Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2023 – 03:48 pm GMT

PDB ID	:	8AJJ
Title	:	Crystal structure of the disulfide reductase MerA from Staphylococcus aureus
Authors	:	Weiland, P.; Altegoer, F.; Bange, G.
Deposited on	:	2022-07-28
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

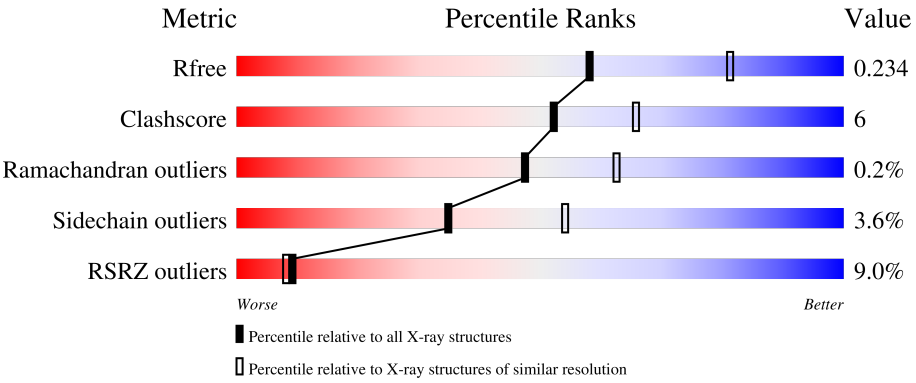
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	446	2% 87% 11%
1	B	446	14% 70% 16% 12%
1	C	446	2% 86% 12%
1	D	446	16% 77% 12% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HIS	A	502	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13403 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 Dihydrolipoamide dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	444	Total	C	N	O	S	0	0	0
			3460	2179	600	674	7			
1	A	442	Total	C	N	O	S	0	0	0
			3440	2167	594	672	7			
1	B	391	Total	C	N	O	S	0	0	0
			3047	1922	526	595	4			
1	D	397	Total	C	N	O	S	0	0	0
			3102	1957	535	606	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP A0A266CGC0
C	2	GLY	-	expression tag	UNP A0A266CGC0
C	441	HIS	-	expression tag	UNP A0A266CGC0
C	442	HIS	-	expression tag	UNP A0A266CGC0
C	443	HIS	-	expression tag	UNP A0A266CGC0
C	444	HIS	-	expression tag	UNP A0A266CGC0
C	445	HIS	-	expression tag	UNP A0A266CGC0
C	446	HIS	-	expression tag	UNP A0A266CGC0
A	1	MET	-	initiating methionine	UNP A0A266CGC0
A	2	GLY	-	expression tag	UNP A0A266CGC0
A	441	HIS	-	expression tag	UNP A0A266CGC0
A	442	HIS	-	expression tag	UNP A0A266CGC0
A	443	HIS	-	expression tag	UNP A0A266CGC0
A	444	HIS	-	expression tag	UNP A0A266CGC0
A	445	HIS	-	expression tag	UNP A0A266CGC0
A	446	HIS	-	expression tag	UNP A0A266CGC0
B	1	MET	-	initiating methionine	UNP A0A266CGC0
B	2	GLY	-	expression tag	UNP A0A266CGC0
B	441	HIS	-	expression tag	UNP A0A266CGC0
B	442	HIS	-	expression tag	UNP A0A266CGC0
B	443	HIS	-	expression tag	UNP A0A266CGC0

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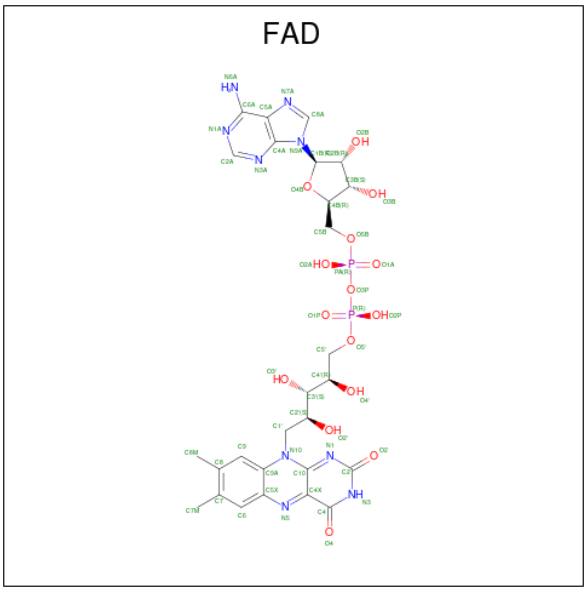
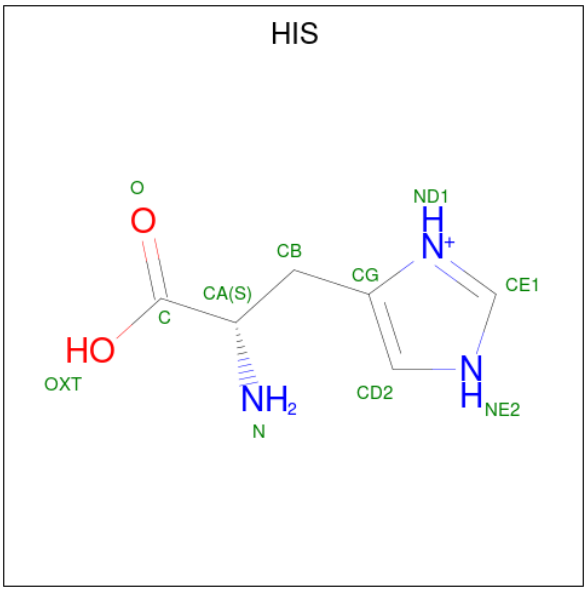
Chain	Residue	Modelled	Actual	Comment	Reference
B	444	HIS	-	expression tag	UNP A0A266CGC0
B	445	HIS	-	expression tag	UNP A0A266CGC0
B	446	HIS	-	expression tag	UNP A0A266CGC0
D	1	MET	-	initiating methionine	UNP A0A266CGC0
D	2	GLY	-	expression tag	UNP A0A266CGC0
D	441	HIS	-	expression tag	UNP A0A266CGC0
D	442	HIS	-	expression tag	UNP A0A266CGC0
D	443	HIS	-	expression tag	UNP A0A266CGC0
D	444	HIS	-	expression tag	UNP A0A266CGC0
D	445	HIS	-	expression tag	UNP A0A266CGC0
D	446	HIS	-	expression tag	UNP A0A266CGC0

- Molecule 2 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
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	1	0
			53	27	9	15	2		

- Molecule 3 is HISTIDINE (three-letter code: HIS) (formula: $C_6H_{10}N_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 6 3 1	0	0
3	A	1	Total C N O 10 6 3 1	0	0

- Molecule 4 is water.

