Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 04:45 PM JST

PDB ID	:	7C3A / pdb_00007c3a
Title	:	Ferredoxin reductase in carbazole 1,9a-dioxygenase
Authors	:	Ashikawa, Y.; Fujimoto, Z.; Nojiri, H.
Deposited on	:	2020-05-11
Resolution	:	2.60 Å(reported)

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

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

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

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

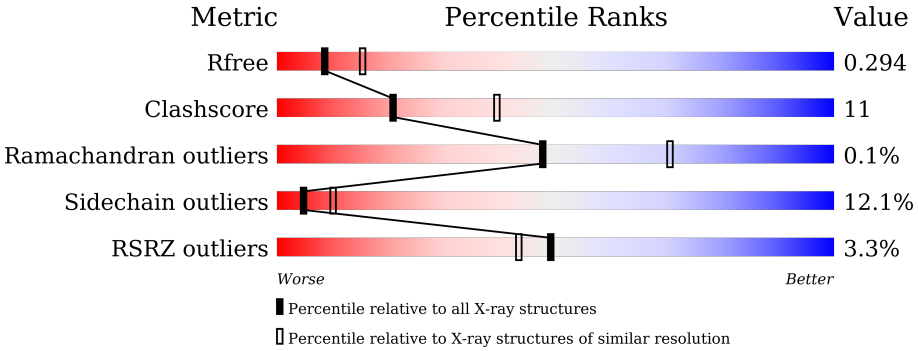
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	335	4%, 65%, 24%, 6%, •
1	B	335	3%, 80%, 18%, ••
1	C	335	2%, 75%, 19%, • •

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
4	IOD	A	1003	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7842 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.

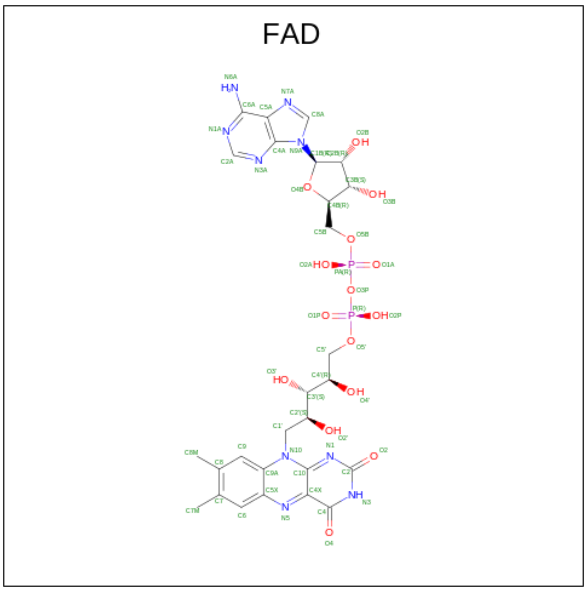
- Molecule 1 is a protein called Ferredoxin reductase component of carbazole.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2482	1585	434	448	15	0	0	0
1	B	332	2562	1633	447	467	15	0	0	0
1	C	329	2536	1621	439	461	15	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

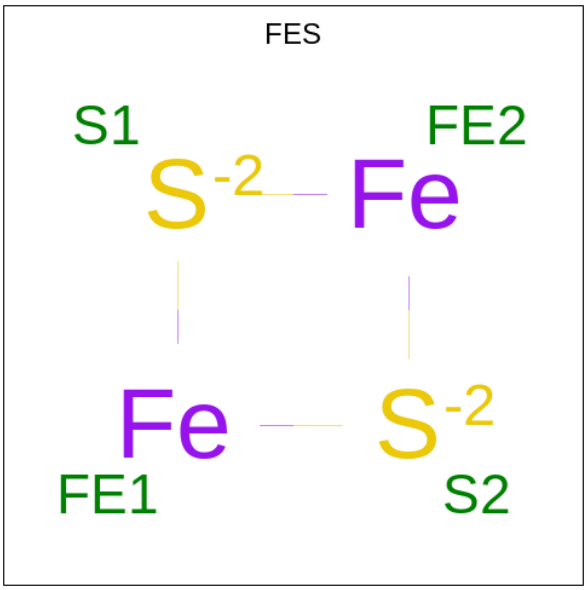
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q84II0
A	-4	HIS	-	expression tag	UNP Q84II0
A	-3	HIS	-	expression tag	UNP Q84II0
A	-2	HIS	-	expression tag	UNP Q84II0
A	-1	HIS	-	expression tag	UNP Q84II0
A	0	HIS	-	expression tag	UNP Q84II0
A	1	HIS	-	expression tag	UNP Q84II0
B	-5	MET	-	expression tag	UNP Q84II0
B	-4	HIS	-	expression tag	UNP Q84II0
B	-3	HIS	-	expression tag	UNP Q84II0
B	-2	HIS	-	expression tag	UNP Q84II0
B	-1	HIS	-	expression tag	UNP Q84II0
B	0	HIS	-	expression tag	UNP Q84II0
B	1	HIS	-	expression tag	UNP Q84II0
C	-5	MET	-	expression tag	UNP Q84II0
C	-4	HIS	-	expression tag	UNP Q84II0
C	-3	HIS	-	expression tag	UNP Q84II0
C	-2	HIS	-	expression tag	UNP Q84II0
C	-1	HIS	-	expression tag	UNP Q84II0
C	0	HIS	-	expression tag	UNP Q84II0
C	1	HIS	-	expression tag	UNP Q84II0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	B	1	4	2	2	0	0
			Total	Fe	S		
3	C	1	4	2	2	0	0

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	4	4	4	0	0
			Total	Cl		
5	B	2	2	2	0	0
			Total	Cl		
5	C	4	4	4	0	0

- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
6	A	1	1	1	0	0

- Molecule 7 is water.

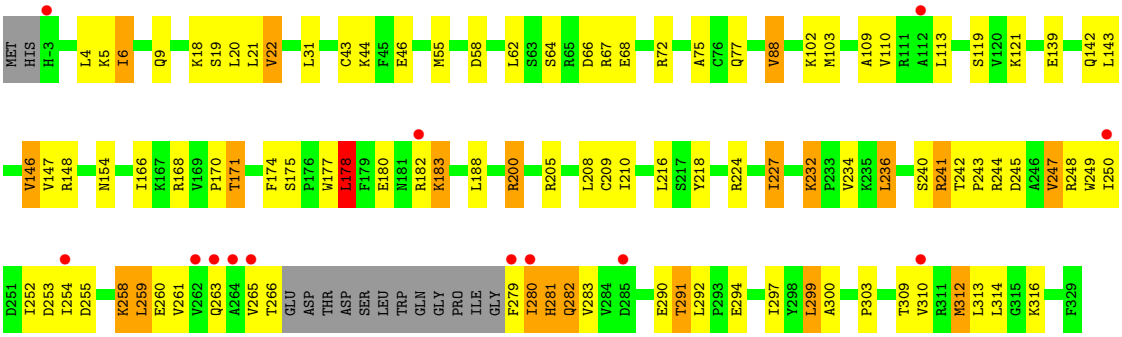
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	20	20	20	0	0
			Total	O		
7	B	29	29	29	0	0
			Total	O		
7	C	28	28	28	0	0

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.

