WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 08:35 PM EDT

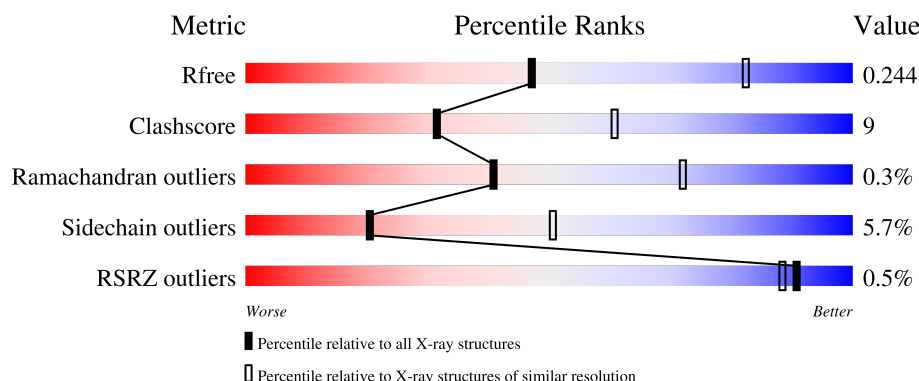|		
PDB ID	:	6MVG
Title	:	Crystal structure of FMN-binding beta-glucuronidase from Ruminococcus gnavus
Authors	:	Pellock, S.J.; Redinbo, M.R.
Deposited on	:	2018-10-25
Resolution	:	2.80 Å(reported)

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	Percentile Ranks	Value
Rfree		0.244
Clashscore		9
Ramachandran outliers		0.3%
Sidechain outliers		5.7%
RSRZ outliers		0.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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.

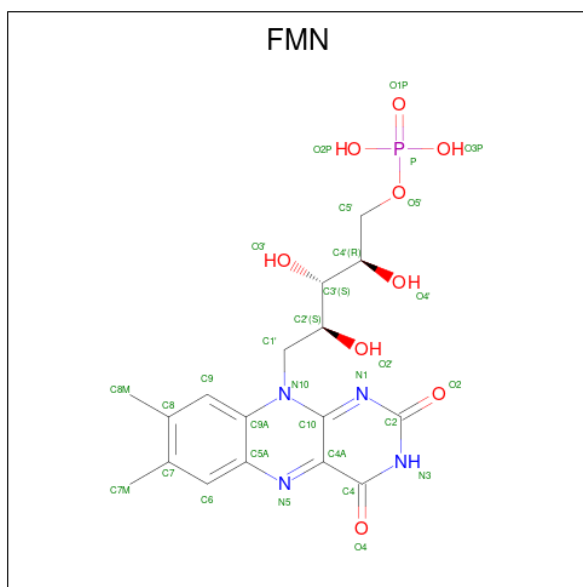| Mol	Chain	Length	Quality of chain
1	A	777	64% 17% • 18%
1	B	777	61% 20% • 18%
1	C	777	% 61% 20% • 18%

2 Entry composition ⓘ

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 (three-letter code: 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		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is CALCIUM ION (three-letter code: 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

3 Residue-property plots ⓘ

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: beta-glucuronidase

Chain A:

- Molecule 1: beta-glucuronidase

Chain B:

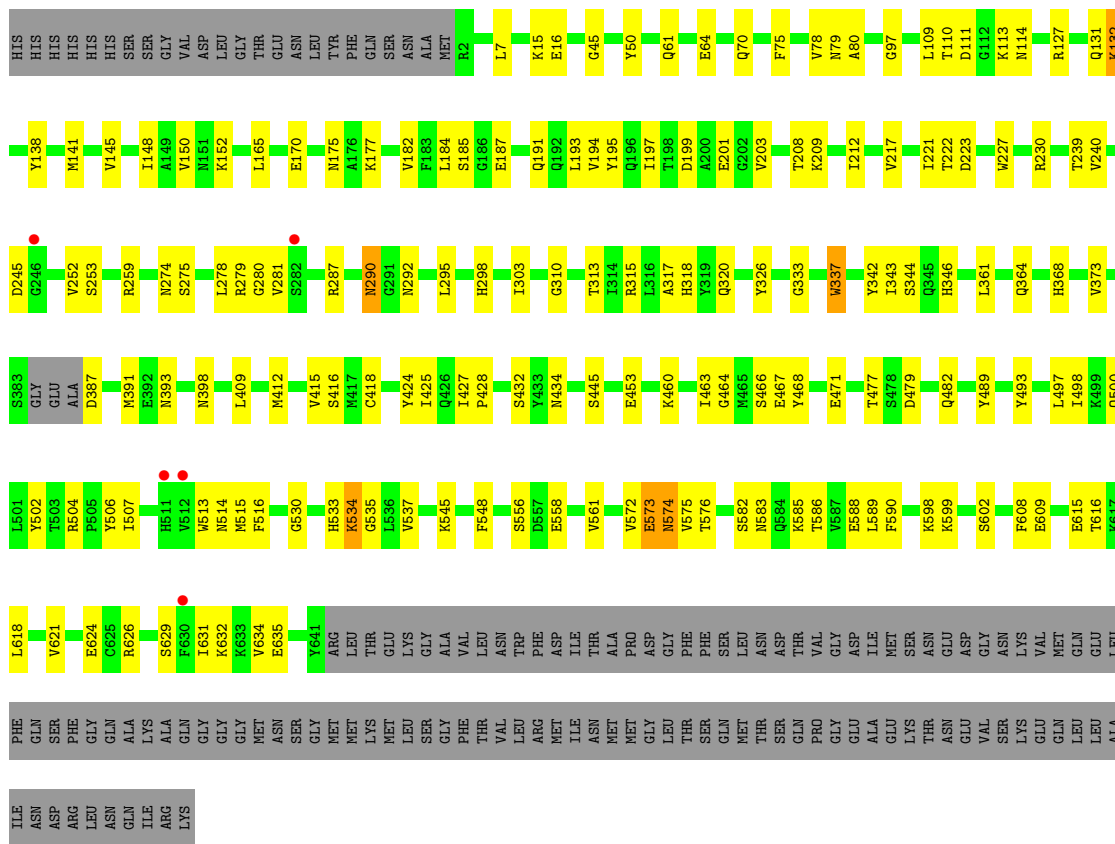I343 S344 S356 Q357 M358 K359 E360 L361 I362 V363 S370 I371 V372 V373 N378 E379 I380 T381 M382 SER GLY ALA D387 N393 H394 N398 D399 L400 E403 M404 D405 P406 T407 R408 L409 M412 A413 V414 V415 D419 M420 H421 N422 P423 Y424 I427 P428 Y433 N434

Y440 D443 T444 S445 M446 E467 E471 H476 E488 I507 H511 V512 W513 N514 M515 F516 N524 M531 N532 H533 K534 G535 L536 V537 K544 V572 E573 T576 V587 E588 K598 K599 S602 F608 E615 A620 V621 A622 G623 E624 C625

R626 V634 L643 THR GLU LYS GLY ALA VAL LEU ASN TRP PHE ASP ILE THR ALA PRO ASP GLY PHE PHE SER LEU ASN ASP THR VAL GLY ASP ILE MET SER ASN GLU ASP GLY VAL LYS VAL MET GLN GLU LEU PHE GLN SER PHE GLN ALA LYS ALA GLN GLY GLY MET

ASN SER GLY MET MET LYS MET LEU SER MET GLY PHE THR VAL LEU ARG MET ILE ASN MET MET GLY LEU THR SER GLN MET THR SER GLN PRO GLU GLY ALA GLU LYS THR ASN GLU VAL LYS GLU LEU LEU LEU ALA ILE ASP ARG ASN GLN ILE ARG LYS

● **Molecule 1: beta-glucuronidase**

Chain C:

61%   20%   ·   18%

HIS HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER ASN ALA MET R2 L7 K15 E16 G45 Y50 Q61 E64 Q70 F75 V78 N79 A80 G97 L109 T110 D111 G112 K113 N114 R127 Q131 K132

Y138 M141 V145 I148 A149 V150 N151 K152 L165 E170 N175 A176 K177 V182 F183 L184 S185 G186 E187 Q191 Q192 L193 V194 Y195 Q196 I197 T198 D199 A200 E201 G202 V203 T208 K209 I212 V217 I221 T222 D223 W227 R230 T239 V240

D245 G246 V252 S253 R259 N274 S275 L278 R279 G280 V281 S282 R287 N290 G291 N292 L295 H298 I303 G310 T313 I314 R315 L316 A317 H318 Y319 Q320 Y326 G333 W337 Y342 I343 S344 Q345 H346 L361 Q364 H368 V373

S383 GLY GLU ALA D387 M391 E392 N393 N398 L409 M412 V415 S416 M417 C418 Y424 I425 Q426 I427 P428 S432 Y433 N434 S445 E453 K460 I463 G464 M465 S466 E467 Y468 E471 T477 S478 D479 Q482 Y489 Y493 L497 I498 K499 Q500

L501 Y502 T503 R504 P505 Y506 I507 H511 V512 W513 N514 M515 F516 G530 H533 K534 G535 L536 V537 K545 F548 S556 D557 E558 V561 V572 E573 N574 V575 T576 S582 N583 Q584 K585 T586 V587 E588 L589 F590 K598 K599 S602 F608 E609 E615 T616 K617

