Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 11:32 AM EDT

PDB ID	:	1ZPT
Title	:	Escherichia coli Methylenetetrahydrofolate Reductase (reduced) complexed with NADH, pH 7.25
Authors	:	Pejchal, R.; Sargeant, R.; Ludwig, M.L.
Deposited on	:	2005-05-17
Resolution	:	1.95 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:

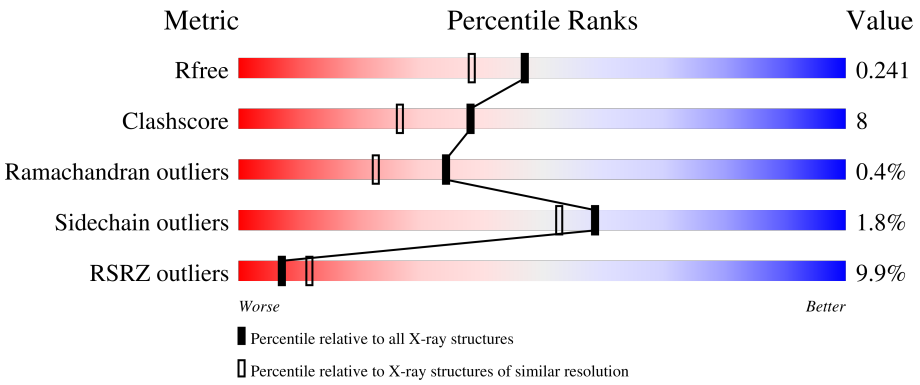
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	304	22% 68% 21% 11%
1	B	304	4% 84% 9% • 6%
1	C	304	% 76% 11% 13%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6953 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 5,10-methylenetetrahydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	271	2068	1314	359	384	11	0	0	0
1	B	285	2184	1380	379	414	11	3	0	0
1	C	265	2064	1310	358	385	11	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	LEU	-	cloning artifact	UNP P00394
A	298	GLU	-	cloning artifact	UNP P00394
A	299	HIS	-	expression tag	UNP P00394
A	300	HIS	-	expression tag	UNP P00394
A	301	HIS	-	expression tag	UNP P00394
A	302	HIS	-	expression tag	UNP P00394
A	303	HIS	-	expression tag	UNP P00394
A	304	HIS	-	expression tag	UNP P00394
B	297	LEU	-	cloning artifact	UNP P00394
B	298	GLU	-	cloning artifact	UNP P00394
B	299	HIS	-	expression tag	UNP P00394
B	300	HIS	-	expression tag	UNP P00394
B	301	HIS	-	expression tag	UNP P00394
B	302	HIS	-	expression tag	UNP P00394
B	303	HIS	-	expression tag	UNP P00394
B	304	HIS	-	expression tag	UNP P00394
C	297	LEU	-	cloning artifact	UNP P00394
C	298	GLU	-	cloning artifact	UNP P00394
C	299	HIS	-	expression tag	UNP P00394
C	300	HIS	-	expression tag	UNP P00394
C	301	HIS	-	expression tag	UNP P00394
C	302	HIS	-	expression tag	UNP P00394
C	303	HIS	-	expression tag	UNP P00394

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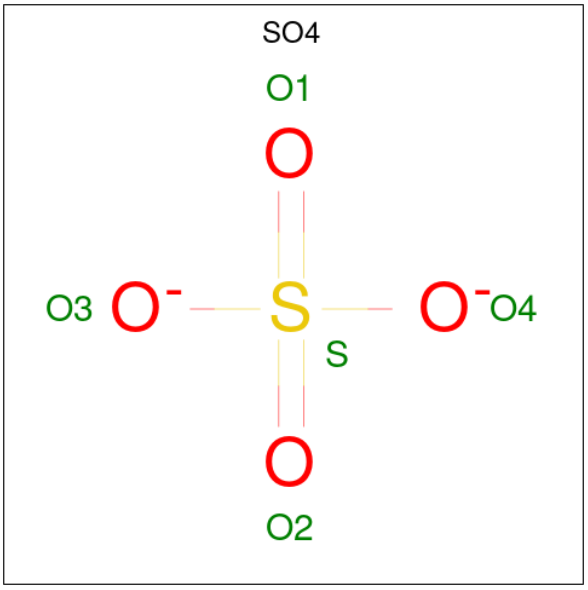
Chain	Residue	Modelled	Actual	Comment	Reference
C	304	HIS	-	expression tag	UNP P00394

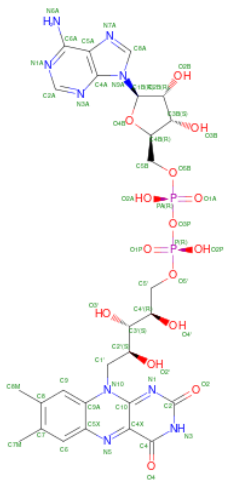
- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			
2	B	1	Total	O	S		0	0
			5	4	1			
2	C	1	Total	O	S		0	0
			5	4	1			

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

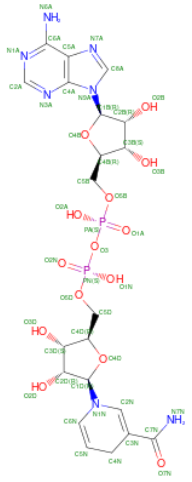
FAD



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

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

NAI



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

- Molecule 5 is water.

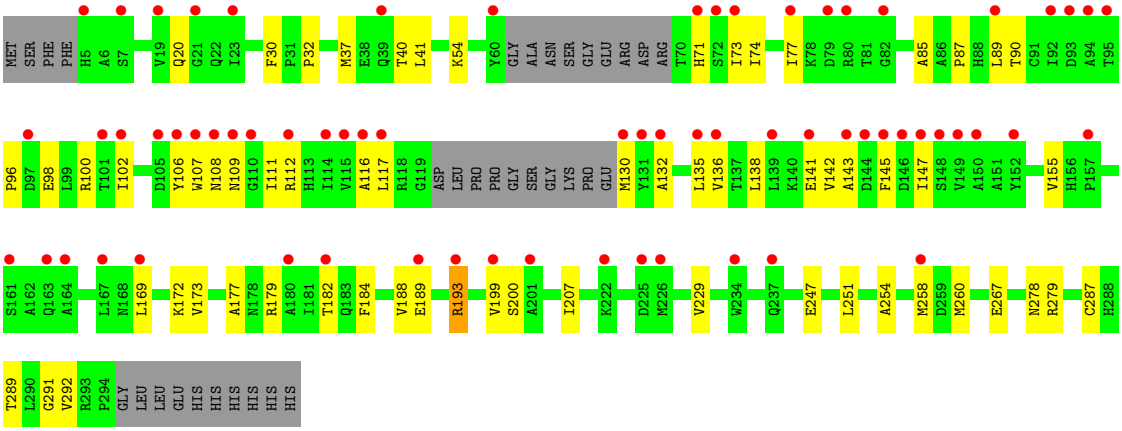
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	42	42	42	0	0
			Total	O		
5	B	128	128	128	0	0
			Total	O		
5	C	156	156	156	0	0

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.

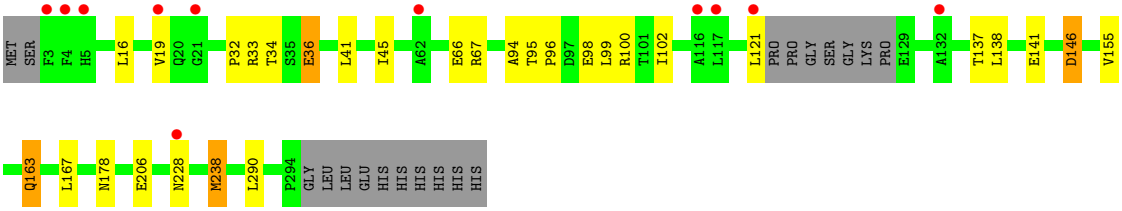
- Molecule 1: 5,10-methylenetetrahydrofolate reductase

Chain A:



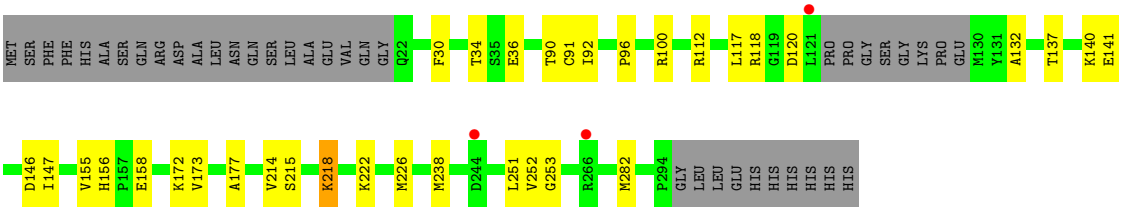
- Molecule 1: 5,10-methylenetetrahydrofolate reductase

