Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 07:34 am GMT

PDB ID	:	2VNK
Title	:	X-RAY STRUCTURE OF THE FERREDOXIN-NADP(H) REDUCTASE FROM RHODOBACTER CAPSULATUS IN COMPLEX WITH NADP. FORM III AT 1.93 ANGSTROMS RESOLUTION
Authors	:	Perez-Dorado, I.; Hermoso, J.A.
Deposited on	:	2008-02-05
Resolution	:	1.93 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:

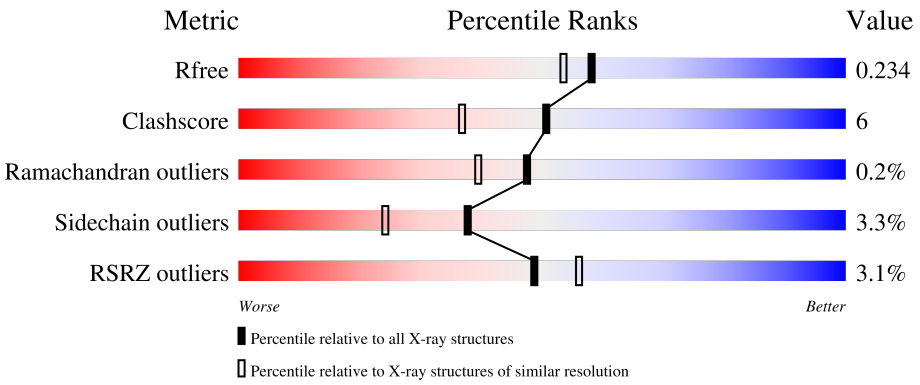
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	272	3% 85% 7% • 6%
1	B	272	2% 81% 10% • 7%
1	C	272	3% 85% 8% • 6%
1	D	272	4% 81% 10% • 7%

2 Entry composition (i)

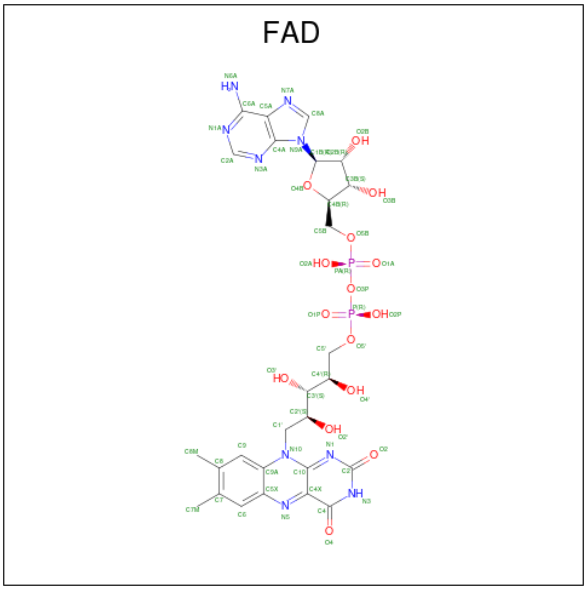
There are 4 unique types of molecules in this entry. The entry contains 9298 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NADPH\:FERREDOXIN REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	257	2031	1297	343	380	11	0	0	0
1	B	254	2009	1284	340	374	11	0	0	0
1	C	257	2031	1297	343	380	11	0	0	0
1	D	254	2009	1284	340	374	11	0	0	0

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

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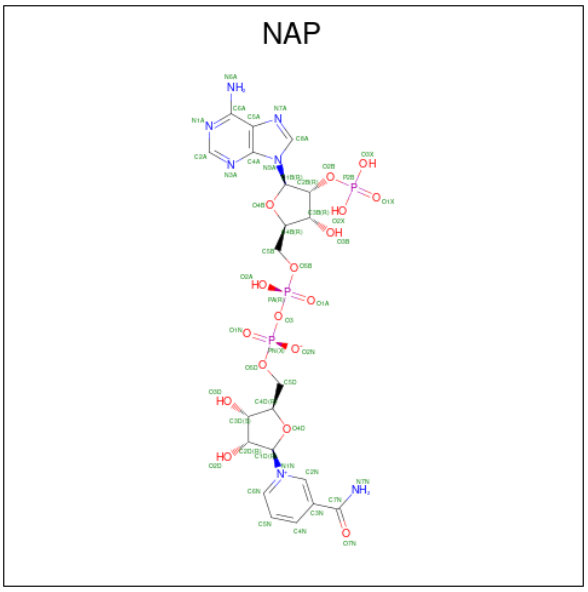
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
2	D	1	53	27	9	15	2	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	B	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	C	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
3	D	1	31	10	5	13	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	221	221	221	0	0
			Total	O		
4	B	215	215	215	0	0
			Total	O		
4	C	236	236	236	0	0

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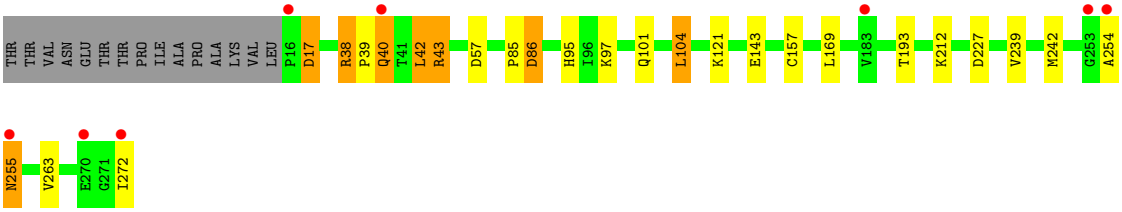
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	210	210	210	0	0

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.

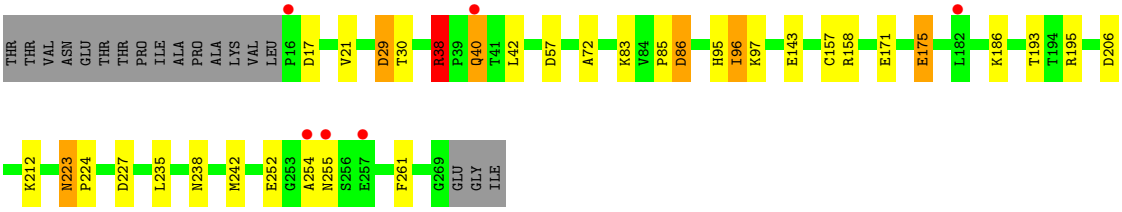
• Molecule 1: NADPH\:FERREDOXIN REDUCTASE

Chain A:



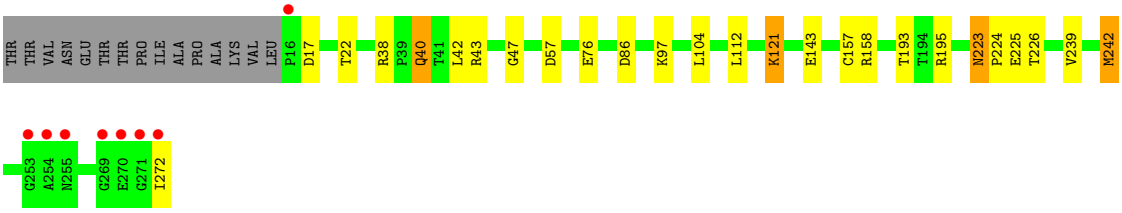
• Molecule 1: NADPH\:FERREDOXIN REDUCTASE

Chain B:



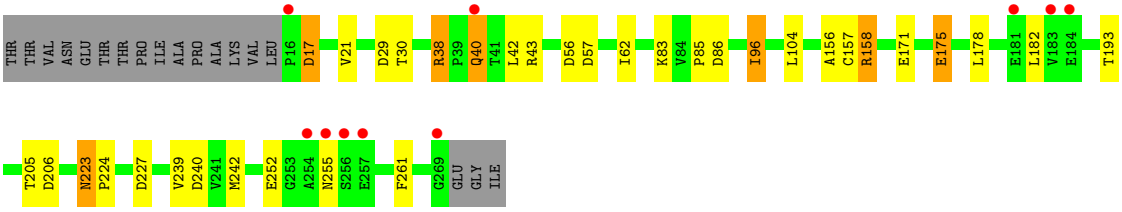
• Molecule 1: NADPH\:FERREDOXIN REDUCTASE

Chain C:



• Molecule 1: NADPH\:FERREDOXIN REDUCTASE

Chain D:


THR
THR
VAL
ASN
GLU
THR
THR
PRO
ILE
ALA
PRO
ALA
LYS
VAL
LEU
P16
D17
V21
D29
T30
R38
P39
Q40
T41
L42
R43
D56
D57
I62
K83
V84
P85
D86
I96
L104
A156
C157
R158
E171
E175
L178
E181
L182
V183
E184
T193
T205
D206
N223
P224
D227
V239
D240
V241
M242
E252
G253
A254
N255
S256
E257
F261
G269
GLU
GLY
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.38Å 93.45Å 104.94Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	49.21 – 1.93 49.21 – 1.50	Depositor EDS
% Data completeness (in resolution range)	94.3 (49.21-1.93) 57.7 (49.21-1.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 1.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.200 , 0.226 0.213 , 0.234	Depositor DCC
R_{free} test set	5899 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	15.3	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9298	wwPDB-VP
Average B, all atoms (Å^2)	17.0	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 57.50 % 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 2.3454e-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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, NAP

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	0.50	0/2077	0.79	5/2812 (0.2%)
1	B	0.48	0/2055	0.81	7/2784 (0.3%)
1	C	0.51	1/2077 (0.0%)	0.79	4/2812 (0.1%)
1	D	0.48	0/2055	0.77	6/2784 (0.2%)
All	All	0.49	1/8264 (0.0%)	0.79	22/11192 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	242	MET	SD-CE	-5.23	1.48	1.77

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	86	ASP	CB-CG-OD2	9.02	126.42	118.30
1	B	38	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	A	38	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	D	38	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	38	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	C	38	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	B	38	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	227	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	17	ASP	CB-CG-OD2	6.47	124.12	118.30
1	D	206	ASP	CB-CG-OD2	6.43	124.09	118.30
1	C	38	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	C	86	ASP	CB-CG-OD2	6.16	123.85	118.30
1	B	206	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	17	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	227	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	38	ARG	NE-CZ-NH2	-5.85	117.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	57	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	17	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	57	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	57	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	227	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	57	ASP	CB-CG-OD2	5.10	122.89	118.30

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	2031	0	2023	18	0
1	B	2009	0	2003	25	0
1	C	2031	0	2023	18	0
1	D	2009	0	2003	27	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	31	0	11	1	0
3	B	31	0	11	2	0
3	C	31	0	11	1	0
3	D	31	0	11	3	0
4	A	221	0	0	8	0
4	B	215	0	0	8	1
4	C	236	0	0	5	1
4	D	210	0	0	8	0
All	All	9298	0	8220	94	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (94) 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)
3:B:274:NAP:H51A	4:B:2104:HOH:O	1.72	0.88
1:A:272:ILE:HG21	4:A:2077:HOH:O	1.80	0.81
1:D:255:ASN:ND2	4:D:2192:HOH:O	2.02	0.81
1:B:255:ASN:ND2	4:B:2194:HOH:O	2.08	0.79
1:D:29:ASP:O	1:D:83:LYS:HD2	1.85	0.77
1:C:239:VAL:HA	1:C:242:MET:HE3	1.68	0.75
1:C:223:ASN:HD22	1:C:224:PRO:HD2	1.53	0.74
1:D:29:ASP:OD2	4:D:2015:HOH:O	2.08	0.72
3:C:274:NAP:O2A	4:C:2236:HOH:O	2.08	0.71
1:D:158:ARG:NH1	4:D:2114:HOH:O	2.23	0.71
1:B:143:GLU:OE2	4:B:2112:HOH:O	2.15	0.64
1:C:239:VAL:HA	1:C:242:MET:CE	2.26	0.64
1:B:212:LYS:HE3	4:B:2146:HOH:O	1.98	0.64
1:C:223:ASN:HD22	1:C:224:PRO:CD	2.10	0.64
1:A:85:PRO:O	1:A:86:ASP:OD1	2.16	0.63
1:B:21:VAL:HG21	1:B:96:ILE:HG12	1.81	0.62
1:A:101:GLN:OE1	4:A:2098:HOH:O	2.16	0.62
1:A:255:ASN:ND2	4:A:2199:HOH:O	2.10	0.61
1:D:156:ALA:HB3	4:D:2100:HOH:O	2.00	0.61
1:A:40:GLN:CD	1:A:40:GLN:H	2.04	0.60
1:D:21:VAL:HG21	1:D:96:ILE:HG12	1.82	0.60
1:B:85:PRO:O	1:B:86:ASP:OD2	2.20	0.60
1:D:30:THR:OG1	4:D:2018:HOH:O	2.16	0.59
1:C:40:GLN:NE2	1:C:40:GLN:H	2.00	0.59
1:D:223:ASN:HD22	1:D:223:ASN:C	2.07	0.58
1:B:223:ASN:C	1:B:223:ASN:HD22	2.07	0.58
1:C:158:ARG:NH1	4:C:2140:HOH:O	2.36	0.58
1:C:272:ILE:HG21	4:C:2078:HOH:O	2.03	0.57
1:B:158:ARG:HG2	1:B:195:ARG:HH11	1.70	0.56
1:B:40:GLN:NE2	1:B:40:GLN:H	2.05	0.55
3:D:274:NAP:H2B	3:D:274:NAP:O1N	2.08	0.54
1:A:40:GLN:H	1:A:40:GLN:NE2	2.05	0.54
1:B:95:HIS:O	1:B:97:LYS:HD2	2.08	0.54
3:D:274:NAP:C5B	4:D:2101:HOH:O	2.57	0.53
1:B:29:ASP:O	1:B:83:LYS:HD2	2.09	0.52
1:D:239:VAL:HA	1:D:242:MET:HE2	1.92	0.52
1:B:29:ASP:OD2	4:B:2011:HOH:O	2.19	0.51
1:D:252:GLU:HB2	1:D:261:PHE:CZ	2.45	0.51
1:C:121:LYS:HB2	1:C:226:THR:HB	1.91	0.51
1:D:223:ASN:HD22	1:D:224:PRO:N	2.08	0.51
1:A:239:VAL:HA	1:A:242:MET:CE	2.42	0.50
1:C:157:CYS:O	1:C:193:THR:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ASN:HD22	1:B:224:PRO:N	2.09	0.50
1:C:121:LYS:HA	1:C:121:LYS:HE2	1.93	0.50
1:D:178:LEU:CD1	1:D:182:LEU:HD11	2.41	0.50
1:D:56:ASP:HB3	1:D:62:ILE:HD11	1.94	0.50
3:D:274:NAP:H52A	4:D:2101:HOH:O	2.11	0.50
1:B:195:ARG:NH2	3:B:274:NAP:O2N	2.44	0.50
1:A:212:LYS:HE3	4:A:2165:HOH:O	2.10	0.50
1:B:171:GLU:O	1:B:175:GLU:HB2	2.11	0.49
1:C:76:GLU:OE2	4:C:2070:HOH:O	2.20	0.48
1:C:17:ASP:HB3	1:C:104:LEU:O	2.14	0.48
1:B:30:THR:HA	1:B:83:LYS:HB2	1.96	0.48
1:A:17:ASP:HB3	1:A:104:LEU:O	2.14	0.48
1:D:158:ARG:HH11	1:D:158:ARG:HB2	1.79	0.47
1:D:252:GLU:HB2	1:D:261:PHE:CE1	2.49	0.47
1:D:157:CYS:O	1:D:193:THR:HA	2.14	0.47
1:C:223:ASN:ND2	1:C:225:GLU:H	2.12	0.47
1:A:39:PRO:HD2	1:A:42:LEU:HD12	1.98	0.46
1:B:186:LYS:NZ	4:B:2141:HOH:O	2.42	0.46
1:D:178:LEU:O	1:D:182:LEU:HD13	2.16	0.46
1:A:95:HIS:O	1:A:97:LYS:HD2	2.16	0.46
1:B:85:PRO:O	1:B:86:ASP:CG	2.54	0.46
1:B:252:GLU:HB2	1:B:261:PHE:CZ	2.51	0.46
1:B:158:ARG:HG3	4:B:2117:HOH:O	2.17	0.45
1:D:30:THR:HA	1:D:83:LYS:HB2	1.99	0.45
1:B:38:ARG:NH2	1:B:72:ALA:O	2.47	0.45
1:A:143:GLU:CD	4:A:2126:HOH:O	2.55	0.45
1:B:254:ALA:HB2	4:B:2193:HOH:O	2.17	0.45
1:C:223:ASN:HD22	1:C:224:PRO:N	2.14	0.44
1:D:171:GLU:O	1:D:175:GLU:HB2	2.16	0.44
1:A:42:LEU:C	1:A:43:ARG:HD2	2.38	0.44
1:A:157:CYS:O	1:A:193:THR:HA	2.18	0.43
1:D:17:ASP:HB3	1:D:104:LEU:O	2.18	0.43
1:B:223:ASN:HD22	1:B:224:PRO:CD	2.32	0.43
1:D:85:PRO:O	1:D:86:ASP:HB2	2.19	0.43
1:A:239:VAL:HA	1:A:242:MET:HE3	2.01	0.43
1:D:223:ASN:HD22	1:D:224:PRO:CD	2.32	0.43
1:A:169:LEU:C	1:A:169:LEU:HD23	2.39	0.43
1:C:40:GLN:H	1:C:40:GLN:CD	2.22	0.43
1:B:238:ASN:O	1:B:242:MET:HG3	2.19	0.43
1:B:157:CYS:O	1:B:193:THR:HA	2.19	0.42
1:D:38:ARG:HD3	4:D:2021:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HD2	4:A:2030:HOH:O	2.18	0.42
1:D:178:LEU:HD11	1:D:182:LEU:HD11	2.00	0.42
1:D:40:GLN:NE2	1:D:40:GLN:H	2.17	0.41
1:A:38:ARG:CD	4:A:2030:HOH:O	2.67	0.41
3:A:274:NAP:O1N	4:A:2219:HOH:O	2.22	0.41
1:D:182:LEU:HD12	1:D:182:LEU:N	2.35	0.41
1:C:47:GLY:HA3	1:C:112:LEU:O	2.20	0.41
1:D:205:THR:HG21	1:D:240:ASP:HB3	2.03	0.41
1:C:22:THR:HG21	1:C:76:GLU:OE1	2.21	0.41
1:B:223:ASN:HD22	1:B:224:PRO:HD2	1.86	0.41
1:C:97:LYS:NZ	4:C:2091:HOH:O	2.53	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2035:HOH:O	4:C:2193:HOH:O[2_545]	1.91	0.29