L618 V621 E624 C625 R626 S629 F630 I631 K632 K633 V634 E635 Y641 ARG LEU THR GLU LYS GLY ALA VAL LEU ASN TRP PHE ASP ILE THR ALA PRO ASP GLY PHE PHE SER LEU ASN ASP THR VAL GLY ASP ILE MET SER ASN GLU ASP GLY VAL LYS VAL MET GLN GLU LEU

PHE GLN SER PHE GLY GLN ALA LYS ALA GLN GLY GLY MET ASN SER GLY MET MET LYS MET LEU SER MET GLY PHE THR VAL LEU ARG MET ILE ASN MET MET GLY LEU THR SER GLN MET THR SER GLN PRO GLU GLY ALA GLU LYS THR ASN GLU VAL LYS GLU LEU LEU LEU ALA

ILE ASN ASP ARG LEU ASN GLN ILE ARG LYS

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) 99.8 (29.88-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (3.14%)	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 , 35.1	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	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.*

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[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, 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	0.47	0/5295	0.63	0/7185
1	B	0.51	0/5292	0.65	1/7182 (0.0%)
1	C	0.46	0/5299	0.62	0/7191
All	All	0.48	0/15886	0.63	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(^{o})	Ideal(^{o})
1	B	424	TYR	CA-CB-CG	5.17	123.22	113.40

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	5153	0	4843	76	0
1	B	5150	0	4844	98	0
1	C	5157	0	4844	96	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	271	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 (271) 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:A:528:GLU:OE2	1:A:531:MET:HG3	1.83	0.79
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLU:OE2	1:B:67:GLU:N	2.32	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:105:MET:HE3	1:B:109:LEU:HD21	1.83	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: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:118:VAL:HG11	1:B:141:MET:HE3	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:141:MET:HE2	1:A:145:VAL:HG21	1.88	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:279:ARG:HB3	1:A:502:TYR:CZ	2.44	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:A:434:ASN:CG	1:A:467:GLU:HB2	2.33	0.48
1:B:34:PRO:HB3	1:B:142:TYR:O	2.13	0.48
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:337:TRP:CD1	1:B:337:TRP:C	2.87	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:573:GLU:CD	1:B:576:THR:HG22	2.35	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:B:412:MET:HE3	1:B:428:PRO:HG3	1.97	0.47
1:C:70:GLN:HG3	1:C:152:LYS:HG2	1.97	0.47
1:C:141:MET:HE2	1:C:145:VAL:HG21	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: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:C:141:MET:CE	1:C:145:VAL:HG21	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:533:HIS:C	1:C:535:GLY:H	2.19	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: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:75:PHE:HE2	1:C:141:MET:HE3	1.80	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:B:363:VAL:HA	2:B:801:FMN:HM72	1.99	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:A:412:MET:HE3	1:A:412:MET:HB3	1.81	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:B:315:ARG:HH12	1:B:467:GLU:HG3	1.82	0.44
1:A:105:MET:HE1	1:A:147:ILE:HD13	2.00	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:B:412:MET:HE3	1:B:412:MET:HB3	1.82	0.44
1:C:513:TRP:HA	1:C:514:ASN:HA	1.72	0.44
1:B:443:ASP:OD1	1:B:446:MET:HG3	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:358:MET:HE2	1:B:362:ILE:HG13	1.99	0.43
1:B:573:GLU:OE2	1:B:576:THR:HG22	2.19	0.43
1:C:75:PHE:CE2	1:C:141:MET:HE3	2.53	0.43
1:C:315:ARG:HG3	1:C:337:TRP:CG	2.53	0.43
1:B:61:GLN:OE1	1:B:113:LYS:HG2	2.18	0.43
1:C:412:MET:HE3	1:C:428:PRO:HG3	2.01	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:A:629:SER:C	1:A:630:PHE:HD2	2.22	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:B:73:LEU:HD13	1:B:75:PHE:CZ	2.54	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PHE:HA	1:A:270:PHE:O	2.20	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: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: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:97:GLY:O	1:A:142:TYR:OH	2.31	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: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: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
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:545:LYS:O	1:C:548:PHE:HB3	2.22	0.40
1:A:478:SER:C	1:A:480:PRO:HD3	2.42	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%)	47	78
1	B	632/777 (81%)	592 (94%)	37 (6%)	3 (0%)	29	61
1	C	633/777 (82%)	591 (93%)	40 (6%)	2 (0%)	41	72
All	All	1898/2331 (81%)	1784 (94%)	108 (6%)	6 (0%)	41	72

