Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 09:01 AM EDT

PDB ID	:	5FA6
Title	:	wild type human CYPOR
Authors	:	Xia, C.; Marohnic, C.; Panda, S.; Masters, B.S.; Kim, J.J.K.
Deposited on	:	2015-12-11
Resolution	:	2.30 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:

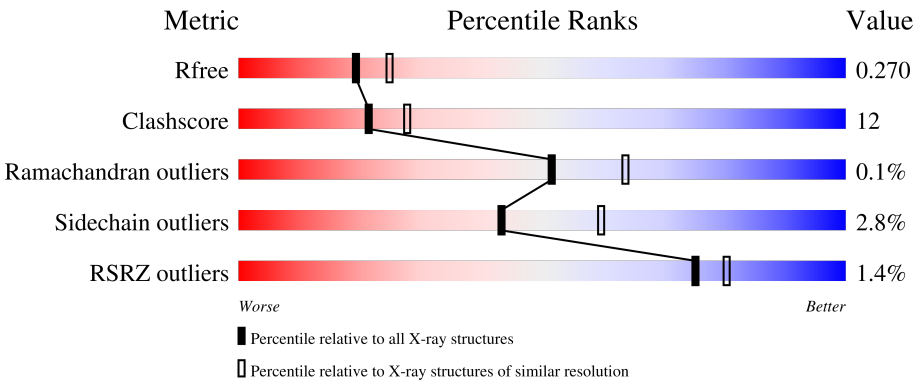
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

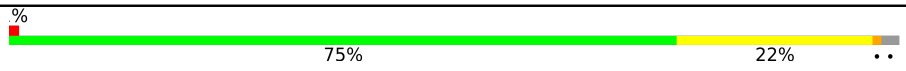
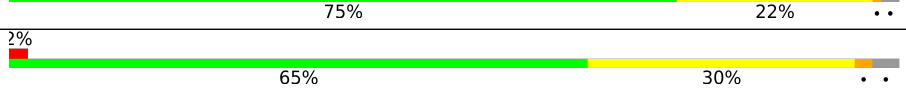
The reported resolution of this entry is 2.30 Å.

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	618	
1	B	618	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10067 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.

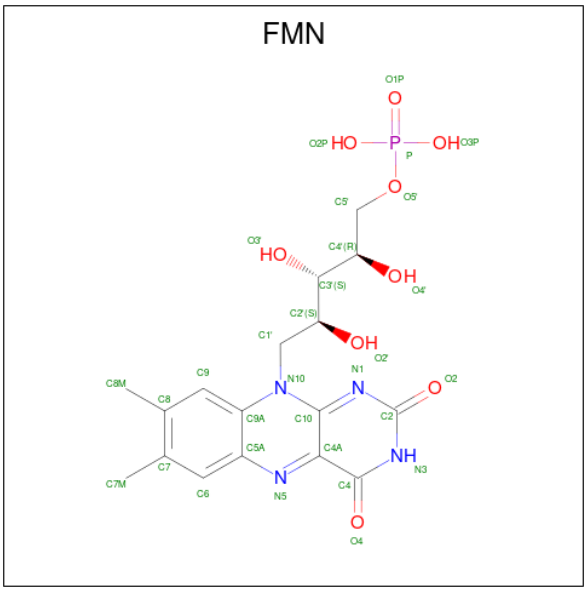
- Molecule 1 is a protein called NADPH–cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	606	4830	3056	836	915	23	0	0	0
1	B	602	4808	3042	835	908	23	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

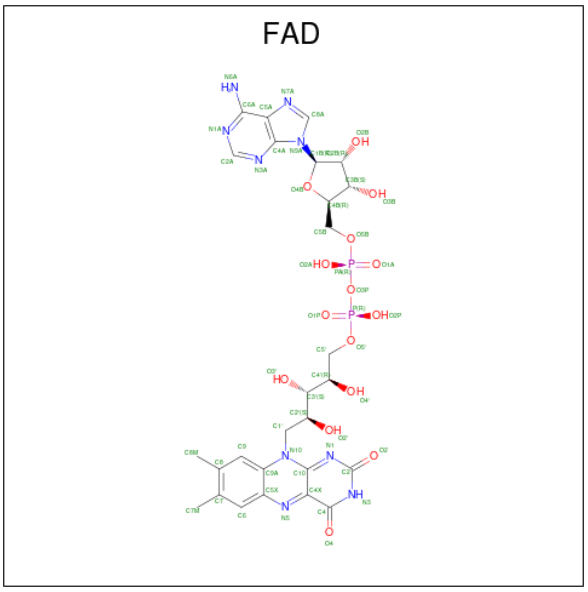
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLY	-	expression tag	UNP P16435
A	64	SER	-	expression tag	UNP P16435
A	65	HIS	-	expression tag	UNP P16435
A	66	MET	-	expression tag	UNP P16435
B	63	GLY	-	expression tag	UNP P16435
B	64	SER	-	expression tag	UNP P16435
B	65	HIS	-	expression tag	UNP P16435
B	66	MET	-	expression tag	UNP P16435

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	17	4	9	1	0	0
2	B	1	31	17	4	9	1	0	0

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



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

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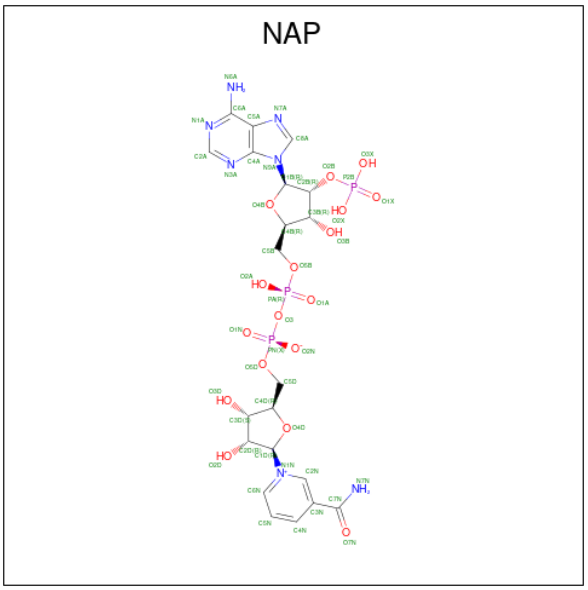
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	53	27	9	15	2	0	0

- Molecule 4 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		
4	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
4	B	1	31	10	5	13	3	0	0

- Molecule 5 is water.

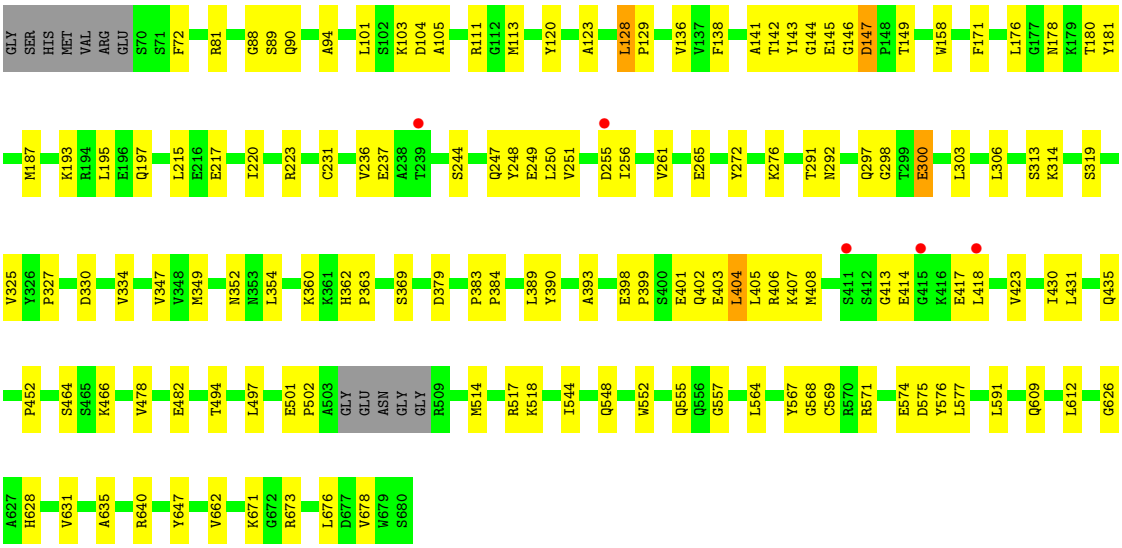
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	139	139	139	0	0
			Total	O		
5	B	60	60	60	0	0

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.

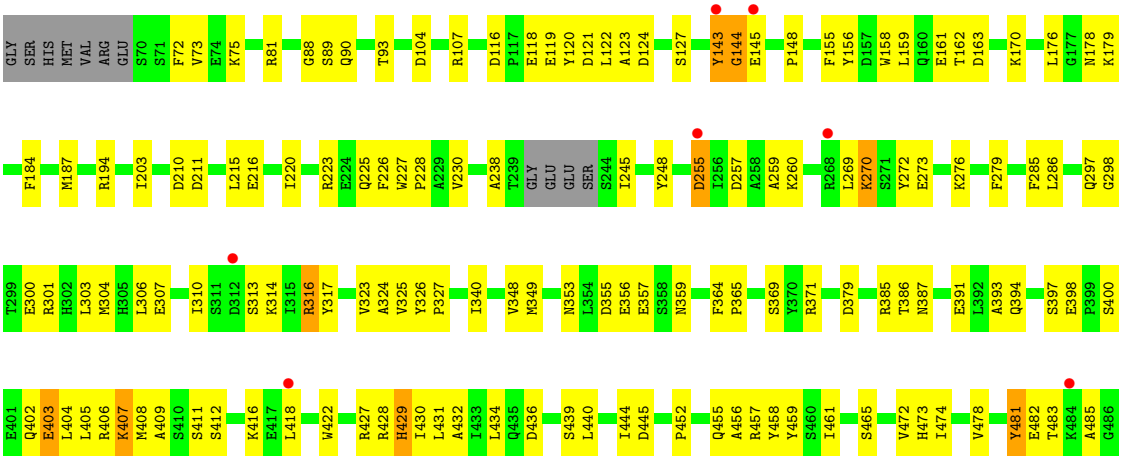
• Molecule 1: NADPH–cytochrome P450 reductase