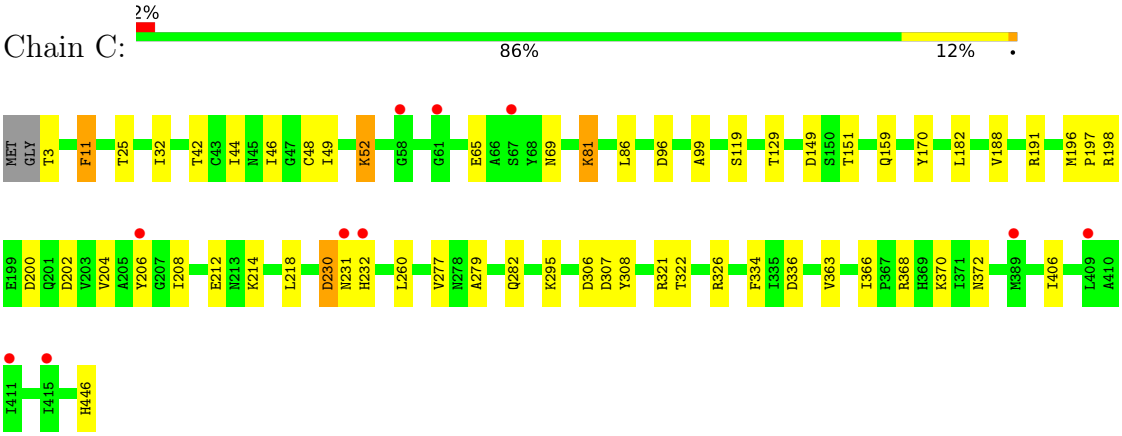
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	44	Total O 44 44	0	0
4	A	24	Total O 24 24	0	0
4	B	35	Total O 35 35	0	0
4	D	19	Total O 19 19	0	0

3 Residue-property plots (i)

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

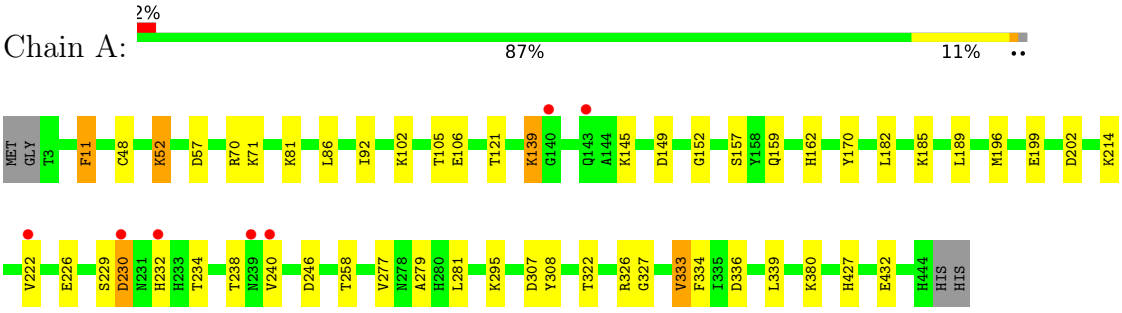
• Molecule 1: Dihydrolipoamide dehydrogenase

Chain C:



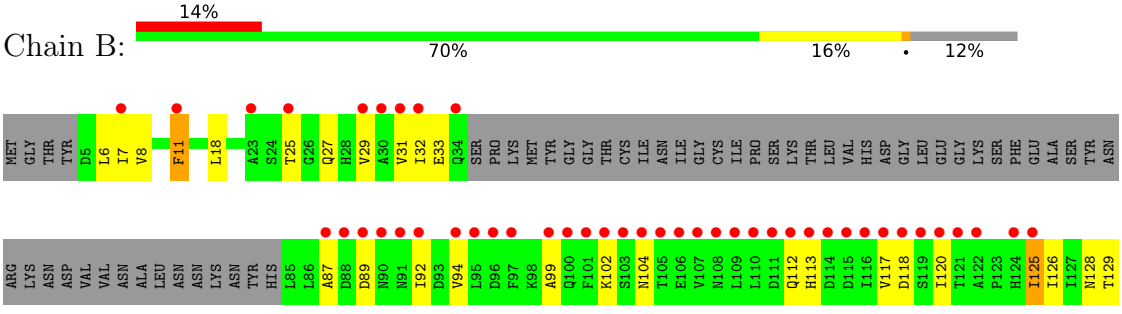
• Molecule 1: Dihydrolipoamide dehydrogenase

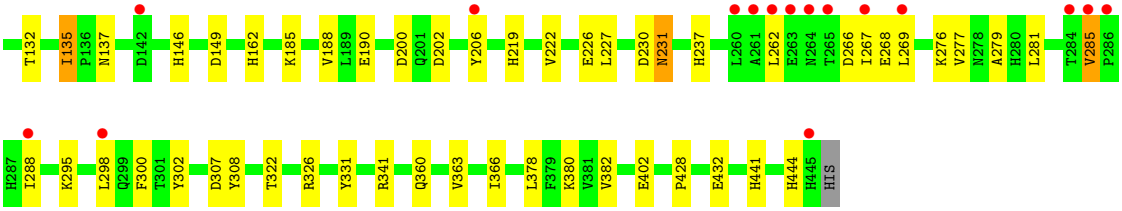
Chain A:



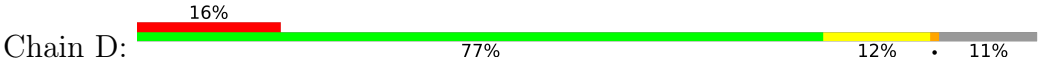
• Molecule 1: Dihydrolipoamide dehydrogenase

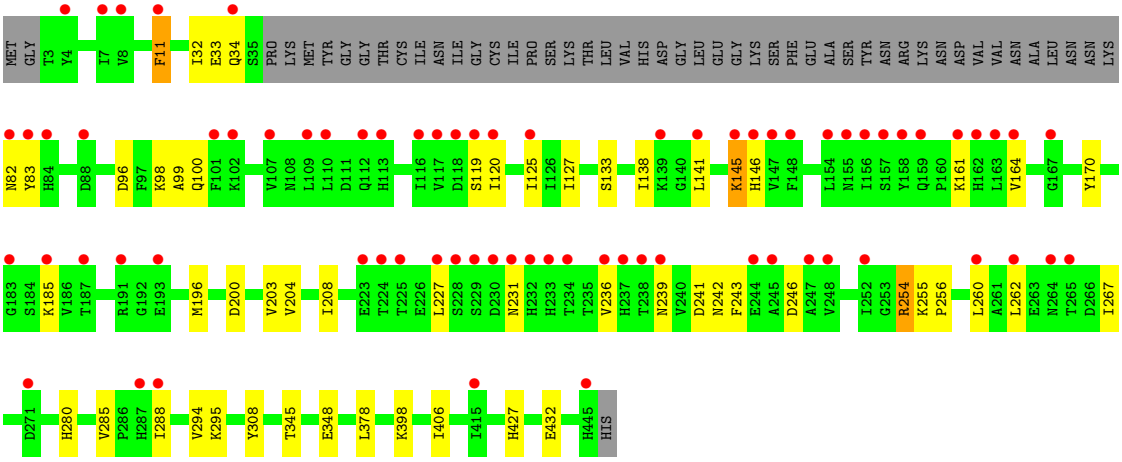
Chain B:





• Molecule 1: Dihydrolipoamide dehydrogenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	250.63Å 250.63Å 141.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.80 – 2.40 49.80 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.80-2.40) 100.0 (49.80-2.40)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.209 , 0.238 0.204 , 0.234	Depositor DCC
R_{free} test set	5055 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.7	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	13403	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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: 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	0.26	0/3508	0.49	0/4770
1	B	0.29	0/3106	0.54	1/4225 (0.0%)
1	C	0.28	0/3530	0.50	0/4800
1	D	0.26	0/3164	0.50	0/4305
All	All	0.27	0/13308	0.51	1/18100 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	125	ILE	CG1-CB-CG2	-5.16	100.06	111.40

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	3440	0	3374	32	0
1	B	3047	0	2991	51	1
1	C	3460	0	3388	32	1
1	D	3102	0	3032	28	0
2	A	53	0	31	0	0
2	B	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	53	0	31	2	0
2	D	53	0	31	1	0
3	A	20	0	13	1	0
4	A	24	0	0	4	0
4	B	35	0	0	2	1
4	C	44	0	0	5	1
4	D	19	0	0	1	0
All	All	13403	0	12922	144	2

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 6.

