



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:12 am BST

PDB ID : 6MVH
Title : Crystal structure of FMN-binding beta-glucuronidase from Roseburia hominis
Authors : Pellock, S.J.; Redinbo, M.R.
Deposited on : 2018-10-25
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

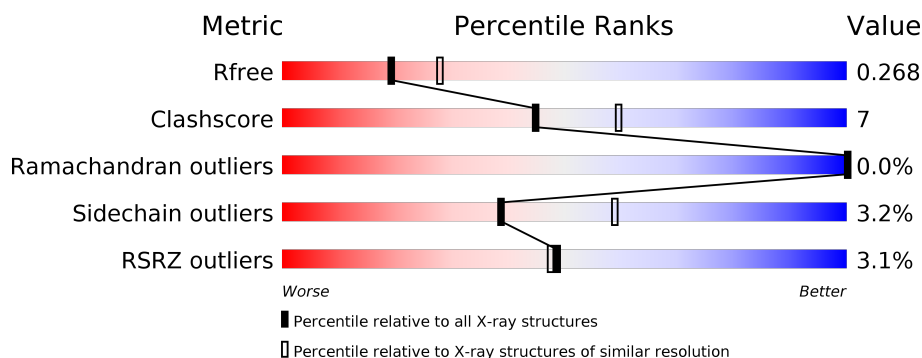
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	780	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>12%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	780	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>12%</div> <div>•</div> <div>18%</div> </div> </div>
1	C	780	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>12%</div> <div>•</div> <div>18%</div> </div> </div>
1	D	780	<div> <div>5%</div> <div> <div></div> <div>29%</div> <div>10%</div> <div>•</div> <div>61%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18964 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-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			5175	3290	865	1000	20			
1	B	638	Total	C	N	O	S	0	0	0
			5167	3286	864	997	20			
1	C	638	Total	C	N	O	S	0	1	0
			5174	3291	866	997	20			
1	D	305	Total	C	N	O	S	0	0	0
			2494	1573	429	480	12			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	HIS	-	expression tag	UNP A0A174HGC0
A	-22	HIS	-	expression tag	UNP A0A174HGC0
A	-21	HIS	-	expression tag	UNP A0A174HGC0
A	-20	HIS	-	expression tag	UNP A0A174HGC0
A	-19	HIS	-	expression tag	UNP A0A174HGC0
A	-18	HIS	-	expression tag	UNP A0A174HGC0
A	-17	SER	-	expression tag	UNP A0A174HGC0
A	-16	SER	-	expression tag	UNP A0A174HGC0
A	-15	GLY	-	expression tag	UNP A0A174HGC0
A	-14	VAL	-	expression tag	UNP A0A174HGC0
A	-13	ASP	-	expression tag	UNP A0A174HGC0
A	-12	LEU	-	expression tag	UNP A0A174HGC0
A	-11	GLY	-	expression tag	UNP A0A174HGC0
A	-10	THR	-	expression tag	UNP A0A174HGC0
A	-9	GLU	-	expression tag	UNP A0A174HGC0
A	-8	ASN	-	expression tag	UNP A0A174HGC0
A	-7	LEU	-	expression tag	UNP A0A174HGC0
A	-6	TYR	-	expression tag	UNP A0A174HGC0
A	-5	PHE	-	expression tag	UNP A0A174HGC0
A	-4	GLN	-	expression tag	UNP A0A174HGC0
A	-3	SER	-	expression tag	UNP A0A174HGC0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ASN	-	expression tag	UNP A0A174HGC0
A	-1	ALA	-	expression tag	UNP A0A174HGC0
B	-23	HIS	-	expression tag	UNP A0A174HGC0
B	-22	HIS	-	expression tag	UNP A0A174HGC0
B	-21	HIS	-	expression tag	UNP A0A174HGC0
B	-20	HIS	-	expression tag	UNP A0A174HGC0
B	-19	HIS	-	expression tag	UNP A0A174HGC0
B	-18	HIS	-	expression tag	UNP A0A174HGC0
B	-17	SER	-	expression tag	UNP A0A174HGC0
B	-16	SER	-	expression tag	UNP A0A174HGC0
B	-15	GLY	-	expression tag	UNP A0A174HGC0
B	-14	VAL	-	expression tag	UNP A0A174HGC0
B	-13	ASP	-	expression tag	UNP A0A174HGC0
B	-12	LEU	-	expression tag	UNP A0A174HGC0
B	-11	GLY	-	expression tag	UNP A0A174HGC0
B	-10	THR	-	expression tag	UNP A0A174HGC0
B	-9	GLU	-	expression tag	UNP A0A174HGC0
B	-8	ASN	-	expression tag	UNP A0A174HGC0
B	-7	LEU	-	expression tag	UNP A0A174HGC0
B	-6	TYR	-	expression tag	UNP A0A174HGC0
B	-5	PHE	-	expression tag	UNP A0A174HGC0
B	-4	GLN	-	expression tag	UNP A0A174HGC0
B	-3	SER	-	expression tag	UNP A0A174HGC0
B	-2	ASN	-	expression tag	UNP A0A174HGC0
B	-1	ALA	-	expression tag	UNP A0A174HGC0
C	-23	HIS	-	expression tag	UNP A0A174HGC0
C	-22	HIS	-	expression tag	UNP A0A174HGC0
C	-21	HIS	-	expression tag	UNP A0A174HGC0
C	-20	HIS	-	expression tag	UNP A0A174HGC0
C	-19	HIS	-	expression tag	UNP A0A174HGC0
C	-18	HIS	-	expression tag	UNP A0A174HGC0
C	-17	SER	-	expression tag	UNP A0A174HGC0
C	-16	SER	-	expression tag	UNP A0A174HGC0
C	-15	GLY	-	expression tag	UNP A0A174HGC0
C	-14	VAL	-	expression tag	UNP A0A174HGC0
C	-13	ASP	-	expression tag	UNP A0A174HGC0
C	-12	LEU	-	expression tag	UNP A0A174HGC0
C	-11	GLY	-	expression tag	UNP A0A174HGC0
C	-10	THR	-	expression tag	UNP A0A174HGC0
C	-9	GLU	-	expression tag	UNP A0A174HGC0
C	-8	ASN	-	expression tag	UNP A0A174HGC0
C	-7	LEU	-	expression tag	UNP A0A174HGC0

Continued on next page...

Continued from previous page...

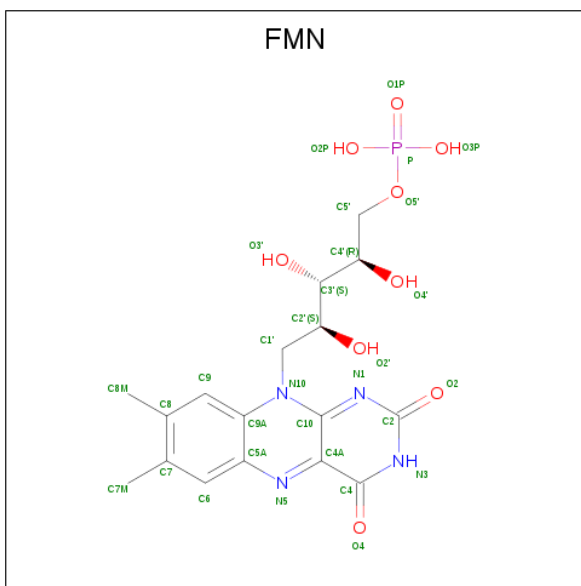
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	TYR	-	expression tag	UNP A0A174HGC0
C	-5	PHE	-	expression tag	UNP A0A174HGC0
C	-4	GLN	-	expression tag	UNP A0A174HGC0
C	-3	SER	-	expression tag	UNP A0A174HGC0
C	-2	ASN	-	expression tag	UNP A0A174HGC0
C	-1	ALA	-	expression tag	UNP A0A174HGC0
D	-23	HIS	-	expression tag	UNP A0A174HGC0
D	-22	HIS	-	expression tag	UNP A0A174HGC0
D	-21	HIS	-	expression tag	UNP A0A174HGC0
D	-20	HIS	-	expression tag	UNP A0A174HGC0
D	-19	HIS	-	expression tag	UNP A0A174HGC0
D	-18	HIS	-	expression tag	UNP A0A174HGC0
D	-17	SER	-	expression tag	UNP A0A174HGC0
D	-16	SER	-	expression tag	UNP A0A174HGC0
D	-15	GLY	-	expression tag	UNP A0A174HGC0
D	-14	VAL	-	expression tag	UNP A0A174HGC0
D	-13	ASP	-	expression tag	UNP A0A174HGC0
D	-12	LEU	-	expression tag	UNP A0A174HGC0
D	-11	GLY	-	expression tag	UNP A0A174HGC0
D	-10	THR	-	expression tag	UNP A0A174HGC0
D	-9	GLU	-	expression tag	UNP A0A174HGC0
D	-8	ASN	-	expression tag	UNP A0A174HGC0
D	-7	LEU	-	expression tag	UNP A0A174HGC0
D	-6	TYR	-	expression tag	UNP A0A174HGC0
D	-5	PHE	-	expression tag	UNP A0A174HGC0
D	-4	GLN	-	expression tag	UNP A0A174HGC0
D	-3	SER	-	expression tag	UNP A0A174HGC0
D	-2	ASN	-	expression tag	UNP A0A174HGC0
D	-1	ALA	-	expression tag	UNP A0A174HGC0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P)

