Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2026 – 09:14 am GMT

PDB ID	:	33QJ / pdb_000033qj
Title	:	Cytochrome P450 Reductases in complex with NADPH from Candida albicans
Authors	:	Opperman, D.J.; Ebrecht, A.C.
Deposited on	:	2026-08-19
Resolution	:	2.15 Å(reported)

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

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

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

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

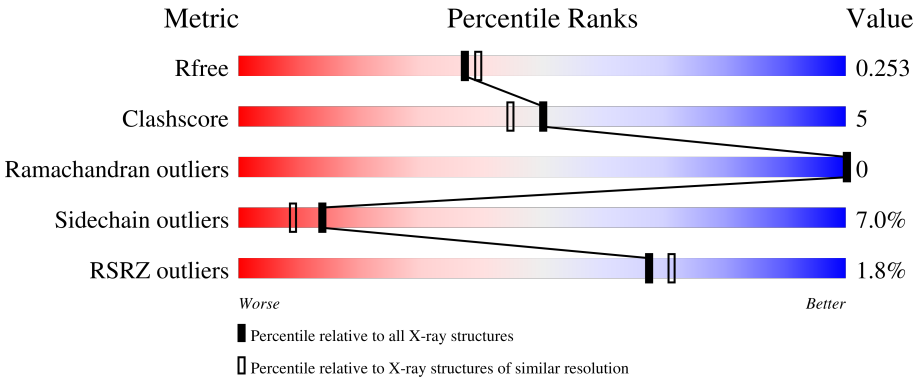
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

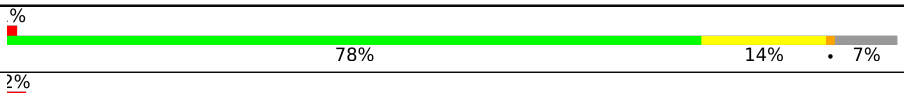
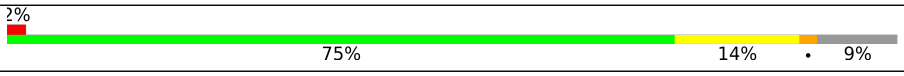
The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	680	
1	B	680	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10475 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.

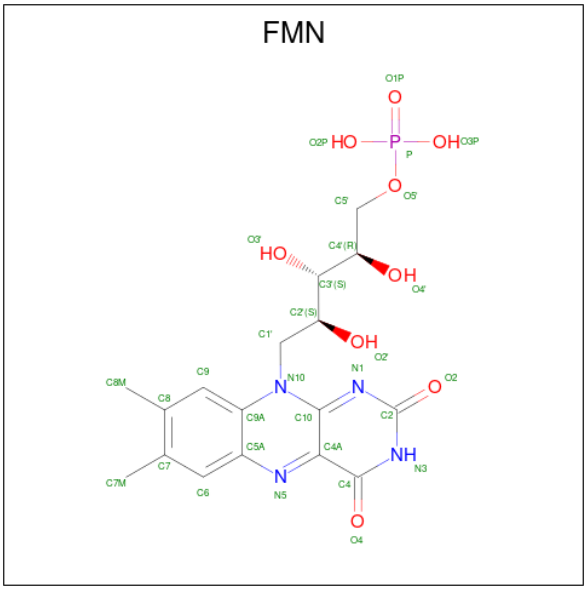
- Molecule 1 is a protein called NADPH–cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	635	Total	C	N	O	S	0	1	0
			5092	3221	862	1002	7			
1	B	617	Total	C	N	O	S	0	0	0
			4944	3131	834	972	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	ASN	HIS	conflict	UNP A0A1D8PLR7
B	238	ASN	HIS	conflict	UNP A0A1D8PLR7

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



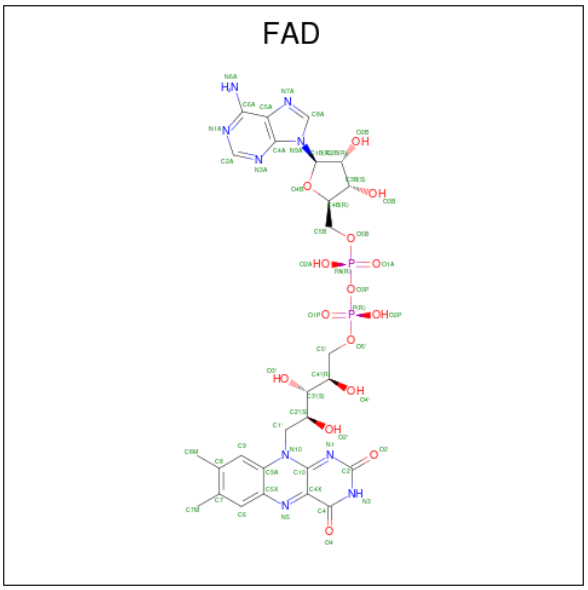
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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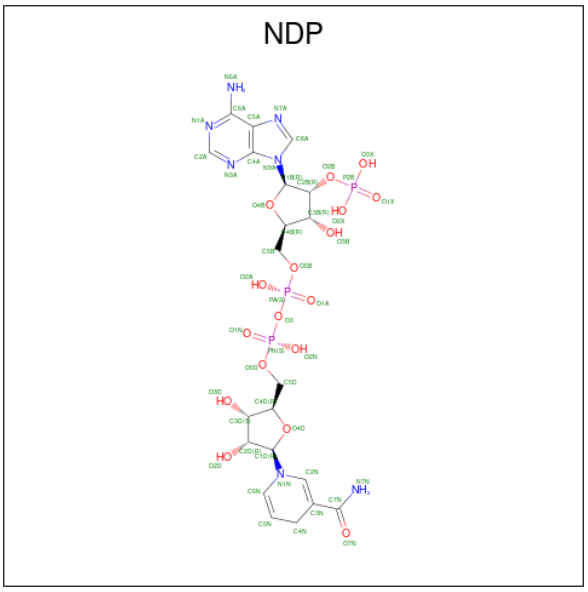
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



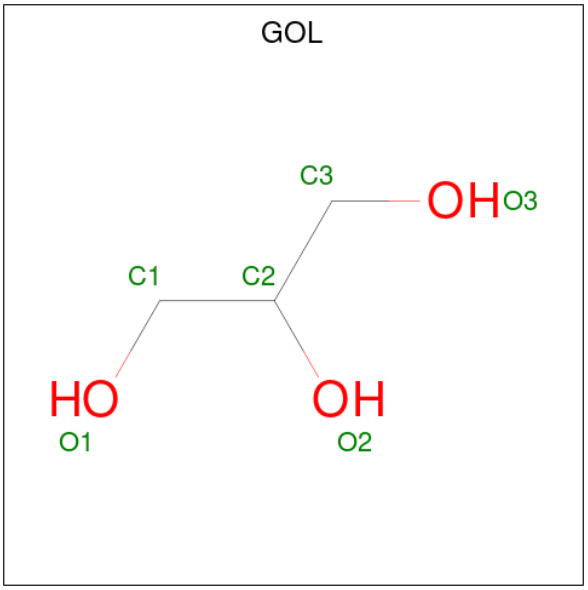
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			6	3	3			
5	B	1	Total	C	O		0	0
			6	3	3			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

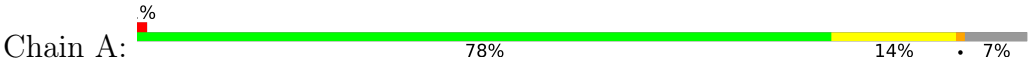
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	106	Total O 106 106	0	0
6	B	79	Total O 79 79	0	0

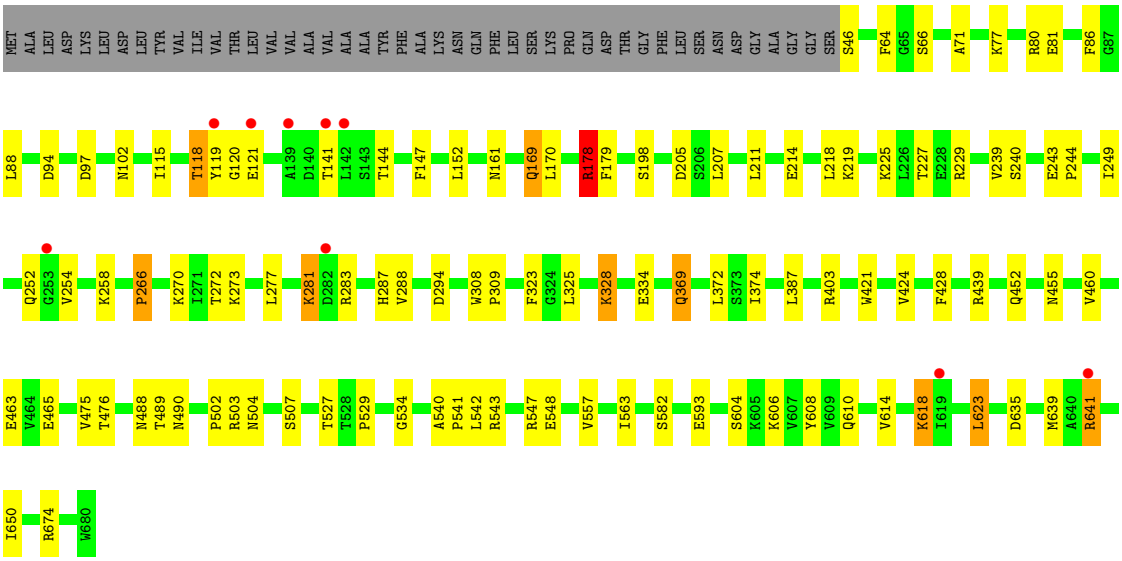
3 Residue-property plots (i)