All (144) 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:C:200:ASP:OD2	4:C:601:HOH:O	1.84	0.95
1:A:92:ILE:O	4:A:601:HOH:O	1.90	0.88
1:B:402:GLU:OE2	4:B:601:HOH:O	1.93	0.86
1:A:199:GLU:OE1	4:A:602:HOH:O	1.92	0.85
1:D:34:GLN:HG2	1:D:98:LYS:HG3	1.63	0.81
1:B:363:VAL:HA	1:B:366:ILE:HD12	1.63	0.80
1:B:146:HIS:NE2	1:B:231:ASN:O	2.18	0.76
1:A:139:LYS:HG2	1:A:226:GLU:HG3	1.68	0.74
1:B:307:ASP:OD1	1:B:326:ARG:NH2	2.21	0.73
1:A:162:HIS:N	1:A:246:ASP:OD1	2.18	0.72
1:A:232:HIS:O	1:A:232:HIS:ND1	2.23	0.71
1:D:164:VAL:HG11	1:D:236:VAL:HG21	1.71	0.71
1:C:368:ARG:HE	1:C:372:ASN:HD21	1.36	0.71
1:C:307:ASP:OD1	1:C:326:ARG:NH2	2.19	0.70
1:A:238:THR:HG22	1:A:240:VAL:H	1.56	0.70
1:A:258:THR:OG1	4:A:603:HOH:O	2.10	0.69
1:B:190:GLU:OE1	4:B:602:HOH:O	2.10	0.69
1:D:280:HIS:HD2	4:D:603:HOH:O	1.76	0.68
1:C:306:ASP:OD1	1:C:321:ARG:NH2	2.25	0.68
1:D:241:ASP:OD1	1:D:242:ASN:N	2.26	0.68
1:C:65:GLU:O	1:C:69:ASN:ND2	2.27	0.66
1:C:3:THR:N	4:C:603:HOH:O	2.30	0.64
1:B:230:ASP:O	1:B:231:ASN:HB2	1.98	0.63
1:D:138:ILE:HD13	1:D:227:LEU:HD13	1.81	0.62
2:C:501:FAD:O4'	4:C:602:HOH:O	2.11	0.61
1:A:149:ASP:HB3	1:A:152:GLY:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:THR:HG23	1:D:348:GLU:H	1.65	0.60
1:A:333:VAL:HG22	1:A:339:LEU:HB3	1.82	0.60
1:A:307:ASP:OD1	1:A:326:ARG:NH2	2.32	0.60
1:C:368:ARG:HE	1:C:372:ASN:ND2	1.98	0.60
2:C:501:FAD:O1A	4:C:602:HOH:O	2.16	0.59
1:C:306:ASP:CG	1:C:321:ARG:HH22	2.06	0.59
1:B:112:GLN:O	1:B:112:GLN:NE2	2.30	0.59
1:A:427:HIS:ND1	1:A:432:GLU:OE1	2.33	0.58
1:B:441:HIS:HB3	1:B:444:HIS:HB2	1.85	0.58
1:D:170:TYR:CE1	1:D:196:MET:HG2	2.39	0.57
1:D:262:LEU:HD12	1:D:267:ILE:HB	1.86	0.56
1:D:285:VAL:HG13	1:D:288:ILE:HB	1.87	0.55
1:C:196:MET:HE3	1:C:204:VAL:HG22	1.89	0.54
1:A:170:TYR:HE1	1:A:196:MET:HG2	1.73	0.54
1:D:32:ILE:HG21	1:D:99:ALA:HB2	1.89	0.54
1:D:203:VAL:HG22	1:D:378:LEU:HD23	1.90	0.54
1:B:18:LEU:HD13	1:B:126:ILE:HG13	1.89	0.54
1:B:7:ILE:HB	1:B:125:ILE:HD12	1.90	0.53
1:B:8:VAL:HG22	1:B:31:VAL:HG12	1.91	0.53
1:B:125:ILE:HG22	1:B:288:ILE:HG12	1.92	0.52
1:D:255:LYS:HG3	1:D:256:PRO:HD2	1.92	0.52
1:B:7:ILE:HB	1:B:125:ILE:CD1	2.41	0.51
1:A:52:LYS:HE2	1:A:334:PHE:CD1	2.46	0.51
1:B:285:VAL:HG11	1:B:288:ILE:HD12	1.90	0.51
1:D:127:ILE:HG22	1:D:294:VAL:HG11	1.92	0.51
1:C:11:PHE:CZ	1:C:86:LEU:HD22	2.46	0.51
1:B:125:ILE:O	1:B:126:ILE:HD13	2.11	0.51
1:D:125:ILE:HB	1:D:288:ILE:HG12	1.93	0.51
1:B:269:LEU:C	1:B:276:LYS:HE2	2.30	0.50
1:C:406:ILE:HG12	1:D:406:ILE:HG12	1.92	0.50
1:B:11:PHE:HD2	1:B:33:GLU:HG2	1.76	0.50
1:C:170:TYR:CE1	1:C:196:MET:HG2	2.46	0.50
1:B:268:GLU:HB3	1:B:276:LYS:HE3	1.92	0.50
1:B:6:LEU:O	1:B:29:VAL:HA	2.12	0.50
1:B:87:ALA:HA	1:B:92:ILE:HD11	1.94	0.49
1:B:89:ASP:O	1:B:92:ILE:HG13	2.13	0.49
1:B:262:LEU:HD13	1:B:269:LEU:HD11	1.94	0.49
1:D:161:LYS:N	1:D:246:ASP:OD2	2.45	0.49
1:C:44:ILE:HD13	1:C:49:ILE:HG13	1.95	0.49
1:B:33:GLU:OE1	2:B:501:FAD:H1B	2.12	0.49
1:B:6:LEU:HB3	1:B:29:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:LYS:HE3	1:D:146:HIS:H	1.77	0.49
1:D:170:TYR:HE1	1:D:196:MET:HG2	1.76	0.49
1:A:102:LYS:HD3	1:A:106:GLU:OE2	2.13	0.48
1:B:285:VAL:HG13	1:B:288:ILE:HB	1.95	0.48
1:B:32:ILE:HG21	1:B:99:ALA:HB2	1.94	0.48
1:C:230:ASP:OD1	1:C:231:ASN:N	2.47	0.48
1:D:138:ILE:HD11	1:D:141:LEU:HD13	1.95	0.48
1:A:229:SER:HA	1:A:234:THR:HA	1.96	0.48
1:B:25:THR:OG1	1:B:27:GLN:HG3	2.14	0.47
1:A:277:VAL:HB	1:A:281:LEU:HA	1.96	0.47
1:C:42:THR:HG23	1:C:46:ILE:HG13	1.96	0.47
1:D:204:VAL:O	1:D:208:ILE:HG12	2.15	0.47
1:A:189:LEU:HB3	1:A:222:VAL:HG11	1.95	0.47
1:B:298:LEU:HB3	1:B:300:PHE:CE2	2.50	0.47
1:C:81:LYS:HB2	1:C:81:LYS:HE2	1.79	0.47
1:C:52:LYS:HE2	1:C:334:PHE:CD2	2.50	0.46
1:A:11:PHE:CZ	1:A:86:LEU:HD22	2.50	0.46
1:A:145:LYS:O	1:A:234:THR:OG1	2.25	0.46
1:B:129:THR:HB	2:B:501:FAD:C8A	2.46	0.46
1:C:159:GLN:NE2	1:C:182:LEU:O	2.41	0.45
1:B:117:VAL:HG12	1:B:118:ASP:OD2	2.16	0.45
1:A:327:GLY:O	4:A:604:HOH:O	2.21	0.45
1:D:241:ASP:HB3	1:D:243:PHE:CZ	2.52	0.45
1:B:360:GLN:HB2	1:B:378:LEU:HD11	1.98	0.45
1:D:200:ASP:O	1:D:204:VAL:HG13	2.16	0.45
1:B:89:ASP:HB3	1:B:92:ILE:HG12	1.98	0.45
1:C:170:TYR:HE1	1:C:196:MET:HG2	1.82	0.45
1:A:170:TYR:CE1	1:A:196:MET:HG2	2.51	0.44
1:A:202:ASP:OD2	1:A:380:LYS:NZ	2.50	0.44
1:B:125:ILE:CG2	1:B:288:ILE:HG12	2.47	0.44
1:C:204:VAL:O	1:C:208:ILE:HG12	2.17	0.44
1:B:331:TYR:CZ	1:B:341:ARG:HG2	2.52	0.44
1:B:219:HIS:HB3	1:B:222:VAL:HG21	2.00	0.44
1:B:200:ASP:HB3	1:B:202:ASP:OD1	2.18	0.44
1:A:279:ALA:HB1	1:A:322:THR:HB	1.98	0.43
1:D:427:HIS:ND1	1:D:432:GLU:OE1	2.50	0.43
1:C:32:ILE:HG21	1:C:99:ALA:HB2	2.00	0.43
1:D:185:LYS:HD2	1:D:185:LYS:HA	1.83	0.43
1:C:3:THR:N	4:C:608:HOH:O	2.51	0.43
1:A:71:LYS:HE3	1:A:71:LYS:HB3	1.86	0.43
1:B:11:PHE:HB2	1:B:33:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:OD1	1:A:70:ARG:NH1	2.52	0.43
1:B:120:ILE:HD12	1:B:120:ILE:HA	1.89	0.43
1:A:159:GLN:NE2	1:A:182:LEU:O	2.52	0.43
1:C:212:GLU:HG3	1:C:218:LEU:HD12	2.00	0.42
1:B:206:TYR:N	1:B:206:TYR:CD1	2.87	0.42
1:D:133:SER:OG	1:D:254:ARG:NH2	2.49	0.42
1:B:279:ALA:HB1	1:B:322:THR:HB	2.01	0.42
1:B:125:ILE:HD12	1:B:125:ILE:HA	1.90	0.42
1:C:46:ILE:HD12	1:C:151:THR:HG21	2.01	0.42
1:C:277:VAL:HA	1:C:282:GLN:O	2.20	0.42
3:A:501:HIS:N	3:A:501:HIS:CD2	2.86	0.42
1:D:120:ILE:HD12	1:D:120:ILE:HA	1.78	0.42
1:C:279:ALA:HB1	1:C:322:THR:HB	2.01	0.42
1:C:363:VAL:HA	1:C:366:ILE:HD12	2.02	0.42
1:A:214:LYS:HZ3	1:A:336:ASP:HB3	1.85	0.42
1:B:135:ILE:H	1:B:135:ILE:HG13	1.47	0.42
1:D:11:PHE:HB2	1:D:33:GLU:OE1	2.20	0.41
1:C:197:PRO:O	1:C:198:ARG:HB2	2.20	0.41
1:B:31:VAL:HG22	1:B:94:VAL:HA	2.03	0.41
1:C:129:THR:HG21	1:C:260:LEU:HD21	2.02	0.41
1:A:222:VAL:HG13	1:A:238:THR:HG23	2.03	0.41
1:B:162:HIS:CD2	1:B:185:LYS:HD3	2.55	0.41
1:D:33:GLU:OE1	2:D:501:FAD:H1B	2.21	0.41
1:C:214:LYS:NZ	1:C:336:ASP:HB3	2.36	0.41
1:B:267:ILE:HD11	1:B:288:ILE:HD13	2.01	0.41
1:C:96:ASP:HB2	1:A:157:SER:HB2	2.03	0.41
1:C:200:ASP:HB3	1:C:202:ASP:OD1	2.21	0.41
1:B:277:VAL:HB	1:B:281:LEU:HA	2.03	0.41
1:A:229:SER:O	1:A:230:ASP:HB2	2.21	0.40
1:B:11:PHE:CD2	1:B:33:GLU:HG2	2.56	0.40
1:B:226:GLU:HB3	1:B:237:HIS:HB2	2.02	0.40
1:A:238:THR:HG22	1:A:240:VAL:N	2.30	0.40
1:B:104:ASN:ND2	1:B:266:ASP:OD2	2.49	0.40
1:B:428:PRO:HA	1:B:432:GLU:OE2	2.20	0.40
1:A:105:THR:O	1:A:121:THR:OG1	2.28	0.40
1:B:202:ASP:OD2	1:B:380:LYS:NZ	2.44	0.40