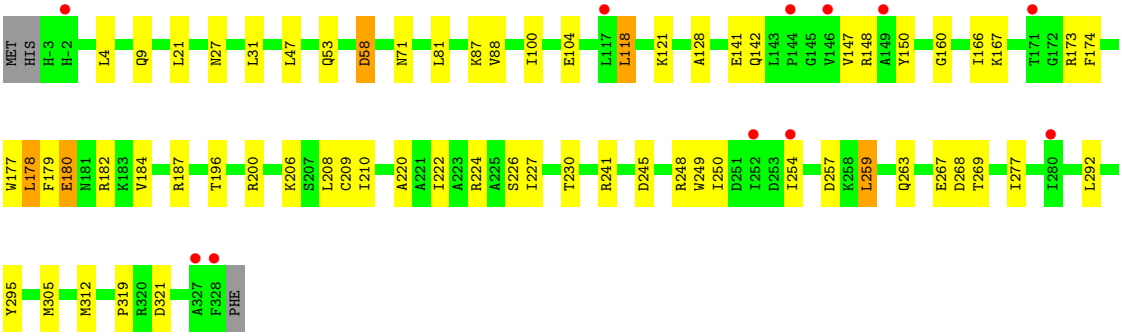
• Molecule 1: Ferredoxin reductase component of carbazole

Chain A:



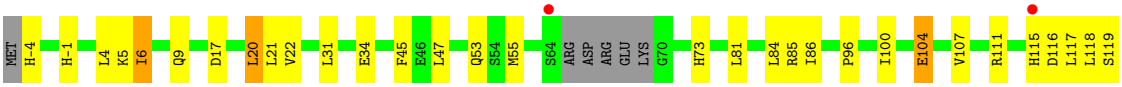
• Molecule 1: Ferredoxin reductase component of carbazole

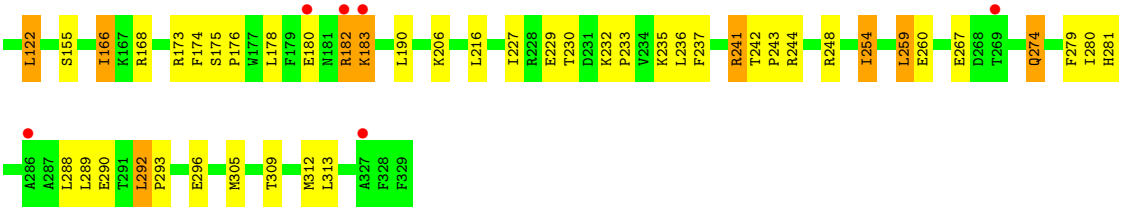
Chain B:



• Molecule 1: Ferredoxin reductase component of carbazole

Chain C:




L122
S155
I166
K167
R168
R173
F174
S175
P176
W177
L178
F179
E180
N181
R182
K183
L190
K206
L216
I227
R228
E229
T230
D231
K232
P233
V234
K235
L236
F237
R241
T242
P243
R244
R248
I254
L259
E260
E267
D268
T269
Q274
F279
I280
H281
A286
A287
L288
L289
E290
T291
L292
P293
E296
M305
T309
M312
L313
A327
F328
F329

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	158.69Å 158.69Å 81.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.67 – 2.60 35.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (35.67-2.60) 99.0 (35.67-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.249 , 0.291 0.250 , 0.294	Depositor DCC
R_{free} test set	1636 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	62.2	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 63.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7842	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, CL, NI, IOD, FES

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	0/2542	0.87	5/3445 (0.1%)
1	B	0.52	0/2625	0.75	0/3563
1	C	0.61	0/2600	0.80	0/3529
All	All	0.59	0/7767	0.81	5/10537 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	253	ASP	N-CA-C	10.39	125.91	113.23
1	A	253	ASP	CB-CA-C	-9.85	94.82	111.26
1	A	178	LEU	N-CA-C	-6.17	104.67	111.82
1	A	6	ILE	CB-CA-C	5.59	117.38	110.73
1	A	303	PRO	N-CA-C	5.47	117.38	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2482	0	2481	84	0
1	B	2562	0	2552	34	0
1	C	2536	0	2518	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	31	2	0
2	B	53	0	31	5	0
2	C	53	0	31	3	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
4	A	2	0	0	3	0
4	C	1	0	0	1	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	4	0	0	0	0
6	A	1	0	0	0	0
7	A	20	0	0	0	0
7	B	29	0	0	1	0
7	C	28	0	0	3	0
All	All	7842	0	7644	171	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 11.