(labeled as "Ligand of Interest" by author).



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

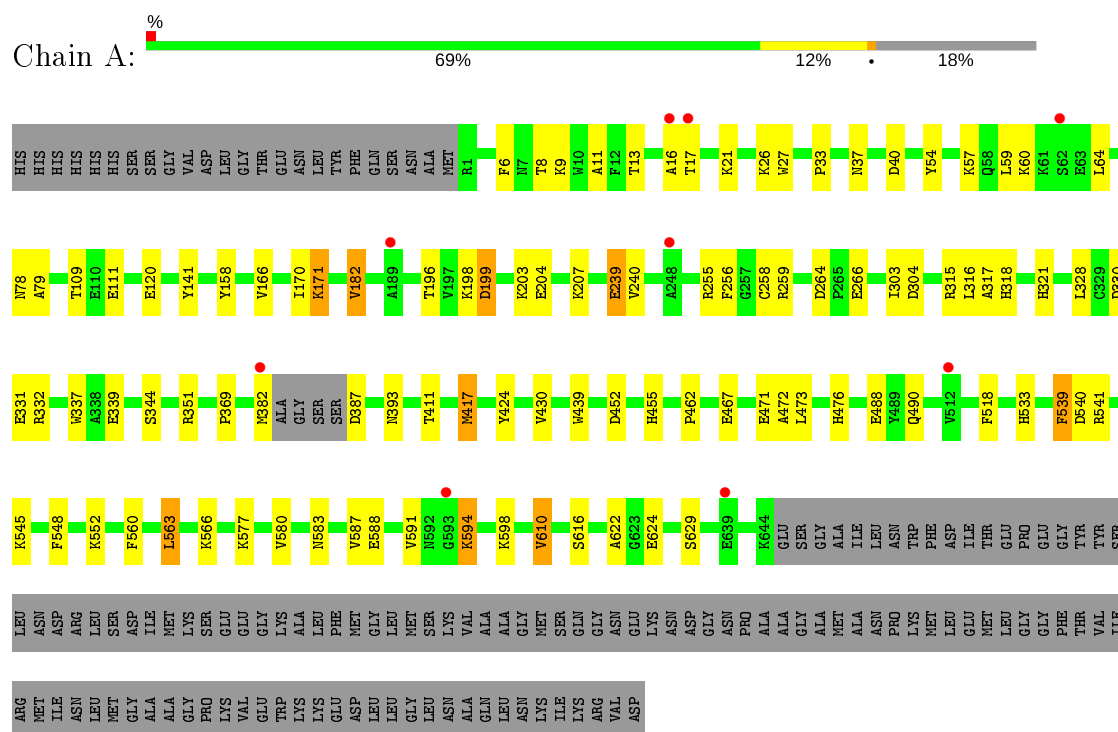
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	296	Total O 296 296	0	0
4	B	224	Total O 224 224	0	0
4	C	234	Total O 234 234	0	0
4	D	72	Total O 72 72	0	0

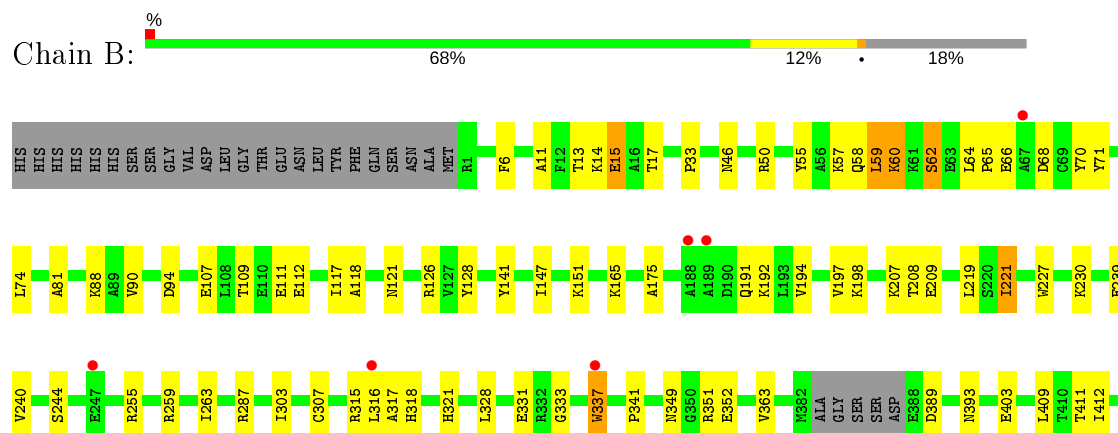
3 Residue-property plots [i](#)

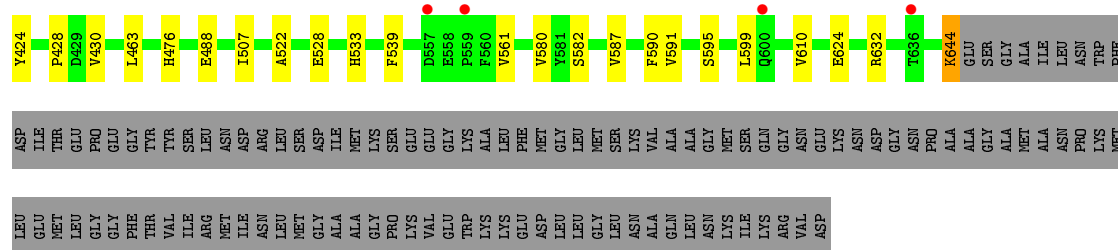
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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-galactosidase

