Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 12:10 PM EDT

PDB ID	:	6CMZ
Title	:	2.3 Angstrom Resolution Crystal Structure of Dihydrolipoamide Dehydrogenase from Burkholderia cenocepacia in Complex with FAD and NAD
Authors	:	Minasov, G.; Shuvalova, L.; Dubrovska, I.; Kiryukhina, O.; Grimshaw, S.; Kwon, K.; Anderson, W.F.; Satchell, K.J.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2018-03-06
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

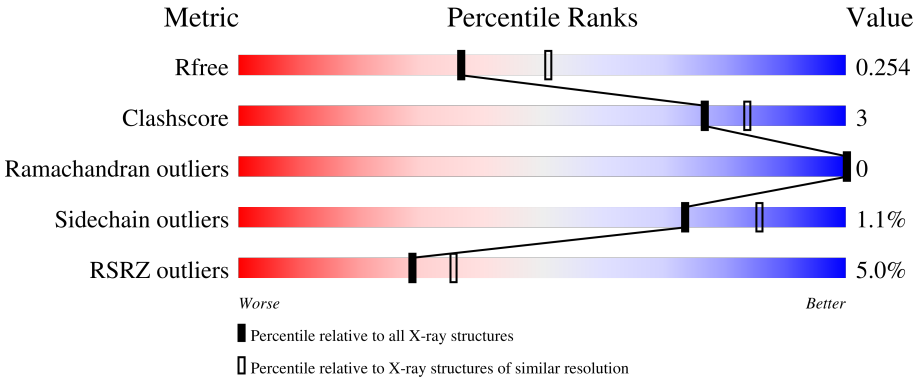
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	466	2% 93% 6% ·
1	B	466	6% 93% 6% ·
1	C	466	4% 90% 8% ·
1	D	466	8% 90% 8% ·

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	FMN	A	505	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14440 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 Dihydrolipoyl dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	4	0
			3442	2155	641	630	16			
1	B	459	Total	C	N	O	S	0	1	0
			3390	2122	633	619	16			
1	C	462	Total	C	N	O	S	0	1	0
			3416	2139	639	622	16			
1	D	459	Total	C	N	O	S	0	1	0
			3389	2122	633	617	17			

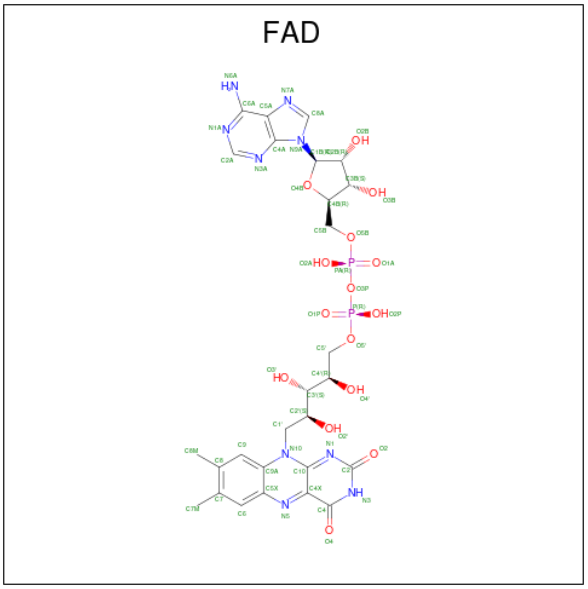
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP B4EEF2
A	-1	ASN	-	expression tag	UNP B4EEF2
A	0	ALA	-	expression tag	UNP B4EEF2
B	-2	SER	-	expression tag	UNP B4EEF2
B	-1	ASN	-	expression tag	UNP B4EEF2
B	0	ALA	-	expression tag	UNP B4EEF2
C	-2	SER	-	expression tag	UNP B4EEF2
C	-1	ASN	-	expression tag	UNP B4EEF2
C	0	ALA	-	expression tag	UNP B4EEF2
D	-2	SER	-	expression tag	UNP B4EEF2
D	-1	ASN	-	expression tag	UNP B4EEF2
D	0	ALA	-	expression tag	UNP B4EEF2

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

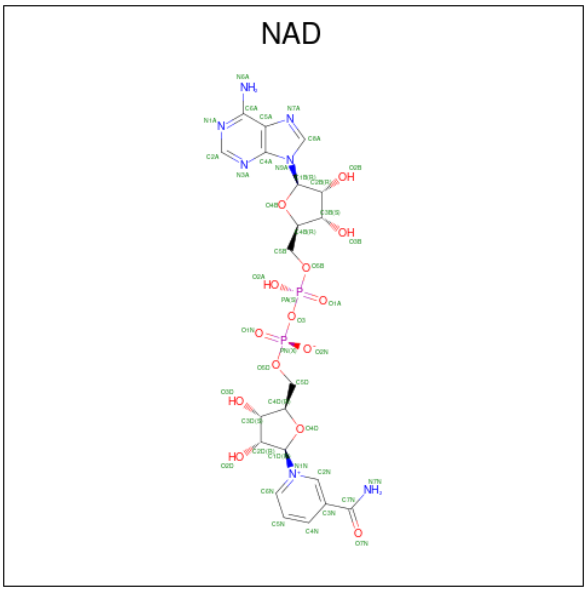
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



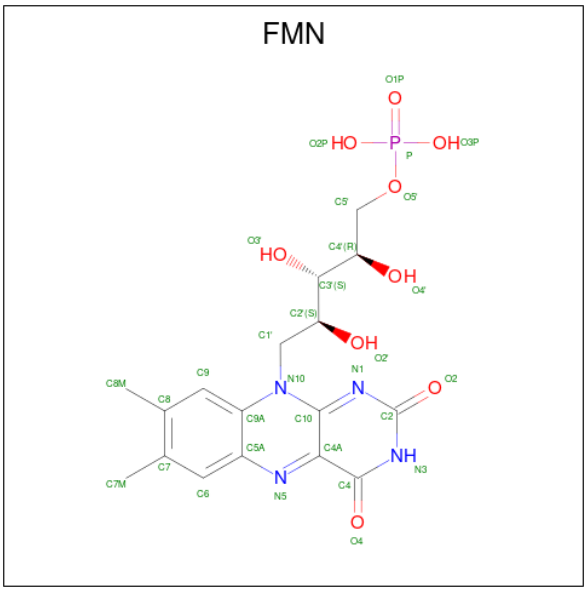
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



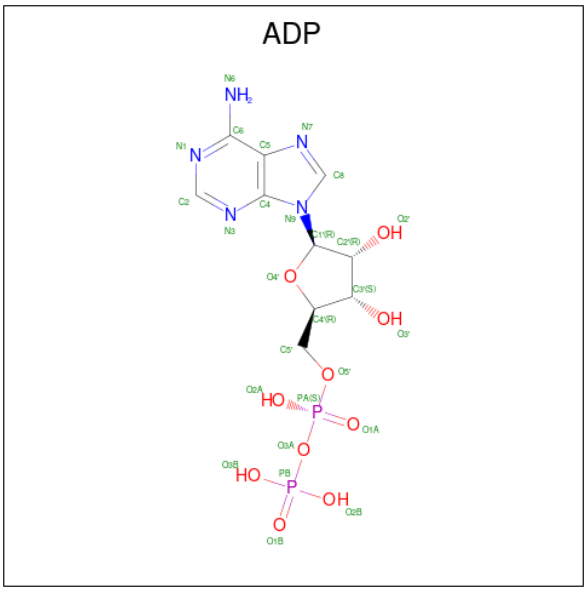
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



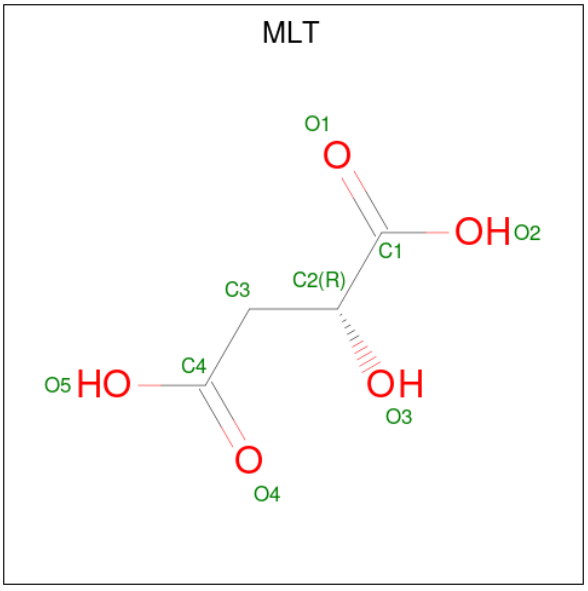
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	O		0	0
			9	4	5			

- Molecule 8 is water.

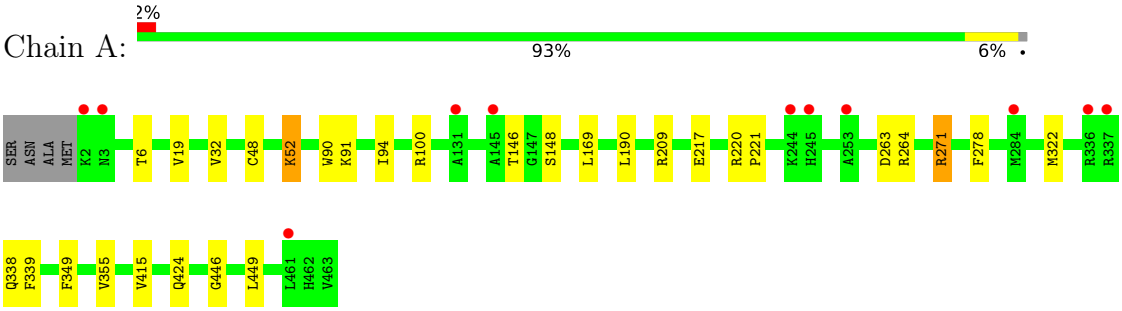
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	115	Total O 117 117	0	2
8	B	90	Total O 92 92	0	2
8	C	79	Total O 82 82	0	3
8	D	76	Total O 80 80	0	4

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.

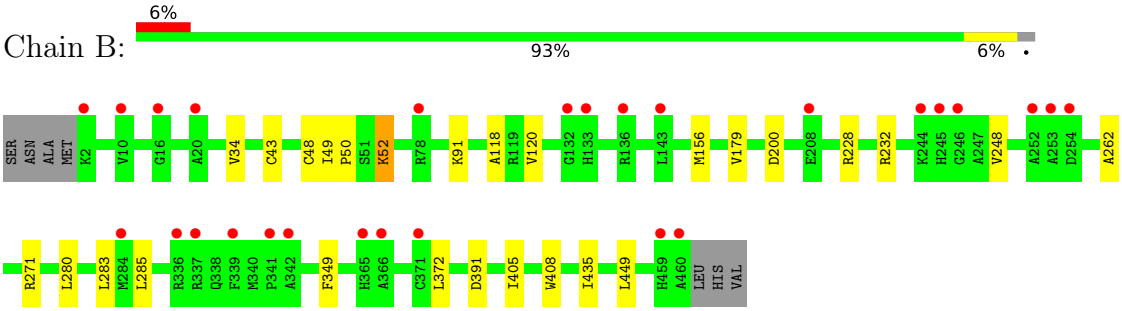
• Molecule 1: Dihydrolipoyl dehydrogenase

Chain A:



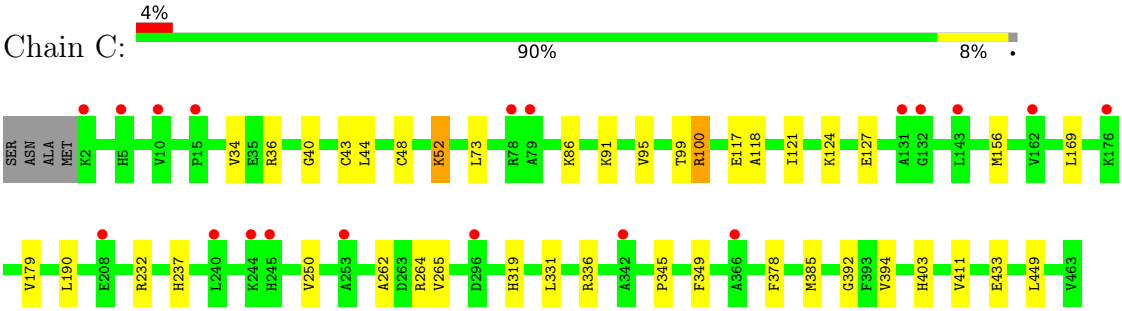
• Molecule 1: Dihydrolipoyl dehydrogenase