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

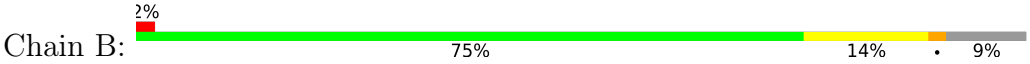
Chain A:

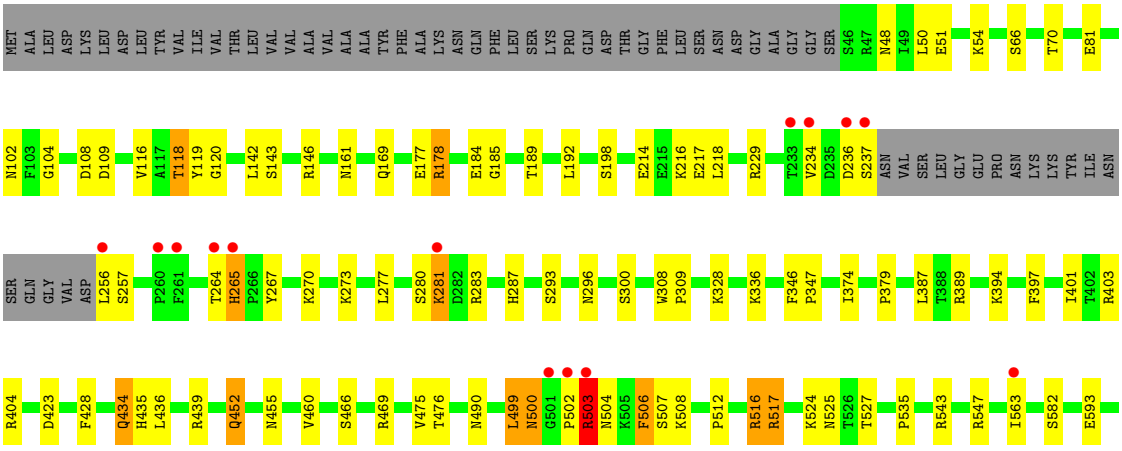


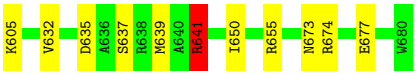


• Molecule 1: NADPH–cytochrome P450 reductase

Chain B:






K605
V632
D635
A636
S637
R638
M639
A640
R641
I650
R655
N673
R674
E677
W680

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.57Å 106.00Å 116.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.61 – 2.15 78.49 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.3 (78.61-2.15) 99.3 (78.49-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.203 , 0.252 0.212 , 0.253	Depositor DCC
R_{free} test set	3525 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10475	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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

5.1 Standard geometry

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

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	0.83	0/5198	1.31	3/7037 (0.0%)
1	B	0.82	0/5047	1.32	1/6832 (0.0%)
All	All	0.83	0/10245	1.32	4/13869 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	11
All	All	0	15

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	674	ARG	N-CA-C	-5.95	106.19	113.50
1	B	674	ARG	N-CA-C	-5.69	106.38	113.38
1	A	179	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	323	PHE	N-CA-CB	-5.43	102.63	110.56

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	ARG	Sidechain
1	A	229	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	283	ARG	Sidechain
1	A	641[A]	ARG	Sidechain
1	B	146	ARG	Sidechain
1	B	178	ARG	Sidechain
1	B	229	ARG	Sidechain
1	B	283	ARG	Sidechain
1	B	404	ARG	Sidechain
1	B	469	ARG	Sidechain
1	B	503	ARG	Sidechain
1	B	516	ARG	Sidechain
1	B	517	ARG	Sidechain
1	B	641	ARG	Sidechain
1	B	655	ARG	Sidechain

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	5092	0	4955	57	0
1	B	4944	0	4808	50	0
2	A	31	0	19	0	0
2	B	31	0	19	2	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	31	0	11	1	0
4	B	31	0	11	1	0
5	A	6	0	8	1	0
5	B	18	0	24	3	0
6	A	106	0	0	3	0
6	B	79	0	0	2	0
All	All	10475	0	9917	108	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 5.

All (108) 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:455:ASN:HD22	1:A:543:ARG:HH12	1.31	0.76
1:B:256:LEU:HB3	1:B:267:TYR:HE1	1.52	0.74
1:B:455:ASN:HD22	1:B:543:ARG:HH12	1.35	0.71
1:B:435:HIS:HD2	1:B:436:LEU:O	1.74	0.69
1:B:379:PRO:O	5:B:706:GOL:H12	1.94	0.68
1:B:118:THR:HG21	1:B:161:ASN:HA	1.79	0.63
1:B:48:ASN:ND2	1:B:51:GLU:HG2	2.16	0.60
1:B:346:PHE:HB2	1:B:347:PRO:HD2	1.84	0.60
1:B:435:HIS:CD2	1:B:436:LEU:O	2.57	0.57
1:A:635:ASP:OD1	5:A:704:GOL:O3	2.23	0.55
1:A:563:ILE:CD1	1:A:593:GLU:HB3	2.37	0.54
1:A:452:GLN:HA	1:A:452:GLN:OE1	2.08	0.54
1:B:277:LEU:HD11	1:B:287:HIS:HB2	1.90	0.54
1:A:118:THR:HG21	1:A:161:ASN:HA	1.91	0.51
1:A:152:LEU:C	1:A:161:ASN:HD21	2.19	0.51
1:A:540:ALA:HB3	1:A:541:PRO:HD3	1.91	0.51
1:B:118:THR:HG21	1:B:161:ASN:CA	2.40	0.51
1:A:325:LEU:HA	1:A:328:LYS:HG3	1.91	0.50
1:A:239:VAL:O	1:A:503:ARG:NH2	2.38	0.50
1:A:610:GLN:OE1	4:A:703:NDP:H2A	2.11	0.50
1:B:374:ILE:HG13	1:B:428:PHE:CE1	2.46	0.50
1:A:240:SER:HB2	1:A:249:ILE:HD11	1.94	0.50
1:A:614:VAL:HA	1:A:650:ILE:HD11	1.93	0.50
1:A:64:PHE:CZ	1:A:94:ASP:HB2	2.47	0.49
1:A:460:VAL:HA	1:A:476:THR:HB	1.94	0.49
1:A:207:LEU:HD23	1:A:211:LEU:HD12	1.93	0.49
1:A:277:LEU:HD11	1:A:287:HIS:HB2	1.95	0.49
1:A:227:THR:HB	1:A:334:GLU:HG2	1.94	0.49
1:A:502:PRO:O	1:A:502:PRO:HG2	2.13	0.49
1:A:543:ARG:O	1:A:547:ARG:HG3	2.12	0.48
1:A:81:GLU:HG3	1:A:218:LEU:HD13	1.95	0.48
1:B:185:GLY:HA3	1:B:192:LEU:HD12	1.95	0.48
1:A:614:VAL:HG23	1:B:189:THR:HG22	1.96	0.48
1:B:293:SER:HA	1:B:452:GLN:HG3	1.95	0.48
1:A:77:LYS:HG2	1:A:80:ARG:HH22	1.78	0.48
1:A:369:GLN:NE2	1:A:372:LEU:HD12	2.29	0.48
1:B:641:ARG:HD2	1:B:641:ARG:HA	1.53	0.47
1:A:374:ILE:HG13	1:A:428:PHE:CE1	2.48	0.47
1:B:346:PHE:HB2	1:B:347:PRO:CD	2.44	0.47
1:A:529:PRO:HB2	1:A:623:LEU:HD13	1.95	0.47
1:A:86:PHE:CB	1:A:88:LEU:CD1	2.93	0.47
1:B:161:ASN:ND2	1:B:184:GLU:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ARG:HD2	1:B:503:ARG:HA	1.56	0.47
1:B:504:ASN:C	1:B:506:PHE:N	2.72	0.47
1:A:86:PHE:HB3	1:A:88:LEU:CD1	2.45	0.46
1:B:460:VAL:HA	1:B:476:THR:HB	1.96	0.46
1:A:489:THR:O	1:A:490:ASN:HB2	2.14	0.46
1:B:256:LEU:HB3	1:B:267:TYR:CE1	2.41	0.46
1:A:452:GLN:HB2	6:A:887:HOH:O	2.14	0.46
1:A:240:SER:HB2	1:A:249:ILE:CD1	2.45	0.46
1:B:308:TRP:HB2	1:B:512:PRO:HB2	1.98	0.46
1:A:266:PRO:HB3	1:A:308:TRP:CE2	2.51	0.45
1:A:77:LYS:HG2	1:A:80:ARG:NH2	2.31	0.45
1:A:328:LYS:HB3	1:A:328:LYS:HE3	1.49	0.45
4:B:703:NDP:H52A	6:B:870:HOH:O	2.17	0.45
1:B:525:ASN:OD1	1:B:527:THR:OG1	2.25	0.45
1:A:97:ASP:OD2	6:A:801:HOH:O	2.20	0.45
1:B:309:PRO:HB3	1:B:475:VAL:HG22	1.99	0.45
1:B:434:GLN:HB3	6:B:821:HOH:O	2.16	0.45
1:B:632:VAL:O	1:B:677:GLU:HA	2.16	0.45
1:A:152:LEU:HD12	1:A:152:LEU:N	2.31	0.44
1:A:281:LYS:HE3	1:A:281:LYS:HB2	1.73	0.44
1:A:169:GLN:HG3	1:A:170:LEU:N	2.33	0.44
1:B:257:SER:HB3	1:B:296:ASN:H	1.83	0.44
1:A:463:GLU:OE2	1:A:465:GLU:OE2	2.35	0.44
1:A:147:PHE:CE2	1:A:178:ARG:HG3	2.53	0.44
1:A:529:PRO:HB2	1:A:623:LEU:CD1	2.48	0.44
1:B:118:THR:CG2	1:B:161:ASN:HA	2.46	0.43
1:B:397:PHE:O	1:B:401:ILE:HB	2.17	0.43
1:A:308:TRP:HA	1:A:309:PRO:HD3	1.90	0.43
1:B:502:PRO:HG2	1:B:507:SER:HB3	2.00	0.43
1:B:639:MET:HE3	1:B:639:MET:HB3	1.94	0.43
1:B:50:LEU:HD12	1:B:102:ASN:ND2	2.33	0.43
1:B:104:GLY:HA2	1:B:142:LEU:HD23	2.00	0.43
1:A:66:SER:HB2	1:A:71:ALA:HB3	2.01	0.43
1:B:81:GLU:HG3	1:B:218:LEU:HD13	1.99	0.43
1:A:618:LYS:HB3	1:A:618:LYS:HE3	1.56	0.43
1:A:421:TRP:HB3	1:A:424:VAL:HG23	1.99	0.43
1:A:102:ASN:ND2	1:A:102:ASN:H	2.16	0.43
1:A:102:ASN:H	1:A:102:ASN:HD22	1.67	0.42
1:B:281:LYS:HA	1:B:281:LYS:HD2	1.32	0.42
1:B:439:ARG:HB2	1:B:475:VAL:HG21	2.01	0.42
1:B:524:LYS:HA	1:B:524:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:ARG:O	1:B:547:ARG:HG3	2.19	0.42
1:B:70:THR:OG1	2:B:701:FMN:O2P	2.28	0.42
1:B:66:SER:OG	2:B:701:FMN:O1P	2.31	0.42
1:A:563:ILE:HD13	1:A:563:ILE:HA	1.65	0.42
1:B:508:LYS:HD3	1:B:508:LYS:HA	1.60	0.42
1:A:225:LYS:HA	6:A:829:HOH:O	2.19	0.42
1:A:374:ILE:CG2	1:A:387:LEU:HD21	2.50	0.42
1:B:535:PRO:HG3	1:B:639:MET:HG3	2.00	0.42
1:A:243:GLU:HA	1:A:244:PRO:HD3	1.94	0.41
1:B:563:ILE:CD1	1:B:593:GLU:HB3	2.49	0.41
1:B:503:ARG:O	1:B:504:ASN:C	2.64	0.41
1:B:499:LEU:O	1:B:500:ASN:C	2.62	0.41
1:A:86:PHE:HB2	1:A:88:LEU:CD1	2.51	0.41
1:A:288:VAL:O	1:A:455:ASN:HA	2.21	0.41
1:A:439:ARG:HB2	1:A:475:VAL:HG21	2.01	0.41
1:A:534:GLY:HA3	1:A:542:LEU:HD12	2.03	0.41
1:B:300:SER:HB2	1:B:517:ARG:HH12	1.86	0.41
1:B:635:ASP:OD1	1:B:637:SER:OG	2.33	0.41
1:A:118:THR:HG21	1:A:161:ASN:CA	2.51	0.41
1:B:119:TYR:O	1:B:120:GLY:C	2.64	0.40
1:B:423:ASP:OD2	5:B:706:GOL:H32	2.21	0.40
1:A:606:LYS:HD2	1:A:608:TYR:CZ	2.57	0.40
1:B:264:THR:O	1:B:265:HIS:C	2.64	0.40
1:A:119:TYR:O	1:A:120:GLY:C	2.64	0.40
5:B:704:GOL:O1	5:B:704:GOL:O3	2.36	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	634/680 (93%)	606 (96%)	28 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	613/680 (90%)	588 (96%)	25 (4%)	0	100 100
All	All	1247/1360 (92%)	1194 (96%)	53 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	562/596 (94%)	525 (93%)	37 (7%)	15 10
1	B	545/596 (91%)	504 (92%)	41 (8%)	12 8
All	All	1107/1192 (93%)	1029 (93%)	78 (7%)	14 9

