43
1:A:216:GLY:HA3	1:A:273:GLY:O	2.19	0.43
2:B:129:THR:HG23	4:B:300:FAD:O1P	2.19	0.43
3:C:156:ILE:HD13	3:C:156:ILE:HA	1.70	0.43
3:C:284:LEU:HA	3:C:284:LEU:HD23	1.50	0.43
3:F:82:THR:HA	3:F:85:ILE:HD12	2.00	0.43
1:A:118:ALA:HA	1:A:158:THR:OG1	2.18	0.43
1:A:46:VAL:HG12	1:A:65:ASP:OD1	2.19	0.43
1:A:136:ARG:HA	1:A:137:PRO:HD3	1.84	0.43
1:A:307:VAL:HG12	1:A:309:ILE:HD13	2.00	0.43
2:B:187:THR:HA	2:B:188:PRO:HD3	1.65	0.43
2:E:53:LEU:HD23	2:E:53:LEU:HA	1.88	0.43
3:F:273:PRO:HG2	3:F:276:LYS:HG2	2.01	0.43
3:C:357:ILE:HG13	3:C:361:TYR:CD1	2.53	0.42
1:D:105:ALA:N	1:D:106:PRO:HD2	2.34	0.42
1:D:129:THR:O	1:D:131:LEU:HD12	2.19	0.42
1:D:279:GLN:NE2	3:F:340:TYR:CZ	2.87	0.42
2:B:254:ILE:O	2:B:258:LYS:HG3	2.19	0.42
3:C:342:TYR:CE1	3:F:357:ILE:HB	2.54	0.42
1:D:50:ILE:H	1:D:50:ILE:HG13	1.55	0.42
2:E:210:VAL:O	2:E:213:ILE:HG12	2.19	0.42
1:A:49:LEU:CD2	1:A:49:LEU:H	2.32	0.42
3:C:66:VAL:O	3:C:70:MET:HG3	2.19	0.42
2:B:107:ALA:HA	2:B:110:LEU:HD12	2.02	0.42
3:C:31:ASP:HB2	3:C:350:ARG:HD3	2.01	0.42
2:E:22:LYS:O	2:E:31:ILE:HG12	2.19	0.42
1:A:186:ASP:C	1:A:188:ASP:H	2.23	0.42
1:D:330:LYS:NZ	1:D:330:LYS:HB3	2.34	0.42
3:C:361:TYR:HD1	3:C:361:TYR:H	1.68	0.42
2:E:125:ILE:HD13	2:E:125:ILE:HG21	1.76	0.42
2:E:162:ARG:O	2:E:168:CYS:HA	2.20	0.42
3:F:29:GLU:OE1	3:F:35:ARG:NH2	2.51	0.42
1:A:56:TYR:CE1	1:A:169:PRO:HD3	2.55	0.41
3:C:273:PRO:HG2	3:C:276:LYS:CG	2.51	0.41
1:D:72:TYR:CE2	1:D:100:ILE:HG23	2.55	0.41
1:A:6:VAL:HG22	1:A:94:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:THR:HG22	4:B:300:FAD:H5'2	2.01	0.41
2:B:248:ALA:CA	2:B:250:THR:HG22	2.45	0.41
1:D:301:ILE:C	1:D:303:LYS:H	2.22	0.41
2:E:221:GLY:O	2:E:225:SER:OG	2.30	0.41
1:A:123:LEU:HB3	1:A:132:LEU:HD21	2.02	0.41
2:B:31:ILE:O	2:B:31:ILE:HG13	2.19	0.41
2:E:18:THR:HA	2:E:21:VAL:HG23	2.02	0.41
3:F:30:LEU:HD23	3:F:35:ARG:HD2	2.02	0.41
2:B:252:ALA:O	2:B:256:ILE:HD12	2.20	0.41
1:D:214:SER:HA	1:D:240:SER:O	2.20	0.41
1:D:313:VAL:HG23	4:D:401:FAD:C2A	2.51	0.41
2:E:262:LYS:O	2:E:263:TYR:CD1	2.73	0.41
3:F:203:ILE:HD13	3:F:203:ILE:HG21	1.81	0.41
2:B:208:TRP:N	2:B:208:TRP:CD1	2.87	0.41
3:C:8:TYR:HA	3:C:11:LEU:HD12	2.01	0.41
3:C:269:GLN:O	3:C:270:PHE:HB2	2.20	0.41
1:D:324:LEU:HD21	2:E:255:ILE:CG2	2.51	0.41
2:E:103:SER:CB	2:E:136:ILE:HG13	2.50	0.41
3:C:195:GLY:HA3	3:C:210:GLU:HB3	2.03	0.41
2:B:181:THR:OG1	2:B:185:MET:SD	2.79	0.41
3:C:106:LYS:O	3:C:110:LEU:HB3	2.21	0.41
1:D:110:ALA:HB3	2:E:138:GLU:HG2	2.02	0.41
3:F:49:MET:H	3:F:49:MET:HG3	1.74	0.41
3:F:357:ILE:HD12	3:F:360:ILE:HB	2.03	0.41
1:A:143:ILE:HD12	1:A:143:ILE:HG23	1.74	0.41
2:E:19:THR:H	2:E:19:THR:HG23	1.67	0.41
3:C:67:GLY:HA2	3:C:70:MET:HG3	2.03	0.41
2:E:30:LEU:HD12	2:E:30:LEU:HA	1.91	0.41
3:F:65:THR:HG21	3:F:305:LYS:HE3	2.02	0.41
1:A:60:GLU:OE2	1:A:62:ILE:HD11	2.20	0.40
2:B:161:LYS:HE2	2:B:170:ASP:OD1	2.22	0.40
3:C:290:LYS:HB3	3:C:325:THR:HG23	2.03	0.40
1:D:50:ILE:HG23	1:D:61:VAL:HG11	2.04	0.40
3:C:162:GLY:O	3:C:187:LYS:HD2	2.22	0.40
1:D:136:ARG:HH11	1:D:136:ARG:HD2	1.74	0.40
2:E:123:GLN:HE21	2:E:128:ASP:HA	1.86	0.40
3:F:333:ALA:O	3:F:337:HIS:HD2	2.04	0.40
3:C:24:LYS:HB2	3:C:78:VAL:HG21	2.02	0.40
1:A:300:PRO:O	1:A:303:LYS:CB	2.69	0.40
1:A:310:VAL:HG23	2:B:244:TYR:O	2.22	0.40
1:D:143:ILE:HD12	1:D:143:ILE:HG23	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:264:VAL:HG13	3:F:275:SER:HB3	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:THR:CG2	6:C:402:COS:C2A[10_455]	2.00	0.20

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	329/331 (99%)	309 (94%)	20 (6%)	0	100	100
1	D	329/331 (99%)	306 (93%)	23 (7%)	0	100	100
2	B	258/260 (99%)	231 (90%)	24 (9%)	3 (1%)	13	44
2	E	258/260 (99%)	232 (90%)	26 (10%)	0	100	100
3	C	376/378 (100%)	348 (93%)	25 (7%)	3 (1%)	19	54
3	F	376/378 (100%)	346 (92%)	29 (8%)	1 (0%)	41	73
All	All	1926/1938 (99%)	1772 (92%)	147 (8%)	7 (0%)	34	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	185	MET
3	C	160	ILE
3	F	160	ILE
2	B	184	ASP
2	B	248	ALA
3	C	159	ALA
3	C	53	PRO

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	266/266 (100%)	258 (97%)	8 (3%)	41 71
1	D	266/266 (100%)	261 (98%)	5 (2%)	57 81
2	B	218/218 (100%)	211 (97%)	7 (3%)	39 69
2	E	218/218 (100%)	216 (99%)	2 (1%)	78 91
3	C	301/301 (100%)	293 (97%)	8 (3%)	44 74
3	F	301/301 (100%)	291 (97%)	10 (3%)	38 69
All	All	1570/1570 (100%)	1530 (98%)	40 (2%)	47 75

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	65	ASP
1	A	107	ARG
1	A	113	HIS
1	A	185	ASN
1	A	199	GLU
1	A	214	SER
1	A	233	GLU
2	B	32	ARG
2	B	163	GLN
2	B	168	CYS
2	B	170	ASP
2	B	189	ARG
2	B	195	ARG
2	B	257	ASP
3	C	2	ASP
3	C	4	ASN
3	C	77	ARG
3	C	91	SER
3	C	200	LYS
3	C	235	MET
3	C	356	LYS