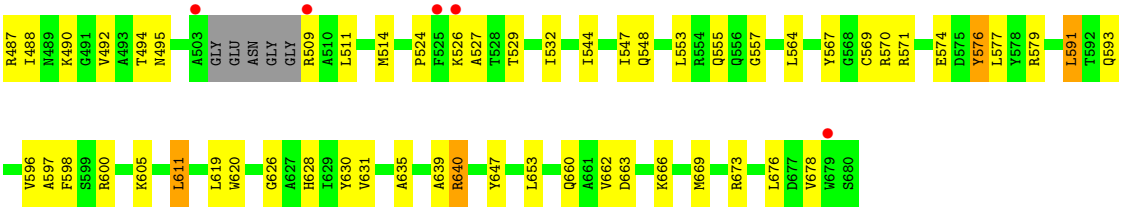
Chain A:



• Molecule 1: NADPH–cytochrome P450 reductase

Chain B:




R487
I488
N489
K490
G491
V492
A493
T494
N495
A503
GLY
GLU
ASN
GLY
GLY
R509
A510
L511
M514
P524
F525
K526
A527
T528
T529
I532
I544
I547
Q548
L553
R554
Q555
Q556
G557
L564
Y567
G568
C569
R570
R571
E574
D575
Y576
L577
Y578
R579
L591
T592
Q593
V596
A597
F598
S599
R600
K605
L611
L619
W620
G626
A627
H628
I629
Y630
V631
A635
A639
R640
Y647
L653
Q660
A661
V662
D663
K666
M669
R673
L676
D677
V678
W679
S680

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.07Å 119.32Å 156.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.32 – 2.30 39.32 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (39.32-2.30) 89.9 (39.32-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.29Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.225 , 0.280 0.220 , 0.270	Depositor DCC
R_{free} test set	2692 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 28.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10067	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% 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: FMN, NAP, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.43	0/4940	0.66	2/6688 (0.0%)
1	B	0.38	0/4917	0.64	7/6654 (0.1%)
All	All	0.41	0/9857	0.65	9/13342 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	244	SER	N-CA-CB	-7.32	99.51	110.50
1	A	88	GLY	N-CA-C	-6.72	96.30	113.10
1	B	245	ILE	N-CA-C	6.47	128.48	111.00
1	B	89	SER	N-CA-CB	6.37	120.06	110.50
1	B	255	ASP	N-CA-CB	-6.22	99.41	110.60
1	B	144	GLY	N-CA-C	5.94	127.94	113.10
1	B	88	GLY	N-CA-C	-5.78	98.66	113.10
1	B	161	GLU	CB-CA-C	-5.16	100.09	110.40
1	B	143	TYR	CB-CA-C	-5.10	100.19	110.40

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	4830	0	4688	93	0
1	B	4808	0	4671	142	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	31	0	11	0	0
4	B	31	0	11	0	0
5	A	139	0	0	5	0
5	B	60	0	0	0	0
All	All	10067	0	9481	233	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 12.