Chain B:



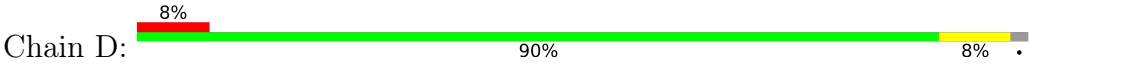
• Molecule 1: Dihydrolipoyl dehydrogenase

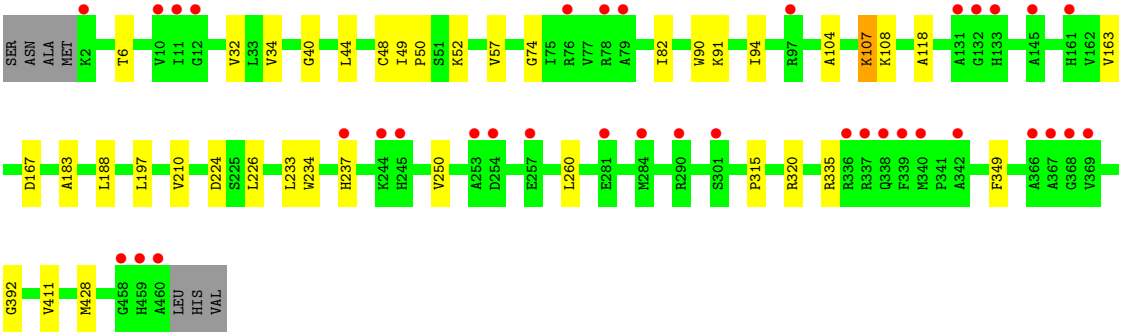
Chain C:



• Molecule 1: Dihydrolipoyl dehydrogenase

Chain D:




SER
ASN
ALA
MET
K2
T6
V10
I11
G12
V32
L33
V34
G40
L44
C48
I49
P50
S51
K52
V57
G74
I75
R76
V77
R78
A79
I82
W90
K91
I94
R97
A104
K107
K108
A118
A131
G132
H133
A145
H161
V162
V163
D167
A183
L188
L197
V210
D224
S225
L226
L233
W234
H237
K244
H245
V250
A253
D254
E257
L260
E281
M284
R290
S301
P315
R320
R335
R336
R337
Q338
F339
M340
P341
A342
F349
A366
A367
G368
V369
G392
V411
M428
G458
H459
A460
LEU
HIS
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.56Å 107.25Å 105.43Å 90.00° 106.09° 90.00°	Depositor
Resolution (Å)	29.21 – 2.30 29.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.21-2.30) 99.8 (29.21-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.199 , 0.253 0.200 , 0.254	Depositor DCC
R_{free} test set	3962 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14440	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, CL, MLT, FMN, ADP, 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	0.44	0/3500	0.75	2/4750 (0.0%)
1	B	0.42	0/3447	0.71	0/4679
1	C	0.42	0/3474	0.70	0/4714
1	D	0.43	0/3446	0.72	0/4676
All	All	0.43	0/13867	0.72	2/18819 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	271	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	271	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3442	0	3496	17	0
1	B	3390	0	3451	20	0
1	C	3416	0	3479	25	0
1	D	3389	0	3451	26	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	A	106	0	62	0	0
3	B	53	0	31	0	0
3	C	53	0	31	0	0
3	D	53	0	31	0	0
4	A	44	0	26	0	0
5	A	31	0	19	0	0
6	B	27	0	12	0	0
6	C	27	0	12	0	0
6	D	27	0	12	0	0
7	D	9	0	4	0	0
8	A	117	0	0	1	0
8	B	92	0	0	1	0
8	C	82	0	0	1	0
8	D	80	0	0	0	0
All	All	14440	0	14117	83	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 3.

All (83) 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:6:THR:HG21	1:A:32:VAL:HG23	1.57	0.84
1:B:43:CYS:HG	1:B:48:CYS:HG	0.83	0.82
1:D:6:THR:HG21	1:D:32:VAL:HG23	1.66	0.77
1:C:43:CYS:HG	1:C:48:CYS:HG	1.38	0.71
1:B:52:LYS:HD2	1:B:349:PHE:CD1	2.30	0.66
1:B:408:TRP:HZ2	1:B:435:ILE:HD13	1.61	0.64
1:D:188:LEU:HD11	1:D:210:VAL:HG22	1.84	0.60
1:A:52:LYS:HD2	1:A:349:PHE:CD1	2.37	0.60
1:C:156:MET:CE	1:C:265:VAL:HG11	2.33	0.59
1:D:163:VAL:HB	1:D:167:ASP:HB2	1.83	0.59
1:D:234:TRP:CZ2	1:D:260:LEU:HD21	2.39	0.58
1:A:90:TRP:CZ2	1:A:94:ILE:HD11	2.39	0.57
1:B:405:ILE:HD12	1:B:435:ILE:HD12	1.86	0.57
1:C:156:MET:HE2	1:C:265:VAL:HG11	1.86	0.56
1:D:52:LYS:HE3	1:D:349:PHE:CD1	2.42	0.54
1:D:52:LYS:N	1:D:52:LYS:HD2	2.21	0.54
1:C:73:LEU:HD22	1:D:57:VAL:HG12	1.90	0.53
1:C:331:LEU:HD23	1:C:336:ARG:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:NH2	1:D:224:ASP:OD1	2.42	0.52
1:D:48:CYS:O	1:D:52:LYS:HD3	2.10	0.52
1:B:120:VAL:HG11	1:B:283:LEU:HD11	1.92	0.52
1:B:48:CYS:O	1:B:52:LYS:HE2	2.10	0.51
1:B:52:LYS:HD2	1:B:349:PHE:CG	2.45	0.51
1:A:217[B]:GLU:OE2	1:A:217[B]:GLU:HA	2.11	0.51
1:B:200:ASP:OD1	1:B:232:ARG:NH2	2.44	0.51
1:C:52:LYS:HD2	1:C:349:PHE:CD1	2.46	0.51
1:B:405:ILE:CD1	1:B:435:ILE:HD12	2.40	0.50
1:B:179:VAL:HG23	1:B:262:ALA:HB2	1.93	0.50
1:C:100:ARG:HA	1:C:100:ARG:HE	1.76	0.50
1:C:403:HIS:ND1	1:C:433:GLU:OE1	2.42	0.49
1:C:52:LYS:HD2	1:C:349:PHE:CG	2.47	0.49
1:C:179:VAL:HG23	1:C:262:ALA:HB2	1.93	0.49
1:C:34:VAL:HG11	1:C:118:ALA:HB2	1.94	0.49
1:D:188:LEU:HD11	1:D:210:VAL:CG2	2.43	0.48
1:C:394:VAL:HG11	1:C:449:LEU:HD22	1.95	0.48
1:D:49:ILE:HB	1:D:50:PRO:HD3	1.95	0.48
1:A:355:VAL:HG23	1:A:415:VAL:HG23	1.95	0.48
8:C:673[A]:HOH:O	1:D:428[A]:MET:HE1	2.13	0.48
1:C:95:VAL:O	1:C:99:THR:HG23	2.14	0.47
1:A:338:GLN:HG3	1:A:339:PHE:CD2	2.49	0.47
1:B:280:LEU:HD21	1:B:285:LEU:HD12	1.96	0.47
1:C:385:MET:HE2	1:D:94:ILE:HG23	1.96	0.47
1:D:90:TRP:CZ2	1:D:94:ILE:HD11	2.50	0.47
1:C:121:ILE:HD11	1:C:127:GLU:HB2	1.96	0.46
1:D:104:ALA:HA	1:D:107:LYS:HE3	1.97	0.46
1:A:169:LEU:HD21	1:A:190:LEU:HD21	1.97	0.46
1:B:49:ILE:HB	1:B:50:PRO:HD3	1.97	0.46
1:C:394:VAL:HG11	1:C:449:LEU:CD2	2.45	0.46
1:C:237:HIS:HB3	1:C:250:VAL:CG1	2.46	0.46
1:C:86:LYS:HD3	1:D:74:GLY:HA2	1.99	0.45
1:A:19:VAL:HG21	1:A:322:MET:HG2	1.99	0.45
1:C:319:HIS:NE2	1:C:345:PRO:O	2.44	0.45
1:D:52:LYS:N	1:D:52:LYS:CD	2.79	0.45
1:A:52:LYS:HD2	1:A:349:PHE:CG	2.52	0.45
1:D:82:ILE:HD13	1:D:197:LEU:HD22	1.99	0.45
1:A:209:ARG:NE	8:A:601:HOH:O	2.49	0.44
1:B:408:TRP:CZ2	1:B:435:ILE:HD13	2.46	0.44
1:B:34:VAL:HG11	1:B:118:ALA:HB2	1.98	0.44
1:A:48:CYS:O	1:A:52:LYS:HE2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLY:HA3	1:C:44:LEU:HD22	2.00	0.43
1:D:34:VAL:HG11	1:D:118:ALA:HB2	1.99	0.43
1:C:156:MET:HE1	1:C:265:VAL:HG11	2.01	0.42
1:A:220:ARG:HB3	1:A:221:PRO:HD3	2.00	0.42
1:B:372:LEU:C	1:B:372:LEU:HD12	2.40	0.42
1:D:183:ALA:HB1	1:D:210:VAL:HG23	2.01	0.42
1:A:146:THR:HG21	1:A:278:PHE:CZ	2.55	0.42
1:D:40:GLY:HA3	1:D:44:LEU:HD12	2.01	0.42
1:D:315:PRO:O	1:D:320:ARG:HD2	2.19	0.42
1:C:36:ARG:HD3	1:C:117:GLU:OE1	2.20	0.41
1:A:148:SER:OG	1:A:271:ARG:NH1	2.53	0.41
1:A:424:GLN:HE22	1:B:449:LEU:HD23	1.85	0.41
1:C:392:GLY:HA3	1:C:411:VAL:O	2.21	0.41
1:B:408:TRP:HZ2	1:B:435:ILE:CD1	2.30	0.41
1:B:228:ARG:NH2	1:B:391:ASP:OD2	2.53	0.41
1:D:392:GLY:HA3	1:D:411:VAL:O	2.20	0.41
1:B:156:MET:HE1	1:B:248:VAL:HG22	2.02	0.41
1:C:169:LEU:HD21	1:C:190:LEU:HD21	2.03	0.41
1:B:271:ARG:HD3	8:B:610:HOH:O	2.22	0.40
1:D:107:LYS:HD2	1:D:108:LYS:N	2.37	0.40
1:A:446:GLY:HA2	1:A:449:LEU:HD13	2.04	0.40
1:C:378:PHE:CZ	1:C:394:VAL:HG23	2.56	0.40
1:D:226:LEU:HD13	1:D:233:LEU:HD21	2.03	0.40
1:D:237:HIS:HB3	1:D:250:VAL:CG1	2.52	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	464/466 (100%)	448 (97%)	16 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	458/466 (98%)	437 (95%)	21 (5%)	0	100	100
1	C	461/466 (99%)	446 (97%)	15 (3%)	0	100	100
1	D	458/466 (98%)	440 (96%)	18 (4%)	0	100	100
All	All	1841/1864 (99%)	1771 (96%)	70 (4%)	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	347/346 (100%)	343 (99%)	4 (1%)	71	84
1	B	341/346 (99%)	339 (99%)	2 (1%)	86	94
1	C	344/346 (99%)	338 (98%)	6 (2%)	60	76
1	D	341/346 (99%)	338 (99%)	3 (1%)	78	89
All	All	1373/1384 (99%)	1358 (99%)	15 (1%)	73	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	91	LYS
1	A	263	ASP
1	A	264	ARG
1	B	52	LYS
1	B	91	LYS
1	C	52	LYS
1	C	91	LYS
1	C	100	ARG
1	C	124	LYS
1	C	232	ARG
1	C	264	ARG
1	D	91	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	107	LYS
1	D	335	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
3	FAD	A	503	-	53,58,58	1.44	7 (13%)	68,89,89	1.36	11 (16%)
7	MLT	D	501	-	8,8,8	1.03	0	10,10,10	1.48	2 (20%)
5	FMN	A	505	-	33,33,33	1.68	6 (18%)	48,50,50	1.35	8 (16%)
3	FAD	C	502	-	53,58,58	1.37	7 (13%)	68,89,89	1.31	10 (14%)
6	ADP	C	503	-	24,29,29	1.06	2 (8%)	29,45,45	1.38	3 (10%)
4	NAD	A	504	-	42,48,48	0.92	4 (9%)	50,73,73	1.28	5 (10%)
3	FAD	B	501	-	53,58,58	1.36	6 (11%)	68,89,89	1.35	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FAD	D	502	-	53,58,58	1.30	4 (7%)	68,89,89	1.33	11 (16%)
6	ADP	B	502	-	24,29,29	1.06	2 (8%)	29,45,45	1.33	3 (10%)
6	ADP	D	503	-	24,29,29	1.03	2 (8%)	29,45,45	1.41	4 (13%)
3	FAD	A	502	-	53,58,58	1.30	5 (9%)	68,89,89	1.36	9 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	503	-	-	5/30/50/50	0/6/6/6
7	MLT	D	501	-	-	5/8/8/8	-
5	FMN	A	505	-	-	3/18/18/18	0/3/3/3
3	FAD	C	502	-	-	2/30/50/50	0/6/6/6
6	ADP	C	503	-	-	6/12/32/32	0/3/3/3
4	NAD	A	504	-	-	11/26/62/62	0/5/5/5
3	FAD	B	501	-	-	2/30/50/50	0/6/6/6
3	FAD	D	502	-	-	3/30/50/50	0/6/6/6
6	ADP	B	502	-	-	0/12/32/32	0/3/3/3
6	ADP	D	503	-	-	3/12/32/32	0/3/3/3
3	FAD	A	502	-	-	2/30/50/50	0/6/6/6