All (2) 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)
1:C:206:TYR:OH	1:B:206:TYR:OH[11_554]	2.07	0.13
4:C:636:HOH:O	4:B:619:HOH:O[11_554]	2.19	0.01

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	440/446 (99%)	432 (98%)	8 (2%)	0	100	100
1	B	387/446 (87%)	376 (97%)	10 (3%)	1 (0%)	41	55
1	C	442/446 (99%)	432 (98%)	9 (2%)	1 (0%)	47	62
1	D	393/446 (88%)	382 (97%)	10 (2%)	1 (0%)	41	55
All	All	1662/1784 (93%)	1622 (98%)	37 (2%)	3 (0%)	47	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	231	ASN
1	C	230	ASP
1	D	231	ASN

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	379/382 (99%)	369 (97%)	10 (3%)	46	66
1	B	335/382 (88%)	320 (96%)	15 (4%)	27	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	381/382 (100%)	367 (96%)	14 (4%)	34 53
1	D	341/382 (89%)	328 (96%)	13 (4%)	33 51
All	All	1436/1528 (94%)	1384 (96%)	52 (4%)	35 54

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	11	PHE
1	C	25	THR
1	C	48	CYS
1	C	52	LYS
1	C	81	LYS
1	C	119	SER
1	C	149	ASP
1	C	188	VAL
1	C	191	ARG
1	C	232	HIS
1	C	295	LYS
1	C	308	TYR
1	C	370	LYS
1	C	446	HIS
1	A	11	PHE
1	A	48	CYS
1	A	52	LYS
1	A	81	LYS
1	A	139	LYS
1	A	185	LYS
1	A	230	ASP
1	A	295	LYS
1	A	308	TYR
1	A	333	VAL
1	B	11	PHE
1	B	102	LYS
1	B	113	HIS
1	B	128	ASN
1	B	132	THR
1	B	135	ILE
1	B	137	ASN
1	B	149	ASP
1	B	188	VAL
1	B	227	LEU

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Mol	Chain	Res	Type
1	B	285	VAL
1	B	295	LYS
1	B	302	TYR
1	B	308	TYR
1	B	382	VAL
1	D	11	PHE
1	D	82	ASN
1	D	83	TYR
1	D	96	ASP
1	D	100	GLN
1	D	119	SER
1	D	145	LYS
1	D	239	ASN
1	D	254	ARG
1	D	260	LEU
1	D	295	LYS
1	D	308	TYR
1	D	398	LYS