Chain B:



- Molecule 1: 5,10-methylenetetrahydrofolate reductase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.61Å 127.73Å 97.83Å 90.00° 121.73° 90.00°	Depositor
Resolution (Å)	19.90 – 1.95 19.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.90-1.95) 97.7 (19.90-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.246 0.211 , 0.241	Depositor DCC
R_{free} test set	3876 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6953	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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, SO4, NAI

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	0.30	0/2109	0.50	0/2866
1	B	0.34	0/2226	0.57	1/3023 (0.0%)
1	C	0.34	0/2106	0.59	1/2856 (0.0%)
All	All	0.33	0/6441	0.55	2/8745 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	146	ASP	N-CA-C	-5.57	95.97	111.00
1	B	146	ASP	N-CA-C	-5.09	97.26	111.00

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	2068	0	1985	53	0
1	B	2184	0	2100	22	0
1	C	2064	0	2017	21	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	31	0	0
3	B	53	0	31	0	0
3	C	53	0	31	0	0
4	A	44	0	27	4	0
4	B	44	0	27	0	0
4	C	44	0	27	2	0
5	A	42	0	0	0	0
5	B	128	0	0	1	0
5	C	156	0	0	0	0
All	All	6953	0	6276	98	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 8.

All (98) 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:258:MET:HE1	1:A:289:THR:HG21	1.40	1.02
1:A:254:ALA:O	1:A:258:MET:HG2	1.61	0.99
1:A:258:MET:HE1	1:A:289:THR:CG2	2.02	0.89
1:A:173:VAL:HA	1:A:177:ALA:HB3	1.64	0.79
1:A:89:LEU:HD23	1:A:135:LEU:HD11	1.67	0.77
1:A:74:ILE:HG13	1:A:87:PRO:HB3	1.68	0.74
1:A:258:MET:CE	1:A:289:THR:HG21	2.17	0.72
1:B:16:LEU:O	1:B:19:VAL:HG12	1.92	0.70
1:A:138:LEU:O	1:A:142:VAL:HG23	1.93	0.68
1:C:112:ARG:HG2	1:C:112:ARG:HH21	1.60	0.67
1:B:34:THR:OG1	1:B:36:GLU:HG2	1.97	0.65
1:B:146:ASP:HA	1:B:178:ASN:HD21	1.60	0.65
1:C:238:MET:HG3	1:C:252:VAL:HG11	1.79	0.64
1:B:137:THR:O	1:B:141:GLU:HG3	1.97	0.64
1:A:247:GLU:H	1:A:247:GLU:CD	2.01	0.63
1:C:156:HIS:CD2	1:C:158:GLU:H	2.18	0.62
1:A:189:GLU:HB3	1:A:193:ARG:HH21	1.65	0.61
1:A:106:TYR:HB3	1:A:111:ILE:HB	1.83	0.61
1:A:258:MET:HE1	1:A:289:THR:CB	2.30	0.60
1:B:67:ARG:HG2	1:B:67:ARG:HH21	1.67	0.59
1:A:100:ARG:HG2	1:A:138:LEU:HD21	1.83	0.59
1:A:258:MET:HE1	1:A:289:THR:OG1	2.03	0.58
1:A:32:PRO:HB3	1:A:37:MET:HG3	1.86	0.58
4:A:895:NAI:O5D	4:A:895:NAI:H6N	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PRO:HD3	1:A:41:LEU:HD22	1.85	0.57
1:A:147:ILE:HD12	1:A:147:ILE:N	2.20	0.57
1:B:32:PRO:HD3	1:B:41:LEU:HD22	1.86	0.56
1:A:73:ILE:HD12	1:A:73:ILE:H	1.70	0.56
1:C:137:THR:O	1:C:141:GLU:HG3	2.05	0.56
1:A:258:MET:HA	1:A:258:MET:HE3	1.89	0.55
1:A:138:LEU:HA	1:A:141:GLU:HG2	1.88	0.55
1:A:54:LYS:HE3	1:A:179:ARG:HH12	1.73	0.54
1:A:73:ILE:HD12	1:A:73:ILE:N	2.22	0.54
1:C:222:LYS:O	1:C:226:MET:HG3	2.08	0.54
1:B:238:MET:HA	1:B:238:MET:CE	2.39	0.53
1:C:120:ASP:OD2	4:C:897:NAI:H4D	2.09	0.53
1:A:143:ALA:HB3	1:A:145:PHE:CE1	2.43	0.53
1:C:238:MET:HG3	1:C:252:VAL:CG1	2.39	0.52
1:B:95:THR:OG1	1:B:98:GLU:HG3	2.08	0.52
1:B:163:GLN:HE21	1:B:163:GLN:H	1.57	0.52
1:C:90:THR:HA	1:C:117:LEU:O	2.10	0.52
1:B:121:LEU:HD22	1:B:121:LEU:H	1.75	0.52
1:C:92:ILE:HG12	1:C:118:ARG:O	2.10	0.52
1:A:30:PHE:HB3	4:A:895:NAI:O2B	2.09	0.51
1:C:132:ALA:HB3	1:C:172:LYS:HD3	1.92	0.51
1:A:107:TRP:HB2	1:A:145:PHE:CZ	2.46	0.51
1:B:36:GLU:H	1:B:36:GLU:CD	2.14	0.51
1:B:163:GLN:H	1:B:163:GLN:NE2	2.09	0.51
1:A:98:GLU:O	1:A:102:ILE:HG12	2.10	0.51
1:A:90:THR:HA	1:A:117:LEU:O	2.11	0.50
1:A:132:ALA:HB3	1:A:172:LYS:HD3	1.94	0.50
1:A:199:VAL:HG23	1:A:200:SER:N	2.26	0.50
1:C:140:LYS:HD3	1:C:147:ILE:HD12	1.94	0.50
1:B:96:PRO:O	1:B:100:ARG:HG3	2.12	0.49
1:A:96:PRO:O	1:A:100:ARG:HG3	2.12	0.49
1:A:138:LEU:C	1:A:138:LEU:HD23	2.33	0.49
1:B:121:LEU:HD22	1:B:121:LEU:N	2.27	0.49
1:B:33:ARG:HD3	5:B:567:HOH:O	2.13	0.49
1:C:156:HIS:HD2	1:C:158:GLU:H	1.61	0.48
1:A:135:LEU:O	1:A:135:LEU:HD13	2.14	0.48
1:A:251:LEU:HD23	1:C:251:LEU:HD23	1.96	0.47
1:A:247:GLU:CD	1:A:247:GLU:N	2.68	0.47
1:C:112:ARG:HG2	1:C:112:ARG:NH2	2.27	0.47
1:C:215:SER:HB3	1:C:282:MET:SD	2.54	0.47
1:A:188:VAL:HG22	1:A:260:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:CYS:HB3	1:A:292:VAL:HB	1.97	0.46
1:B:138:LEU:C	1:B:138:LEU:HD23	2.35	0.46
1:B:16:LEU:HD11	1:B:290:LEU:HD23	1.98	0.46
1:A:138:LEU:O	1:A:141:GLU:HG2	2.16	0.46
1:C:34:THR:OG1	1:C:36:GLU:HG2	2.16	0.46
1:A:40:THR:HG21	1:A:279:ARG:HH11	1.80	0.46
1:B:94:ALA:HB3	1:B:99:LEU:HD21	1.98	0.45
1:A:41:LEU:HD13	1:A:278:ASN:CG	2.37	0.45
1:A:108:ASN:C	1:A:109:ASN:HD22	2.21	0.44
1:A:116:ALA:HB1	1:A:135:LEU:HD12	2.00	0.44
4:A:895:NAI:H2B	4:A:895:NAI:H42N	2.00	0.43
1:A:73:ILE:O	1:A:77:ILE:HG13	2.19	0.43
1:A:182:THR:CG2	1:A:207:ILE:HG22	2.48	0.43
1:B:32:PRO:HD3	1:B:41:LEU:CD2	2.49	0.43
1:C:218:LYS:HA	1:C:218:LYS:HE3	2.00	0.42
1:A:107:TRP:HB2	1:A:145:PHE:CE2	2.54	0.42
1:B:41:LEU:O	1:B:45:ILE:HG12	2.19	0.42
1:A:267:GLU:HA	1:A:267:GLU:OE1	2.20	0.42
1:C:96:PRO:O	1:C:100:ARG:HG3	2.18	0.42
1:A:169:LEU:O	1:A:173:VAL:HG23	2.20	0.42
1:A:184:PHE:CE1	1:A:229:VAL:HG11	2.55	0.42
1:B:67:ARG:NH2	1:B:102:ILE:HD11	2.34	0.41
1:A:20:GLN:HA	1:A:291:GLY:HA3	2.01	0.41
1:A:193:ARG:HG2	1:A:193:ARG:HH11	1.85	0.41
4:A:895:NAI:O5B	4:A:895:NAI:H8A	2.20	0.41
1:C:30:PHE:HB3	4:C:897:NAI:O2B	2.20	0.41
1:B:33:ARG:HH12	1:B:66:GLU:CD	2.22	0.41
1:C:173:VAL:HA	1:C:177:ALA:HB3	2.02	0.41
1:A:73:ILE:H	1:A:73:ILE:CD1	2.32	0.41
1:A:74:ILE:HG23	1:A:85:ALA:HB3	2.03	0.41
1:A:136:VAL:HG13	1:A:147:ILE:HG21	2.02	0.41
1:A:116:ALA:CB	1:A:135:LEU:HD12	2.51	0.41
1:C:214:VAL:O	1:C:253:GLY:HA3	2.21	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	265/304 (87%)	259 (98%)	5 (2%)	1 (0%)	34	22
1	B	281/304 (92%)	278 (99%)	2 (1%)	1 (0%)	34	22
1	C	261/304 (86%)	253 (97%)	7 (3%)	1 (0%)	34	22
All	All	807/912 (88%)	790 (98%)	14 (2%)	3 (0%)	34	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	VAL
1	B	155	VAL
1	C	155	VAL