All (171) 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:210:ILE:CD1	1:A:280:ILE:HD11	1.87	1.05
1:C:178:LEU:O	1:C:182:ARG:HB2	1.59	0.99
1:A:210:ILE:HG13	1:A:280:ILE:HD11	1.43	0.99
1:A:210:ILE:CG1	1:A:280:ILE:HD11	1.94	0.98
1:A:210:ILE:HG13	1:A:280:ILE:CD1	2.02	0.89
1:A:247:VAL:HG11	1:A:263:GLN:OE1	1.73	0.86
1:A:249:TRP:NE1	1:A:261:VAL:HG21	1.97	0.79
1:A:247:VAL:CG1	1:A:263:GLN:OE1	2.32	0.77
1:B:179:PHE:O	1:B:182:ARG:NE	2.21	0.74
1:A:249:TRP:CZ2	1:A:261:VAL:HG11	2.23	0.73
1:C:6:ILE:HG12	1:C:9:GLN:HB2	1.71	0.72
1:B:249:TRP:HZ2	1:B:263:GLN:HB3	1.54	0.71
1:A:178:LEU:H	1:A:178:LEU:HD23	1.56	0.70
1:C:178:LEU:O	1:C:182:ARG:CB	2.38	0.69
1:C:182:ARG:O	1:C:183:LYS:HG2	1.93	0.68
1:A:249:TRP:CE2	1:A:261:VAL:HG11	2.29	0.67
1:A:178:LEU:HD22	1:A:182:ARG:NH1	2.10	0.67
1:C:288:LEU:HB2	1:C:292:LEU:HD13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ILE:HD11	1:B:259:LEU:HB3	1.78	0.65
1:A:210:ILE:HD11	1:A:280:ILE:HD11	1.76	0.64
1:C:166:ILE:HG13	1:C:178:LEU:HD23	1.81	0.63
1:A:254:ILE:HG13	1:A:255:ASP:N	2.13	0.63
1:A:183:LYS:HB3	4:A:1003:IOD:I	2.69	0.63
1:A:110:VAL:HG21	4:A:1003:IOD:I	2.69	0.62
1:A:168:ARG:HA	1:A:175:SER:OG	2.00	0.61
1:C:118:LEU:HD21	1:C:182:ARG:HD3	1.82	0.61
1:A:200:ARG:CG	1:A:200:ARG:HH11	2.14	0.61
1:B:148:ARG:NH2	2:B:1001:FAD:O4B	2.34	0.61
1:A:178:LEU:HD23	1:A:178:LEU:N	2.15	0.60
1:C:104:GLU:H	1:C:104:GLU:CD	2.10	0.60
1:A:299:LEU:HD11	1:A:309:THR:HB	1.84	0.59
1:A:208:LEU:HD23	1:A:297:ILE:HG12	1.85	0.59
1:A:254:ILE:HD12	1:A:255:ASP:H	1.69	0.58
1:A:210:ILE:CG1	1:A:280:ILE:CD1	2.71	0.58
2:C:1001:FAD:C6A	7:C:1104:HOH:O	2.50	0.58
1:A:248:ARG:NE	1:A:248:ARG:HA	2.18	0.57
1:C:176:PRO:O	1:C:180:GLU:HG2	2.03	0.57
1:C:-1:HIS:CE1	1:C:17:ASP:HB3	2.40	0.57
1:A:247:VAL:CB	1:A:263:GLN:OE1	2.53	0.57
1:C:254:ILE:HD11	1:C:259:LEU:HD11	1.87	0.57
1:C:6:ILE:CG1	1:C:9:GLN:HB2	2.34	0.57
1:A:210:ILE:HD12	1:A:280:ILE:HD11	1.86	0.57
1:A:210:ILE:CD1	1:A:280:ILE:CD1	2.74	0.56
1:C:175:SER:HB2	1:C:176:PRO:HD3	1.87	0.56
1:C:237:PHE:HB3	1:C:280:ILE:HD11	1.88	0.56
1:A:19:SER:OG	1:A:22:VAL:HG12	2.06	0.56
1:A:240:SER:OG	1:A:245:ASP:HB2	2.06	0.56
1:A:174:PHE:CE2	1:A:178:LEU:HD21	2.41	0.55
1:A:241:ARG:HG2	1:A:242:THR:N	2.22	0.55
1:B:148:ARG:HB3	1:B:150:TYR:CE2	2.42	0.55
1:C:227:ILE:HD11	1:C:259:LEU:HD23	1.89	0.55
1:B:179:PHE:O	1:B:182:ARG:CZ	2.54	0.55
1:A:254:ILE:CG1	1:A:255:ASP:N	2.69	0.55
1:A:281:HIS:CD2	1:A:281:HIS:C	2.85	0.54
1:A:18:LYS:HB2	4:A:1004:IOD:I	2.78	0.54
1:B:147:VAL:O	1:B:148:ARG:HD2	2.09	0.53
1:A:254:ILE:CD1	1:A:255:ASP:H	2.21	0.53
1:A:210:ILE:HD11	1:A:280:ILE:CD1	2.37	0.53
1:A:249:TRP:HA	1:A:249:TRP:CE3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:TRP:HE1	1:A:261:VAL:HG21	1.74	0.52
1:B:142:GLN:HB3	1:B:177:TRP:HZ2	1.74	0.52
1:A:62:LEU:H	1:A:62:LEU:HD23	1.74	0.52
1:A:46:GLU:HB3	1:A:72:ARG:HD3	1.90	0.52
1:B:104:GLU:N	1:B:104:GLU:OE1	2.42	0.52
1:A:55:MET:HE3	1:A:77:GLN:HA	1.92	0.51
1:C:174:PHE:CE2	1:C:178:LEU:HD22	2.46	0.51
1:C:5:LYS:O	1:C:85:ARG:HA	2.10	0.51
1:C:20:LEU:HD11	1:C:84:LEU:HD12	1.93	0.51
1:A:297:ILE:HD13	1:A:313:LEU:HD11	1.93	0.51
1:C:309:THR:O	1:C:313:LEU:HB2	2.11	0.50
1:C:182:ARG:O	1:C:183:LYS:CG	2.59	0.50
1:C:6:ILE:H	1:C:6:ILE:HD13	1.77	0.50
1:A:182:ARG:NH1	1:A:188:LEU:HD21	2.26	0.49
1:A:6:ILE:HG23	1:A:9:GLN:HB2	1.94	0.49
1:B:196:THR:O	1:B:200:ARG:NH2	2.45	0.49
1:B:268:ASP:HB3	1:B:277:ILE:HG23	1.94	0.49
1:B:104:GLU:H	1:B:104:GLU:CD	2.20	0.49
1:B:226:SER:C	1:B:230:THR:HG22	2.38	0.49
1:A:247:VAL:HB	1:A:263:GLN:OE1	2.13	0.48
1:B:128:ALA:HB2	1:B:160:GLY:HA2	1.95	0.48
1:C:241:ARG:HD2	1:C:242:THR:HG23	1.96	0.48
1:A:43:CYS:HB2	1:A:75:ALA:HB3	1.94	0.48
1:B:226:SER:O	1:B:230:THR:HG22	2.12	0.48
1:C:279:PHE:HB3	1:C:281:HIS:NE2	2.28	0.48
1:B:173:ARG:HG2	2:B:1001:FAD:O2A	2.13	0.48
1:C:296:GLU:HA	1:C:296:GLU:OE1	2.14	0.48
1:A:31:LEU:CD1	1:A:88:VAL:HG11	2.44	0.48
1:A:254:ILE:HG21	1:A:259:LEU:HD12	1.95	0.48
1:C:111:ARG:HB2	1:C:119:SER:HB3	1.95	0.48
1:A:232:LYS:O	1:A:234:VAL:HG23	2.13	0.48
1:C:206:LYS:HD3	1:C:233:PRO:HB2	1.96	0.47
1:A:64:SER:HA	1:A:67:ARG:HB2	1.97	0.47
1:A:258:LYS:HD2	1:A:258:LYS:N	2.28	0.47
2:B:1001:FAD:O4'	2:B:1001:FAD:O2'	2.30	0.47
1:A:113:LEU:HD11	1:A:119:SER:HB2	1.96	0.47
1:A:154:ASN:HA	1:A:224:ARG:NH2	2.29	0.47
1:A:280:ILE:CG1	1:A:281:HIS:N	2.77	0.47
1:A:148:ARG:NE	2:A:1001:FAD:O1P	2.46	0.47
1:B:226:SER:O	1:B:230:THR:N	2.46	0.46
1:C:-4:HIS:O	1:C:-4:HIS:ND1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:CG1	1:A:255:ASP:H	2.28	0.46
1:B:58:ASP:OD1	1:B:58:ASP:N	2.48	0.46
1:C:235:LYS:HG2	1:C:260:GLU:HB3	1.98	0.46
1:B:241:ARG:NH2	7:B:1101:HOH:O	2.23	0.46
1:A:227:ILE:CD1	1:A:254:ILE:HD11	2.45	0.46
1:A:280:ILE:O	1:A:282:GLN:N	2.49	0.45
1:A:312:MET:C	1:A:312:MET:SD	3.00	0.45
1:A:200:ARG:HH11	1:A:200:ARG:HG3	1.79	0.45
1:B:173:ARG:NE	2:B:1001:FAD:O2A	2.50	0.45
1:A:291:THR:O	1:A:294:GLU:HG2	2.17	0.45
1:C:168:ARG:HD2	7:C:1109:HOH:O	2.16	0.45
1:C:182:ARG:C	1:C:183:LYS:CG	2.90	0.45
1:C:305:MET:C	1:C:305:MET:SD	2.99	0.45
1:A:244:ARG:HA	1:A:244:ARG:HD2	1.68	0.45
1:B:178:LEU:O	1:B:182:ARG:HB3	2.17	0.45
1:B:319:PRO:HB2	1:B:321:ASP:OD1	2.17	0.44
1:C:242:THR:HB	1:C:243:PRO:CD	2.47	0.44
1:C:274:GLN:H	1:C:274:GLN:CD	2.25	0.44
1:B:148:ARG:HG3	2:B:1001:FAD:O3'	2.17	0.44
1:C:6:ILE:HG22	1:C:86:ILE:HG13	1.99	0.44
1:B:174:PHE:CD1	1:B:174:PHE:C	2.96	0.44
1:C:53:GLN:HB2	1:C:81:LEU:HD11	1.99	0.44
1:C:230:THR:C	1:C:232:LYS:H	2.25	0.44
1:C:242:THR:HB	1:C:243:PRO:HD2	2.00	0.44
1:A:170:PRO:O	1:A:171:THR:HB	2.18	0.43
1:A:209:CYS:HB2	1:A:236:LEU:HD23	2.00	0.43
1:A:243:PRO:CG	1:A:265:VAL:HG11	2.48	0.43
1:A:243:PRO:CA	1:A:265:VAL:HG11	2.48	0.43
1:A:281:HIS:ND1	1:A:309:THR:HA	2.33	0.43
1:A:279:PHE:CD1	1:A:279:PHE:N	2.86	0.43
1:A:243:PRO:CB	1:A:265:VAL:HG11	2.49	0.43
1:A:174:PHE:O	1:A:177:TRP:HB2	2.19	0.42
1:B:220:ALA:O	1:B:224:ARG:HG2	2.19	0.42
1:B:53:GLN:HB2	1:B:81:LEU:HD21	2.01	0.42
1:A:280:ILE:O	1:A:283:VAL:HG22	2.18	0.42
1:C:104:GLU:CD	1:C:104:GLU:N	2.74	0.42
1:A:182:ARG:C	1:A:183:LYS:HG3	2.44	0.42
1:C:45:PHE:CZ	1:C:73:HIS:HB2	2.54	0.42
1:C:96:PRO:CG	1:C:100:ILE:HD11	2.49	0.42
1:B:27:ASN:N	1:B:27:ASN:HD22	2.16	0.42
1:A:143:LEU:HB3	1:A:146:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:LEU:HD12	1:C:190:LEU:HD11	2.02	0.42
1:C:183:LYS:NZ	7:C:1102:HOH:O	2.53	0.42
2:C:1001:FAD:N1	2:C:1001:FAD:C2'	2.82	0.42
1:C:55:MET:HA	1:C:55:MET:HE2	2.01	0.42
1:A:310:VAL:O	1:A:314:LEU:HB2	2.19	0.42
1:A:18:LYS:HD3	1:A:22:VAL:HG22	2.02	0.42
1:A:218:TYR:CD1	1:A:300:ALA:HB2	2.54	0.42
1:C:107:VAL:HG22	1:C:122:LEU:HD22	2.00	0.42
1:C:183:LYS:HA	4:C:1003:IOD:I	2.90	0.42
1:A:243:PRO:HG3	1:A:265:VAL:HG11	2.02	0.41
1:A:102:LYS:NZ	1:A:139:GLU:OE1	2.52	0.41
1:A:248:ARG:O	1:A:252:ILE:HD13	2.20	0.41
1:C:292:LEU:N	1:C:293:PRO:CD	2.83	0.41
2:C:1001:FAD:N1	2:C:1001:FAD:H2'	2.33	0.41
2:A:1001:FAD:H9	2:A:1001:FAD:H1'1	1.91	0.41
1:A:170:PRO:O	1:A:171:THR:CB	2.68	0.41
1:C:206:LYS:HG2	1:C:233:PRO:O	2.20	0.41
1:A:44:LYS:HD2	1:A:66:ASP:OD2	2.21	0.41
1:B:179:PHE:C	1:B:180:GLU:OE1	2.64	0.41
1:B:206:LYS:O	1:B:295:TYR:HA	2.21	0.41
1:B:249:TRP:CZ2	1:B:263:GLN:HB3	2.44	0.41
1:B:268:ASP:O	1:B:269:THR:C	2.62	0.41
1:A:200:ARG:CG	1:A:200:ARG:NH1	2.77	0.40
1:B:208:LEU:HD22	1:B:210:ILE:HG13	2.02	0.40
1:B:209:CYS:SG	1:B:222:ILE:HG22	2.61	0.40
1:A:280:ILE:C	1:A:282:GLN:H	2.29	0.40
1:C:115:HIS:NE2	1:C:116:ASP:OD2	2.53	0.40
1:A:168:ARG:HA	1:A:175:SER:HG	1.85	0.40
1:A:109:ALA:HB3	1:A:121:LYS:HB3	2.04	0.40
1:B:118:LEU:HD13	1:B:179:PHE:CZ	2.57	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	317/335 (95%)	293 (92%)	24 (8%)	0	100	100
1	B	330/335 (98%)	304 (92%)	26 (8%)	0	100	100
1	C	325/335 (97%)	301 (93%)	23 (7%)	1 (0%)	36	58
All	All	972/1005 (97%)	898 (92%)	73 (8%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	289	LEU