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Mol	Chain	Res	Type
3	C	361	TYR
1	D	34	ASP
1	D	107	ARG
1	D	113	HIS
1	D	153	ARG
1	D	265	ARG
2	E	33	ASP
2	E	168	CYS
3	F	4	ASN
3	F	77	ARG
3	F	79	CYS
3	F	91	SER
3	F	152	SER
3	F	200	LYS
3	F	235	MET
3	F	272	ARG
3	F	356	LYS
3	F	361	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	169	HIS
3	F	337	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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	FAD	C	401	-	53,58,58	0.80	1 (1%)	68,89,89	0.86	2 (2%)
4	FAD	D	401	1	53,58,58	1.26	4 (7%)	68,89,89	1.12	6 (8%)
4	FAD	F	401	-	53,58,58	0.83	2 (3%)	68,89,89	1.10	7 (10%)
4	FAD	E	301	-	53,58,58	0.76	2 (3%)	68,89,89	0.79	2 (2%)
4	FAD	A	401	-	53,58,58	0.57	0	68,89,89	0.83	5 (7%)
6	COS	C	402	3,2	42,51,51	4.39	17 (40%)	54,76,76	2.34	15 (27%)
4	FAD	B	300	-	53,58,58	0.63	2 (3%)	68,89,89	1.00	5 (7%)
6	COS	F	402	-	42,51,51	4.19	15 (35%)	54,76,76	2.07	12 (22%)

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	FAD	C	401	-	-	5/30/50/50	0/6/6/6
4	FAD	D	401	1	-	15/30/50/50	0/6/6/6
4	FAD	F	401	-	-	4/30/50/50	0/6/6/6
4	FAD	E	301	-	-	1/30/50/50	0/6/6/6
4	FAD	A	401	-	-	13/30/50/50	0/6/6/6
6	COS	C	402	3,2	-	22/44/65/65	0/3/3/3
4	FAD	B	300	-	-	5/30/50/50	0/6/6/6
6	COS	F	402	-	-	10/44/65/65	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	402	COS	O4B-C1B	18.70	1.67	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	402	COS	O4B-C1B	18.53	1.66	1.41
6	C	402	COS	C2B-C1B	-12.26	1.35	1.53
6	F	402	COS	C2B-C1B	-12.02	1.35	1.53
6	C	402	COS	C9P-N8P	8.15	1.51	1.33
6	C	402	COS	C5P-N4P	7.55	1.50	1.33
6	F	402	COS	C9P-N8P	7.32	1.49	1.33
6	F	402	COS	C5P-N4P	6.25	1.47	1.33
6	F	402	COS	P3B-O3B	6.01	1.70	1.59
6	F	402	COS	O4B-C4B	-5.40	1.32	1.45
4	D	401	FAD	C10-N1	5.37	1.44	1.33
6	C	402	COS	O4B-C4B	-5.08	1.33	1.45
6	C	402	COS	P3B-O3B	4.87	1.68	1.59
6	C	402	COS	C6P-C5P	4.84	1.60	1.51
4	D	401	FAD	O2-C2	4.63	1.32	1.24
6	C	402	COS	C2A-N3A	3.88	1.38	1.32
6	C	402	COS	C6A-N6A	3.69	1.47	1.34
6	F	402	COS	C3B-C4B	3.63	1.62	1.52
6	F	402	COS	C6A-N6A	3.44	1.46	1.34
6	C	402	COS	O5P-C5P	3.43	1.30	1.23
4	F	401	FAD	P-O2P	-3.10	1.40	1.55
6	C	402	COS	C3B-C4B	2.98	1.60	1.52
6	F	402	COS	C2A-N3A	2.90	1.36	1.32
6	C	402	COS	C7P-N8P	2.79	1.52	1.46
6	C	402	COS	C2A-N1A	2.77	1.39	1.33
4	C	401	FAD	P-O2P	-2.69	1.42	1.55
4	E	301	FAD	P-O2P	-2.61	1.43	1.55
4	D	401	FAD	C10-N10	2.57	1.42	1.37
6	C	402	COS	P1A-O5B	2.43	1.69	1.59
6	C	402	COS	O3B-C3B	-2.39	1.35	1.44
6	F	402	COS	P1A-O5B	2.38	1.68	1.59
6	F	402	COS	O2B-C2B	2.36	1.48	1.43
6	C	402	COS	O9P-C9P	-2.34	1.18	1.23
6	C	402	COS	O2B-C2B	2.33	1.48	1.43
6	F	402	COS	C2B-C3B	2.30	1.58	1.52
6	F	402	COS	O9P-C9P	-2.29	1.18	1.23
4	F	401	FAD	PA-O5B	-2.20	1.50	1.59
4	D	401	FAD	P-O2P	-2.16	1.45	1.55
4	B	300	FAD	P-O2P	-2.16	1.45	1.55
6	F	402	COS	O5P-C5P	-2.12	1.19	1.23
4	E	301	FAD	C8A-N7A	-2.09	1.31	1.34
6	F	402	COS	C5B-C4B	2.03	1.57	1.51
4	B	300	FAD	C8A-N7A	-2.02	1.31	1.34

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	402	COS	C5A-C6A-N6A	7.85	132.28	120.35
6	C	402	COS	C7P-C6P-C5P	7.23	124.40	112.36
6	C	402	COS	C5A-C6A-N6A	6.40	130.07	120.35
6	F	402	COS	N6A-C6A-N1A	-5.63	106.88	118.57
6	F	402	COS	N3A-C2A-N1A	-5.51	120.07	128.68
6	C	402	COS	C6P-C5P-N4P	-5.21	107.65	116.42
6	C	402	COS	N6A-C6A-N1A	-4.80	108.61	118.57
6	C	402	COS	N3A-C2A-N1A	-4.42	121.77	128.68
6	C	402	COS	CAP-C9P-N8P	4.18	124.91	116.58
6	C	402	COS	C2P-S1P-S'P	4.05	121.93	103.44
6	C	402	COS	O4B-C1B-C2B	-3.91	101.21	106.93
6	C	402	COS	O6A-CCP-CBP	3.74	116.55	110.55
6	C	402	COS	O5P-C5P-C6P	3.73	128.84	122.02
6	F	402	COS	O4B-C1B-C2B	-3.73	101.48	106.93
4	B	300	FAD	O3'-C3'-C4'	-3.54	100.26	108.81
4	D	401	FAD	O2-C2-N1	3.43	127.52	121.83
6	F	402	COS	C2P-S1P-S'P	3.25	118.25	103.44
4	F	401	FAD	O4'-C4'-C3'	3.09	116.62	109.10
6	F	402	COS	C7P-N8P-C9P	-2.99	117.25	122.59
6	C	402	COS	O5B-C5B-C4B	2.98	119.25	108.99
4	F	401	FAD	O4'-C4'-C5'	-2.96	103.28	109.92
4	A	401	FAD	O5B-PA-O1A	-2.95	97.55	109.07
6	F	402	COS	O5B-C5B-C4B	2.93	119.09	108.99
6	C	402	COS	O9P-C9P-N8P	-2.93	116.71	122.99
4	C	401	FAD	O2A-PA-O1A	2.87	126.42	112.24
4	F	401	FAD	O2A-PA-O1A	2.86	126.37	112.24
4	E	301	FAD	O3'-C3'-C4'	-2.83	101.97	108.81
4	B	300	FAD	O2P-P-O1P	2.81	126.12	112.24
6	F	402	COS	C3B-C2B-C1B	2.75	105.98	99.89
6	F	402	COS	CEP-CBP-CAP	2.70	113.51	108.82
6	F	402	COS	C7P-C6P-C5P	-2.66	107.93	112.36
4	F	401	FAD	O4B-C1B-C2B	-2.63	103.08	106.93
4	B	300	FAD	O5'-P-O1P	-2.63	98.79	109.07
4	F	401	FAD	C4'-C3'-C2'	2.56	118.68	113.36
4	D	401	FAD	C4'-C3'-C2'	-2.52	108.12	113.36
6	C	402	COS	C3B-C2B-C1B	2.47	105.37	99.89
4	A	401	FAD	O2A-PA-O5B	2.44	119.09	107.75
4	B	300	FAD	O2'-C2'-C3'	-2.44	103.18	109.10
4	E	301	FAD	C4'-C3'-C2'	2.43	118.41	113.36
4	D	401	FAD	O5B-PA-O1A	-2.40	99.70	109.07
4	D	401	FAD	C3B-C2B-C1B	-2.33	97.47	100.98
4	D	401	FAD	O4B-C1B-C2B	-2.32	103.54	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	401	FAD	C5A-C6A-N6A	2.31	123.86	120.35
4	B	300	FAD	O4'-C4'-C3'	-2.30	103.50	109.10
4	A	401	FAD	C5A-C6A-N6A	2.30	123.85	120.35
4	F	401	FAD	P-O3P-PA	-2.29	124.98	132.83
4	F	401	FAD	O2A-PA-O5B	-2.27	97.18	107.75
4	A	401	FAD	O5'-P-O1P	2.20	117.67	109.07
6	C	402	COS	C4A-C5A-N7A	-2.18	107.13	109.40
6	F	402	COS	O5P-C5P-C6P	-2.16	118.07	122.02
6	F	402	COS	CDP-CBP-CCP	2.09	111.63	108.23
6	C	402	COS	OAP-CAP-CBP	-2.07	105.37	110.25
4	D	401	FAD	C5A-C6A-N6A	2.01	123.41	120.35
4	A	401	FAD	O3B-C3B-C4B	-2.01	105.23	111.05