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	505	FMN	C9A-C5A	6.04	1.51	1.41
3	A	503	FAD	C9A-C5X	5.91	1.51	1.41
3	C	502	FAD	C9A-C5X	5.48	1.50	1.41
3	B	501	FAD	C9A-C5X	5.40	1.50	1.41
3	D	502	FAD	C9A-C5X	5.29	1.50	1.41
3	A	502	FAD	C9A-C5X	5.14	1.49	1.41
3	A	503	FAD	C8-C7	3.63	1.49	1.40
3	D	502	FAD	C8-C7	3.47	1.49	1.40
3	C	502	FAD	C8-C7	3.44	1.49	1.40
5	A	505	FMN	C8-C7	3.42	1.49	1.40
3	B	501	FAD	C8-C7	3.41	1.49	1.40
3	A	502	FAD	C8-C7	3.34	1.49	1.40
5	A	505	FMN	C10-N10	2.88	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	NAD	C5A-C4A	2.60	1.47	1.40
3	A	503	FAD	C4X-N5	2.57	1.35	1.30
3	B	501	FAD	C4X-N5	2.52	1.35	1.30
6	C	503	ADP	C5-C4	2.49	1.47	1.40
3	A	503	FAD	C5A-C4A	2.48	1.47	1.40
3	A	502	FAD	C4X-N5	2.44	1.35	1.30
6	D	503	ADP	C5-C4	2.44	1.47	1.40
3	A	502	FAD	C2A-N3A	2.43	1.36	1.32
3	B	501	FAD	C4-N3	-2.42	1.34	1.38
3	C	502	FAD	C10-N10	2.41	1.42	1.37
6	B	502	ADP	C5-C4	2.41	1.47	1.40
3	D	502	FAD	C4X-N5	2.39	1.35	1.30
6	C	503	ADP	C2-N3	2.38	1.35	1.32
3	C	502	FAD	C4X-N5	2.38	1.35	1.30
5	A	505	FMN	C4A-N5	2.37	1.35	1.30
3	A	503	FAD	C10-N10	2.34	1.42	1.37
4	A	504	NAD	C2A-N3A	2.32	1.35	1.32
3	B	501	FAD	C5A-C4A	2.29	1.47	1.40
3	C	502	FAD	C4-N3	-2.29	1.34	1.38
3	A	503	FAD	C4-N3	-2.27	1.34	1.38
3	D	502	FAD	C5A-C4A	2.27	1.46	1.40
6	B	502	ADP	C2-N3	2.26	1.35	1.32
3	B	501	FAD	C10-N10	2.23	1.42	1.37
3	A	502	FAD	C5A-C4A	2.23	1.46	1.40
3	C	502	FAD	C5A-C4A	2.22	1.46	1.40
5	A	505	FMN	C4-N3	-2.21	1.34	1.38
4	A	504	NAD	O4D-C1D	2.20	1.44	1.41
6	D	503	ADP	C2-N3	2.20	1.35	1.32
4	A	504	NAD	O4B-C1B	2.09	1.44	1.41
5	A	505	FMN	C9A-N10	2.08	1.44	1.41
3	A	503	FAD	C2A-N3A	2.06	1.35	1.32
3	C	502	FAD	C2A-N3A	2.06	1.35	1.32

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	502	ADP	N3-C2-N1	-3.91	122.56	128.68
4	A	504	NAD	N3A-C2A-N1A	-3.80	122.73	128.68
3	A	502	FAD	N3A-C2A-N1A	-3.80	122.73	128.68
3	A	503	FAD	N3A-C2A-N1A	-3.80	122.74	128.68
6	D	503	ADP	N3-C2-N1	-3.75	122.81	128.68
3	C	502	FAD	N3A-C2A-N1A	-3.73	122.84	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502	FAD	N3A-C2A-N1A	-3.73	122.84	128.68
6	C	503	ADP	N3-C2-N1	-3.73	122.85	128.68
3	B	501	FAD	N3A-C2A-N1A	-3.72	122.86	128.68
4	A	504	NAD	C3D-C2D-C1D	3.70	106.54	100.98
5	A	505	FMN	C4A-C10-N1	-3.35	116.95	124.73
3	B	501	FAD	C4-C4X-N5	3.22	122.82	118.23
3	A	502	FAD	C4-C4X-N5	3.16	122.73	118.23
3	C	502	FAD	C4X-C10-N1	-3.11	117.52	124.73
4	A	504	NAD	C3B-C2B-C1B	3.08	105.62	100.98
3	A	503	FAD	C4X-C10-N1	-3.07	117.60	124.73
3	A	503	FAD	C4A-C5A-N7A	-3.02	106.25	109.40
3	D	502	FAD	C4-C4X-N5	2.99	122.48	118.23
6	C	503	ADP	C4-C5-N7	-2.97	106.31	109.40
3	A	502	FAD	O2-C2-N1	-2.95	116.94	121.83
3	B	501	FAD	C4X-C10-N1	-2.93	117.94	124.73
5	A	505	FMN	C10-N1-C2	2.89	122.68	116.90
6	D	503	ADP	C4-C5-N7	-2.88	106.40	109.40
3	C	502	FAD	C4A-C5A-N7A	-2.80	106.48	109.40
3	A	502	FAD	O4-C4-C4X	-2.78	119.21	126.60
3	C	502	FAD	C4-C4X-N5	2.78	122.19	118.23
3	C	502	FAD	C10-N1-C2	2.74	122.37	116.90
3	A	503	FAD	C10-N1-C2	2.71	122.33	116.90
3	A	503	FAD	C4-C4X-N5	2.71	122.09	118.23
4	A	504	NAD	PN-O3-PA	-2.70	123.58	132.83
6	D	503	ADP	PA-O3A-PB	-2.68	123.64	132.83
6	B	502	ADP	C4-C5-N7	-2.67	106.62	109.40
3	B	501	FAD	C4A-C5A-N7A	-2.66	106.63	109.40
4	A	504	NAD	C4A-C5A-N7A	-2.66	106.63	109.40
3	D	502	FAD	O2-C2-N1	-2.60	117.52	121.83
3	D	502	FAD	O4-C4-C4X	-2.57	119.79	126.60
3	A	502	FAD	C4X-C10-N1	-2.47	118.99	124.73
3	D	502	FAD	C4X-C10-N1	-2.46	119.02	124.73
5	A	505	FMN	C4A-C10-N10	2.46	120.07	116.48
3	D	502	FAD	C4A-C5A-N7A	-2.46	106.84	109.40
3	B	501	FAD	C10-N1-C2	2.41	121.73	116.90
3	A	502	FAD	C4X-C4-N3	2.41	119.32	113.19
3	D	502	FAD	C10-N1-C2	2.41	121.72	116.90
3	A	502	FAD	C10-N1-C2	2.41	121.71	116.90
3	C	502	FAD	C4X-C4-N3	2.39	119.26	113.19
6	B	502	ADP	PA-O3A-PB	-2.37	124.70	132.83
3	B	501	FAD	C4X-C4-N3	2.37	119.20	113.19
7	D	501	MLT	O2-C1-C2	2.36	117.90	112.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	FAD	C4A-C5A-N7A	-2.35	106.95	109.40
3	A	503	FAD	P-O3P-PA	-2.32	124.88	132.83
6	D	503	ADP	C3'-C2'-C1'	2.31	104.46	100.98
3	D	502	FAD	C4X-C4-N3	2.30	119.02	113.19
5	A	505	FMN	C4-C4A-N5	2.29	121.50	118.23
3	A	503	FAD	C4X-C10-N10	2.29	119.83	116.48
3	A	503	FAD	C4X-C4-N3	2.26	118.94	113.19
5	A	505	FMN	C9A-N10-C10	-2.26	117.25	120.77
3	A	502	FAD	C4-N3-C2	-2.24	121.50	125.64
6	C	503	ADP	PA-O3A-PB	-2.23	125.16	132.83
3	C	502	FAD	O4-C4-C4X	-2.22	120.71	126.60
3	B	501	FAD	C5X-N5-C4X	2.22	121.76	118.07
7	D	501	MLT	O5-C4-C3	2.21	121.17	114.07
3	A	503	FAD	O4-C4-C4X	-2.20	120.76	126.60
5	A	505	FMN	C4A-C4-N3	2.15	118.66	113.19
3	C	502	FAD	C5X-N5-C4X	2.15	121.65	118.07
3	D	502	FAD	C1'-N10-C9A	2.14	124.08	120.51
3	D	502	FAD	C4X-C10-N10	2.13	119.59	116.48
3	C	502	FAD	C4X-C10-N10	2.12	119.58	116.48
3	C	502	FAD	C4-N3-C2	-2.10	121.77	125.64
3	A	503	FAD	C4-N3-C2	-2.07	121.81	125.64
3	D	502	FAD	C4-N3-C2	-2.06	121.83	125.64
3	A	503	FAD	O2-C2-N1	-2.06	118.42	121.83
3	B	501	FAD	C2A-N1A-C6A	2.02	122.21	118.75
3	B	501	FAD	O4-C4-C4X	-2.01	121.26	126.60
5	A	505	FMN	O2-C2-N1	-2.01	118.50	121.83
5	A	505	FMN	C4-N3-C2	-2.00	121.94	125.64

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	FAD	PA-O3P-P-O5'
3	A	503	FAD	C5'-O5'-P-O1P
3	A	503	FAD	C5'-O5'-P-O2P
4	A	504	NAD	C5B-O5B-PA-O2A
4	A	504	NAD	C5B-O5B-PA-O3
5	A	505	FMN	C2'-C1'-N10-C10
5	A	505	FMN	N10-C1'-C2'-O2'
5	A	505	FMN	N10-C1'-C2'-C3'
6	C	503	ADP	PA-O3A-PB-O3B
6	C	503	ADP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	503	ADP	C5'-O5'-PA-O3A
7	D	501	MLT	O3-C2-C3-C4
3	B	501	FAD	O4B-C4B-C5B-O5B
3	C	502	FAD	O4B-C4B-C5B-O5B
4	A	504	NAD	O4B-C4B-C5B-O5B
4	A	504	NAD	C3B-C4B-C5B-O5B
6	C	503	ADP	O4'-C4'-C5'-O5'
6	C	503	ADP	C3'-C4'-C5'-O5'
7	D	501	MLT	C1-C2-C3-C4
3	B	501	FAD	C3B-C4B-C5B-O5B
3	C	502	FAD	C3B-C4B-C5B-O5B
3	D	502	FAD	O4B-C4B-C5B-O5B
6	D	503	ADP	O4'-C4'-C5'-O5'
7	D	501	MLT	O2-C1-C2-C3
3	D	502	FAD	PA-O3P-P-O5'
4	A	504	NAD	PA-O3-PN-O2N
4	A	504	NAD	C5B-O5B-PA-O1A
7	D	501	MLT	O2-C1-C2-O3
4	A	504	NAD	C4B-C5B-O5B-PA
4	A	504	NAD	C2N-C3N-C7N-O7N
3	A	502	FAD	O4B-C4B-C5B-O5B
3	A	503	FAD	O4B-C4B-C5B-O5B
7	D	501	MLT	O1-C1-C2-C3
4	A	504	NAD	C2N-C3N-C7N-N7N
3	D	502	FAD	C3B-C4B-C5B-O5B
6	D	503	ADP	C3'-C4'-C5'-O5'
6	C	503	ADP	PA-O3A-PB-O2B
3	A	503	FAD	C5'-O5'-P-O3P
3	A	503	FAD	P-O3P-PA-O1A
6	D	503	ADP	C5'-O5'-PA-O1A
4	A	504	NAD	C4N-C3N-C7N-N7N
4	A	504	NAD	C4N-C3N-C7N-O7N

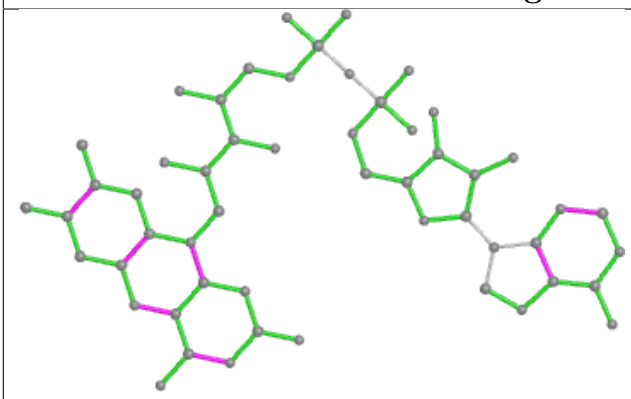
There are no ring outliers.