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	A	115	ILE
1	A	118	THR
1	A	121	GLU
1	A	141	THR
1	A	144	THR
1	A	169	GLN
1	A	178	ARG
1	A	198	SER
1	A	205	ASP
1	A	214	GLU
1	A	219	LYS
1	A	252	GLN
1	A	254	VAL
1	A	258	LYS
1	A	266	PRO
1	A	270	LYS
1	A	272	THR

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Mol	Chain	Res	Type
1	A	273	LYS
1	A	281	LYS
1	A	294	ASP
1	A	328	LYS
1	A	369	GLN
1	A	403	ARG
1	A	488	ASN
1	A	504	ASN
1	A	507	SER
1	A	527	THR
1	A	548	GLU
1	A	557	VAL
1	A	582	SER
1	A	604	SER
1	A	618	LYS
1	A	623	LEU
1	A	639	MET
1	A	641[A]	ARG
1	A	641[B]	ARG
1	B	54	LYS
1	B	108	ASP
1	B	109	ASP
1	B	116	VAL
1	B	118	THR
1	B	143	SER
1	B	169	GLN
1	B	177	GLU
1	B	178	ARG
1	B	198	SER
1	B	214	GLU
1	B	216	LYS
1	B	217	GLU
1	B	234	VAL
1	B	236	ASP
1	B	237	SER
1	B	265	HIS
1	B	270	LYS
1	B	273	LYS
1	B	280	SER
1	B	281	LYS
1	B	328	LYS
1	B	336	LYS

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Mol	Chain	Res	Type
1	B	387	LEU
1	B	389	ARG
1	B	394	LYS
1	B	403	ARG
1	B	434	GLN
1	B	452	GLN
1	B	466	SER
1	B	490	ASN
1	B	499	LEU
1	B	500	ASN
1	B	503	ARG
1	B	506	PHE
1	B	516	ARG
1	B	582	SER
1	B	605	LYS
1	B	641	ARG
1	B	650	ILE
1	B	673	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	102	ASN
1	A	161	ASN
1	A	210	ASN
1	A	284	ASN
1	A	359	HIS
1	A	369	GLN
1	A	392	ASN
1	A	435	HIS
1	A	455	ASN
1	A	490	ASN
1	A	579	GLN
1	A	621	ASN
1	A	625	ASN
1	B	76	ASN
1	B	83	HIS
1	B	169	GLN
1	B	209	ASN
1	B	223	ASN
1	B	435	HIS

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Mol	Chain	Res	Type
1	B	455	ASN
1	B	486	GLN
1	B	500	ASN
1	B	514	HIS
1	B	621	ASN
1	B	625	ASN
1	B	626	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	FMN	A	701	-	33,33,33	0.70	0	48,50,50	0.68	1 (2%)
5	GOL	B	705	-	5,5,5	0.06	0	5,5,5	0.28	0
4	NDP	A	703	-	31,33,52	0.81	0	48,52,80	1.58	10 (20%)
5	GOL	A	704	-	5,5,5	0.13	0	5,5,5	0.67	0
5	GOL	B	706	-	5,5,5	0.28	0	5,5,5	0.81	0
4	NDP	B	703	-	31,33,52	0.97	2 (6%)	48,52,80	1.72	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FAD	A	702	-	56,58,58	0.69	0	81,89,89	1.11	7 (8%)
2	FMN	B	701	-	33,33,33	1.72	3 (9%)	48,50,50	1.13	4 (8%)
3	FAD	B	702	-	56,58,58	0.68	0	81,89,89	1.00	5 (6%)
5	GOL	B	704	-	5,5,5	0.08	0	5,5,5	0.51	0