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	FAD	C1'-C2'-C3'-C4'
4	A	401	FAD	C5'-O5'-P-O1P
4	B	300	FAD	C5B-O5B-PA-O3P
4	C	401	FAD	C1'-C2'-C3'-O3'
4	C	401	FAD	C1'-C2'-C3'-C4'
4	D	401	FAD	P-O3P-PA-O5B
4	D	401	FAD	C5'-O5'-P-O1P
4	D	401	FAD	C5'-O5'-P-O3P
4	F	401	FAD	C5B-O5B-PA-O1A
6	C	402	COS	C5B-O5B-P1A-O1A
6	C	402	COS	C5B-O5B-P1A-O2A
6	C	402	COS	CCP-O6A-P2A-O4A
6	C	402	COS	CCP-O6A-P2A-O5A
6	C	402	COS	CBP-CCP-O6A-P2A
6	C	402	COS	CEP-CBP-CCP-O6A
6	C	402	COS	CAP-CBP-CCP-O6A
6	C	402	COS	OAP-CAP-CBP-CCP
6	C	402	COS	C9P-CAP-CBP-CCP
6	C	402	COS	OAP-CAP-CBP-CDP
6	C	402	COS	C9P-CAP-CBP-CDP
6	C	402	COS	C9P-CAP-CBP-CEP
6	F	402	COS	C3B-O3B-P3B-O7A
6	F	402	COS	C3B-C4B-C5B-O5B
6	F	402	COS	O4B-C4B-C5B-O5B
6	F	402	COS	CCP-O6A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
6	F	402	COS	CCP-O6A-P2A-O5A
6	F	402	COS	S1P-C2P-C3P-N4P
4	F	401	FAD	O4B-C4B-C5B-O5B
6	C	402	COS	C3B-C4B-C5B-O5B
6	C	402	COS	O4B-C4B-C5B-O5B
4	F	401	FAD	C3B-C4B-C5B-O5B
4	A	401	FAD	C2'-C3'-C4'-C5'
4	D	401	FAD	C2'-C3'-C4'-C5'
6	C	402	COS	CDP-CBP-CCP-O6A
4	C	401	FAD	O2'-C2'-C3'-C4'
4	A	401	FAD	O3'-C3'-C4'-C5'
4	A	401	FAD	O2'-C2'-C3'-O3'
4	C	401	FAD	O2'-C2'-C3'-O3'
4	A	401	FAD	O2'-C2'-C3'-C4'
4	D	401	FAD	O2'-C2'-C3'-O3'
4	D	401	FAD	O3'-C3'-C4'-C5'
4	D	401	FAD	O2'-C2'-C3'-C4'
6	C	402	COS	OAP-CAP-CBP-CEP
6	C	402	COS	O9P-C9P-CAP-CBP
4	B	300	FAD	C4'-C5'-O5'-P
6	C	402	COS	C3B-O3B-P3B-O7A
6	C	402	COS	N8P-C9P-CAP-OAP
4	F	401	FAD	C5B-O5B-PA-O3P
6	C	402	COS	CCP-O6A-P2A-O3A
6	F	402	COS	C5B-O5B-P1A-O3A
4	C	401	FAD	PA-O3P-P-O1P
4	E	301	FAD	C4'-C5'-O5'-P
4	B	300	FAD	C5B-O5B-PA-O1A
4	D	401	FAD	C5'-O5'-P-O2P
6	F	402	COS	C5B-O5B-P1A-O1A
6	C	402	COS	S1P-C2P-C3P-N4P
4	D	401	FAD	C3B-C4B-C5B-O5B
4	A	401	FAD	C4'-C5'-O5'-P
4	B	300	FAD	C2'-C3'-C4'-C5'
4	B	300	FAD	PA-O3P-P-O1P
4	A	401	FAD	O3'-C3'-C4'-O4'
4	D	401	FAD	C4'-C5'-O5'-P
4	D	401	FAD	O4'-C4'-C5'-O5'
6	C	402	COS	C5B-O5B-P1A-O3A
6	F	402	COS	C3B-O3B-P3B-O9A
6	F	402	COS	CCP-O6A-P2A-O3A
4	A	401	FAD	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
4	A	401	FAD	PA-O3P-P-O1P
4	D	401	FAD	PA-O3P-P-O2P
4	D	401	FAD	C2'-C3'-C4'-O4'
4	D	401	FAD	C5B-O5B-PA-O1A
4	A	401	FAD	O4B-C4B-C5B-O5B
4	A	401	FAD	C1'-C2'-C3'-O3'
4	D	401	FAD	C1'-C2'-C3'-O3'
4	A	401	FAD	N10-C1'-C2'-O2'

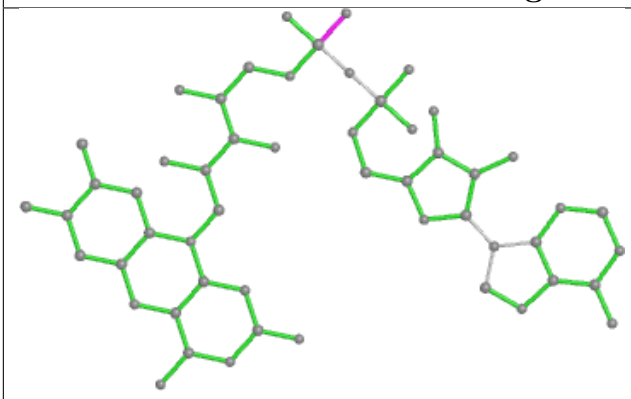
There are no ring outliers.

8 monomers are involved in 25 short contacts:

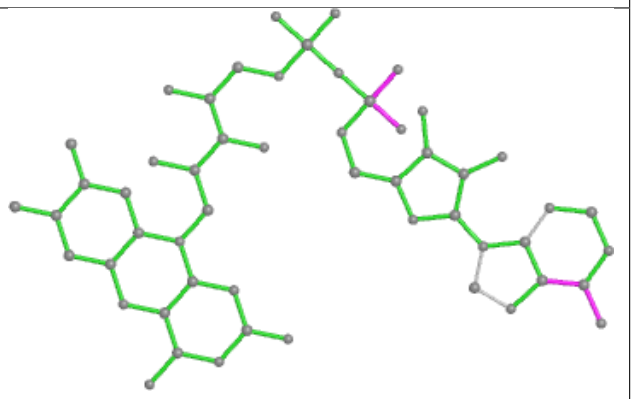
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	FAD	3	0
4	D	401	FAD	7	0
4	F	401	FAD	1	0
4	E	301	FAD	1	0
4	A	401	FAD	4	0
6	C	402	COS	3	1
4	B	300	FAD	4	0
6	F	402	COS	2	0