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%)	514 (94%)	33 (6%)	19	48
1	B	547/665 (82%)	512 (94%)	35 (6%)	17	45
1	C	548/665 (82%)	522 (95%)	26 (5%)	26	59
All	All	1642/1995 (82%)	1548 (94%)	94 (6%)	20	50

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
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	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	259	ARG
1	A	275	SER
1	A	337	TRP
1	A	393	ASN
1	A	400	LEU
1	A	407	THR
1	A	412	MET
1	A	416	SER
1	A	424	TYR
1	A	443	ASP
1	A	470	CYS
1	A	482	GLN
1	A	539	PHE
1	A	576	THR
1	A	596	LEU
1	A	613	HIS
1	A	631	ILE
1	A	636	LYS
1	B	103	VAL
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

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Mol	Chain	Res	Type
1	B	203	VAL
1	B	212	ILE
1	B	213	SER
1	B	225	HIS
1	B	247	VAL
1	B	248	CYS
1	B	259	ARG
1	B	260	THR
1	B	262	THR
1	B	266	ASP
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	424	TYR
1	B	444	THR
1	B	488	GLU
1	B	524	ASN
1	B	544	LYS
1	B	602	SER
1	B	615	GLU
1	C	132	LYS
1	C	185	SER
1	C	187	GLU
1	C	193	LEU
1	C	195	TYR
1	C	245	ASP
1	C	259	ARG
1	C	274	ASN
1	C	275	SER
1	C	287	ARG
1	C	290	ASN
1	C	337	TRP
1	C	344	SER
1	C	393	ASN
1	C	415	VAL
1	C	418	CYS

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Mol	Chain	Res	Type
1	C	424	TYR
1	C	425	ILE
1	C	453	GLU
1	C	460	LYS
1	C	556	SER
1	C	574	ASN
1	C	590	PHE
1	C	602	SER
1	C	616	THR
1	C	624	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	394	HIS
1	C	175	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	801	-	33,33,33	1.02	2 (6%)	48,50,50	1.41	9 (18%)
2	FMN	B	801	-	33,33,33	1.16	3 (9%)	48,50,50	1.65	11 (22%)
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	A	801	-	-	0/18/18/18	0/3/3/3
2	FMN	B	801	-	-	7/18/18/18	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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.
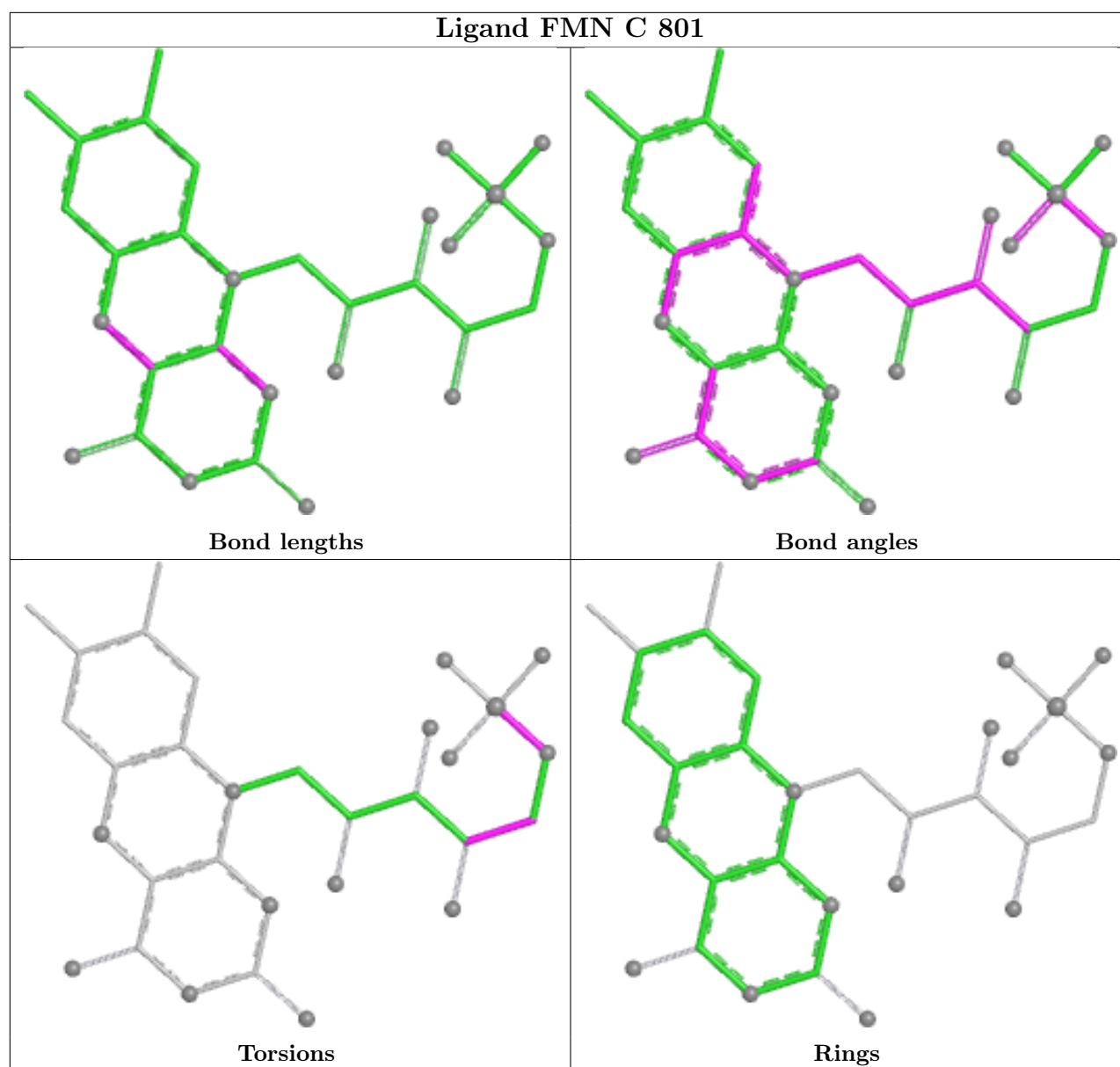
2 monomers are involved in 3 short contacts:

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 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 801

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN B 801

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN C 801

Bond lengths

Bond angles

Torsions

Rings
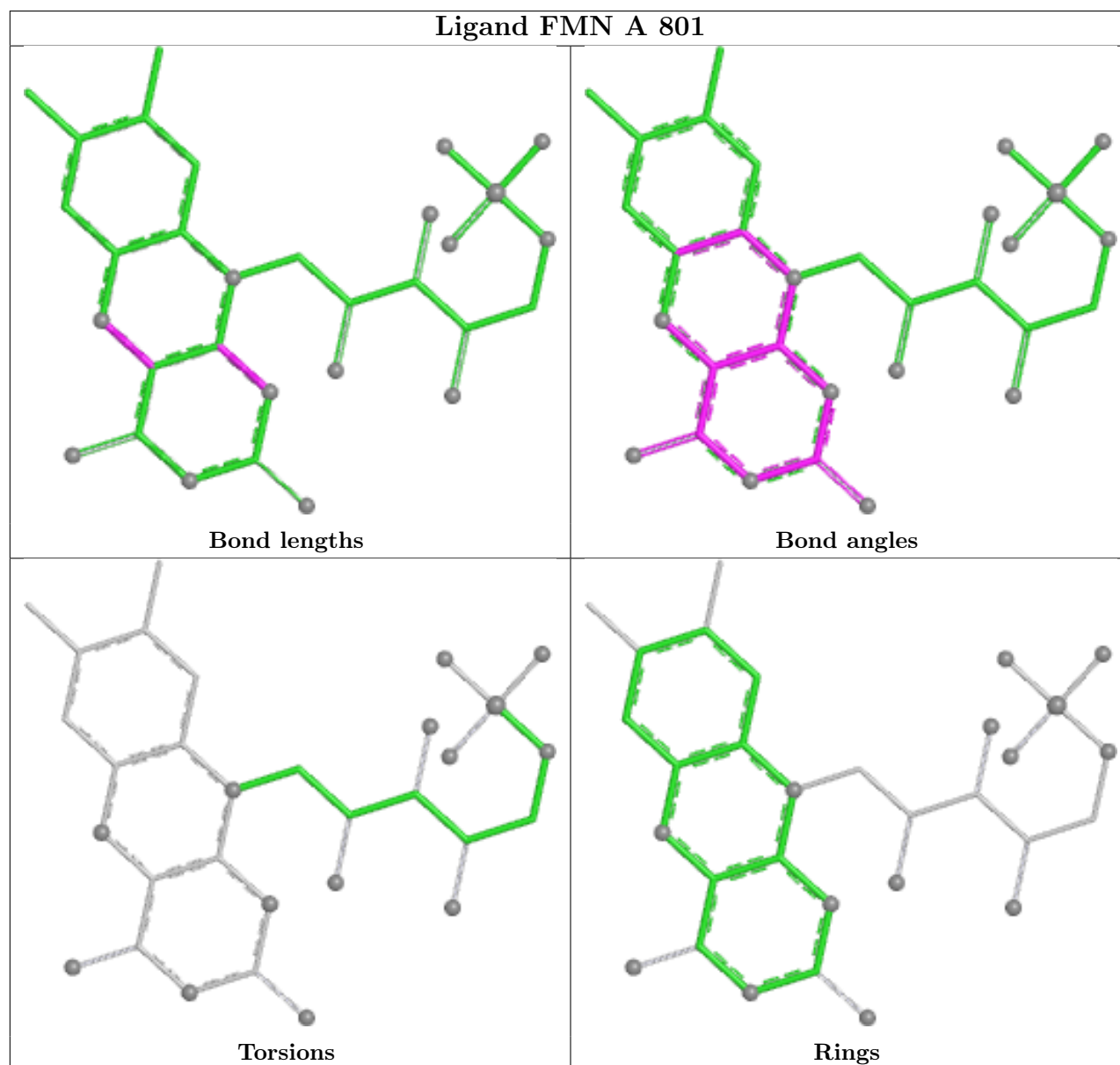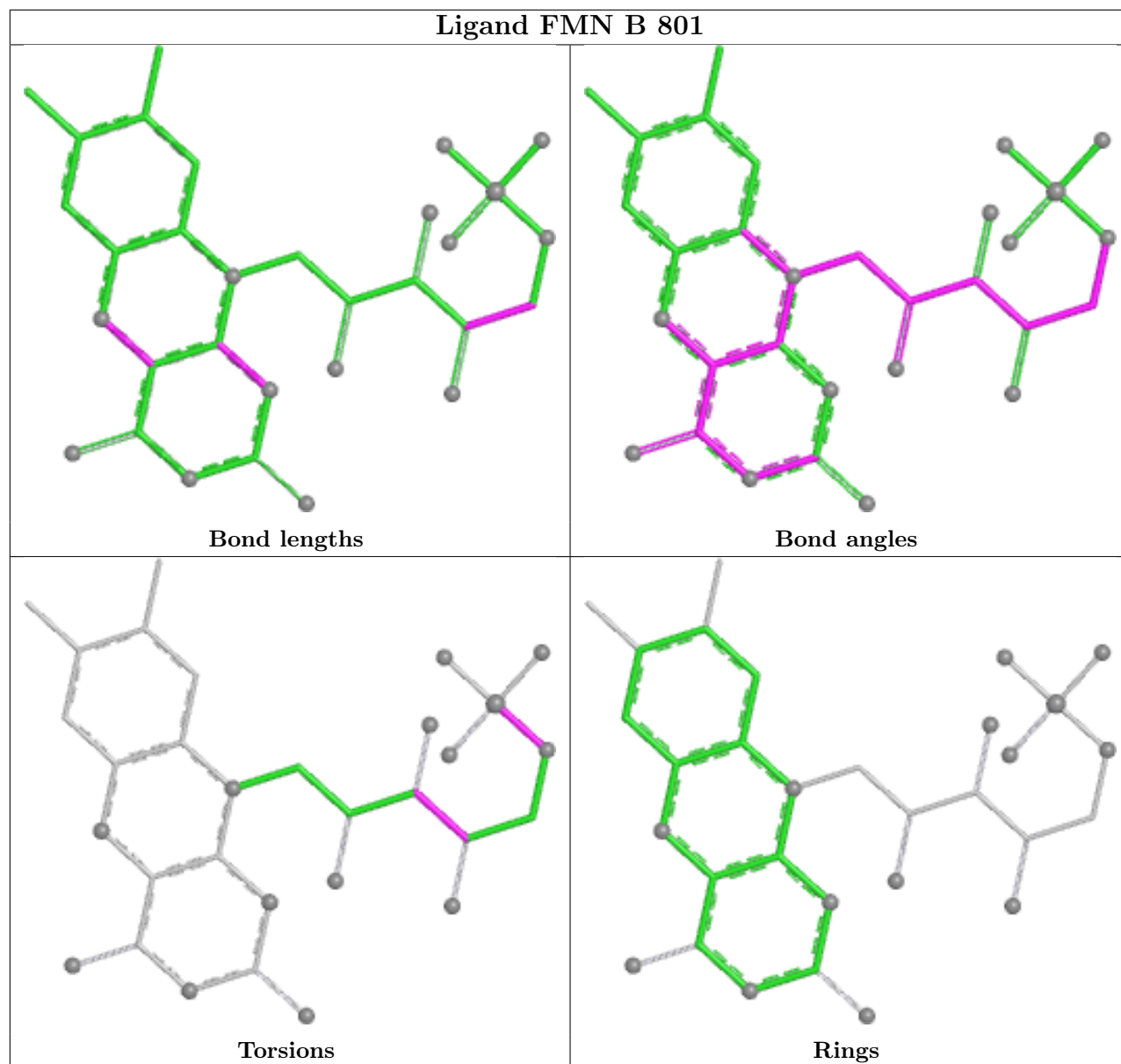
5.7 Other polymers (i)