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	210/258 (81%)	206 (98%)	4 (2%)	57	50
1	B	225/258 (87%)	219 (97%)	6 (3%)	44	34
1	C	217/258 (84%)	215 (99%)	2 (1%)	78	77
All	All	652/774 (84%)	640 (98%)	12 (2%)	59	53

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	112	ARG
1	A	130	MET
1	A	193	ARG
1	B	36	GLU
1	B	163	GLN
1	B	167	LEU
1	B	206	GLU
1	B	228	ASN
1	B	238	MET
1	C	91	CYS
1	C	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	43	ASN
1	A	108	ASN
1	A	109	ASN
1	A	178	ASN
1	A	228	ASN
1	B	14	GLN
1	B	20	GLN
1	B	163	GLN
1	B	178	ASN
1	B	219	GLN
1	B	228	ASN
1	C	156	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	C	397	-	53,58,58	1.67	9 (16%)	68,89,89	1.35	8 (11%)
2	SO4	A	900	-	4,4,4	0.25	0	6,6,6	0.04	0
4	NAI	B	896	-	42,48,48	1.69	8 (19%)	47,73,73	1.22	3 (6%)
3	FAD	B	396	-	53,58,58	1.64	8 (15%)	68,89,89	1.39	14 (20%)
2	SO4	A	899	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	C	902	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	B	901	-	4,4,4	0.26	0	6,6,6	0.06	0
4	NAI	C	897	-	42,48,48	1.67	8 (19%)	47,73,73	1.30	4 (8%)
3	FAD	A	395	-	53,58,58	1.82	11 (20%)	68,89,89	1.56	13 (19%)
4	NAI	A	895	-	42,48,48	1.68	8 (19%)	47,73,73	1.29	4 (8%)

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	C	397	-	-	2/30/50/50	0/6/6/6
4	NAI	B	896	-	-	4/25/72/72	0/5/5/5
3	FAD	B	396	-	-	3/30/50/50	0/6/6/6
4	NAI	C	897	-	-	8/25/72/72	0/5/5/5
3	FAD	A	395	-	-	5/30/50/50	0/6/6/6
4	NAI	A	895	-	-	5/25/72/72	0/5/5/5

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	896	NAI	O4B-C1B	5.56	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	395	FAD	C10-N10	5.54	1.49	1.37
4	C	897	NAI	O4B-C1B	5.53	1.48	1.41
4	A	895	NAI	O4B-C1B	5.51	1.48	1.41
3	C	397	FAD	C4X-N5	5.15	1.40	1.30
3	B	396	FAD	C4X-N5	5.08	1.40	1.30
3	A	395	FAD	C4X-N5	4.99	1.40	1.30
3	A	395	FAD	C9A-N10	4.71	1.49	1.41
3	C	397	FAD	C10-N10	4.49	1.47	1.37
4	B	896	NAI	C4N-C3N	-4.48	1.41	1.49
4	A	895	NAI	C4N-C3N	-4.45	1.41	1.49
4	C	897	NAI	C4N-C3N	-4.45	1.41	1.49
3	B	396	FAD	C10-N10	4.30	1.46	1.37
3	B	396	FAD	C9A-N10	4.21	1.48	1.41
4	B	896	NAI	C6N-C5N	4.05	1.40	1.33
4	C	897	NAI	C6N-C5N	3.98	1.40	1.33
4	A	895	NAI	C6N-C5N	3.96	1.40	1.33
3	A	395	FAD	C9-C9A	3.92	1.46	1.39
3	C	397	FAD	C9A-N10	3.79	1.47	1.41
3	C	397	FAD	C9-C9A	3.59	1.45	1.39
3	B	396	FAD	C6-C5X	3.28	1.45	1.40
3	A	395	FAD	O4B-C1B	3.25	1.45	1.41
3	B	396	FAD	C9-C9A	3.22	1.44	1.39
4	A	895	NAI	C4N-C5N	-3.08	1.40	1.48
3	B	396	FAD	C8-C7	3.08	1.48	1.40
4	C	897	NAI	C4N-C5N	-3.06	1.40	1.48
4	B	896	NAI	C4N-C5N	-3.02	1.41	1.48
3	A	395	FAD	C8-C7	2.94	1.48	1.40
3	A	395	FAD	C5'-C4'	2.90	1.55	1.51
3	A	395	FAD	C6-C5X	2.88	1.44	1.40
4	B	896	NAI	O4D-C1D	2.86	1.48	1.42
3	C	397	FAD	C6-C5X	2.80	1.44	1.40
3	C	397	FAD	C8-C7	2.78	1.47	1.40
3	C	397	FAD	C8A-N7A	-2.73	1.29	1.34
3	A	395	FAD	C1'-C2'	2.70	1.56	1.52
4	A	895	NAI	C7N-C3N	2.54	1.54	1.48
4	B	896	NAI	C7N-C3N	2.51	1.54	1.48
4	A	895	NAI	O4D-C1D	2.46	1.47	1.42
3	A	395	FAD	C8A-N7A	-2.43	1.30	1.34
4	C	897	NAI	C7N-C3N	2.39	1.53	1.48
3	B	396	FAD	C9A-C5X	2.37	1.45	1.41
3	A	395	FAD	C10-N1	2.34	1.38	1.33
3	C	397	FAD	C9A-C5X	2.30	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	897	NAI	O4D-C1D	2.19	1.47	1.42
3	B	396	FAD	C7M-C7	2.18	1.55	1.51
4	C	897	NAI	C6N-N1N	2.15	1.42	1.37
4	A	895	NAI	C2N-C3N	2.14	1.40	1.34
4	A	895	NAI	C6N-N1N	2.12	1.42	1.37
4	B	896	NAI	C6N-N1N	2.12	1.42	1.37
4	B	896	NAI	C2N-C3N	2.04	1.40	1.34
4	C	897	NAI	C2N-C3N	2.04	1.40	1.34
3	C	397	FAD	C2'-C3'	2.01	1.57	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	896	NAI	N3A-C2A-N1A	-5.24	120.48	128.68
4	A	895	NAI	N3A-C2A-N1A	-5.20	120.55	128.68
4	C	897	NAI	N3A-C2A-N1A	-5.18	120.58	128.68
3	A	395	FAD	C5'-C4'-C3'	4.82	121.51	112.20
3	A	395	FAD	C9-C9A-N10	3.85	127.05	121.84
3	A	395	FAD	C9A-C5X-N5	3.68	126.43	122.43
3	C	397	FAD	C9-C9A-N10	3.56	126.64	121.84
3	C	397	FAD	C5X-C9A-N10	-3.46	114.39	117.95
4	A	895	NAI	PN-O3-PA	-3.44	121.01	132.83
3	A	395	FAD	C5X-C9A-N10	-3.42	114.42	117.95
4	C	897	NAI	PN-O3-PA	-3.33	121.40	132.83
3	B	396	FAD	O2-C2-N3	3.19	124.85	118.65
4	C	897	NAI	O4D-C1D-N1N	3.17	114.26	108.06
4	B	896	NAI	PN-O3-PA	-3.10	122.20	132.83
3	B	396	FAD	C5X-C9A-N10	-2.87	114.99	117.95
3	A	395	FAD	C4'-C3'-C2'	2.85	119.29	113.36
4	A	895	NAI	O4D-C1D-N1N	2.82	113.57	108.06
3	C	397	FAD	C9A-C5X-N5	2.74	125.42	122.43
3	B	396	FAD	C5'-C4'-C3'	2.73	117.48	112.20
3	B	396	FAD	C9-C9A-N10	2.70	125.48	121.84
3	C	397	FAD	O2-C2-N3	2.67	123.85	118.65
3	B	396	FAD	O5'-C5'-C4'	2.64	116.40	109.36
3	C	397	FAD	O5'-C5'-C4'	2.61	116.33	109.36
3	A	395	FAD	O2'-C2'-C3'	2.54	115.28	109.10
3	B	396	FAD	C9A-C5X-N5	2.49	125.14	122.43
3	B	396	FAD	N3-C2-N1	-2.45	114.57	119.38
4	A	895	NAI	C3N-C2N-N1N	-2.45	119.60	123.10
3	B	396	FAD	C8M-C8-C9	-2.43	114.99	119.49
3	B	396	FAD	C8M-C8-C7	2.43	125.71	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	395	FAD	O5'-C5'-C4'	2.38	115.72	109.36
3	C	397	FAD	N3-C2-N1	-2.38	114.72	119.38
3	B	396	FAD	O5B-C5B-C4B	2.37	117.17	108.99
4	C	897	NAI	C3N-C2N-N1N	-2.37	119.71	123.10
3	B	396	FAD	C10-N1-C2	2.36	121.61	116.90
3	B	396	FAD	O3'-C3'-C4'	2.34	114.46	108.81
3	C	397	FAD	C8M-C8-C7	2.33	125.51	120.74
3	A	395	FAD	C8M-C8-C7	2.33	125.51	120.74
3	C	397	FAD	C10-N1-C2	2.27	121.45	116.90
4	B	896	NAI	C3N-C2N-N1N	-2.26	119.86	123.10
3	B	396	FAD	C1B-N9A-C4A	-2.23	122.72	126.64
3	A	395	FAD	C7M-C7-C8	2.20	125.24	120.74
3	A	395	FAD	C6-C5X-N5	-2.16	114.74	118.51
3	B	396	FAD	O2'-C2'-C3'	2.09	114.19	109.10
3	A	395	FAD	C7M-C7-C6	-2.07	115.66	119.49
3	A	395	FAD	C8M-C8-C9	-2.05	115.70	119.49
3	A	395	FAD	C4-C4X-N5	-2.02	115.36	118.23