All (233) 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:B:144:GLY:O	1:B:145:GLU:HG2	1.50	1.12
1:B:379:ASP:HB3	1:B:452:PRO:HG2	1.43	0.99
1:A:407:LYS:HD3	1:A:414:GLU:HG3	1.53	0.89
1:A:609:GLN:HA	1:A:612:LEU:HD12	1.63	0.80
1:B:303:LEU:HD22	1:B:577:LEU:HD21	1.64	0.79
1:B:397:SER:HB2	1:B:439:SER:HB2	1.64	0.78
1:A:276:LYS:NZ	1:A:276:LYS:HB3	1.99	0.78
1:A:379:ASP:HB3	1:A:452:PRO:HG2	1.66	0.76
1:A:399:PRO:O	1:A:403:GLU:HG2	1.86	0.76
1:B:407:LYS:HD3	1:B:418:LEU:HD23	1.67	0.75
1:B:270:LYS:HE3	1:B:270:LYS:HA	1.69	0.74
1:B:406:ARG:HG2	1:B:406:ARG:HH11	1.54	0.73
1:B:81:ARG:HH11	1:B:81:ARG:HG3	1.54	0.72
1:B:323:VAL:HG13	1:B:459:TYR:HB2	1.72	0.69
1:B:569:CYS:O	1:B:598:PHE:HA	1.92	0.69
1:A:628:HIS:NE2	1:A:673:ARG:HG2	2.07	0.69
1:A:144:GLY:O	1:A:147:ASP:HB2	1.93	0.69
1:A:389:LEU:HD11	1:A:423:VAL:HG21	1.74	0.69
1:A:298:GLY:HA3	1:A:300:GLU:OE2	1.92	0.69
1:A:635:ALA:HB2	1:A:678:VAL:HB	1.74	0.68
1:B:405:LEU:HA	1:B:408:MET:HE3	1.76	0.68
1:B:404:LEU:CD1	1:B:418:LEU:HD21	2.25	0.67
1:A:111:ARG:HG2	1:A:111:ARG:HH11	1.60	0.66
1:B:620:TRP:HB2	1:B:653:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:HD21	1:B:276:LYS:HB3	1.79	0.65
1:B:144:GLY:O	1:B:145:GLU:CG	2.38	0.64
1:B:436:ASP:OD1	1:B:487:ARG:NH1	2.31	0.64
1:B:429:HIS:CE1	1:B:432:ALA:HB2	2.33	0.63
1:A:306:LEU:HD11	1:A:497:LEU:HB3	1.81	0.63
1:B:640:ARG:HA	1:B:640:ARG:HH11	1.64	0.62
1:B:532:ILE:HD13	1:B:619:LEU:HD22	1.81	0.62
1:B:544:ILE:O	1:B:548:GLN:HG3	1.99	0.61
1:A:89:SER:HB2	1:A:94:ALA:HB3	1.81	0.61
1:A:393:ALA:O	1:A:402:GLN:HG3	2.00	0.61
1:B:404:LEU:HD12	1:B:418:LEU:HD21	1.83	0.60
1:B:300:GLU:HG3	1:B:301:ARG:H	1.65	0.60
1:A:111:ARG:HG2	1:A:111:ARG:NH1	2.16	0.60
1:B:148:PRO:HB3	1:B:187:MET:SD	2.42	0.60
1:A:276:LYS:HB3	1:A:276:LYS:HZ2	1.66	0.60
1:B:298:GLY:HA3	1:B:574:GLU:OE1	2.02	0.59
1:A:569:CYS:HB2	1:A:575:ASP:OD1	2.02	0.59
1:A:193:LYS:O	1:A:197:GLN:HG3	2.02	0.59
1:A:571:ARG:HD3	1:A:574:GLU:OE1	2.03	0.59
1:B:179:LYS:HE3	1:B:184:PHE:CE2	2.38	0.58
1:B:482:GLU:HA	1:B:488:ILE:HD13	1.83	0.58
1:B:270:LYS:HE2	1:B:273:GLU:OE2	2.03	0.58
1:A:564:LEU:N	1:A:564:LEU:HD12	2.18	0.58
1:B:123:ALA:HA	1:B:158:TRP:CZ2	2.39	0.58
1:B:406:ARG:HG2	1:B:406:ARG:NH1	2.17	0.57
1:B:626:GLY:HA2	1:B:673:ARG:NH2	2.20	0.57
1:A:671:LYS:NZ	5:A:804:HOH:O	2.36	0.57
1:B:576:TYR:CD1	1:B:579:ARG:HB2	2.40	0.57
1:B:304:MET:HG3	1:B:306:LEU:HD11	1.87	0.57
1:A:178:ASN:HB3	1:A:181:TYR:HD2	1.68	0.57
1:B:631:VAL:HB	1:B:676:LEU:HD23	1.87	0.57
1:A:628:HIS:CD2	1:A:673:ARG:HG2	2.39	0.57
1:A:101:LEU:O	1:A:104:ASP:HB2	2.05	0.57
1:B:104:ASP:HB2	1:B:227:TRP:CZ2	2.39	0.56
1:A:631:VAL:HB	1:A:676:LEU:HD23	1.88	0.56
1:B:386:THR:HB	1:B:409:ALA:HA	1.88	0.56
1:A:466:LYS:HD3	1:A:552:TRP:CZ3	2.40	0.56
1:B:260:LYS:HA	1:B:269:LEU:HD21	1.88	0.55
1:B:325:VAL:HG12	1:B:514:MET:HB3	1.88	0.55
1:A:145:GLU:N	5:A:803:HOH:O	2.36	0.55
1:B:326:TYR:CE1	1:B:456:ALA:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:ARG:HG2	1:A:640:ARG:HH11	1.72	0.54
1:B:526:LYS:HE3	1:B:529:THR:OG1	2.08	0.54
1:B:666:LYS:O	1:B:669:MET:HB2	2.08	0.54
1:A:231:CYS:HA	1:A:236:VAL:HG23	1.89	0.54
1:A:103:LYS:HE2	1:A:247:GLN:OE1	2.08	0.54
1:B:304:MET:HG3	1:B:306:LEU:CD1	2.38	0.54
1:B:404:LEU:HG	1:B:408:MET:HE2	1.90	0.54
1:B:407:LYS:NZ	1:B:407:LYS:HB3	2.22	0.54
1:B:490:LYS:HB3	1:B:495:ASN:ND2	2.23	0.54
1:B:547:ILE:HD13	1:B:591:LEU:HG	1.90	0.54
1:A:231:CYS:HA	1:A:236:VAL:CG2	2.39	0.53
1:B:158:TRP:O	1:B:162:THR:HG22	2.08	0.53
1:B:571:ARG:HB2	1:B:574:GLU:HB3	1.91	0.52
1:A:265:GLU:HA	1:A:272:TYR:CZ	2.43	0.52
1:B:524:PRO:HG3	1:B:628:HIS:CD2	2.44	0.52
1:A:390:TYR:HE1	1:A:406:ARG:HG2	1.73	0.52
1:B:628:HIS:HB3	1:B:630:TYR:CE1	2.45	0.52
1:A:330:ASP:O	1:A:334:VAL:HG23	2.10	0.52
1:A:81:ARG:HH11	1:A:113:MET:HB3	1.76	0.51
1:A:398:GLU:OE1	1:A:399:PRO:HD2	2.10	0.51
1:B:148:PRO:HB3	1:B:187:MET:CE	2.41	0.51
1:B:73:VAL:HG21	1:B:127:SER:HB2	1.92	0.51
1:B:122:LEU:HG	1:B:155:PHE:CD1	2.44	0.51
1:B:478:VAL:HA	1:B:494:THR:HB	1.93	0.51
1:B:310:ILE:HD13	1:B:472:VAL:HG23	1.93	0.51
1:B:639:ALA:HB2	1:B:678:VAL:HG11	1.92	0.51
1:B:340:ILE:HG12	1:B:340:ILE:O	2.11	0.51
1:A:544:ILE:O	1:A:548:GLN:HG3	2.11	0.50
1:B:407:LYS:C	1:B:409:ALA:H	2.15	0.50
1:B:597:ALA:HB2	1:B:611:LEU:HD22	1.94	0.50
1:A:407:LYS:HD3	1:A:414:GLU:CG	2.33	0.50
1:B:286:LEU:HD23	1:B:511:LEU:HD23	1.92	0.50
1:A:256:ILE:HD13	1:A:261:VAL:HG22	1.94	0.50
1:A:128:LEU:N	1:A:129:PRO:CD	2.74	0.49
1:B:391:GLU:O	1:B:394:GLN:HG2	2.12	0.49
1:B:398:GLU:H	1:B:439:SER:CB	2.26	0.49
1:B:226:PHE:O	1:B:230:VAL:HG23	2.12	0.49
1:B:72:PHE:HB3	1:B:120:TYR:CD1	2.47	0.49
1:B:576:TYR:CG	1:B:579:ARG:HB2	2.48	0.49
1:A:217:GLU:OE1	1:A:220:ILE:HD11	2.14	0.48
1:A:236:VAL:O	1:A:237:GLU:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:ARG:HB2	1:B:574:GLU:CB	2.43	0.48
1:B:407:LYS:HD3	1:B:418:LEU:CD2	2.41	0.48
1:B:481:TYR:CD1	1:B:481:TYR:N	2.82	0.48
1:A:143:TYR:CD1	1:A:149:THR:HG22	2.48	0.48
1:B:90:GLN:HG2	1:B:143:TYR:CZ	2.49	0.48
1:B:427:ARG:HG3	1:B:481:TYR:HE2	1.77	0.48
1:A:430:ILE:HG23	1:A:431:LEU:N	2.29	0.48
1:A:404:LEU:HD22	1:A:408:MET:HE2	1.96	0.48
1:A:413:GLY:O	1:A:417:GLU:HG2	2.14	0.48
1:B:81:ARG:HG3	1:B:81:ARG:NH1	2.22	0.47
1:B:227:TRP:HB2	1:B:228:PRO:HD3	1.95	0.47
1:B:257:ASP:C	1:B:259:ALA:N	2.67	0.47
1:B:524:PRO:HG3	1:B:628:HIS:CG	2.48	0.47
1:A:517:ARG:HH21	1:A:517:ARG:HG3	1.80	0.47
1:A:555:GLN:C	1:A:557:GLY:H	2.18	0.47
1:B:272:TYR:O	1:B:286:LEU:HD22	2.14	0.47
1:B:303:LEU:CD2	1:B:577:LEU:HD21	2.38	0.47
1:B:434:LEU:HD23	1:B:440:LEU:HD23	1.97	0.47
1:A:141:ALA:HA	1:A:176:LEU:O	2.14	0.47
1:A:313:SER:O	1:A:314:LYS:HB2	2.13	0.47
1:B:159:LEU:HB3	1:B:194:ARG:HG2	1.96	0.46
1:B:303:LEU:N	1:B:303:LEU:HD12	2.30	0.46
1:B:591:LEU:HD22	1:B:593:GLN:O	2.15	0.46
1:B:635:ALA:HB2	1:B:678:VAL:HB	1.97	0.46
1:A:431:LEU:O	1:A:435:GLN:HG3	2.16	0.46
1:B:324:ALA:HA	1:B:457:ARG:O	2.15	0.46
1:B:570:ARG:O	1:B:571:ARG:HG3	2.15	0.46
1:B:323:VAL:HG11	1:B:474:ILE:HG12	1.97	0.46
1:B:364:PHE:HB2	1:B:365:PRO:HD2	1.97	0.46
1:A:250:LEU:HD12	1:A:251:VAL:H	1.80	0.46
1:A:567:TYR:CG	1:A:568:GLY:N	2.84	0.46
1:A:631:VAL:HB	1:A:676:LEU:CD2	2.46	0.46
1:B:93:THR:HG21	1:B:215:LEU:HD23	1.97	0.46
1:A:352:ASN:OD1	1:A:362:HIS:CE1	2.68	0.45
1:A:236:VAL:C	1:A:237:GLU:HG3	2.37	0.45
1:A:249:GLU:HB3	1:A:354:LEU:HD21	1.98	0.45
1:A:303:LEU:HD22	1:A:577:LEU:HD21	1.99	0.45
1:B:660:GLN:O	1:B:663:ASP:HB2	2.17	0.45
1:A:647:TYR:CE1	1:A:662:VAL:HA	2.52	0.45
1:B:170:LYS:HB3	1:B:203:ILE:CG1	2.46	0.45
1:B:211:ASP:OD1	1:B:211:ASP:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:TRP:CB	1:B:653:LEU:HD23	2.44	0.45
1:A:217:GLU:CD	1:A:220:ILE:HD11	2.37	0.45
1:A:390:TYR:CE1	1:A:406:ARG:HG2	2.51	0.45
1:A:482:GLU:OE2	1:B:509:ARG:HG2	2.17	0.45
1:B:600:ARG:HG2	1:B:605:LYS:HZ3	1.80	0.45
1:A:180:THR:HB	1:A:635:ALA:O	2.17	0.45
1:A:352:ASN:OD1	1:A:362:HIS:HE1	1.99	0.45
1:B:316:ARG:HG2	1:B:316:ARG:HH11	1.80	0.45
1:B:324:ALA:HB2	1:B:458:TYR:CD1	2.52	0.45
1:A:347:VAL:O	1:A:369:SER:HA	2.17	0.45
1:A:398:GLU:HG2	1:A:401:GLU:HG3	1.99	0.45
1:A:291:THR:HG22	1:A:292:ASN:N	2.32	0.44
1:A:319:SER:OG	1:A:464:SER:HA	2.17	0.44
1:A:123:ALA:HA	1:A:158:TRP:CZ2	2.53	0.44
1:A:248:TYR:CD2	1:A:363:PRO:HD3	2.52	0.44
1:B:600:ARG:HG2	1:B:605:LYS:NZ	2.33	0.44
1:A:360:LYS:NZ	5:A:809:HOH:O	2.48	0.44
1:B:220:ILE:HG22	1:B:411:SER:HB3	1.98	0.44
1:A:105:ALA:HB3	5:A:884:HOH:O	2.18	0.44
1:B:107:ARG:O	1:B:238:ALA:HA	2.18	0.44
1:B:483:THR:HG23	1:B:485:ALA:H	1.81	0.44
1:B:248:TYR:CD2	1:B:353:ASN:HA	2.53	0.44
1:A:178:ASN:HB3	1:A:181:TYR:CD2	2.50	0.44
1:B:371:ARG:HG3	1:B:371:ARG:HH11	1.83	0.44
1:B:444:ILE:HG23	1:B:445:ASP:N	2.33	0.44
1:A:517:ARG:HG3	1:A:517:ARG:NH2	2.33	0.44
1:B:404:LEU:HG	1:B:408:MET:CE	2.48	0.43
1:B:75:LYS:HE2	1:B:357:GLU:O	2.18	0.43
1:B:327:PRO:HB2	1:B:492:VAL:HG12	2.00	0.43
1:B:323:VAL:CG1	1:B:459:TYR:HB2	2.43	0.43
1:A:383:PRO:HA	1:A:384:PRO:HD3	1.92	0.43
1:B:411:SER:HA	1:B:416:LYS:HD3	2.00	0.43
1:B:412:SER:CA	1:B:416:LYS:HG3	2.49	0.43
1:B:81:ARG:HH22	1:B:355:ASP:CG	2.22	0.43
1:B:116:ASP:HB3	1:B:119:GLU:HG2	2.01	0.43
1:B:220:ILE:CG2	1:B:411:SER:HB3	2.48	0.43
1:B:176:LEU:N	1:B:176:LEU:HD12	2.34	0.43
1:B:398:GLU:H	1:B:439:SER:HB2	1.83	0.43
1:B:393:ALA:HA	1:B:405:LEU:HD12	2.00	0.43
1:B:422:TRP:CD1	1:B:428:ARG:NH1	2.87	0.43
1:A:72:PHE:HB3	1:A:120:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LEU:HD23	1:A:215:LEU:HD21	2.01	0.42
1:B:307:GLU:HG2	1:B:473:HIS:CD2	2.55	0.42
1:B:526:LYS:HE3	1:B:526:LYS:HB2	1.76	0.42
1:A:276:LYS:HB3	1:A:276:LYS:HZ3	1.81	0.42
1:B:407:LYS:HB3	1:B:407:LYS:HZ3	1.84	0.42
1:B:121:ASP:HB3	1:B:124:ASP:OD2	2.19	0.42
1:A:138:PHE:CE2	1:A:195:LEU:HD11	2.55	0.42
1:A:478:VAL:HA	1:A:494:THR:HB	2.00	0.42
1:A:405:LEU:HD23	1:A:408:MET:CE	2.50	0.42
1:A:501:GLU:HA	1:A:502:PRO:HD3	1.89	0.42
1:B:317:TYR:O	1:B:465:SER:HB3	2.19	0.42
1:B:178:ASN:HA	1:B:210:ASP:OD1	2.20	0.42
1:A:325:VAL:HG12	1:A:514:MET:HB3	2.02	0.42
1:B:527:ALA:HB2	1:B:553:LEU:HD13	2.02	0.42
1:A:142:THR:CG2	1:A:146:GLY:HA2	2.50	0.41
1:A:144:GLY:HA2	5:A:803:HOH:O	2.19	0.41
1:B:155:PHE:CZ	1:B:159:LEU:HD11	2.55	0.41
1:B:404:LEU:HD12	1:B:418:LEU:CD2	2.47	0.41
1:B:118:GLU:O	1:B:118:GLU:HG3	2.19	0.41
1:B:317:TYR:CE2	1:B:461:ILE:HG21	2.55	0.41
1:B:567:TYR:O	1:B:596:VAL:HA	2.20	0.41
1:A:90:GLN:HB3	1:A:143:TYR:CZ	2.55	0.41
1:B:348:VAL:HA	1:B:369:SER:HA	2.03	0.41
1:A:404:LEU:HD22	1:A:408:MET:CE	2.50	0.41
1:B:148:PRO:HG3	1:B:156:TYR:CB	2.51	0.41
1:B:400:SER:C	1:B:402:GLN:H	2.23	0.41
1:B:555:GLN:C	1:B:557:GLY:H	2.24	0.41
1:B:455:GLN:O	1:B:457:ARG:NH2	2.48	0.41
1:A:398:GLU:CG	1:A:401:GLU:HG3	2.50	0.41
1:A:626:GLY:HA2	1:A:673:ARG:NH2	2.35	0.41
1:B:324:ALA:HB2	1:B:458:TYR:CE1	2.55	0.41
1:B:430:ILE:HG23	1:B:431:LEU:N	2.36	0.41
1:B:647:TYR:CE1	1:B:662:VAL:HA	2.56	0.41
1:B:81:ARG:NH1	1:B:81:ARG:CG	2.84	0.41
1:B:279:PHE:CG	1:B:285:PHE:HB2	2.56	0.41
1:A:104:ASP:OD2	1:A:223:ARG:HD2	2.21	0.40
1:B:404:LEU:HA	1:B:407:LYS:HD2	2.03	0.40
1:B:406:ARG:NH1	1:B:406:ARG:CG	2.84	0.40
1:B:107:ARG:NH2	1:B:223:ARG:HH21	2.19	0.40
1:B:403:GLU:HA	1:B:406:ARG:HD2	2.03	0.40
1:A:136:VAL:O	1:A:171:PHE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LYS:HE3	1:A:518:LYS:HB2	1.96	0.40
1:B:216:GLU:OE1	1:B:385:ARG:HD3	2.21	0.40
1:B:313:SER:O	1:B:314:LYS:HB2	2.21	0.40
1:B:364:PHE:HB2	1:B:365:PRO:CD	2.51	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	602/618 (97%)	570 (95%)	32 (5%)	0	100	100
1	B	596/618 (96%)	547 (92%)	48 (8%)	1 (0%)	47	58
All	All	1198/1236 (97%)	1117 (93%)	80 (7%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	356	GLU