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	263/275 (96%)	224 (85%)	39 (15%)	3	6
1	B	272/275 (99%)	243 (89%)	29 (11%)	6	14
1	C	269/275 (98%)	240 (89%)	29 (11%)	6	13
All	All	804/825 (98%)	707 (88%)	97 (12%)	5	10

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	LYS
1	A	20	LEU
1	A	21	LEU
1	A	22	VAL
1	A	58	ASP
1	A	68	GLU
1	A	88	VAL
1	A	103	MET

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Mol	Chain	Res	Type
1	A	142	GLN
1	A	146	VAL
1	A	147	VAL
1	A	166	ILE
1	A	171	THR
1	A	178	LEU
1	A	180	GLU
1	A	183	LYS
1	A	200	ARG
1	A	205	ARG
1	A	216	LEU
1	A	227	ILE
1	A	232	LYS
1	A	236	LEU
1	A	241	ARG
1	A	247	VAL
1	A	250	ILE
1	A	258	LYS
1	A	259	LEU
1	A	260	GLU
1	A	266	THR
1	A	280	ILE
1	A	281	HIS
1	A	282	GLN
1	A	290	GLU
1	A	291	THR
1	A	292	LEU
1	A	299	LEU
1	A	312	MET
1	A	316	LYS
1	B	4	LEU
1	B	9	GLN
1	B	21	LEU
1	B	31	LEU
1	B	47	LEU
1	B	58	ASP
1	B	71	ASN
1	B	87	LYS
1	B	88	VAL
1	B	100	ILE
1	B	118	LEU
1	B	121	LYS

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Mol	Chain	Res	Type
1	B	141	GLU
1	B	166	ILE
1	B	167	LYS
1	B	178	LEU
1	B	180	GLU
1	B	184	VAL
1	B	187	ARG
1	B	245	ASP
1	B	248	ARG
1	B	250	ILE
1	B	254	ILE
1	B	257	ASP
1	B	259	LEU
1	B	267	GLU
1	B	292	LEU
1	B	305	MET
1	B	312	MET
1	C	4	LEU
1	C	6	ILE
1	C	20	LEU
1	C	21	LEU
1	C	22	VAL
1	C	31	LEU
1	C	34	GLU
1	C	47	LEU
1	C	104	GLU
1	C	117	LEU
1	C	122	LEU
1	C	155	SER
1	C	166	ILE
1	C	173	ARG
1	C	182	ARG
1	C	183	LYS
1	C	216	LEU
1	C	229	GLU
1	C	236	LEU
1	C	241	ARG
1	C	244	ARG
1	C	248	ARG
1	C	254	ILE
1	C	259	LEU
1	C	267	GLU

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Mol	Chain	Res	Type
1	C	274	GLN
1	C	290	GLU
1	C	292	LEU
1	C	312	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	9	GLN
1	A	77	GLN
1	A	282	GLN
1	B	3	GLN
1	B	71	ASN
1	B	181	ASN
1	C	9	GLN
1	C	27	ASN
1	C	73	HIS
1	C	181	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 14 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	A	1001	-	56,58,58	1.49	8 (14%)	81,89,89	1.73	20 (24%)
3	FES	A	1002	1	0,4,4	-	-	-		
3	FES	B	1002	1	0,4,4	-	-	-		
2	FAD	C	1001	-	56,58,58	1.48	11 (19%)	81,89,89	1.77	20 (24%)
3	FES	C	1002	1	0,4,4	-	-	-		
2	FAD	B	1001	-	56,58,58	1.53	7 (12%)	81,89,89	1.74	17 (20%)