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	895	NAI	C5B-O5B-PA-O1A
4	A	895	NAI	C5B-O5B-PA-O2A
4	B	896	NAI	C5B-O5B-PA-O1A
4	B	896	NAI	C5B-O5B-PA-O2A
4	B	896	NAI	O4D-C1D-N1N-C2N
4	C	897	NAI	C5B-O5B-PA-O1A
4	C	897	NAI	C5B-O5B-PA-O2A
3	A	395	FAD	O4'-C4'-C5'-O5'
3	A	395	FAD	O2'-C2'-C3'-C4'
4	C	897	NAI	O4D-C1D-N1N-C2N
3	B	396	FAD	O2'-C2'-C3'-C4'
4	A	895	NAI	C5B-O5B-PA-O3
4	A	895	NAI	O4D-C1D-N1N-C2N
4	C	897	NAI	C5D-O5D-PN-O1N
3	C	397	FAD	O2'-C2'-C3'-C4'
3	A	395	FAD	PA-O3P-P-O2P
3	B	396	FAD	P-O3P-PA-O1A
3	C	397	FAD	C2'-C3'-C4'-O4'
3	B	396	FAD	P-O3P-PA-O2A
3	A	395	FAD	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
4	B	896	NAI	C5B-O5B-PA-O3
4	C	897	NAI	C5B-O5B-PA-O3
4	C	897	NAI	C5D-O5D-PN-O3
3	A	395	FAD	C5B-O5B-PA-O1A
4	A	895	NAI	C2N-C3N-C7N-N7N
4	C	897	NAI	C5D-O5D-PN-O2N
4	C	897	NAI	C2N-C3N-C7N-N7N

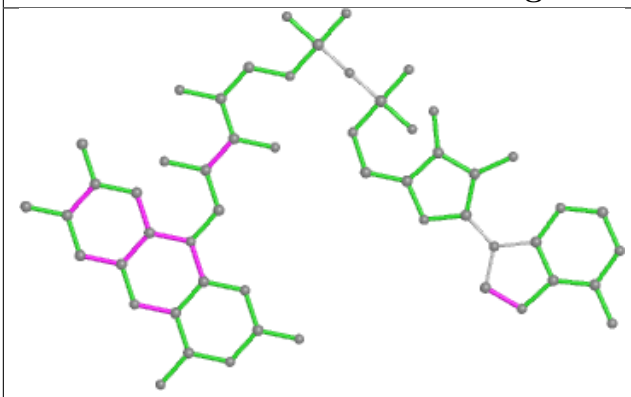
There are no ring outliers.

2 monomers are involved in 6 short contacts:

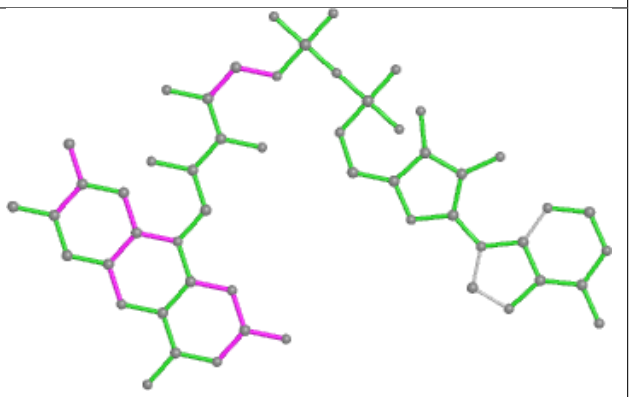
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	897	NAI	2	0
4	A	895	NAI	4	0

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.