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	512/525 (98%)	501 (98%)	11 (2%)	53	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	510/525 (97%)	492 (96%)	18 (4%)	36	50
All	All	1022/1050 (97%)	993 (97%)	29 (3%)	43	60

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

Mol	Chain	Res	Type
1	A	128	LEU
1	A	147	ASP
1	A	187	MET
1	A	255	ASP
1	A	297	GLN
1	A	300	GLU
1	A	327	PRO
1	A	349	MET
1	A	404	LEU
1	A	576	TYR
1	A	591	LEU
1	B	163	ASP
1	B	225	GLN
1	B	255	ASP
1	B	270	LYS
1	B	297	GLN
1	B	316	ARG
1	B	349	MET
1	B	359	ASN
1	B	387	ASN
1	B	403	GLU
1	B	407	LYS
1	B	429	HIS
1	B	481	TYR
1	B	564	LEU
1	B	576	TYR
1	B	591	LEU
1	B	611	LEU
1	B	640	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	468	HIS

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Mol	Chain	Res	Type
1	B	160	GLN
1	B	470	ASN
1	B	495	ASN
1	B	595	ASN
1	B	628	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)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FAD	B	702	-	53,58,58	2.14	11 (20%)	68,89,89	1.54	11 (16%)
2	FMN	A	701	-	33,33,33	2.73	14 (42%)	48,50,50	1.58	11 (22%)
3	FAD	A	702	-	53,58,58	2.13	11 (20%)	68,89,89	1.51	11 (16%)
4	NAP	A	703	-	27,33,52	1.71	5 (18%)	35,52,80	1.66	5 (14%)
2	FMN	B	701	-	33,33,33	2.58	13 (39%)	48,50,50	1.65	15 (31%)
4	NAP	B	703	-	27,33,52	1.71	5 (18%)	35,52,80	1.77	5 (14%)

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	B	702	-	-	1/30/50/50	0/6/6/6
2	FMN	A	701	-	-	0/18/18/18	0/3/3/3
3	FAD	A	702	-	-	3/30/50/50	0/6/6/6
4	NAP	A	703	-	-	4/17/37/67	0/3/3/5
2	FMN	B	701	-	-	0/18/18/18	0/3/3/3
4	NAP	B	703	-	-	5/17/37/67	0/3/3/5

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	FAD	C8A-N7A	7.55	1.48	1.34
3	A	702	FAD	C8A-N7A	7.49	1.48	1.34
2	B	701	FMN	C8M-C8	-6.69	1.37	1.51
2	A	701	FMN	C8M-C8	-6.20	1.38	1.51
3	B	702	FAD	C8M-C8	-5.77	1.39	1.51
3	A	702	FAD	C8M-C8	-5.77	1.39	1.51
3	B	702	FAD	C7M-C7	-5.76	1.39	1.51
2	A	701	FMN	C10-N10	5.74	1.49	1.37
3	A	702	FAD	C7M-C7	-5.72	1.39	1.51
2	A	701	FMN	C4A-N5	5.65	1.41	1.30
2	B	701	FMN	C4A-N5	5.55	1.41	1.30
2	A	701	FMN	C9-C9A	5.20	1.48	1.39
4	B	703	NAP	C2A-N3A	5.17	1.40	1.32
3	A	702	FAD	C2A-N3A	5.17	1.40	1.32
4	A	703	NAP	C2A-N3A	5.16	1.40	1.32
3	B	702	FAD	C2A-N3A	5.14	1.40	1.32
2	B	701	FMN	C10-N10	4.98	1.48	1.37
2	B	701	FMN	C9-C9A	4.51	1.47	1.39
2	A	701	FMN	C9A-N10	4.35	1.48	1.41
2	B	701	FMN	C9A-C5A	4.09	1.48	1.41
2	B	701	FMN	C9A-N10	3.91	1.48	1.41
2	A	701	FMN	C9A-C5A	3.86	1.47	1.41
2	A	701	FMN	C8-C7	3.84	1.50	1.40
2	B	701	FMN	C8-C7	3.76	1.50	1.40
3	B	702	FAD	C9A-N10	-3.70	1.34	1.41
3	A	702	FAD	C9A-N10	-3.69	1.34	1.41
3	B	702	FAD	C10-N1	3.54	1.40	1.33
3	A	702	FAD	C10-N1	3.52	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	FAD	C2A-N1A	3.49	1.40	1.33
4	A	703	NAP	C2A-N1A	3.47	1.40	1.33
2	A	701	FMN	C10-N1	3.45	1.40	1.33
3	A	702	FAD	C2A-N1A	3.41	1.40	1.33
4	B	703	NAP	C2A-N1A	3.41	1.40	1.33
2	A	701	FMN	C1'-C2'	3.22	1.57	1.52
2	B	701	FMN	C4'-C3'	3.18	1.59	1.53
2	B	701	FMN	C10-N1	3.17	1.39	1.33
2	A	701	FMN	C4'-C3'	2.95	1.59	1.53
2	A	701	FMN	C6-C5A	2.85	1.44	1.40
4	B	703	NAP	C5A-C4A	-2.78	1.33	1.40
4	A	703	NAP	C5A-C4A	-2.75	1.33	1.40
3	A	702	FAD	C5A-C4A	-2.69	1.33	1.40
3	B	702	FAD	C5A-C4A	-2.67	1.33	1.40
4	B	703	NAP	C6A-C5A	-2.64	1.33	1.43
4	A	703	NAP	C6A-C5A	-2.63	1.33	1.43
3	A	702	FAD	C6A-C5A	-2.62	1.33	1.43
3	B	702	FAD	C5X-N5	-2.60	1.34	1.39
3	B	702	FAD	C6A-C5A	-2.60	1.33	1.43
3	A	702	FAD	C5X-N5	-2.57	1.34	1.39
2	B	701	FMN	C6-C5A	2.48	1.43	1.40
2	B	701	FMN	C1'-C2'	2.47	1.56	1.52
2	A	701	FMN	O2'-C2'	2.44	1.48	1.43
3	A	702	FAD	O4B-C1B	2.37	1.44	1.41
3	B	702	FAD	O4B-C1B	2.32	1.44	1.41
2	A	701	FMN	C6-C7	2.24	1.42	1.39
2	A	701	FMN	C7M-C7	2.19	1.55	1.51
4	A	703	NAP	O4B-C1B	2.12	1.44	1.41
2	B	701	FMN	C7M-C7	2.10	1.55	1.51
2	B	701	FMN	O2'-C2'	2.03	1.47	1.43
4	B	703	NAP	O4B-C1B	2.01	1.43	1.41

