



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:40 AM UTC

PDB ID : 6MVG / pdb_00006mvg
Title : Crystal structure of FMN-binding beta-glucuronidase from *Ruminococcus gnavus*
Authors : Pellock, S.J.; Redinbo, M.R.
Deposited on : 2018-10-25
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

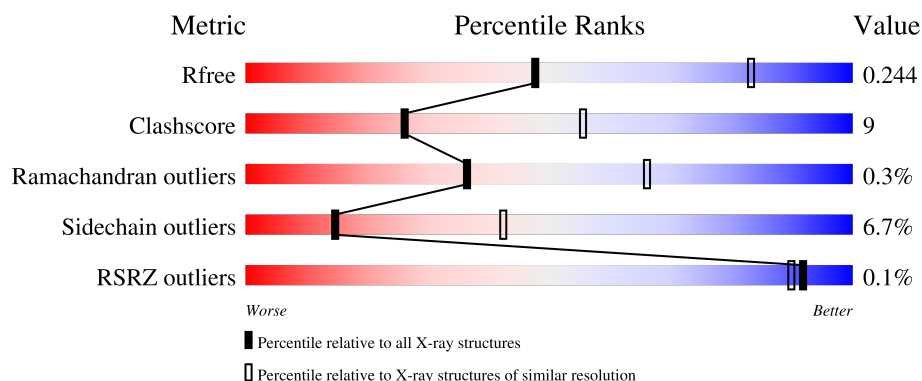
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	777	 64% 18% 18%
1	B	777	 60% 20% 18%
1	C	777	 60% 20% 18%

2 Entry composition [i](#)

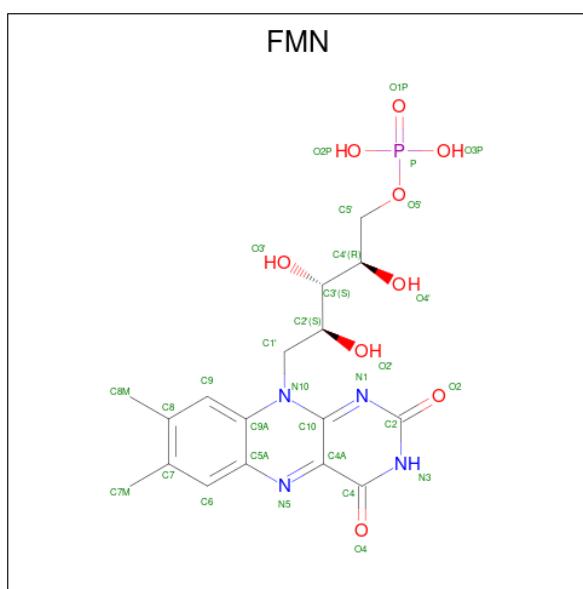
There are 4 unique types of molecules in this entry. The entry contains 15660 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	0	0	0
			5153	3271	871	984	27			
1	B	636	Total	C	N	O	S	0	0	0
			5150	3271	870	982	27			
1	C	637	Total	C	N	O	S	0	0	0
			5157	3273	871	986	27			

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

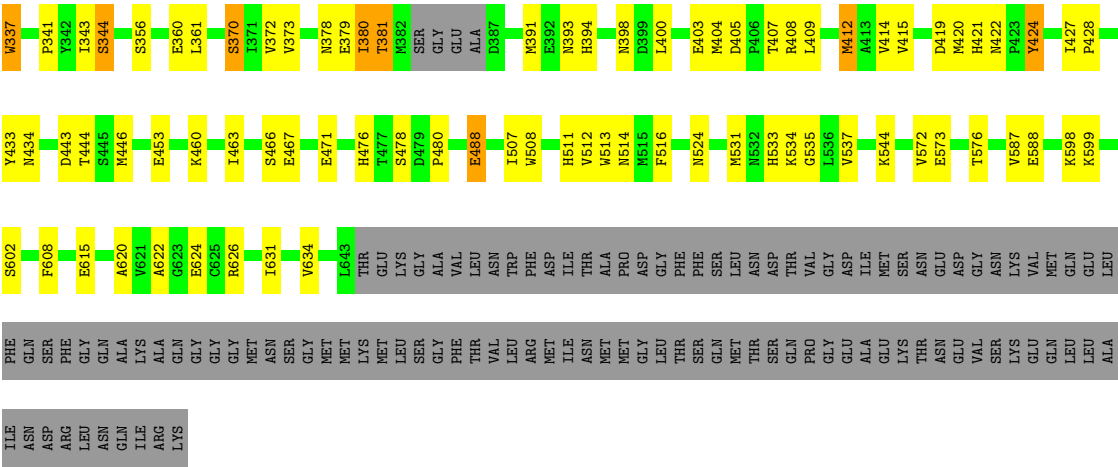


- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

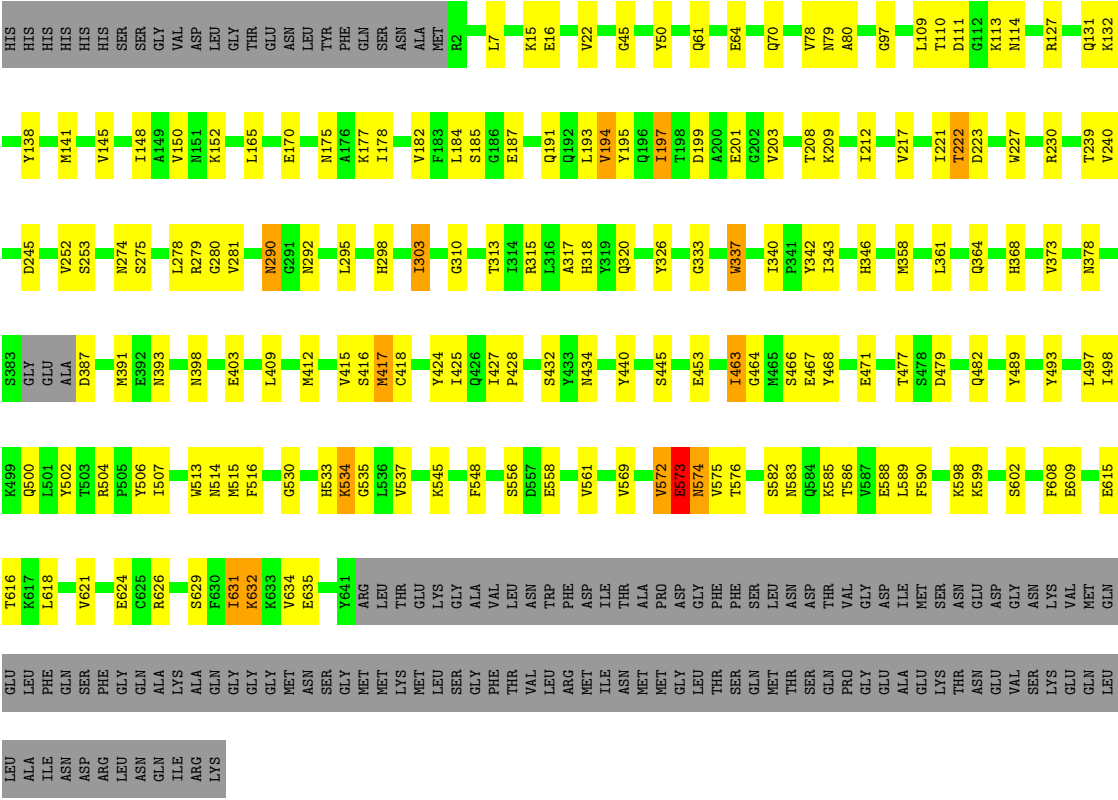
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total 27	O 27	0	0
4	B	41	Total 41	O 41	0	0
4	C	36	Total 36	O 36	0	0