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	A	1001	-	-	14/34/50/50	0/6/6/6
3	FES	A	1002	1	-	-	0/1/1/1
3	FES	B	1002	1	-	-	0/1/1/1
2	FAD	C	1001	-	-	19/34/50/50	0/6/6/6
3	FES	C	1002	1	-	-	0/1/1/1
2	FAD	B	1001	-	-	16/34/50/50	0/6/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	FAD	C9A-C5X	5.38	1.50	1.41
2	A	1001	FAD	C9A-C5X	5.18	1.49	1.41
2	A	1001	FAD	C5A-C4A	4.95	1.48	1.39
2	B	1001	FAD	C5A-C4A	4.88	1.48	1.39
2	C	1001	FAD	C5A-C4A	4.80	1.48	1.39
2	C	1001	FAD	C9A-C5X	4.56	1.48	1.41
2	B	1001	FAD	C8-C7	3.62	1.49	1.40
2	C	1001	FAD	C4'-C3'	-3.14	1.47	1.53
2	A	1001	FAD	C8-C7	3.06	1.48	1.40
2	A	1001	FAD	C5A-C6A	2.88	1.49	1.41
2	B	1001	FAD	C5A-C6A	2.84	1.49	1.41
2	C	1001	FAD	C8-C7	2.80	1.47	1.40
2	B	1001	FAD	C4X-N5	2.77	1.36	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	FAD	C8A-N7A	2.59	1.36	1.31
2	A	1001	FAD	C4X-N5	2.54	1.35	1.30
2	B	1001	FAD	C8A-N7A	2.40	1.36	1.31
2	C	1001	FAD	C4X-N5	2.37	1.35	1.30
2	C	1001	FAD	C5X-N5	-2.36	1.34	1.39
2	A	1001	FAD	C10-N10	2.35	1.42	1.37
2	C	1001	FAD	C5A-C6A	2.34	1.47	1.41
2	C	1001	FAD	C8A-N7A	2.28	1.35	1.31
2	C	1001	FAD	C4-N3	-2.27	1.34	1.38
2	C	1001	FAD	C5A-N7A	-2.26	1.34	1.39
2	A	1001	FAD	C4-N3	-2.21	1.34	1.38
2	B	1001	FAD	C10-N10	2.07	1.41	1.37
2	C	1001	FAD	C10-N10	2.06	1.41	1.37

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	FAD	C5A-C4A-N3A	-6.24	118.61	126.75
2	B	1001	FAD	C5A-C4A-N3A	-6.21	118.65	126.75
2	A	1001	FAD	C5A-C4A-N3A	-5.54	119.52	126.75
2	C	1001	FAD	N3A-C4A-N9A	5.12	135.51	127.08
2	B	1001	FAD	N3A-C4A-N9A	4.80	134.99	127.08
2	A	1001	FAD	N3A-C4A-N9A	4.63	134.72	127.08
2	B	1001	FAD	C2A-N3A-C4A	4.06	121.35	111.75
2	A	1001	FAD	C4-C4X-N5	4.03	123.96	118.23
2	A	1001	FAD	C2A-N3A-C4A	3.89	120.93	111.75
2	B	1001	FAD	N3A-C2A-N1A	-3.76	122.72	128.60
2	A	1001	FAD	N3A-C2A-N1A	-3.76	122.73	128.60
2	C	1001	FAD	C2A-N3A-C4A	3.72	120.55	111.75
2	C	1001	FAD	N3A-C2A-N1A	-3.29	123.46	128.60
2	B	1001	FAD	C4A-C5A-N7A	-3.28	106.63	110.62
2	C	1001	FAD	C4'-C3'-C2'	-3.23	106.65	113.36
2	B	1001	FAD	C5A-N7A-C8A	3.17	108.01	103.51
2	B	1001	FAD	C4-C4X-N5	3.11	122.66	118.23
2	C	1001	FAD	C4-C4X-N5	3.07	122.60	118.23
2	A	1001	FAD	C4A-N9A-C8A	3.06	109.05	105.73
2	A	1001	FAD	C5A-N7A-C8A	3.02	107.79	103.51
2	A	1001	FAD	C4A-C5A-N7A	-2.96	107.02	110.62
2	B	1001	FAD	P-O3P-PA	-2.95	122.70	132.83
2	C	1001	FAD	C5'-C4'-C3'	-2.87	106.67	112.20
2	A	1001	FAD	C4X-C10-N1	-2.84	118.15	124.73
2	C	1001	FAD	O5'-C5'-C4'	-2.78	101.93	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	FAD	C10-N1-C2	2.78	122.46	116.90
2	A	1001	FAD	O2-C2-N1	-2.73	117.31	121.83
2	B	1001	FAD	C4X-C10-N1	-2.69	118.49	124.73
2	B	1001	FAD	C10-N1-C2	2.66	122.22	116.90
2	C	1001	FAD	C4A-C5A-N7A	-2.64	107.40	110.62
2	C	1001	FAD	C4X-C10-N1	-2.64	118.61	124.73
2	C	1001	FAD	C5A-N7A-C8A	2.64	107.25	103.51
2	A	1001	FAD	C4X-C10-N10	2.62	120.31	116.48
2	C	1001	FAD	O4-C4-C4X	-2.61	119.67	126.60
2	A	1001	FAD	C5X-N5-C4X	2.61	122.41	118.07
2	A	1001	FAD	N9A-C8A-N7A	-2.59	110.38	113.91
2	C	1001	FAD	O2'-C2'-C3'	2.56	115.31	109.10
2	B	1001	FAD	C4X-C10-N10	2.55	120.20	116.48
2	B	1001	FAD	O3'-C3'-C4'	2.50	114.84	108.81
2	A	1001	FAD	C10-C4X-N5	-2.48	119.59	124.86
2	C	1001	FAD	C5X-N5-C4X	2.44	122.14	118.07
2	A	1001	FAD	P-O3P-PA	-2.41	124.54	132.83
2	C	1001	FAD	O3'-C3'-C2'	2.37	114.54	108.81
2	A	1001	FAD	C4-N3-C2	-2.31	121.38	125.64
2	A	1001	FAD	C4X-C4-N3	2.29	119.01	113.19
2	C	1001	FAD	C10-N1-C2	2.28	121.46	116.90
2	B	1001	FAD	N9A-C8A-N7A	-2.27	110.81	113.91
2	B	1001	FAD	C4A-N9A-C8A	2.27	108.18	105.73
2	C	1001	FAD	P-O3P-PA	-2.24	125.13	132.83
2	C	1001	FAD	C4A-N9A-C8A	2.24	108.15	105.73
2	B	1001	FAD	C2A-N1A-C6A	2.17	122.48	118.77
2	B	1001	FAD	O2-C2-N1	-2.16	118.25	121.83
2	B	1001	FAD	C6A-C5A-N7A	2.16	136.04	132.02
2	C	1001	FAD	C10-C4X-N5	-2.13	120.33	124.86
2	A	1001	FAD	C6A-C5A-N7A	2.13	135.99	132.02
2	C	1001	FAD	C4X-C4-N3	2.05	118.39	113.19
2	A	1001	FAD	O2A-PA-O1A	2.00	122.15	112.24