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	FAD	N3A-C2A-N1A	-7.23	117.38	128.68
3	A	702	FAD	N3A-C2A-N1A	-7.13	117.53	128.68
4	B	703	NAP	N3A-C2A-N1A	-6.98	117.76	128.68
4	A	703	NAP	N3A-C2A-N1A	-6.91	117.88	128.68
4	B	703	NAP	PA-O3-PN	4.00	146.57	132.83
2	B	701	FMN	C9A-C5A-N5	3.99	126.77	122.43
2	A	701	FMN	C9A-C5A-N5	3.80	126.56	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	FAD	P-O3P-PA	-3.72	120.07	132.83
2	A	701	FMN	O4'-C4'-C3'	-3.56	100.45	109.10
2	A	701	FMN	P-O5'-C5'	3.46	127.83	118.30
3	A	702	FAD	P-O3P-PA	-3.35	121.33	132.83
2	B	701	FMN	O4'-C4'-C3'	-3.10	101.56	109.10
4	A	703	NAP	C3B-C2B-C1B	-3.00	97.24	102.89
3	B	702	FAD	C5A-C6A-N6A	-2.94	115.88	120.35
3	B	702	FAD	C4-N3-C2	-2.94	120.20	125.64
3	A	702	FAD	C5A-C6A-N6A	-2.94	115.88	120.35
2	B	701	FMN	P-O5'-C5'	2.93	126.36	118.30
3	B	702	FAD	C2B-C3B-C4B	-2.90	97.01	102.64
3	A	702	FAD	C10-C4X-N5	-2.89	118.73	124.86
3	A	702	FAD	C4-N3-C2	-2.87	120.35	125.64
2	A	701	FMN	O4-C4-N3	-2.74	114.86	120.12
2	B	701	FMN	C8M-C8-C7	2.64	126.15	120.74
3	B	702	FAD	C4X-C4-N3	2.64	119.89	113.19
2	B	701	FMN	O4-C4-N3	-2.62	115.10	120.12
3	A	702	FAD	C4X-C4-N3	2.61	119.82	113.19
4	B	703	NAP	C5A-C6A-N6A	-2.60	116.40	120.35
2	B	701	FMN	C4'-C3'-C2'	-2.60	107.96	113.36
2	B	701	FMN	O4'-C4'-C5'	-2.58	104.13	109.92
2	A	701	FMN	C8M-C8-C7	2.53	125.92	120.74
4	B	703	NAP	C3B-C2B-C1B	-2.51	98.18	102.89
4	A	703	NAP	C5A-C6A-N6A	-2.49	116.57	120.35
3	B	702	FAD	C10-C4X-N5	-2.47	119.62	124.86
2	B	701	FMN	C5A-N5-C4A	-2.44	114.02	118.07
3	B	702	FAD	C4X-C10-N10	2.37	119.95	116.48
2	B	701	FMN	C8M-C8-C9	-2.33	115.19	119.49
2	A	701	FMN	O2P-P-O1P	2.32	119.77	110.68
3	B	702	FAD	O4-C4-C4X	-2.29	120.52	126.60
2	B	701	FMN	C5A-C9A-N10	-2.25	115.63	117.95
3	A	702	FAD	C2B-C3B-C4B	-2.23	98.32	102.64
3	A	702	FAD	C9A-C5X-N5	-2.21	120.03	122.43
3	A	702	FAD	O4-C4-C4X	-2.21	120.75	126.60
2	B	701	FMN	O2P-P-O1P	2.19	119.26	110.68
3	B	702	FAD	C9A-C5X-N5	-2.16	120.08	122.43
4	A	703	NAP	O2N-PN-O1N	2.13	119.03	110.68
3	A	702	FAD	C4'-C3'-C2'	-2.11	108.97	113.36
2	A	701	FMN	C5A-N5-C4A	-2.11	114.57	118.07
3	A	702	FAD	C4-C4X-C10	2.10	120.32	116.79
2	B	701	FMN	O3P-P-O5'	-2.09	101.17	106.73
2	B	701	FMN	C5'-C4'-C3'	2.09	116.24	112.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	FMN	C7M-C7-C6	-2.09	115.63	119.49
2	A	701	FMN	C5A-C9A-N10	-2.08	115.80	117.95
4	B	703	NAP	O2N-PN-O1N	2.07	118.78	110.68
4	A	703	NAP	O4B-C1B-C2B	-2.06	103.02	106.59
2	B	701	FMN	C9-C9A-N10	2.05	124.61	121.84
2	A	701	FMN	C8M-C8-C9	-2.04	115.71	119.49
2	A	701	FMN	C5'-C4'-C3'	2.04	116.14	112.20
3	B	702	FAD	C4-C4X-C10	2.02	120.18	116.79
2	A	701	FMN	O4'-C4'-C5'	-2.01	105.40	109.92

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	NAP	C2B-O2B-P2B-O1X
4	A	703	NAP	PA-O3-PN-O2N
4	B	703	NAP	C2B-O2B-P2B-O1X
4	A	703	NAP	PA-O3-PN-O1N
4	B	703	NAP	PA-O3-PN-O1N
4	B	703	NAP	PA-O3-PN-O2N
3	A	702	FAD	PA-O3P-P-O1P
3	A	702	FAD	PA-O3P-P-O2P
3	B	702	FAD	PA-O3P-P-O1P
4	B	703	NAP	PA-O3-PN-O5D
4	A	703	NAP	C2B-O2B-P2B-O3X
4	B	703	NAP	PN-O3-PA-O2A
3	A	702	FAD	C5'-O5'-P-O1P

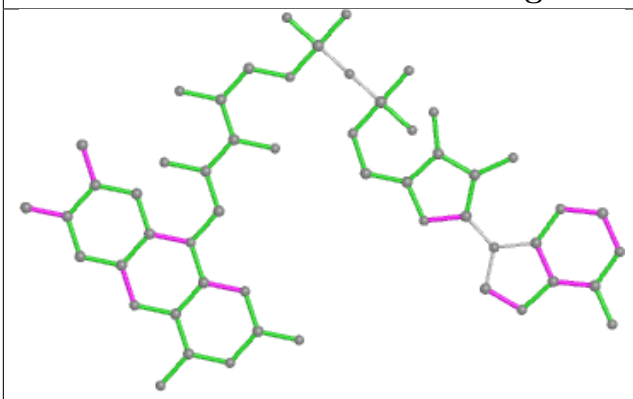
There are no ring outliers.

No monomer is involved in short contacts.

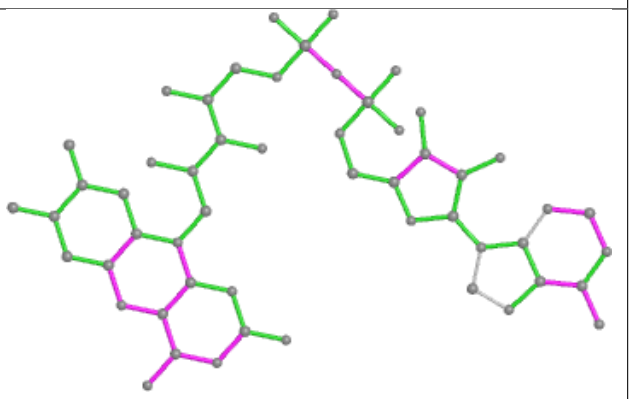
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

