Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:13 am BST

PDB ID	:	2OK8
Title	:	Ferredoxin-NADP+ reductase from Plasmodium falciparum
Authors	:	Milani, M.; Mastrangelo, E.; Bolognesi, M.
Deposited on	:	2007-01-16
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 following versions of software and data (see references ⓘ) were used in the production of this report:

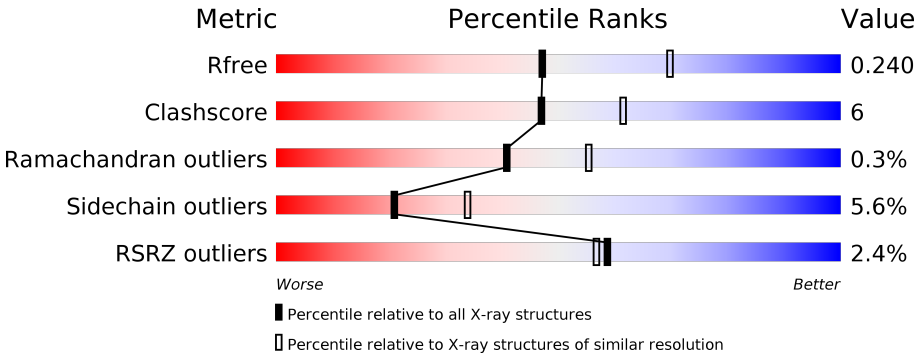
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 on 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	316	69% 14% 17%
1	B	316	3% 67% 15% • 17%
1	C	316	2% 66% 15% • 19%
1	D	316	3% 66% 15% • 17%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	A	9002	-	-	-	X

2 Entry composition

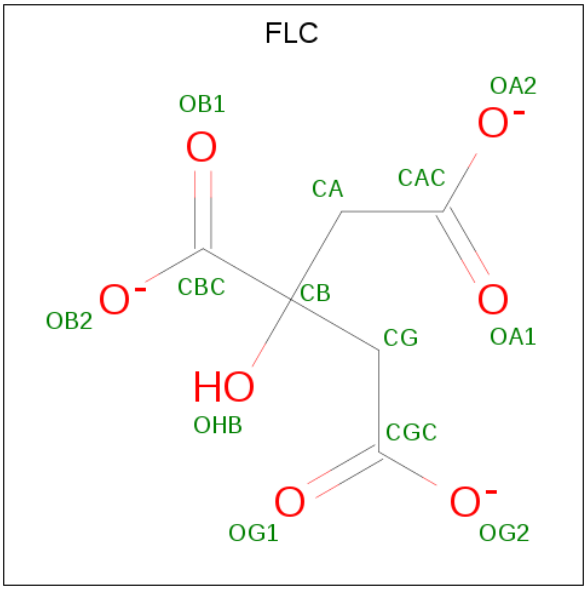
There are 4 unique types of molecules in this entry. The entry contains 9261 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative ferredoxin–NADP reductase.

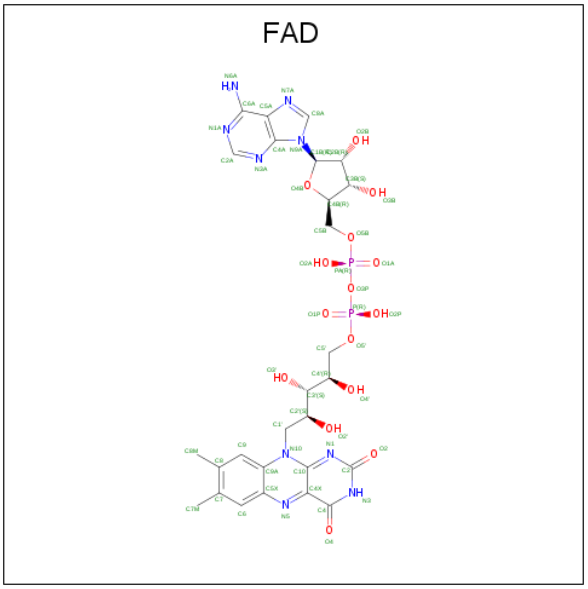
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2201	1427	361	404	9			
1	B	262	Total	C	N	O	S	0	1	0
			2199	1430	358	402	9			
1	C	257	Total	C	N	O	S	0	0	0
			2146	1397	349	391	9			
1	D	261	Total	C	N	O	S	0	0	0
			2186	1423	357	397	9			

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 water.

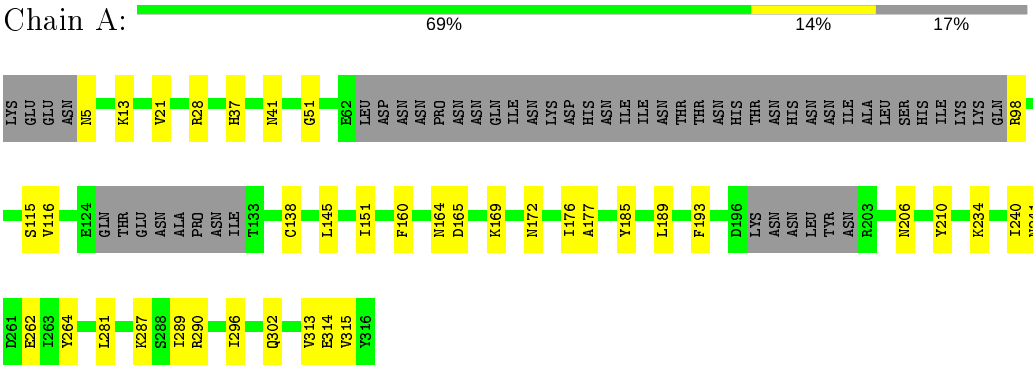
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	88	Total	O	0	0
			88	88		
4	C	73	Total	O	0	0
			73	73		
4	D	39	Total	O	0	0
			39	39		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

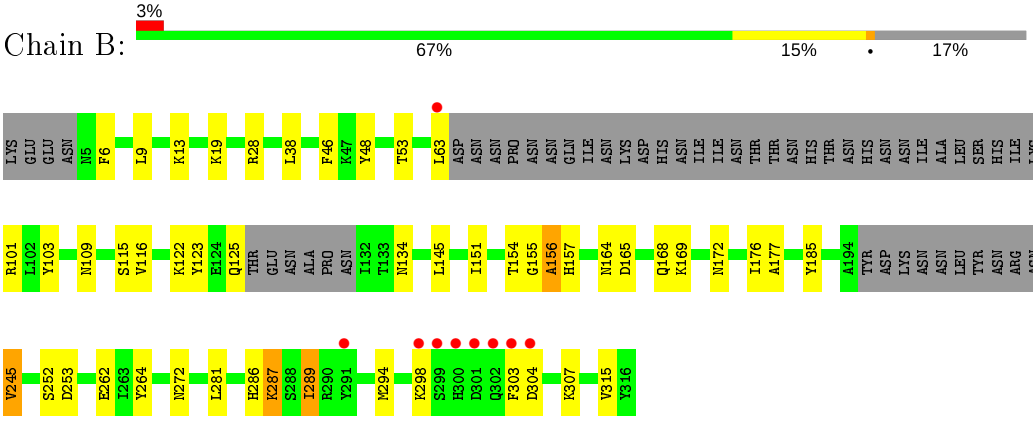
- Molecule 1: Putative ferredoxin–NADP reductase