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	FMN	A	701	-	-	0/18/18/18	0/3/3/3
5	GOL	B	705	-	-	1/4/4/4	-
4	NDP	A	703	-	-	6/21/37/77	0/3/3/5
5	GOL	A	704	-	-	0/4/4/4	-
5	GOL	B	706	-	-	2/4/4/4	-
4	NDP	B	703	-	-	10/21/37/77	0/3/3/5
3	FAD	A	702	-	-	4/34/50/50	0/6/6/6
2	FMN	B	701	-	-	0/18/18/18	0/3/3/3
3	FAD	B	702	-	-	4/34/50/50	0/6/6/6
5	GOL	B	704	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FMN	C1'-C2'	8.68	1.64	1.52
4	B	703	NDP	P2B-O2B	3.04	1.65	1.59
4	B	703	NDP	O5B-C5B	-2.68	1.34	1.44
2	B	701	FMN	C4A-N5	2.32	1.35	1.30
2	B	701	FMN	O2'-C2'	2.05	1.47	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	703	NDP	O5D-PN-O3	-6.69	82.19	104.64
4	A	703	NDP	O5D-PN-O3	-4.83	88.43	104.64
2	B	701	FMN	C4'-C3'-C2'	4.02	121.73	113.36
4	A	703	NDP	O3B-C3B-C4B	3.90	122.34	111.05
3	A	702	FAD	O2'-C2'-C1'	3.89	119.19	109.80
3	B	702	FAD	C5'-C4'-C3'	-3.58	105.29	112.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	703	NDP	O2N-PN-O1N	3.53	124.48	110.68
4	B	703	NDP	O4B-C4B-C5B	-3.52	97.78	109.37
3	A	702	FAD	C5'-C4'-C3'	-3.50	105.44	112.20
4	B	703	NDP	O3B-C3B-C4B	3.00	119.71	111.05
4	B	703	NDP	O4B-C1B-C2B	2.93	111.71	106.57
4	A	703	NDP	O4B-C1B-N9A	2.90	113.78	108.06
4	B	703	NDP	C2B-C1B-N9A	2.84	118.32	113.53
4	B	703	NDP	O2N-PN-O1N	2.82	121.70	110.68
4	A	703	NDP	O2B-C2B-C1B	2.73	119.92	110.10
3	A	702	FAD	P-O3P-PA	-2.62	123.82	132.83
3	B	702	FAD	O4'-C4'-C5'	2.62	115.81	109.92
4	B	703	NDP	C4A-N9A-C1B	-2.58	120.45	126.59
4	B	703	NDP	C3B-C2B-C1B	-2.55	98.09	102.89
3	A	702	FAD	C4A-N9A-C1B	2.54	132.66	126.59
4	A	703	NDP	PA-O5B-C5B	-2.51	106.98	121.68
3	B	702	FAD	O4B-C1B-C2B	-2.49	101.22	106.64
3	B	702	FAD	O2B-C2B-C1B	2.44	118.18	110.02
3	A	702	FAD	C1B-N9A-C8A	-2.42	121.66	127.14
3	B	702	FAD	O2A-PA-O1A	2.36	123.91	112.24
4	A	703	NDP	C4B-O4B-C1B	-2.34	104.31	109.47
4	B	703	NDP	O2B-C2B-C3B	-2.32	103.29	111.68
4	A	703	NDP	O4B-C4B-C5B	-2.29	101.82	109.37
2	B	701	FMN	C4-N3-C2	-2.18	121.61	125.64
4	A	703	NDP	O4B-C1B-C2B	2.17	110.38	106.57
3	A	702	FAD	O2'-C2'-C3'	-2.13	103.91	109.10
2	B	701	FMN	C4A-C4-N3	2.12	118.57	113.19
4	B	703	NDP	O2A-PA-O1A	2.05	122.35	112.24
2	B	701	FMN	C4-C4A-N5	2.03	121.12	118.23
3	A	702	FAD	O4B-C1B-C2B	-2.02	102.23	106.64
4	A	703	NDP	C3B-C2B-C1B	-2.02	99.10	102.89
2	A	701	FMN	C4-N3-C2	-2.01	121.93	125.64

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	NDP	C3B-C4B-C5B-O5B
4	A	703	NDP	C2B-C1B-N9A-C8A
4	B	703	NDP	C5B-O5B-PA-O2A
4	B	703	NDP	C5B-O5B-PA-O3
4	A	703	NDP	O4B-C4B-C5B-O5B
4	B	703	NDP	C2B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
5	B	704	GOL	C1-C2-C3-O3
5	B	706	GOL	C1-C2-C3-O3
5	B	704	GOL	O2-C2-C3-O3
5	B	706	GOL	O2-C2-C3-O3
3	B	702	FAD	C2B-C1B-N9A-C8A
3	A	702	FAD	C2B-C1B-N9A-C8A
3	A	702	FAD	O2'-C2'-C3'-C4'
4	B	703	NDP	C2B-O2B-P2B-O2X
4	B	703	NDP	C5B-O5B-PA-O1A
3	A	702	FAD	C2B-C1B-N9A-C4A
5	B	705	GOL	C1-C2-C3-O3
4	B	703	NDP	O4B-C1B-N9A-C8A
3	B	702	FAD	C2B-C1B-N9A-C4A
4	B	703	NDP	C2B-C1B-N9A-C4A
3	B	702	FAD	O4B-C1B-N9A-C8A
4	B	703	NDP	PA-O3-PN-O1N
4	B	703	NDP	O4B-C4B-C5B-O5B
4	A	703	NDP	C2B-O2B-P2B-O3X
4	B	703	NDP	C2B-O2B-P2B-O3X
3	A	702	FAD	O4B-C1B-N9A-C8A
3	B	702	FAD	PA-O3P-P-O2P
4	A	703	NDP	C5B-O5B-PA-O1A
4	A	703	NDP	C2B-C1B-N9A-C4A

There are no ring outliers.

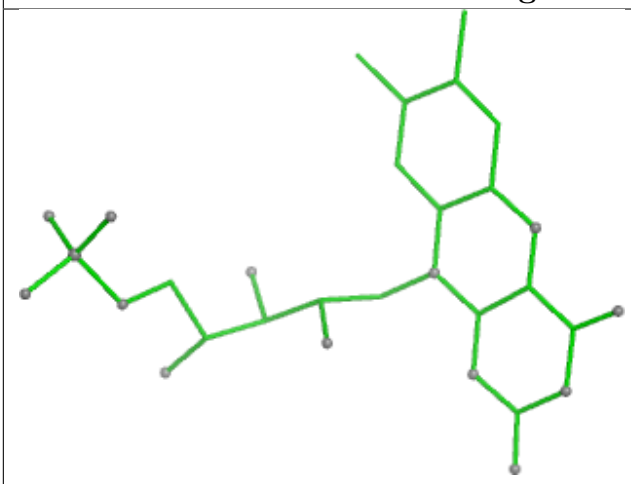
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	NDP	1	0
5	A	704	GOL	1	0
5	B	706	GOL	2	0
4	B	703	NDP	1	0
2	B	701	FMN	2	0
5	B	704	GOL	1	0

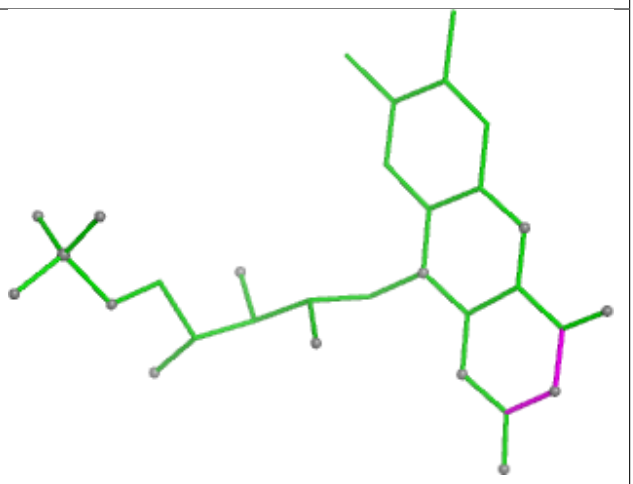
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