● Molecule 1: beta-glucuronidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	236.03Å 127.08Å 88.82Å 90.00° 98.49° 90.00°	Depositor
Resolution (Å)	29.88 – 2.80 29.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.88-2.80) 99.7 (29.88-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.80Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.185 , 0.246 0.187 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15660	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, CA

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	0.41	0/5295	0.60	0/7185
1	B	0.43	0/5292	0.63	1/7182 (0.0%)
1	C	0.40	0/5299	0.61	0/7191
All	All	0.41	0/15886	0.62	1/21558 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	424	TYR	CA-CB-CG	5.18	123.22	113.90

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	5153	0	4843	81	0
1	B	5150	0	4844	103	0
1	C	5157	0	4844	97	0
2	A	31	0	19	0	0
2	B	31	0	19	2	0
2	C	31	0	19	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	27	0	0	2	0
4	B	41	0	0	2	0
4	C	36	0	0	2	0
All	All	15660	0	14588	283	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 9.

All (283) 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:471:GLU:HG2	1:B:534:LYS:HG2	1.48	0.91
1:B:624:GLU:OE2	1:B:624:GLU:N	2.14	0.80
1:C:141:MET:HE2	1:C:145:VAL:HG21	1.65	0.79
1:A:528:GLU:OE2	1:A:531:MET:HG3	1.83	0.79
1:A:141:MET:HE2	1:A:145:VAL:HG21	1.64	0.78
1:C:561:VAL:HG23	1:C:582:SER:HB2	1.67	0.77
1:B:281:VAL:HG12	1:B:512:VAL:HB	1.68	0.75
1:A:616:THR:HB	1:A:631:ILE:HG22	1.71	0.72
1:C:175:ASN:HD22	1:C:222:THR:HA	1.54	0.71
1:C:175:ASN:ND2	1:C:222:THR:HA	2.06	0.71
1:B:78:VAL:HG22	1:B:141:MET:HG2	1.74	0.70
1:A:9:GLU:O	1:A:58:LYS:NZ	2.23	0.70
1:C:621:VAL:HG12	1:C:626:ARG:HG2	1.74	0.70
1:B:372:VAL:HG23	1:B:373:VAL:HG13	1.74	0.69
1:B:330:ASP:OD1	1:B:370:SER:OG	2.09	0.69
1:B:381:THR:O	1:B:381:THR:OG1	2.05	0.68
1:A:76:LEU:HD22	1:A:144:ASP:HB2	1.76	0.68
1:C:165:LEU:HD22	1:C:252:VAL:HG13	1.74	0.68
1:B:171:VAL:HG11	1:B:260:THR:HG22	1.74	0.67
1:B:192:GLN:HA	1:B:211:GLY:HA2	1.75	0.67
1:C:477:THR:HG23	1:C:479:ASP:H	1.62	0.65
1:A:131:GLN:OE1	4:A:901:HOH:O	2.15	0.65
1:C:468:TYR:CD2	1:C:497:LEU:HD23	2.33	0.64
1:B:533:HIS:HD2	4:B:912:HOH:O	1.80	0.64
1:C:199:ASP:HB3	1:C:201:GLU:H	1.63	0.64
1:C:138:TYR:HB2	1:C:292:ASN:ND2	2.14	0.63
1:C:295:LEU:H	1:C:298:HIS:HD2	1.45	0.62
1:B:398:ASN:HD22	1:B:427:ILE:HG22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LEU:HB3	1:B:321:HIS:CD2	2.34	0.62
1:C:182:VAL:HG11	1:C:240:VAL:HG11	1.82	0.62
1:B:67:GLU:OE2	1:B:67:GLU:N	2.32	0.61
1:B:105:MET:HE3	1:B:109:LEU:HD21	1.82	0.61
1:A:15:LYS:HE3	1:A:50:TYR:CG	2.36	0.60
1:B:343:ILE:HG23	1:B:378:ASN:HD22	1.66	0.60
1:B:227:TRP:CZ2	1:B:333:GLY:HA2	2.36	0.60
1:A:571:ARG:HD2	1:A:576:THR:HG21	1.84	0.60
1:C:573:GLU:OE2	1:C:576:THR:HG22	2.02	0.60
1:A:141:MET:CE	1:A:145:VAL:HG21	2.31	0.60
1:B:412:MET:HE3	1:B:428:PRO:HG3	1.84	0.59
1:A:306:ILE:HG21	1:A:314:ILE:HD11	1.85	0.59
1:C:110:THR:HG22	1:C:111:ASP:O	2.01	0.59
1:C:317:ALA:HB1	1:C:318:HIS:ND1	2.17	0.58
1:A:33:LEU:HD23	1:A:145:VAL:HG23	1.86	0.58
1:B:434:ASN:HB3	1:B:467:GLU:HB2	1.86	0.58
1:C:280:GLY:HA3	1:C:313:THR:O	2.04	0.58
1:A:433:TYR:HB3	1:A:435:HIS:CD2	2.39	0.57
1:A:514:ASN:O	1:A:535:GLY:HA2	2.05	0.56
1:A:573:GLU:OE1	1:A:576:THR:HG23	2.05	0.56
1:C:445:SER:HA	1:C:500:GLN:HE22	1.70	0.56
1:C:558:GLU:O	1:C:583:ASN:ND2	2.37	0.55
1:B:154:HIS:HE1	4:B:929:HOH:O	1.90	0.55
1:A:317:ALA:HB1	1:A:318:HIS:ND1	2.21	0.55
1:B:588:GLU:HB2	1:B:598:LYS:HG3	1.87	0.55
1:C:342:TYR:OH	1:C:346:HIS:ND1	2.33	0.55
1:A:194:VAL:HG22	1:A:209:LYS:HD3	1.88	0.55
1:A:181:GLU:HG3	1:A:216:GLN:HG2	1.89	0.54
1:A:76:LEU:O	1:A:143:ARG:HD2	2.07	0.54
1:A:226:LEU:O	4:A:902:HOH:O	2.18	0.54
1:C:197:ILE:HG21	1:C:221:ILE:HD11	1.90	0.54
1:A:182:VAL:HG11	1:A:240:VAL:HG11	1.88	0.54
1:B:405:ASP:OD2	1:B:408:ARG:HD2	2.08	0.54
1:A:571:ARG:CD	1:A:576:THR:HG21	2.38	0.54
1:C:504:ARG:HB3	1:C:506:TYR:CE1	2.43	0.54
1:C:290:ASN:N	1:C:290:ASN:HD22	2.06	0.53
1:A:334:LEU:O	1:A:370:SER:HB2	2.07	0.53
1:A:473:LEU:HD21	1:A:533:HIS:CE1	2.43	0.53
1:B:531:MET:HB2	1:B:533:HIS:NE2	2.24	0.53
1:A:434:ASN:CG	1:A:467:GLU:HB2	2.33	0.53
1:A:279:ARG:HB3	1:A:502:TYR:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ASP:OD1	1:B:407:THR:HB	2.07	0.53
1:A:343:ILE:HG13	1:A:378:ASN:HD22	1.73	0.53
1:C:387:ASP:O	1:C:391:MET:HG2	2.08	0.53
1:A:243:MET:HG3	1:A:248:CYS:HA	1.90	0.52
1:C:514:ASN:O	1:C:535:GLY:HA2	2.09	0.52
1:C:589:LEU:HD11	1:C:618:LEU:HD23	1.91	0.52
1:B:378:ASN:ND2	1:B:379:GLU:HG3	2.24	0.52
1:C:295:LEU:H	1:C:298:HIS:CD2	2.27	0.52
1:B:337:TRP:CD1	1:B:337:TRP:C	2.87	0.52
