Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:39 pm BST

PDB ID	:	2BGJ
Title	:	X-Ray Structure of the Ferredoxin-NADP(H) Reductase from Rhodobacter capsulatus at 2.1 Angstroms
Authors	:	Perez-Dorado, J.I.; Hermoso, J.A.; Nogues, I.; Frago, S.; Bittel, C.; Mayhew, S.G.; Gomez-Moreno, C.; Medina, M.; Cortez, N.; Carrillo, N.
Deposited on	:	2004-12-23
Resolution	:	2.10 Å(reported)

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

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

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

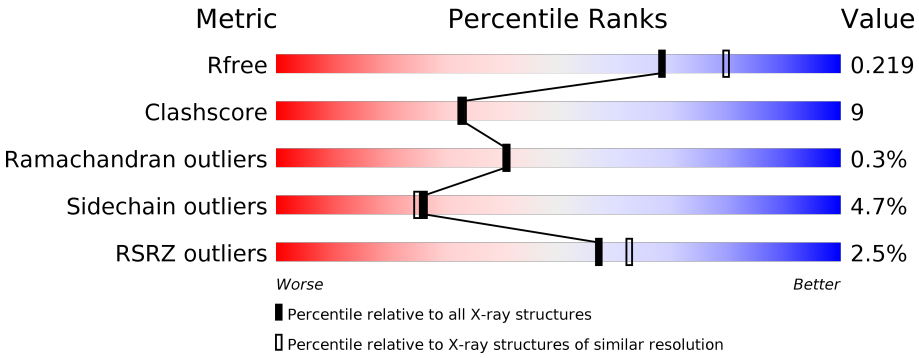
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	272	3% 76% 17%
1	B	272	3% 73% 19% 6%
1	C	272	2% 74% 18% 6%
1	D	272	2% 78% 15% 6%

2 Entry composition

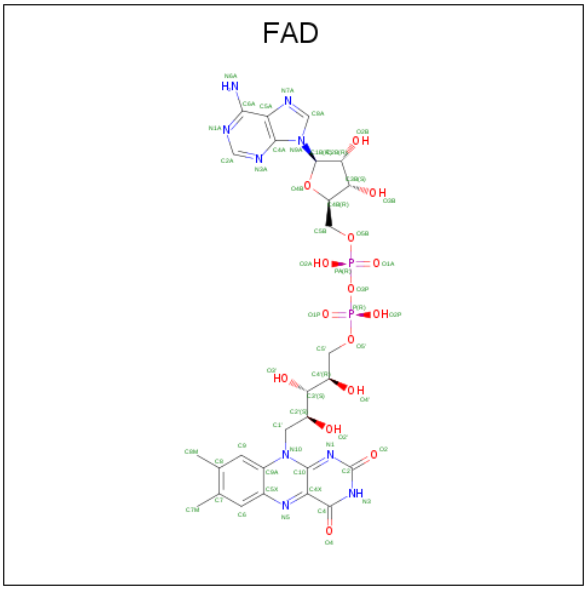
There are 3 unique types of molecules in this entry. The entry contains 8711 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FERREDOXIN-NADP(H) REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2055	1314	347	383	11			
1	B	257	Total	C	N	O	S	0	0	0
			2031	1297	343	380	11			
1	C	257	Total	C	N	O	S	0	0	0
			2031	1297	343	380	11			
1	D	257	Total	C	N	O	S	0	0	0
			2031	1297	343	380	11			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is water.

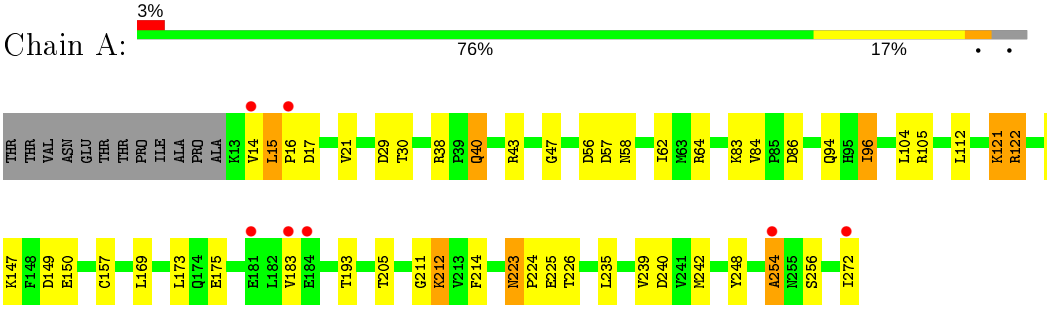
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total	O	0	0
			91	91		
3	B	85	Total	O	0	0
			85	85		
3	C	81	Total	O	0	0
			81	81		
3	D	94	Total	O	0	0
			94	94		

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.

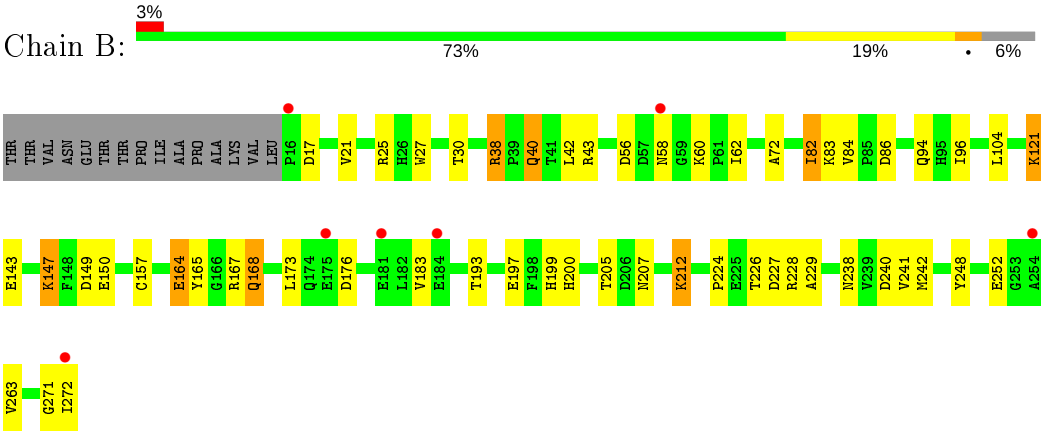
- Molecule 1: FERREDOXIN-NADP(H) REDUCTASE

Chain A:



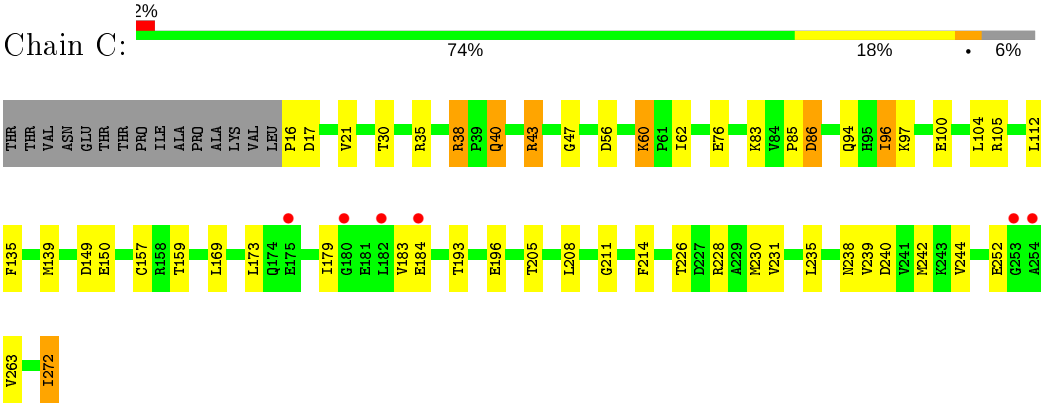
- Molecule 1: FERREDOXIN-NADP(H) REDUCTASE