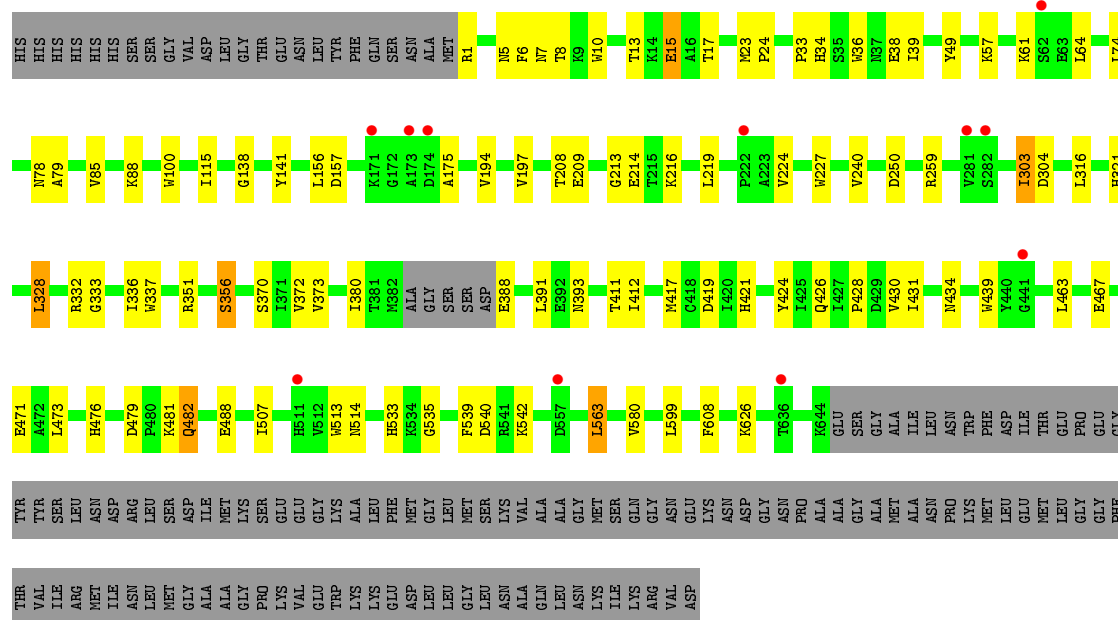


• Molecule 1: Beta-galactosidase

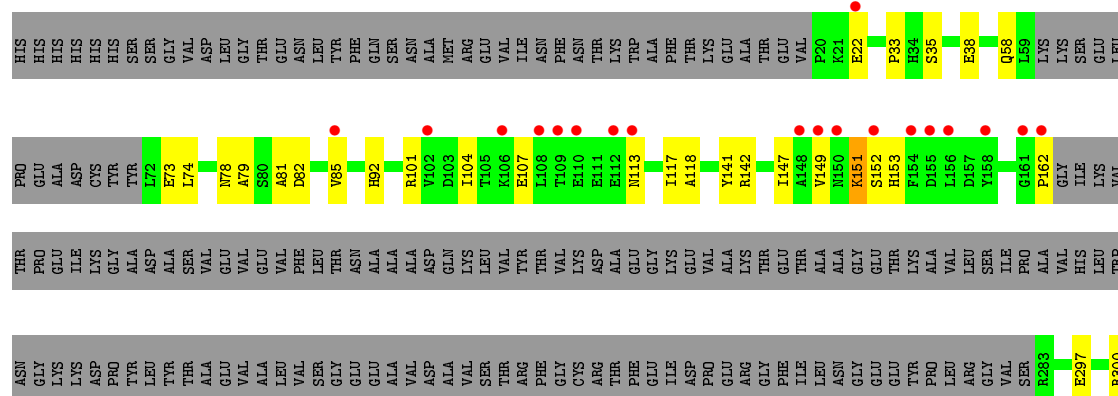




• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.42Å 137.41Å 108.83Å 90.00° 91.88° 90.00°	Depositor
Resolution (Å)	29.27 – 2.40 29.27 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.27-2.40) 98.3 (29.27-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.14 _3260: ???)	Depositor
R, R_{free}	0.209 , 0.268 0.209 , 0.268	Depositor DCC
R_{free} test set	1996 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18964	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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	0.49	0/5317	0.64	2/7226 (0.0%)
1	B	0.44	0/5309	0.60	0/7215
1	C	0.46	0/5320	0.61	0/7230
1	D	0.41	0/2560	0.59	0/3468
All	All	0.46	0/18506	0.61	2/25139 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ASP	N-CA-CB	-5.95	99.90	110.60
1	A	198	LYS	C-N-CA	5.41	135.22	121.70

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	5175	0	4870	64	0
1	B	5167	0	4866	56	0
1	C	5174	0	4873	60	0
1	D	2494	0	2279	50	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	19	3	0
3	B	31	0	19	1	0
3	C	31	0	19	2	0
3	D	31	0	19	2	0
4	A	296	0	0	8	0
4	B	224	0	0	6	0
4	C	234	0	0	8	0
4	D	72	0	0	2	0
All	All	18964	0	16964	229	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 7.