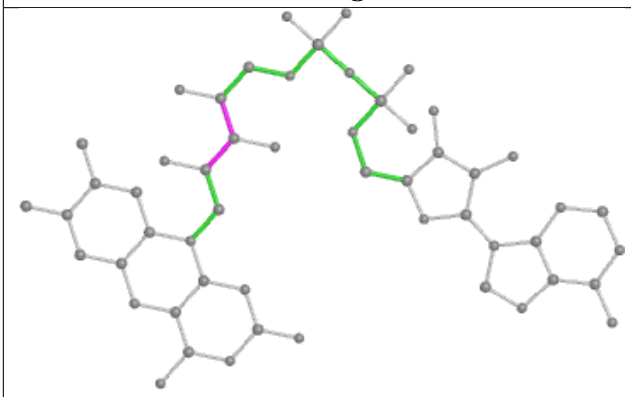
Ligand FAD C 397



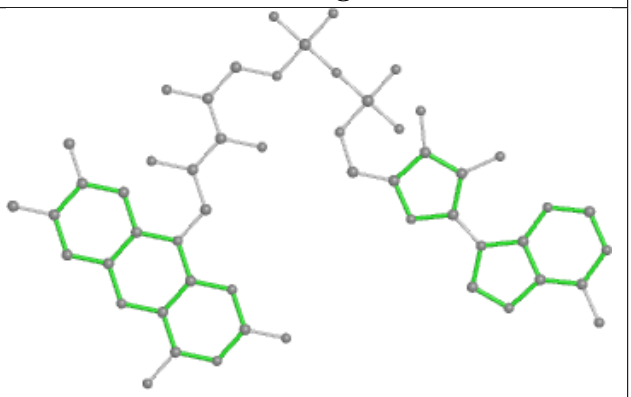
Bond lengths



Bond angles

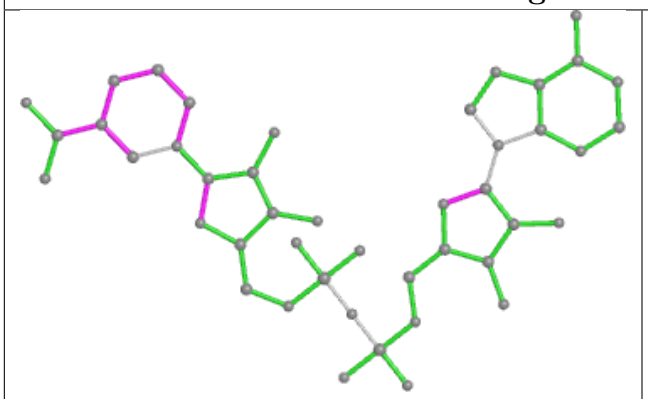


Torsions



Rings

Ligand NAI B 896



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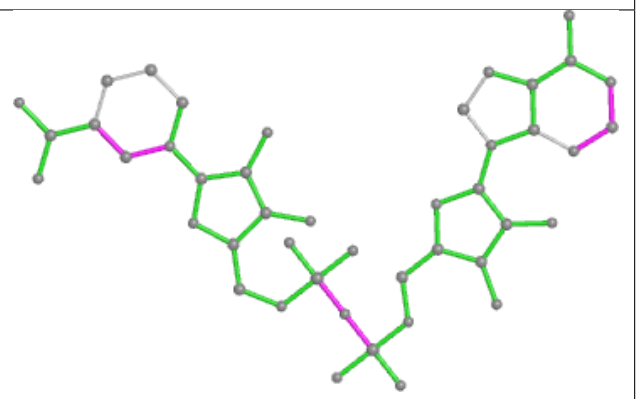
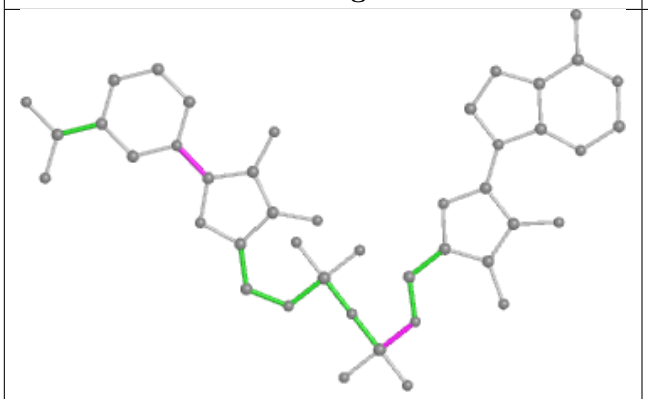
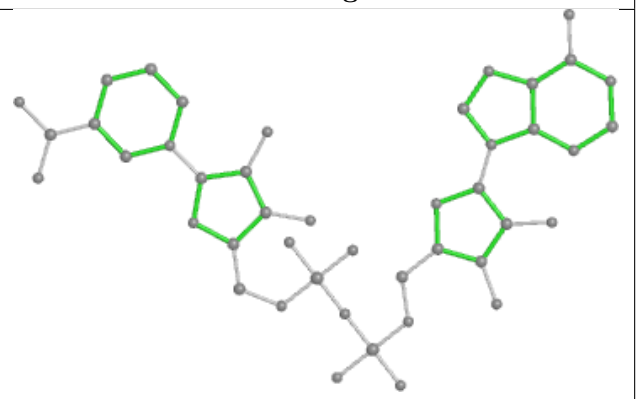