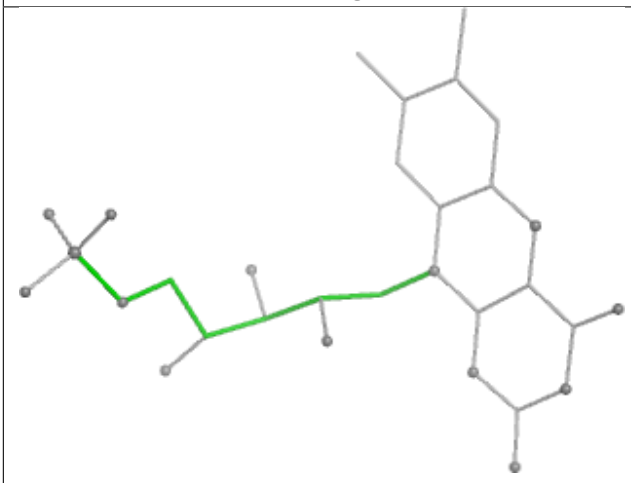
Ligand FMN A 701



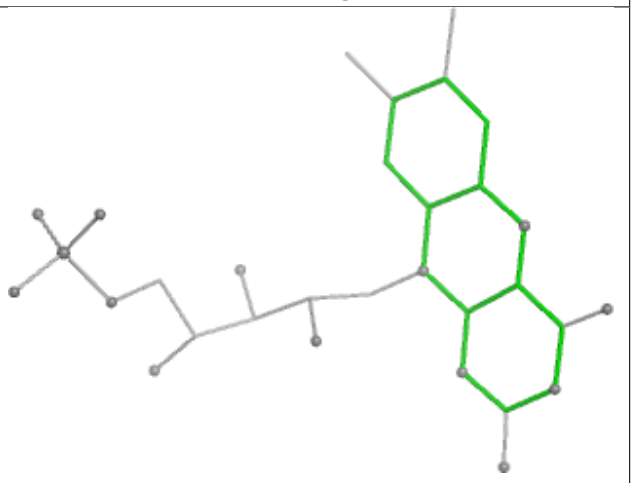
Bond lengths



Bond angles

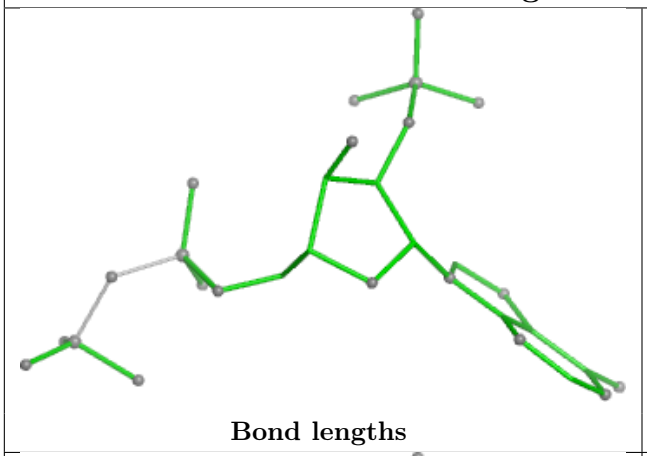


Torsions

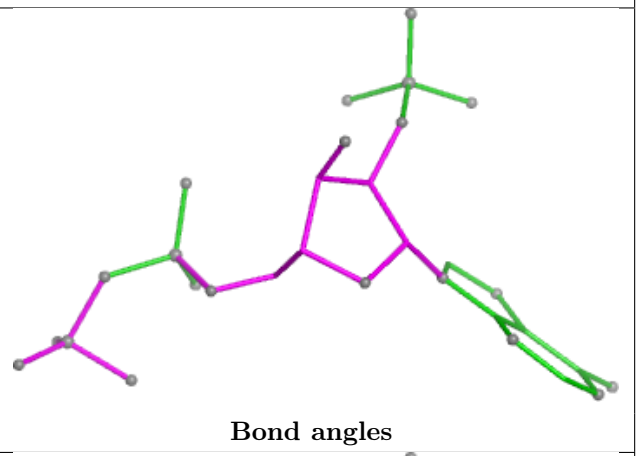


Rings

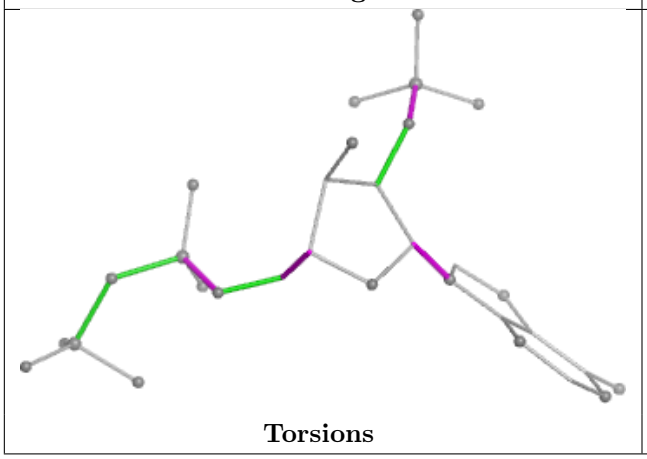
Ligand NDP A 703



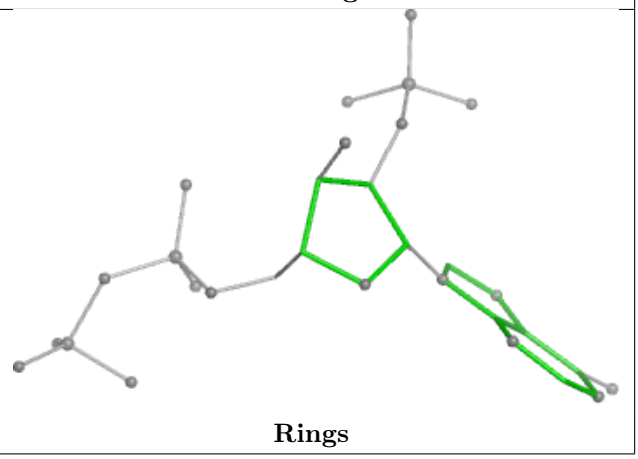
Bond lengths



Bond angles

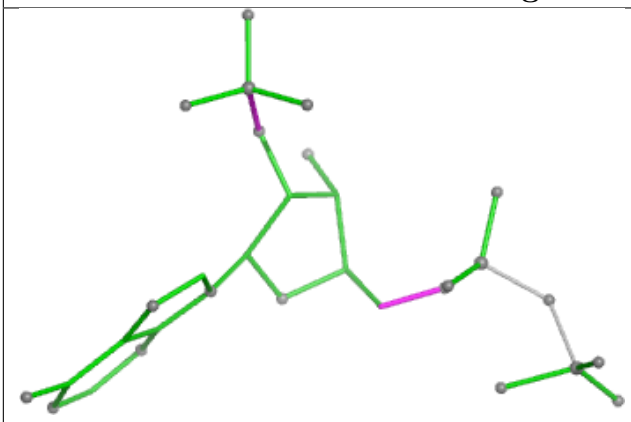


Torsions

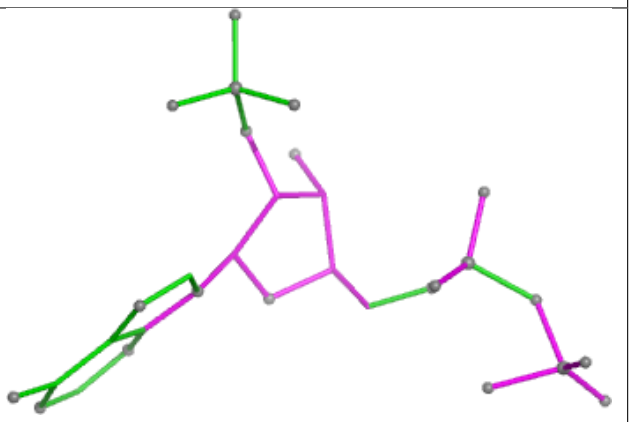


Rings

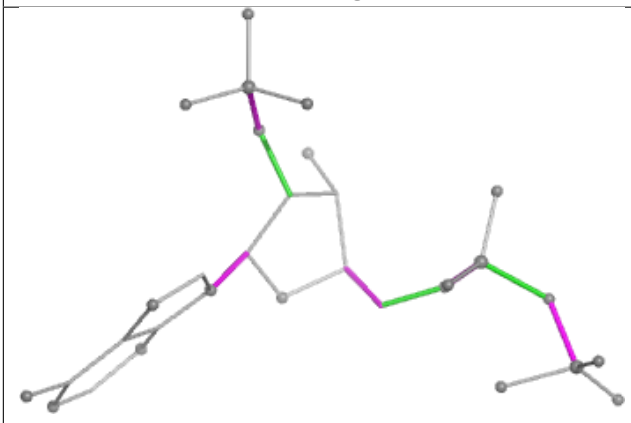
Ligand NDP B 703



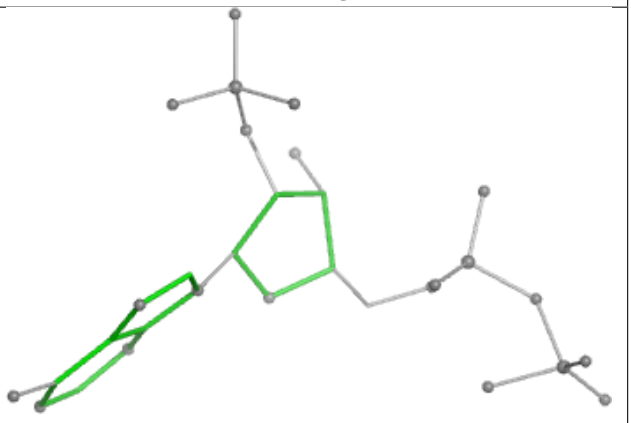
Bond lengths



Bond angles

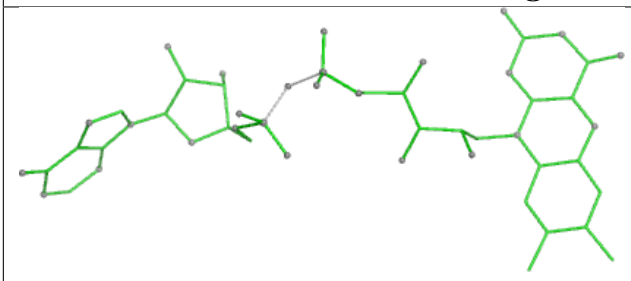


Torsions

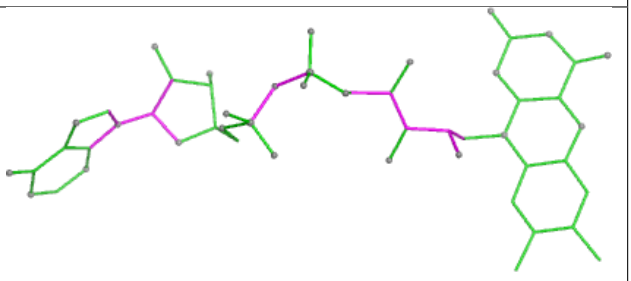


Rings

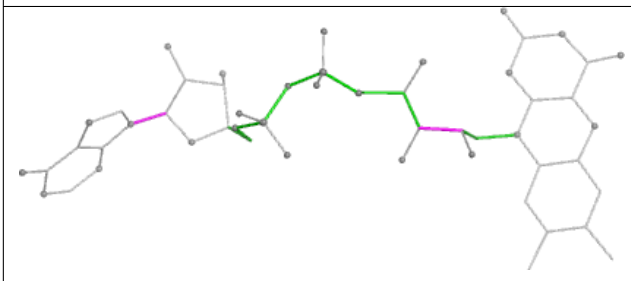
Ligand FAD A 702



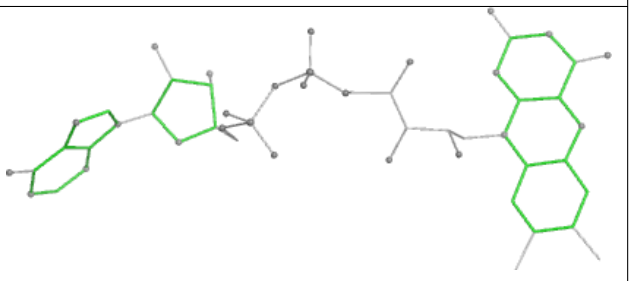
Bond lengths



Bond angles

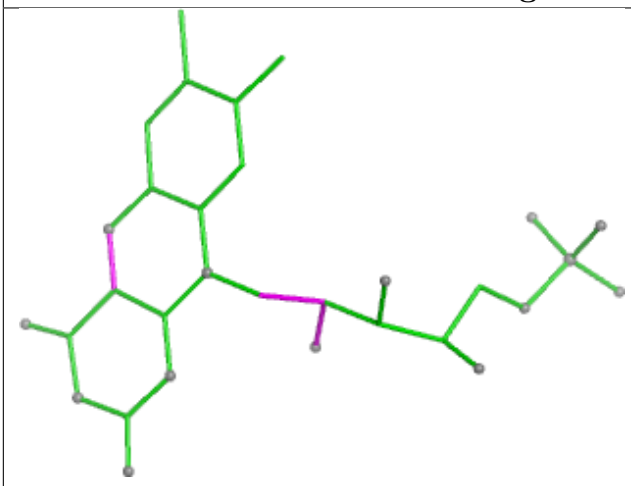


Torsions

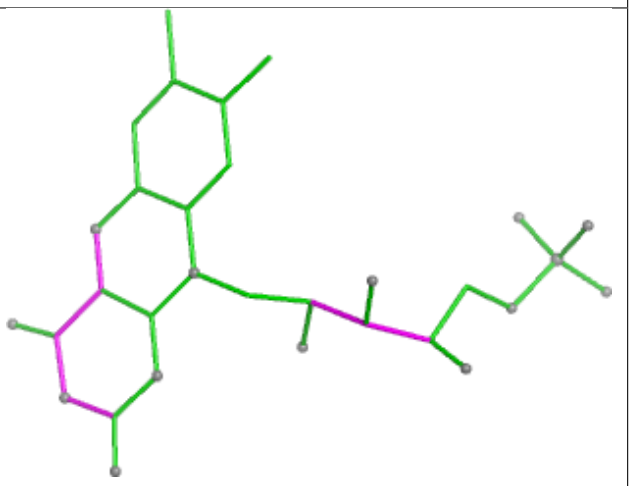


Rings

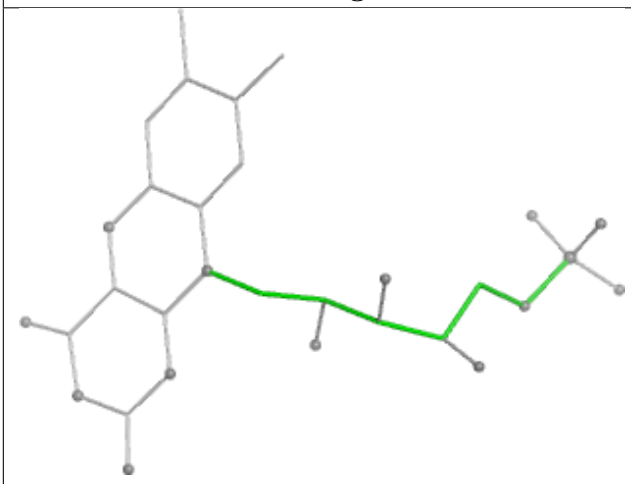
Ligand FMN B 701