All (229) 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:C:157:ASP:OD2	4:C:901:HOH:O	1.92	0.88
1:A:196:THR:HG22	1:A:207:LYS:HG3	1.65	0.79
1:D:162:PRO:HD3	1:D:364:GLN:HA	1.65	0.77
1:C:61:LYS:HA	1:C:64:LEU:HD12	1.71	0.72
1:B:349:ASN:ND2	4:B:901:HOH:O	2.12	0.70
1:B:13:THR:HB	1:B:15:GLU:H	1.57	0.70
1:A:120:GLU:OE1	4:A:901:HOH:O	2.09	0.70
1:A:16:ALA:HB3	1:A:54:TYR:HD2	1.56	0.70
1:C:479:ASP:OD2	1:C:481:LYS:HE2	1.92	0.70
3:D:802:FMN:H9	3:D:802:FMN:H2'	1.74	0.69
1:C:213:GLY:O	4:C:902:HOH:O	2.11	0.68
1:C:304:ASP:OD1	1:C:332:ARG:NH2	2.27	0.68
1:B:227:TRP:CZ2	1:B:333:GLY:HA2	2.29	0.67
1:B:165:LYS:NZ	4:B:904:HOH:O	2.27	0.67
1:A:59:LEU:HD21	1:A:64:LEU:HD11	1.77	0.66
1:B:68:ASP:OD2	1:B:151:LYS:HG2	1.96	0.66
1:C:388:GLU:HA	1:C:391:LEU:HD12	1.79	0.65
1:B:263:ILE:HD12	1:B:409:LEU:HD12	1.80	0.64
1:D:458:PHE:HB3	1:D:461:ILE:HD12	1.80	0.64
1:B:192:LYS:HE3	1:B:209:GLU:OE2	1.99	0.63
1:A:16:ALA:HB3	1:A:54:TYR:CD2	2.33	0.63
1:D:420:ILE:HG22	1:D:458:PHE:HE2	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:THR:O	1:A:57:LYS:HE2	1.98	0.62
1:B:88:LYS:HE2	1:B:107:GLU:OE2	1.99	0.61
1:C:316:LEU:HB3	1:C:321:HIS:CD2	2.36	0.61
1:C:356:SER:OG	4:C:903:HOH:O	2.14	0.60
1:C:439:TRP:CZ2	1:C:471:GLU:HG3	2.37	0.60
1:D:73:GLU:HG3	1:D:101:ARG:HG2	1.82	0.60
1:D:324:TYR:CE2	1:D:328:LEU:HD11	2.35	0.60
1:D:356:SER:OG	4:D:902:HOH:O	2.16	0.60
1:C:13:THR:OG1	1:C:15:GLU:HG3	2.02	0.60
1:D:420:ILE:HG22	1:D:458:PHE:CE2	2.37	0.59
1:C:6:PHE:CZ	1:C:57:LYS:HD3	2.37	0.59
1:A:13:THR:HG21	1:A:16:ALA:HB2	1.84	0.59
1:A:563:LEU:HD13	1:A:580:VAL:HG22	1.84	0.59
1:D:317:ALA:HB1	1:D:318:HIS:CG	2.38	0.58
1:D:325:PHE:HA	1:D:328:LEU:HD12	1.85	0.58
3:D:802:FMN:O4'	3:D:802:FMN:O2'	2.18	0.58
1:A:316:LEU:HB3	1:A:321:HIS:CD2	2.38	0.58
1:D:454:PHE:CD2	1:D:463:LEU:HD22	2.39	0.58
1:A:591:VAL:O	1:A:594:LYS:HE3	2.04	0.57
1:D:360:GLU:O	1:D:364:GLN:HG2	2.04	0.57
1:C:540:ASP:OD2	1:C:542:LYS:HD2	2.04	0.56
1:D:142:ARG:HD3	4:D:937:HOH:O	2.06	0.56
1:C:175:ALA:HB2	1:C:224:VAL:HG11	1.88	0.56
1:D:85:VAL:HG21	1:D:104:ILE:HD11	1.87	0.56
1:D:318:HIS:HA	1:D:339:GLU:OE2	2.06	0.56
1:D:398:ASN:ND2	1:D:427:ILE:O	2.39	0.55
1:C:411:THR:HA	1:C:430:VAL:O	2.06	0.55
1:B:126:ARG:NH2	4:B:916:HOH:O	2.38	0.55
1:D:85:VAL:HG21	1:D:104:ILE:CD1	2.37	0.55
1:B:580:VAL:HG11	1:B:587:VAL:HG11	1.89	0.55
1:B:59:LEU:HD21	1:B:64:LEU:HD21	1.89	0.54
1:C:214:GLU:OE2	1:C:216:LYS:HE2	2.07	0.54
1:A:304:ASP:OD1	1:A:332:ARG:NH2	2.34	0.54
1:C:194:VAL:HG22	1:C:209:GLU:HG2	1.89	0.54
1:B:128:TYR:HB3	1:B:341:PRO:O	2.08	0.54
1:C:412:ILE:HG12	1:C:428:PRO:HG3	1.89	0.54
1:B:94:ASP:OD1	4:B:902:HOH:O	2.19	0.53
1:B:197:VAL:HG23	1:B:219:LEU:HD22	1.90	0.53
1:A:588:GLU:HB2	1:A:598:LYS:HG2	1.91	0.53
1:B:198:LYS:NZ	1:B:239:GLU:OE2	2.32	0.53
1:B:58:GLN:HB2	1:B:60:LYS:HE2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ALA:HB1	1:D:318:HIS:ND1	2.24	0.52
1:A:203:LYS:HD3	1:A:204:GLU:O	2.10	0.52
1:D:320:GLN:NE2	1:D:364:GLN:OE1	2.35	0.52
1:C:426:GLN:HB3	1:D:403:GLU:OE1	2.09	0.52
1:A:170:ILE:HD11	1:A:258:CYS:HB3	1.92	0.52
1:C:15:GLU:OE2	1:C:17:THR:HG23	2.10	0.52
1:D:398:ASN:HD21	1:D:428:PRO:HA	1.75	0.52
1:C:303:ILE:HD13	1:C:328:LEU:HB3	1.92	0.52
1:A:577:LYS:H	1:A:577:LYS:HD2	1.76	0.51
1:A:6:PHE:CZ	1:A:57:LYS:HD3	2.46	0.51
1:C:33:PRO:HB3	1:C:141:TYR:O	2.10	0.51
1:B:65:PRO:O	1:B:70:TYR:OH	2.21	0.51
1:C:563:LEU:HD13	1:C:580:VAL:HG22	1.91	0.51
1:B:17:THR:HG21	1:D:351:ARG:HG2	1.92	0.51
1:D:402:HIS:NE2	1:D:429:ASP:OD2	2.27	0.51
1:C:476:HIS:HA	1:C:488:GLU:OE2	2.11	0.50
1:B:175:ALA:HB3	1:B:221:ILE:HG23	1.93	0.50
1:A:37:ASN:HA	1:A:40:ASP:OD1	2.11	0.50
1:C:1:ARG:NH1	1:C:156:LEU:HD21	2.26	0.50
1:C:419:ASP:OD2	1:C:421:HIS:N	2.39	0.50
1:C:514:ASN:O	1:C:535:GLY:HA2	2.11	0.50
1:C:599:LEU:HD12	1:C:608:PHE:CE1	2.47	0.50
1:A:411:THR:HA	1:A:430:VAL:O	2.11	0.50
1:A:315:ARG:HH12	1:A:467:GLU:HG3	1.76	0.50
1:D:82:ASP:OD2	1:D:92:HIS:HB2	2.12	0.50
1:D:35:SER:O	1:D:38:GLU:HG3	2.12	0.49
1:D:398:ASN:HD22	1:D:427:ILE:HG22	1.77	0.49
1:B:62:SER:HB3	1:B:111:GLU:OE2	2.12	0.49
1:B:14:LYS:NZ	4:B:906:HOH:O	2.30	0.49
1:C:8:THR:O	1:C:57:LYS:HE2	2.13	0.49
1:D:316:LEU:HD12	1:D:326:TYR:HE1	1.78	0.49
1:B:60:LYS:NZ	1:B:112:GLU:OE1	2.42	0.49
1:A:266:GLU:OE1	1:A:455:HIS:NE2	2.33	0.49
1:A:439:TRP:CZ2	1:A:471:GLU:HG3	2.47	0.49
1:A:33:PRO:HB3	1:A:141:TYR:O	2.13	0.49
1:A:351:ARG:HH11	1:C:17:THR:HG22	1.78	0.48
1:A:344:SER:O	1:A:382:MET:HB2	2.13	0.48
1:B:561:VAL:HG23	1:B:582:SER:HB2	1.94	0.48
1:A:182:VAL:HG21	1:A:240:VAL:HG11	1.95	0.48
1:A:21:LYS:HG3	3:C:802:FMN:O1P	2.13	0.48
1:A:616:SER:OG	4:A:902:HOH:O	2.19	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:GLN:NE2	4:C:909:HOH:O	2.33	0.48
1:B:191:GLN:NE2	1:B:244:SER:OG	2.44	0.48
1:D:514:ASN:O	1:D:535:GLY:HA2	2.14	0.48
1:A:239:GLU:HG3	4:A:1176:HOH:O	2.14	0.47
1:B:316:LEU:HB3	1:B:321:HIS:CD2	2.49	0.47
1:A:330:ASP:CG	1:A:369:PRO:HD2	2.34	0.47
1:A:315:ARG:NH1	1:A:467:GLU:HG3	2.29	0.47
1:C:10:TRP:CE3	1:C:57:LYS:HB2	2.49	0.47
1:B:411:THR:HA	1:B:430:VAL:O	2.14	0.47
1:A:109:THR:O	4:A:904:HOH:O	2.20	0.47
1:C:197:VAL:HG23	1:C:219:LEU:HD22	1.95	0.47
1:A:583:ASN:O	4:A:903:HOH:O	2.20	0.47
1:A:318:HIS:HA	1:A:339:GLU:OE2	2.14	0.47