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

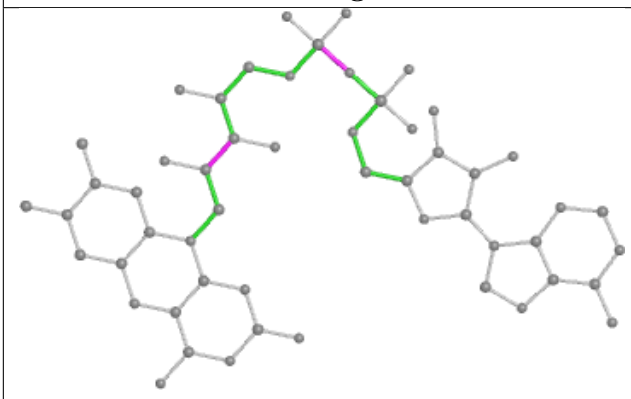
Ligand FAD C 401



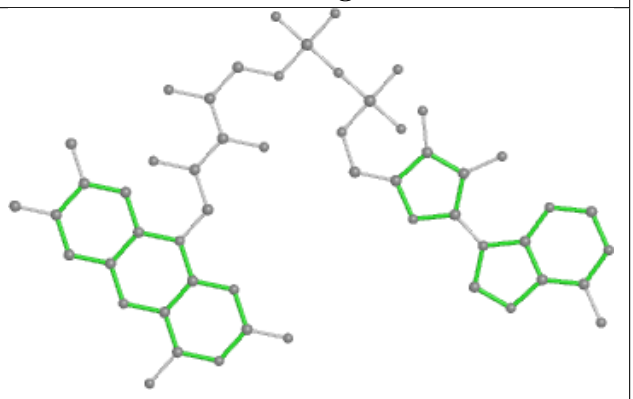
Bond lengths



Bond angles

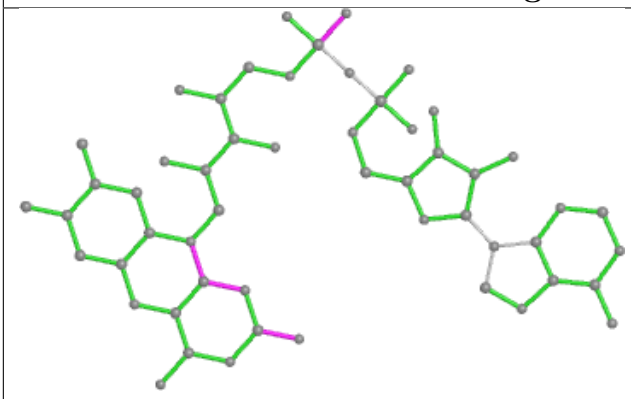


Torsions

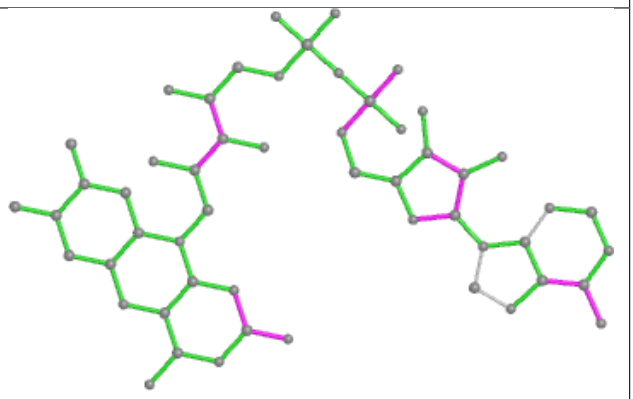


Rings

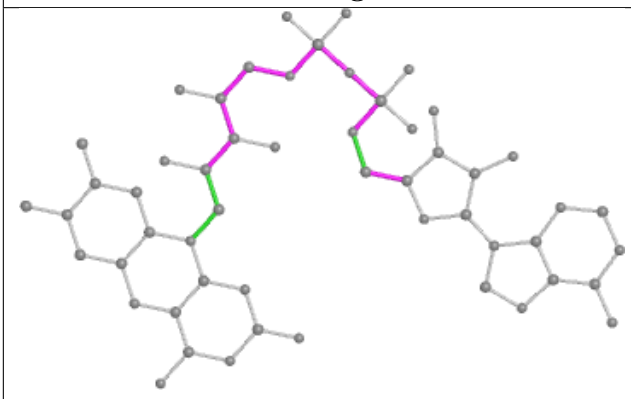
Ligand FAD D 401



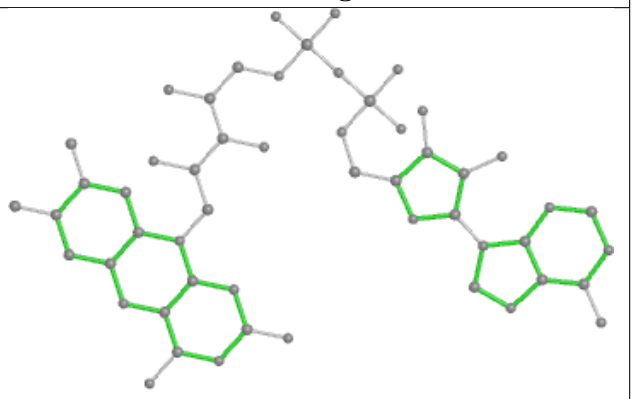
Bond lengths



Bond angles

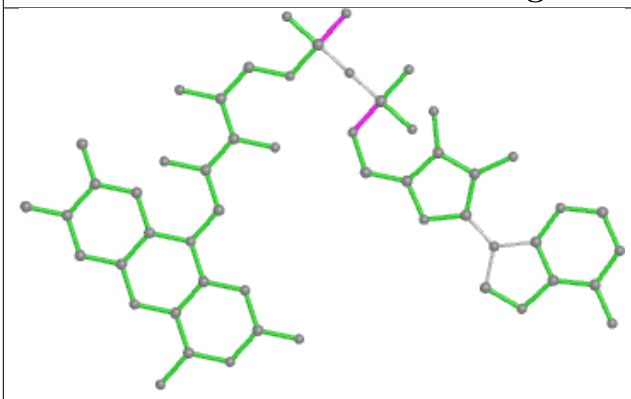


Torsions

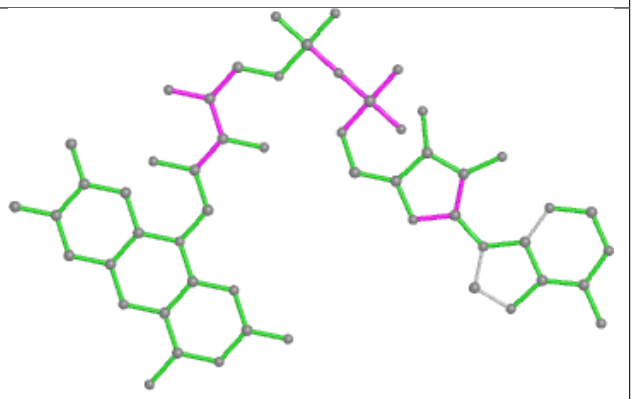


Rings

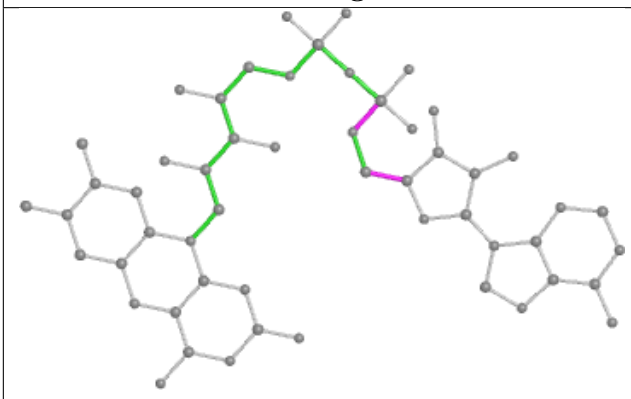
Ligand FAD F 401



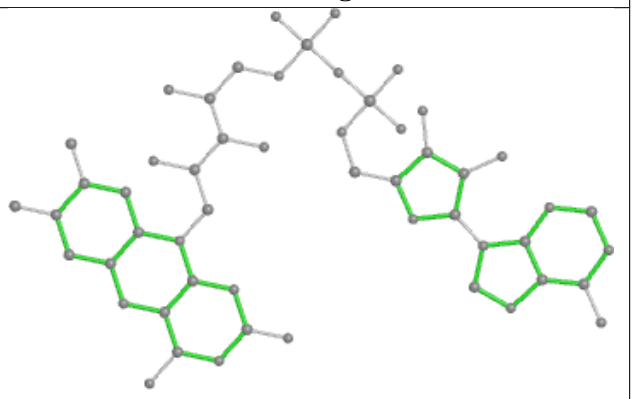