1:C:239:THR:HG23	1:C:253:SER:HB3	1.90	0.52
1:B:381:THR:HG23	1:B:415:VAL:HG12	1.91	0.52
1:B:573:GLU:CD	1:B:576:THR:HG22	2.35	0.52
1:A:105:MET:HE1	1:A:147:ILE:HD13	1.92	0.51
1:C:533:HIS:C	1:C:535:GLY:H	2.19	0.51
1:B:476:HIS:ND1	1:B:488:GLU:OE1	2.38	0.51
1:C:615:GLU:HG3	1:C:632:LYS:HG3	1.93	0.51
1:B:263:ILE:HD12	1:B:409:LEU:HD12	1.92	0.51
1:B:336:LEU:HD22	1:B:370:SER:HB2	1.93	0.51
1:A:439:TRP:CZ2	1:A:471:GLU:HG3	2.46	0.51
1:B:194:VAL:HG12	1:B:209:LYS:HG2	1.93	0.51
1:C:599:LYS:HD2	1:C:608:PHE:CE1	2.46	0.51
1:C:78:VAL:O	1:C:97:GLY:HA2	2.11	0.50
1:C:170:GLU:HG2	1:C:177:LYS:O	2.11	0.50
1:B:74:GLU:HB3	1:B:146:ASN:HB2	1.93	0.50
1:A:228:ASN:OD1	1:A:231:LYS:HD2	2.12	0.50
1:A:110:THR:H	1:A:114:ASN:HD21	1.60	0.50
1:C:373:VAL:HA	1:C:409:LEU:O	2.12	0.50
1:C:440:TYR:OH	1:C:534:LYS:NZ	2.33	0.50
1:C:416:SER:HB2	1:C:434:ASN:O	2.12	0.50
1:B:178:ILE:HG21	1:B:197:ILE:HD11	1.93	0.49
1:B:343:ILE:HG22	1:B:344:SER:OG	2.12	0.49
1:C:574:ASN:N	1:C:574:ASN:OD1	2.45	0.49
1:A:75:PHE:CE2	1:A:141:MET:HE3	2.48	0.49
1:C:326:TYR:HB3	1:C:368:HIS:CD2	2.47	0.49
1:C:471:GLU:HG2	1:C:534:LYS:HG2	1.94	0.49
1:B:171:VAL:HG21	1:B:260:THR:HG21	1.93	0.49
1:B:178:ILE:HG22	1:B:180:VAL:HG23	1.95	0.49
1:B:285:GLN:HG2	1:B:319:TYR:CE1	2.46	0.49
1:B:414:VAL:HG12	1:B:415:VAL:O	2.12	0.49
1:B:398:ASN:HD22	1:B:427:ILE:CG2	2.25	0.49
1:B:34:PRO:HB3	1:B:142:TYR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:O	1:B:143:ARG:HD2	2.13	0.48
1:B:341:PRO:O	1:B:343:ILE:HG12	2.14	0.48
1:B:141:MET:HE2	1:B:145:VAL:HG21	1.96	0.48
1:B:434:ASN:CB	1:B:467:GLU:HB2	2.43	0.48
1:C:493:TYR:CE1	1:C:497:LEU:HD22	2.49	0.48
1:B:20:PRO:HB3	1:B:117:VAL:HG11	1.96	0.48
1:B:102:ARG:NH1	1:B:162:GLY:O	2.44	0.48
1:B:419:ASP:OD2	1:B:421:HIS:HB2	2.14	0.48
1:C:493:TYR:CZ	1:C:497:LEU:HD22	2.49	0.48
1:A:500:GLN:O	1:A:504:ARG:NH1	2.44	0.48
1:B:12:ALA:HB1	1:B:28:TRP:HB2	1.96	0.48
1:B:514:ASN:O	1:B:535:GLY:HA2	2.14	0.48
1:C:61:GLN:O	1:C:64:GLU:HG2	2.14	0.48
1:B:171:VAL:HG21	1:B:260:THR:CG2	2.44	0.48
1:B:398:ASN:ND2	1:B:427:ILE:HG22	2.29	0.48
1:C:184:LEU:HD13	1:C:212:ILE:HD11	1.94	0.48
1:A:452:ASP:O	1:A:456:LYS:HG3	2.14	0.47
1:B:51:ARG:HB3	1:B:123:SER:HA	1.97	0.47
1:C:79:ASN:ND2	1:C:138:TYR:O	2.42	0.47
1:B:587:VAL:HG22	1:B:622:ALA:HB2	1.95	0.47
1:C:572:VAL:HB	1:C:634:VAL:HG23	1.97	0.47
1:A:34:PRO:HB3	1:A:142:TYR:O	2.14	0.47
1:B:206:ALA:HB3	1:B:219:LEU:HD23	1.96	0.47
1:C:70:GLN:HG3	1:C:152:LYS:HG2	1.97	0.47
1:C:199:ASP:HB2	1:C:203:VAL:H	1.79	0.47
1:C:588:GLU:HG3	1:C:598:LYS:HG2	1.97	0.47
1:A:7:LEU:HD11	1:A:60:VAL:HG11	1.96	0.47
1:A:319:TYR:HB3	1:A:341:PRO:HG3	1.96	0.47
1:C:227:TRP:CZ2	1:C:333:GLY:HA2	2.50	0.47
1:A:316:LEU:HD22	1:A:321:HIS:CE1	2.50	0.47
1:B:167:VAL:HG22	1:B:180:VAL:HG22	1.96	0.47
1:B:380:ILE:HG21	1:B:394:HIS:CE1	2.50	0.47
1:A:571:ARG:NE	1:A:631:ILE:HD11	2.30	0.46
1:C:618:LEU:HB2	1:C:629:SER:HB2	1.97	0.46
1:C:191:GLN:O	1:C:212:ILE:N	2.48	0.46
1:C:317:ALA:HA	1:C:318:HIS:HA	1.78	0.46
1:A:629:SER:C	1:A:630:PHE:HD2	2.22	0.46
1:C:575:VAL:CG1	1:C:609:GLU:HB3	2.45	0.46
1:C:7:LEU:HD12	1:C:7:LEU:HA	1.79	0.46
1:A:227:TRP:CZ2	1:A:333:GLY:HA2	2.50	0.46
1:B:98:TYR:HB3	1:B:320:GLN:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:GLN:HB2	1:C:361:LEU:HD13	1.97	0.46
2:B:801:FMN:H9	2:B:801:FMN:O2'	2.16	0.46
1:B:320:GLN:HB2	1:B:361:LEU:HD13	1.98	0.46
1:A:353:ASN:OD1	1:A:357:GLN:NE2	2.47	0.46
1:B:221:ILE:HG21	1:B:224:VAL:HG23	1.96	0.46
1:A:279:ARG:HD2	1:A:502:TYR:CD1	2.51	0.45
1:B:471:GLU:CG	1:B:534:LYS:HG2	2.34	0.45
1:C:131:GLN:O	1:C:132:LYS:HD3	2.16	0.45
1:B:316:LEU:HD21	1:B:325:PHE:CE2	2.51	0.45
1:C:572:VAL:HG21	1:C:635:GLU:O	2.16	0.45
1:B:15:LYS:HE3	1:B:50:TYR:CG	2.51	0.45
1:B:171:VAL:HG23	1:B:171:VAL:O	2.17	0.45
1:B:380:ILE:HG21	1:B:394:HIS:HE1	1.80	0.45
1:B:400:LEU:O	1:B:404:MET:HG3	2.16	0.45
1:A:41:ASP:O	1:A:49:TYR:HB3	2.15	0.45
1:B:315:ARG:HB2	1:B:511:HIS:CD2	2.52	0.45
1:B:420:MET:HA	1:B:433:TYR:OH	2.17	0.45
1:B:118:VAL:HG11	1:B:141:MET:HE3	1.98	0.45
1:B:184:LEU:HD21	1:B:242:LEU:HD13	1.98	0.45
1:B:516:PHE:HD2	1:B:537:VAL:HB	1.82	0.45
1:C:281:VAL:HB	1:C:515:MET:HB2	1.99	0.45
1:C:194:VAL:HB	1:C:209:LYS:HG2	1.98	0.45
1:C:109:LEU:HD23	1:C:114:ASN:OD1	2.17	0.45
1:A:478:SER:C	1:A:480:PRO:HD3	2.42	0.45
1:C:230:ARG:HH12	1:C:310:GLY:HA2	1.82	0.45
1:A:279:ARG:HD2	1:A:502:TYR:CE1	2.52	0.44
1:B:151:ASN:O	1:B:154:HIS:HD2	2.01	0.44
1:A:434:ASN:OD1	1:A:467:GLU:HB2	2.17	0.44
1:C:127:ARG:NH2	4:C:904:HOH:O	2.46	0.44
1:C:417:MET:HE3	1:C:417:MET:HB2	1.84	0.44
1:B:315:ARG:HH12	1:B:467:GLU:HG3	1.82	0.44
1:B:531:MET:HE3	1:B:531:MET:HB3	1.83	0.44
1:C:412:MET:HE3	1:C:428:PRO:HG3	1.99	0.44
1:A:244:GLU:O	1:A:247:VAL:HG23	2.18	0.44