1:B:68:ASP:HB2	1:B:151:LYS:N	2.29	0.47
1:B:46:ASN:HB2	1:B:522:ALA:HA	1.97	0.47
1:A:430:VAL:HG12	1:A:462:PRO:HG2	1.98	0.46
1:A:587:VAL:HG22	1:A:622:ALA:HB2	1.96	0.46
1:C:372:VAL:HG23	1:C:373:VAL:HG13	1.97	0.46
1:A:158:TYR:OH	3:A:802:FMN:H5'2	2.15	0.46
1:C:74:LEU:HD22	1:C:100:TRP:CZ2	2.51	0.46
1:A:591:VAL:HG21	1:A:610:VAL:HG22	1.97	0.46
1:B:33:PRO:HB3	1:B:141:TYR:O	2.15	0.46
1:A:171:LYS:HD3	1:A:171:LYS:HA	1.62	0.46
1:A:26:LYS:NZ	1:D:389:ASP:OD2	2.31	0.46
1:D:33:PRO:HB3	1:D:141:TYR:O	2.15	0.45
1:A:552:LYS:HG2	1:A:560:PHE:CE1	2.52	0.45
1:C:351:ARG:HB2	4:C:965:HOH:O	2.16	0.45
1:A:417:MET:SD	1:A:417:MET:N	2.87	0.45
1:B:71:TYR:HB2	1:B:147:ILE:HB	1.97	0.45
1:C:1:ARG:HB2	1:C:250:ASP:OD1	2.16	0.45
1:A:166:VAL:HG11	1:A:256:PHE:CG	2.52	0.45
1:A:9:LYS:NZ	4:A:935:HOH:O	2.49	0.45
1:C:38:GLU:HG3	1:C:39:ILE:HG13	1.98	0.45
1:A:60:LYS:HA	1:A:111:GLU:O	2.17	0.45
1:C:463:LEU:O	1:C:507:ILE:HA	2.16	0.45
1:B:303:ILE:HD13	1:B:328:LEU:HB3	1.98	0.45
1:D:151:LYS:O	1:D:153:HIS:ND1	2.50	0.45
1:D:531:GLN:OE1	1:D:539:PHE:HB2	2.17	0.45
1:A:518:PHE:HA	1:A:539:PHE:CE1	2.52	0.44
1:B:230:LYS:NZ	1:B:307:CYS:SG	2.87	0.44
1:B:476:HIS:HA	1:B:488:GLU:OE2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:CG2	1:A:16:ALA:HB2	2.46	0.44
1:B:255:ARG:HH12	1:B:331:GLU:HG2	1.82	0.44
1:A:476:HIS:HA	1:A:488:GLU:OE2	2.17	0.44
1:D:457:GLU:HB3	1:D:458:PHE:CD2	2.52	0.44
1:D:513:TRP:HA	1:D:514:ASN:HA	1.59	0.44
1:B:60:LYS:HA	1:B:111:GLU:O	2.17	0.44
1:B:11:ALA:O	1:B:55:TYR:HA	2.16	0.44
1:D:300:ARG:O	1:D:303:ILE:HG22	2.17	0.44
1:A:540:ASP:O	1:A:541:ARG:HB2	2.18	0.44
1:B:528:GLU:O	1:B:533:HIS:HE1	2.01	0.44
1:C:5:ASN:HD21	1:C:7:ASN:HB2	1.82	0.44
1:B:352:GLU:H	1:B:352:GLU:CD	2.21	0.44
1:A:264:ASP:O	4:A:905:HOH:O	2.21	0.43
1:A:328:LEU:O	1:A:332:ARG:HG2	2.18	0.43
1:C:214:GLU:OE2	1:C:216:LYS:HG2	2.18	0.43
1:C:49:TYR:OH	4:C:904:HOH:O	2.20	0.43
1:D:81:ALA:HA	1:D:118:ALA:O	2.18	0.43
1:D:316:LEU:HD12	1:D:326:TYR:CE1	2.53	0.43
1:D:346:HIS:NE2	1:D:389:ASP:OD1	2.37	0.43
1:B:6:PHE:CZ	1:B:57:LYS:HD3	2.54	0.43
1:B:88:LYS:HE3	1:B:90:VAL:HG12	1.99	0.43
1:C:23:MET:HA	1:C:24:PRO:HD3	1.89	0.43
1:C:78:ASN:HA	1:C:79:ALA:HA	1.61	0.43
1:B:207:LYS:HG2	1:B:208:THR:N	2.33	0.43
1:B:315:ARG:HG3	1:B:337:TRP:CD1	2.53	0.43
1:D:320:GLN:HB2	1:D:361:LEU:HD13	2.00	0.43
1:A:11:ALA:HB1	1:A:27:TRP:HB2	2.00	0.43
1:C:15:GLU:O	1:C:15:GLU:OE2	2.36	0.43
1:C:434:ASN:HB3	1:C:467:GLU:HB2	2.00	0.43
1:B:590:PHE:CE1	1:B:595:SER:HB2	2.54	0.43
1:C:36:TRP:CZ2	1:C:138:GLY:HA3	2.53	0.43
1:C:10:TRP:CE2	1:C:57:LYS:HD2	2.54	0.43
1:A:158:TYR:OH	3:A:802:FMN:H2'	2.19	0.42
1:B:74:LEU:HD21	1:B:117:ILE:HD13	2.00	0.42
1:C:513:TRP:HE3	4:C:905:HOH:O	2.02	0.42
1:A:78:ASN:HA	1:A:79:ALA:HA	1.62	0.42
1:A:199:ASP:HB3	1:A:203:LYS:H	1.84	0.42
1:B:412:ILE:HG12	1:B:428:PRO:HG3	2.01	0.42
1:B:644:LYS:HD3	1:B:644:LYS:H	1.84	0.42
1:C:85:VAL:HG22	1:C:115:ILE:HD12	2.02	0.42
1:C:336:ILE:HG12	1:C:370:SER:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:THR:HG22	1:D:412:ILE:N	2.34	0.42
1:C:434:ASN:CB	1:C:467:GLU:HB2	2.49	0.42
1:B:351:ARG:NH2	1:B:389:ASP:OD1	2.49	0.42
1:B:363:VAL:HA	3:B:802:FMN:HM72	2.02	0.42
1:D:413:ALA:HA	1:D:432:SER:O	2.20	0.42
1:C:316:LEU:HD23	1:C:316:LEU:HA	1.93	0.42
1:C:380:ILE:HD12	1:C:380:ILE:HA	1.86	0.42
1:D:446:MET:O	1:D:450:TRP:HB2	2.20	0.42
1:B:317:ALA:HB1	1:B:318:HIS:ND1	2.34	0.41
1:D:324:TYR:O	1:D:327:ASP:HB2	2.20	0.41
1:B:591:VAL:HG21	1:B:610:VAL:HG13	2.02	0.41
1:D:78:ASN:HA	1:D:79:ALA:HA	1.65	0.41
1:A:472:ALA:HB2	1:A:490:GLN:HB2	2.02	0.41
1:B:81:ALA:HA	1:B:118:ALA:O	2.21	0.41
1:C:1:ARG:HD2	1:C:250:ASP:OD1	2.21	0.41
1:A:158:TYR:CZ	3:A:802:FMN:H2'	2.55	0.41
1:A:545:LYS:O	1:A:548:PHE:HB3	2.21	0.41
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.87	0.41
1:A:317:ALA:HB1	1:A:318:HIS:CG	2.56	0.41
1:A:317:ALA:HB1	1:A:318:HIS:ND1	2.35	0.41
1:B:194:VAL:O	1:B:240:VAL:HA	2.20	0.41
1:D:74:LEU:HD21	1:D:117:ILE:HD13	2.03	0.41
1:C:34:HIS:H	1:C:141:TYR:HA	1.86	0.41
1:D:147:ILE:HG22	1:D:149:VAL:HG13	2.03	0.41
1:D:420:ILE:HD12	1:D:420:ILE:H	1.84	0.41
1:B:463:LEU:O	1:B:507:ILE:HA	2.21	0.41
1:D:420:ILE:HD11	1:D:450:TRP:CZ2	2.56	0.41
1:A:473:LEU:HD21	1:A:533:HIS:CE1	2.56	0.41
1:C:332:ARG:NH1	4:C:915:HOH:O	2.37	0.41
1:D:104:ILE:CD1	1:D:107:GLU:HB2	2.52	0.41
1:A:255:ARG:HH22	1:A:331:GLU:HG3	1.85	0.40
1:D:401:VAL:HG13	1:D:402:HIS:N	2.36	0.40
1:B:287:ARG:HD3	4:B:1082:HOH:O	2.22	0.40
1:B:50:ARG:HA	1:B:121:ASN:OD1	2.20	0.40
1:C:194:VAL:O	1:C:240:VAL:HA	2.21	0.40
1:C:473:LEU:HD21	1:C:533:HIS:CE1	2.56	0.40
1:C:88:LYS:HB2	1:C:88:LYS:HE2	1.96	0.40
1:A:452:ASP:O	4:A:906:HOH:O	2.22	0.40
1:A:566:LYS:HG2	1:A:629:SER:HB3	2.04	0.40
1:B:175:ALA:HB3	1:B:221:ILE:CG2	2.51	0.40
1:C:227:TRP:CZ2	1:C:333:GLY:HA2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:802:FMN:H9	3:C:802:FMN:H1'2	1.42	0.40
1:D:58:GLN:HA	1:D:113:ASN:O	2.22	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	635/780 (81%)	614 (97%)	21 (3%)	0	100	100
1	B	634/780 (81%)	607 (96%)	27 (4%)	0	100	100
1	C	635/780 (81%)	609 (96%)	26 (4%)	0	100	100
1	D	287/780 (37%)	267 (93%)	19 (7%)	1 (0%)	41	55
All	All	2191/3120 (70%)	2097 (96%)	93 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	330	ASP