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	FAD	O4B-C4B-C5B-O5B
2	A	1001	FAD	C3B-C4B-C5B-O5B
2	A	1001	FAD	N10-C1'-C2'-O2'
2	A	1001	FAD	N10-C1'-C2'-C3'
2	A	1001	FAD	C1'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
2	A	1001	FAD	C1'-C2'-C3'-C4'
2	A	1001	FAD	O4'-C4'-C5'-O5'
2	B	1001	FAD	O4B-C4B-C5B-O5B
2	B	1001	FAD	C3B-C4B-C5B-O5B
2	B	1001	FAD	C2'-C1'-N10-C10
2	B	1001	FAD	N10-C1'-C2'-O2'
2	B	1001	FAD	N10-C1'-C2'-C3'
2	B	1001	FAD	C1'-C2'-C3'-O3'
2	B	1001	FAD	C1'-C2'-C3'-C4'
2	B	1001	FAD	O2'-C2'-C3'-O3'
2	B	1001	FAD	O2'-C2'-C3'-C4'
2	B	1001	FAD	C5'-O5'-P-O2P
2	B	1001	FAD	C5'-O5'-P-O3P
2	C	1001	FAD	C5B-O5B-PA-O1A
2	C	1001	FAD	C5B-O5B-PA-O2A
2	C	1001	FAD	P-O3P-PA-O5B
2	C	1001	FAD	N10-C1'-C2'-O2'
2	C	1001	FAD	N10-C1'-C2'-C3'
2	C	1001	FAD	C1'-C2'-C3'-O3'
2	C	1001	FAD	C1'-C2'-C3'-C4'
2	C	1001	FAD	O2'-C2'-C3'-O3'
2	C	1001	FAD	O2'-C2'-C3'-C4'
2	C	1001	FAD	C5'-O5'-P-O2P
2	A	1001	FAD	C2'-C3'-C4'-C5'
2	A	1001	FAD	O2'-C2'-C3'-O3'
2	A	1001	FAD	C2'-C3'-C4'-O4'
2	A	1001	FAD	O2'-C2'-C3'-C4'
2	C	1001	FAD	C2B-C1B-N9A-C8A
2	A	1001	FAD	O3'-C3'-C4'-O4'
2	C	1001	FAD	O4B-C4B-C5B-O5B
2	C	1001	FAD	C2'-C1'-N10-C10
2	A	1001	FAD	O3'-C3'-C4'-C5'
2	B	1001	FAD	P-O3P-PA-O5B
2	C	1001	FAD	C5B-O5B-PA-O3P
2	C	1001	FAD	C5'-O5'-P-O3P
2	B	1001	FAD	PA-O3P-P-O1P
2	C	1001	FAD	C5'-O5'-P-O1P
2	C	1001	FAD	C2B-C1B-N9A-C4A
2	C	1001	FAD	C3B-C4B-C5B-O5B
2	B	1001	FAD	C2B-C1B-N9A-C8A
2	B	1001	FAD	C5B-O5B-PA-O3P
2	C	1001	FAD	O4B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
2	A	1001	FAD	PA-O3P-P-O2P
2	B	1001	FAD	PA-O3P-P-O2P

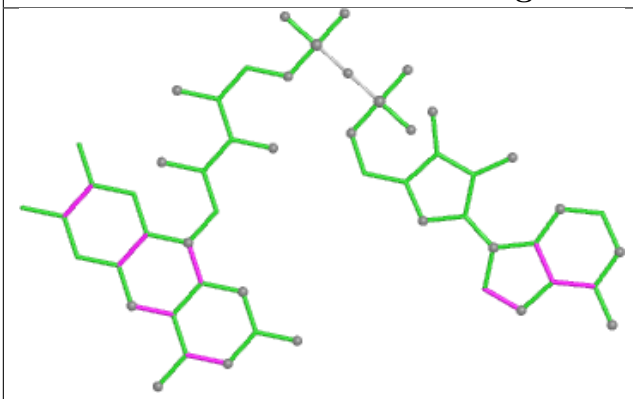
There are no ring outliers.

3 monomers are involved in 10 short contacts:

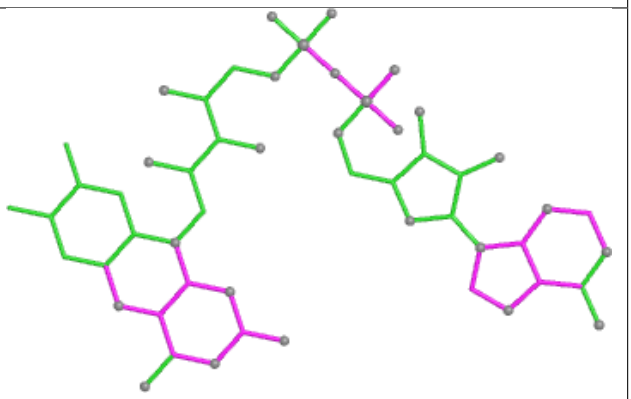
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	FAD	2	0
2	C	1001	FAD	3	0
2	B	1001	FAD	5	0

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.