1:B:51:ARG:HA	1:B:122:ASN:OD1	2.17	0.44
1:C:482:GLN:HA	1:C:489:TYR:CE1	2.52	0.44
1:B:188:LYS:HA	1:B:188:LYS:HD2	1.89	0.44
1:B:281:VAL:O	1:B:314:ILE:HA	2.17	0.44
1:C:513:TRP:HA	1:C:514:ASN:HA	1.72	0.44
1:A:97:GLY:O	1:A:142:TYR:OH	2.31	0.44
1:B:443:ASP:OD1	1:B:446:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:ILE:C	1:B:508:TRP:HD1	2.25	0.44
1:C:15:LYS:HE2	1:C:50:TYR:CD1	2.53	0.44
1:A:12:ALA:HB1	1:A:28:TRP:HB2	2.01	0.43
1:A:303:ILE:HG13	1:A:328:LEU:HD13	1.99	0.43
1:C:61:GLN:OE1	1:C:113:LYS:HG3	2.18	0.43
1:C:498:ILE:HG23	1:C:502:TYR:CD2	2.53	0.43
2:C:801:FMN:H9	2:C:801:FMN:H1'1	1.79	0.43
1:A:531:MET:HB2	1:A:533:HIS:CE1	2.53	0.43
1:B:513:TRP:HA	1:B:514:ASN:HA	1.79	0.43
1:A:405:ASP:OD2	1:A:408:ARG:HD2	2.19	0.43
1:A:561:VAL:HG23	1:A:582:SER:HB2	2.00	0.43
1:B:281:VAL:HA	1:B:512:VAL:H	1.83	0.43
1:B:573:GLU:OE2	1:B:576:THR:HG22	2.19	0.43
1:C:315:ARG:HG3	1:C:337:TRP:CG	2.53	0.43
1:A:391:MET:HE3	1:A:391:MET:HB3	1.67	0.43
1:B:61:GLN:OE1	1:B:113:LYS:HG2	2.18	0.43
1:C:432:SER:HB3	1:C:466:SER:CB	2.49	0.43
1:C:575:VAL:HG12	1:C:609:GLU:HB3	2.01	0.43
1:A:411:THR:OG1	1:A:412:MET:N	2.52	0.43
1:A:456:LYS:O	1:A:459:PRO:HD3	2.19	0.43
1:C:79:ASN:HA	1:C:80:ALA:HA	1.69	0.43
1:B:168:THR:HB	1:B:179:ALA:HB3	2.00	0.42
1:C:398:ASN:ND2	1:C:427:ILE:O	2.52	0.42
1:A:129:TYR:CE1	1:A:347:MET:HE2	2.54	0.42
1:B:73:LEU:HD13	1:B:75:PHE:CZ	2.54	0.42
1:B:337:TRP:C	1:B:337:TRP:HD1	2.26	0.42
1:C:434:ASN:OD1	1:C:467:GLU:HB2	2.19	0.42
1:C:631:ILE:HD12	1:C:631:ILE:HA	1.86	0.42
1:B:620:ALA:O	1:B:626:ARG:HA	2.20	0.42
1:C:175:ASN:ND2	1:C:223:ASP:H	2.17	0.42
1:C:278:LEU:O	1:C:279:ARG:HD3	2.20	0.42
1:A:27:ASN:ND2	1:C:16:GLU:HG2	2.35	0.42
1:B:79:ASN:HA	1:B:80:ALA:HA	1.72	0.42
1:C:45:GLY:N	1:C:530:GLY:HA3	2.34	0.42
1:A:380:ILE:HD12	1:A:380:ILE:HA	1.91	0.42
1:B:270:PHE:HD2	1:B:273:GLY:O	2.02	0.42
1:C:290:ASN:HD22	1:C:290:ASN:H	1.67	0.42
1:B:599:LYS:HE3	1:B:608:PHE:CD1	2.55	0.42
1:C:340:ILE:HD13	1:C:358:MET:HE2	2.00	0.42
1:C:432:SER:HB3	1:C:466:SER:OG	2.20	0.42
1:A:478:SER:O	1:A:480:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:LEU:HA	1:B:305:LEU:HD23	1.84	0.42
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.90	0.42
1:C:320:GLN:NE2	1:C:364:GLN:OE1	2.44	0.42
1:C:463:ILE:O	1:C:507:ILE:HA	2.20	0.42
1:A:471:GLU:OE1	1:A:533:HIS:HB2	2.20	0.42
1:A:261:PHE:HA	1:A:270:PHE:O	2.20	0.42
1:B:378:ASN:CG	1:B:379:GLU:HG3	2.44	0.42
2:B:801:FMN:HM73	2:B:801:FMN:HM81	1.75	0.42
1:C:585:LYS:HB2	1:C:586:THR:HG23	2.01	0.42
1:B:317:ALA:HB1	1:B:318:HIS:ND1	2.35	0.41
1:A:241:ARG:HD2	1:A:248:CYS:SG	2.60	0.41
1:C:303:ILE:HA	1:C:303:ILE:HD13	1.80	0.41
1:A:327:ASP:OD1	1:A:368:HIS:HE1	2.03	0.41
1:B:356:SER:O	1:B:360:GLU:HG3	2.20	0.41
1:B:572:VAL:HG12	1:B:634:VAL:HG23	2.03	0.41
1:A:337:TRP:CD1	1:A:337:TRP:C	2.98	0.41
1:A:592:ASN:OD1	1:A:616:THR:HA	2.20	0.41
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.76	0.41
1:B:280:GLY:HA3	1:B:313:THR:O	2.20	0.41
1:B:478:SER:C	1:B:480:PRO:HD3	2.46	0.41
1:C:315:ARG:NH1	1:C:467:GLU:HG3	2.36	0.41
1:C:464:GLY:HA2	1:C:507:ILE:HG23	2.02	0.41
1:A:411:THR:HB	1:A:430:VAL:CG2	2.51	0.41
1:A:572:VAL:O	1:A:573:GLU:HG3	2.20	0.41
1:C:222:THR:OG1	4:C:901:HOH:O	2.22	0.41
1:A:545:LYS:O	1:A:548:PHE:HB3	2.21	0.41
1:A:75:PHE:HE2	1:A:141:MET:HE3	1.86	0.41
1:A:193:LEU:HG	1:A:212:ILE:HD12	2.03	0.41
1:B:315:ARG:NH1	1:B:467:GLU:HG3	2.35	0.41
1:B:412:MET:HE2	1:B:412:MET:HB3	1.81	0.41
1:C:317:ALA:HB1	1:C:318:HIS:CE1	2.56	0.41
1:A:514:ASN:OD1	1:A:515:MET:N	2.54	0.41
1:A:632:LYS:HB3	1:A:632:LYS:HE2	1.91	0.41
1:B:391:MET:HE3	1:B:391:MET:HB3	1.72	0.41
1:C:516:PHE:CD1	1:C:537:VAL:HB	2.56	0.41
1:A:98:TYR:CG	1:A:319:TYR:HB2	2.56	0.40
1:B:471:GLU:HA	1:B:534:LYS:HA	2.02	0.40
1:C:208:THR:HG21	1:C:217:VAL:HG11	2.01	0.40
1:A:110:THR:HG23	1:A:111:ASP:O	2.20	0.40
1:B:516:PHE:CD2	1:B:537:VAL:HB	2.56	0.40
1:C:279:ARG:HB3	1:C:502:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:H	1:A:63:GLU:CD	2.29	0.40
1:C:148:ILE:HG22	1:C:150:VAL:HG13	2.03	0.40
1:A:143:ARG:NH2	1:A:285:GLN:OE1	2.54	0.40
1:A:317:ALA:HB1	1:A:318:HIS:CG	2.57	0.40
1:C:318:HIS:CD2	1:C:343:ILE:HD11	2.56	0.40
1:C:391:MET:HE3	1:C:391:MET:HB3	1.92	0.40
1:C:545:LYS:O	1:C:548:PHE:HB3	2.22	0.40
1:A:520:ALA:O	1:A:530:GLY:HA2	2.22	0.40
1:B:531:MET:HB2	1:B:533:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	633/777 (82%)	601 (95%)	31 (5%)	1 (0%)	43	72
1	B	632/777 (81%)	592 (94%)	37 (6%)	3 (0%)	24	55
1	C	633/777 (82%)	591 (93%)	40 (6%)	2 (0%)	36	66
All	All	1898/2331 (81%)	1784 (94%)	108 (6%)	6 (0%)	36	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	SER
1	B	507	ILE
1	B	422	ASN
1	C	573	GLU
1	B	245	ASP
1	C	534	LYS