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	550/662 (83%)	534 (97%)	16 (3%)	42	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	549/662 (83%)	532 (97%)	17 (3%)	40	60
1	C	550/662 (83%)	535 (97%)	15 (3%)	44	65
1	D	265/662 (40%)	251 (95%)	14 (5%)	22	37
All	All	1914/2648 (72%)	1852 (97%)	62 (3%)	39	59

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	171	LYS
1	A	182	VAL
1	A	239	GLU
1	A	259	ARG
1	A	303	ILE
1	A	337	TRP
1	A	387	ASP
1	A	393	ASN
1	A	417	MET
1	A	424	TYR
1	A	539	PHE
1	A	563	LEU
1	A	594	LYS
1	A	610	VAL
1	A	624	GLU
1	B	15	GLU
1	B	59	LEU
1	B	60	LYS
1	B	62	SER
1	B	66	GLU
1	B	109	THR
1	B	221	ILE
1	B	259	ARG
1	B	337	TRP
1	B	393	ASN
1	B	403	GLU
1	B	424	TYR
1	B	539	PHE
1	B	599	LEU
1	B	624	GLU
1	B	632	ARG
1	B	644	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	15	GLU
1	C	208	THR
1	C	259	ARG
1	C	303	ILE
1	C	328	LEU
1	C	337	TRP
1	C	356	SER
1	C	393	ASN
1	C	417	MET
1	C	424	TYR
1	C	431	ILE
1	C	482	GLN
1	C	539	PHE
1	C	563	LEU
1	C	626	LYS
1	D	22	GLU
1	D	151	LYS
1	D	152	SER
1	D	297	GLU
1	D	356	SER
1	D	362	VAL
1	D	377	SER
1	D	393	ASN
1	D	424	TYR
1	D	431	ILE
1	D	432	SER
1	D	456	LYS
1	D	516	PHE
1	D	539	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
3	FMN	A	802	-	31,33,33	1.54	4 (12%)	40,50,50	1.64	6 (15%)
3	FMN	B	802	-	31,33,33	1.47	4 (12%)	40,50,50	1.99	7 (17%)
3	FMN	C	802	-	31,33,33	1.58	5 (16%)	40,50,50	2.40	8 (20%)
3	FMN	D	802	-	31,33,33	1.72	6 (19%)	40,50,50	3.10	10 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	A	802	-	-	11/18/18/18	0/3/3/3
3	FMN	B	802	-	-	6/18/18/18	0/3/3/3
3	FMN	C	802	-	-	15/18/18/18	0/3/3/3
3	FMN	D	802	-	-	17/18/18/18	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	FMN	C1'-N10	5.31	1.53	1.48
3	B	802	FMN	C10-N1	4.68	1.39	1.33
3	C	802	FMN	C10-N1	4.47	1.39	1.33
3	D	802	FMN	C10-N1	4.16	1.38	1.33
3	A	802	FMN	C10-N1	3.85	1.38	1.33
3	A	802	FMN	C1'-N10	3.77	1.52	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	FMN	C1'-N10	3.63	1.52	1.48
3	A	802	FMN	C4-N3	3.61	1.39	1.33
3	C	802	FMN	C4A-N5	3.42	1.38	1.33
3	C	802	FMN	C4-N3	3.33	1.38	1.33
3	A	802	FMN	C4A-N5	3.32	1.38	1.33
3	D	802	FMN	C4A-N5	3.29	1.38	1.33
3	D	802	FMN	C4-N3	3.28	1.38	1.33
3	B	802	FMN	C1'-N10	3.21	1.51	1.48
3	B	802	FMN	C4-N3	3.20	1.38	1.33
3	B	802	FMN	C4A-N5	2.80	1.37	1.33
3	D	802	FMN	C9A-N10	2.71	1.42	1.38
3	C	802	FMN	C4A-C10	2.11	1.40	1.38
3	D	802	FMN	C5A-N5	2.01	1.38	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	802	FMN	C1'-N10-C9A	15.33	130.36	118.29
3	C	802	FMN	C1'-N10-C10	9.82	127.20	118.41
3	D	802	FMN	C1'-N10-C10	-7.29	111.88	118.41
3	B	802	FMN	C4-N3-C2	7.03	121.08	115.14
3	B	802	FMN	C1'-N10-C9A	6.27	123.23	118.29
3	C	802	FMN	C1'-N10-C9A	-5.53	113.94	118.29
3	C	802	FMN	C5A-C9A-N10	5.20	121.49	117.72
3	A	802	FMN	C4-N3-C2	5.12	119.46	115.14
3	C	802	FMN	C4-N3-C2	5.06	119.42	115.14
3	A	802	FMN	C1'-N10-C9A	4.99	122.22	118.29
3	D	802	FMN	C4-N3-C2	4.70	119.11	115.14
3	B	802	FMN	C4A-C4-N3	-3.62	118.48	123.43
3	B	802	FMN	C4A-N5-C5A	3.57	120.34	116.77
3	D	802	FMN	C4A-N5-C5A	3.28	120.05	116.77
3	B	802	FMN	C5A-C9A-N10	3.17	120.01	117.72
3	D	802	FMN	C9A-N10-C10	-3.17	117.76	121.91
3	A	802	FMN	C4A-C4-N3	-2.97	119.37	123.43
3	D	802	FMN	C10-C4A-N5	-2.82	119.31	121.26
3	B	802	FMN	P-O5'-C5'	2.72	125.79	118.30
3	A	802	FMN	C9A-N10-C10	-2.69	118.38	121.91
3	A	802	FMN	C4A-N5-C5A	2.69	119.46	116.77
3	A	802	FMN	C5A-C9A-N10	2.63	119.62	117.72
3	C	802	FMN	C9A-N10-C10	-2.50	118.64	121.91
3	C	802	FMN	C4A-C4-N3	-2.49	120.02	123.43
3	B	802	FMN	C9A-N10-C10	-2.48	118.66	121.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	FMN	C4A-N5-C5A	2.35	119.12	116.77
3	D	802	FMN	C4A-C4-N3	-2.22	120.40	123.43
3	D	802	FMN	C4A-C10-N10	2.15	122.51	120.30
3	C	802	FMN	O2'-C2'-C3'	2.12	114.26	109.10
3	D	802	FMN	C6-C5A-N5	-2.10	116.74	119.05
3	D	802	FMN	C6-C5A-C9A	2.07	121.76	119.05

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	802	FMN	C2'-C1'-N10-C9A
3	D	802	FMN	C2'-C1'-N10-C10
3	D	802	FMN	N10-C1'-C2'-O2'
3	D	802	FMN	C1'-C2'-C3'-O3'
3	D	802	FMN	C1'-C2'-C3'-C4'
3	D	802	FMN	O2'-C2'-C3'-O3'
3	D	802	FMN	O2'-C2'-C3'-C4'
3	D	802	FMN	C2'-C3'-C4'-O4'
3	D	802	FMN	O3'-C3'-C4'-O4'
3	D	802	FMN	C3'-C4'-C5'-O5'
3	D	802	FMN	C5'-O5'-P-O1P
3	D	802	FMN	C5'-O5'-P-O2P
3	D	802	FMN	C5'-O5'-P-O3P
3	B	802	FMN	C2'-C3'-C4'-O4'
3	B	802	FMN	C2'-C3'-C4'-C5'
3	B	802	FMN	O3'-C3'-C4'-O4'
3	B	802	FMN	O3'-C3'-C4'-C5'
3	B	802	FMN	C3'-C4'-C5'-O5'
3	B	802	FMN	O4'-C4'-C5'-O5'
3	A	802	FMN	C1'-C2'-C3'-O3'
3	A	802	FMN	C1'-C2'-C3'-C4'
3	A	802	FMN	O2'-C2'-C3'-O3'
3	A	802	FMN	C3'-C4'-C5'-O5'
3	A	802	FMN	O4'-C4'-C5'-O5'
3	C	802	FMN	C2'-C1'-N10-C9A
3	C	802	FMN	C2'-C1'-N10-C10
3	C	802	FMN	N10-C1'-C2'-O2'
3	C	802	FMN	N10-C1'-C2'-C3'
3	C	802	FMN	C1'-C2'-C3'-O3'
3	C	802	FMN	C1'-C2'-C3'-C4'
3	C	802	FMN	O2'-C2'-C3'-O3'

Continued on next page...

Continued from previous page...