Chain B:



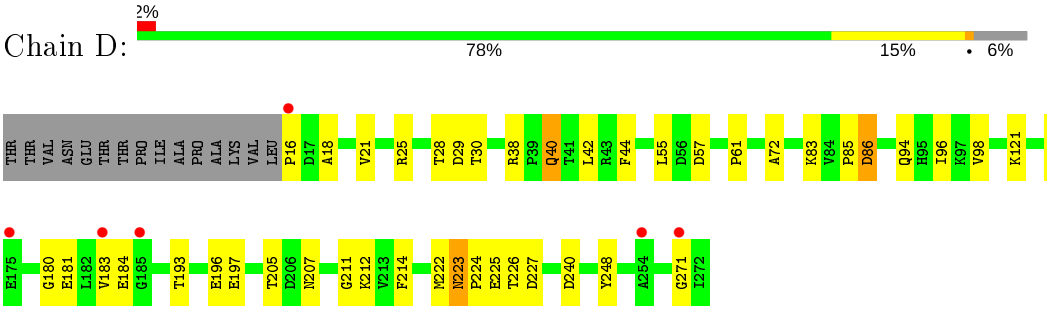
- Molecule 1: FERREDOXIN-NADP(H) REDUCTASE

Chain C:



• Molecule 1: FERREDOXIN-NADP(H) REDUCTASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.29Å 93.63Å 103.43Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	105.41 – 2.10 22.83 – 1.92	Depositor EDS
% Data completeness (in resolution range)	79.1 (105.41-2.10) 72.7 (22.83-1.92)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 1.92Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.243 0.214 , 0.219	Depositor DCC
R_{free} test set	4187 reflections (5.71%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.459 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8711	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5923e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.62	0/2101	0.78	3/2845 (0.1%)
1	B	0.62	0/2077	0.79	2/2812 (0.1%)
1	C	0.64	0/2077	0.78	2/2812 (0.1%)
1	D	0.62	0/2077	0.77	1/2812 (0.0%)
All	All	0.62	0/8332	0.78	8/11281 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	86	ASP	CB-CG-OD2	6.60	124.24	118.30
1	D	86	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	86	ASP	CB-CG-OD2	5.76	123.48	118.30
1	C	86	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	149	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	149	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	176	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	57	ASP	CB-CG-OD2	5.13	122.92	118.30

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	2055	0	2055	39	0
1	B	2031	0	2023	35	0
1	C	2031	0	2023	38	0
1	D	2031	0	2023	31	0
2	A	53	0	31	2	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
3	A	91	0	0	4	0
3	B	85	0	0	1	0
3	C	81	0	0	2	0
3	D	94	0	0	2	0
All	All	8711	0	8248	144	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 9.