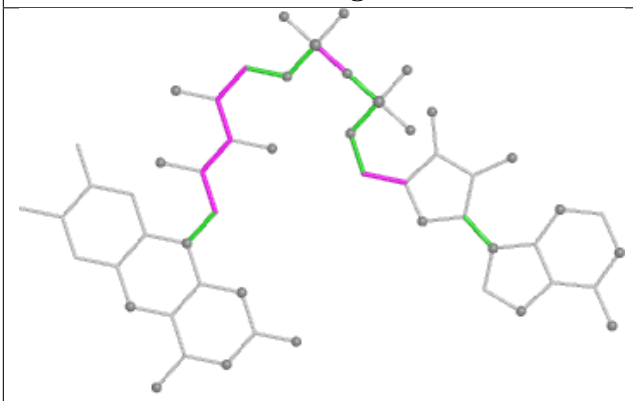
Ligand FAD A 1001



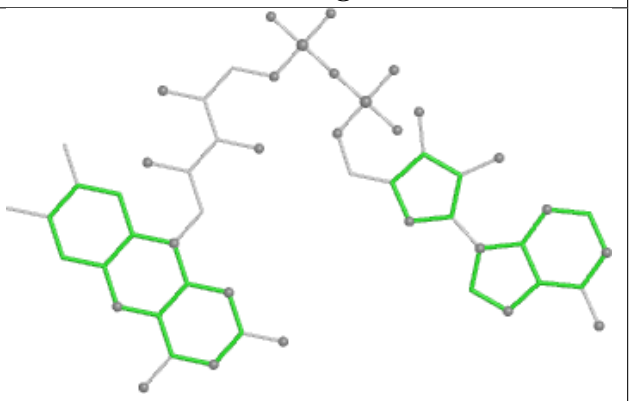
Bond lengths



Bond angles

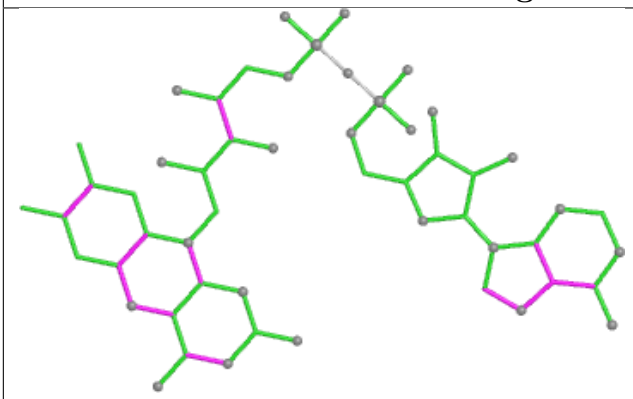


Torsions

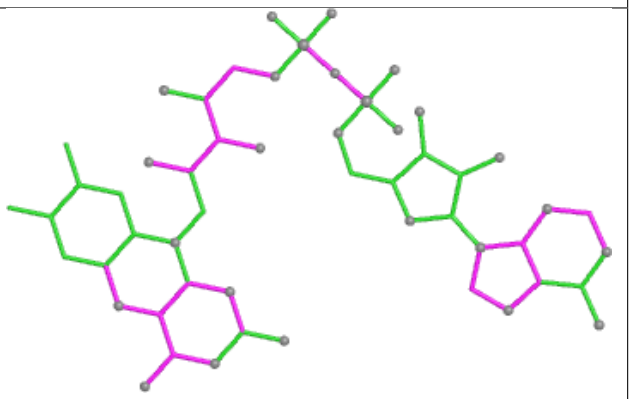


Rings

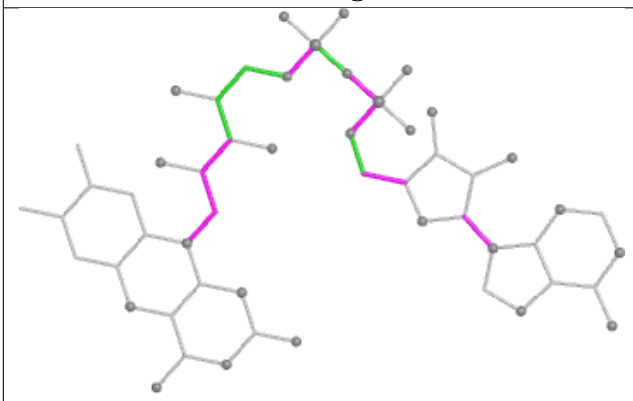
Ligand FAD C 1001



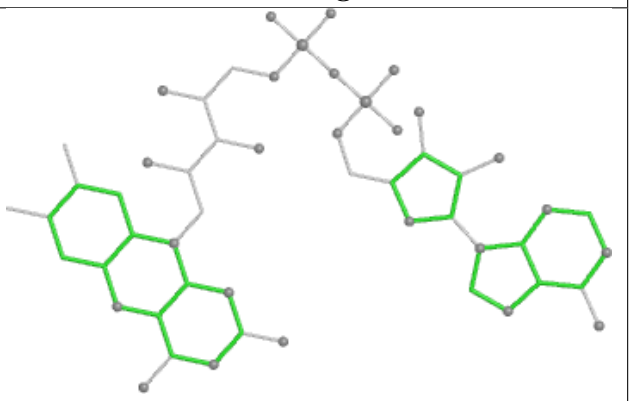
Bond lengths



Bond angles

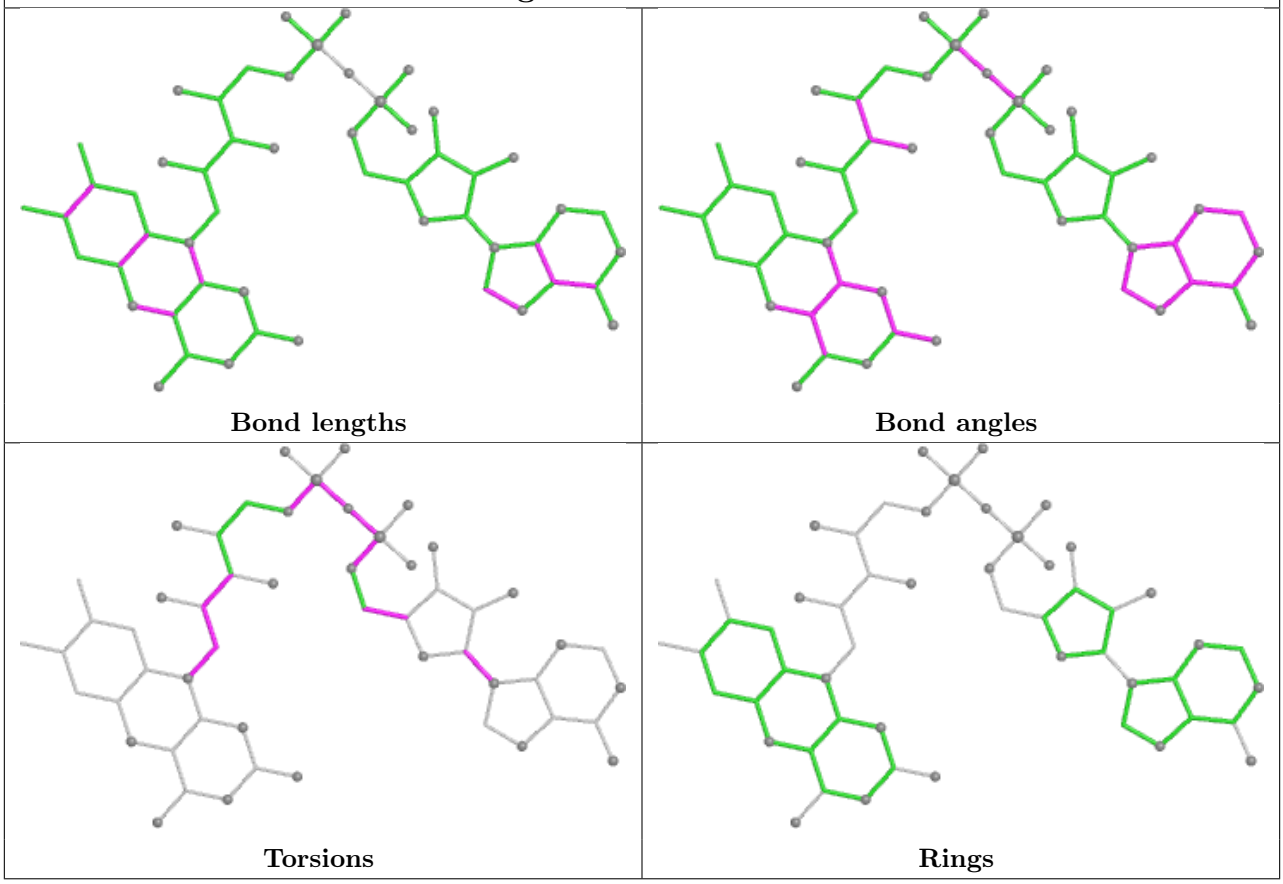


Torsions



Rings

Ligand FAD B 1001



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	321/335 (95%)	0.46	13 (4%)	42	37	51, 86, 143, 167	0
1	B	332/335 (99%)	0.53	11 (3%)	49	43	61, 95, 130, 151	0
1	C	329/335 (98%)	0.31	8 (2%)	59	54	46, 81, 117, 142	0
All	All	982/1005 (97%)	0.43	32 (3%)	49	43	46, 88, 132, 167	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	ARG	5.3
1	B	327	ALA	4.6
1	A	262	VAL	4.6
1	B	254	ILE	3.6
1	A	279	PHE	3.5
1	B	328	PHE	3.2
1	A	310	VAL	3.2
1	C	115	HIS	2.9
1	A	265	VAL	2.7
1	A	254	ILE	2.6
1	A	264	ALA	2.6
1	A	263	GLN	2.6
1	B	280	ILE	2.6
1	A	112	ALA	2.6
1	A	280	ILE	2.5
1	C	64	SER	2.4
1	C	327	ALA	2.4
1	C	269	THR	2.4
1	B	117	LEU	2.3
1	A	285	ASP	2.3
1	B	144	PRO	2.3
1	C	182	ARG	2.3
1	B	252	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	-3	HIS	2.2
1	A	250	ILE	2.2
1	B	149	ALA	2.1
1	C	183	LYS	2.1
1	C	286	ALA	2.1
1	B	171	THR	2.0
1	B	146	VAL	2.0
1	C	180	GLU	2.0
1	B	-2	HIS	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 oligosaccharides 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, 95th 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	1001	53/53	0.82	0.11	55,70,84,91	0