5.3.2 Protein sidechains ⓘ

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	547/665 (82%)	515 (94%)	32 (6%)	18	48
1	B	547/665 (82%)	505 (92%)	42 (8%)	12	36
1	C	548/665 (82%)	512 (93%)	36 (7%)	15	43
All	All	1642/1995 (82%)	1532 (93%)	110 (7%)	15	42

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	22	VAL
1	A	61	GLN
1	A	147	ILE
1	A	192	GLN
1	A	198	THR
1	A	199	ASP
1	A	201	GLU
1	A	210	THR
1	A	217	VAL
1	A	218	ASN
1	A	225	HIS
1	A	239	THR
1	A	243	MET
1	A	247	VAL
1	A	251	SER
1	A	252	VAL
1	A	275	SER
1	A	337	TRP
1	A	400	LEU
1	A	407	THR
1	A	412	MET
1	A	415	VAL
1	A	424	TYR
1	A	443	ASP
1	A	460	LYS

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Mol	Chain	Res	Type
1	A	482	GLN
1	A	576	THR
1	A	596	LEU
1	A	613	HIS
1	A	631	ILE
1	A	636	LYS
1	B	91	LEU
1	B	103	VAL
1	B	113	LYS
1	B	128	VAL
1	B	150	VAL
1	B	157	LEU
1	B	174	LYS
1	B	184	LEU
1	B	187	GLU
1	B	188	LYS
1	B	192	GLN
1	B	203	VAL
1	B	212	ILE
1	B	213	SER
1	B	217	VAL
1	B	247	VAL
1	B	248	CYS
1	B	252	VAL
1	B	259	ARG
1	B	260	THR
1	B	262	THR
1	B	287	ARG
1	B	336	LEU
1	B	337	TRP
1	B	344	SER
1	B	370	SER
1	B	380	ILE
1	B	381	THR
1	B	393	ASN
1	B	403	GLU
1	B	412	MET
1	B	424	TYR
1	B	444	THR
1	B	453	GLU
1	B	460	LYS
1	B	466	SER