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:A:122:ARG:HG2	1:A:150:GLU:HB3	1.57	0.86
1:A:15:LEU:H	1:A:16:PRO:HD2	1.42	0.82
1:A:15:LEU:H	1:A:16:PRO:CD	1.92	0.81
1:B:199:HIS:CD2	1:B:200:HIS:ND1	2.50	0.80
1:D:205:THR:HG21	1:D:240:ASP:HB3	1.65	0.79
1:C:40:GLN:H	1:C:40:GLN:CD	1.87	0.78
1:C:122:ARG:HG2	1:C:150:GLU:HB3	1.63	0.77
1:A:256:SER:HB3	3:A:2081:HOH:O	1.85	0.76
1:B:205:THR:HG21	1:B:240:ASP:HB3	1.69	0.75
1:D:40:GLN:CD	1:D:40:GLN:H	1.92	0.73
1:B:30:THR:HA	1:B:83:LYS:HB2	1.71	0.72
1:B:205:THR:HG23	3:B:2065:HOH:O	1.88	0.72
1:A:223:ASN:HD22	1:A:224:PRO:HD2	1.53	0.72
1:D:121:LYS:HG2	1:D:226:THR:HB	1.72	0.71
1:B:21:VAL:HG21	1:B:96:ILE:HG12	1.72	0.71
1:C:43:ARG:HD2	3:C:2014:HOH:O	1.90	0.70
1:D:224:PRO:HG3	1:D:248:TYR:O	1.91	0.70
1:C:43:ARG:HD3	1:C:43:ARG:O	1.92	0.69
1:C:21:VAL:HG21	1:C:96:ILE:HG12	1.75	0.69
1:D:30:THR:HA	1:D:83:LYS:HB2	1.75	0.68
1:A:40:GLN:H	1:A:40:GLN:CD	1.95	0.68
1:B:199:HIS:HD2	1:B:200:HIS:ND1	1.91	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:TRP:CH2	1:B:168:GLN:HG2	2.30	0.66
1:B:40:GLN:H	1:B:40:GLN:CD	1.99	0.66
1:C:173:LEU:HD23	1:C:179:ILE:HG21	1.78	0.66
1:A:223:ASN:HD22	1:A:224:PRO:CD	2.08	0.65
1:A:17:ASP:HB3	1:A:104:LEU:O	1.96	0.65
1:A:15:LEU:N	1:A:16:PRO:HD2	2.11	0.65
1:D:223:ASN:HD22	1:D:224:PRO:HD2	1.61	0.65
1:A:83:LYS:HD3	1:A:94:GLN:HE21	1.61	0.65
1:A:121:LYS:HG2	1:A:226:THR:HB	1.80	0.62
1:C:56:ASP:HB3	1:C:62:ILE:HD11	1.79	0.62
1:D:223:ASN:HD22	1:D:224:PRO:CD	2.12	0.62
1:A:205:THR:HG21	1:A:240:ASP:HB3	1.80	0.61
1:D:207:ASN:OD1	1:D:212:LYS:HE2	1.99	0.61
1:A:84:VAL:HG13	1:A:272:ILE:HD11	1.83	0.61
1:A:56:ASP:HB3	1:A:62:ILE:HD11	1.83	0.60
1:B:183:VAL:O	1:B:183:VAL:HG12	2.02	0.59
1:C:121:LYS:HG2	1:C:226:THR:HB	1.82	0.59
1:A:224:PRO:HG3	1:A:248:TYR:O	2.02	0.59
1:A:15:LEU:N	1:A:16:PRO:CD	2.60	0.58
1:C:157:CYS:O	1:C:193:THR:HA	2.03	0.58
1:B:121:LYS:HG2	1:B:226:THR:HB	1.86	0.58
1:C:30:THR:HA	1:C:83:LYS:HB2	1.85	0.58
1:B:56:ASP:HB3	1:B:62:ILE:HD11	1.84	0.57
1:D:157:CYS:O	1:D:193:THR:HA	2.04	0.57
1:C:83:LYS:HD3	1:C:94:GLN:HE21	1.68	0.57
1:C:173:LEU:CD2	1:C:179:ILE:HG21	2.35	0.57
1:D:181:GLU:C	1:D:183:VAL:H	2.09	0.56
1:C:135:PHE:O	1:C:139:MET:HB2	2.05	0.56
1:B:82:ILE:HG13	1:B:83:LYS:N	2.20	0.56
1:D:223:ASN:HD22	1:D:224:PRO:N	2.04	0.56
1:A:169:LEU:C	1:A:169:LEU:HD23	2.27	0.55
1:B:224:PRO:HG3	1:B:248:TYR:O	2.07	0.55
1:B:83:LYS:HD3	1:B:94:GLN:HE21	1.72	0.55
1:C:205:THR:HG21	1:C:240:ASP:HB3	1.88	0.55
1:D:85:PRO:O	1:D:86:ASP:HB2	2.06	0.55
1:C:238:ASN:O	1:C:242:MET:HG3	2.06	0.54
1:D:98:VAL:HG23	3:D:2033:HOH:O	2.07	0.54
1:A:21:VAL:HG21	1:A:96:ILE:HG12	1.88	0.54
1:D:222:MET:HA	1:D:227:ASP:OD1	2.08	0.54
1:A:143:GLU:O	1:A:147:LYS:HG2	2.08	0.54
1:A:14:VAL:HG23	3:A:2017:HOH:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:NH2	1:B:72:ALA:O	2.41	0.54
1:D:38:ARG:NH2	1:D:72:ALA:O	2.41	0.54
1:A:140:ARG:HG2	1:A:173:LEU:HD21	1.91	0.54
1:B:157:CYS:O	1:B:193:THR:HA	2.08	0.53
1:A:254:ALA:HB3	3:A:2081:HOH:O	2.08	0.53
1:D:180:GLY:O	1:D:184:GLU:HB3	2.09	0.53
1:C:183:VAL:HG12	1:C:183:VAL:O	2.09	0.53
1:D:83:LYS:HD3	1:D:94:GLN:HE21	1.72	0.52
1:B:82:ILE:HG13	1:B:83:LYS:H	1.75	0.52
1:C:169:LEU:HD23	1:C:169:LEU:C	2.30	0.52
1:B:121:LYS:HE3	1:B:149:ASP:HB2	1.92	0.52
1:D:28:THR:HG21	3:D:2008:HOH:O	2.09	0.52
1:C:38:ARG:HD3	3:C:2013:HOH:O	2.09	0.51
1:A:223:ASN:HD21	1:A:225:GLU:HB2	1.75	0.51
1:A:183:VAL:HG12	1:A:183:VAL:O	2.11	0.51
1:C:122:ARG:CG	1:C:150:GLU:HB3	2.35	0.51
1:B:143:GLU:O	1:B:147:LYS:HG2	2.11	0.51
1:B:140:ARG:HG2	1:B:173:LEU:HD21	1.91	0.51
1:A:83:LYS:HD3	1:A:94:GLN:NE2	2.26	0.50
1:A:29:ASP:HA	1:D:196:GLU:OE1	2.10	0.50
1:D:29:ASP:O	1:D:83:LYS:HD2	2.12	0.50
1:D:223:ASN:HD22	1:D:223:ASN:C	2.14	0.50
1:C:56:ASP:OD2	1:C:60:LYS:HB2	2.12	0.50
1:C:159:THR:HB	1:C:196:GLU:OE2	2.12	0.49
1:B:17:ASP:HB3	1:B:104:LEU:O	2.12	0.49
1:C:83:LYS:HD3	1:C:94:GLN:NE2	2.28	0.49
1:C:252:GLU:HB2	1:C:261:PHE:CZ	2.48	0.49
1:A:157:CYS:O	1:A:193:THR:HA	2.13	0.49
1:C:47:GLY:HA3	1:C:112:LEU:O	2.15	0.47
1:B:84:VAL:HG22	1:B:272:ILE:HD13	1.96	0.47
1:C:85:PRO:O	1:C:86:ASP:HB2	2.15	0.47
1:B:205:THR:HG22	1:B:241:VAL:HG22	1.96	0.47
1:D:21:VAL:HG21	1:D:96:ILE:HG12	1.97	0.47
1:A:211:GLY:HA2	1:A:214:PHE:CD2	2.50	0.47
1:A:223:ASN:HD22	1:A:224:PRO:N	2.11	0.46
1:B:84:VAL:HG22	1:B:272:ILE:CD1	2.46	0.46
1:D:211:GLY:HA2	1:D:214:PHE:CD2	2.51	0.45
1:D:121:LYS:HE3	1:D:149:ASP:HB2	1.98	0.45
1:D:223:ASN:ND2	1:D:224:PRO:HD2	2.30	0.45
1:B:252:GLU:HB2	1:B:261:PHE:CZ	2.51	0.45
1:C:43:ARG:C	1:C:43:ARG:HD3	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HA	1:A:242:MET:CE	2.47	0.45
1:D:55:LEU:HD23	1:D:61:PRO:HA	1.99	0.45
1:B:164:GLU:OE1	1:B:167:ARG:CZ	2.65	0.45
1:C:97:LYS:HB2	1:C:100:GLU:OE1	2.16	0.45
1:B:165:TYR:O	1:B:168:GLN:HG3	2.17	0.44
1:B:207:ASN:OD1	1:B:212:LYS:HE2	2.17	0.44
1:A:47:GLY:HA3	1:A:112:LEU:O	2.17	0.44
1:D:271:GLY:HA2	2:D:1273:FAD:H1B	1.99	0.44
1:C:231:VAL:HB	1:C:263:VAL:HG12	2.00	0.44
1:B:238:ASN:O	1:B:242:MET:HG3	2.17	0.44
1:B:56:ASP:OD2	1:B:60:LYS:HB2	2.17	0.43
1:B:122:ARG:HB3	1:B:227:ASP:OD2	2.18	0.43
1:C:85:PRO:HD2	1:C:272:ILE:HD11	2.01	0.43
1:C:112:LEU:HD22	1:C:230:MET:HB3	2.00	0.43
1:C:211:GLY:HA2	1:C:214:PHE:CD2	2.53	0.43
1:A:212:LYS:HE3	3:A:2058:HOH:O	2.19	0.42
1:C:235:LEU:O	1:C:239:VAL:HG23	2.19	0.42
1:A:223:ASN:HD22	1:A:223:ASN:C	2.21	0.42
1:B:271:GLY:O	1:B:272:ILE:HG13	2.19	0.42
2:A:1273:FAD:H9	2:A:1273:FAD:H1'1	1.79	0.42
1:A:64:ARG:HD2	2:A:1273:FAD:H3'	2.00	0.42
1:A:223:ASN:ND2	1:A:223:ASN:C	2.73	0.42
1:A:235:LEU:O	1:A:239:VAL:HG23	2.20	0.42
1:D:223:ASN:ND2	1:D:225:GLU:H	2.18	0.42
1:D:44:PHE:CZ	1:D:72:ALA:HA	2.55	0.42
1:C:17:ASP:HB3	1:C:104:LEU:O	2.20	0.41
2:C:1273:FAD:H9	2:C:1273:FAD:H1'1	1.84	0.41
1:C:35:ARG:NH2	1:C:76:GLU:HB2	2.35	0.41
1:C:205:THR:HG21	1:C:240:ASP:CB	2.51	0.41
1:C:40:GLN:CD	1:C:40:GLN:N	2.67	0.41
1:B:228:ARG:HA	1:B:260:GLU:O	2.21	0.41
1:C:208:LEU:HB3	1:C:244:VAL:HG11	2.03	0.41
1:C:228:ARG:HA	1:C:260:GLU:O	2.21	0.41
1:D:223:ASN:C	1:D:223:ASN:ND2	2.75	0.41
1:A:239:VAL:HA	1:A:242:MET:HE3	2.02	0.40
1:A:223:ASN:ND2	1:A:225:GLU:H	2.19	0.40
1:B:122:ARG:HG3	1:B:150:GLU:HB3	2.03	0.40
1:B:229:ALA:O	1:B:261:PHE:HA	2.22	0.40
1:D:16:PRO:HD2	1:D:18:ALA:HB2	2.03	0.40
1:A:30:THR:HA	1:A:83:LYS:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	258/272 (95%)	247 (96%)	9 (4%)	2 (1%)	19	15
1	B	255/272 (94%)	246 (96%)	9 (4%)	0	100	100
1	C	255/272 (94%)	245 (96%)	9 (4%)	1 (0%)	34	32
1	D	255/272 (94%)	243 (95%)	12 (5%)	0	100	100
All	All	1023/1088 (94%)	981 (96%)	39 (4%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	184	GLU
1	A	15	LEU
1	A	254	ALA