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	255/272 (94%)	249 (98%)	4 (2%)	2 (1%)	19 9
1	B	252/272 (93%)	248 (98%)	4 (2%)	0	100 100
1	C	255/272 (94%)	251 (98%)	4 (2%)	0	100 100
1	D	252/272 (93%)	250 (99%)	2 (1%)	0	100 100
All	All	1014/1088 (93%)	998 (98%)	14 (1%)	2 (0%)	47 39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ASN
1	A	254	ALA

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	219/232 (94%)	212 (97%)	7 (3%)	39	25
1	B	217/232 (94%)	209 (96%)	8 (4%)	34	19
1	C	219/232 (94%)	212 (97%)	7 (3%)	39	25
1	D	217/232 (94%)	210 (97%)	7 (3%)	39	25
All	All	872/928 (94%)	843 (97%)	29 (3%)	38	24

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	42	LEU
1	A	43	ARG
1	A	86	ASP
1	A	104	LEU
1	A	121	LYS
1	A	263	VAL
1	B	29	ASP
1	B	38	ARG
1	B	40	GLN
1	B	42	LEU
1	B	96	ILE
1	B	175	GLU
1	B	223	ASN
1	B	235	LEU
1	C	40	GLN
1	C	42	LEU
1	C	43	ARG
1	C	121	LYS
1	C	143	GLU

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Mol	Chain	Res	Type
1	C	195	ARG
1	C	223	ASN
1	D	40	GLN
1	D	42	LEU
1	D	43	ARG
1	D	96	ILE
1	D	158	ARG
1	D	175	GLU
1	D	223	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	B	40	GLN
1	B	94	GLN
1	B	223	ASN
1	C	40	GLN
1	C	223	ASN
1	D	94	GLN
1	D	199	HIS
1	D	223	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	D	273	-	53,58,58	1.25	5 (9%)	68,89,89	2.04	14 (20%)
3	NAP	B	274	-	27,33,52	1.89	5 (18%)	35,52,80	1.82	7 (20%)
2	FAD	C	273	-	53,58,58	1.26	6 (11%)	68,89,89	2.48	18 (26%)
3	NAP	D	274	-	27,33,52	1.78	5 (18%)	35,52,80	1.65	7 (20%)
2	FAD	B	273	-	53,58,58	1.26	4 (7%)	68,89,89	1.92	17 (25%)
3	NAP	A	274	-	27,33,52	1.86	5 (18%)	35,52,80	1.64	6 (17%)
2	FAD	A	273	-	53,58,58	1.12	4 (7%)	68,89,89	1.89	17 (25%)
3	NAP	C	274	-	27,33,52	1.85	5 (18%)	35,52,80	1.73	7 (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	D	273	-	-	4/30/50/50	0/6/6/6
3	NAP	B	274	-	-	6/17/37/67	0/3/3/5
2	FAD	C	273	-	-	4/30/50/50	0/6/6/6
3	NAP	D	274	-	-	3/17/37/67	0/3/3/5
2	FAD	B	273	-	-	4/30/50/50	0/6/6/6
3	NAP	A	274	-	-	7/17/37/67	0/3/3/5
2	FAD	A	273	-	-	4/30/50/50	0/6/6/6
3	NAP	C	274	-	-	2/17/37/67	0/3/3/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	274	NAP	C4A-N3A	6.68	1.44	1.35
3	A	274	NAP	C4A-N3A	6.55	1.44	1.35
3	C	274	NAP	C4A-N3A	6.47	1.44	1.35
3	D	274	NAP	C4A-N3A	6.34	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	273	FAD	C4X-N5	4.39	1.39	1.30
2	D	273	FAD	C4X-N5	4.23	1.39	1.30
2	D	273	FAD	C2A-N3A	4.15	1.38	1.32
2	B	273	FAD	C2A-N3A	4.11	1.38	1.32
2	C	273	FAD	C4X-N5	4.07	1.38	1.30
2	A	273	FAD	C4X-N5	3.88	1.38	1.30
2	A	273	FAD	C2A-N3A	3.84	1.38	1.32
2	C	273	FAD	C2A-N3A	3.82	1.38	1.32
3	B	274	NAP	PN-O1N	3.05	1.60	1.50
3	A	274	NAP	PN-O1N	2.89	1.59	1.50
2	B	273	FAD	C10-N1	2.85	1.39	1.33
3	C	274	NAP	PN-O1N	2.84	1.59	1.50
2	C	273	FAD	C6-C7	2.83	1.43	1.39
2	D	273	FAD	C10-N1	2.75	1.38	1.33
3	B	274	NAP	P2B-O1X	2.75	1.59	1.50
3	A	274	NAP	P2B-O1X	2.75	1.59	1.50
3	D	274	NAP	PN-O1N	2.71	1.59	1.50
3	C	274	NAP	P2B-O1X	2.70	1.59	1.50
2	D	273	FAD	C2A-N1A	2.69	1.38	1.33
3	C	274	NAP	O4B-C1B	2.68	1.44	1.41
2	C	273	FAD	C10-N1	2.64	1.38	1.33
3	D	274	NAP	P2B-O1X	2.57	1.58	1.50
3	A	274	NAP	PA-O1A	2.55	1.60	1.50
3	C	274	NAP	PA-O1A	2.54	1.59	1.50
2	B	273	FAD	C2A-N1A	2.51	1.38	1.33
3	B	274	NAP	O4B-C1B	2.49	1.44	1.41
3	D	274	NAP	PA-O1A	2.42	1.59	1.50
2	A	273	FAD	C2A-N1A	2.41	1.38	1.33
2	C	273	FAD	C2A-N1A	2.40	1.38	1.33
2	A	273	FAD	C10-N1	2.40	1.38	1.33
3	B	274	NAP	PA-O1A	2.31	1.59	1.50
3	A	274	NAP	O4B-C1B	2.29	1.44	1.41
3	D	274	NAP	O4B-C1B	2.24	1.44	1.41
2	C	273	FAD	C7M-C7	2.24	1.55	1.51
2	D	273	FAD	O4B-C4B	-2.05	1.40	1.45