Chain A:



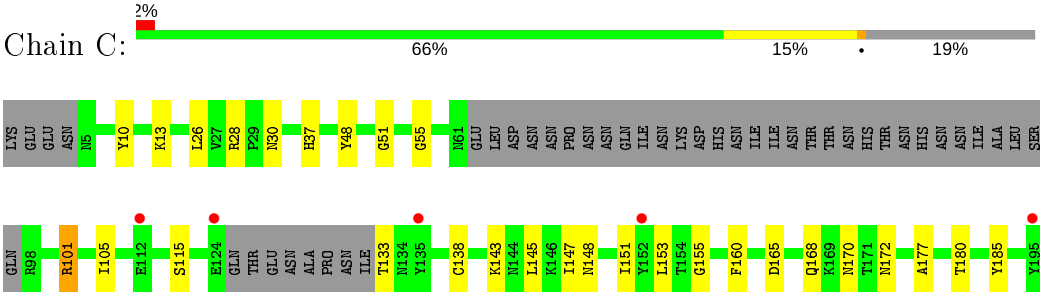
- Molecule 1: Putative ferredoxin–NADP reductase

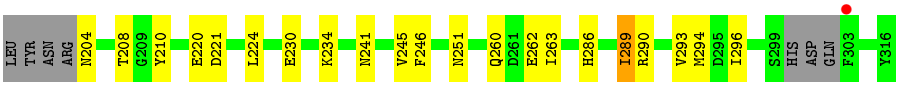
Chain B:



- Molecule 1: Putative ferredoxin–NADP reductase

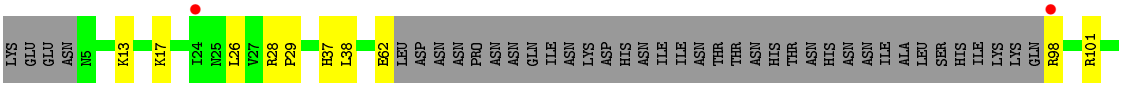
Chain C:

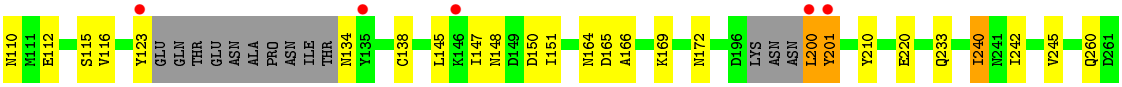


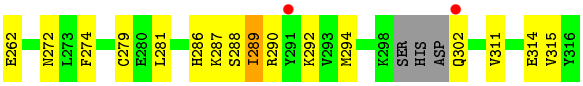


• Molecule 1: Putative ferredoxin–NADP reductase

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.04Å 138.04Å 147.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 69.02 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.40) 99.4 (69.02-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.195 , 0.246 0.192 , 0.240	Depositor DCC
R_{free} test set	3197 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	41.7	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9261	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: FLC, 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	0.52	0/2256	0.62	0/3045
1	B	0.52	0/2254	0.63	0/3043
1	C	0.50	0/2199	0.59	0/2967
1	D	0.48	0/2240	0.60	0/3022
All	All	0.50	0/8949	0.61	0/12077

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
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	154	THR	Peptide

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	2201	0	2144	22	0
1	B	2199	0	2150	24	0
1	C	2146	0	2101	34	0
1	D	2186	0	2136	25	0
2	A	13	0	5	0	0
2	B	13	0	5	0	0
3	A	53	0	31	0	0
3	B	53	0	31	2	0
3	C	53	0	31	3	0
3	D	53	0	31	0	0
4	A	91	0	0	0	0
4	B	88	0	0	6	0
4	C	73	0	0	3	0
4	D	39	0	0	2	0
All	All	9261	0	8665	109	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 6.