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, 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%)	-0.33	2 (0%)	94	93	40, 62, 93, 111	0
1	B	636/777 (81%)	-0.37	3 (0%)	91	88	35, 60, 83, 98	0
1	C	637/777 (81%)	-0.27	5 (0%)	86	81	38, 67, 90, 104	0
All	All	1910/2331 (81%)	-0.33	10 (0%)	91	88	35, 62, 89, 111	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	GLY	3.3
1	B	221	ILE	3.1
1	A	441	GLY	2.7
1	C	282	SER	2.5
1	C	246	GLY	2.3
1	A	640	ALA	2.3
1	C	512	VAL	2.2
1	C	630	PHE	2.1
1	B	440	TYR	2.1
1	C	511	HIS	2.0

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

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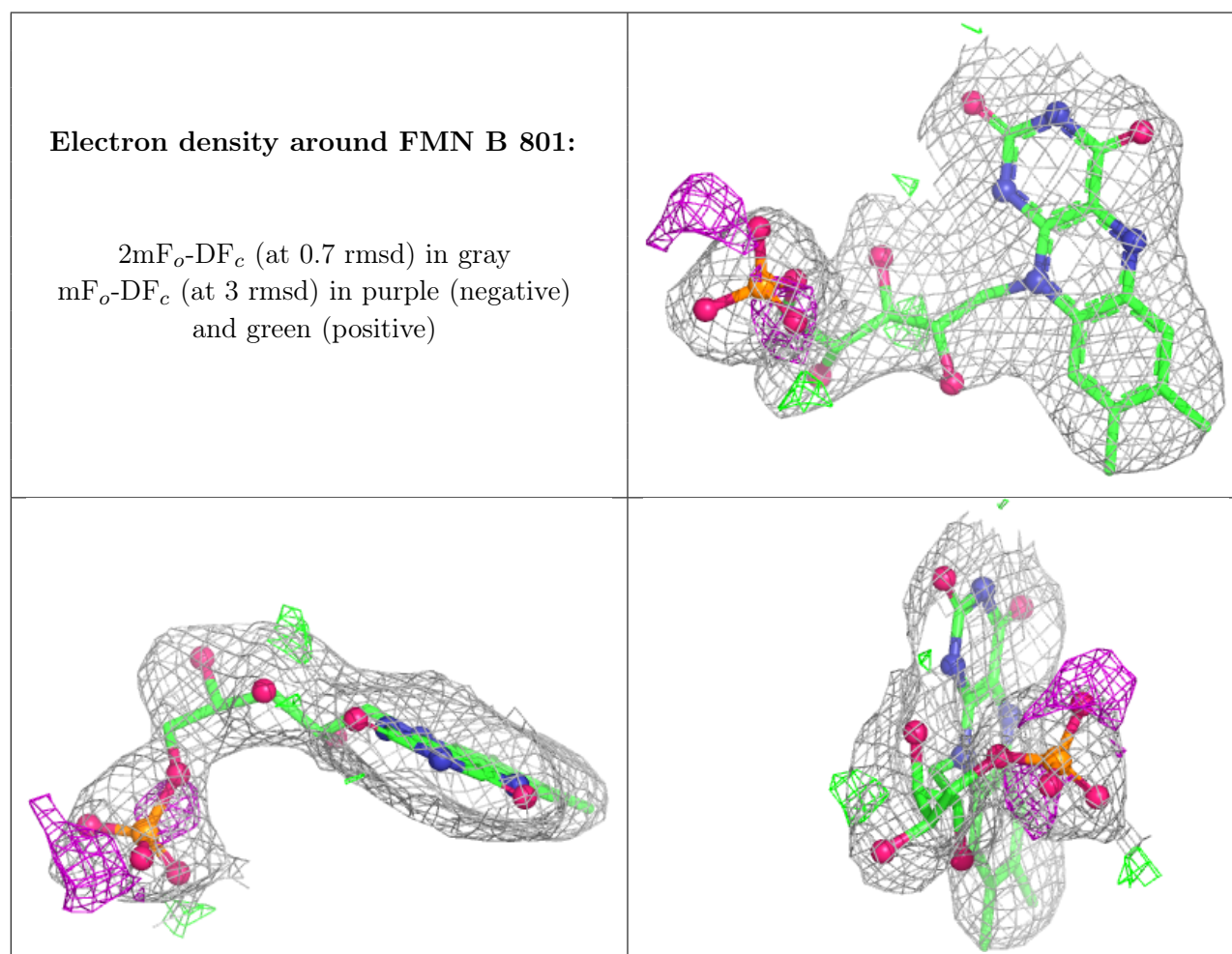
6.3 Carbohydrates ⓘ