No monomer is involved in short contacts.

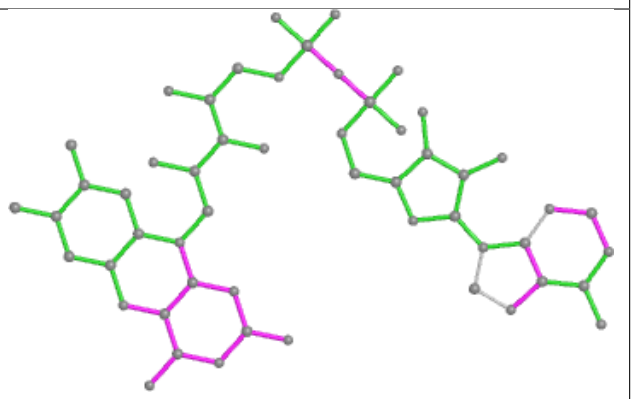
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

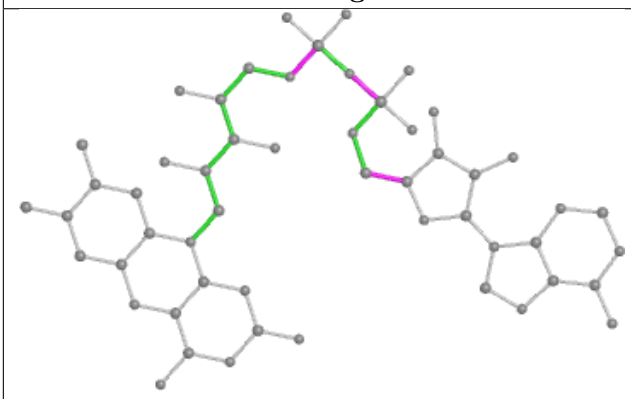
Ligand FAD A 503



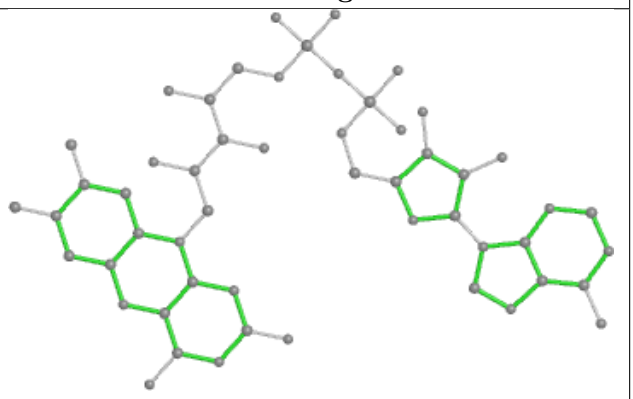
Bond lengths



Bond angles

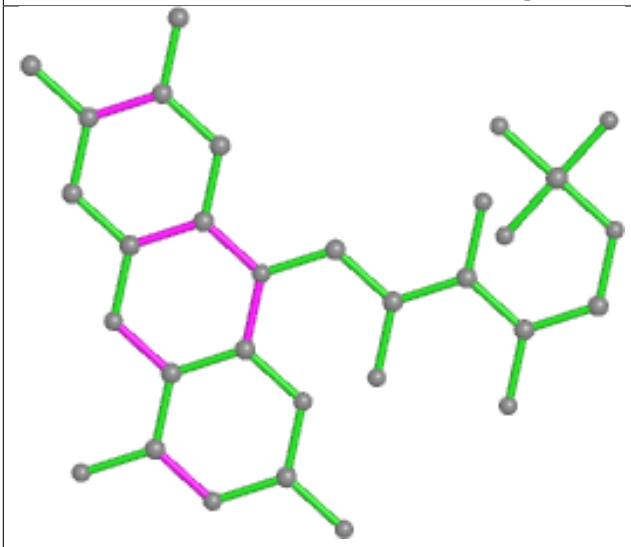


Torsions

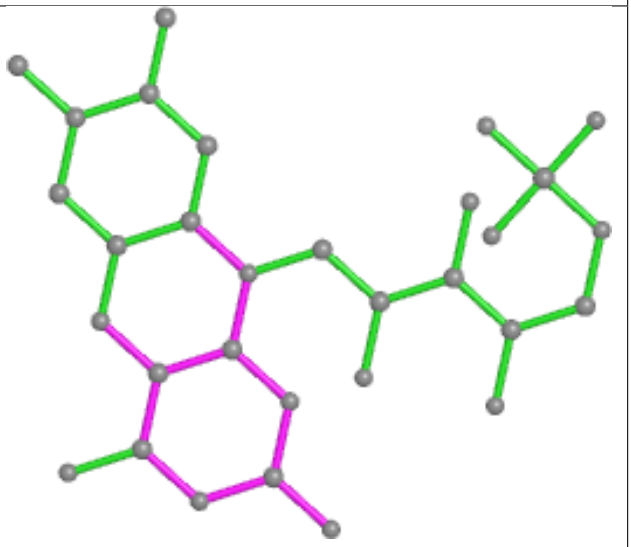


Rings

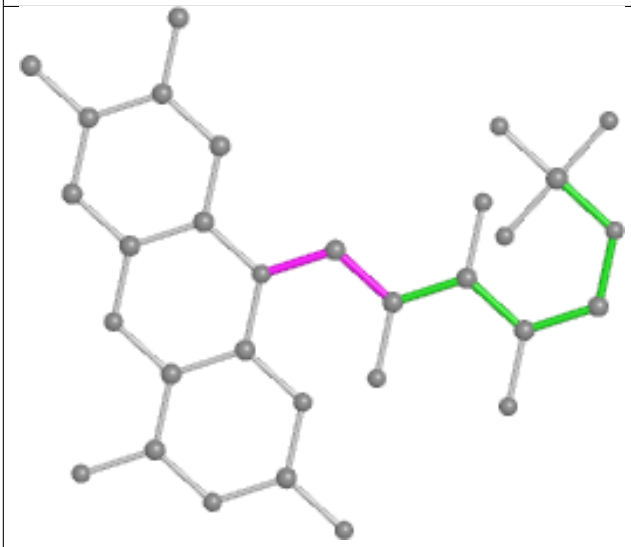
Ligand FMN A 505



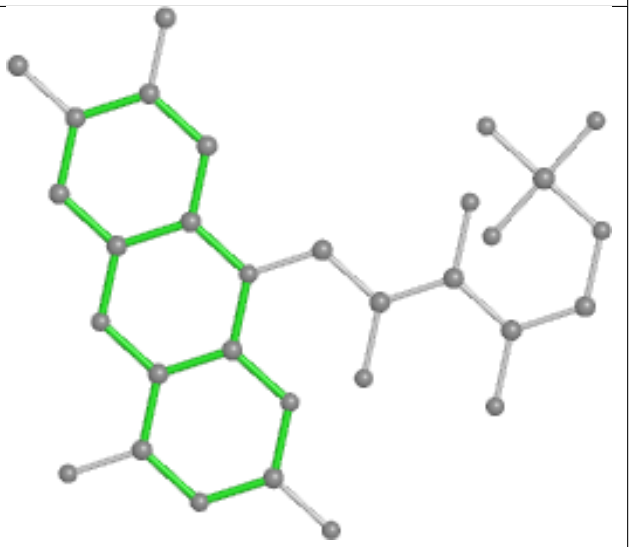
Bond lengths



Bond angles

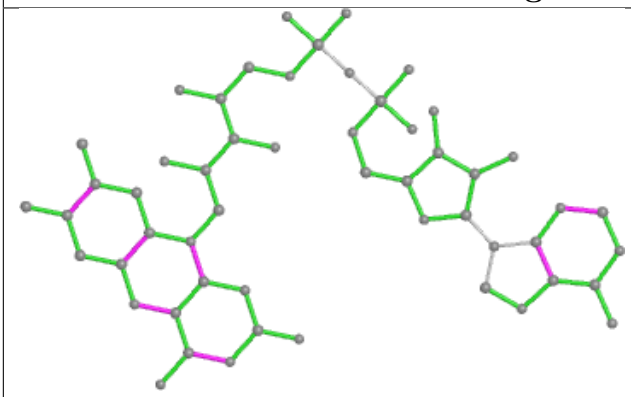


Torsions

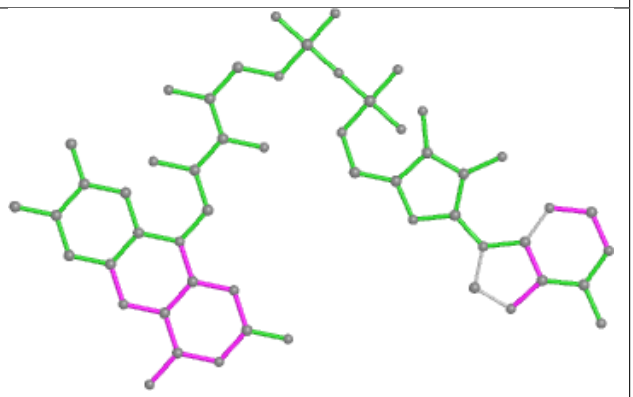


Rings

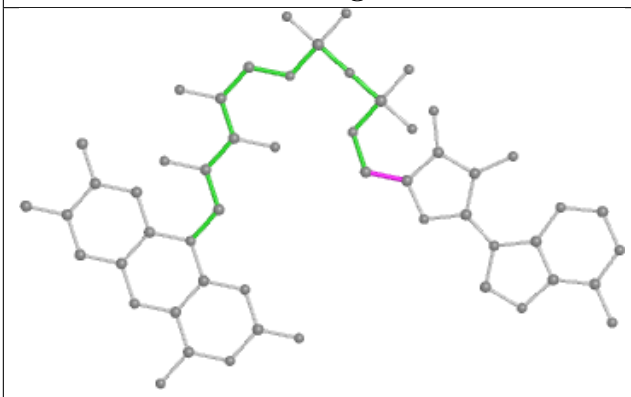
Ligand FAD C 502



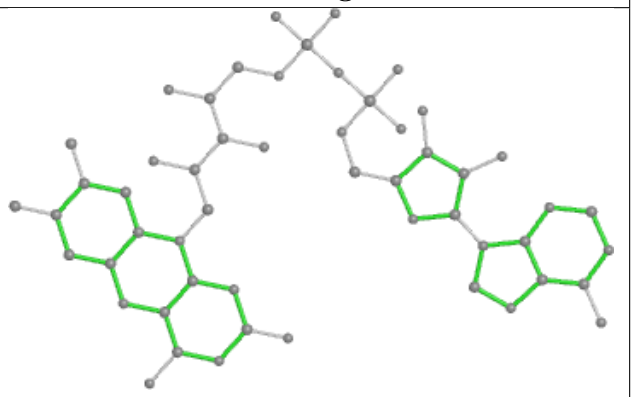
Bond lengths



Bond angles

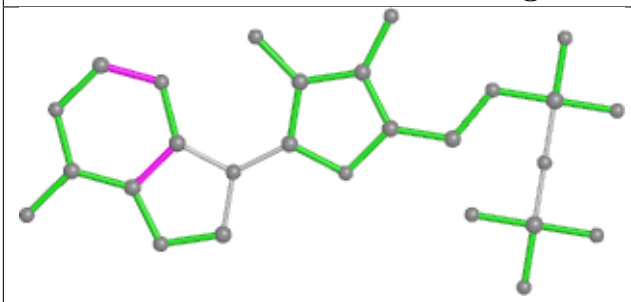


Torsions

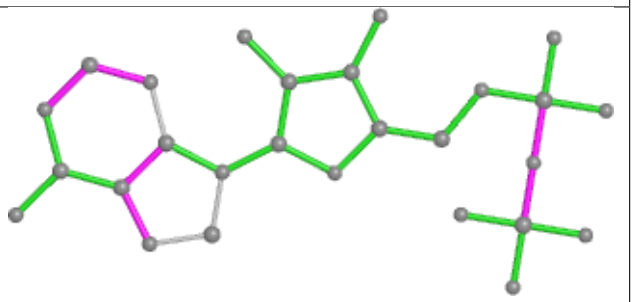


Rings

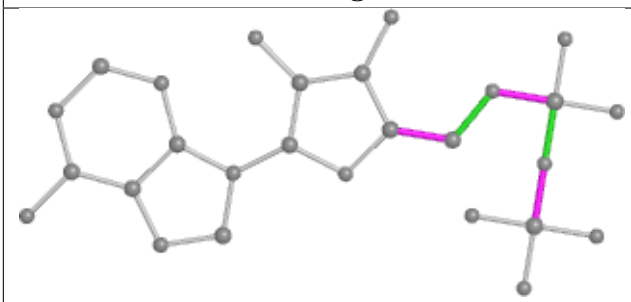
Ligand ADP C 503



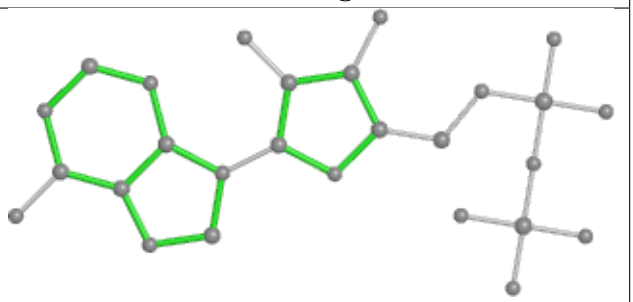
Bond lengths



Bond angles

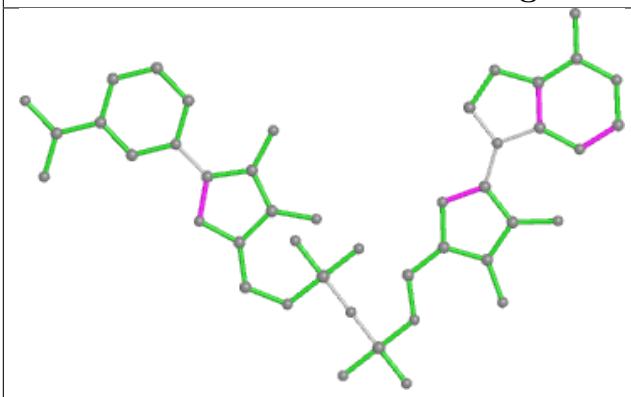


Torsions

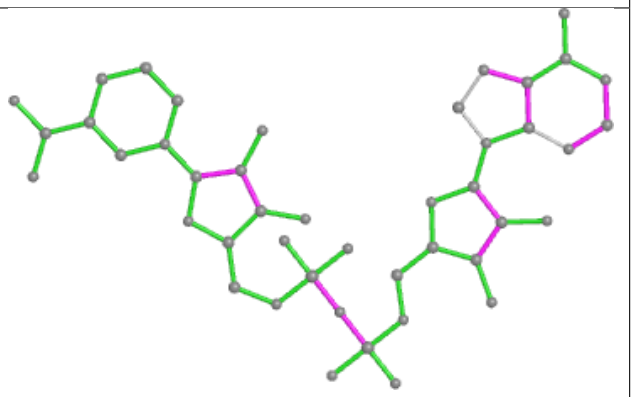


Rings

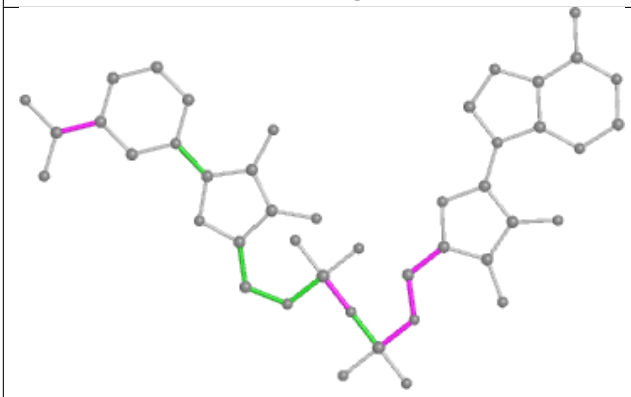
Ligand NAD A 504



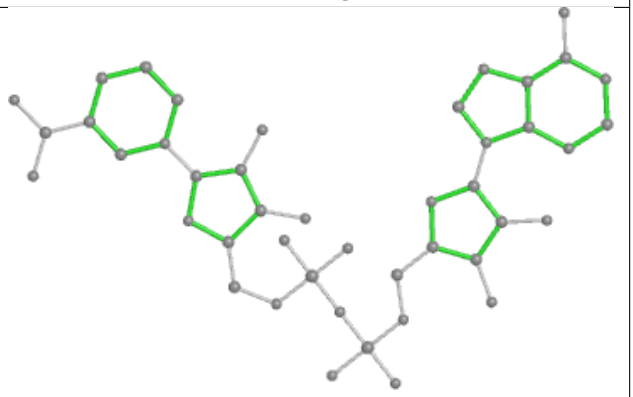
Bond lengths



Bond angles

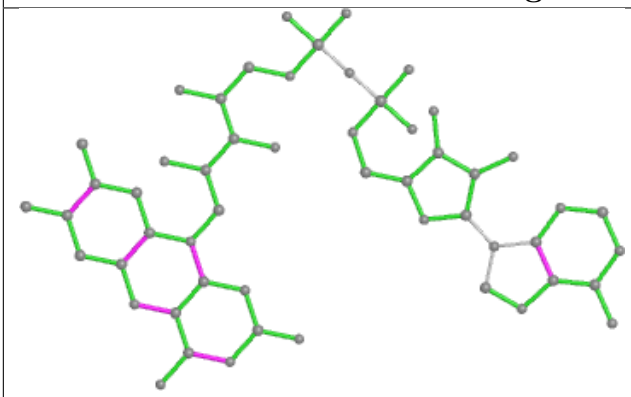


Torsions

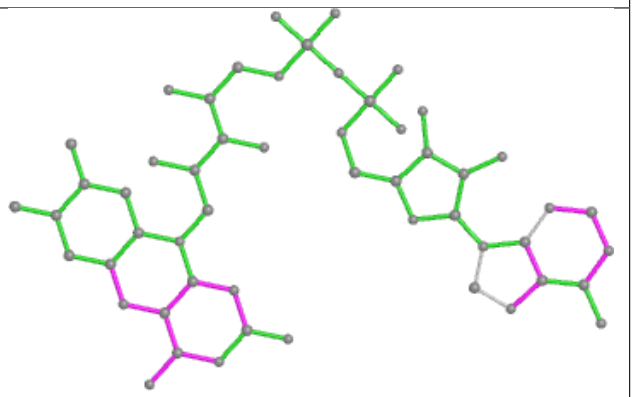


Rings

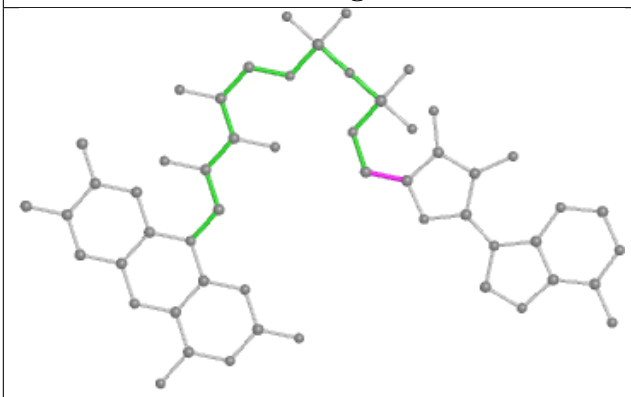
Ligand FAD B 501



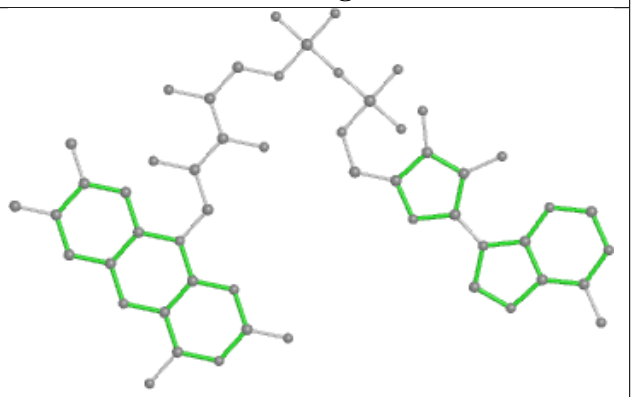
Bond lengths



Bond angles