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Mol	Chain	Res	Type
1	B	488	GLU
1	B	524	ASN
1	B	544	LYS
1	B	602	SER
1	B	615	GLU
1	B	631	ILE
1	C	22	VAL
1	C	178	ILE
1	C	185	SER
1	C	187	GLU
1	C	193	LEU
1	C	194	VAL
1	C	195	TYR
1	C	197	ILE
1	C	222	THR
1	C	245	ASP
1	C	274	ASN
1	C	275	SER
1	C	290	ASN
1	C	303	ILE
1	C	337	TRP
1	C	378	ASN
1	C	393	ASN
1	C	403	GLU
1	C	415	VAL
1	C	417	MET
1	C	418	CYS
1	C	424	TYR
1	C	425	ILE
1	C	453	GLU
1	C	463	ILE
1	C	556	SER
1	C	569	VAL
1	C	572	VAL
1	C	573	GLU
1	C	574	ASN
1	C	590	PHE
1	C	602	SER
1	C	616	THR
1	C	624	GLU
1	C	631	ILE
1	C	632	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	323	GLN
1	A	365	ASN
1	A	584	GLN
1	B	89	ASN
1	B	292	ASN
1	B	320	GLN
1	B	323	GLN
1	B	394	HIS
1	B	482	GLN
1	B	492	HIS
1	B	584	GLN
1	C	90	HIS
1	C	292	ASN
1	C	323	GLN
1	C	592	ASN
1	C	604	HIS
1	C	612	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	B	801	-	33,33,33	1.16	3 (9%)	48,50,50	1.65	11 (22%)
2	FMN	A	801	-	33,33,33	1.02	2 (6%)	48,50,50	1.41	9 (18%)
2	FMN	C	801	-	33,33,33	1.13	2 (6%)	48,50,50	1.41	10 (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	FMN	B	801	-	-	7/18/18/18	0/3/3/3
2	FMN	A	801	-	-	0/18/18/18	0/3/3/3
2	FMN	C	801	-	-	3/18/18/18	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FMN	C4A-N5	4.08	1.39	1.30
2	B	801	FMN	C4A-N5	3.56	1.38	1.30
2	C	801	FMN	C10-N1	3.41	1.40	1.33
2	A	801	FMN	C4A-N5	3.30	1.37	1.30
2	B	801	FMN	C10-N1	2.84	1.39	1.33
2	A	801	FMN	C10-N1	2.52	1.38	1.33
2	B	801	FMN	C5'-C4'	2.18	1.54	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FMN	C1'-N10-C9A	3.55	127.53	120.63
2	C	801	FMN	C5A-C9A-N10	3.36	121.01	117.97
2	B	801	FMN	C5'-C4'-C3'	3.34	118.53	112.22
2	B	801	FMN	C2'-C1'-N10	3.34	125.99	110.20
2	A	801	FMN	C4-N3-C2	-3.29	119.80	125.64
2	B	801	FMN	C4A-C10-N10	3.19	121.05	116.48
2	B	801	FMN	O4-C4-C4A	-3.03	118.53	126.53
2	C	801	FMN	C9A-C5A-N5	-2.88	119.40	122.45
2	B	801	FMN	C4-N3-C2	-2.81	120.64	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FMN	O4-C4-C4A	-2.77	119.23	126.53
2	A	801	FMN	C4A-C10-N10	2.75	120.41	116.48
2	C	801	FMN	C4-N3-C2	-2.73	120.80	125.64
2	B	801	FMN	C4A-C4-N3	2.66	120.03	113.25
2	C	801	FMN	C4A-C4-N3	2.65	119.99	113.25
2	C	801	FMN	O4-C4-C4A	-2.61	119.64	126.53
2	B	801	FMN	O5'-C5'-C4'	2.44	115.89	109.36
2	C	801	FMN	C1'-C2'-C3'	-2.41	103.13	109.66
2	C	801	FMN	O3P-P-O5'	2.39	112.89	106.67
2	A	801	FMN	C4-C4A-C10	2.33	120.92	116.93
2	A	801	FMN	C4A-C4-N3	2.33	119.17	113.25
2	A	801	FMN	C10-C4A-N5	-2.29	120.14	124.81
2	C	801	FMN	O3'-C3'-C4'	2.25	114.05	108.93
2	B	801	FMN	O2'-C2'-C3'	2.23	114.46	109.25
2	A	801	FMN	C4A-C10-N1	-2.18	119.24	124.59
2	A	801	FMN	C5A-C9A-N10	2.16	119.92	117.97
2	C	801	FMN	C2'-C1'-N10	2.10	120.11	110.20
2	C	801	FMN	C9-C9A-N10	-2.04	119.11	121.85
2	B	801	FMN	C10-C4A-N5	-2.04	120.64	124.81
2	B	801	FMN	C1'-C2'-C3'	-2.04	104.13	109.66
2	A	801	FMN	O2-C2-N1	-2.02	118.45	121.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

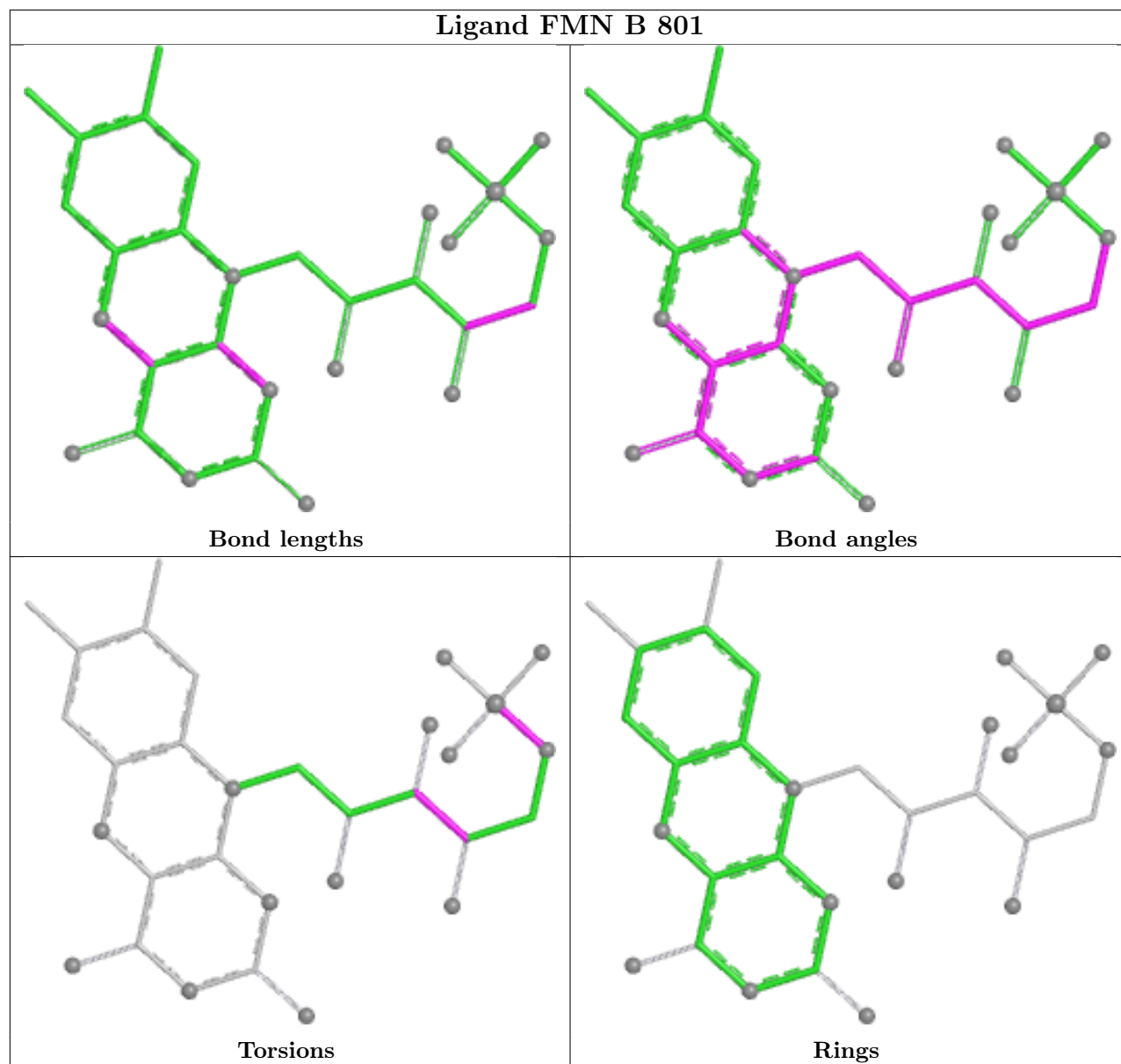
Mol	Chain	Res	Type	Atoms
2	B	801	FMN	C2'-C3'-C4'-O4'
2	B	801	FMN	C2'-C3'-C4'-C5'
2	B	801	FMN	O3'-C3'-C4'-O4'
2	B	801	FMN	O3'-C3'-C4'-C5'
2	B	801	FMN	C5'-O5'-P-O2P
2	B	801	FMN	C5'-O5'-P-O3P
2	C	801	FMN	C5'-O5'-P-O2P
2	C	801	FMN	C5'-O5'-P-O3P
2	C	801	FMN	C3'-C4'-C5'-O5'
2	B	801	FMN	C5'-O5'-P-O1P