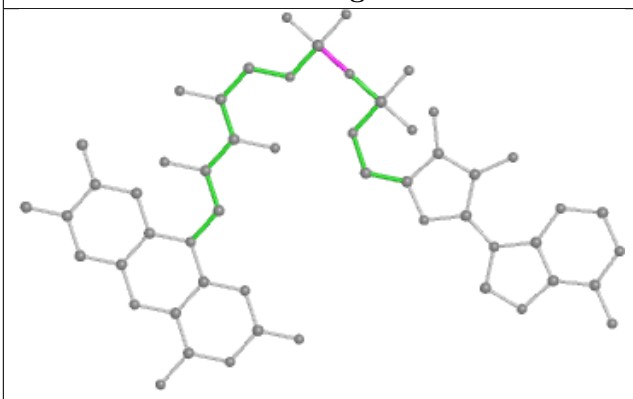
Ligand FAD B 702



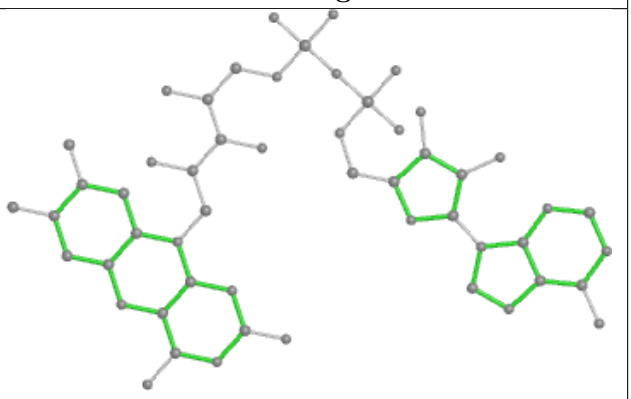
Bond lengths



Bond angles

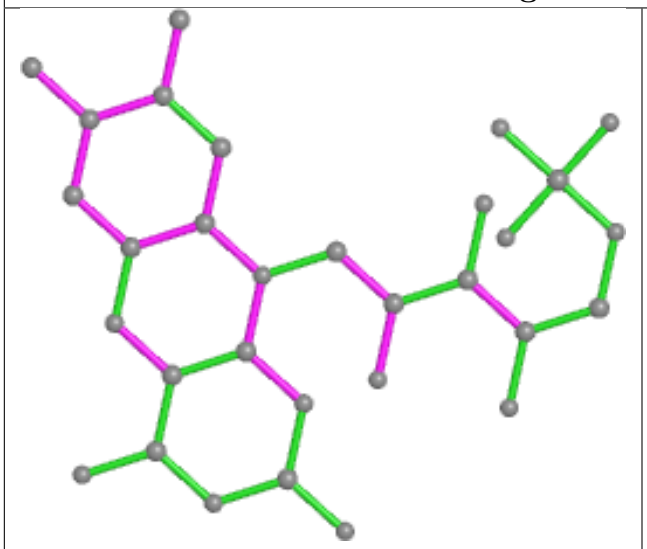


Torsions

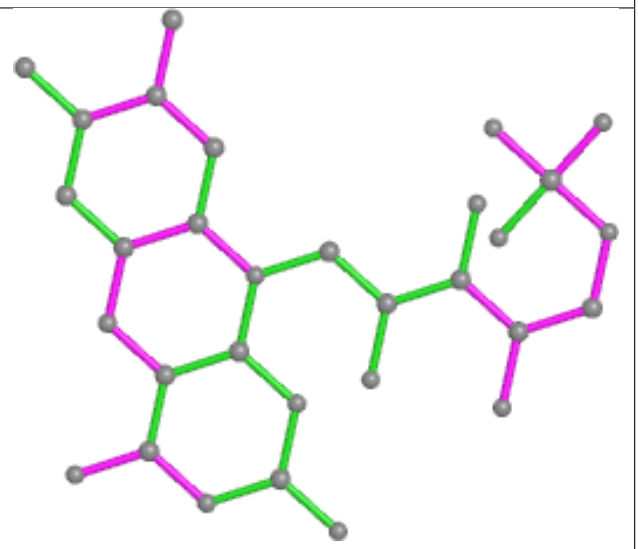


Rings

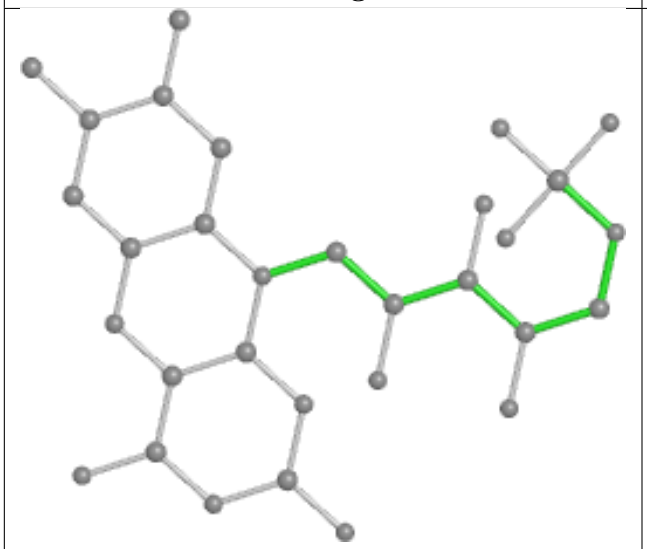
Ligand FMN A 701



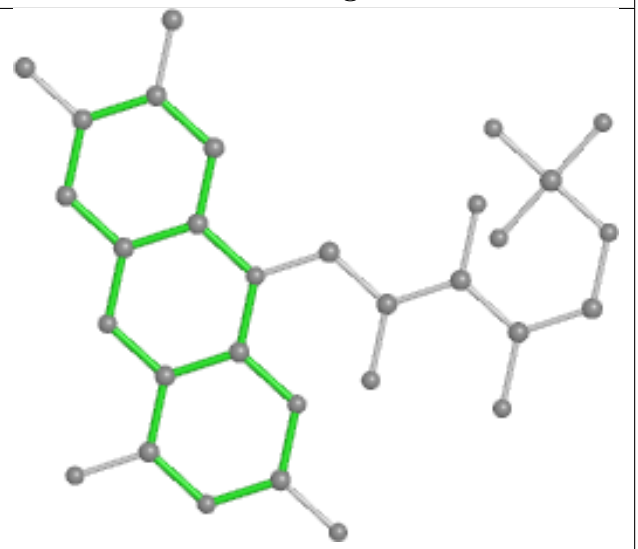
Bond lengths



Bond angles

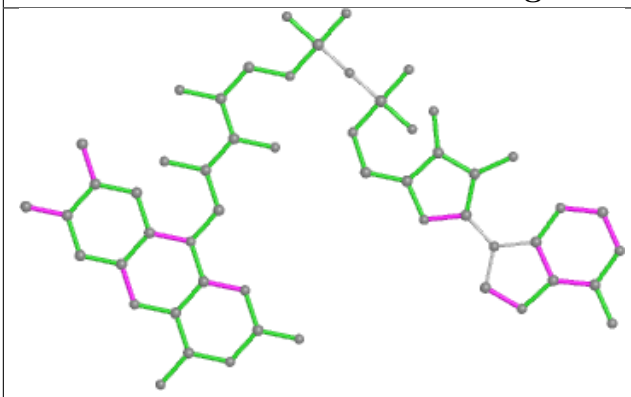


Torsions

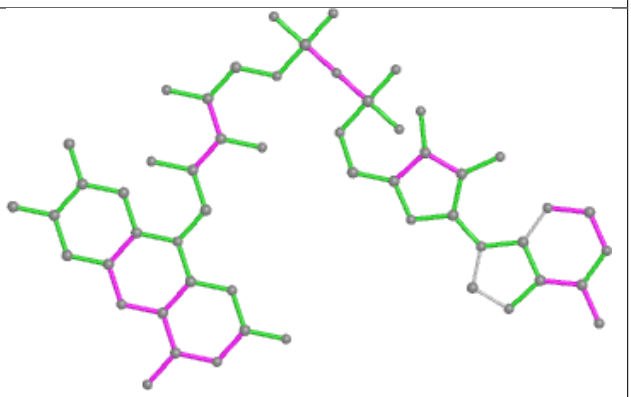


Rings

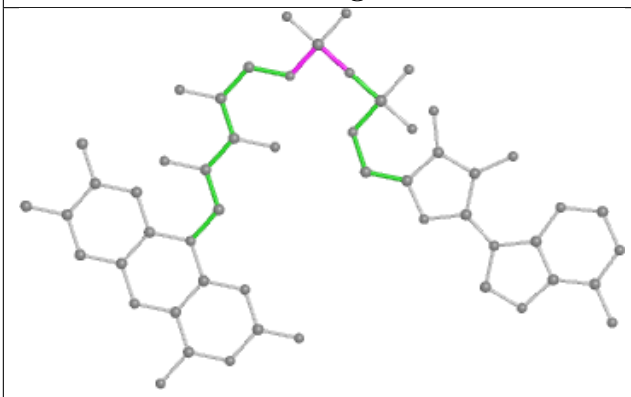
Ligand FAD A 702



Bond lengths



Bond angles



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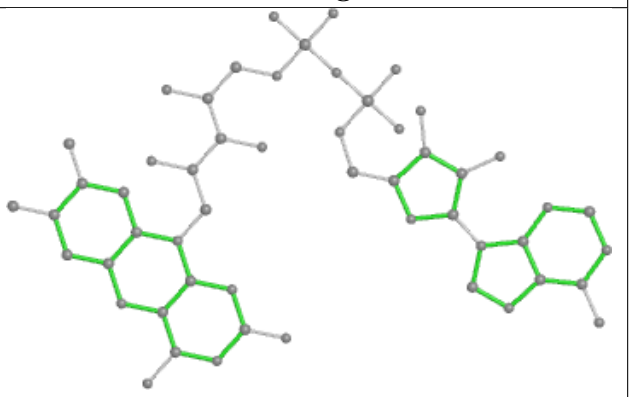
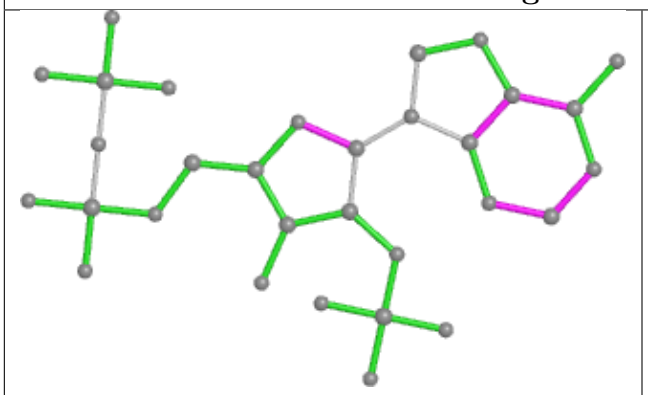
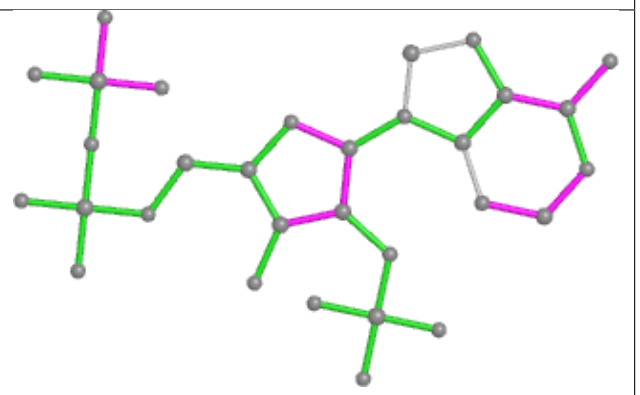