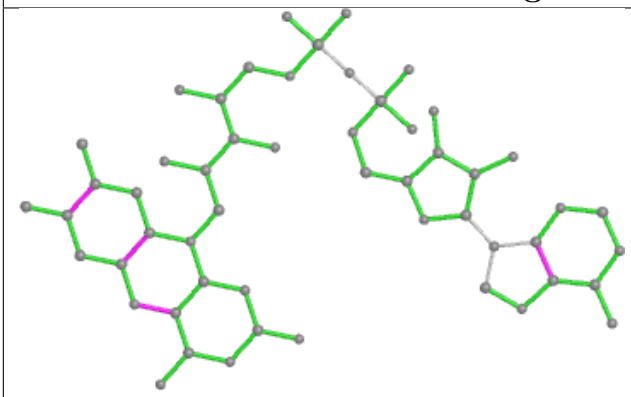


Torsions

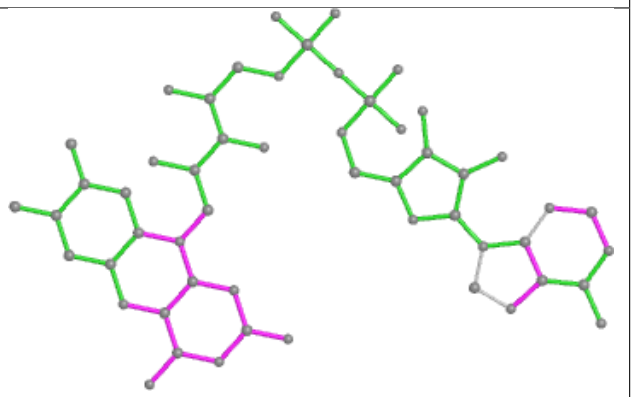


Rings

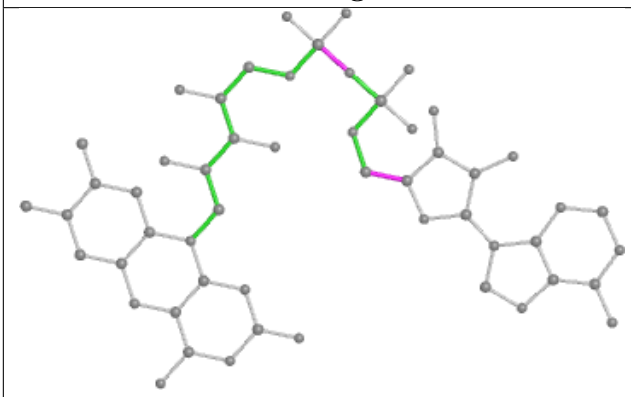
Ligand FAD D 502



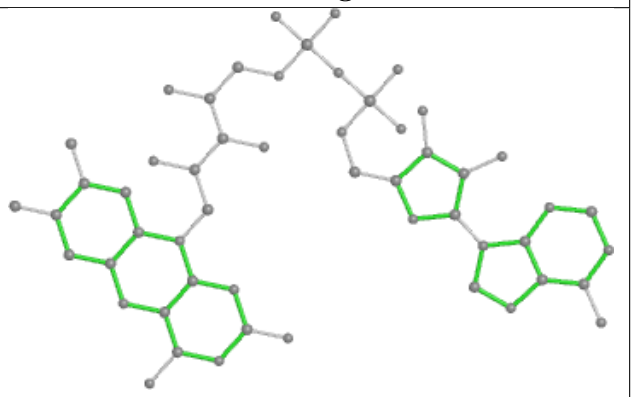
Bond lengths



Bond angles

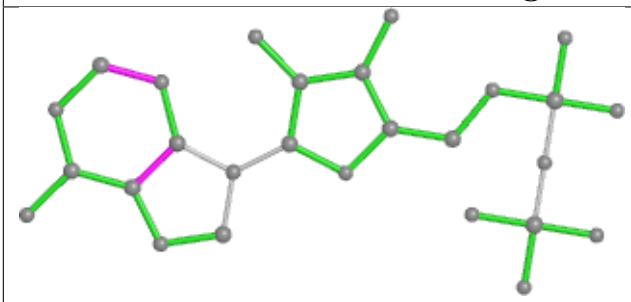


Torsions

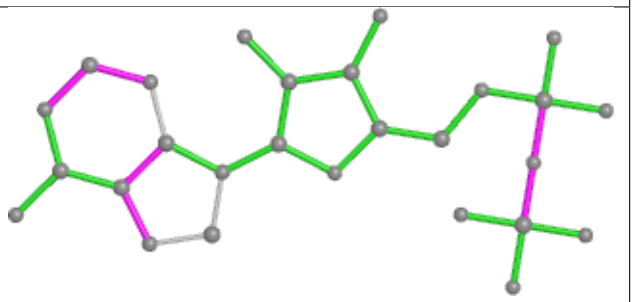


Rings

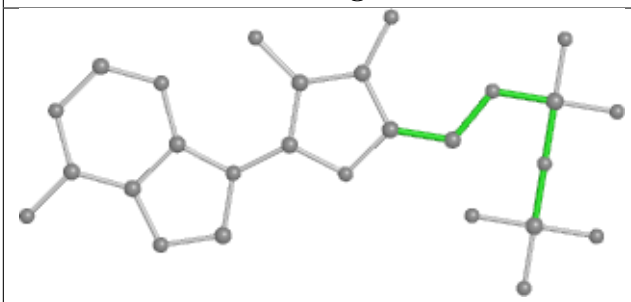
Ligand ADP B 502



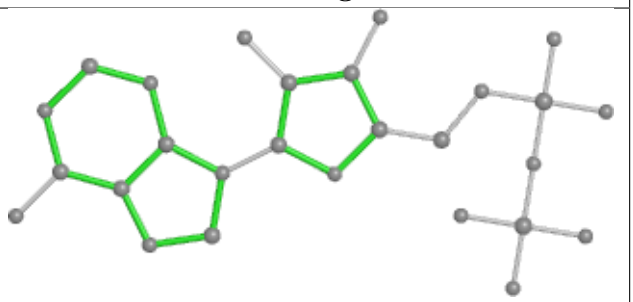
Bond lengths



Bond angles

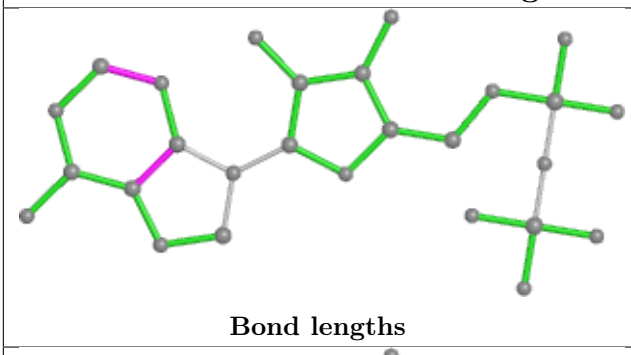


Torsions

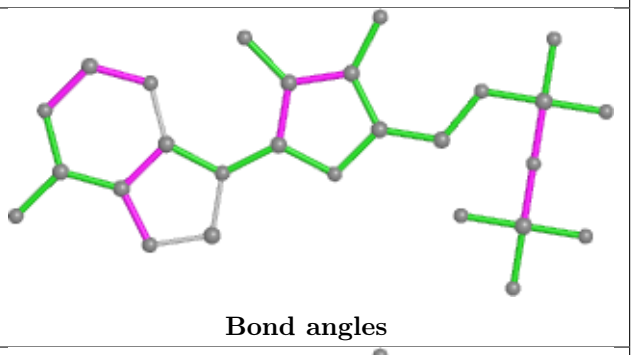


Rings

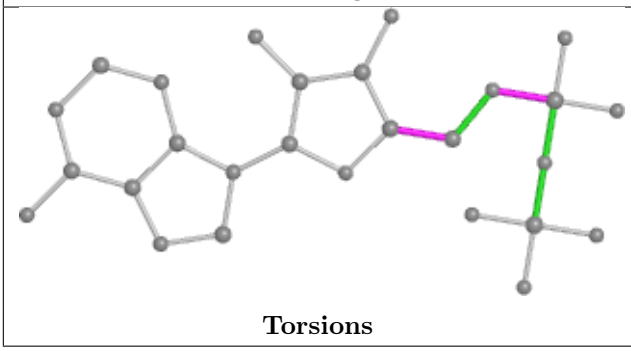
Ligand ADP D 503



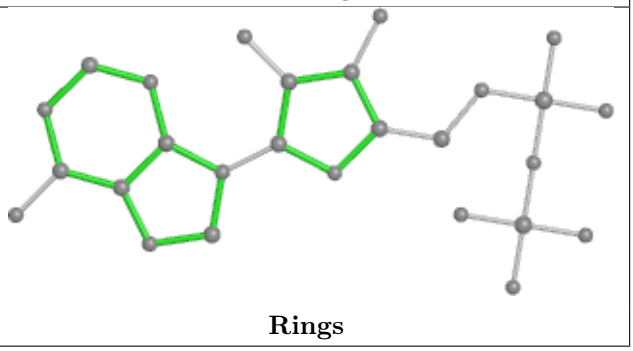
Bond lengths



Bond angles

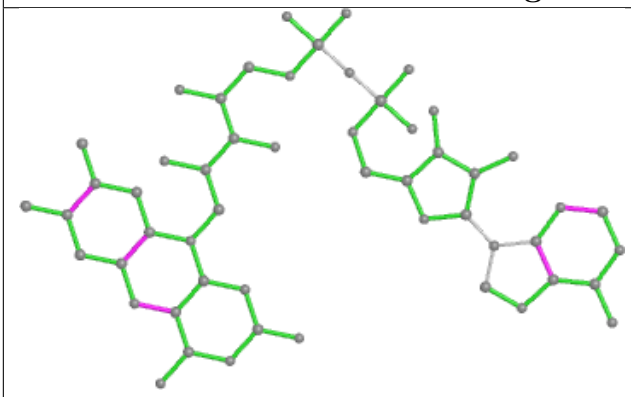


Torsions

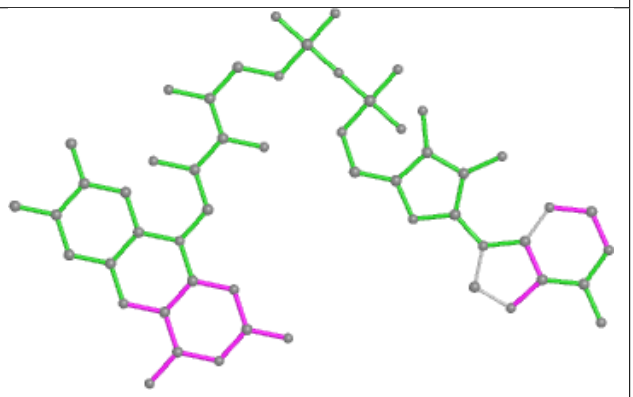


Rings

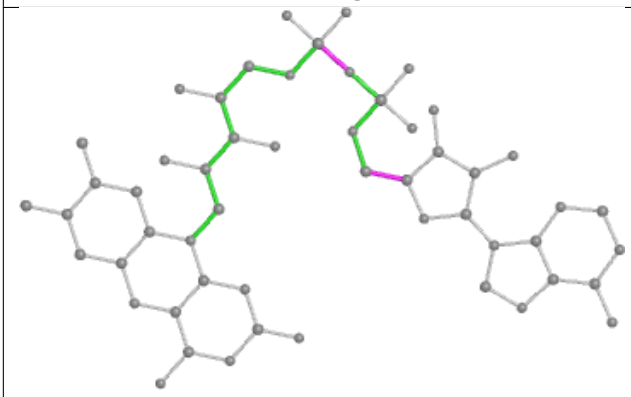
Ligand FAD A 502



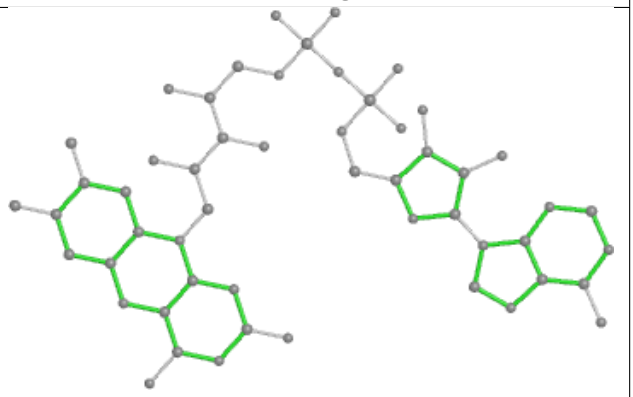
Bond lengths



Bond angles



Torsions



Rings

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	462/466 (99%)	0.05	11 (2%)	59	66	27, 42, 71, 103	0
1	B	459/466 (98%)	0.24	27 (5%)	22	28	27, 45, 85, 116	0
1	C	462/466 (99%)	0.11	19 (4%)	37	44	32, 49, 77, 120	0
1	D	459/466 (98%)	0.29	36 (7%)	13	17	30, 49, 93, 123	0
All	All	1842/1864 (98%)	0.17	93 (5%)	28	35	27, 47, 81, 123	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	342	ALA	8.2
1	D	254	ASP	6.9
1	B	253	ALA	6.8
1	B	460	ALA	6.7
1	B	337	ARG	6.2
1	D	132	GLY	5.7
1	D	459	HIS	5.6
1	B	133	HIS	5.5
1	C	244	LYS	5.2