5.3.2 Protein sidechains

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	222/232 (96%)	211 (95%)	11 (5%)	24	23
1	B	219/232 (94%)	205 (94%)	14 (6%)	17	14
1	C	219/232 (94%)	209 (95%)	10 (5%)	27	26
1	D	219/232 (94%)	213 (97%)	6 (3%)	44	48
All	All	879/928 (95%)	838 (95%)	41 (5%)	26	25

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	40	GLN
1	A	43	ARG
1	A	58	ASN
1	A	96	ILE
1	A	105	ARG
1	A	121	LYS
1	A	122	ARG
1	A	175	GLU
1	A	212	LYS
1	A	223	ASN
1	B	25	ARG
1	B	38	ARG
1	B	40	GLN
1	B	42	LEU
1	B	43	ARG
1	B	58	ASN
1	B	82	ILE
1	B	121	LYS
1	B	147	LYS
1	B	164	GLU
1	B	168	GLN
1	B	197	GLU
1	B	212	LYS
1	B	263	VAL
1	C	16	PRO
1	C	38	ARG
1	C	40	GLN
1	C	43	ARG
1	C	60	LYS
1	C	96	ILE
1	C	105	ARG
1	C	121	LYS
1	C	122	ARG
1	C	272	ILE
1	D	25	ARG
1	D	40	GLN
1	D	42	LEU
1	D	57	ASP
1	D	197	GLU
1	D	223	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	199	HIS
1	A	200	HIS
1	A	223	ASN
1	B	94	GLN
1	B	168	GLN
1	B	174	GLN
1	B	199	HIS
1	C	94	GLN
1	C	174	GLN
1	D	94	GLN
1	D	174	GLN
1	D	199	HIS
1	D	200	HIS
1	D	223	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 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	C	1273	-	51,58,58	1.43	8 (15%)	60,89,89	1.82	13 (21%)
2	FAD	D	1273	-	51,58,58	1.29	5 (9%)	60,89,89	1.69	11 (18%)
2	FAD	A	1273	-	51,58,58	1.36	6 (11%)	60,89,89	1.75	8 (13%)
2	FAD	B	1273	-	51,58,58	1.28	5 (9%)	60,89,89	1.71	9 (15%)

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	C	1273	-	-	6/30/50/50	0/6/6/6
2	FAD	D	1273	-	-	1/30/50/50	0/6/6/6
2	FAD	A	1273	-	-	6/30/50/50	0/6/6/6
2	FAD	B	1273	-	-	4/30/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1273	FAD	C4X-N5	4.27	1.39	1.33
2	A	1273	FAD	C2A-N3A	4.02	1.38	1.32
2	D	1273	FAD	C4X-N5	3.90	1.38	1.33
2	C	1273	FAD	C2A-N3A	3.76	1.38	1.32
2	D	1273	FAD	C10-N1	3.71	1.38	1.33
2	C	1273	FAD	C1'-N10	3.70	1.52	1.48
2	A	1273	FAD	C4X-N5	3.62	1.38	1.33
2	B	1273	FAD	C4X-N5	3.62	1.38	1.33
2	B	1273	FAD	C10-N1	3.61	1.37	1.33
2	C	1273	FAD	C4-N3	3.46	1.39	1.33
2	D	1273	FAD	C2A-N3A	3.35	1.37	1.32
2	D	1273	FAD	C4-N3	3.32	1.38	1.33
2	B	1273	FAD	C1'-N10	3.32	1.51	1.48
2	A	1273	FAD	C4-N3	3.31	1.38	1.33
2	B	1273	FAD	C2A-N3A	3.23	1.37	1.32
2	A	1273	FAD	C10-N1	3.19	1.37	1.33
2	A	1273	FAD	C1'-N10	3.07	1.51	1.48
2	B	1273	FAD	C4-N3	3.05	1.38	1.33
2	C	1273	FAD	C10-N1	2.62	1.36	1.33
2	C	1273	FAD	C4X-C10	2.51	1.41	1.38
2	C	1273	FAD	C2A-N1A	2.39	1.38	1.33
2	D	1273	FAD	C1'-N10	2.20	1.50	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1273	FAD	C2A-N1A	2.11	1.37	1.33
2	C	1273	FAD	C5X-N5	2.00	1.38	1.35

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1273	FAD	C4-N3-C2	6.35	120.50	115.14
2	A	1273	FAD	C4-N3-C2	6.22	120.39	115.14
2	B	1273	FAD	C4-N3-C2	6.14	120.33	115.14
2	B	1273	FAD	N3A-C2A-N1A	-6.11	119.12	128.68
2	D	1273	FAD	C4-N3-C2	6.04	120.24	115.14
2	A	1273	FAD	N3A-C2A-N1A	-5.79	119.62	128.68
2	C	1273	FAD	N3A-C2A-N1A	-5.76	119.68	128.68
2	D	1273	FAD	N3A-C2A-N1A	-5.35	120.32	128.68
2	A	1273	FAD	C5X-C9A-N10	4.22	120.77	117.72
2	D	1273	FAD	C4X-N5-C5X	4.11	120.87	116.77
2	D	1273	FAD	C4X-C4-N3	-3.57	118.54	123.43
2	C	1273	FAD	C5X-C9A-N10	3.54	120.28	117.72
2	C	1273	FAD	C4X-C4-N3	-3.53	118.60	123.43
2	A	1273	FAD	P-O3P-PA	-3.51	120.77	132.83
2	C	1273	FAD	P-O3P-PA	-3.40	121.17	132.83
2	B	1273	FAD	C4X-C4-N3	-3.35	118.84	123.43
2	D	1273	FAD	C5X-C9A-N10	3.34	120.14	117.72
2	A	1273	FAD	C4X-C4-N3	-3.34	118.87	123.43
2	B	1273	FAD	C1'-N10-C9A	3.31	120.90	118.29
2	B	1273	FAD	C4X-N5-C5X	3.25	120.02	116.77
2	B	1273	FAD	C5X-C9A-N10	3.21	120.04	117.72
2	B	1273	FAD	P-O3P-PA	-3.18	121.93	132.83
2	A	1273	FAD	C4X-N5-C5X	2.96	119.73	116.77
2	D	1273	FAD	C10-C4X-N5	-2.86	119.28	121.26
2	C	1273	FAD	C9A-N10-C10	-2.79	118.25	121.91
2	C	1273	FAD	C1'-N10-C9A	2.76	120.46	118.29
2	A	1273	FAD	C9A-N10-C10	-2.73	118.33	121.91
2	C	1273	FAD	C10-C4X-N5	-2.71	119.39	121.26
2	A	1273	FAD	C1'-N10-C10	2.68	120.81	118.41
2	D	1273	FAD	C1'-N10-C9A	2.65	120.38	118.29
2	B	1273	FAD	C2B-C3B-C4B	2.62	107.74	102.64
2	C	1273	FAD	C3B-C2B-C1B	2.56	104.83	100.98
2	B	1273	FAD	C9A-N10-C10	-2.40	118.76	121.91
2	D	1273	FAD	P-O3P-PA	-2.40	124.60	132.83
2	C	1273	FAD	C4X-N5-C5X	2.34	119.11	116.77
2	D	1273	FAD	C2B-C3B-C4B	2.27	107.06	102.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1273	FAD	C1'-C2'-C3'	2.16	115.83	109.79
2	D	1273	FAD	C9A-N10-C10	-2.14	119.11	121.91
2	C	1273	FAD	C7M-C7-C6	-2.10	115.32	120.34
2	D	1273	FAD	C3B-C2B-C1B	2.05	104.07	100.98
2	C	1273	FAD	C1'-N10-C10	2.02	120.22	118.41