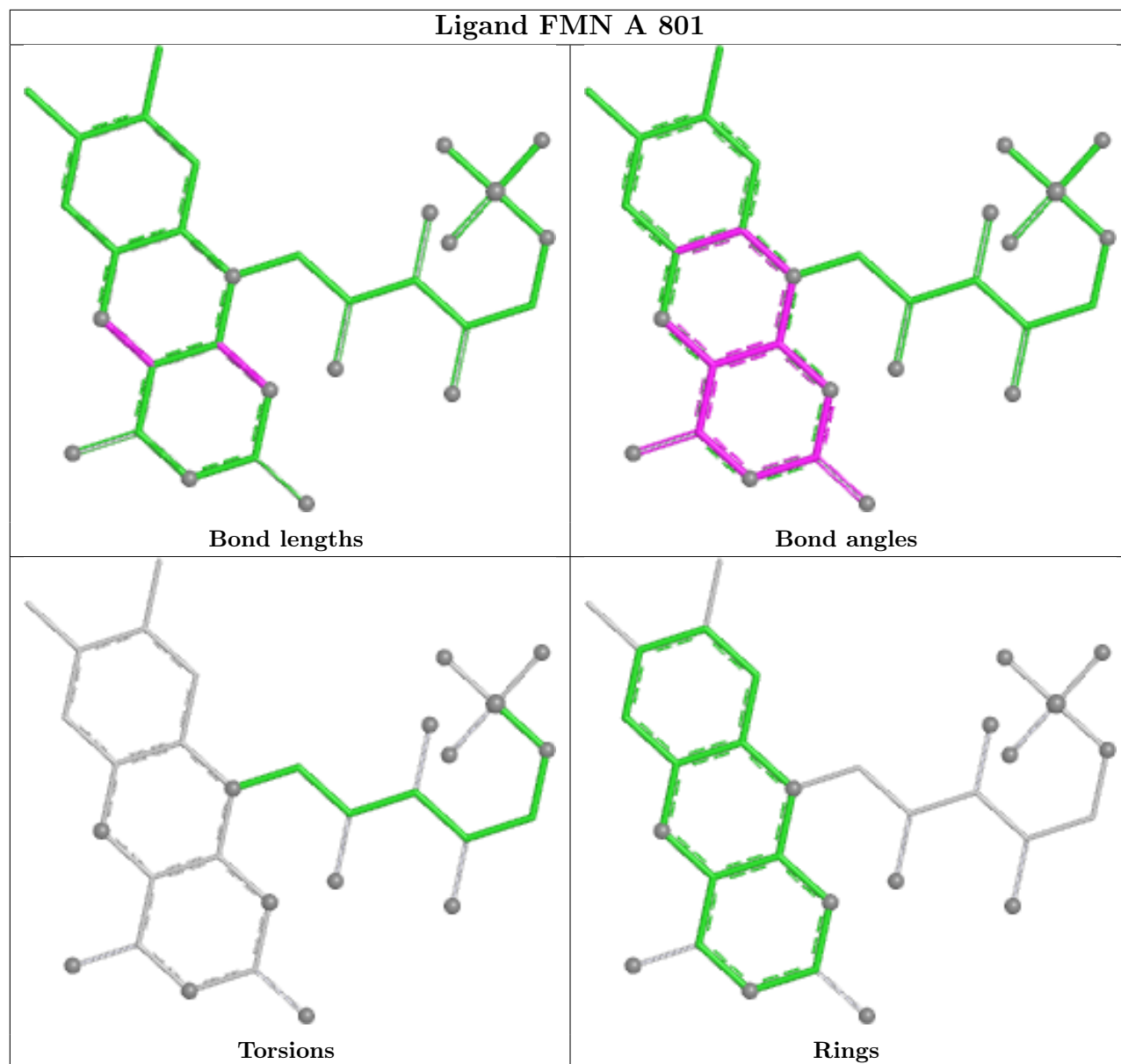
There are no ring outliers.

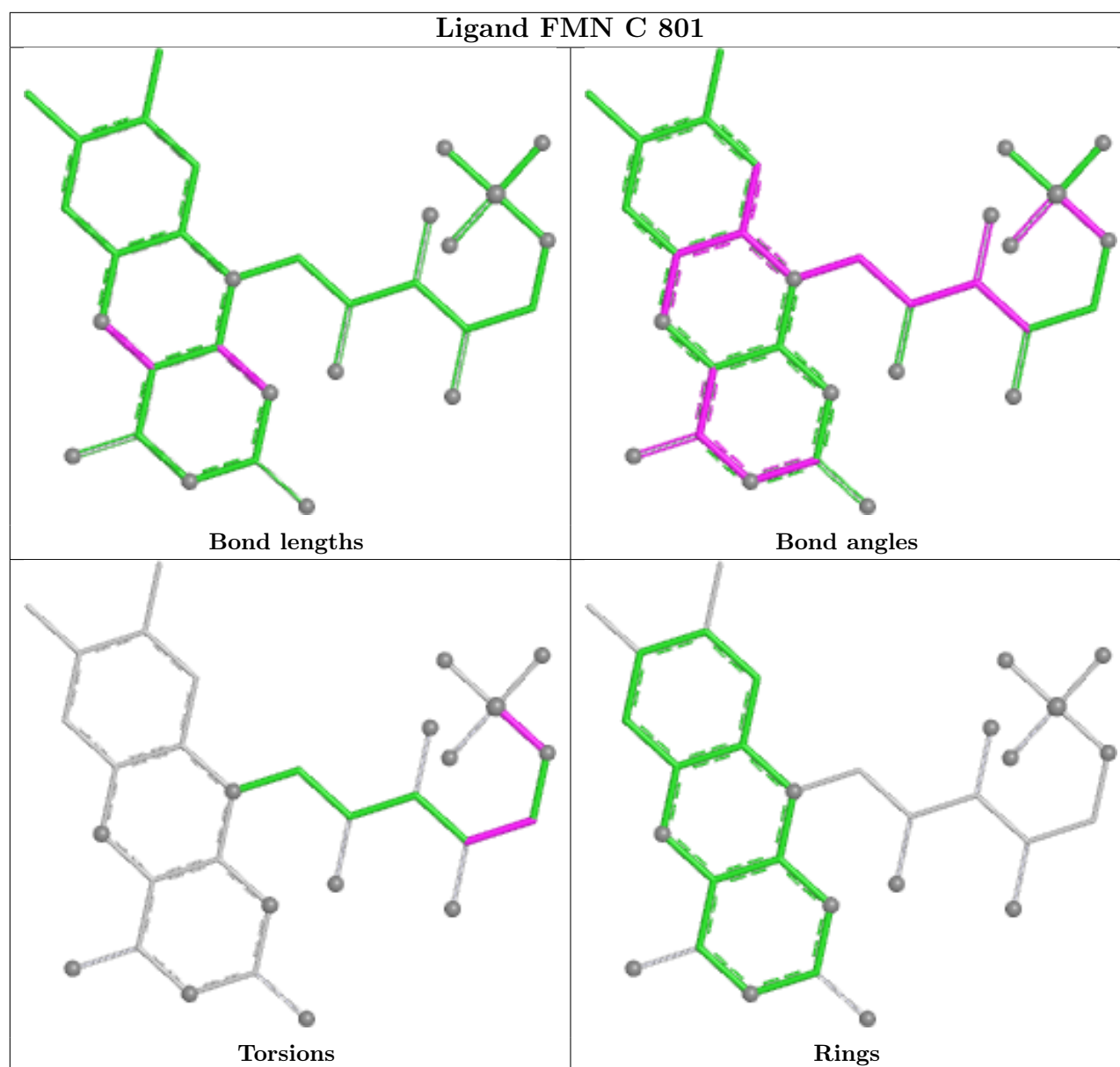
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	FMN	2	0
2	C	801	FMN	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 than 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.