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	273	FAD	C5X-C6-C7	-8.03	105.97	120.71
2	C	273	FAD	C6-C5X-C9A	7.38	129.38	118.94
2	B	273	FAD	C5X-C6-C7	6.86	133.31	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	273	FAD	C5X-C6-C7	6.70	133.01	120.71
2	A	273	FAD	O3B-C3B-C4B	-6.28	92.88	111.05
2	C	273	FAD	O2B-C2B-C1B	6.12	133.44	110.85
2	C	273	FAD	O3B-C3B-C4B	-6.11	93.37	111.05
2	C	273	FAD	C6-C7-C8	5.99	128.25	119.67
2	C	273	FAD	N3A-C2A-N1A	-5.92	119.43	128.68
2	D	273	FAD	N3A-C2A-N1A	-5.85	119.53	128.68
2	B	273	FAD	N3A-C2A-N1A	-5.70	119.77	128.68
2	A	273	FAD	N3A-C2A-N1A	-5.69	119.79	128.68
2	B	273	FAD	C6-C7-C8	-5.68	111.53	119.67
2	D	273	FAD	O2B-C2B-C1B	5.57	131.44	110.85
2	D	273	FAD	C6-C7-C8	-5.46	111.85	119.67
2	D	273	FAD	O3B-C3B-C4B	-5.12	96.25	111.05
2	A	273	FAD	C6-C5X-C9A	4.55	125.37	118.94
3	B	274	NAP	PA-O3-PN	-4.54	117.24	132.83
2	A	273	FAD	C5X-C6-C7	-4.42	112.59	120.71
3	D	274	NAP	N3A-C2A-N1A	-4.36	121.86	128.68
3	A	274	NAP	PA-O3-PN	-4.33	117.96	132.83
3	C	274	NAP	N3A-C2A-N1A	-4.26	122.02	128.68
3	B	274	NAP	N3A-C2A-N1A	-4.20	122.11	128.68
3	A	274	NAP	N3A-C2A-N1A	-4.20	122.12	128.68
2	C	273	FAD	C6-C5X-N5	-4.20	111.19	118.51
3	C	274	NAP	PA-O3-PN	-4.16	118.55	132.83
2	B	273	FAD	O3B-C3B-C4B	-4.09	99.23	111.05
2	C	273	FAD	O3B-C3B-C2B	-3.91	99.17	111.82
3	D	274	NAP	PA-O3-PN	-3.88	119.51	132.83
2	D	273	FAD	C6-C5X-C9A	-3.65	113.77	118.94
2	B	273	FAD	C6-C5X-C9A	-3.63	113.81	118.94
2	C	273	FAD	C7M-C7-C6	-3.57	112.88	119.49
3	B	274	NAP	O3B-C3B-C4B	-3.55	100.78	111.05
3	C	274	NAP	C4A-C5A-N7A	-3.53	105.72	109.40
3	C	274	NAP	O3B-C3B-C4B	-3.46	101.04	111.05
2	A	273	FAD	C6-C7-C8	3.37	124.49	119.67
2	B	273	FAD	C4X-C10-N10	3.17	121.12	116.48
2	A	273	FAD	C4X-C10-N10	3.15	121.08	116.48
2	D	273	FAD	C4X-C10-N10	3.12	121.04	116.48
2	C	273	FAD	C4X-C10-N10	3.10	121.02	116.48
3	D	274	NAP	C4A-C5A-N7A	-3.08	106.19	109.40
2	D	273	FAD	C1B-N9A-C4A	-3.04	121.29	126.64
2	A	273	FAD	O3B-C3B-C2B	-3.02	102.05	111.82
3	B	274	NAP	C2B-C3B-C4B	2.97	108.44	101.99
3	B	274	NAP	C4A-C5A-N7A	-2.95	106.33	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	273	FAD	C7M-C7-C6	-2.89	114.14	119.49
3	A	274	NAP	C4A-C5A-N7A	-2.87	106.40	109.40
3	D	274	NAP	O3B-C3B-C4B	-2.87	102.75	111.05
3	A	274	NAP	O3B-C3B-C4B	-2.77	103.03	111.05
3	D	274	NAP	C2A-N1A-C6A	2.77	123.49	118.75
3	A	274	NAP	C2B-C3B-C4B	2.76	108.00	101.99
2	C	273	FAD	C9A-C5X-N5	-2.76	119.43	122.43
2	A	273	FAD	C3B-C2B-C1B	2.67	104.99	100.98
2	B	273	FAD	O3B-C3B-C2B	-2.64	103.28	111.82
2	C	273	FAD	C10-C4X-N5	-2.64	119.26	124.86
2	A	273	FAD	C6-C5X-N5	-2.63	113.92	118.51
3	C	274	NAP	C2A-N1A-C6A	2.62	123.24	118.75
2	B	273	FAD	C1B-N9A-C4A	-2.60	122.06	126.64
3	A	274	NAP	C2A-N1A-C6A	2.60	123.21	118.75
3	B	274	NAP	C2A-N1A-C6A	2.59	123.18	118.75
3	C	274	NAP	C2B-C3B-C4B	2.57	107.58	101.99
2	D	273	FAD	C6-C5X-N5	2.54	122.95	118.51
2	B	273	FAD	C2B-C3B-C4B	2.54	107.57	102.64
2	D	273	FAD	C2B-C3B-C4B	2.52	107.54	102.64
2	A	273	FAD	C10-C4X-N5	-2.48	119.59	124.86
2	C	273	FAD	C2B-C3B-C4B	2.48	107.46	102.64
2	C	273	FAD	C1B-N9A-C4A	-2.46	122.33	126.64
2	B	273	FAD	C6-C5X-N5	2.44	122.78	118.51
2	D	273	FAD	O4B-C1B-C2B	2.39	110.42	106.93
2	A	273	FAD	O4B-C4B-C5B	2.32	117.02	109.37
3	D	274	NAP	C2B-C3B-C4B	2.31	107.01	101.99
3	B	274	NAP	C5B-C4B-C3B	-2.30	106.58	115.18
2	C	273	FAD	O4B-C4B-C5B	2.28	116.89	109.37
2	B	273	FAD	C10-C4X-N5	-2.20	120.18	124.86
3	D	274	NAP	O3X-P2B-O2B	2.20	115.83	105.99
2	A	273	FAD	C4-C4X-C10	2.19	120.47	116.79
2	B	273	FAD	C7M-C7-C8	2.19	125.22	120.74
2	A	273	FAD	C2B-C3B-C4B	2.19	106.89	102.64
2	A	273	FAD	C4-N3-C2	-2.17	121.63	125.64
2	D	273	FAD	P-O3P-PA	-2.13	125.53	132.83
3	C	274	NAP	C1B-N9A-C4A	-2.12	122.91	126.64
2	B	273	FAD	O2B-C2B-C1B	2.10	118.60	110.85
2	C	273	FAD	P-O3P-PA	-2.10	125.64	132.83
2	A	273	FAD	P-O3P-PA	-2.08	125.68	132.83
2	D	273	FAD	C10-C4X-N5	-2.07	120.46	124.86
2	B	273	FAD	O4B-C1B-C2B	2.06	109.94	106.93
2	B	273	FAD	C4X-C4-N3	2.03	118.36	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	273	FAD	C4X-C10-N1	-2.03	120.01	124.73
2	B	273	FAD	P-O3P-PA	-2.03	125.86	132.83
2	C	273	FAD	C4-C4X-C10	2.03	120.20	116.79
2	B	273	FAD	O4B-C4B-C5B	2.02	116.02	109.37
2	D	273	FAD	C7M-C7-C8	2.00	124.84	120.74
2	C	273	FAD	C4-N3-C2	-2.00	121.94	125.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	273	FAD	C1'-C2'-C3'-C4'
2	B	273	FAD	C1'-C2'-C3'-C4'
2	C	273	FAD	C1'-C2'-C3'-C4'
2	D	273	FAD	C1'-C2'-C3'-C4'
3	A	274	NAP	C5B-O5B-PA-O1A
3	A	274	NAP	C5B-O5B-PA-O2A
3	B	274	NAP	C5B-O5B-PA-O1A
3	C	274	NAP	C5B-O5B-PA-O3
3	D	274	NAP	C5B-O5B-PA-O3
3	A	274	NAP	O4B-C4B-C5B-O5B
3	B	274	NAP	O4B-C4B-C5B-O5B
3	A	274	NAP	C3B-C4B-C5B-O5B
3	B	274	NAP	C3B-C4B-C5B-O5B
2	A	273	FAD	O2'-C2'-C3'-C4'
2	B	273	FAD	O2'-C2'-C3'-C4'
2	C	273	FAD	O2'-C2'-C3'-C4'
2	D	273	FAD	O2'-C2'-C3'-C4'
3	A	274	NAP	C4B-C5B-O5B-PA
2	A	273	FAD	O2'-C2'-C3'-O3'
2	B	273	FAD	O2'-C2'-C3'-O3'
2	C	273	FAD	O2'-C2'-C3'-O3'
2	D	273	FAD	O2'-C2'-C3'-O3'
3	B	274	NAP	C5B-O5B-PA-O3
3	B	274	NAP	C5B-O5B-PA-O2A
3	C	274	NAP	C5B-O5B-PA-O1A
3	D	274	NAP	C5B-O5B-PA-O1A
3	A	274	NAP	C5B-O5B-PA-O3
3	A	274	NAP	C2B-O2B-P2B-O2X
3	B	274	NAP	C2B-O2B-P2B-O2X
3	D	274	NAP	C2B-O2B-P2B-O2X
2	A	273	FAD	C1'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
2	B	273	FAD	C1'-C2'-C3'-O3'
2	C	273	FAD	C1'-C2'-C3'-O3'
2	D	273	FAD	C1'-C2'-C3'-O3'