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1273	FAD	C1'-C2'-C3'-C4'
2	A	1273	FAD	C1'-C2'-C3'-C4'
2	B	1273	FAD	C1'-C2'-C3'-C4'
2	C	1273	FAD	O2'-C2'-C3'-C4'
2	C	1273	FAD	O2'-C2'-C3'-O3'
2	A	1273	FAD	O2'-C2'-C3'-C4'
2	A	1273	FAD	O2'-C2'-C3'-O3'
2	D	1273	FAD	O2'-C2'-C3'-C4'
2	B	1273	FAD	O2'-C2'-C3'-C4'
2	A	1273	FAD	O4B-C4B-C5B-O5B
2	C	1273	FAD	O4B-C4B-C5B-O5B
2	A	1273	FAD	C3B-C4B-C5B-O5B
2	B	1273	FAD	C3B-C4B-C5B-O5B
2	B	1273	FAD	O4B-C4B-C5B-O5B
2	C	1273	FAD	C3B-C4B-C5B-O5B
2	C	1273	FAD	C1'-C2'-C3'-O3'
2	A	1273	FAD	C1'-C2'-C3'-O3'

There are no ring outliers.

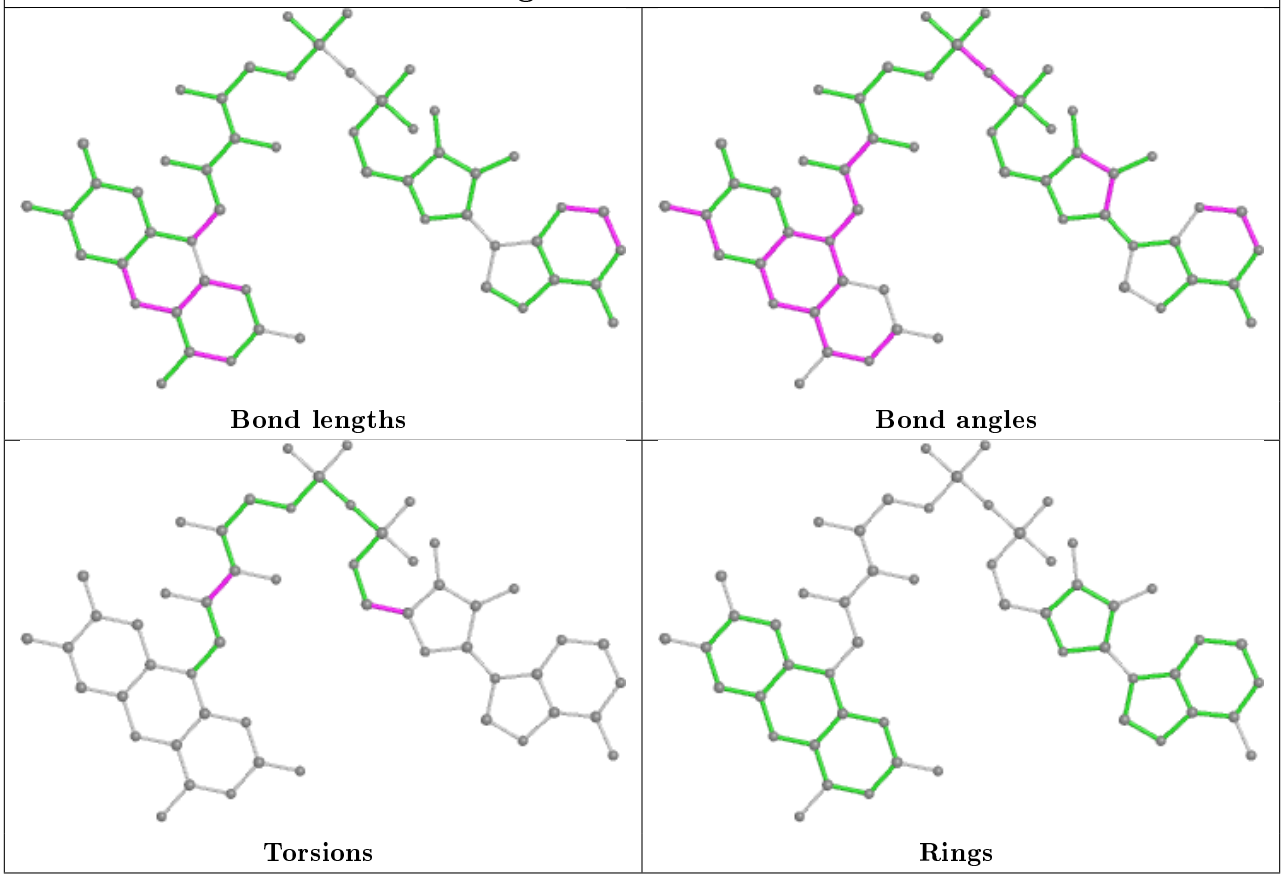
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1273	FAD	1	0
2	D	1273	FAD	1	0
2	A	1273	FAD	2	0

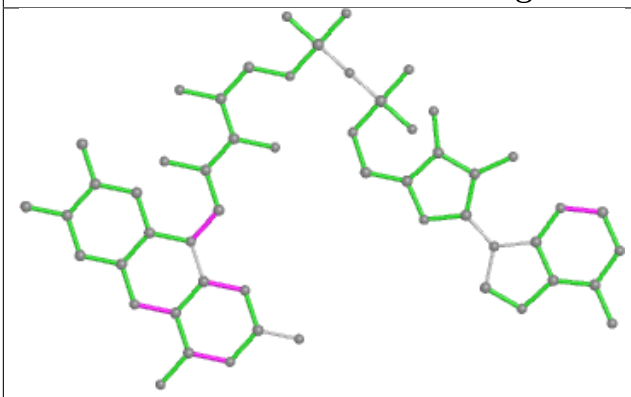
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