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	637/777 (81%)	-0.25	2 (0%) 90 86	40, 62, 93, 111	0
1	B	636/777 (81%)	-0.30	0 100 100	35, 60, 83, 98	0
1	C	637/777 (81%)	-0.20	0 100 100	38, 67, 90, 104	0
All	All	1910/2331 (81%)	-0.25	2 (0%) 92 90	35, 62, 89, 111	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	384	GLY	2.8
1	A	641	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMN	B	801	31/31	0.86	0.11	52,62,85,93	0

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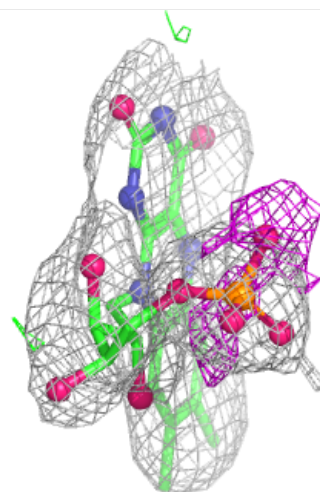
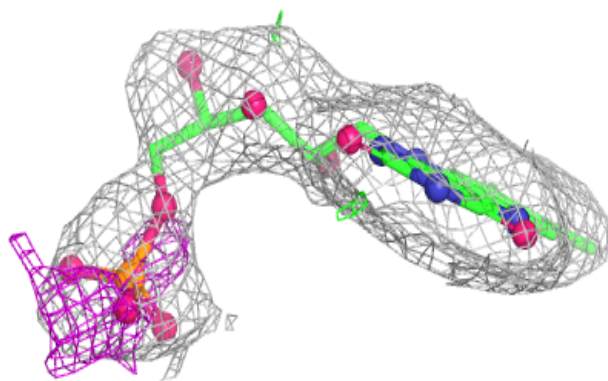
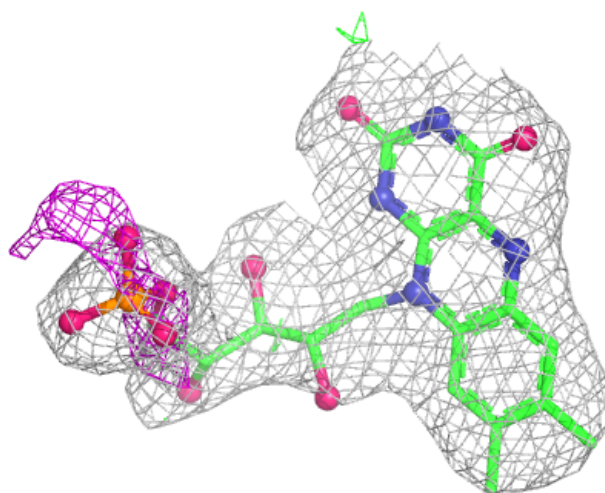
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	C	801	31/31	0.90	0.09	61,69,76,90	0
2	FMN	A	801	31/31	0.93	0.07	58,68,78,93	0
3	CA	C	802	1/1	0.98	0.05	70,70,70,70	0
3	CA	A	802	1/1	0.99	0.02	65,65,65,65	0
3	CA	B	802	1/1	1.00	0.03	63,63,63,63	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.

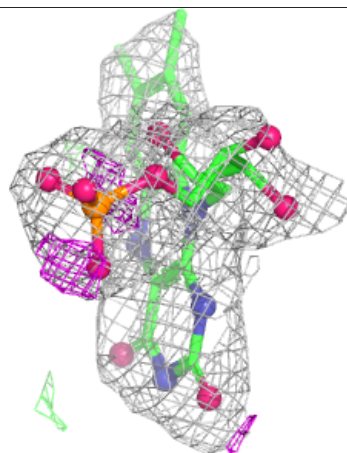
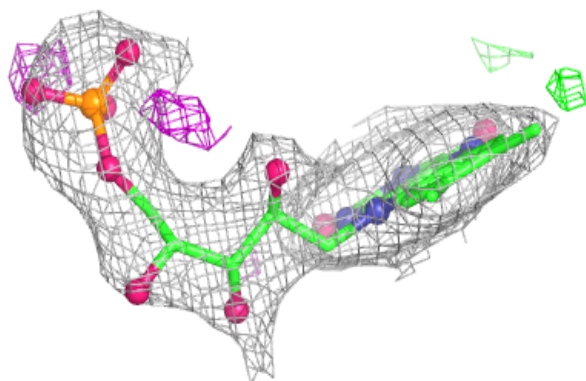
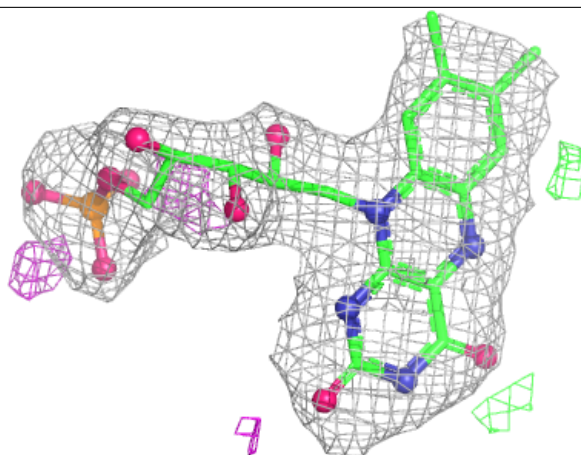
Electron density around FMN B 801:

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



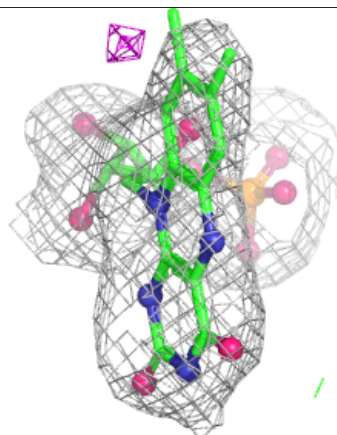
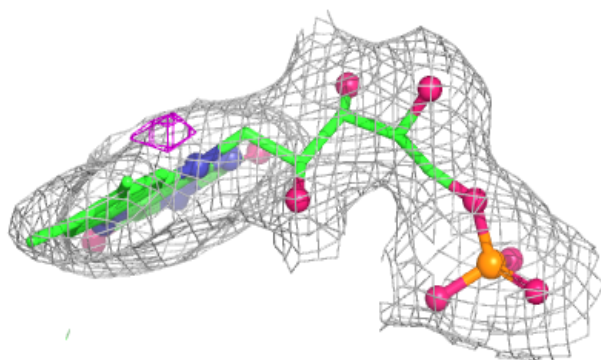
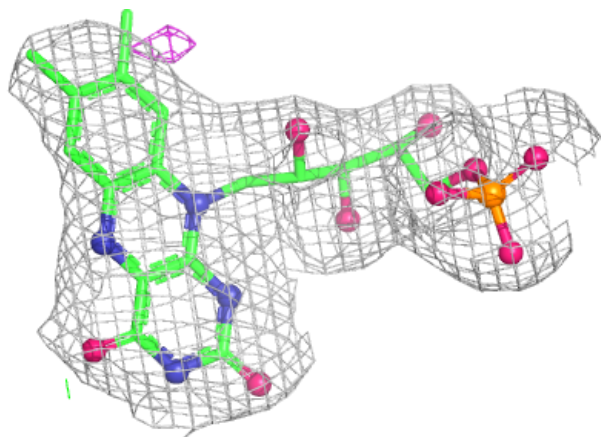
Electron density around FMN C 801:

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



Electron density around FMN A 801:

$2mF_o - DF_c$ (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.