Bond angles

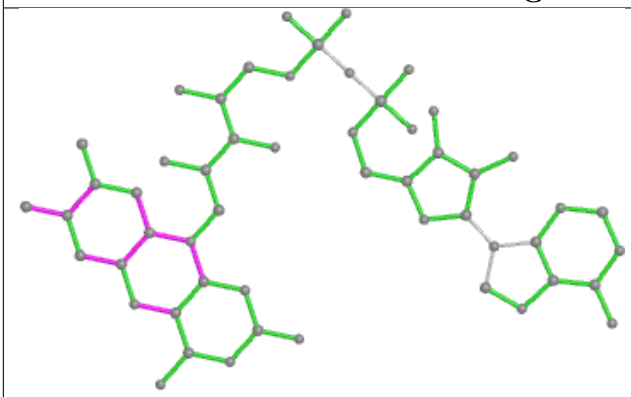


Torsions

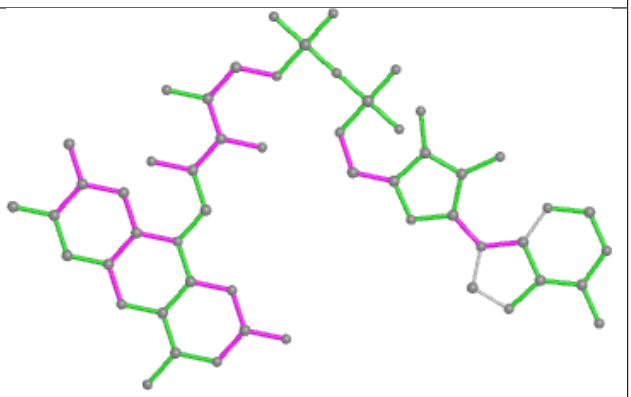


Rings

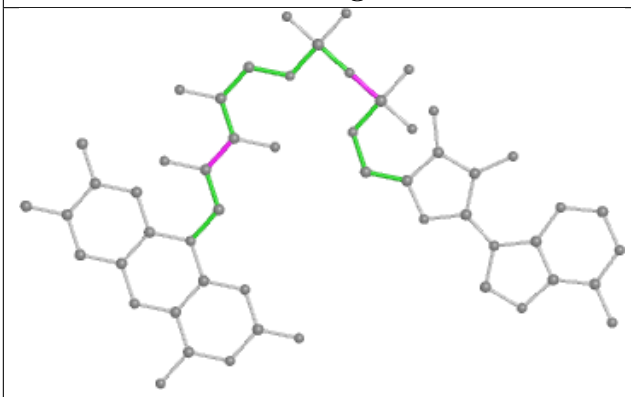
Ligand FAD B 396



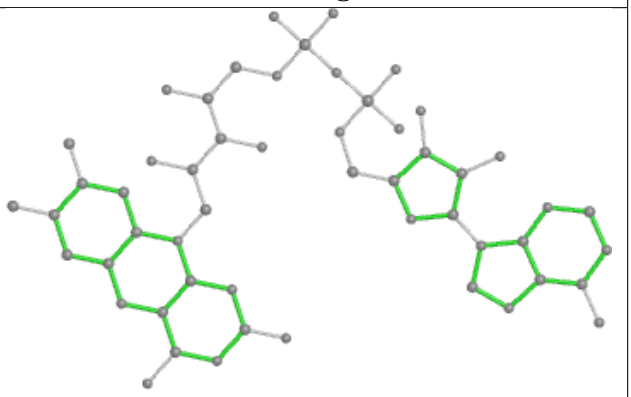
Bond lengths



Bond angles

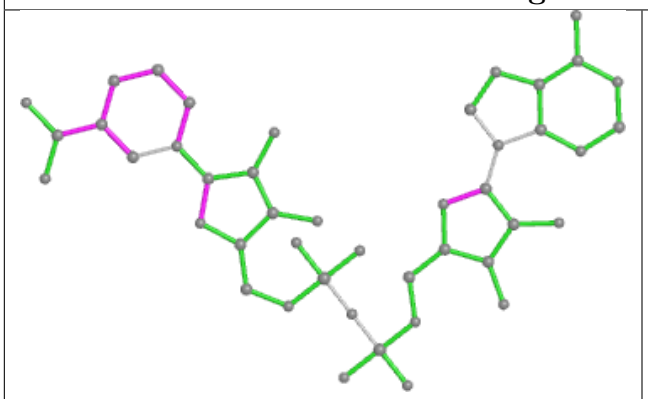


Torsions

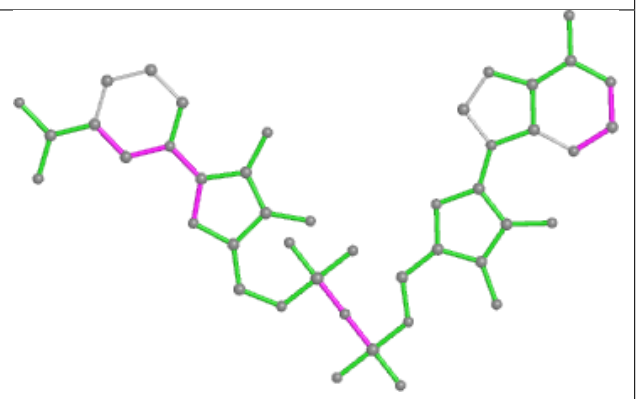


Rings

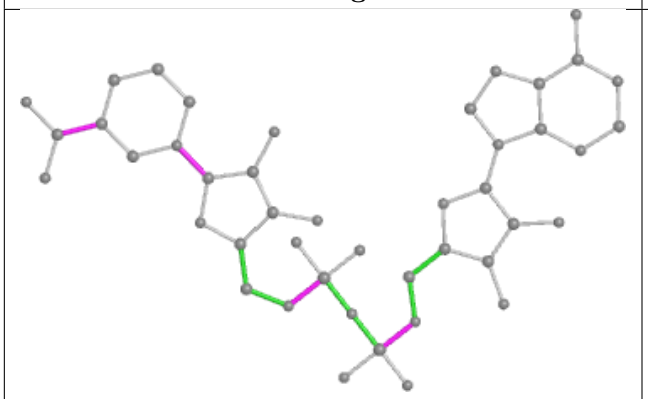
Ligand NAI C 897



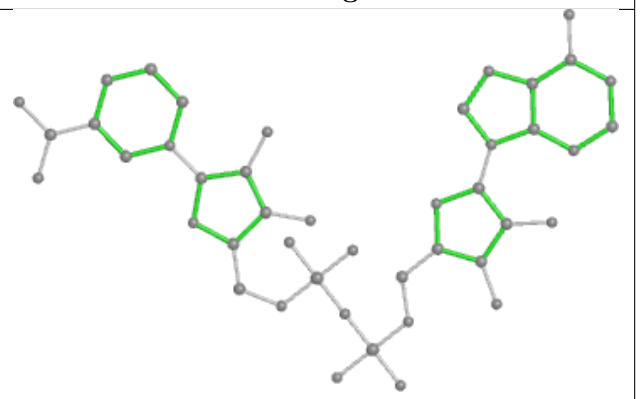
Bond lengths



Bond angles

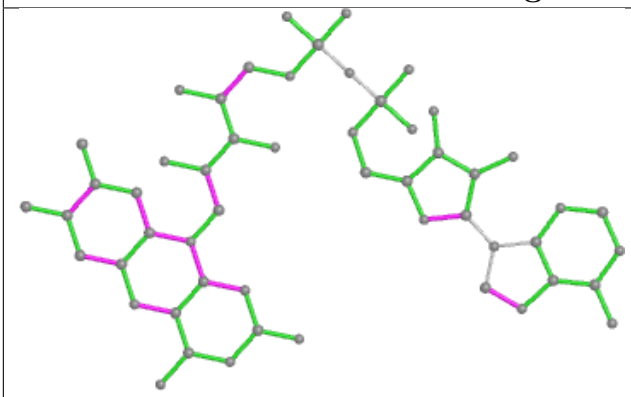


Torsions

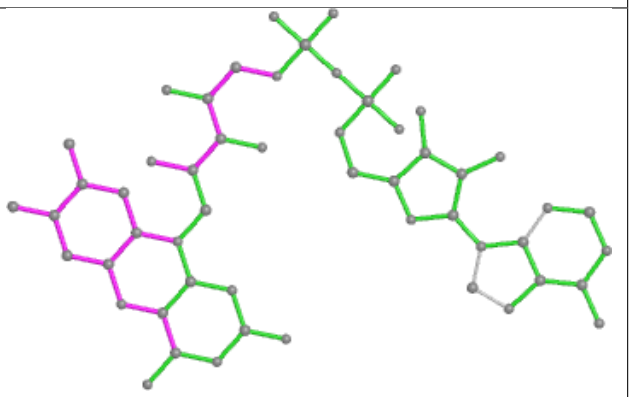


Rings

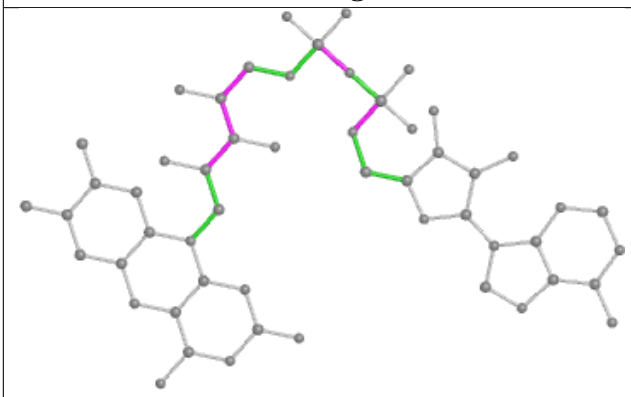
Ligand FAD A 395



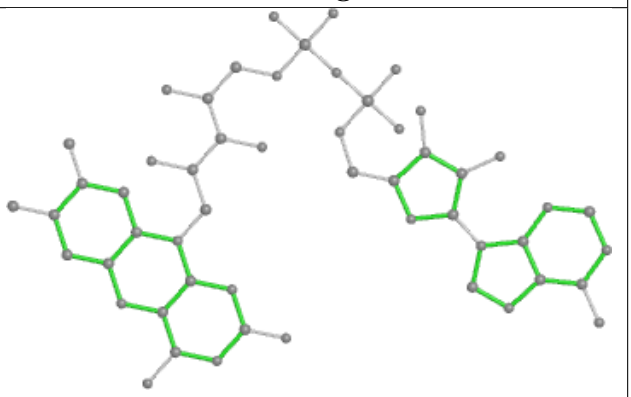
Bond lengths



Bond angles

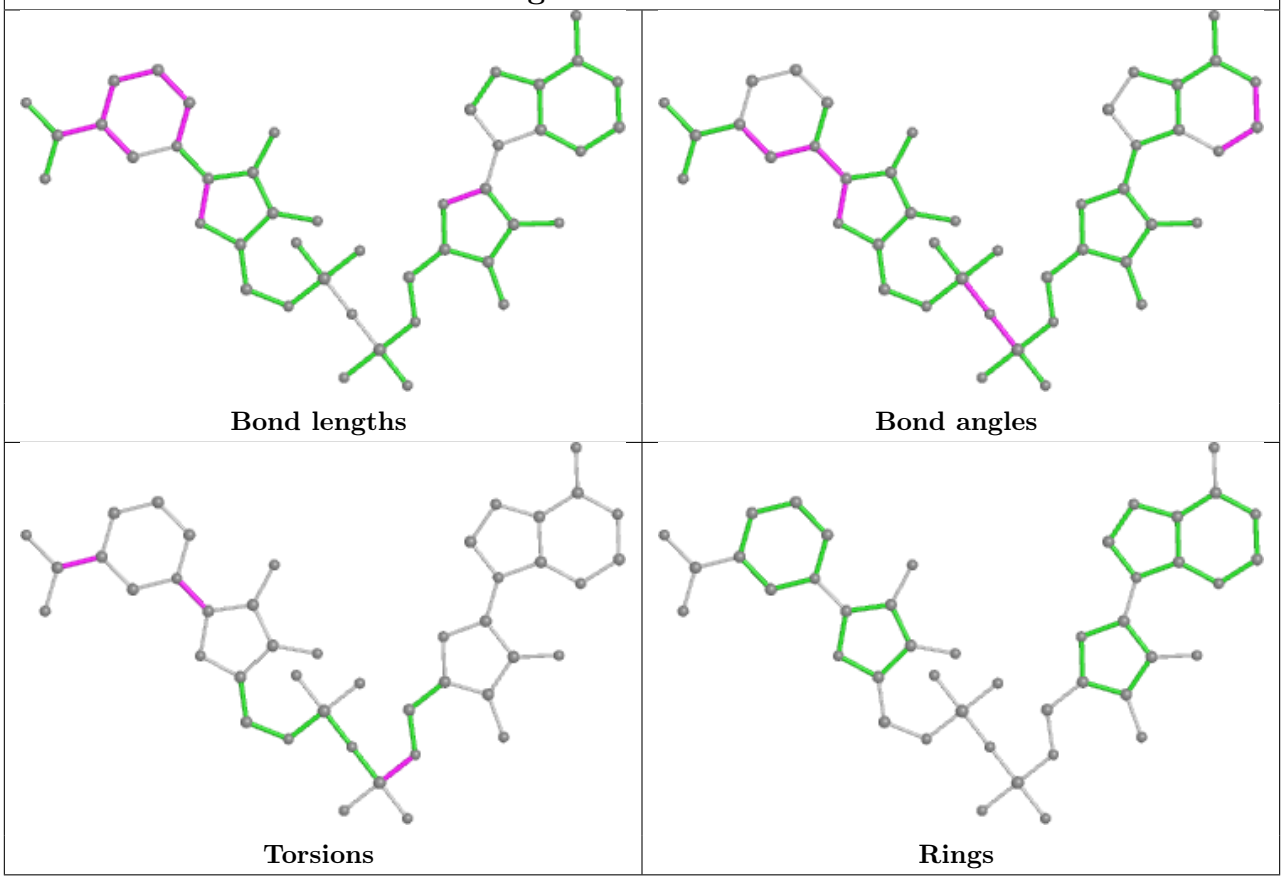


Torsions



Rings

Ligand NAI A 895



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	271/304 (89%)	1.29	67 (24%) 0 0	22, 45, 72, 80	0
1	B	285/304 (93%)	0.26	11 (3%) 39 49	16, 27, 41, 49	1 (0%)
1	C	265/304 (87%)	0.04	3 (1%) 80 85	16, 24, 36, 47	0
All	All	821/912 (90%)	0.53	81 (9%) 7 12	16, 30, 62, 80	1 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	ALA	6.0
1	A	60	TYR	5.9
1	A	93	ASP	5.9
1	A	21	GLY	5.6
1	A	102	ILE	5.4
1	B	121	LEU	5.0
1	A	143	ALA	4.8
1	A	92	ILE	4.8
1	A	226	MET	4.4
1	A	108	ASN	4.4
1	A	144	ASP	4.4
1	A	114	ILE	4.3
1	A	19	VAL	4.3
1	A	146	ASP	4.3
1	B	21	GLY	4.2
1	A	80	ARG	4.1
1	A	141	GLU	4.0
1	A	161	SER	4.0
1	A	112	ARG	3.9
1	A	115	VAL	3.9
1	A	145	PHE	3.8
1	B	3	PHE	3.7
1	B	62	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	107	TRP	3.6
1	A	95	THR	3.6
1	A	147	ILE	3.4
1	C	121	LEU	3.4
1	A	116	ALA	3.4
1	A	89	LEU	3.4
1	A	130	MET	3.4
1	A	135	LEU	3.3