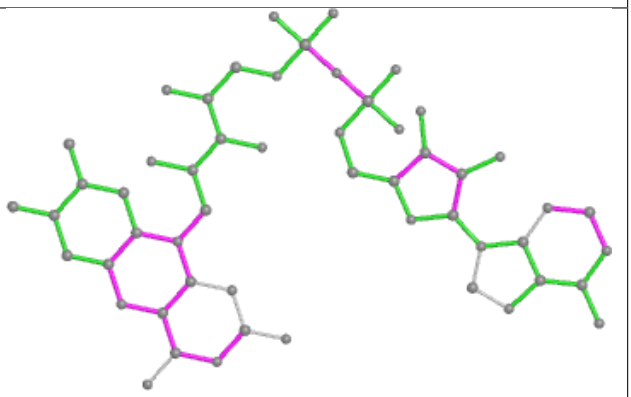
Ligand FAD C 1273



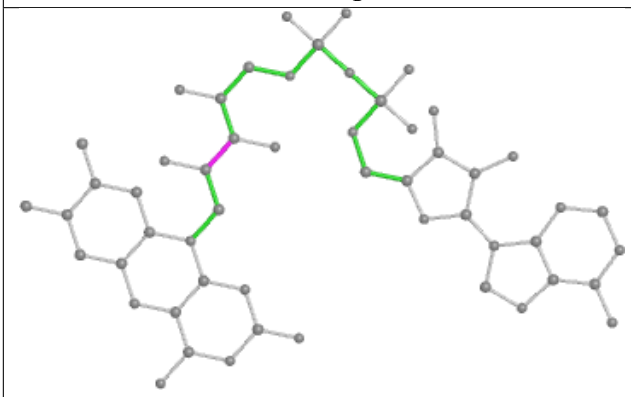
Ligand FAD D 1273



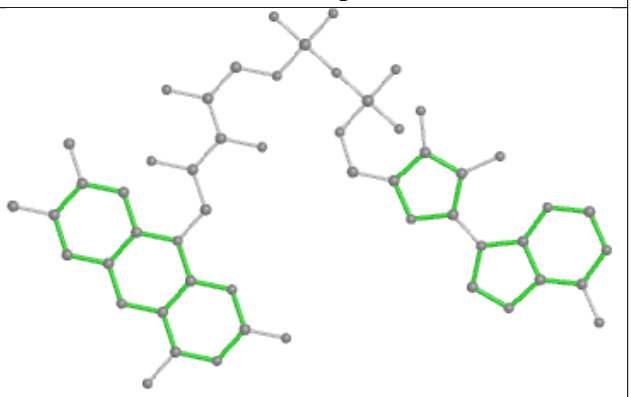
Bond lengths



Bond angles

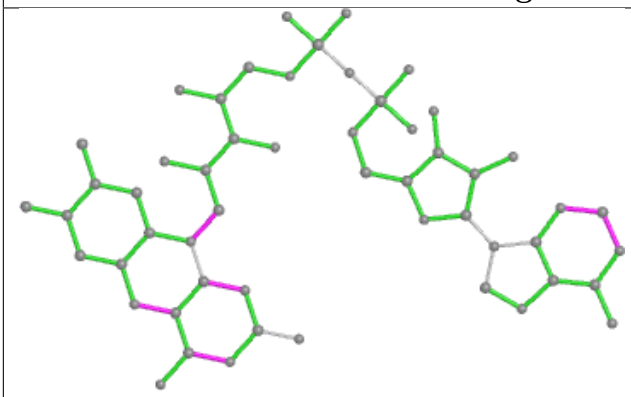


Torsions

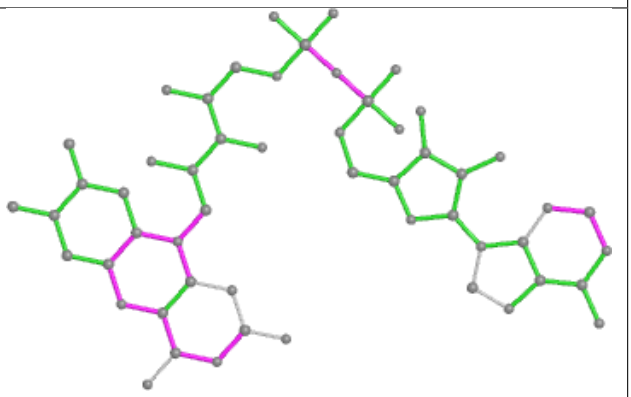


Rings

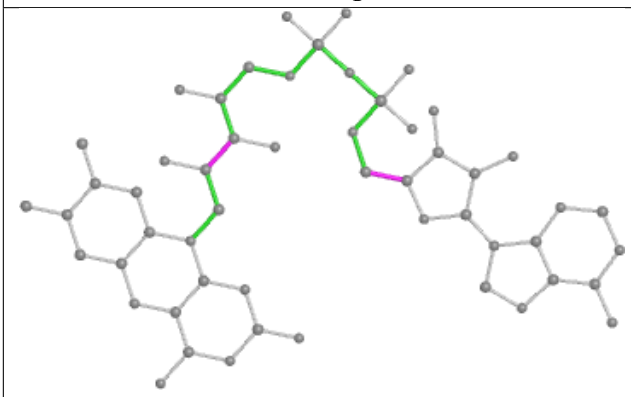
Ligand FAD A 1273



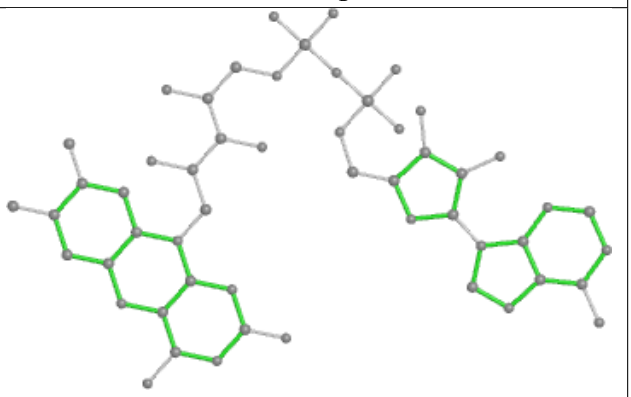
Bond lengths



Bond angles

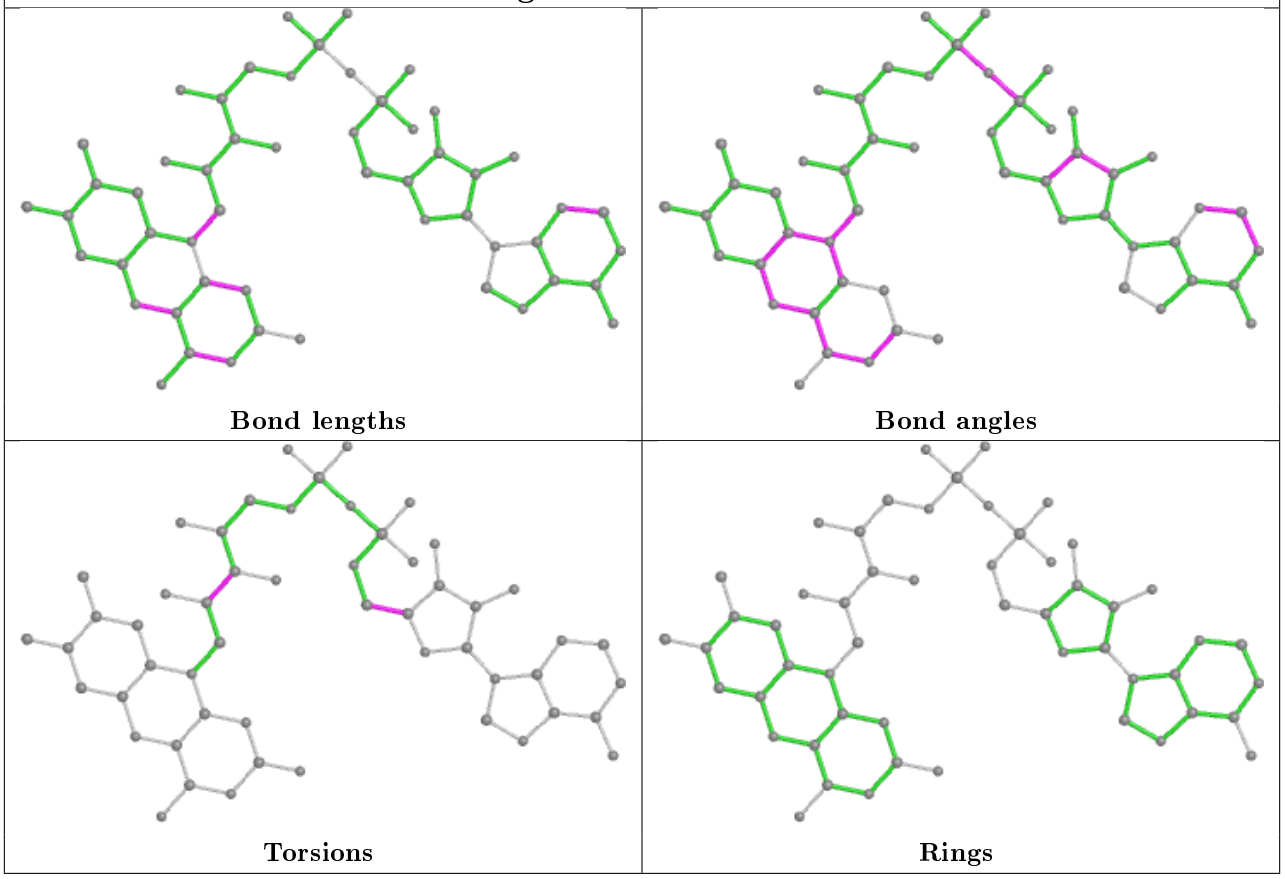


Torsions



Rings

Ligand FAD B 1273



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	260/272 (95%)	-0.10	7 (2%)	54	60	29, 39, 66, 81	0
1	B	257/272 (94%)	-0.09	7 (2%)	54	60	29, 39, 65, 76	0
1	C	257/272 (94%)	-0.14	6 (2%)	60	65	29, 39, 64, 76	0
1	D	257/272 (94%)	-0.10	6 (2%)	60	65	29, 39, 65, 76	0
All	All	1031/1088 (94%)	-0.11	26 (2%)	57	62	29, 39, 65, 81	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	254	ALA	6.5
1	B	254	ALA	5.9