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

Mol	Chain	Res	Type
1	C	372	ASN
1	B	91	ASN
1	B	137	ASN
1	D	162	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	D	501	1	53,58,58	0.47	0	68,89,89	0.53	2 (2%)
3	HIS	A	501	-	5,10,11	0.60	0	3,12,14	1.27	1 (33%)
2	FAD	B	501	-	53,58,58	0.45	0	68,89,89	0.57	2 (2%)
3	HIS	A	502	-	5,10,11	0.56	0	3,12,14	1.61	1 (33%)
2	FAD	C	501	-	53,58,58	0.44	0	68,89,89	0.51	1 (1%)
2	FAD	A	503	-	53,58,58	0.45	0	68,89,89	0.50	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	501	1	-	11/30/50/50	0/6/6/6
3	HIS	A	501	-	-	1/5/6/8	0/1/1/1
2	FAD	B	501	-	-	10/30/50/50	0/6/6/6
3	HIS	A	502	-	-	1/5/6/8	0/1/1/1
2	FAD	C	501	-	-	7/30/50/50	0/6/6/6
2	FAD	A	503	-	-	6/30/50/50	0/6/6/6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	FAD	P-O3P-PA	-2.64	123.76	132.83
2	C	501	FAD	C5A-C6A-N6A	2.35	123.92	120.35
2	D	501	FAD	C5A-C6A-N6A	2.30	123.84	120.35
2	B	501	FAD	C5A-C6A-N6A	2.29	123.84	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	503	FAD	C5A-C6A-N6A	2.28	123.81	120.35
2	D	501	FAD	P-O3P-PA	-2.20	125.27	132.83
3	A	502	HIS	CD2-NE2-CE1	2.02	108.94	105.78
3	A	501	HIS	CD2-NE2-CE1	2.02	108.94	105.78

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	FAD	C5'-O5'-P-O1P
2	C	501	FAD	C5'-O5'-P-O2P
2	A	503	FAD	C5'-O5'-P-O2P
2	B	501	FAD	C3'-C4'-C5'-O5'
2	B	501	FAD	O4'-C4'-C5'-O5'
2	B	501	FAD	PA-O3P-P-O5'
2	D	501	FAD	O4'-C4'-C5'-O5'
2	D	501	FAD	C5'-O5'-P-O1P
2	D	501	FAD	C5'-O5'-P-O2P
3	A	501	HIS	CA-CB-CG-ND1
3	A	502	HIS	CA-CB-CG-ND1
2	B	501	FAD	O2'-C2'-C3'-O3'
2	C	501	FAD	PA-O3P-P-O5'
2	A	503	FAD	PA-O3P-P-O5'
2	D	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	O2'-C2'-C3'-C4'
2	A	503	FAD	C5'-O5'-P-O3P
2	B	501	FAD	C5B-O5B-PA-O3P
2	A	503	FAD	C5'-O5'-P-O1P
2	B	501	FAD	C1'-C2'-C3'-O3'
2	C	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	C1'-C2'-C3'-C4'
2	A	503	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	O2'-C2'-C3'-O3'
2	B	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	O4B-C4B-C5B-O5B
2	C	501	FAD	O4'-C4'-C5'-O5'
2	C	501	FAD	C5'-O5'-P-O3P
2	D	501	FAD	C5'-O5'-P-O3P
2	D	501	FAD	O2'-C2'-C3'-C4'
2	A	503	FAD	PA-O3P-P-O1P
2	B	501	FAD	PA-O3P-P-O2P
2	D	501	FAD	PA-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
2	D	501	FAD	C3'-C4'-C5'-O5'
2	C	501	FAD	C1'-C2'-C3'-O3'
2	D	501	FAD	C1'-C2'-C3'-O3'

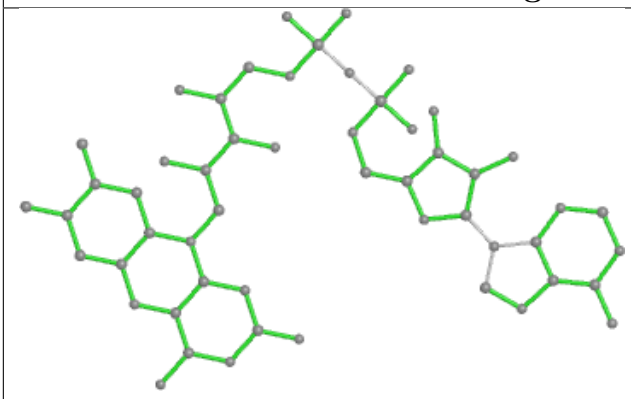
There are no ring outliers.

4 monomers are involved in 6 short contacts:

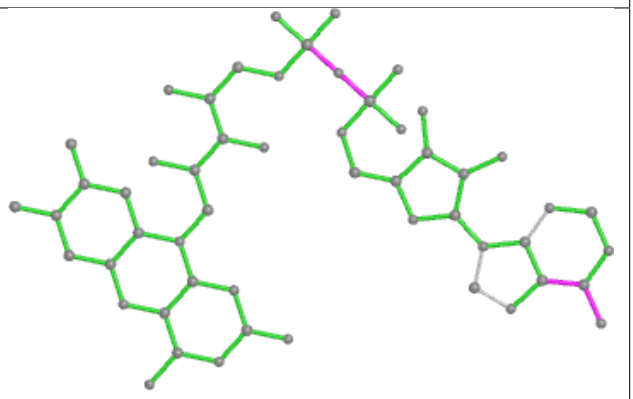
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	FAD	1	0
3	A	501	HIS	1	0
2	B	501	FAD	2	0
2	C	501	FAD	2	0

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.