1	B	459	HIS	5.1
1	D	337	ARG	4.9
1	B	2	LYS	4.9
1	B	244	LYS	4.4
1	D	339	PHE	4.4
1	B	132	GLY	4.4
1	A	253	ALA	4.2
1	D	253	ALA	4.1
1	D	244	LYS	4.1
1	D	290	ARG	4.1
1	D	2	LYS	4.1
1	A	336	ARG	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	458	GLY	3.8
1	C	131	ALA	3.8
1	B	342	ALA	3.7
1	C	78	ARG	3.6
1	A	284	MET	3.6
1	B	366	ALA	3.5
1	B	339	PHE	3.5
1	D	133	HIS	3.5
1	C	79	ALA	3.4
1	B	254	ASP	3.4
1	A	2	LYS	3.3
1	A	244	LYS	3.3
1	B	365	HIS	3.2
1	D	76	ARG	3.2
1	D	245	HIS	3.2
1	D	366	ALA	3.2
1	C	240	LEU	3.1
1	D	161	HIS	3.1
1	D	367	ALA	3.1
1	C	366	ALA	3.0
1	B	78	ARG	3.0
1	C	208	GLU	3.0
1	C	342	ALA	3.0
1	D	336	ARG	2.9
1	D	369	VAL	2.9
1	C	5	HIS	2.9
1	A	337	ARG	2.9
1	D	368	GLY	2.8
1	D	338	GLN	2.8
1	D	79	ALA	2.7
1	C	253	ALA	2.7
1	D	97	ARG	2.7
1	B	336	ARG	2.6
1	D	10	VAL	2.6
1	A	131	ALA	2.6
1	B	341	PRO	2.5
1	C	2	LYS	2.5
1	C	176	LYS	2.5
1	B	245	HIS	2.5
1	C	132	GLY	2.5
1	C	296	ASP	2.5
1	D	284	MET	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	143	LEU	2.5
1	B	252	ALA	2.4
1	D	131	ALA	2.4
1	A	145	ALA	2.3
1	B	284	MET	2.3
1	D	281	GLU	2.3
1	D	257	GLU	2.3
1	B	10	VAL	2.3
1	A	245	HIS	2.3
1	B	371	CYS	2.2
1	D	301	SER	2.2
1	A	3	ASN	2.2
1	B	16	GLY	2.2
1	B	246	GLY	2.2
1	B	20	ALA	2.2
1	C	143	LEU	2.2
1	B	208	GLU	2.2
1	D	11	ILE	2.1
1	A	461	LEU	2.1
1	D	78	ARG	2.1
1	C	245	HIS	2.1
1	C	162	VAL	2.1
1	D	340	MET	2.1
1	D	237	HIS	2.1
1	C	10	VAL	2.1
1	C	15	PRO	2.1
1	B	136	ARG	2.1
1	D	460	ALA	2.0
1	D	12	GLY	2.0
1	D	145	ALA	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)