All (109) 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:165:ASP:HB3	1:A:169:LYS:HG3	1.36	1.05
1:A:245:VAL:HG22	1:A:262:GLU:HG3	1.61	0.83
1:C:172:ASN:HD22	1:C:210:TYR:H	1.26	0.81
1:D:245:VAL:HG22	1:D:262:GLU:HG3	1.64	0.80
1:B:272:ASN:HB3	4:B:9033:HOH:O	1.81	0.78
1:A:172:ASN:HD22	1:A:210:TYR:H	1.32	0.75
1:B:176:ILE:HD12	1:B:281:LEU:HD11	1.70	0.73
1:B:172:ASN:HD22	1:B:210[B]:TYR:H	1.39	0.71
1:C:170:ASN:ND2	1:C:208:THR:OG1	2.26	0.69
3:B:415:FAD:H8A	3:B:415:FAD:H51A	1.74	0.69
1:C:101:ARG:HG3	1:C:138:CYS:HB2	1.75	0.68
1:B:172:ASN:HD22	1:B:210[A]:TYR:H	1.44	0.66
1:C:234:LYS:HE2	4:C:476:HOH:O	1.96	0.66
1:C:220:GLU:HG3	1:C:246:PHE:CZ	2.30	0.66
1:B:98:ARG:HD3	4:B:9084:HOH:O	1.96	0.66
1:C:172:ASN:ND2	1:C:210:TYR:H	1.93	0.65
1:D:101:ARG:HG3	1:D:138:CYS:HB2	1.79	0.64
3:C:415:FAD:H51A	3:C:415:FAD:H8A	1.80	0.63
1:B:294:MET:O	1:B:298:LYS:HG2	1.99	0.61
1:B:46:PHE:CE1	1:B:155:GLY:HA2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:415:FAD:C8A	3:B:415:FAD:H51A	2.30	0.60
1:C:10:TYR:HB2	1:C:155:GLY:H	1.65	0.60
1:B:286:HIS:O	1:B:289:ILE:HG13	2.01	0.60
1:B:122:LYS:HE2	4:B:9078:HOH:O	2.01	0.58
1:C:220:GLU:HG3	1:C:246:PHE:CE1	2.40	0.57
1:D:172:ASN:ND2	1:D:210:TYR:H	2.03	0.57
1:B:122:LYS:HD2	4:B:9057:HOH:O	2.06	0.56
1:A:172:ASN:ND2	1:A:210:TYR:H	2.02	0.55
1:C:294:MET:HG3	4:C:464:HOH:O	2.06	0.55
1:A:101:ARG:HG3	1:A:138:CYS:HB2	1.89	0.54
1:A:37:HIS:CE1	1:A:115:SER:HB2	2.43	0.54
1:A:177:ALA:HB2	1:A:185:TYR:HE2	1.73	0.53
1:A:165:ASP:CB	1:A:169:LYS:HG3	2.24	0.52
1:D:38:LEU:O	1:D:115:SER:HA	2.09	0.52
1:C:286:HIS:O	1:C:289:ILE:HG13	2.10	0.52
1:D:123:TYR:CZ	1:D:134:ASN:HB2	2.45	0.52
1:B:303:PHE:HA	1:B:307:LYS:HD2	1.92	0.52
1:C:145:LEU:HD11	1:C:151:ILE:HD12	1.92	0.51
1:B:19:LYS:HE2	4:B:9072:HOH:O	2.09	0.51
1:C:10:TYR:H	1:C:155:GLY:HA3	1.76	0.50
1:B:48:TYR:O	1:B:109:ASN:OD1	2.30	0.50
1:D:200:LEU:O	1:D:201:TYR:CG	2.64	0.50
1:B:122:LYS:HE3	4:B:9007:HOH:O	2.12	0.49
1:C:230:GLU:O	1:C:234:LYS:HG3	2.11	0.49
1:B:287:LYS:HA	1:B:315:VAL:HB	1.94	0.49
1:D:272:ASN:HB3	4:D:439:HOH:O	2.11	0.49
1:A:98:ARG:HA	1:B:98:ARG:NH1	2.28	0.48
1:A:145:LEU:HD11	1:A:151:ILE:HD12	1.95	0.48
1:B:245:VAL:HG22	1:B:262:GLU:HG3	1.95	0.48
1:D:147:ILE:O	1:D:148:ASN:HB2	2.14	0.48
1:D:98:ARG:O	1:D:101:ARG:NH1	2.44	0.47
1:D:26:LEU:HG	1:D:37:HIS:HB2	1.95	0.47
1:C:37:HIS:CE1	1:C:115:SER:HB2	2.50	0.47
1:C:10:TYR:HB2	1:C:155:GLY:N	2.27	0.47
3:C:415:FAD:C8A	3:C:415:FAD:H51A	2.44	0.46
1:D:240:ILE:HD11	1:D:242:ILE:HD11	1.97	0.46
1:C:10:TYR:O	1:C:155:GLY:N	2.49	0.46
1:C:26:LEU:HG	1:C:37:HIS:HB2	1.96	0.46
1:A:177:ALA:HB2	1:A:185:TYR:CE2	2.49	0.46
1:B:38:LEU:O	1:B:115:SER:HA	2.16	0.45
1:C:147:ILE:O	1:C:148:ASN:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:LYS:HA	1:D:315:VAL:HB	1.98	0.45
1:C:263:ILE:CG2	1:C:296:ILE:HD13	2.47	0.45
1:C:48:TYR:CE2	1:C:105:ILE:HG21	2.52	0.45
1:A:193:PHE:CE2	1:A:240:ILE:HD11	2.52	0.45
1:A:290:ARG:HG3	1:A:313:VAL:HG11	1.99	0.45
1:B:101:ARG:HB2	1:B:103:TYR:CE1	2.52	0.45
1:A:176:ILE:HD12	1:A:281:LEU:HD11	1.99	0.44
1:D:112:GLU:HG2	4:D:427:HOH:O	2.16	0.44
1:C:290:ARG:NH1	4:C:464:HOH:O	2.50	0.44
1:D:37:HIS:CE1	1:D:115:SER:HB2	2.52	0.44
1:C:290:ARG:O	1:C:294:MET:HG2	2.18	0.44
1:D:233:GLN:HA	1:D:240:ILE:HG12	2.00	0.44
1:C:101:ARG:HG3	1:C:138:CYS:CB	2.46	0.44
1:D:17:LYS:HE2	1:D:150:ASP:OD1	2.16	0.44
1:D:286:HIS:O	1:D:289:ILE:HG13	2.18	0.44
1:D:145:LEU:HD11	1:D:151:ILE:HD12	1.99	0.43
1:C:165:ASP:HA	1:C:168:GLN:OE1	2.17	0.43
1:A:264:TYR:CZ	1:A:296:ILE:HG12	2.52	0.43
1:D:288:SER:HB2	1:D:292:LYS:HZ2	1.83	0.43
1:A:165:ASP:HB3	1:A:169:LYS:CG	2.27	0.43
1:C:245:VAL:HG22	1:C:262:GLU:HG3	2.01	0.43
1:A:260:GLN:HG3	1:A:296:ILE:HD11	2.01	0.43
3:C:415:FAD:H1'1	3:C:415:FAD:H9	1.79	0.43
1:B:123:TYR:CZ	1:B:134:ASN:HB2	2.54	0.42
1:D:200:LEU:O	1:D:201:TYR:CB	2.65	0.42
1:D:281:LEU:HD23	1:D:311:VAL:HG13	2.01	0.42
1:C:147:ILE:HD12	1:C:147:ILE:H	1.83	0.42
1:A:21:VAL:CG2	1:A:41:ASN:HB2	2.49	0.42
1:D:172:ASN:HD22	1:D:210:TYR:H	1.66	0.42
1:A:109:ASN:HA	1:A:109:ASN:HD22	1.62	0.42
1:A:51:GLY:HA3	1:A:160:PHE:O	2.19	0.42
1:C:289:ILE:H	1:C:289:ILE:HG13	1.62	0.42
1:C:263:ILE:HG21	1:C:296:ILE:HD13	2.01	0.42
1:B:145:LEU:HD11	1:B:151:ILE:HD12	2.01	0.41
1:B:177:ALA:HB2	1:B:185:TYR:HE2	1.85	0.41
1:C:51:GLY:HA3	1:C:160:PHE:O	2.20	0.41
1:C:55:GLY:O	1:C:153:LEU:HA	2.20	0.41
1:D:165:ASP:HB3	1:D:169:LYS:HB2	2.02	0.41
1:C:180:THR:HA	1:C:224:LEU:HD12	2.03	0.41
1:D:274:PHE:HA	1:D:279:CYS:HB2	2.03	0.41
1:D:290:ARG:O	1:D:294:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ALA:HB2	1:C:185:TYR:CE2	2.56	0.41
1:A:185:TYR:O	1:A:189:LEU:HG	2.21	0.41
1:B:53:THR:OG1	1:B:157:HIS:HB2	2.21	0.41
1:C:30:ASN:HB2	1:C:221:ASP:OD2	2.20	0.40
1:C:293:VAL:HA	1:C:296:ILE:HD12	2.02	0.40
1:B:6:PHE:O	1:B:156:ALA:HB3	2.21	0.40
1:A:287:LYS:HA	1:A:315:VAL:HB	2.03	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	255/316 (81%)	252 (99%)	3 (1%)	0	100	100
1	B	255/316 (81%)	247 (97%)	7 (3%)	1 (0%)	34	48
1	C	247/316 (78%)	234 (95%)	13 (5%)	0	100	100
1	D	251/316 (79%)	240 (96%)	9 (4%)	2 (1%)	19	29
All	All	1008/1264 (80%)	973 (96%)	32 (3%)	3 (0%)	41	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	ALA
1	D	166	ALA
1	D	29	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	244/295 (83%)	231 (95%)	13 (5%)	22	37
1	B	244/295 (83%)	227 (93%)	17 (7%)	15	24
1	C	238/295 (81%)	228 (96%)	10 (4%)	30	47
1	D	241/295 (82%)	227 (94%)	14 (6%)	20	32
All	All	967/1180 (82%)	913 (94%)	54 (6%)	21	34

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	13	LYS
1	A	28	ARG
1	A	109	ASN
1	A	110	ASN
1	A	116	VAL
1	A	164	ASN
1	A	206	ASN
1	A	234	LYS
1	A	241	ASN
1	A	289	ILE
1	A	302	GLN
1	A	314	GLU
1	B	9	LEU
1	B	13	LYS
1	B	28	ARG
1	B	63	LEU
1	B	116	VAL
1	B	125	GLN
1	B	164	ASN
1	B	165	ASP
1	B	168	GLN
1	B	169	LYS
1	B	245	VAL
1	B	252	SER
1	B	253	ASP
1	B	264	TYR
1	B	287	LYS