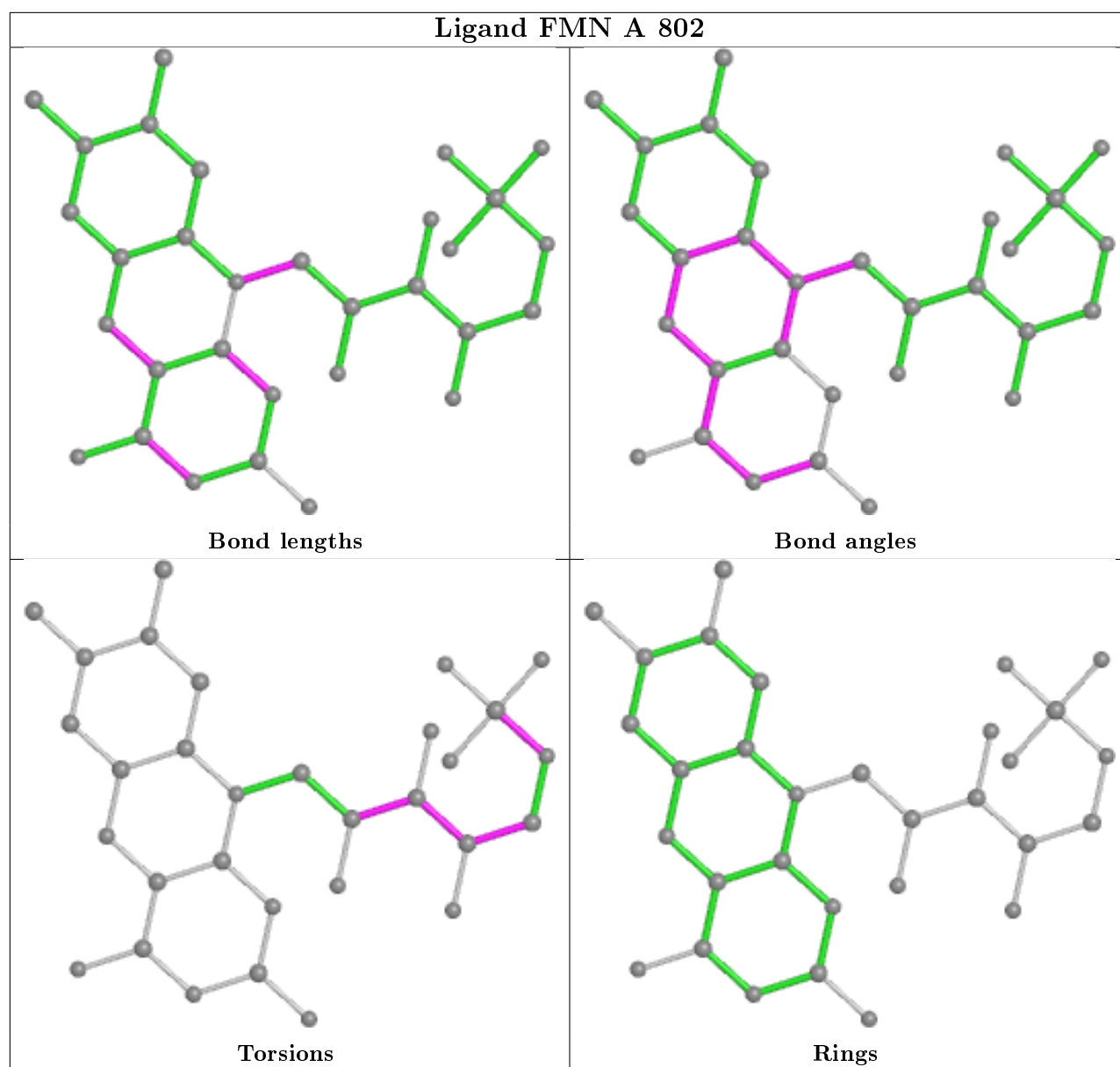
Mol	Chain	Res	Type	Atoms
3	C	802	FMN	O2'-C2'-C3'-C4'
3	C	802	FMN	C2'-C3'-C4'-O4'
3	C	802	FMN	O3'-C3'-C4'-O4'
3	C	802	FMN	O3'-C3'-C4'-C5'
3	C	802	FMN	C5'-O5'-P-O2P
3	C	802	FMN	C5'-O5'-P-O3P
3	A	802	FMN	O2'-C2'-C3'-C4'
3	D	802	FMN	O3'-C3'-C4'-C5'
3	D	802	FMN	C2'-C3'-C4'-C5'
3	C	802	FMN	C2'-C3'-C4'-C5'
3	A	802	FMN	C2'-C3'-C4'-O4'
3	A	802	FMN	O3'-C3'-C4'-O4'
3	C	802	FMN	C5'-O5'-P-O1P
3	A	802	FMN	C2'-C3'-C4'-C5'
3	D	802	FMN	O4'-C4'-C5'-O5'
3	D	802	FMN	N10-C1'-C2'-C3'
3	A	802	FMN	C5'-O5'-P-O1P
3	A	802	FMN	O3'-C3'-C4'-C5'

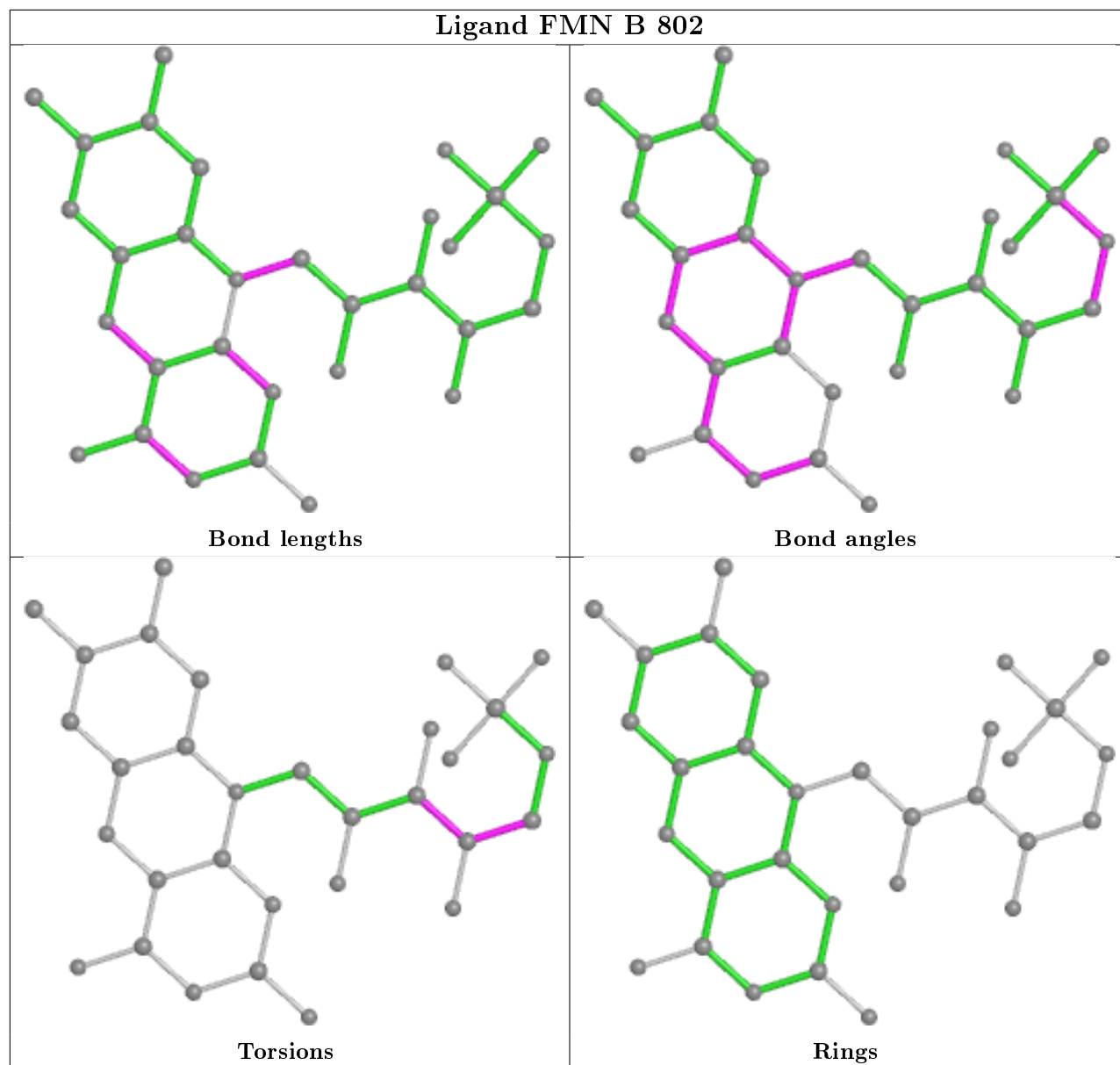
There are no ring outliers.