2	FAD	A	1001	53/53	0.89	0.09	32,57,86,92	0
5	CL	A	1007	1/1	0.90	0.11	64,64,64,64	0
5	CL	A	1006	1/1	0.91	0.17	58,58,58,58	0
5	CL	B	1004	1/1	0.91	0.09	58,58,58,58	0
2	FAD	C	1001	53/53	0.92	0.09	42,52,78,80	0
5	CL	B	1003	1/1	0.93	0.17	44,44,44,44	0
5	CL	A	1005	1/1	0.93	0.12	51,51,51,51	0
5	CL	C	1005	1/1	0.93	0.09	59,59,59,59	0
5	CL	C	1007	1/1	0.93	0.12	60,60,60,60	0
5	CL	C	1006	1/1	0.94	0.17	62,62,62,62	0
5	CL	A	1008	1/1	0.94	0.10	57,57,57,57	0
4	IOD	A	1004	1/1	0.95	0.13	75,75,75,75	0
5	CL	C	1004	1/1	0.97	0.06	63,63,63,63	0

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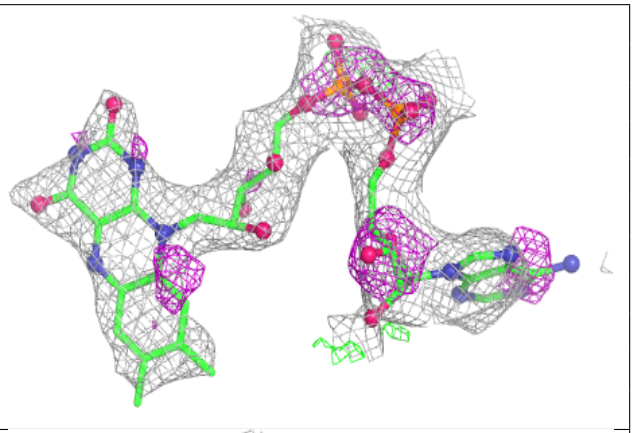
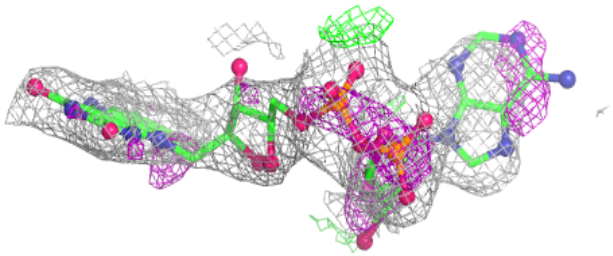
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	IOD	C	1003	1/1	0.97	0.05	65,65,65,65	1
3	FES	A	1002	4/4	0.98	0.04	47,52,52,55	0
4	IOD	A	1003	1/1	0.98	0.10	73,73,73,73	0
6	NI	A	1009	1/1	0.98	0.04	61,61,61,61	0
3	FES	B	1002	4/4	0.99	0.04	45,49,54,54	0
3	FES	C	1002	4/4	0.99	0.04	42,44,50,52	0

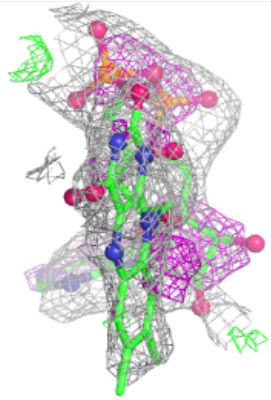
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 1001:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

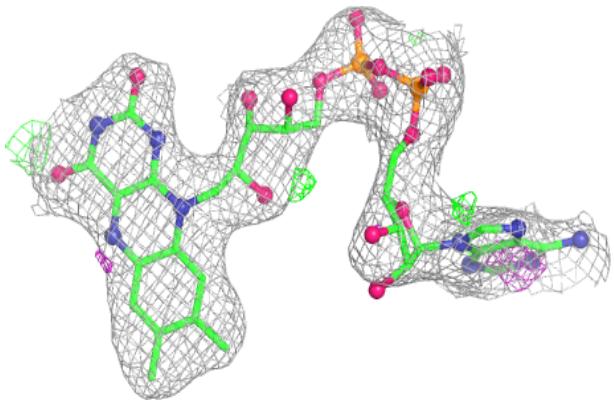


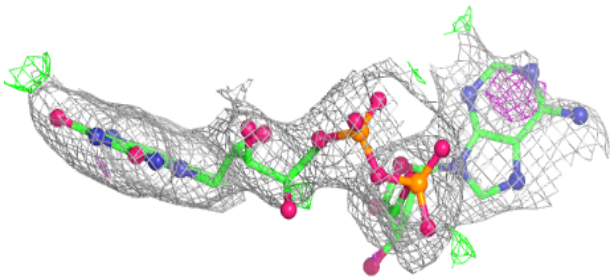


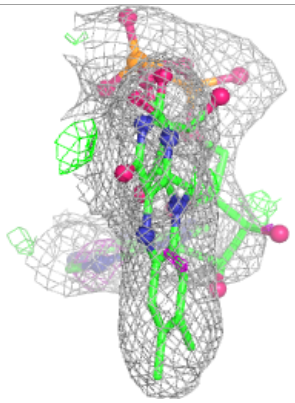


Electron density around FAD A 1001:

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

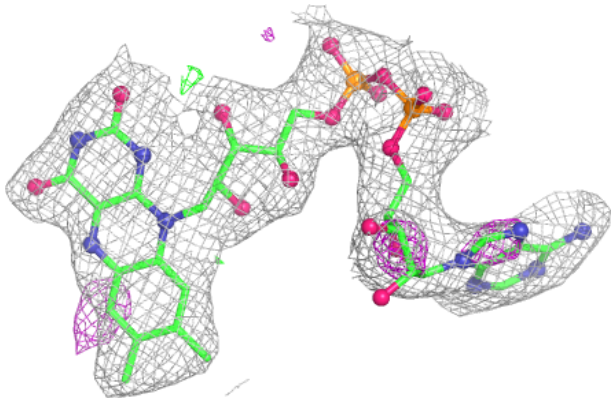


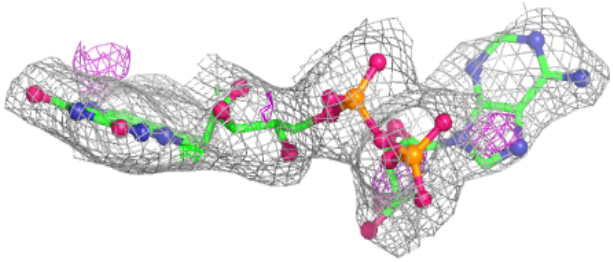


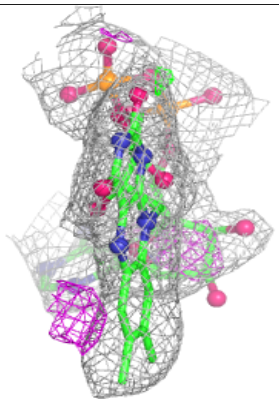


Electron density around FAD C 1001:

$2mF_o$-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.