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Mol	Chain	Res	Type
1	B	289	ILE
1	B	304	ASP
1	C	13	LYS
1	C	28	ARG
1	C	101	ARG
1	C	133	THR
1	C	143	LYS
1	C	204	ASN
1	C	241	ASN
1	C	251	ASN
1	C	260	GLN
1	C	289	ILE
1	D	13	LYS
1	D	28	ARG
1	D	62	GLU
1	D	110	ASN
1	D	116	VAL
1	D	164	ASN
1	D	200	LEU
1	D	201	TYR
1	D	220	GLU
1	D	240	ILE
1	D	260	GLN
1	D	289	ILE
1	D	302	GLN
1	D	314	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	241	ASN
1	A	300	HIS
1	B	5	ASN
1	B	8	ASN
1	B	109	ASN
1	B	125	GLN
1	B	172	ASN
1	B	241	ASN
1	B	260	GLN
1	B	300	HIS
1	C	8	ASN

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Mol	Chain	Res	Type
1	C	30	ASN
1	C	134	ASN
1	C	170	ASN
1	C	172	ASN
1	C	241	ASN
1	C	251	ASN
1	D	172	ASN
1	D	241	ASN

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 carbohydrates 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	$\#\|Z\| > 2$
3	FAD	D	415	-	51,58,58	1.48	8 (15%)	60,89,89	1.83	16 (26%)
3	FAD	A	415	-	51,58,58	1.40	7 (13%)	60,89,89	2.10	15 (25%)
3	FAD	C	415	-	51,58,58	1.46	6 (11%)	60,89,89	1.76	9 (15%)
2	FLC	A	9002	-	3,12,12	0.98	0	3,17,17	1.11	0
2	FLC	B	9001	-	3,12,12	0.91	0	3,17,17	2.27	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FAD	B	415	-	51,58,58	1.45	7 (13%)	60,89,89	2.17	15 (25%)

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	D	415	-	-	12/30/50/50	0/6/6/6
3	FAD	A	415	-	-	10/30/50/50	0/6/6/6
3	FAD	C	415	-	-	12/30/50/50	0/6/6/6
2	FLC	A	9002	-	-	6/6/16/16	-
2	FLC	B	9001	-	-	0/6/16/16	-
3	FAD	B	415	-	-	12/30/50/50	0/6/6/6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	415	FAD	C10-N1	5.02	1.39	1.33
3	D	415	FAD	C10-N1	4.64	1.39	1.33
3	C	415	FAD	C2A-N3A	4.35	1.39	1.32
3	A	415	FAD	C10-N1	4.25	1.38	1.33
3	B	415	FAD	C10-N1	4.15	1.38	1.33
3	D	415	FAD	C2A-N3A	4.10	1.38	1.32
3	B	415	FAD	C2A-N3A	4.08	1.38	1.32
3	D	415	FAD	C4X-N5	4.07	1.39	1.33
3	A	415	FAD	C4X-N5	4.07	1.39	1.33
3	A	415	FAD	C2A-N3A	3.90	1.38	1.32
3	B	415	FAD	C4X-N5	3.87	1.38	1.33
3	C	415	FAD	C4X-N5	3.72	1.38	1.33
3	D	415	FAD	C4-N3	3.35	1.38	1.33
3	C	415	FAD	C4-N3	2.99	1.38	1.33
3	D	415	FAD	C2A-N1A	2.90	1.39	1.33
3	A	415	FAD	C2A-N1A	2.85	1.39	1.33
3	B	415	FAD	C4-N3	2.84	1.38	1.33
3	C	415	FAD	C2A-N1A	2.82	1.39	1.33
3	B	415	FAD	C2A-N1A	2.75	1.39	1.33
3	A	415	FAD	C4-N3	2.69	1.37	1.33
3	B	415	FAD	C4'-C3'	-2.49	1.48	1.53
3	A	415	FAD	C4'-C3'	-2.37	1.49	1.53
3	D	415	FAD	C4'-C3'	-2.32	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	415	FAD	C5X-N5	2.25	1.39	1.35
3	D	415	FAD	C5X-N5	2.18	1.38	1.35
3	B	415	FAD	C1'-N10	2.17	1.50	1.48
3	A	415	FAD	C5X-N5	2.06	1.38	1.35
3	D	415	FAD	C1'-N10	2.06	1.50	1.48

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	415	FAD	C4-N3-C2	7.92	121.83	115.14
3	B	415	FAD	C4-N3-C2	6.83	120.91	115.14
3	D	415	FAD	C4-N3-C2	6.42	120.56	115.14
3	C	415	FAD	C4-N3-C2	6.41	120.55	115.14
3	C	415	FAD	N3A-C2A-N1A	-6.19	119.00	128.68
3	B	415	FAD	N3A-C2A-N1A	-5.99	119.32	128.68
3	A	415	FAD	N3A-C2A-N1A	-5.83	119.56	128.68
3	D	415	FAD	N3A-C2A-N1A	-5.74	119.70	128.68
3	B	415	FAD	O5'-C5'-C4'	-5.68	94.20	109.36
3	A	415	FAD	O3'-C3'-C2'	4.60	119.92	108.81
3	C	415	FAD	C4X-N5-C5X	4.40	121.17	116.77
3	A	415	FAD	C4X-N5-C5X	4.40	121.17	116.77
3	B	415	FAD	C1'-N10-C9A	4.24	121.63	118.29
3	B	415	FAD	C4X-N5-C5X	3.90	120.67	116.77
3	B	415	FAD	O4'-C4'-C5'	3.90	118.67	109.92
3	B	415	FAD	O3'-C3'-C2'	3.84	118.09	108.81
3	A	415	FAD	C1'-N10-C9A	3.66	121.17	118.29
3	A	415	FAD	C5'-C4'-C3'	-3.65	105.14	112.20
3	D	415	FAD	C4X-N5-C5X	3.55	120.31	116.77
3	D	415	FAD	O3'-C3'-C2'	3.30	116.78	108.81
3	A	415	FAD	C10-C4X-N5	-3.26	119.00	121.26
3	B	415	FAD	C4'-C3'-C2'	-3.26	106.58	113.36
3	D	415	FAD	O5'-C5'-C4'	-3.26	100.67	109.36
3	A	415	FAD	C4X-C4-N3	-3.25	118.98	123.43
3	D	415	FAD	C1'-N10-C9A	3.23	120.84	118.29
2	B	9001	FLC	CB-CA-CAC	-3.16	109.92	114.98
3	A	415	FAD	O5'-C5'-C4'	-3.16	100.93	109.36
3	C	415	FAD	C5X-C9A-N10	3.15	120.00	117.72
3	C	415	FAD	O2'-C2'-C3'	2.87	116.08	109.10
3	B	415	FAD	C5X-C9A-N10	2.76	119.72	117.72
3	D	415	FAD	C5X-C9A-N10	2.75	119.71	117.72
3	B	415	FAD	O2A-PA-O5B	2.74	120.46	107.75
3	B	415	FAD	O2'-C2'-C3'	2.69	115.63	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	415	FAD	O2'-C2'-C3'	2.67	115.60	109.10
3	D	415	FAD	C5'-C4'-C3'	-2.65	107.09	112.20
3	A	415	FAD	C4-C4X-N5	2.61	121.58	118.60
3	B	415	FAD	O4B-C4B-C5B	-2.58	100.87	109.37
3	C	415	FAD	C1'-N10-C9A	2.57	120.32	118.29
3	C	415	FAD	C4X-C4-N3	-2.55	119.94	123.43
3	A	415	FAD	O4'-C4'-C5'	2.52	115.58	109.92
3	A	415	FAD	C4'-C3'-C2'	-2.51	108.14	113.36
3	C	415	FAD	O3'-C3'-C2'	2.46	114.76	108.81
3	B	415	FAD	C5'-C4'-C3'	-2.44	107.50	112.20
3	D	415	FAD	O2A-PA-O5B	2.42	119.00	107.75
3	B	415	FAD	C4X-C4-N3	-2.41	120.14	123.43
3	D	415	FAD	O2'-C2'-C3'	2.36	114.85	109.10
3	D	415	FAD	O4'-C4'-C5'	2.32	115.12	109.92
3	D	415	FAD	P-O3P-PA	-2.26	125.07	132.83
2	B	9001	FLC	CB-CG-CGC	-2.23	111.41	114.98
3	D	415	FAD	C4-C4X-N5	2.23	121.14	118.60
3	B	415	FAD	C4-C4X-N5	2.23	121.14	118.60
3	D	415	FAD	C4X-C4-N3	-2.21	120.40	123.43
3	D	415	FAD	C4'-C3'-C2'	-2.21	108.77	113.36
3	C	415	FAD	C9A-C5X-N5	-2.19	118.94	122.36
3	A	415	FAD	C5A-C6A-N6A	-2.06	117.22	120.35
3	A	415	FAD	P-O3P-PA	-2.06	125.76	132.83
3	D	415	FAD	C4-C4X-C10	-2.06	118.59	119.95