Rings

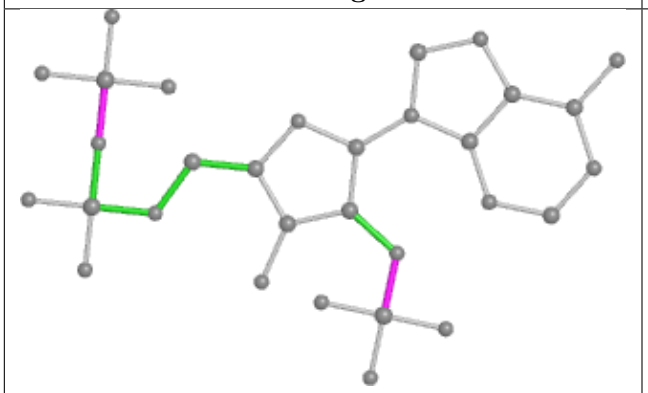
Ligand NAP A 703



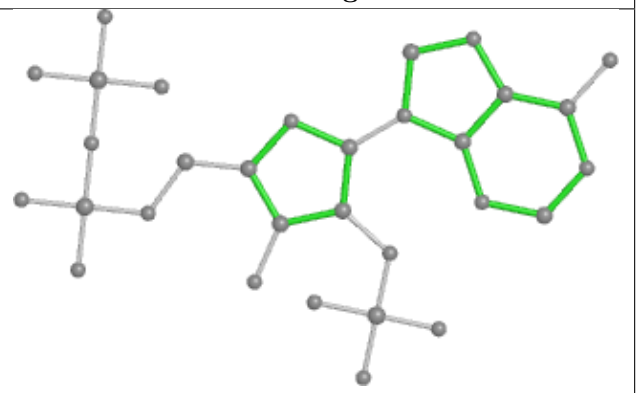
Bond lengths



Bond angles

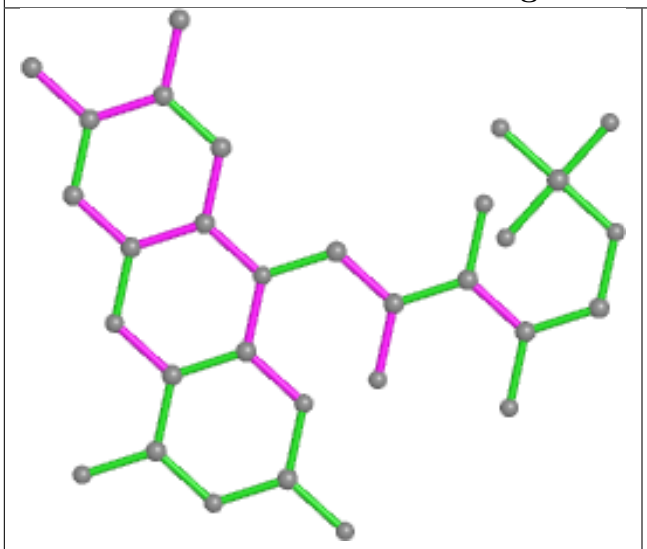


Torsions

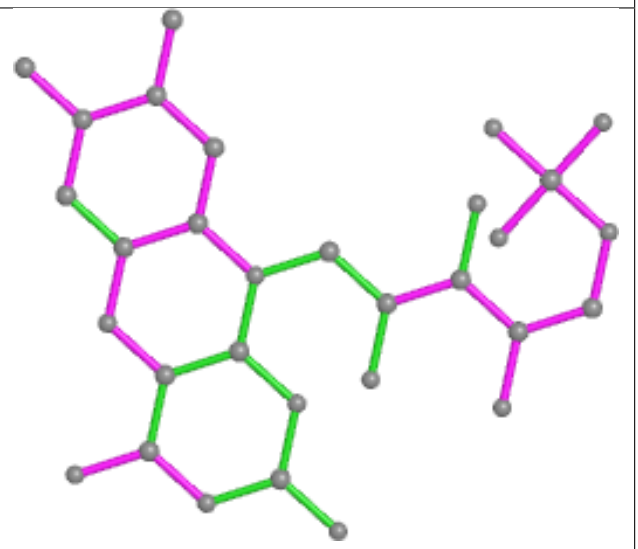


Rings

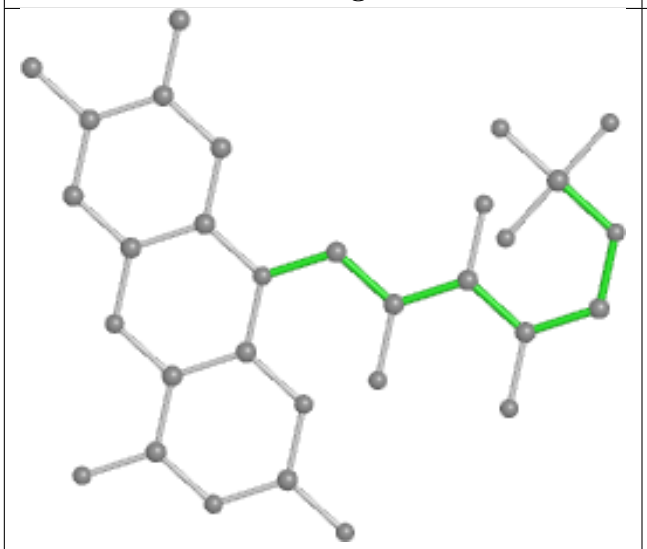
Ligand FMN B 701



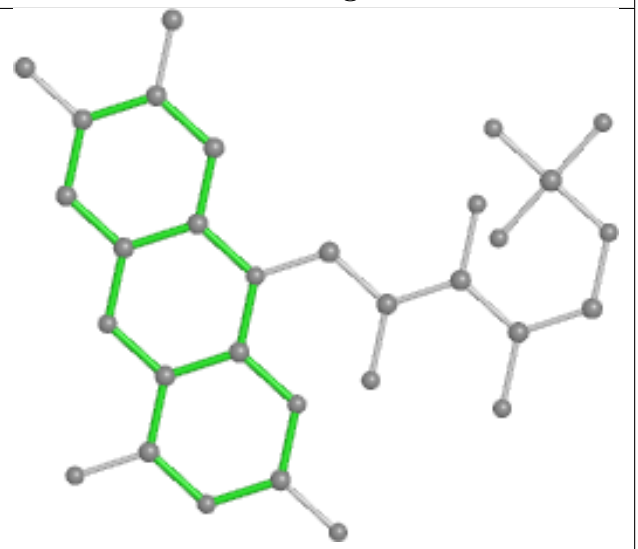
Bond lengths



Bond angles

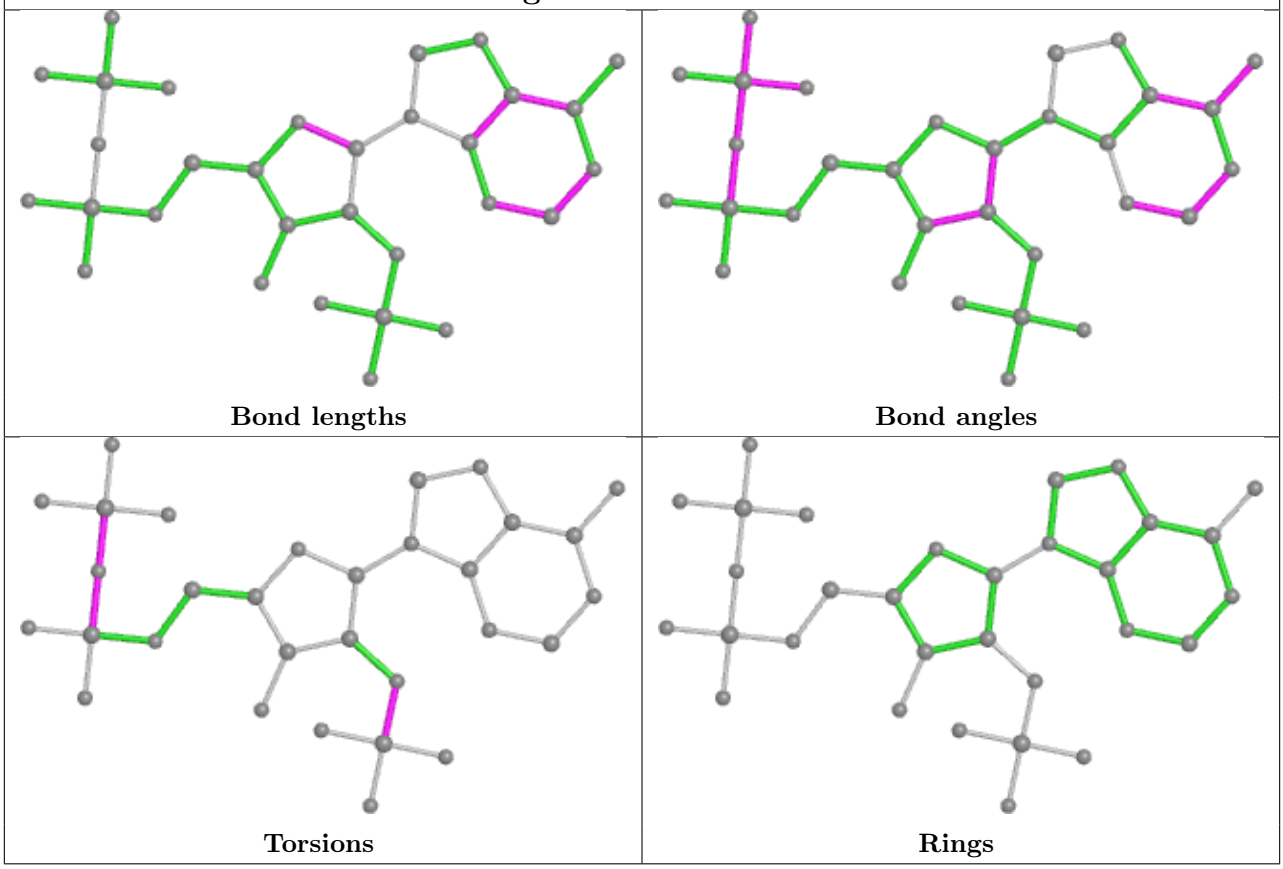


Torsions



Rings

Ligand NAP B 703



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	606/618 (98%)	-0.07	5 (0%)	86	89	30, 47, 72, 95	0
1	B	602/618 (97%)	0.16	12 (1%)	65	71	36, 60, 83, 91	0
All	All	1208/1236 (97%)	0.04	17 (1%)	75	80	30, 53, 80, 95	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	525	PHE	4.4
1	B	418	LEU	4.0
1	A	415	GLY	3.3
1	A	239	THR	3.0
1	B	143	TYR	2.9
1	B	484	LYS	2.6
1	B	503	ALA	2.6
1	A	411	SER	2.5
1	B	526	LYS	2.5
1	B	255	ASP	2.4
1	A	418	LEU	2.4
1	B	509	ARG	2.3
1	B	268	ARG	2.3
1	B	312	ASP	2.2
1	B	679	TRP	2.1
1	A	255	ASP	2.1
1	B	145	GLU	2.1

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)

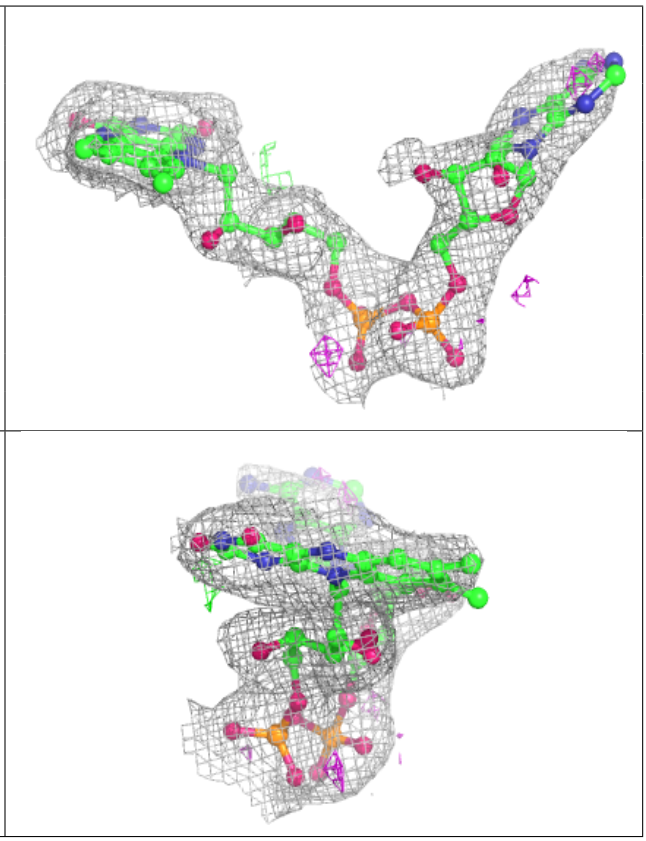
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

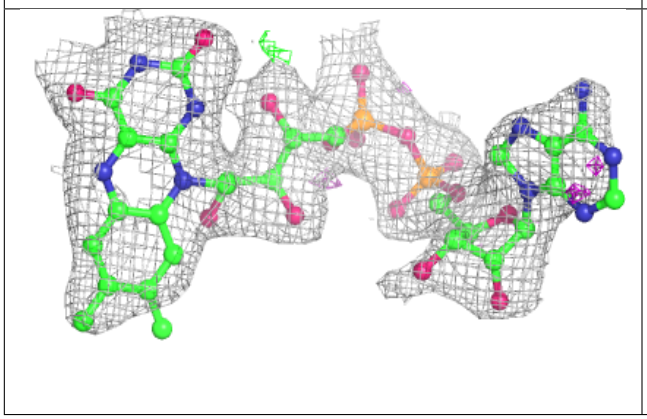
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FAD	B	702	53/53	0.93	0.19	49,68,83,85	0
4	NAP	A	703	31/48	0.95	0.10	43,54,77,85	0
4	NAP	B	703	31/48	0.95	0.15	56,61,84,90	0
2	FMN	B	701	31/31	0.96	0.20	47,61,64,65	0
3	FAD	A	702	53/53	0.97	0.15	32,37,50,52	0
2	FMN	A	701	31/31	0.97	0.17	35,43,47,50	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 702:

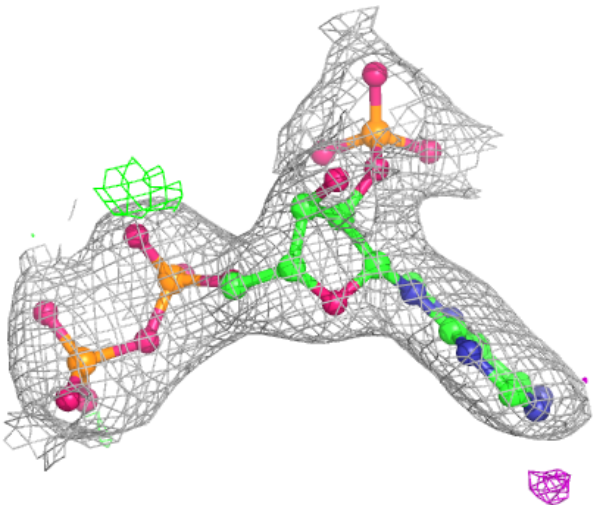
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

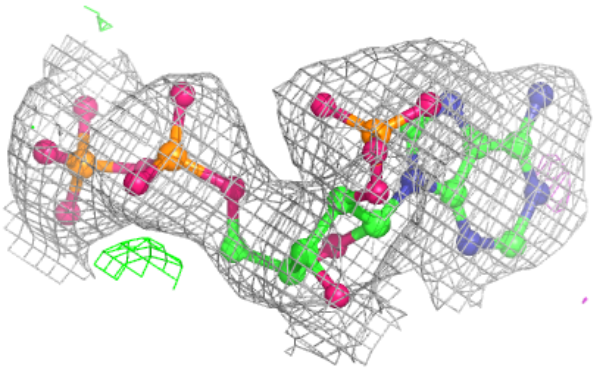


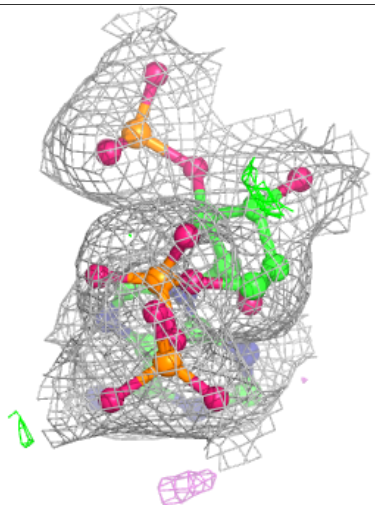


Electron density around NAP A 703:

$2mF_o$-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 703:

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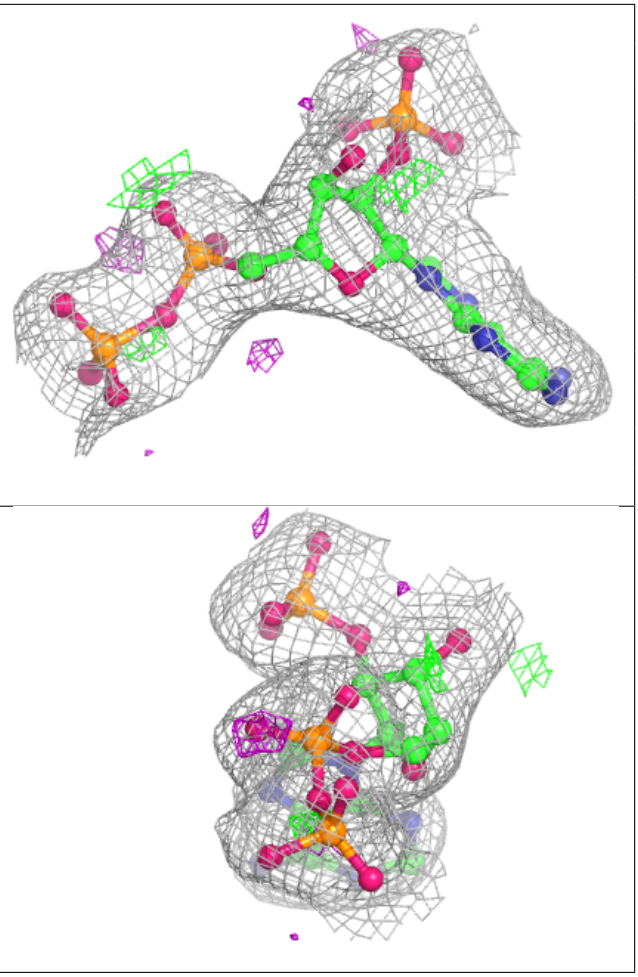
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN B 701:

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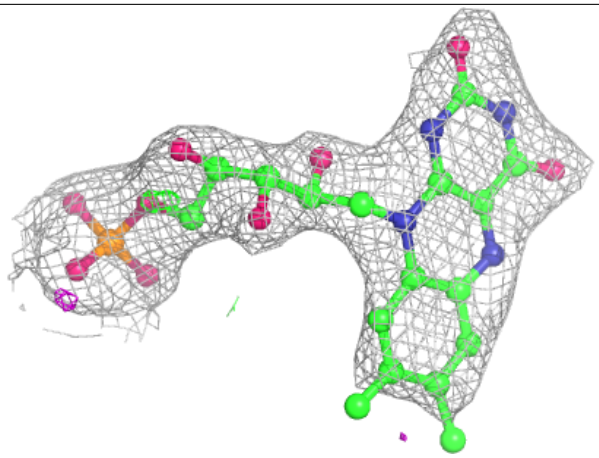
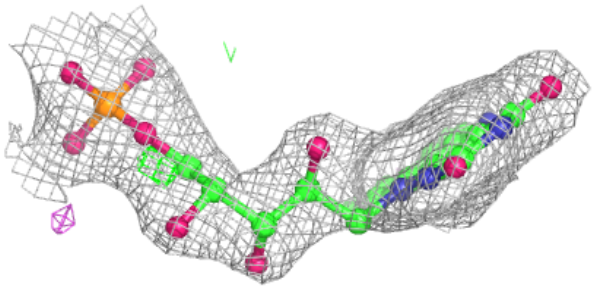
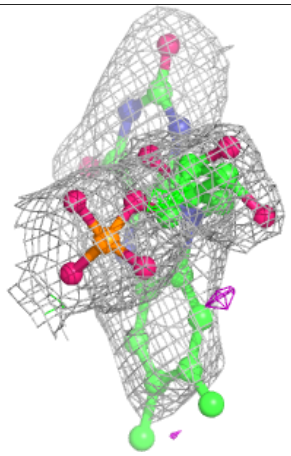
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

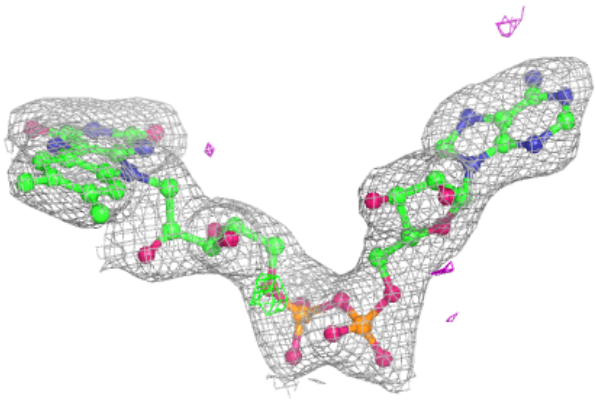


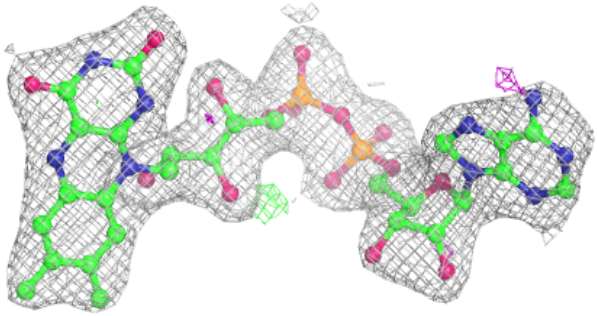


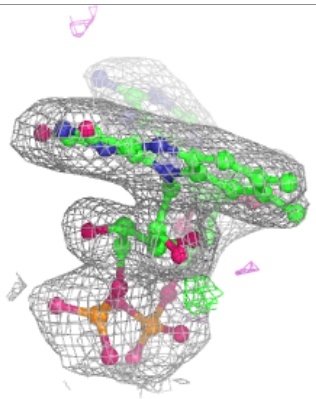


Electron density around FAD A 702:

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

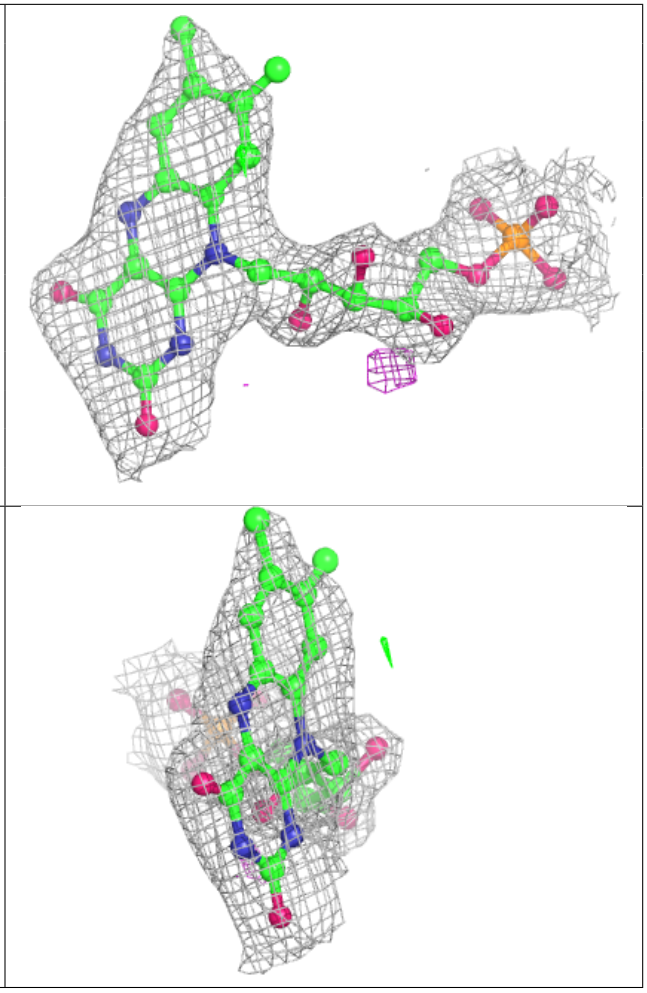






Electron density around FMN A 701:

$2mF_o$-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.