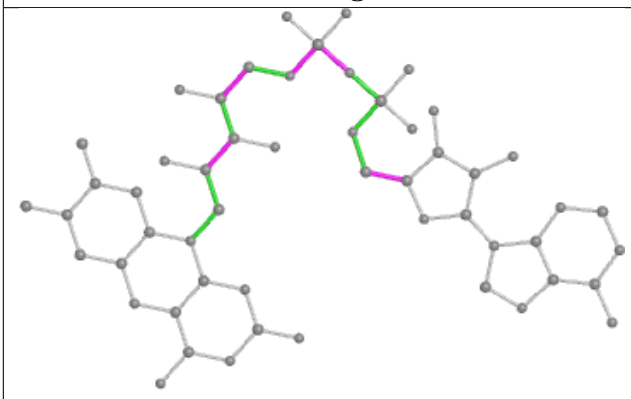
Ligand FAD D 501



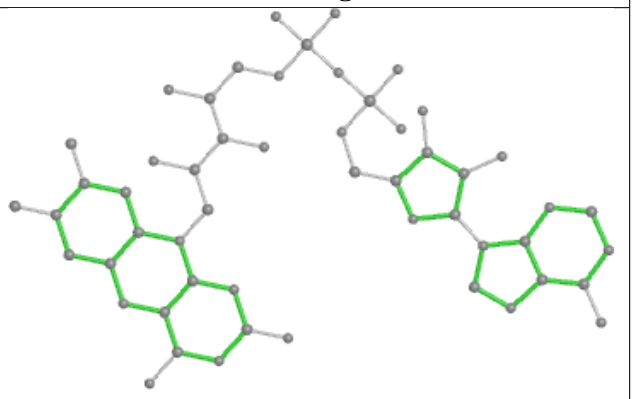
Bond lengths



Bond angles

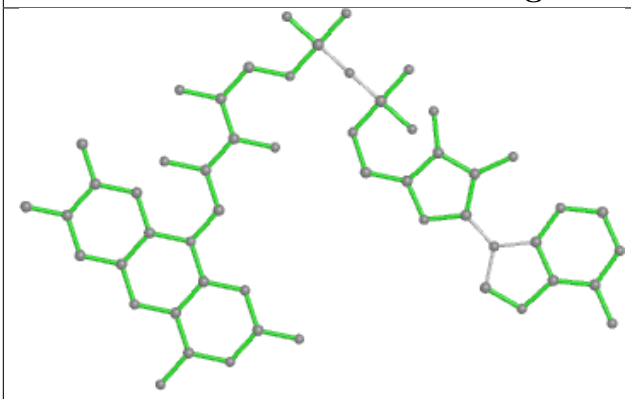


Torsions

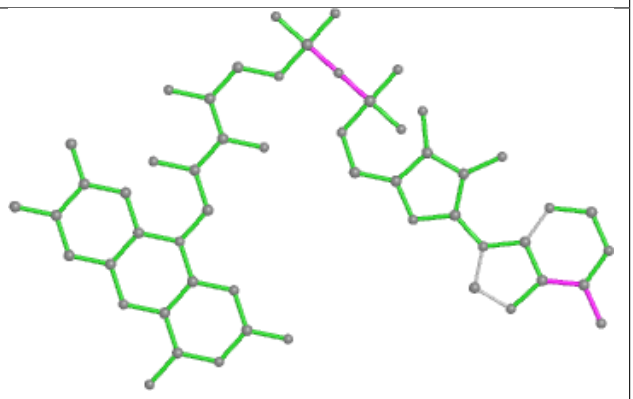


Rings

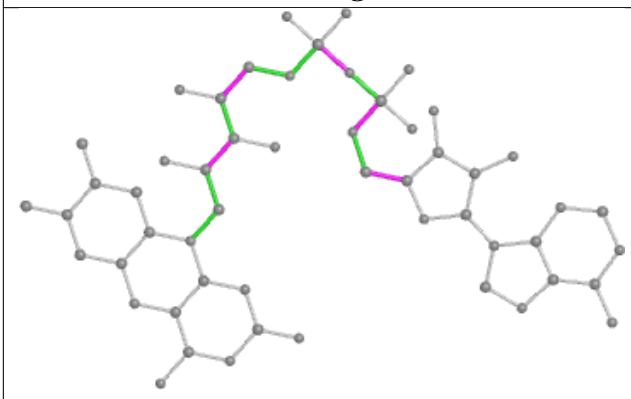
Ligand FAD B 501



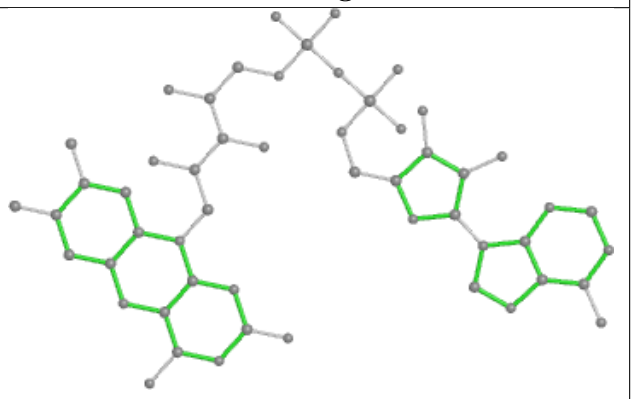
Bond lengths



Bond angles

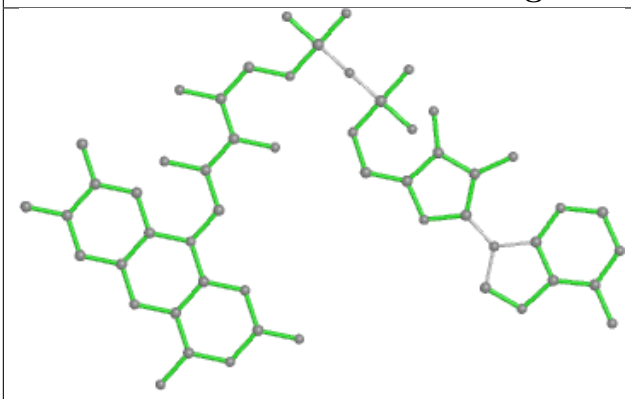


Torsions

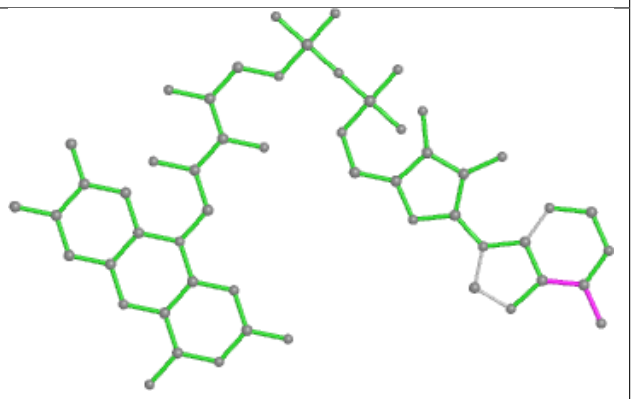


Rings

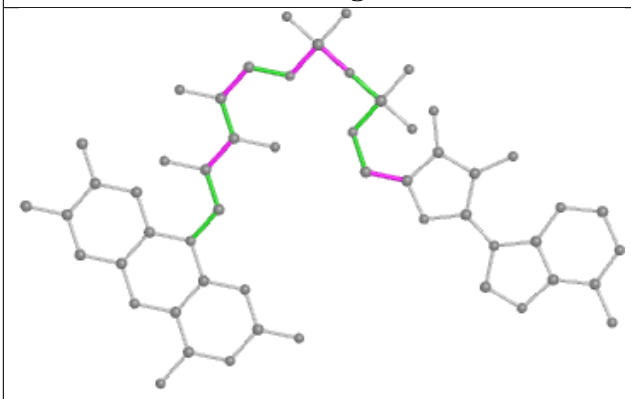
Ligand FAD C 501



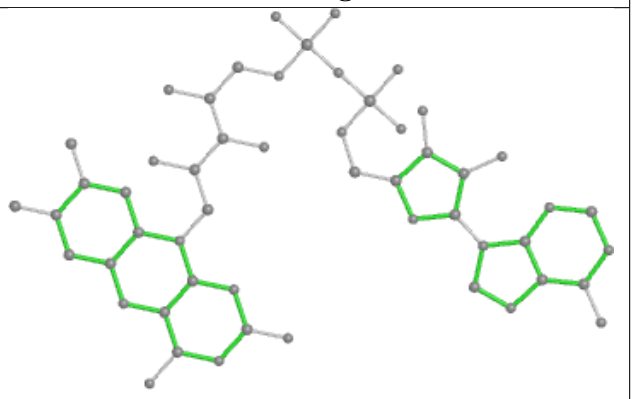
Bond lengths



Bond angles

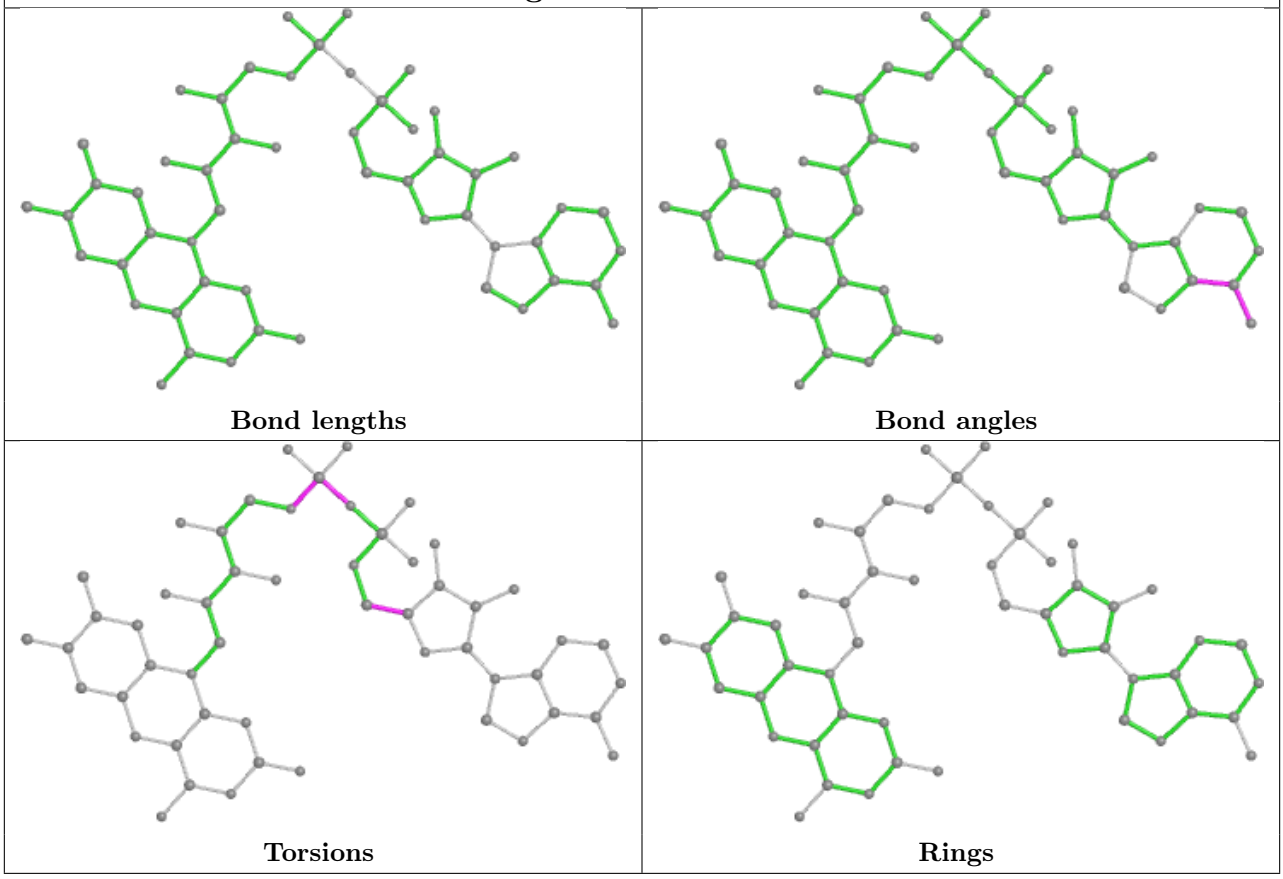


Torsions



Rings

Ligand FAD A 503



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	442/446 (99%)	0.13	7 (1%) 72 70	49, 70, 100, 131	0
1	B	391/446 (87%)	0.80	61 (15%) 2 1	44, 73, 133, 153	0
1	C	444/446 (99%)	0.17	10 (2%) 60 58	40, 61, 86, 116	0
1	D	397/446 (89%)	0.86	73 (18%) 1 1	43, 86, 132, 150	0
All	All	1674/1784 (93%)	0.47	151 (9%) 9 8	40, 70, 125, 153	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	95	LEU	8.5
1	B	109	LEU	7.1
1	B	101	PHE	6.9
1	B	115	ASP	6.5
1	B	110	LEU	6.5
1	B	107	VAL	6.5
1	B	111	ASP	6.4
1	B	99	ALA	6.2
1	B	117	VAL	6.1
1	B	97	PHE	6.1
1	D	107	VAL	5.8
1	D	84	HIS	5.6
1	D	113	HIS	5.4
1	B	89	ASP	5.4
1	D	82	ASN	5.3
1	B	30	ALA	5.2
1	D	101	PHE	5.2
1	D	109	LEU	5.2
1	D	112	GLN	5.1
1	D	232	HIS	5.1
1	B	113	HIS	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	262	LEU	4.9
1	D	248	VAL	4.8
1	B	11	PHE	4.7
1	B	29	VAL	4.7
1	B	92	ILE	4.7
1	D	236	VAL	4.6
1	D	147	VAL	4.6
1	D	116	ILE	4.5
1	B	23	ALA	4.5
1	B	103	SER	4.4
1	B	264	ASN	4.4
1	B	88	ASP	4.3
1	D	227	LEU	4.2
1	B	142	ASP	4.2
1	D	146	HIS	4.1
1	B	118	ASP	4.1
1	A	232	HIS	4.1
1	D	141	LEU	4.0
1	D	155	ASN	4.0
1	B	445	HIS	3.9
1	D	154	LEU	3.9
1	B	125	ILE	3.9
1	D	260	LEU	3.9
1	B	102	LYS	3.9
1	B	31	VAL	3.9