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	415	FAD	C5B-O5B-PA-O1A
3	D	415	FAD	C5B-O5B-PA-O2A
3	D	415	FAD	C1'-C2'-C3'-O3'
3	D	415	FAD	C1'-C2'-C3'-C4'
3	D	415	FAD	C3'-C4'-C5'-O5'
3	D	415	FAD	O4'-C4'-C5'-O5'
3	A	415	FAD	C1'-C2'-C3'-O3'
3	A	415	FAD	C1'-C2'-C3'-C4'
3	A	415	FAD	O2'-C2'-C3'-O3'
3	A	415	FAD	C5'-O5'-P-O3P
3	C	415	FAD	C5B-O5B-PA-O2A
3	C	415	FAD	C1'-C2'-C3'-O3'
3	C	415	FAD	C1'-C2'-C3'-C4'

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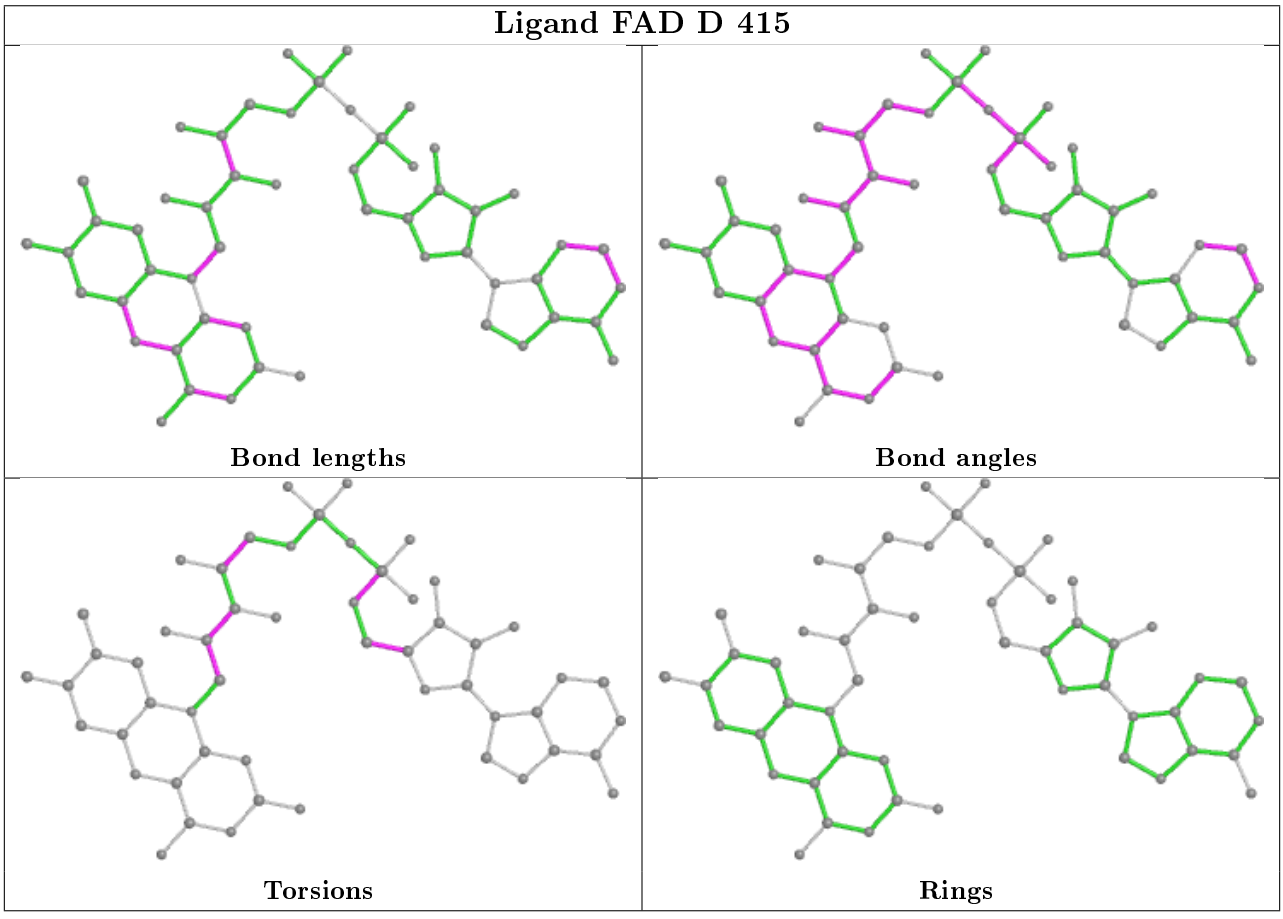
Mol	Chain	Res	Type	Atoms
3	C	415	FAD	C5'-O5'-P-O3P
2	A	9002	FLC	CAC-CA-CB-CBC
2	A	9002	FLC	CA-CB-CG-CGC
2	A	9002	FLC	CBC-CB-CG-CGC
2	A	9002	FLC	OHB-CB-CG-CGC
3	B	415	FAD	C5B-O5B-PA-O1A
3	B	415	FAD	C5B-O5B-PA-O2A
3	B	415	FAD	N10-C1'-C2'-C3'
3	B	415	FAD	C1'-C2'-C3'-O3'
3	B	415	FAD	C1'-C2'-C3'-C4'
3	B	415	FAD	C3'-C4'-C5'-O5'
3	B	415	FAD	O4'-C4'-C5'-O5'
3	D	415	FAD	O2'-C2'-C3'-C4'
3	A	415	FAD	O2'-C2'-C3'-C4'
3	B	415	FAD	O2'-C2'-C3'-C4'
3	C	415	FAD	O2'-C2'-C3'-C4'
3	D	415	FAD	O2'-C2'-C3'-O3'
3	C	415	FAD	O2'-C2'-C3'-O3'
3	B	415	FAD	O2'-C2'-C3'-O3'
2	A	9002	FLC	CAC-CA-CB-OHB
3	A	415	FAD	C3'-C4'-C5'-O5'
2	A	9002	FLC	CAC-CA-CB-CG
3	C	415	FAD	C5B-O5B-PA-O3P
3	A	415	FAD	C5'-O5'-P-O1P
3	A	415	FAD	C5'-O5'-P-O2P
3	C	415	FAD	C5B-O5B-PA-O1A
3	C	415	FAD	C5'-O5'-P-O1P
3	D	415	FAD	N10-C1'-C2'-C3'
3	D	415	FAD	O4B-C4B-C5B-O5B
3	C	415	FAD	O4B-C4B-C5B-O5B
3	D	415	FAD	C5B-O5B-PA-O3P
3	B	415	FAD	C5B-O5B-PA-O3P
3	B	415	FAD	O4B-C4B-C5B-O5B
3	A	415	FAD	PA-O3P-P-O1P
3	A	415	FAD	PA-O3P-P-O2P
3	C	415	FAD	PA-O3P-P-O2P
3	C	415	FAD	C5'-O5'-P-O2P
3	D	415	FAD	N10-C1'-C2'-O2'
3	B	415	FAD	N10-C1'-C2'-O2'