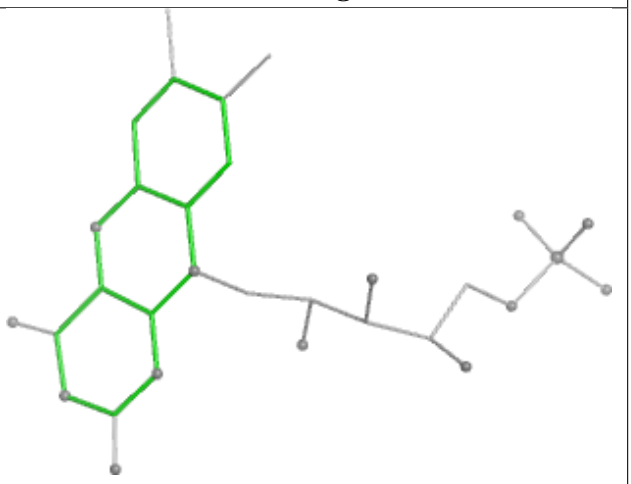
Bond lengths



Bond angles

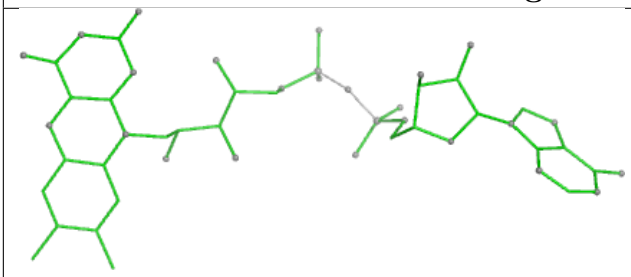


Torsions

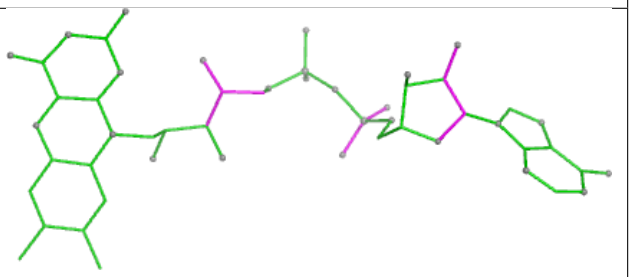


Rings

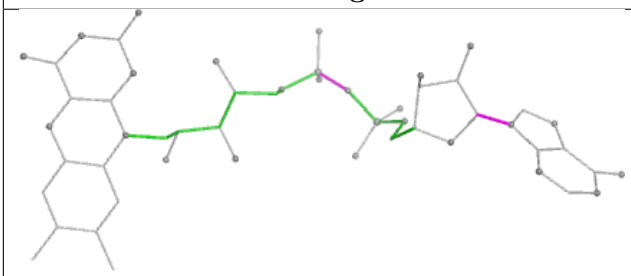
Ligand FAD B 702



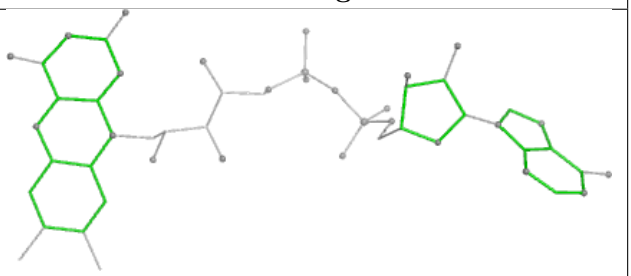
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	635/680 (93%)	0.11	9 (1%)	73	77	20, 52, 81, 124	1 (0%)
1	B	617/680 (90%)	0.13	14 (2%)	61	64	30, 49, 79, 195	0
All	All	1252/1360 (92%)	0.12	23 (1%)	67	71	20, 50, 81, 195	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	VAL	3.5
1	A	119	TYR	3.4
1	B	256	LEU	3.2
1	A	282	ASP	3.0
1	A	619	ILE	3.0
1	B	264	THR	2.9
1	B	260	PRO	2.9
1	B	503	ARG	2.9
1	B	237	SER	2.9
1	B	261	PHE	2.9
1	B	502	PRO	2.8
1	B	233	THR	2.5
1	A	253	GLY	2.5
1	A	121	GLU	2.4
1	B	236	ASP	2.4
1	B	501	GLY	2.3
1	A	641[A]	ARG	2.2
1	A	142	LEU	2.2
1	B	265	HIS	2.2
1	B	563	ILE	2.1
1	A	141	THR	2.1
1	B	281	LYS	2.1
1	A	139	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 oligosaccharides in this entry.