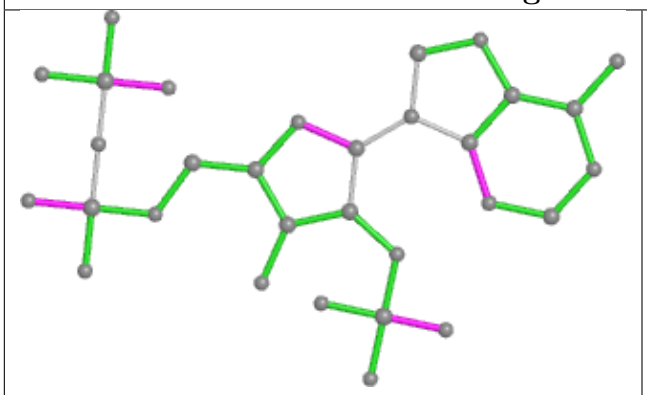
There are no ring outliers.

4 monomers are involved in 7 short contacts:

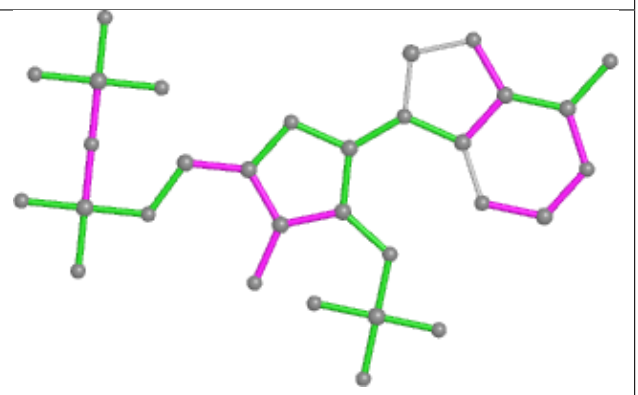
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	274	NAP	2	0
3	D	274	NAP	3	0
3	A	274	NAP	1	0
3	C	274	NAP	1	0

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.