1	D	88	ASP	3.8
1	B	32	ILE	3.8
1	B	120	ILE	3.8
1	B	105	THR	3.8
1	D	245	ALA	3.7
1	B	116	ILE	3.7
1	B	262	LEU	3.7
1	D	239	ASN	3.6
1	B	94	VAL	3.6
1	C	61	GLY	3.6
1	D	11	PHE	3.6
1	B	100	GLN	3.6
1	D	148	PHE	3.6
1	D	265	THR	3.5
1	D	231	ASN	3.5
1	D	191	ARG	3.5
1	B	122	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	104	ASN	3.4
1	B	263	GLU	3.4
1	B	265	THR	3.4
1	B	112	GLN	3.4
1	B	96	ASP	3.4
1	B	267	ILE	3.4
1	B	288	ILE	3.4
1	A	140	GLY	3.4
1	A	239	ASN	3.3
1	D	288	ILE	3.3
1	D	102	LYS	3.3
1	B	119	SER	3.3
1	D	159	GLN	3.3
1	D	163	LEU	3.2
1	B	25	THR	3.2
1	B	106	GLU	3.2
1	B	121	THR	3.1
1	D	158	TYR	3.0
1	D	162	HIS	3.0
1	A	240	VAL	3.0
1	D	187	THR	2.9
1	D	117	VAL	2.9
1	D	185	LYS	2.9
1	B	124	HIS	2.9
1	B	108	ASN	2.9
1	B	298	LEU	2.9
1	C	389	MET	2.9
1	B	7	ILE	2.9
1	D	225	THR	2.9
1	D	145	LYS	2.9
1	B	269	LEU	2.9
1	D	223	GLU	2.8
1	D	164	VAL	2.8
1	D	233	HIS	2.8
1	B	90	ASN	2.8
1	B	34	GLN	2.8
1	D	110	LEU	2.8
1	D	120	ILE	2.8
1	D	183	GLY	2.8
1	B	260	LEU	2.7
1	D	264	ASN	2.7
1	D	445	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	247	ALA	2.6
1	D	83	TYR	2.6
1	A	222	VAL	2.6
1	D	156	ILE	2.6
1	D	224	THR	2.6
1	D	118	ASP	2.6
1	A	230	ASP	2.6
1	C	232	HIS	2.6
1	B	87	ALA	2.6
1	D	244	GLU	2.5
1	C	206	TYR	2.5
1	B	261	ALA	2.4
1	D	161	LYS	2.4
1	D	237	HIS	2.4
1	D	193	GLU	2.4
1	C	409	LEU	2.4
1	D	157	SER	2.4
1	B	286	PRO	2.4
1	D	252	ILE	2.4
1	D	229	SER	2.4
1	D	271	ASP	2.3
1	C	415	ILE	2.3
1	B	114	ASP	2.3
1	D	228	SER	2.3
1	B	206	TYR	2.3
1	D	4	TYR	2.3
1	D	287	HIS	2.3
1	D	34	GLN	2.3
1	D	119	SER	2.3
1	D	415	ILE	2.3
1	B	284	THR	2.3
1	C	411	ILE	2.2
1	D	139	LYS	2.2
1	D	125	ILE	2.2
1	D	7	ILE	2.2
1	D	230	ASP	2.2
1	C	58	GLY	2.2
1	B	285	VAL	2.1
1	A	143	GLN	2.1
1	B	91	ASN	2.1
1	D	238	THR	2.1
1	C	231	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	167	GLY	2.1
1	D	234	THR	2.0
1	C	67	SER	2.0
1	D	8	VAL	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)