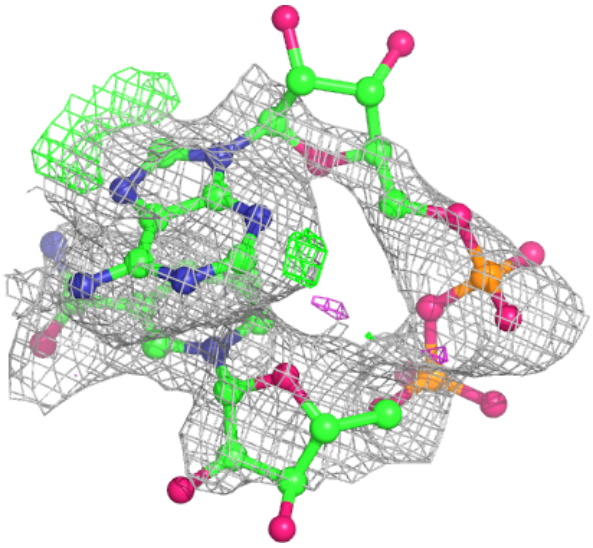
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

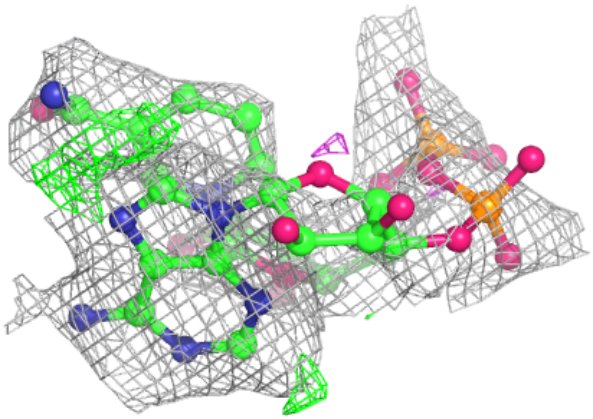
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAD	A	504	44/44	0.63	0.31	85,122,155,161	0
5	FMN	A	505	31/31	0.68	0.48	82,101,136,141	0
6	ADP	B	502	27/27	0.69	0.34	98,117,130,138	0
2	CL	C	501	1/1	0.76	0.09	81,81,81,81	0
7	MLT	D	501	9/9	0.85	0.20	61,69,77,79	0
6	ADP	D	503	27/27	0.89	0.22	60,68,85,91	0
3	FAD	A	503	53/53	0.90	0.19	48,64,85,86	0
6	ADP	C	503	27/27	0.90	0.15	56,60,89,94	0
2	CL	A	501	1/1	0.94	0.12	64,64,64,64	0
3	FAD	D	502	53/53	0.95	0.15	31,36,53,57	0
3	FAD	C	502	53/53	0.96	0.12	36,41,47,47	0
3	FAD	A	502	53/53	0.96	0.15	28,33,40,45	0
3	FAD	B	501	53/53	0.97	0.12	31,38,42,43	0

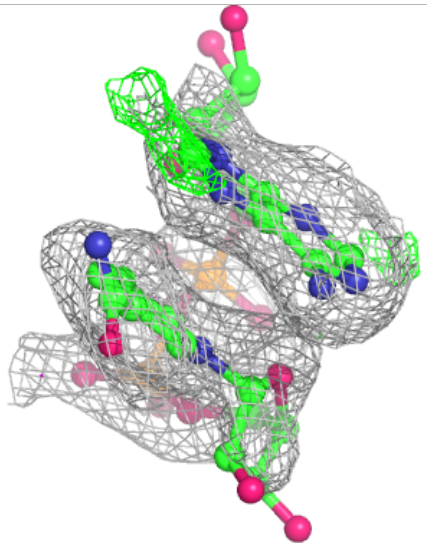
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 504:

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

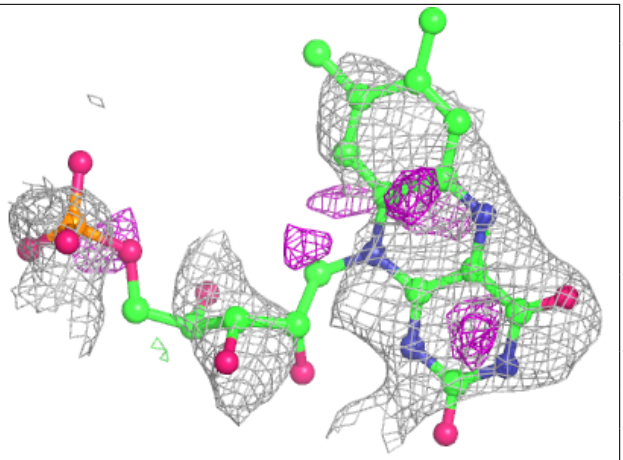


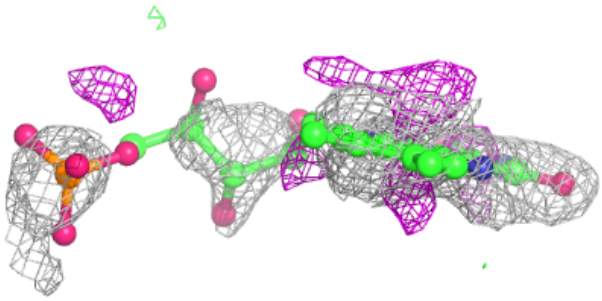


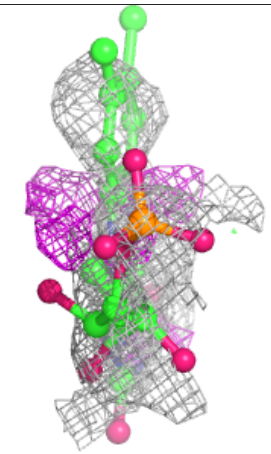


Electron density around FMN A 505:

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

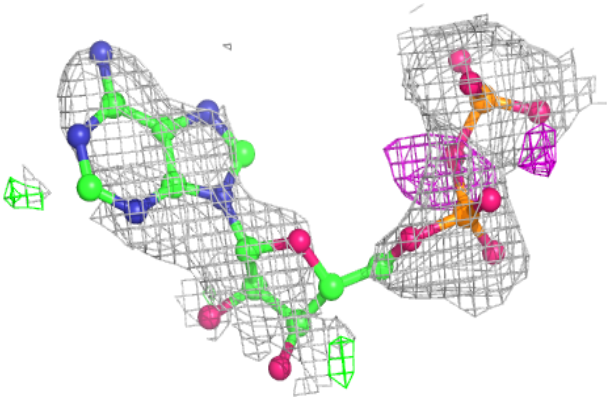


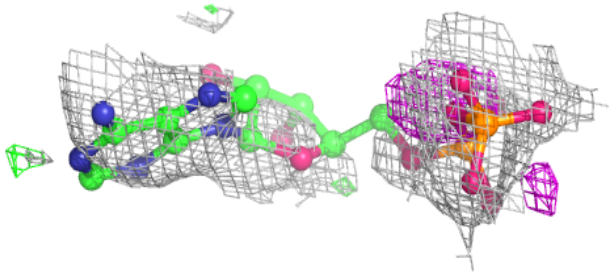


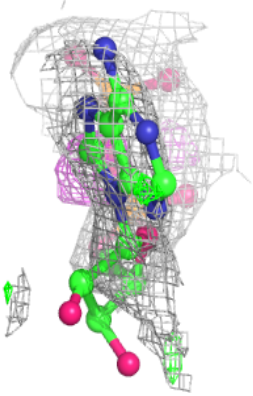


Electron density around ADP B 502:

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

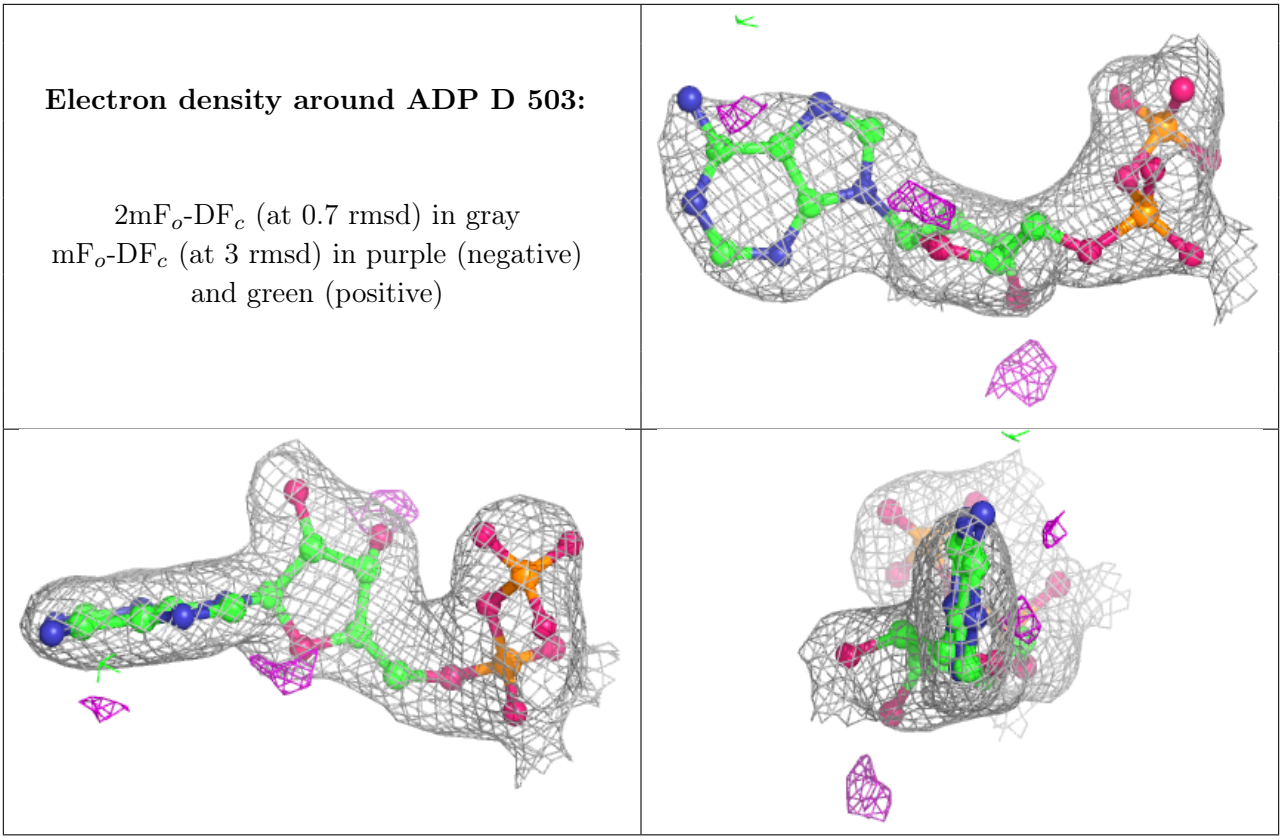






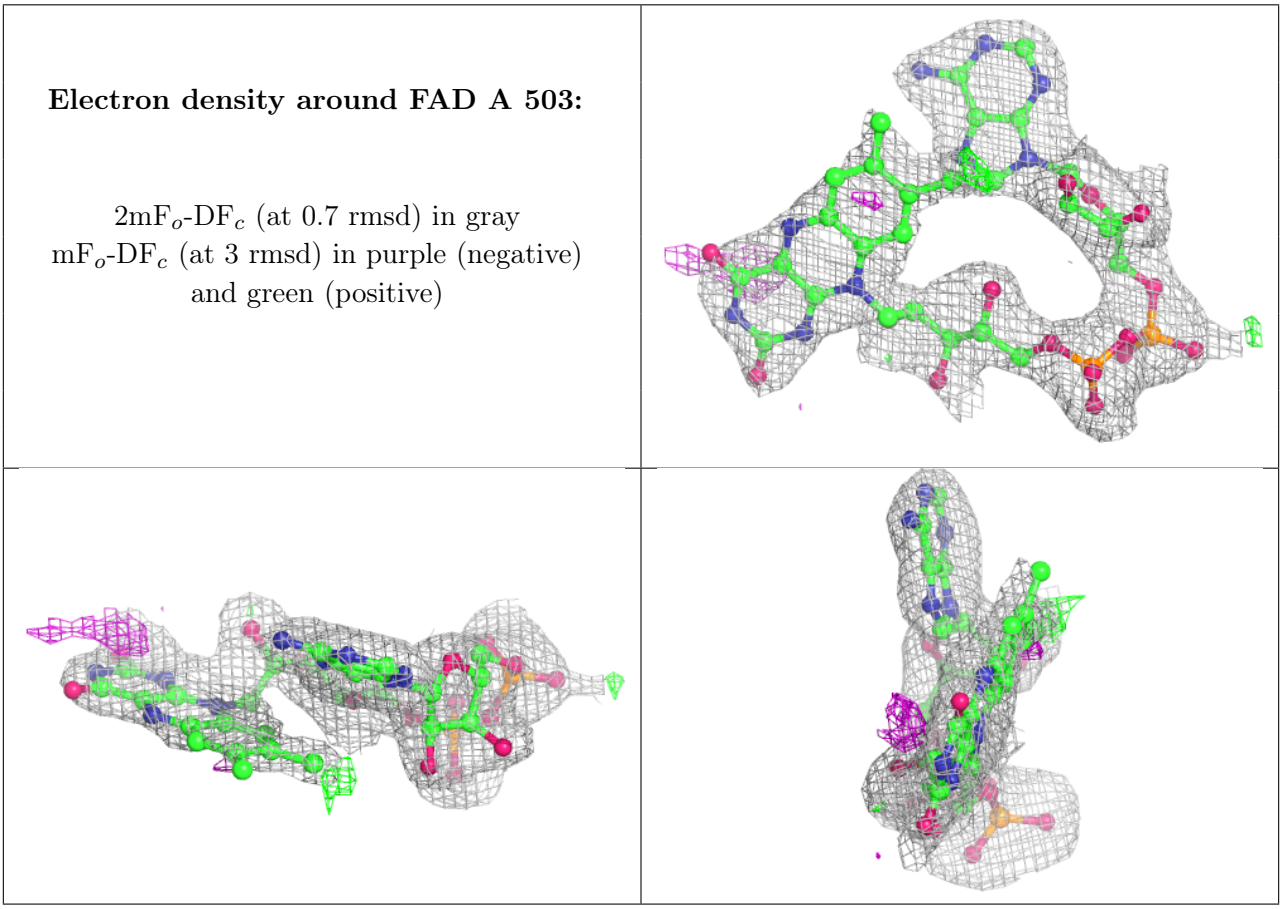
Electron density around ADP D 503:

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



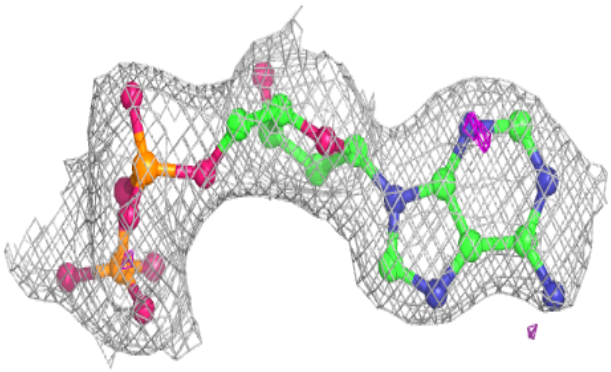
Electron density around FAD A 503:

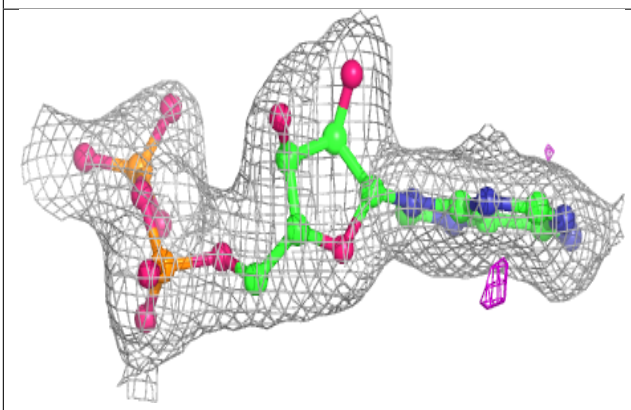
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

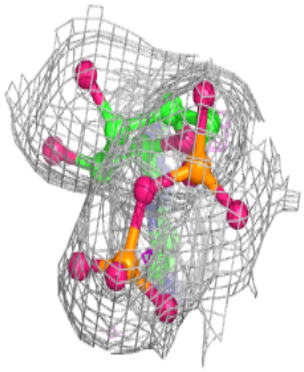


Electron density around ADP C 503:

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

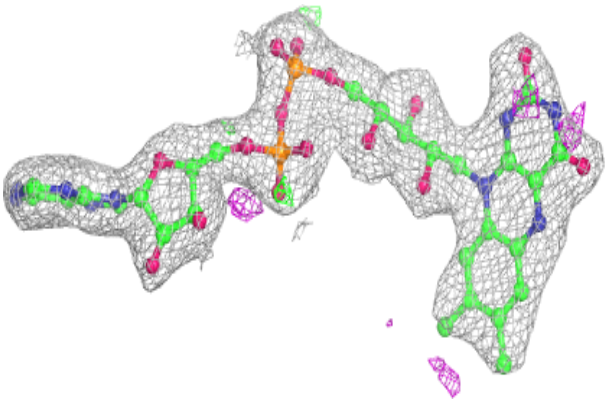


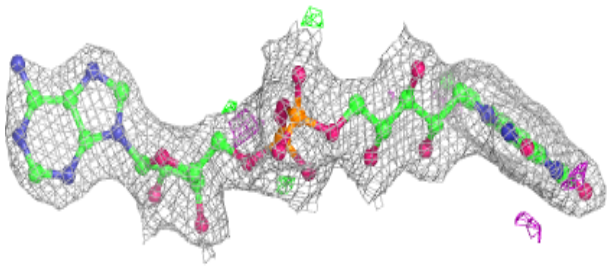


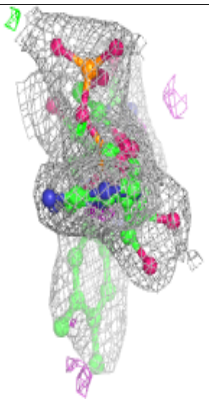


Electron density around FAD D 502:

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

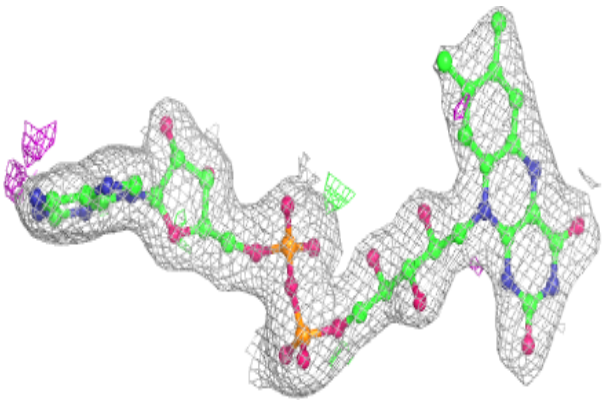


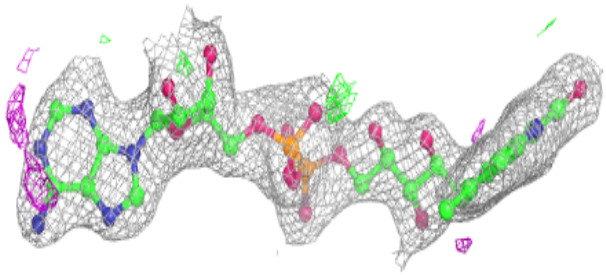


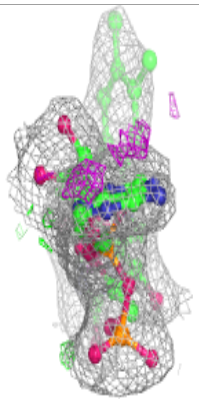


Electron density around FAD C 502:

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

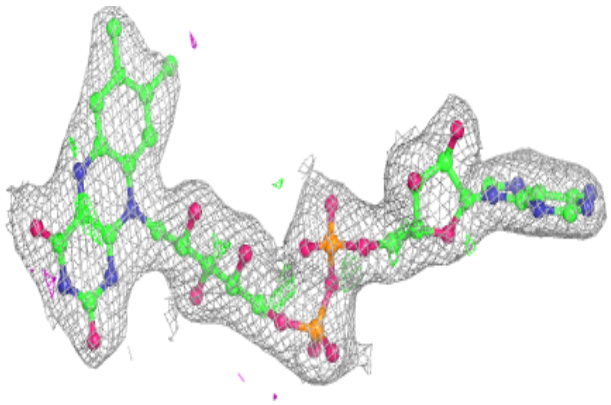


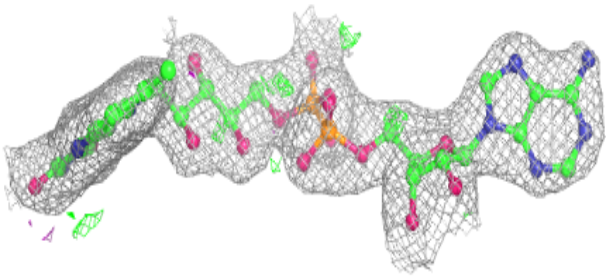


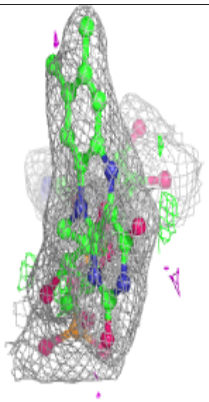


Electron density around FAD A 502:

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

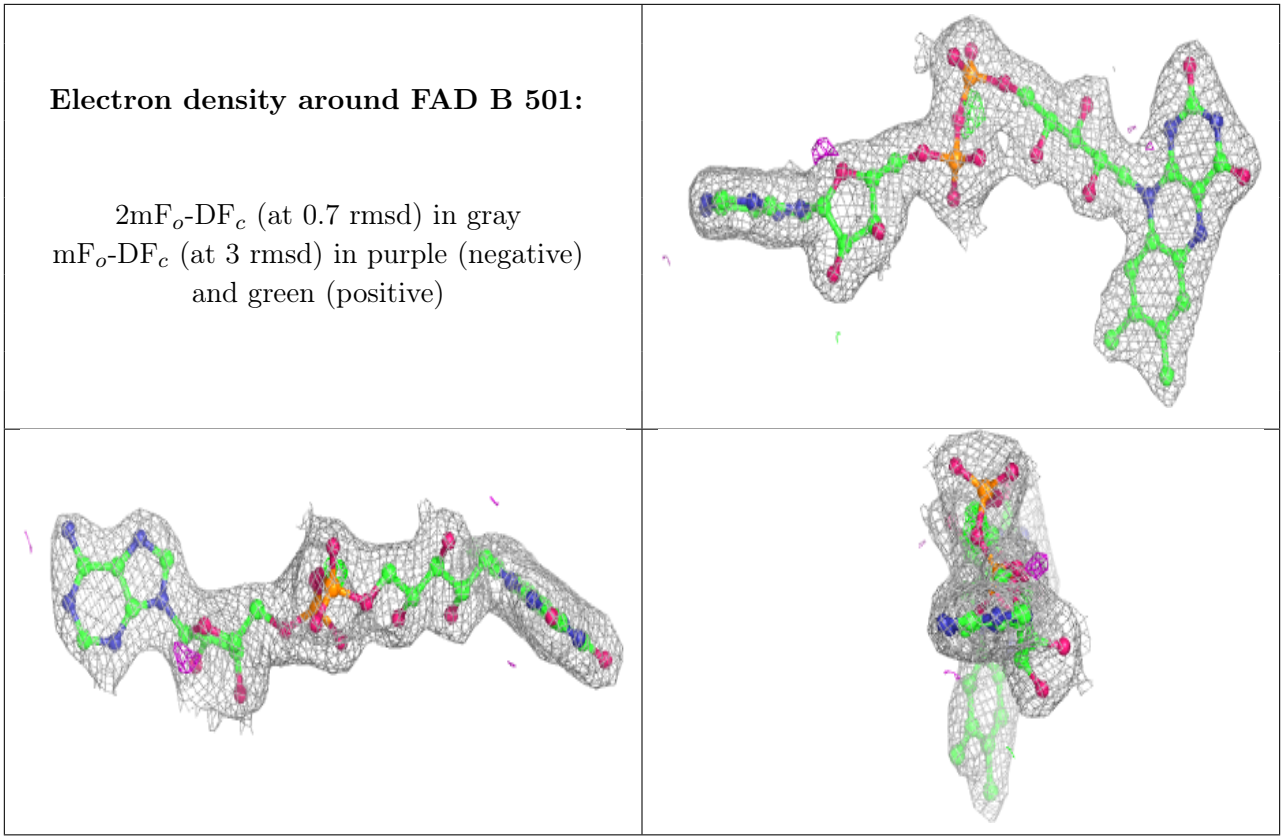






Electron density around FAD B 501:

$2mF_o$-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.