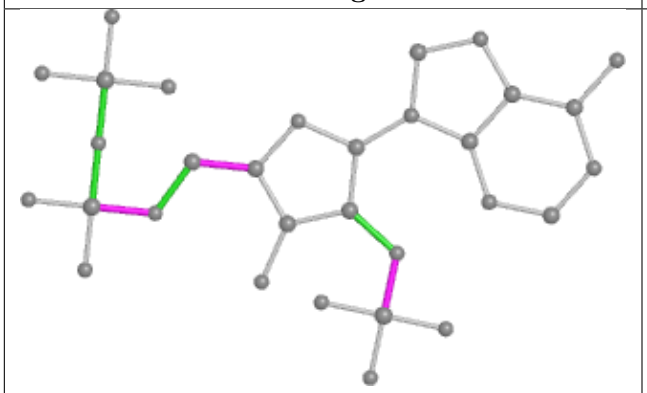
Ligand NAP B 274



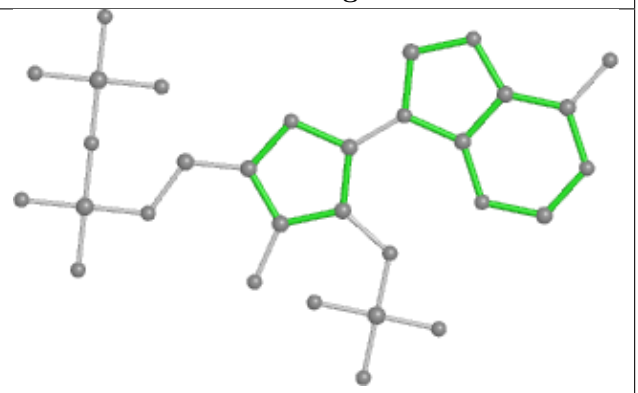
Bond lengths



Bond angles

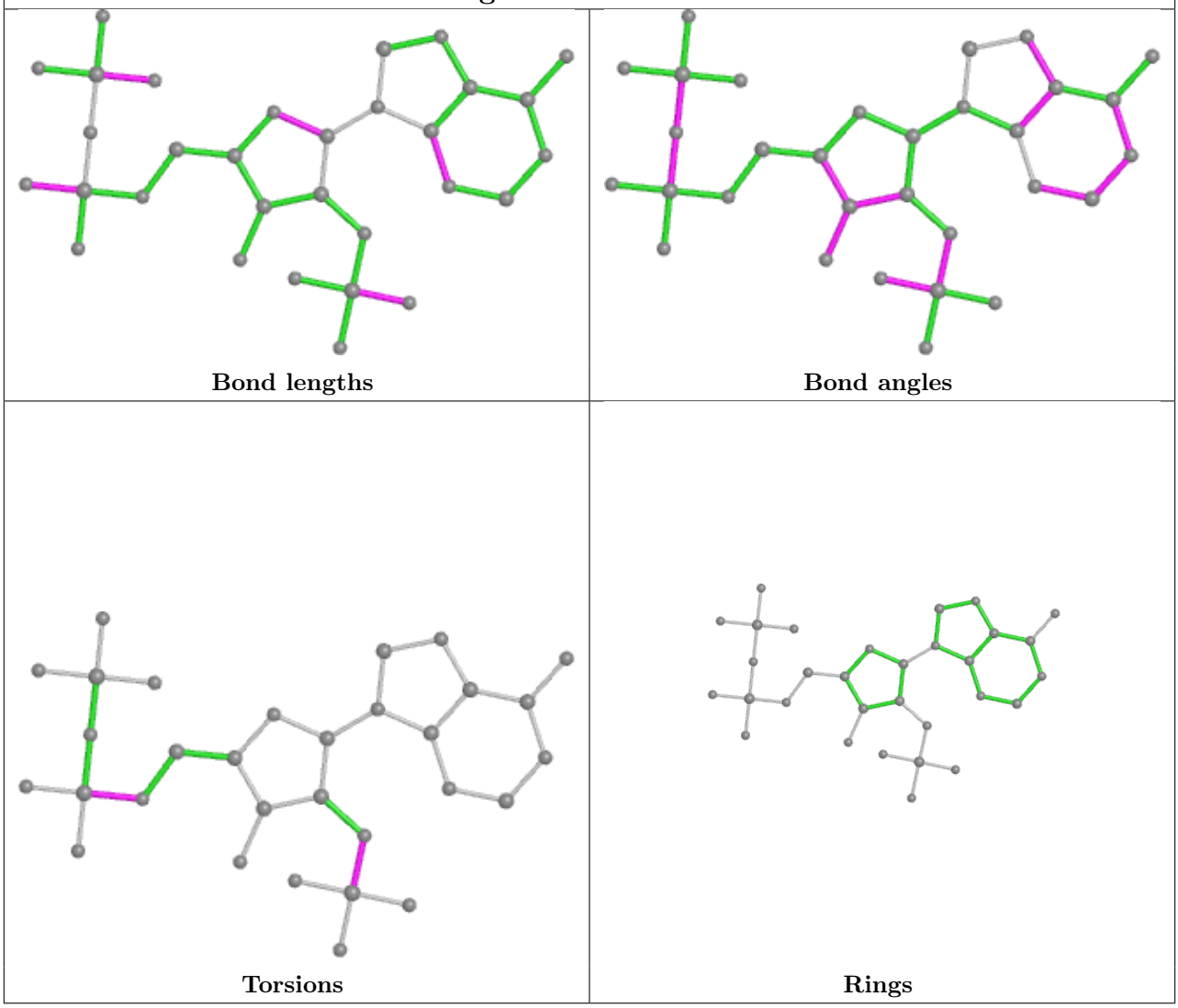


Torsions



Rings

Ligand NAP D 274



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	257/272 (94%)	-0.26	8 (3%)	49	56	7, 14, 30, 46	0
1	B	254/272 (93%)	-0.32	6 (2%)	59	66	7, 14, 28, 42	0
1	C	257/272 (94%)	-0.30	8 (3%)	49	56	7, 13, 30, 45	0
1	D	254/272 (93%)	-0.30	10 (3%)	39	47	8, 14, 29, 42	0
All	All	1022/1088 (93%)	-0.29	32 (3%)	49	56	7, 14, 30, 46	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	PRO	7.4
1	A	254	ALA	7.4
1	A	255	ASN	5.9
1	D	16	PRO	5.3
1	C	272	ILE	5.2
1	A	16	PRO	5.1
1	B	254	ALA	5.1
1	B	255	ASN	4.7
1	D	255	ASN	4.3
1	C	270	GLU	4.3
1	C	255	ASN	4.2
1	A	272	ILE	4.2
1	C	254	ALA	3.7
1	A	270	GLU	3.6
1	C	16	PRO	3.0
1	D	257	GLU	2.9
1	D	269	GLY	2.9
1	D	183	VAL	2.8
1	D	254	ALA	2.8
1	C	253	GLY	2.8
1	D	256	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	181	GLU	2.7
1	A	253	GLY	2.7
1	C	271	GLY	2.6
1	B	40	GLN	2.5
1	B	257	GLU	2.3
1	D	184	GLU	2.2
1	A	183	VAL	2.2
1	C	269	GLY	2.2
1	D	40	GLN	2.1
1	A	40	GLN	2.0
1	B	182	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

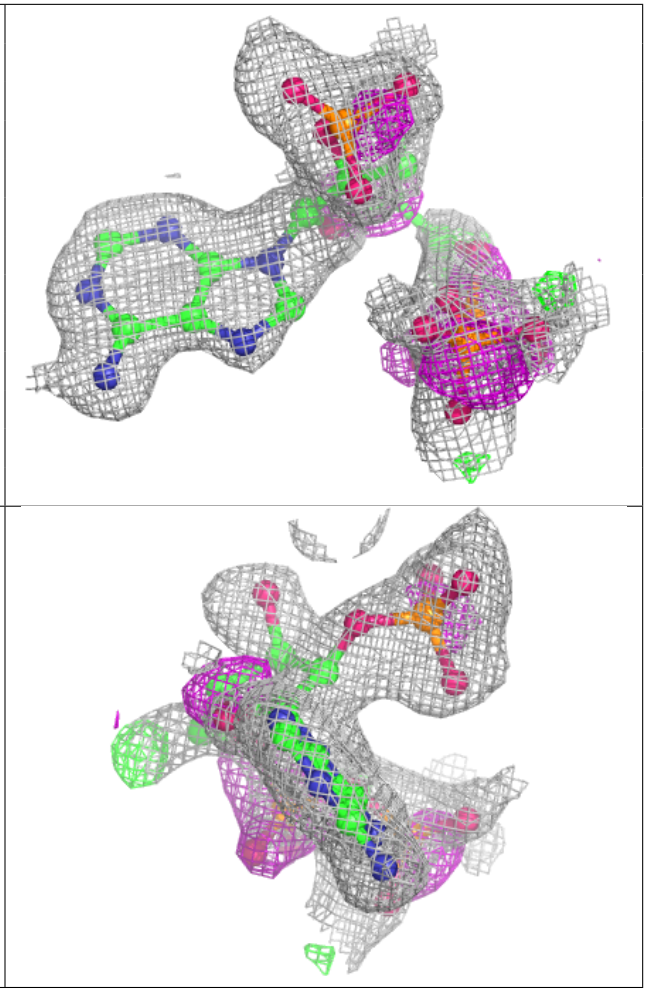
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAP	A	274	31/48	0.72	0.22	21,28,43,44	0
3	NAP	B	274	31/48	0.77	0.19	19,24,44,44	0
3	NAP	C	274	31/48	0.81	0.17	20,31,50,51	0
3	NAP	D	274	31/48	0.81	0.17	20,24,42,43	0
2	FAD	B	273	53/53	0.94	0.09	9,12,18,22	0
2	FAD	D	273	53/53	0.95	0.09	9,12,20,25	0
2	FAD	C	273	53/53	0.96	0.08	10,12,21,25	0
2	FAD	A	273	53/53	0.96	0.08	10,12,19,23	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.