There are no ring outliers.

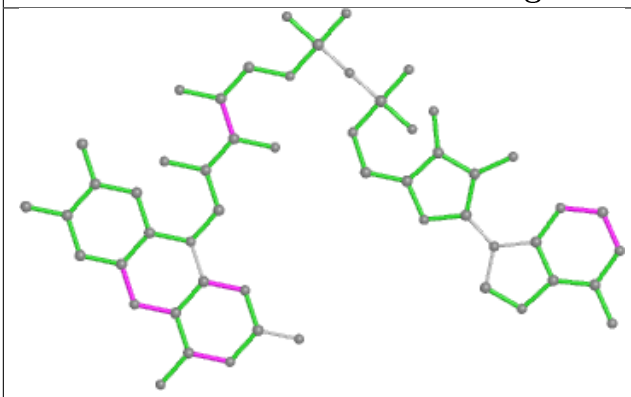
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	415	FAD	3	0
3	B	415	FAD	2	0

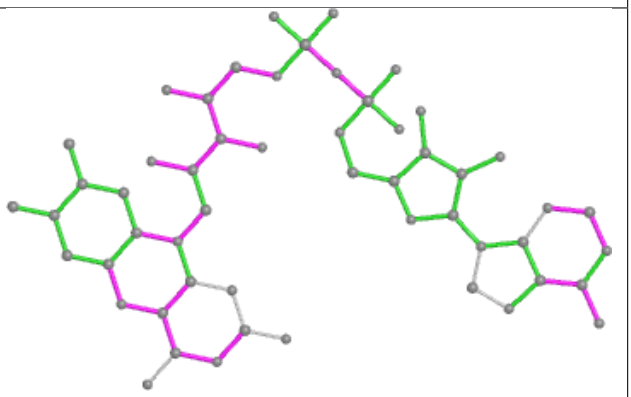
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