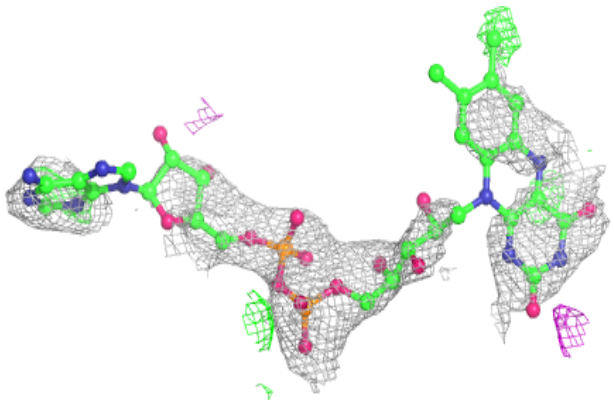
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

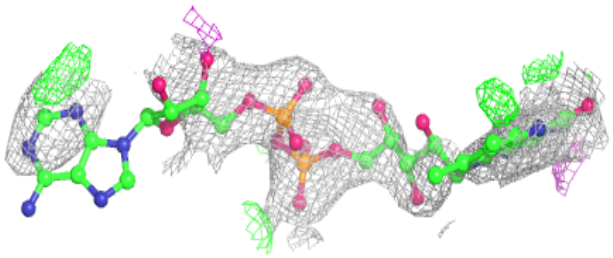
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HIS	A	502	10/11	0.49	0.46	112,128,137,137	0
3	HIS	A	501	10/11	0.76	0.25	99,103,111,115	0
2	FAD	B	501	53/53	0.81	0.28	95,122,141,187	27
2	FAD	D	501	53/53	0.88	0.22	86,114,134,159	25
2	FAD	C	501	53/53	0.95	0.15	49,61,71,77	0
2	FAD	A	503	53/53	0.96	0.18	52,65,73,78	0

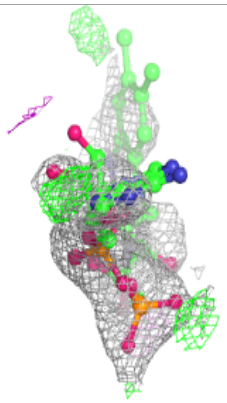
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

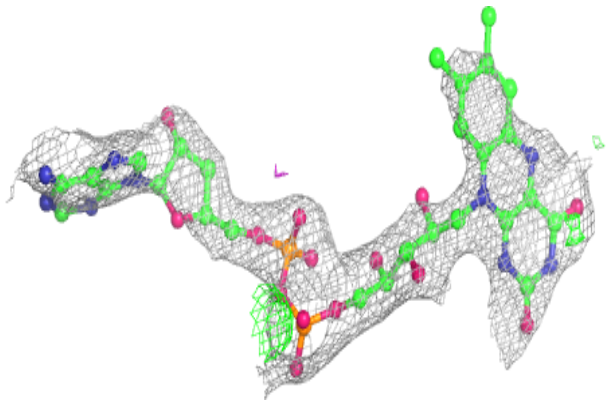


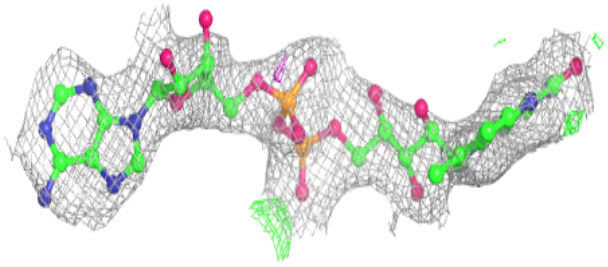


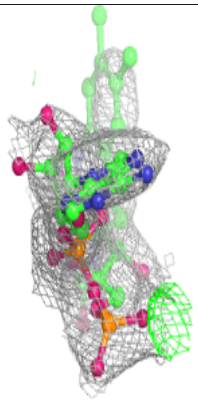


Electron density around FAD D 501:

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

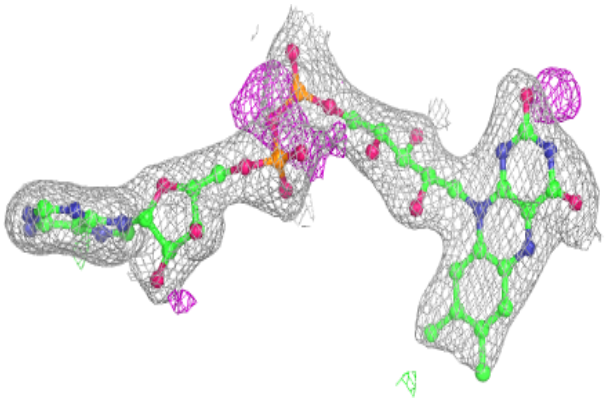


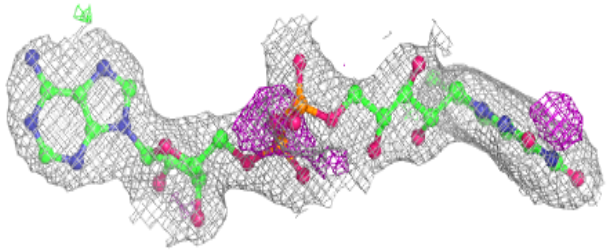


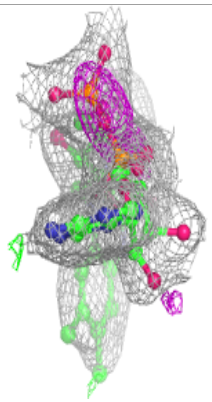


Electron density around FAD C 501:

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

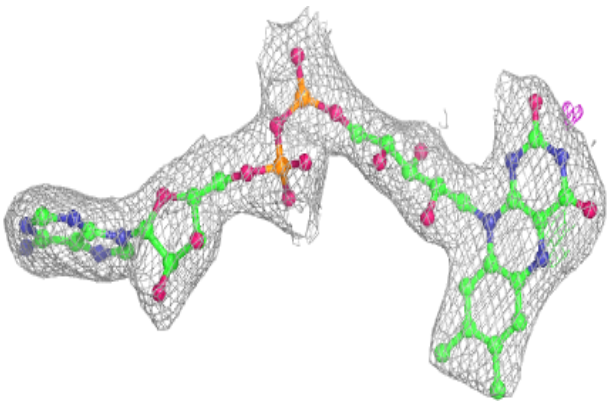


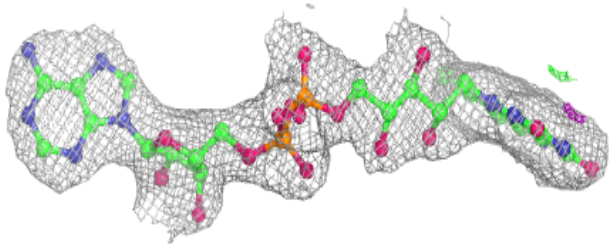


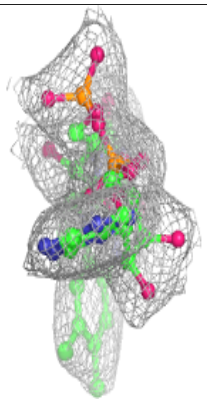


Electron density around FAD A 503:

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







6.5 Other polymers (i)

There are no such residues in this entry.