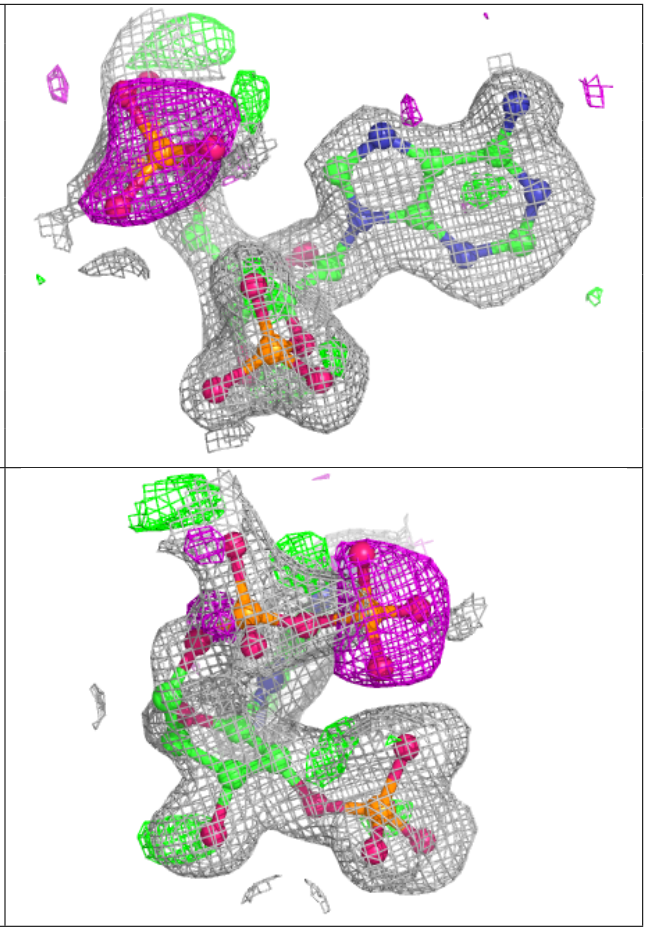
Electron density around NAP A 274:

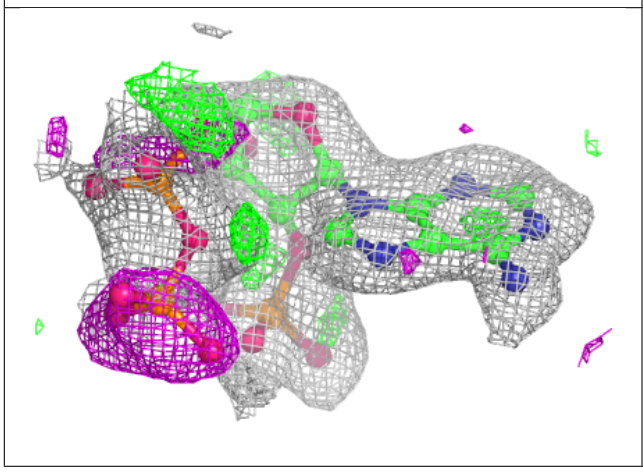
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAP B 274:

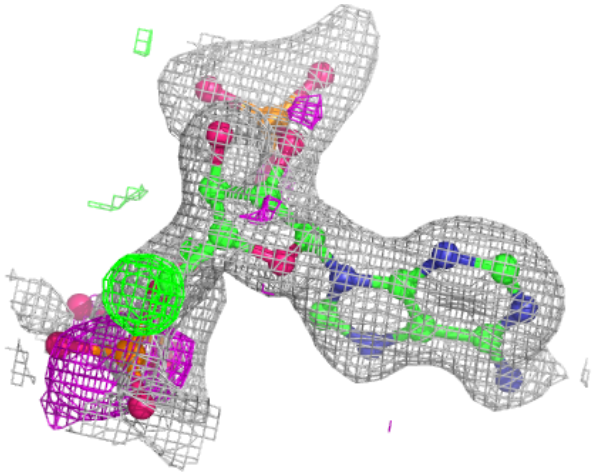
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

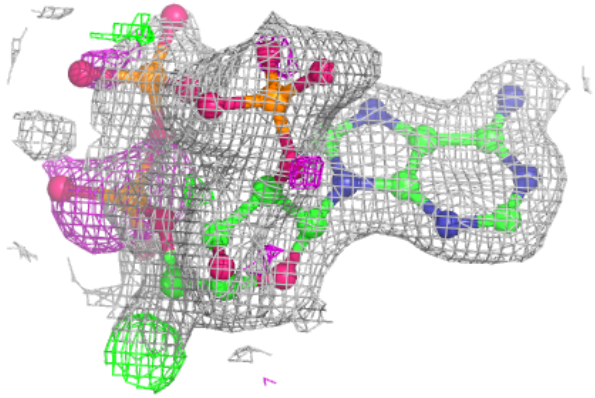


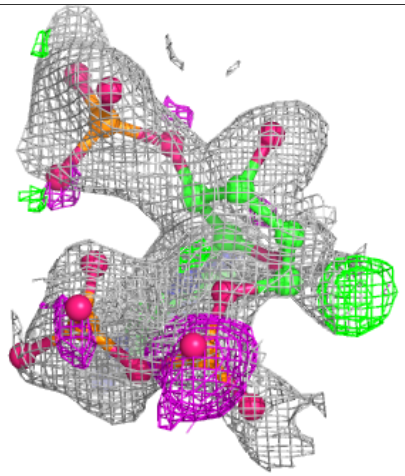


Electron density around NAP C 274:

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

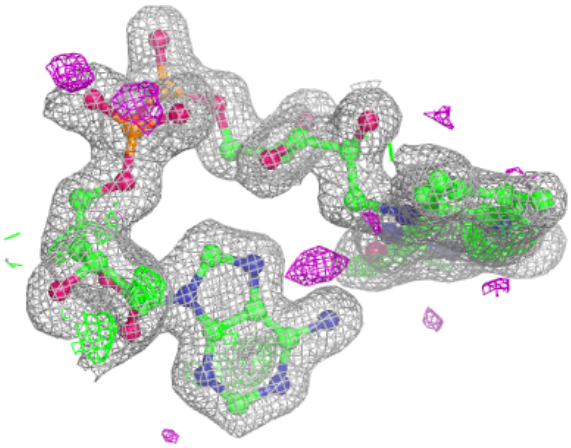


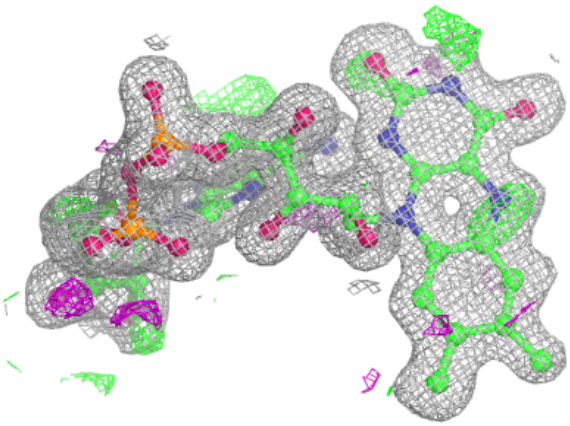


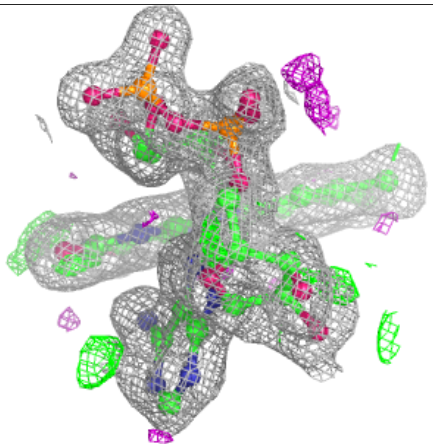


Electron density around FAD B 273:

$2mF_o$-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 273:

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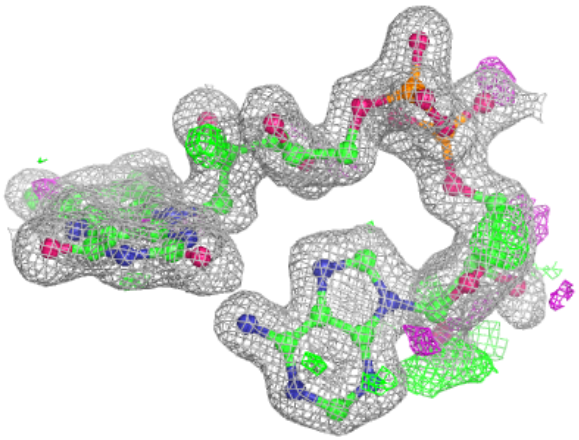
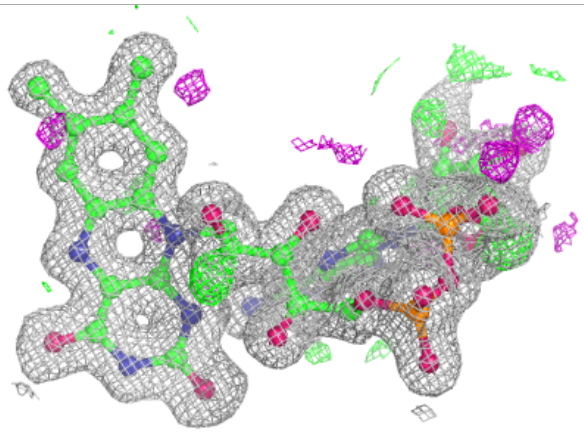
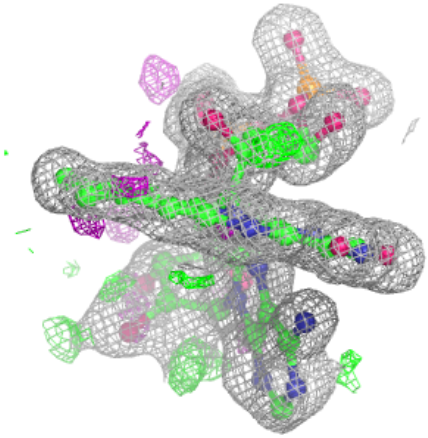
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around FAD C 273:

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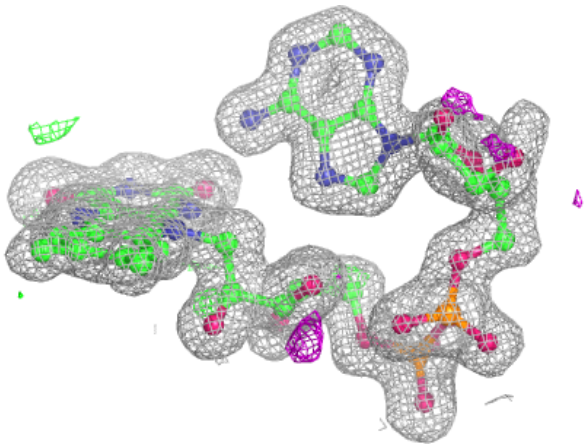
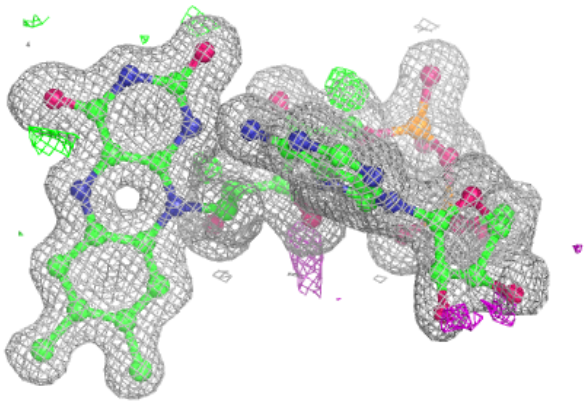
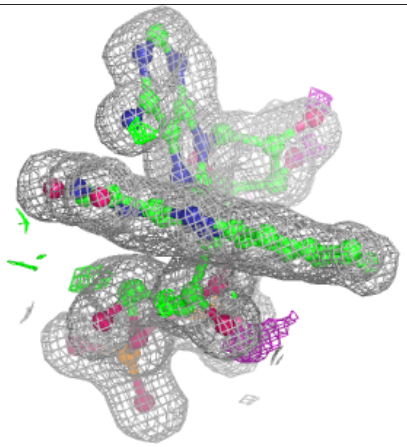
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

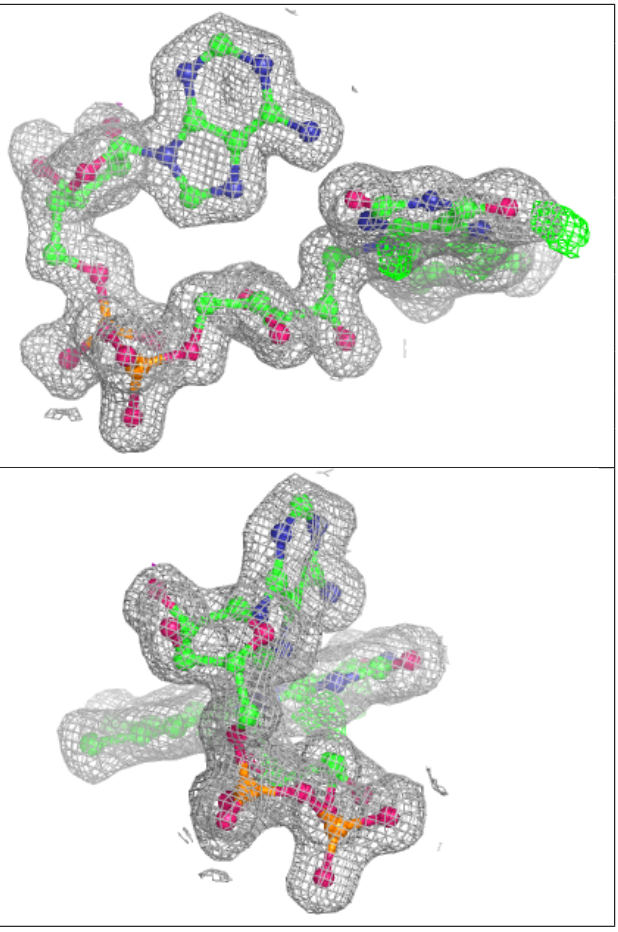


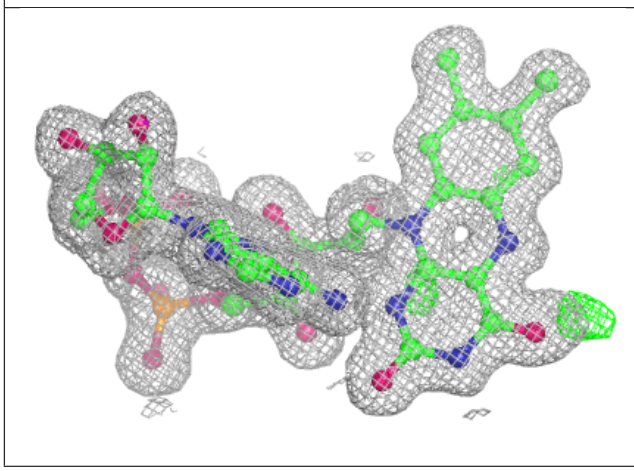




Electron density around FAD A 273:

$2mF_o$-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.