1	A	82	GLY	3.3
1	A	101	THR	3.3
1	A	234	TRP	3.3
1	A	77	ILE	3.2
1	A	71	HIS	3.1
1	A	201	ALA	3.1
1	A	39	GLN	3.0
1	A	109	ASN	3.0
1	A	225	ASP	3.0
1	C	266	ARG	3.0
1	A	131	TYR	3.0
1	B	228	ASN	2.9
1	A	258	MET	2.9
1	A	105	ASP	2.9
1	A	167	LEU	2.8
1	A	106	TYR	2.8
1	B	117	LEU	2.8
1	A	7	SER	2.7
1	A	79	ASP	2.7
1	A	73	ILE	2.7
1	A	139	LEU	2.6
1	A	193	ARG	2.6
1	A	5	HIS	2.6
1	B	19	VAL	2.5
1	A	150	ALA	2.5
1	A	149	VAL	2.5
1	A	132	ALA	2.5
1	B	116	ALA	2.5
1	A	148	SER	2.5
1	A	110	GLY	2.4
1	A	189	GLU	2.4
1	A	237	GLN	2.4
1	A	23	ILE	2.4
1	A	222	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	97	ASP	2.3
1	A	180	ALA	2.3
1	A	169	LEU	2.3
1	B	4	PHE	2.2
1	B	5	HIS	2.2
1	A	136	VAL	2.2
1	A	163	GLN	2.1
1	A	72	SER	2.1
1	A	152	TYR	2.1
1	C	244	ASP	2.1
1	A	117	LEU	2.1
1	A	157	PRO	2.1
1	A	199	VAL	2.1
1	A	164	ALA	2.1
1	A	182	THR	2.0
1	B	132	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	NAI	A	895	44/44	0.55	0.32	72,74,79,79	44
4	NAI	C	897	44/44	0.73	0.20	40,45,55,56	44
4	NAI	B	896	44/44	0.75	0.20	37,46,55,56	44
3	FAD	A	395	53/53	0.80	0.18	39,46,59,60	0
2	SO4	A	900	5/5	0.89	0.19	62,62,62,62	5
2	SO4	B	901	5/5	0.93	0.18	45,46,46,46	5
3	FAD	B	396	53/53	0.94	0.10	21,25,33,33	0

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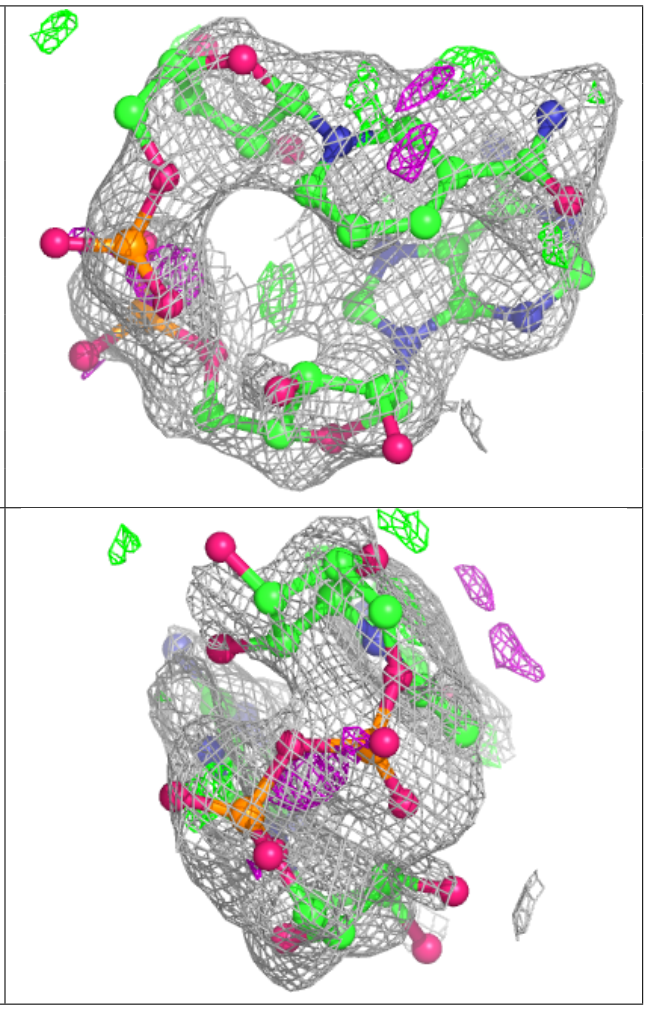
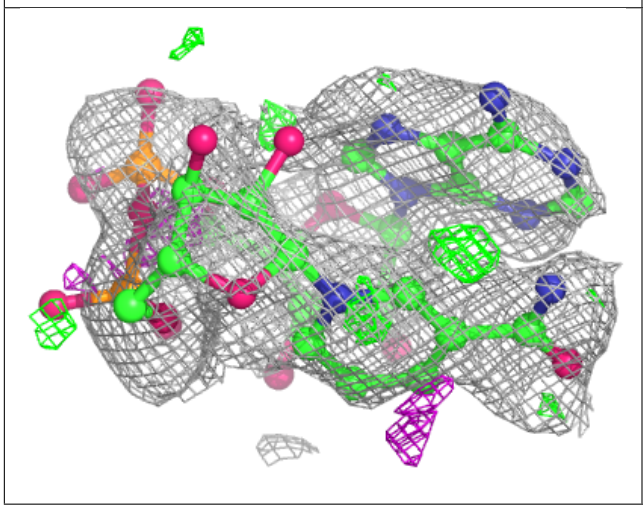
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	902	5/5	0.94	0.15	50,50,51,51	5
2	SO4	A	899	5/5	0.95	0.10	56,56,56,56	5
3	FAD	C	397	53/53	0.96	0.09	18,21,29,29	0

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 NAI A 895:

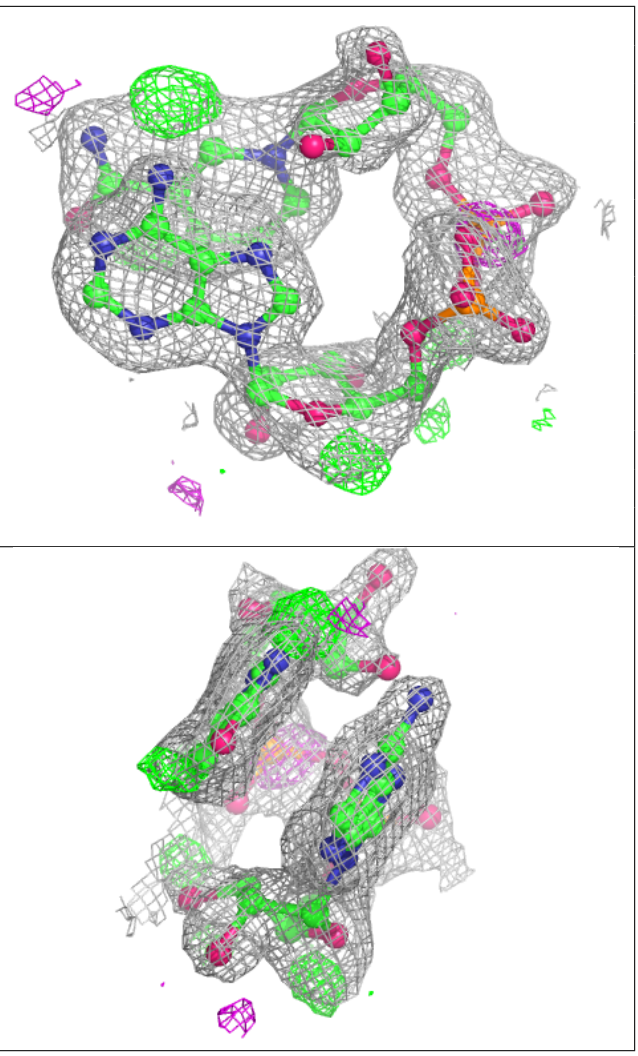
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