Bond lengths



Bond angles

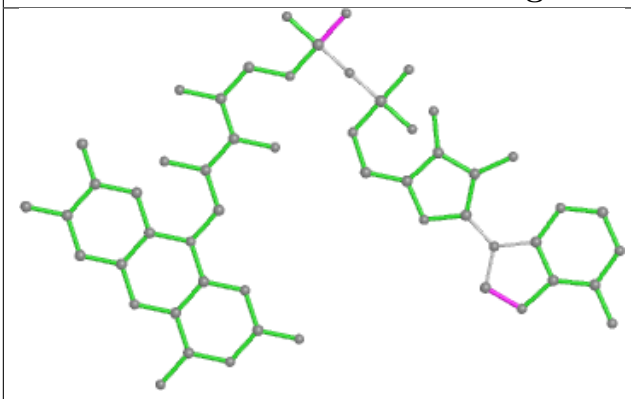


Torsions

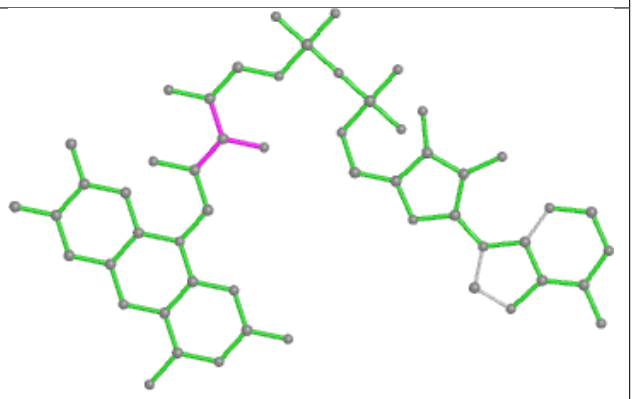


Rings

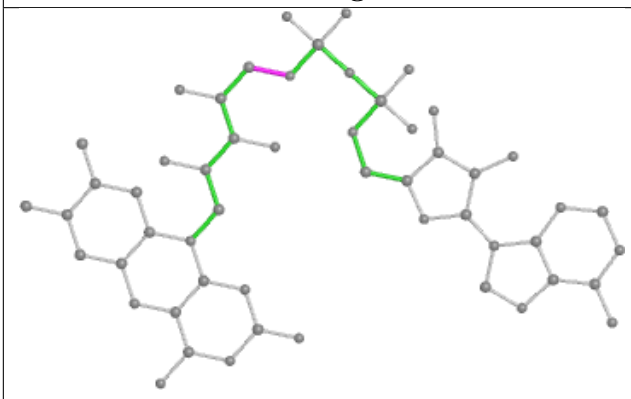
Ligand FAD E 301



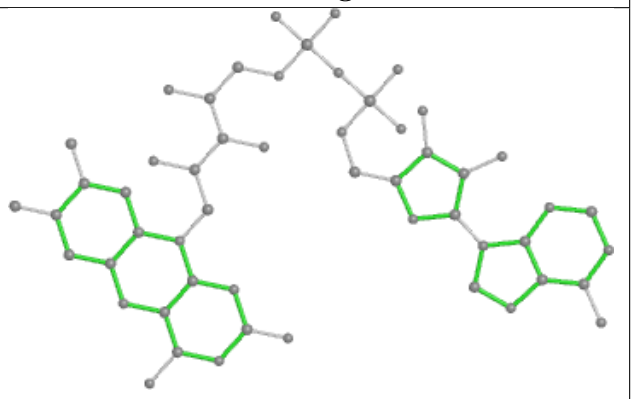
Bond lengths



Bond angles

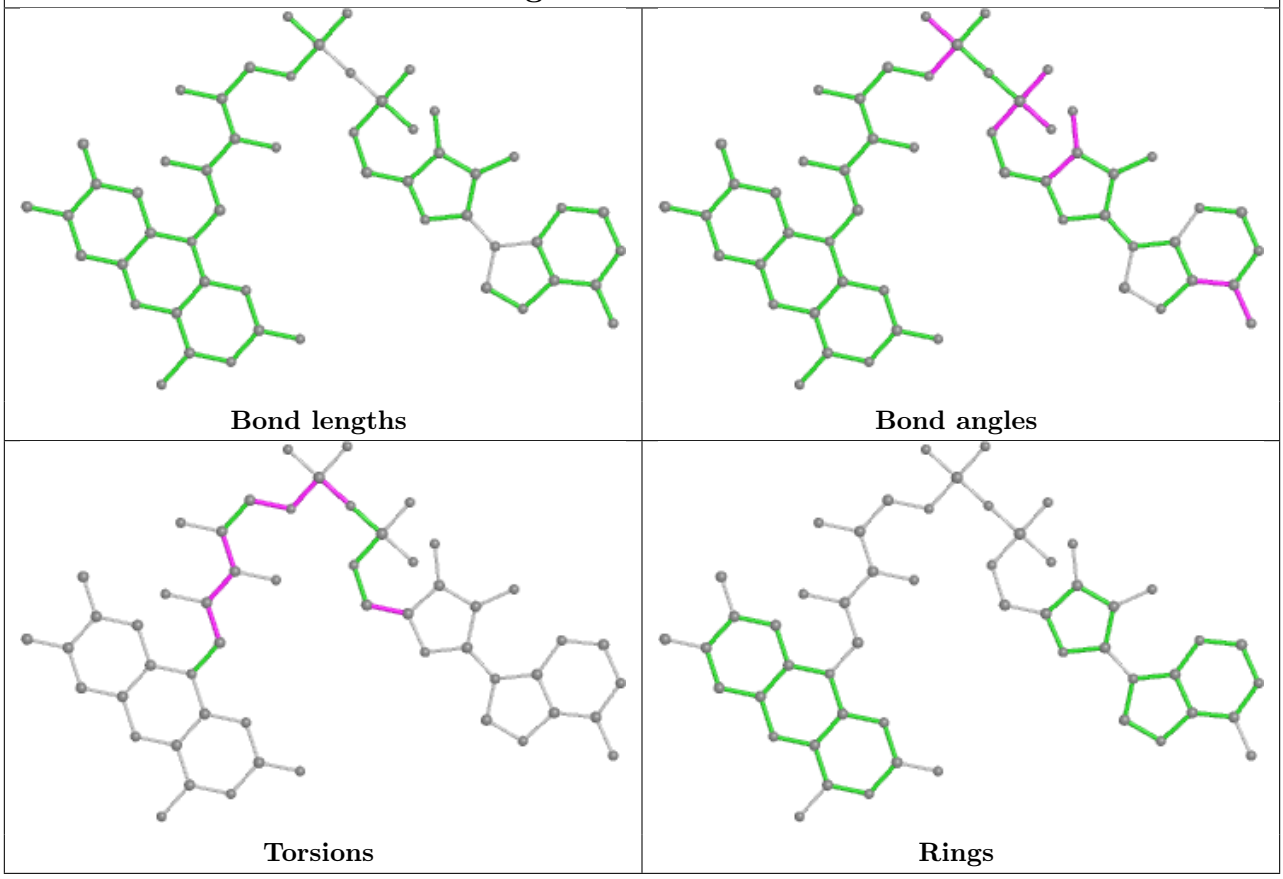


Torsions

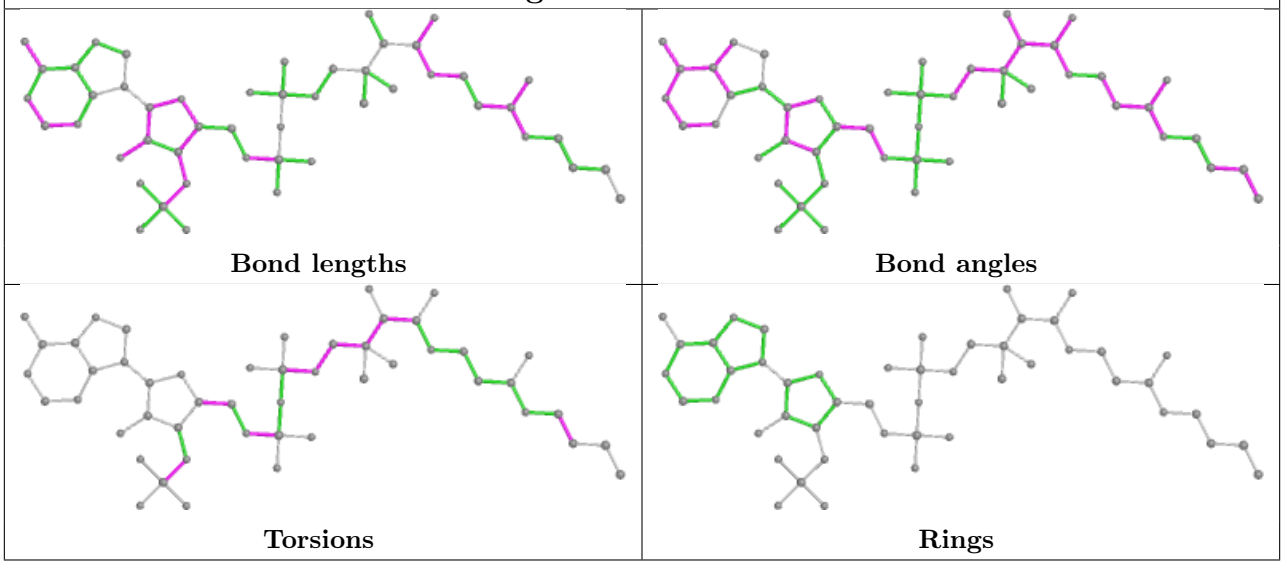


Rings

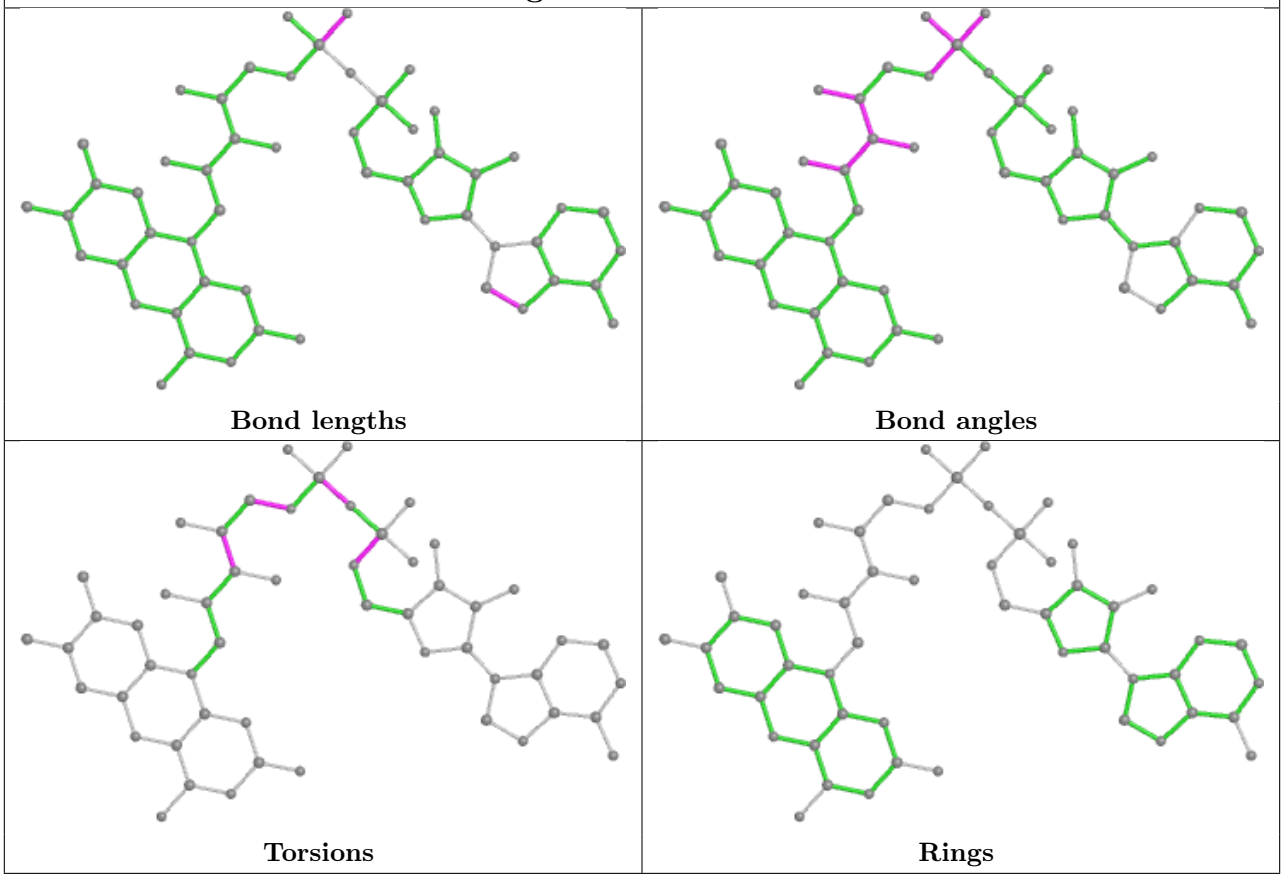
Ligand FAD A 401



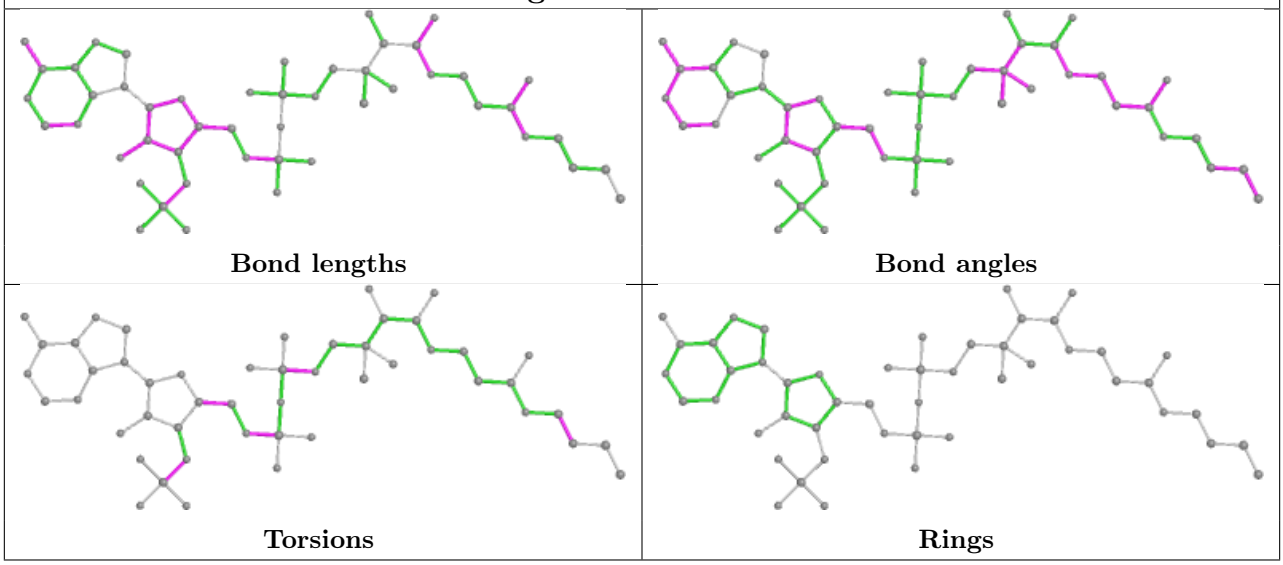
Ligand COS C 402



Ligand FAD B 300



Ligand COS F 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	331/331 (100%)	-0.12	4 (1%) 79 61	103, 134, 181, 244	0
1	D	331/331 (100%)	-0.19	4 (1%) 79 61	107, 143, 190, 243	0
2	B	260/260 (100%)	-0.31	0 100 100	103, 126, 177, 261	0
2	E	260/260 (100%)	-0.29	1 (0%) 92 84	98, 126, 184, 233	0
3	C	378/378 (100%)	-0.48	0 100 100	81, 113, 146, 197	0
3	F	378/378 (100%)	-0.43	0 100 100	82, 113, 143, 174	0
All	All	1938/1938 (100%)	-0.31	9 (0%) 91 81	81, 126, 176, 261	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	141	ASN	3.0
1	A	272	CYS	2.7
1	D	219	MET	2.3
1	D	324	LEU	2.2
1	D	330	LYS	2.1
1	A	61	VAL	2.1
1	A	329	GLU	2.1
1	A	219	MET	2.1
1	D	145	ALA	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