6.4 Ligands (i)

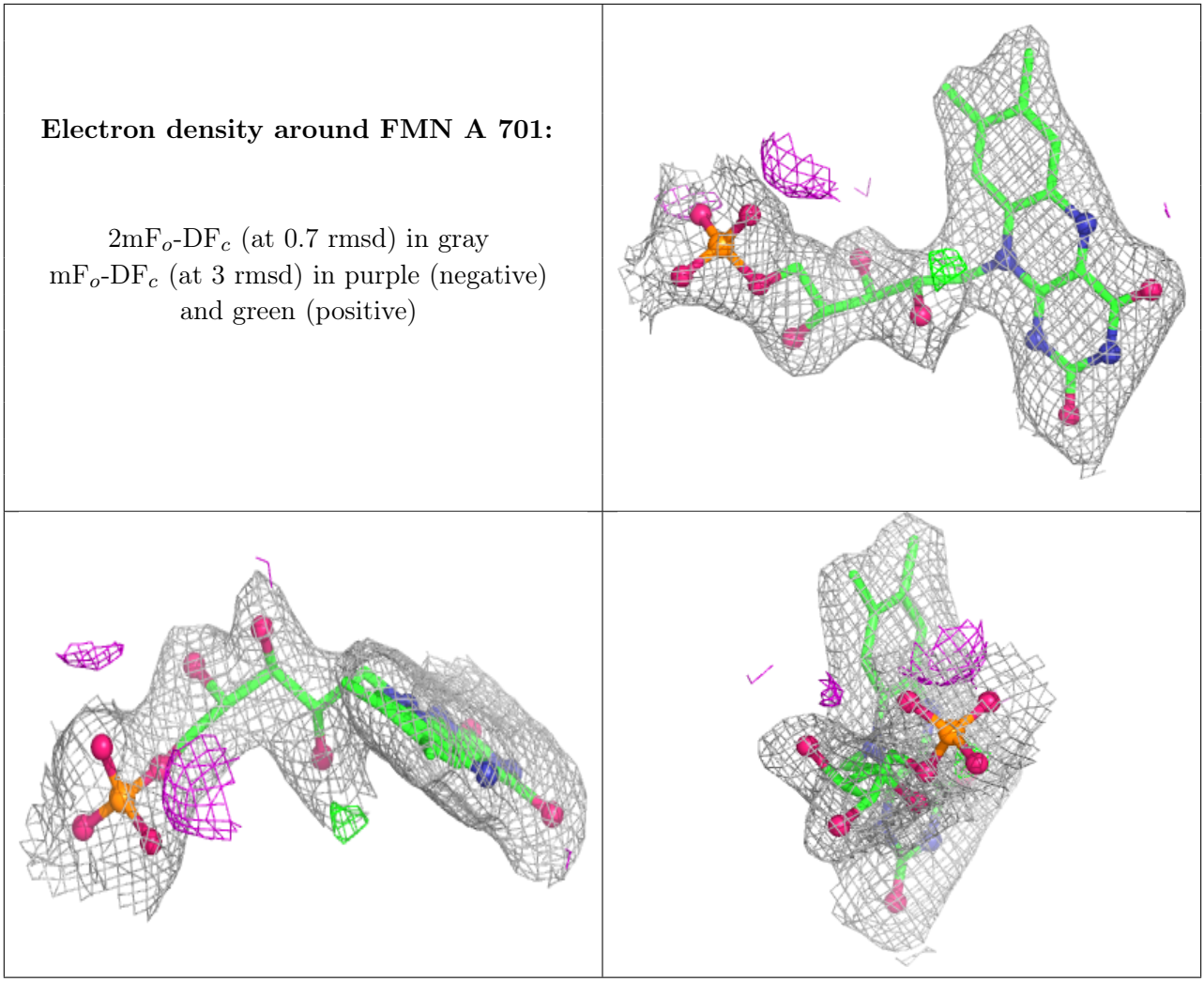
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	B	705	6/6	0.75	0.15	69,70,73,76	0
5	GOL	A	704	6/6	0.81	0.12	49,67,69,74	0
5	GOL	B	706	6/6	0.83	0.10	68,73,76,81	0
5	GOL	B	704	6/6	0.90	0.09	42,55,60,72	0
2	FMN	A	701	31/31	0.94	0.07	38,43,47,57	0
4	NDP	B	703	31/48	0.95	0.07	32,41,50,54	0
4	NDP	A	703	31/48	0.97	0.06	33,37,53,55	0
2	FMN	B	701	31/31	0.97	0.05	32,38,40,48	0
3	FAD	B	702	53/53	0.97	0.05	26,33,38,45	0
3	FAD	A	702	53/53	0.98	0.05	29,33,41,45	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.

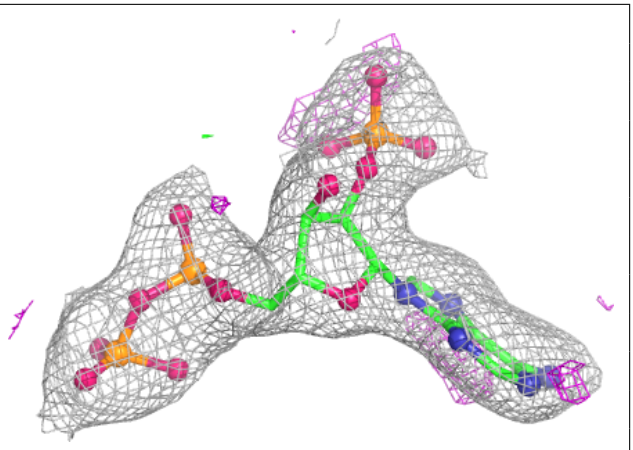
Electron density around FMN A 701:

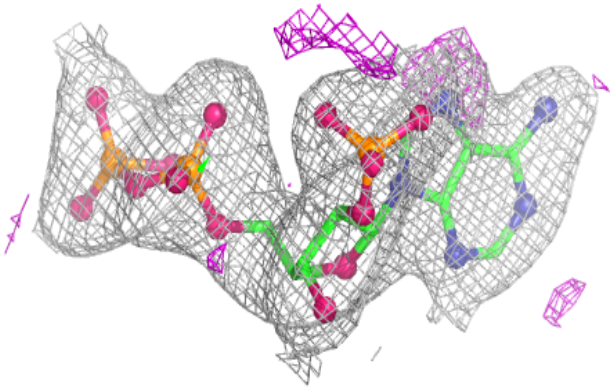
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

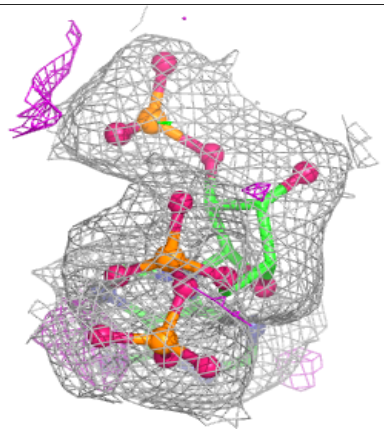


Electron density around NDP B 703:

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

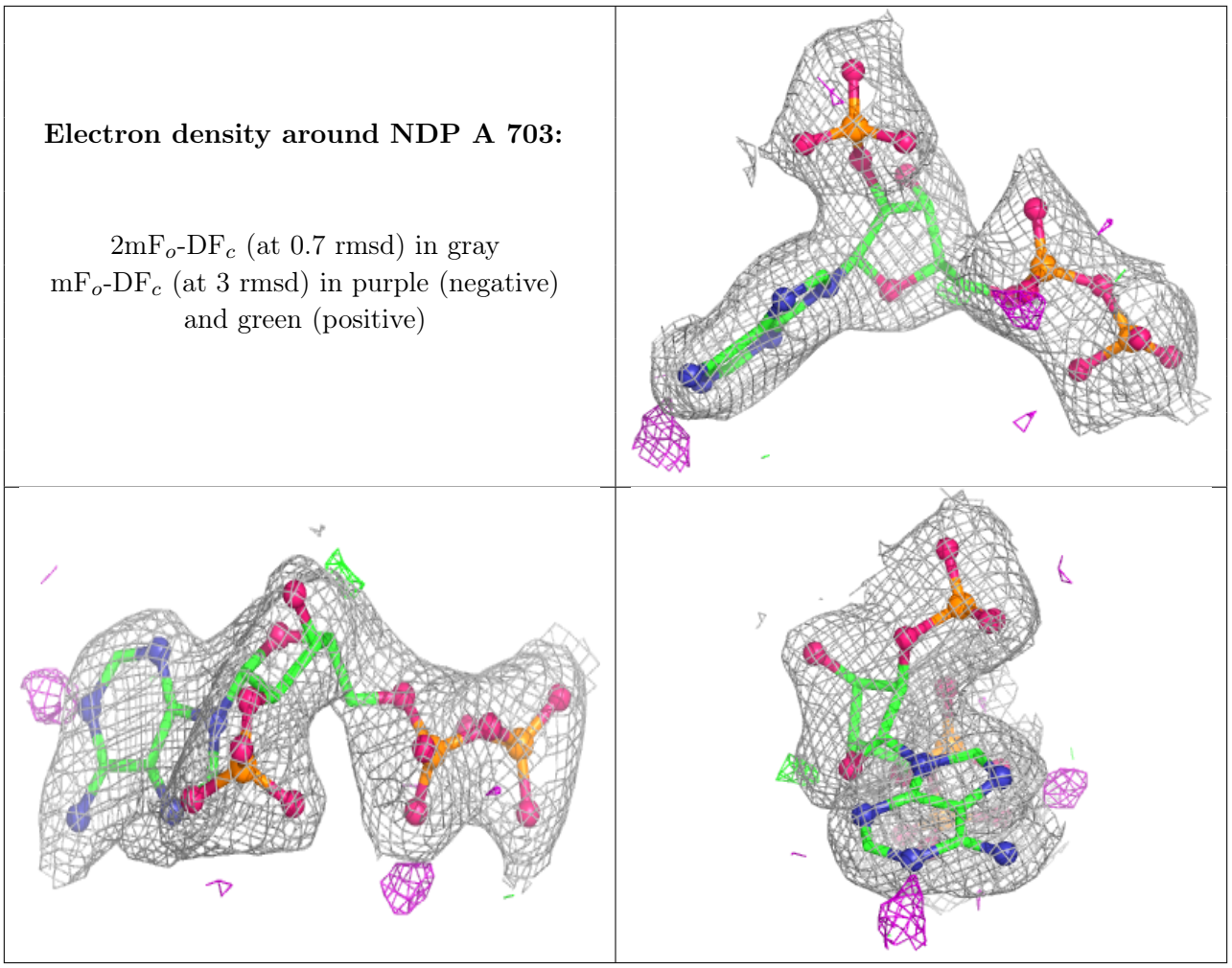






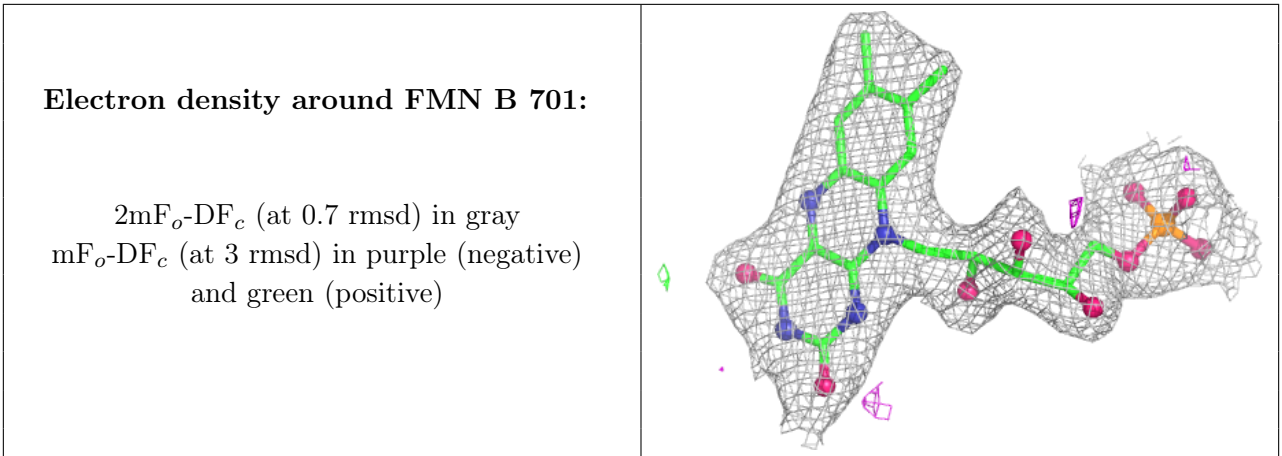
Electron density around NDP A 703:

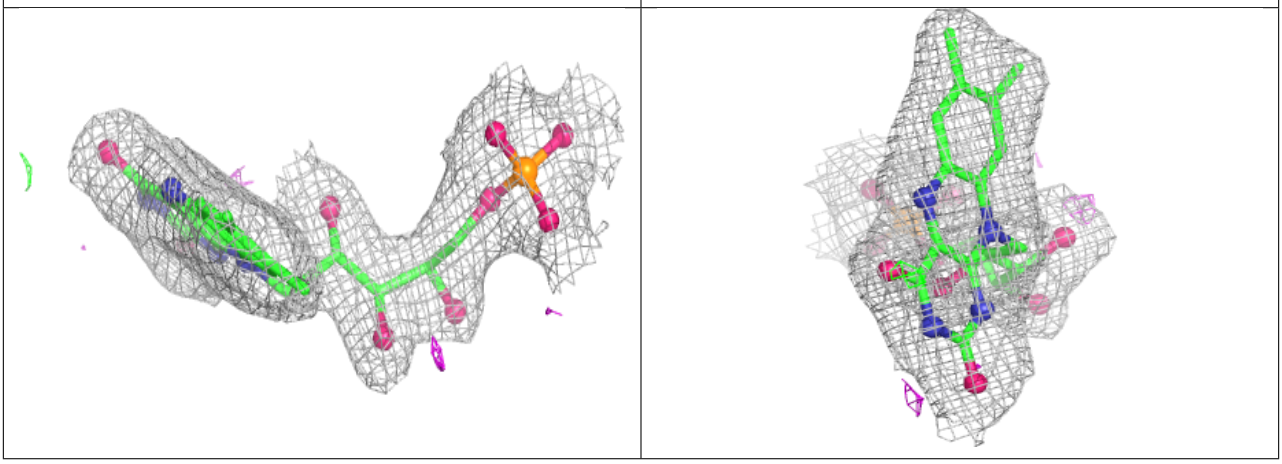
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FMN B 701:

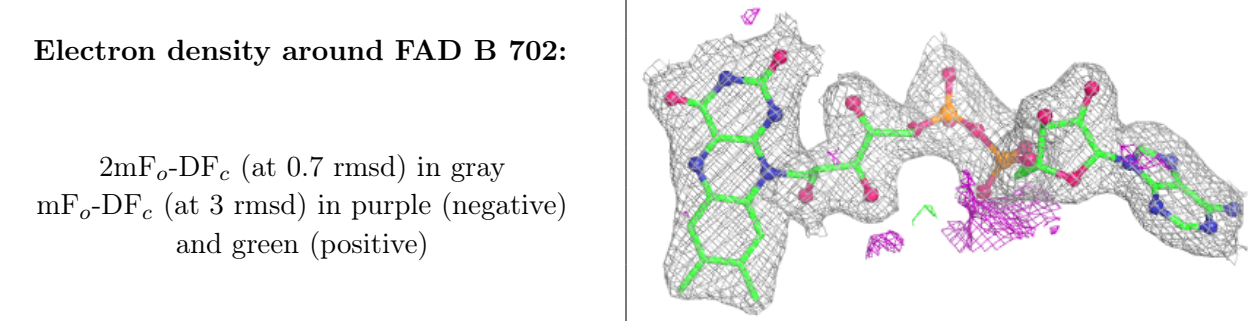
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

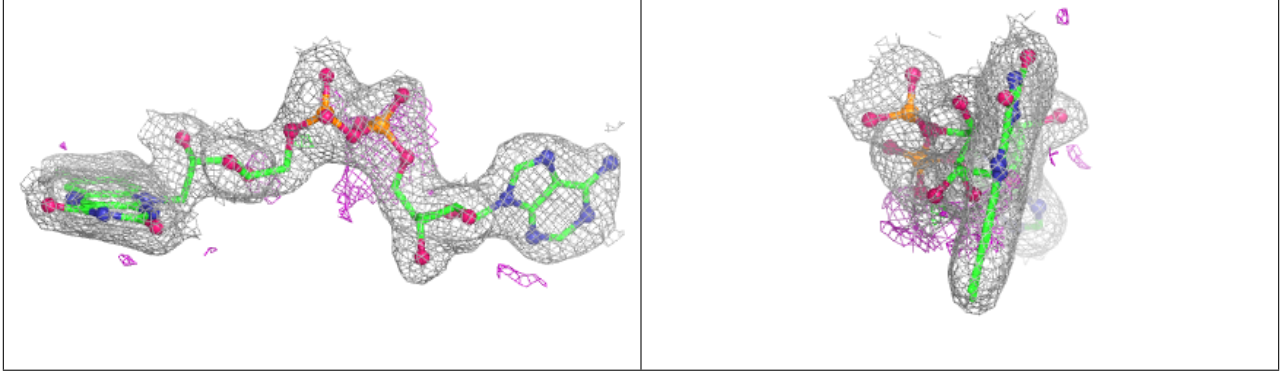




Electron density around FAD B 702:

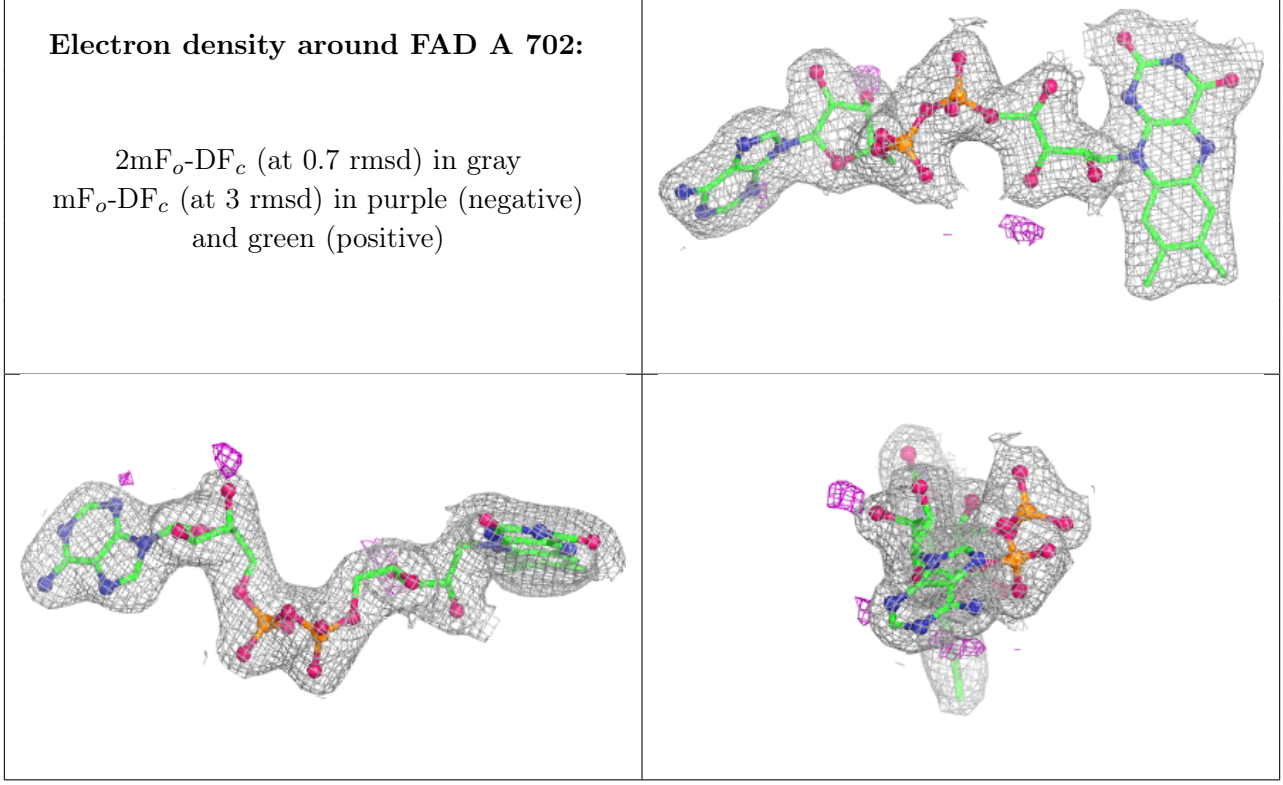
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around 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)



6.5 Other polymers (i)

There are no such residues in this entry.