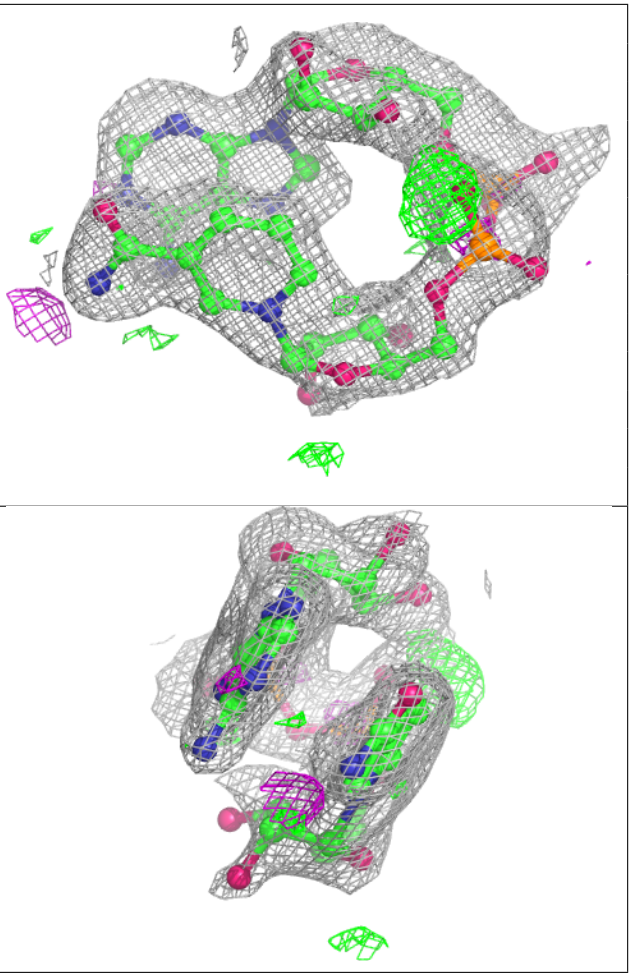
Electron density around NAI C 897:

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



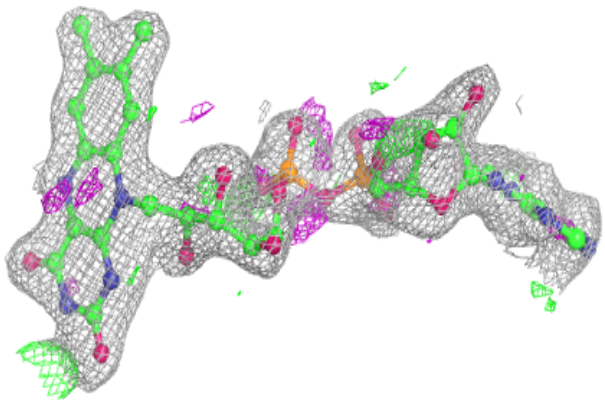
Electron density around NAI B 896:

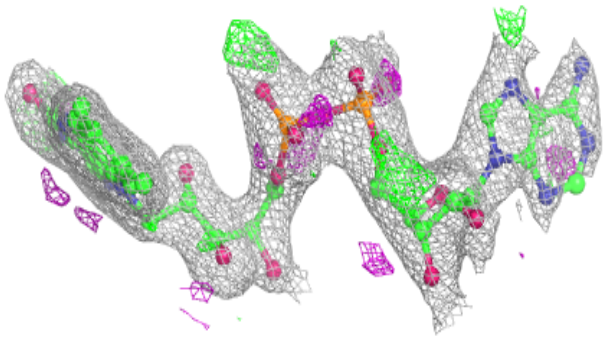
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

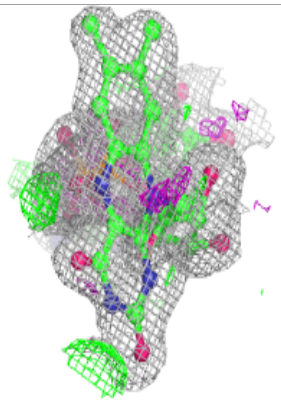


Electron density around FAD A 395:

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

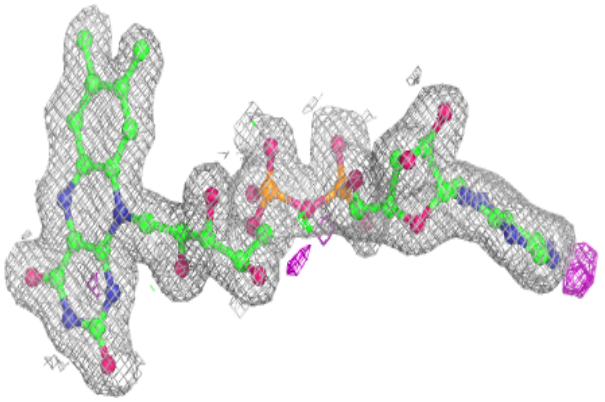


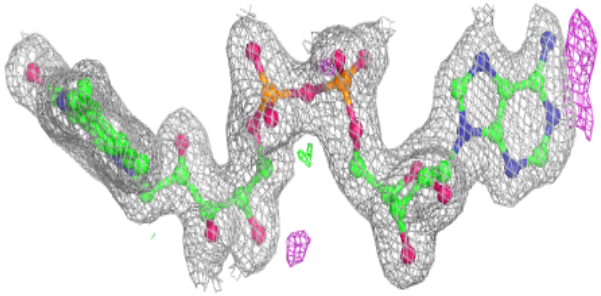


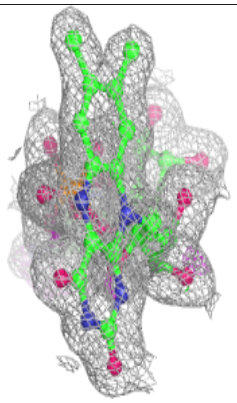


Electron density around FAD B 396:

$2mF_o$-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 397:

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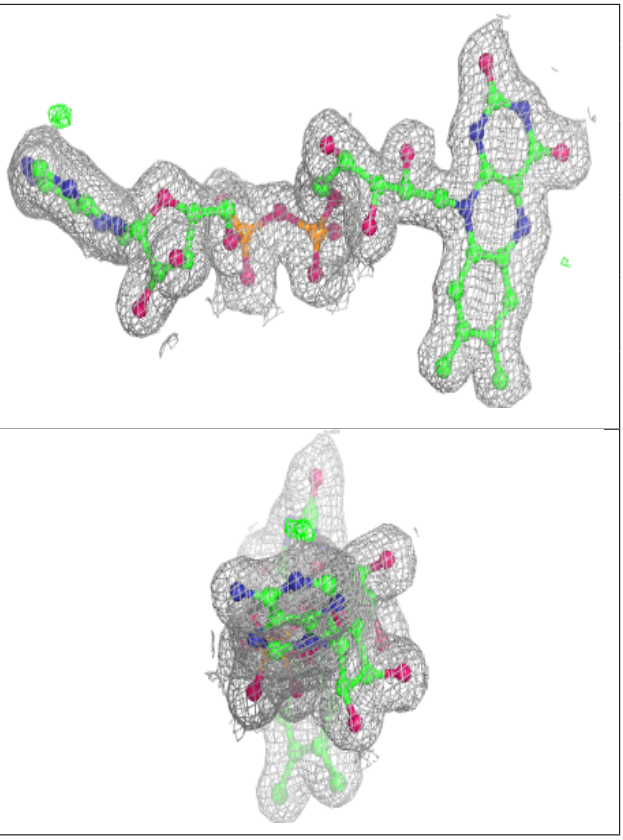
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.