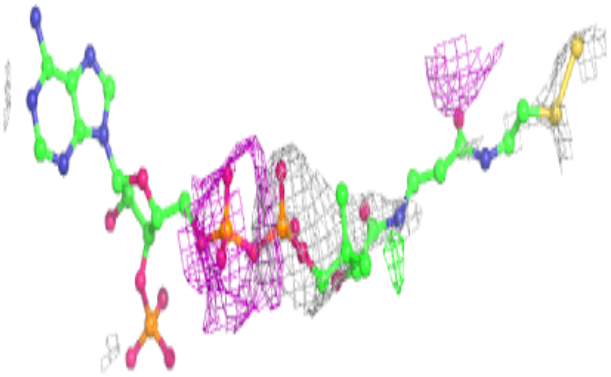
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

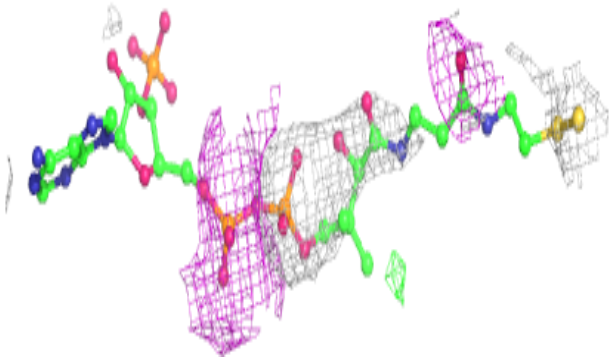
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	E	302	1/1	0.31	2.26	319,319,319,319	0
5	CA	F	403	1/1	0.49	0.10	159,159,159,159	0
6	COS	C	402	49/49	0.61	0.67	145,258,325,330	0
6	COS	F	402	49/49	0.68	0.64	162,272,312,316	0
5	CA	A	402	1/1	0.76	0.36	108,108,108,108	0
5	CA	C	403	1/1	0.88	0.08	146,146,146,146	0
4	FAD	A	401	53/53	0.95	0.15	95,126,144,160	0
4	FAD	D	401	53/53	0.95	0.15	98,136,166,175	0
5	CA	D	402	1/1	0.96	0.58	122,122,122,122	0
4	FAD	F	401	53/53	0.97	0.21	79,103,126,132	0
4	FAD	C	401	53/53	0.97	0.17	81,102,130,133	0
4	FAD	B	300	53/53	0.97	0.16	101,112,148,169	0
4	FAD	E	301	53/53	0.97	0.17	92,114,142,146	0

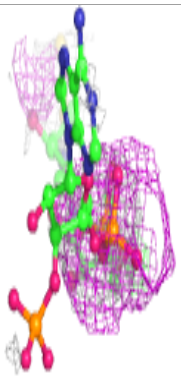
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COS C 402:

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

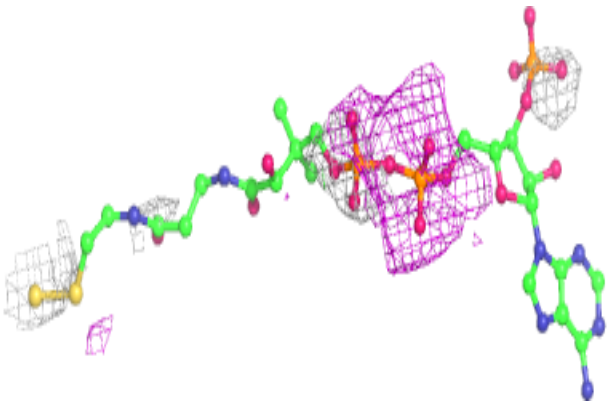


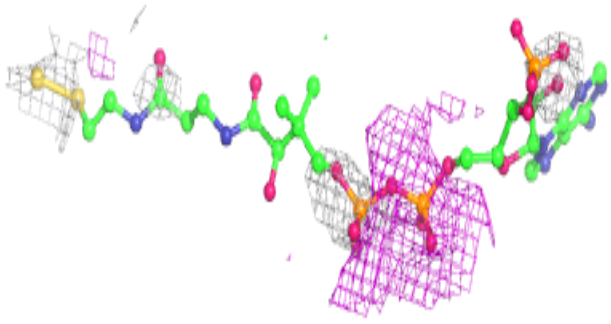


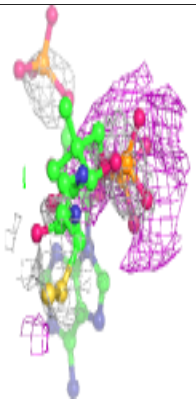


Electron density around COS F 402:

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

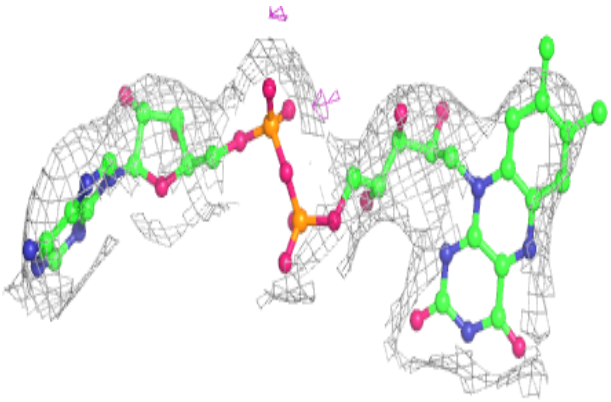


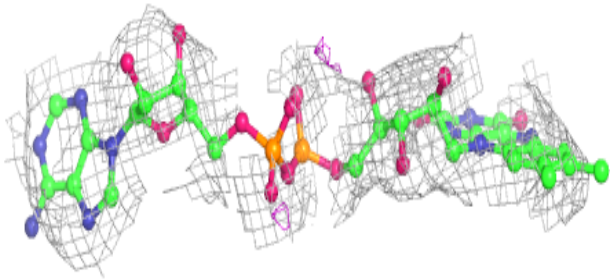


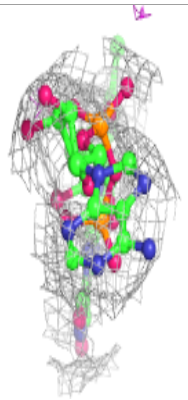


Electron density around FAD A 401:

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

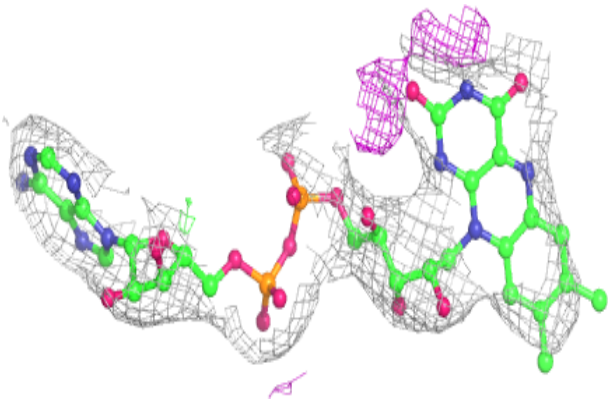


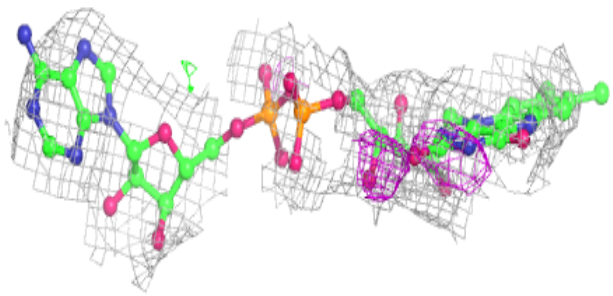


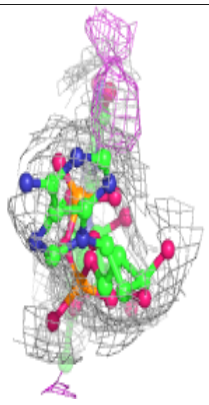


Electron density around FAD D 401:

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

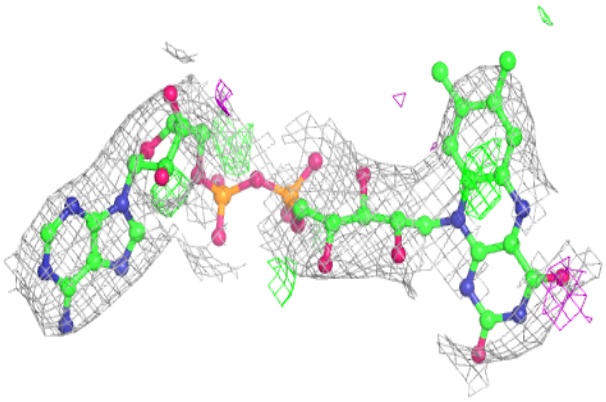


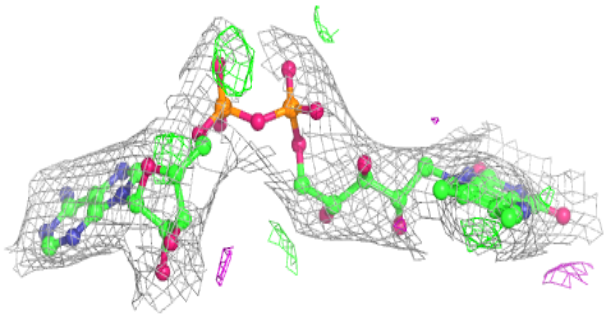


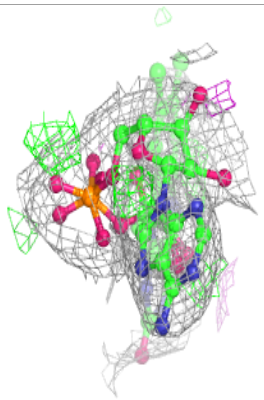


Electron density around FAD F 401:

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

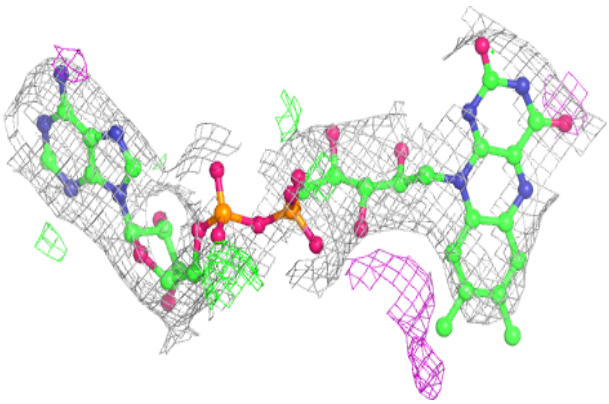


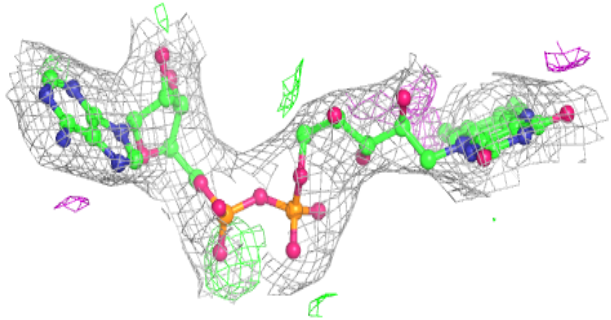


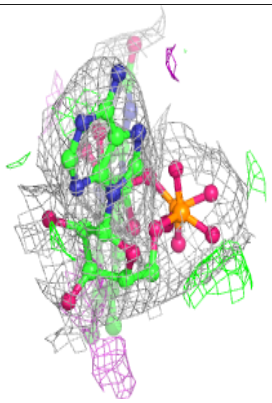


Electron density around FAD C 401:

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

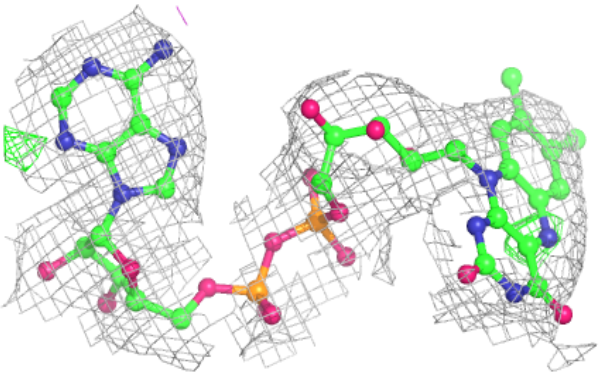


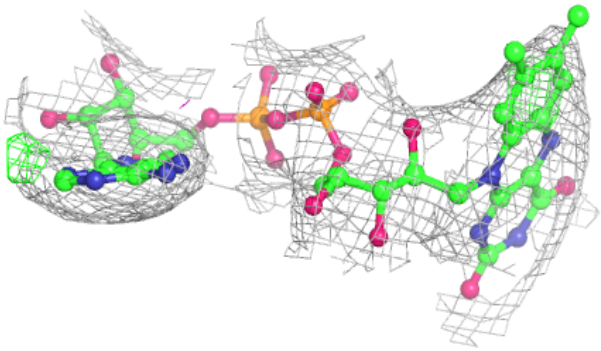


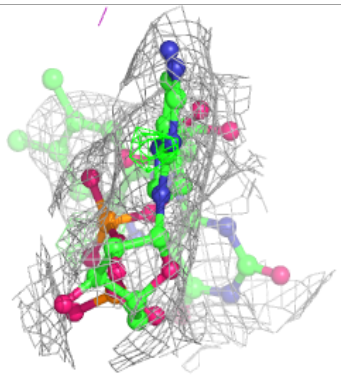


Electron density around FAD B 300:

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

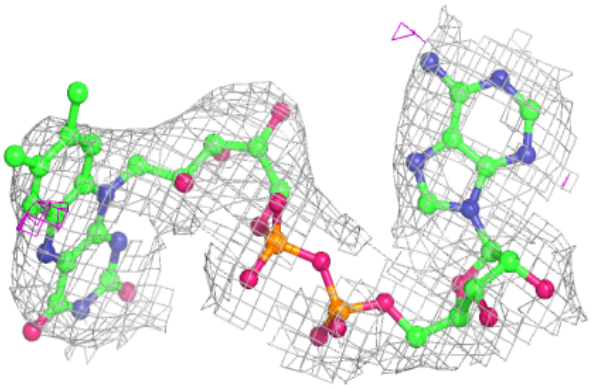


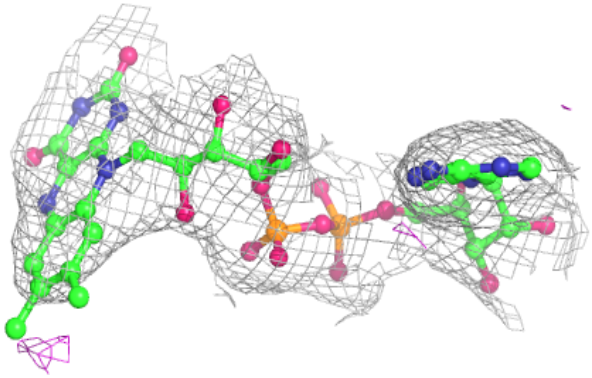


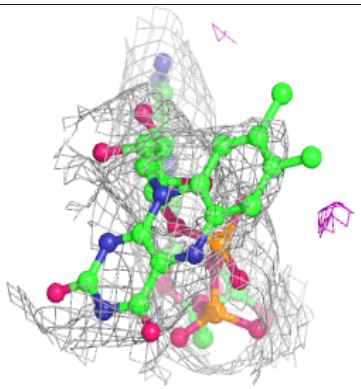


Electron density around FAD E 301:

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







6.5 Other polymers (i)

There are no such residues in this entry.