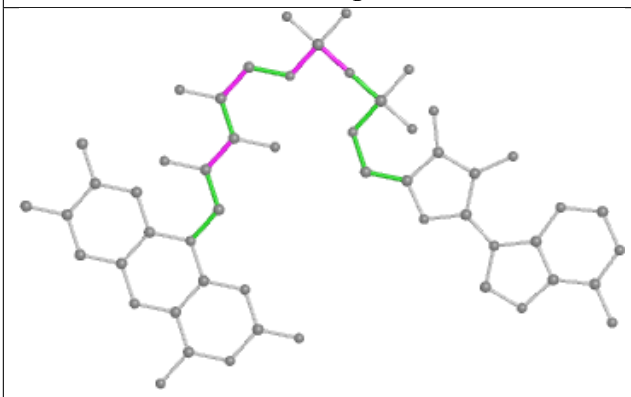
Ligand FAD A 415



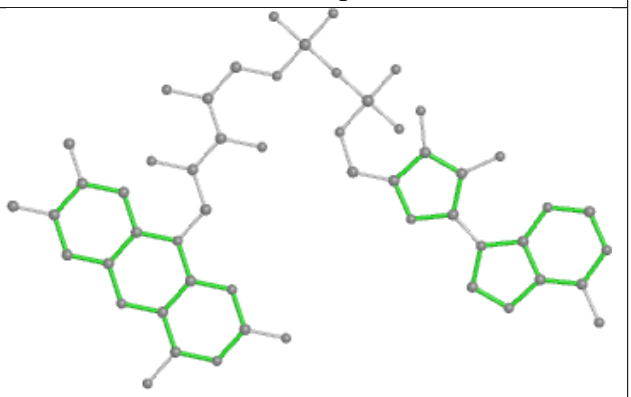
Bond lengths



Bond angles

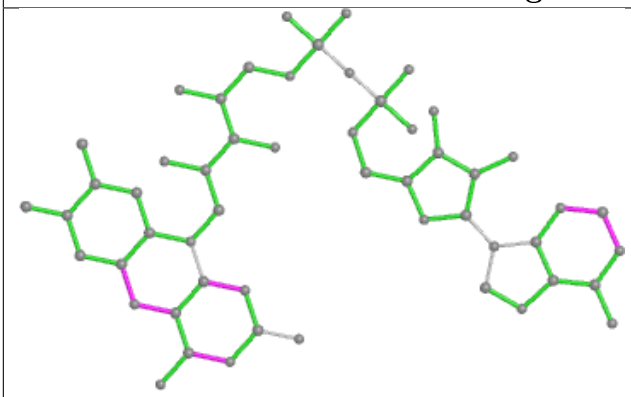


Torsions

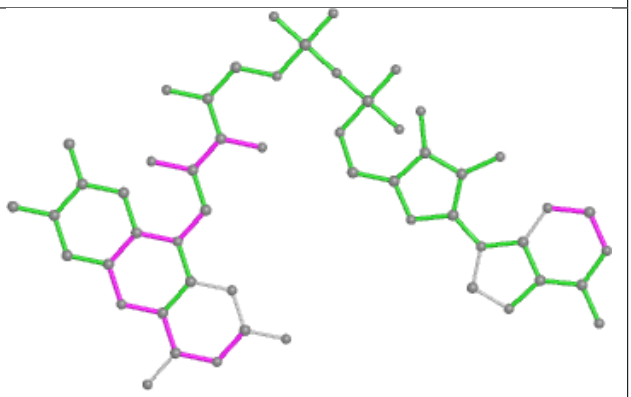


Rings

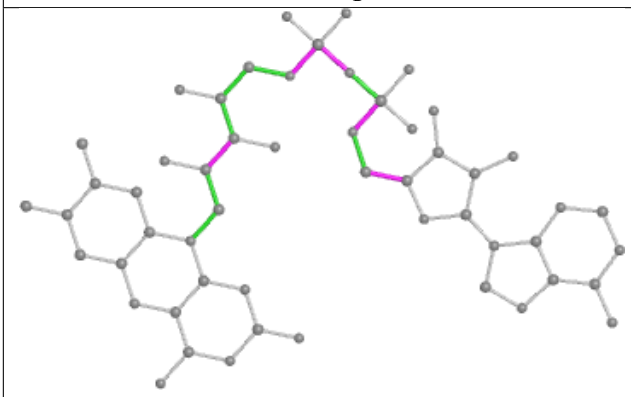
Ligand FAD C 415



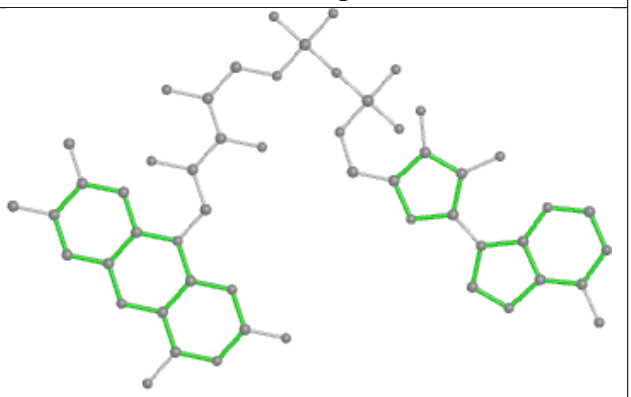
Bond lengths



Bond angles

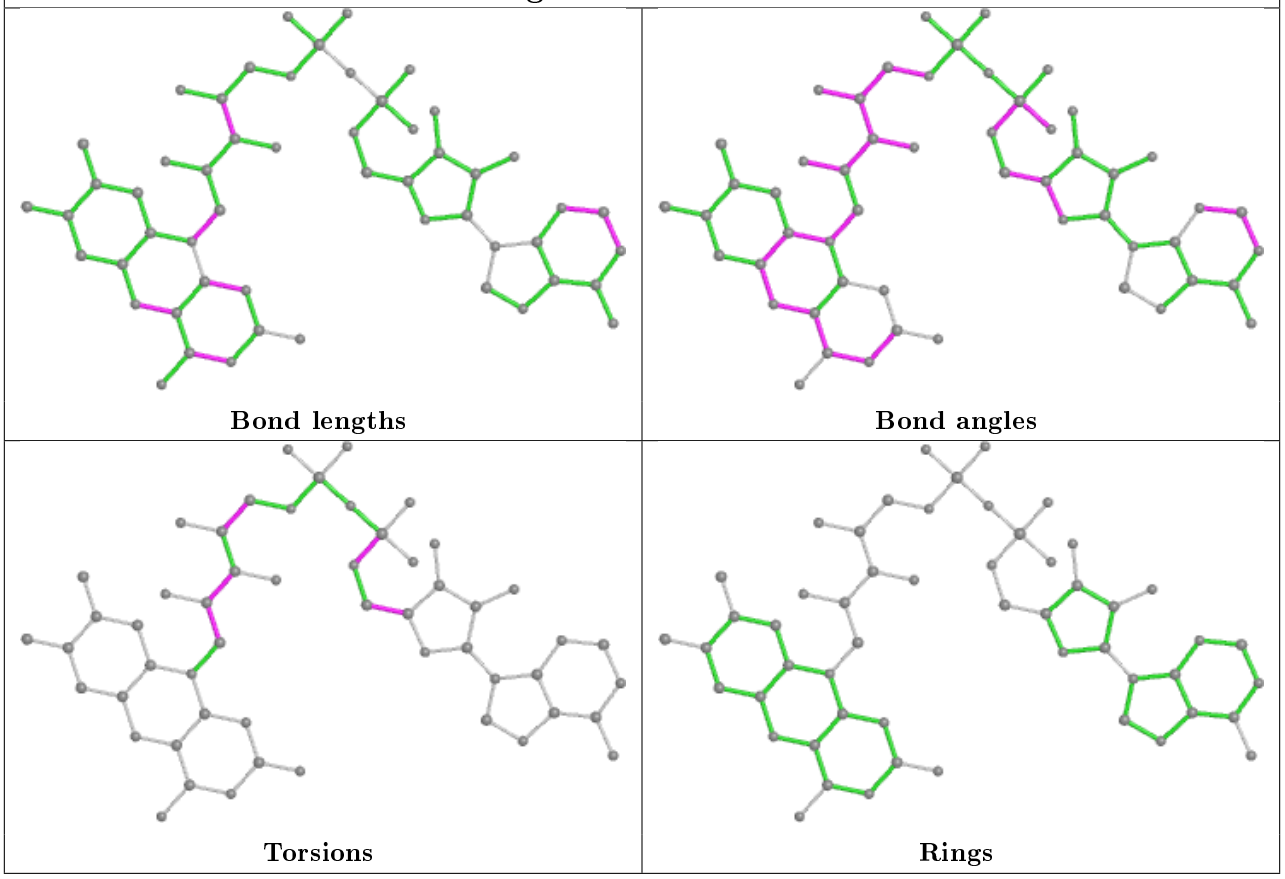


Torsions



Rings

Ligand FAD B 415



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	263/316 (83%)	0.08	0 100 100	17, 31, 58, 93	0
1	B	262/316 (82%)	0.21	10 (3%) 40 39	18, 35, 72, 115	1 (0%)
1	C	257/316 (81%)	0.24	6 (2%) 60 58	21, 41, 69, 94	1 (0%)
1	D	261/316 (82%)	0.32	9 (3%) 45 44	32, 54, 86, 124	2 (0%)
All	All	1043/1264 (82%)	0.21	25 (2%) 59 57	17, 40, 78, 124	4 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	ARG	5.3
1	D	200	LEU	4.5
1	D	123	TYR	4.2
1	B	299	SER	4.0
1	B	300	HIS	3.8
1	B	301	ASP	3.8
1	B	302	GLN	3.7
1	D	135	TYR	3.2
1	B	303	PHE	3.1
1	B	298	LYS	2.9
1	D	98	ARG	2.5
1	C	195	TYR	2.4
1	B	304	ASP	2.4
1	D	146	LYS	2.4
1	C	112	GLU	2.3
1	C	124	GLU	2.3
1	D	201	TYR	2.2
1	C	135	TYR	2.2
1	D	302	GLN	2.1
1	C	303	PHE	2.1
1	C	152	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	291	TYR	2.0
1	D	24	ILE	2.0
1	D	291	TYR	2.0
1	B	63	LEU	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 carbohydrates in this entry.