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
2	FMN	B	801	31/31	0.89	0.18	52,62,85,93	0
2	FMN	C	801	31/31	0.93	0.18	61,69,76,90	0
2	FMN	A	801	31/31	0.94	0.13	58,68,78,93	0
3	CA	B	802	1/1	0.98	0.03	63,63,63,63	0
3	CA	C	802	1/1	0.98	0.04	70,70,70,70	0
3	CA	A	802	1/1	0.99	0.09	65,65,65,65	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.
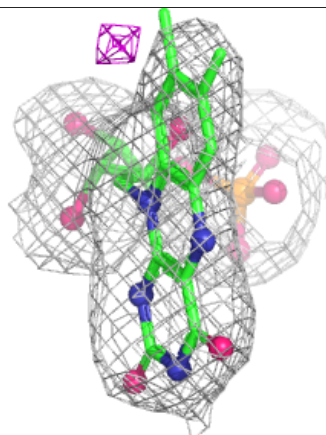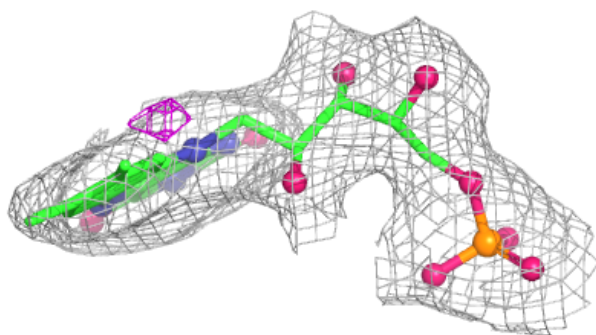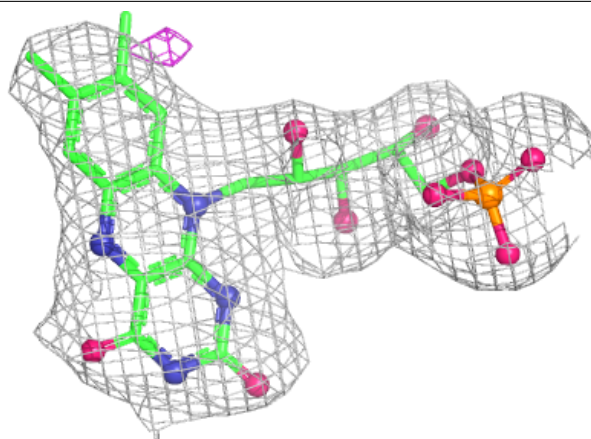

Electron density around FMN B 801:

$2mF_o$-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)
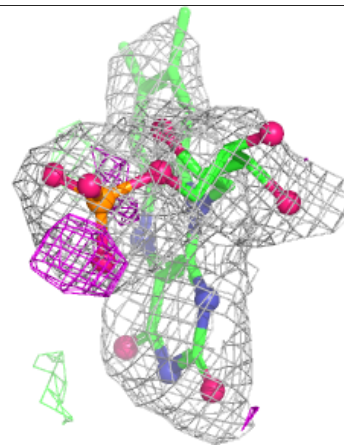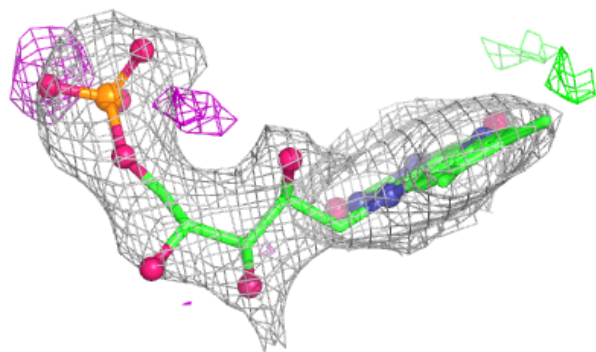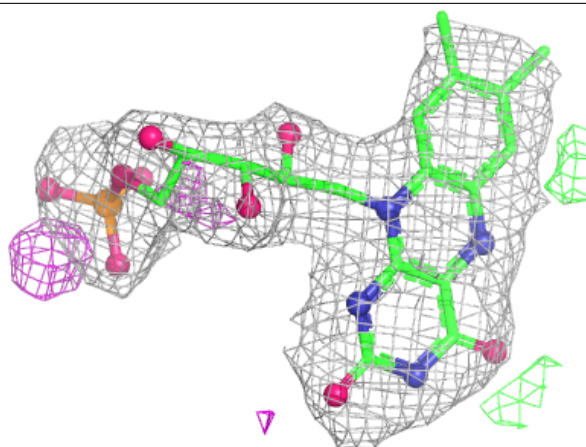
Electron density around FMN A 801:

$2mF_o$-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 ⓘ

There are no such residues in this entry.