1	D	16	PRO	5.5
1	A	254	ALA	5.3
1	B	272	ILE	3.9
1	D	254	ALA	3.5
1	B	16	PRO	3.5
1	B	175	GLU	3.5
1	A	14	VAL	3.4
1	D	183	VAL	3.2
1	A	181	GLU	3.1
1	C	180	GLY	2.9
1	A	184	GLU	2.9
1	A	16	PRO	2.7
1	C	182	LEU	2.7
1	B	58	ASN	2.6
1	D	271	GLY	2.6
1	C	184	GLU	2.5
1	C	175	GLU	2.4
1	A	183	VAL	2.3
1	A	272	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	184	GLU	2.2
1	D	185	GLY	2.2
1	B	181	GLU	2.0
1	D	175	GLU	2.0
1	C	253	GLY	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)

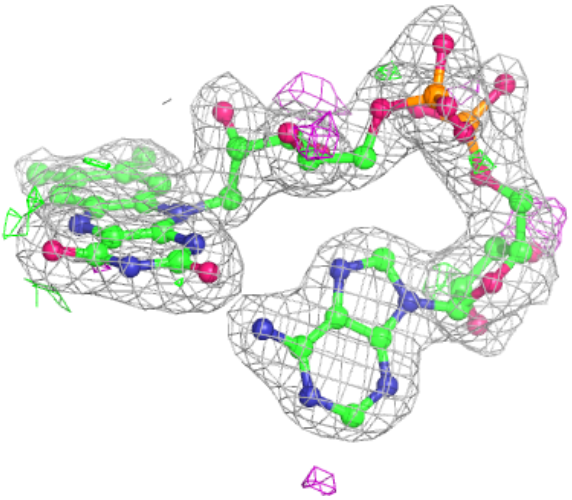
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

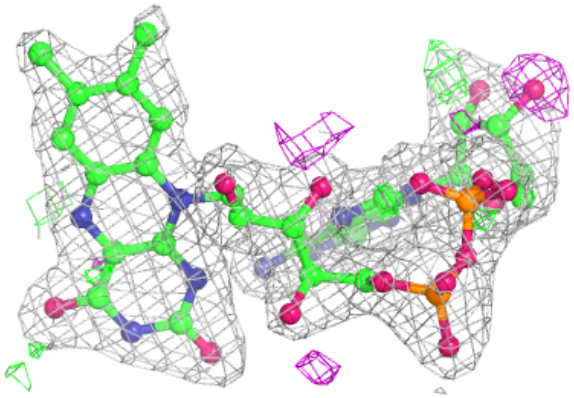
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	B	1273	53/53	0.94	0.12	38,43,56,63	0
2	FAD	A	1273	53/53	0.95	0.11	36,42,54,59	0
2	FAD	C	1273	53/53	0.96	0.12	33,41,55,60	0
2	FAD	D	1273	53/53	0.96	0.12	36,41,57,62	0

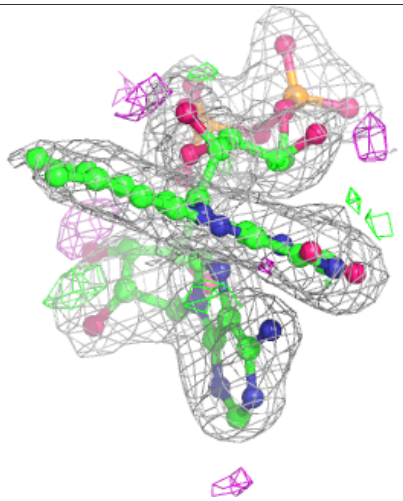
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 1273:

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

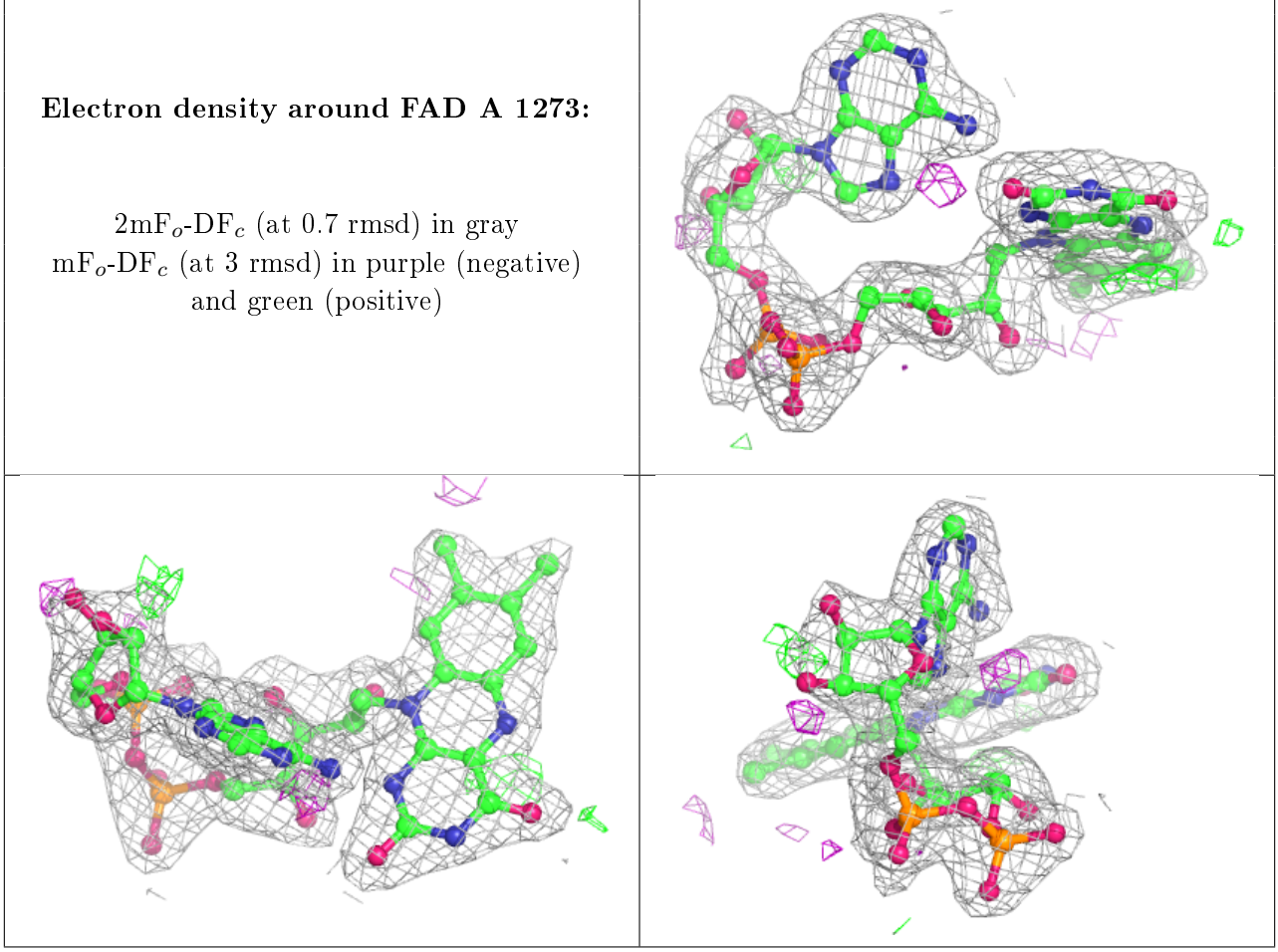






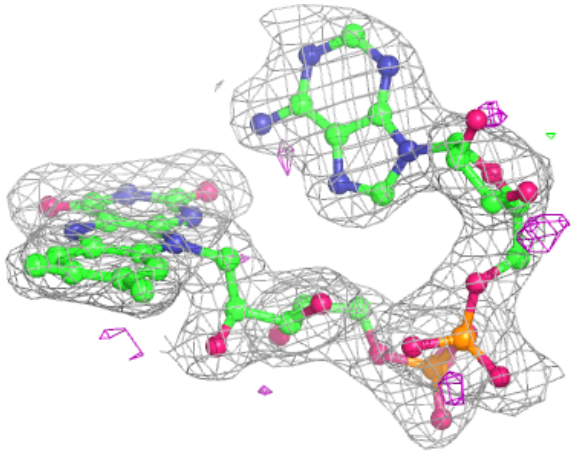
Electron density around FAD A 1273:

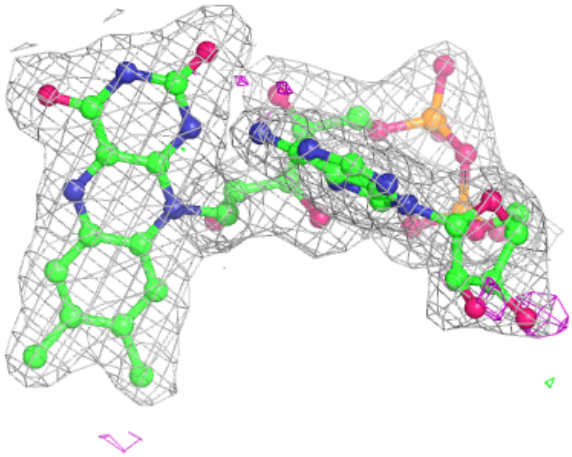
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

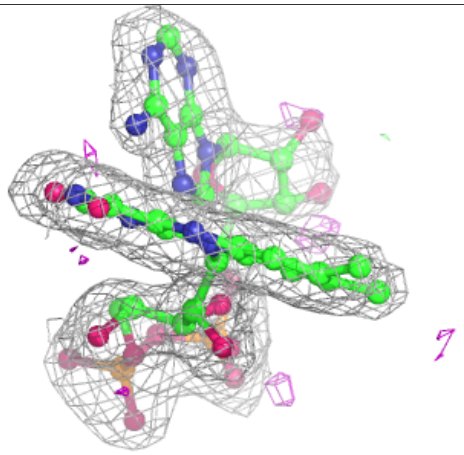


Electron density around FAD C 1273:

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

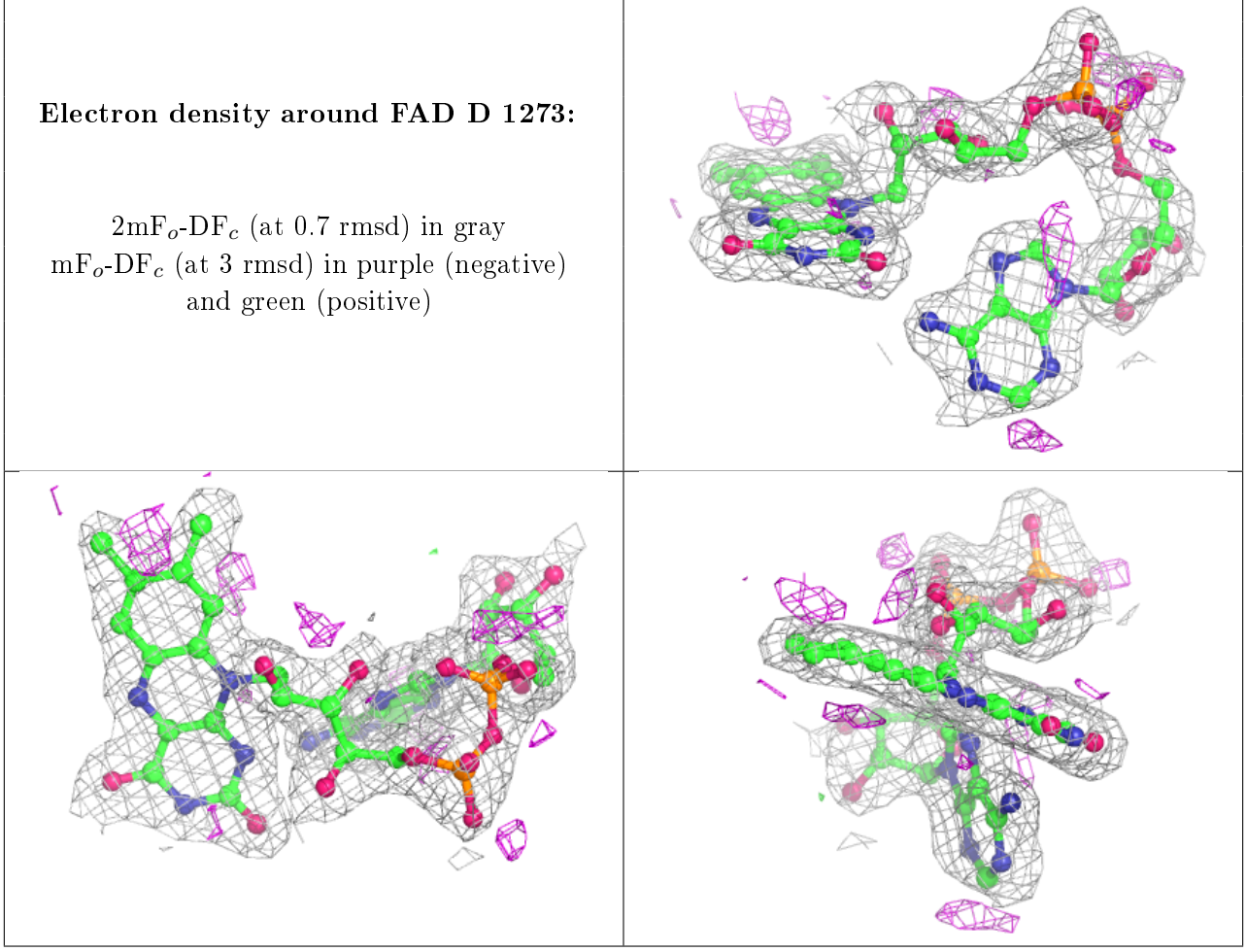






Electron density around FAD D 1273:

$2mF_o$-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

There are no such residues in this entry.