6.4 Ligands (i)

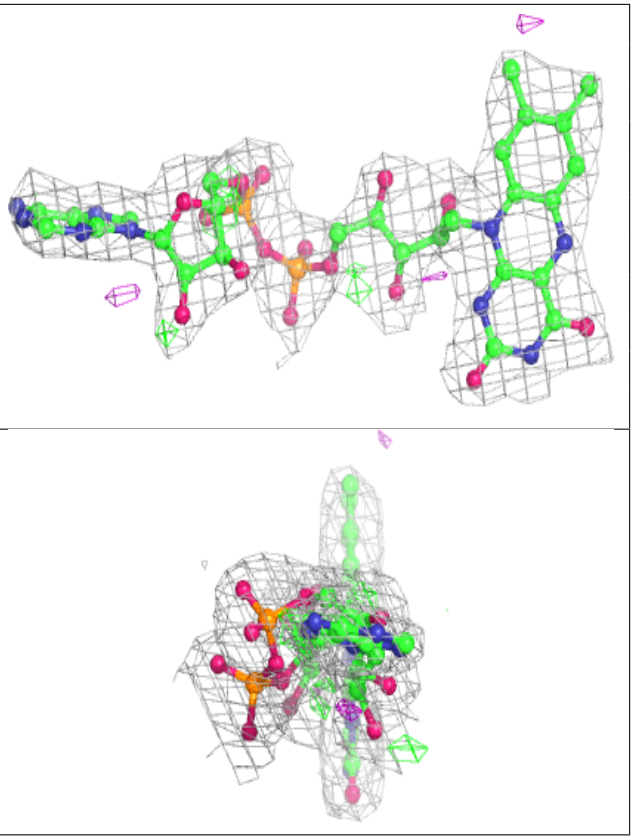
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	FLC	A	9002	13/13	0.59	0.48	45,59,62,65	12
3	FAD	C	415	53/53	0.96	0.15	25,37,68,68	0
3	FAD	D	415	53/53	0.96	0.18	25,39,84,85	0
2	FLC	B	9001	13/13	0.97	0.13	42,44,48,48	0
3	FAD	B	415	53/53	0.97	0.16	14,23,43,45	0
3	FAD	A	415	53/53	0.98	0.14	17,24,59,60	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.

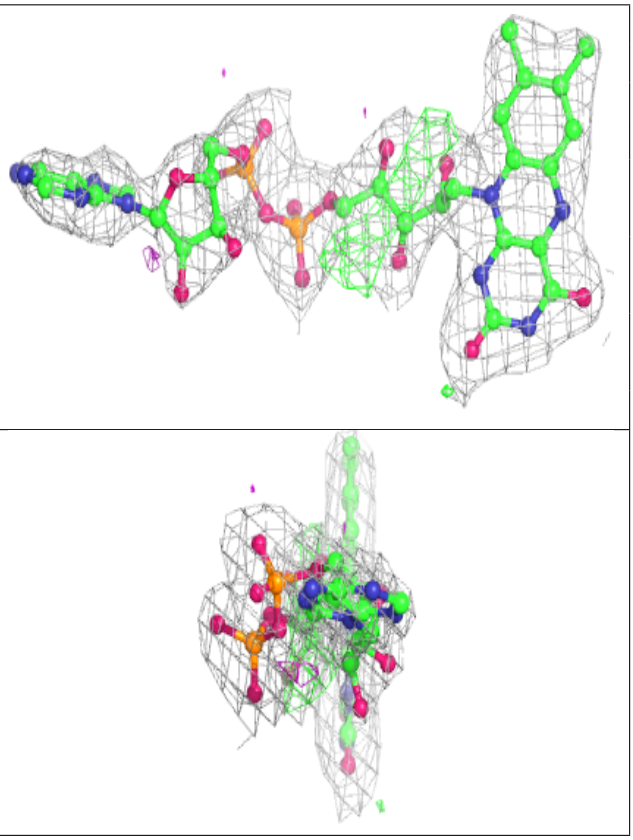
Electron density around FAD C 415:

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



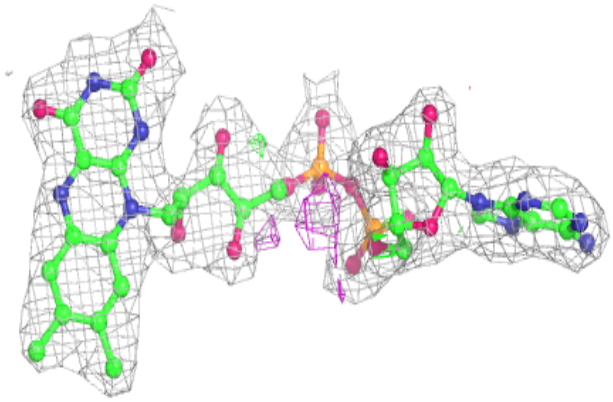
Electron density around FAD D 415:

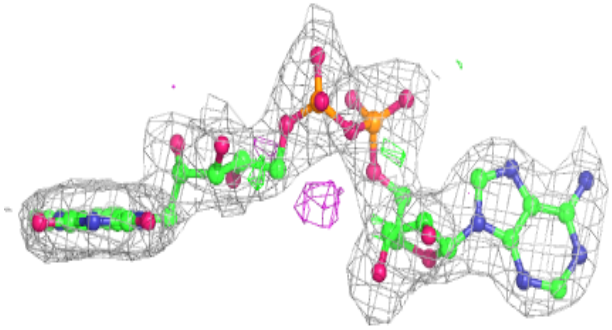
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

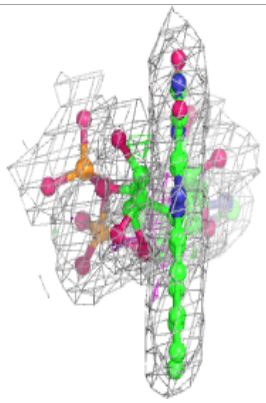


Electron density around FAD B 415:

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

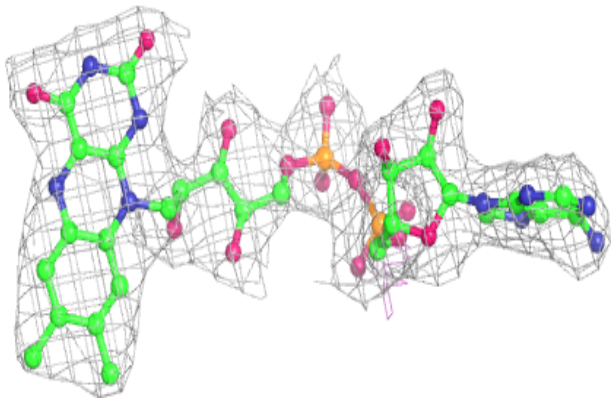


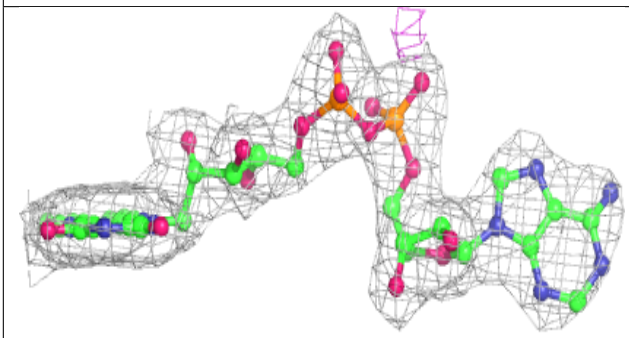


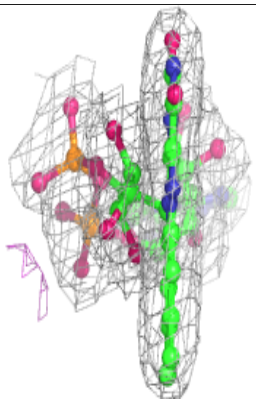


Electron density around FAD A 415:

$2mF_o$-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.