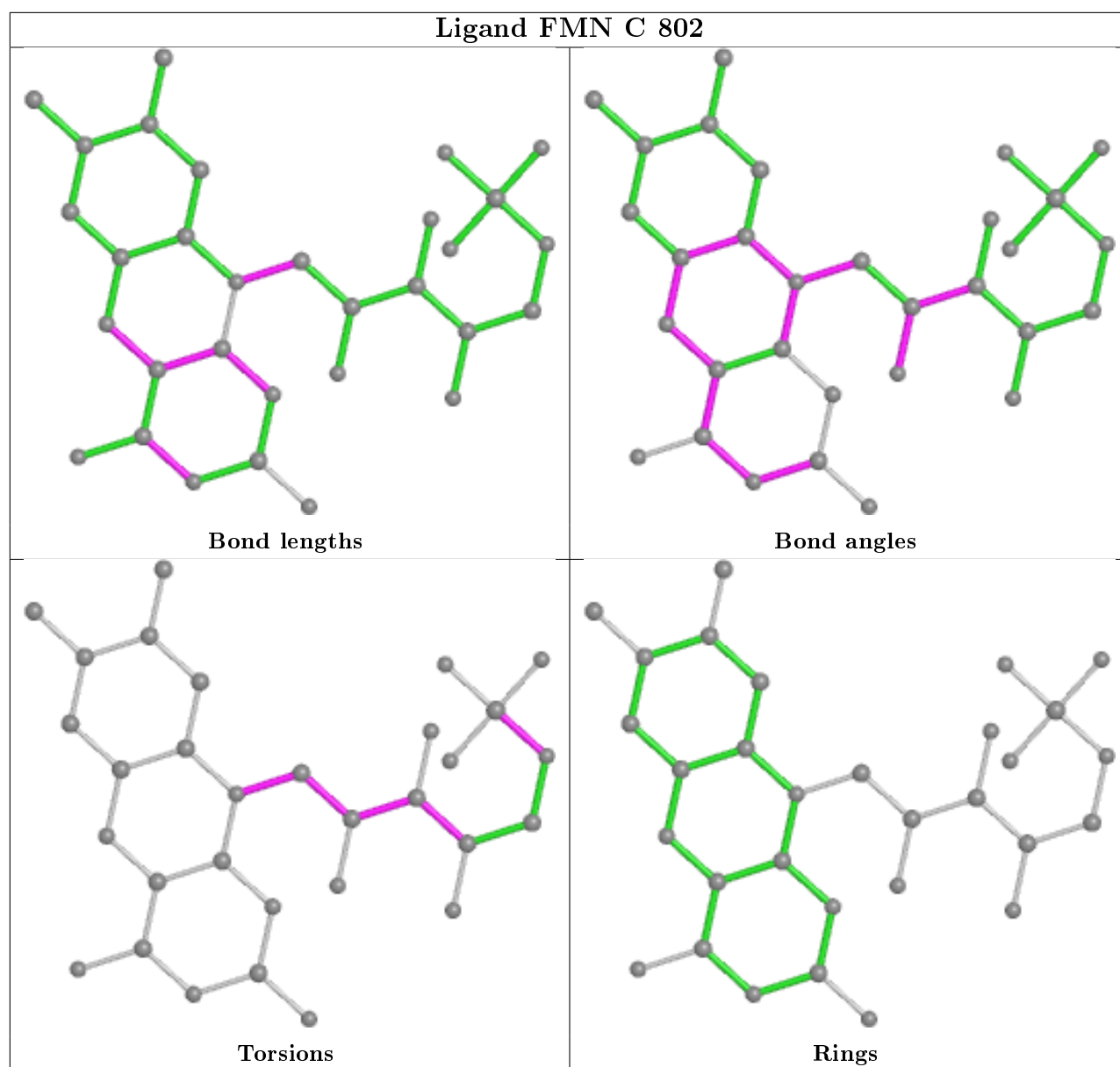
4 monomers are involved in 8 short contacts:

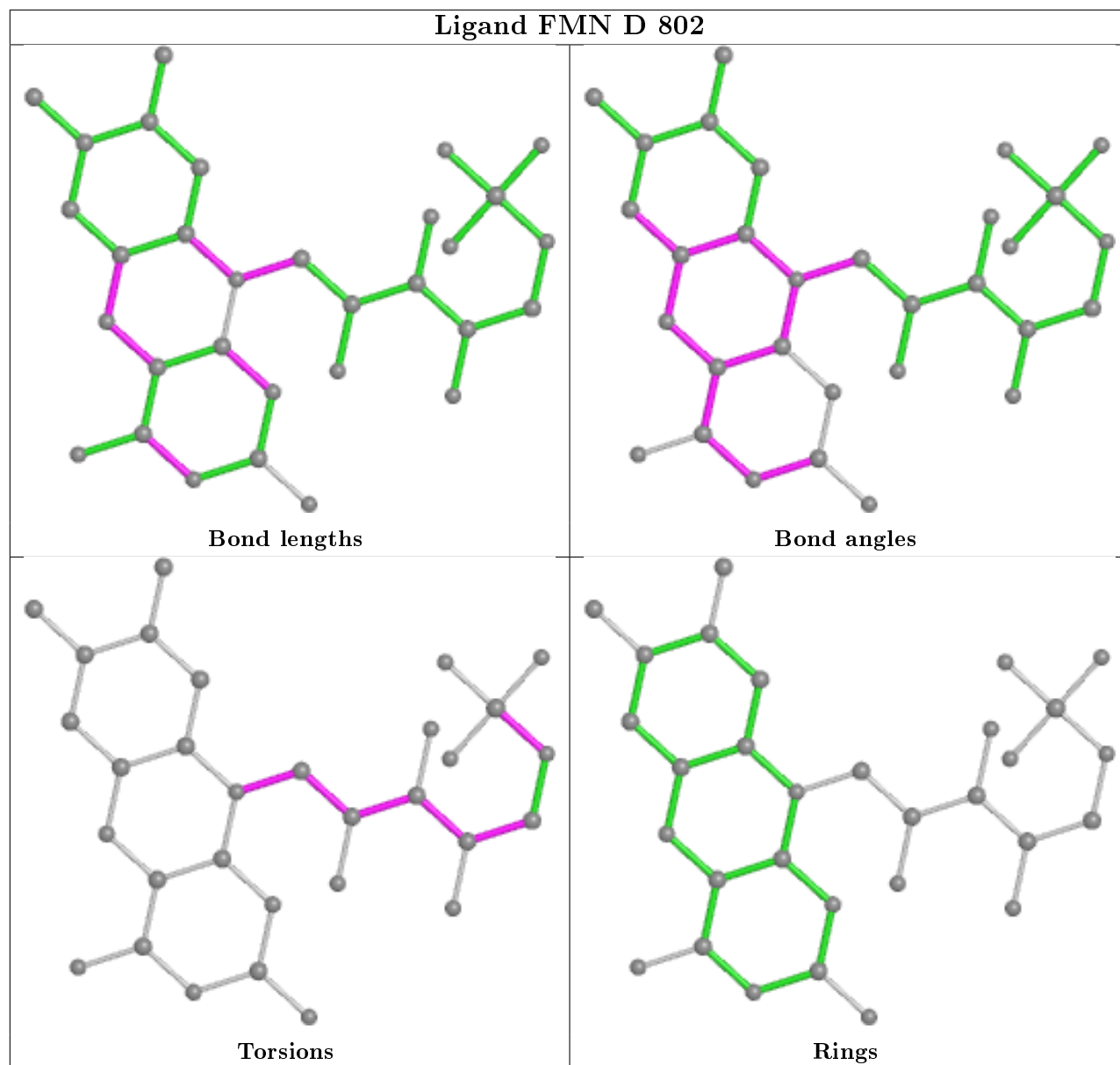
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	FMN	3	0
3	B	802	FMN	1	0
3	C	802	FMN	2	0
3	D	802	FMN	2	0

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 ⓘ

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	639/780 (81%)	-0.18	9 (1%) 75 73	19, 28, 46, 59	0
1	B	638/780 (81%)	-0.08	10 (1%) 72 70	22, 32, 56, 72	0
1	C	638/780 (81%)	-0.12	11 (1%) 70 68	19, 32, 52, 62	0
1	D	305/780 (39%)	0.61	39 (12%) 3 3	25, 46, 64, 80	0
All	All	2220/3120 (71%)	-0.02	69 (3%) 49 47	19, 32, 56, 80	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	162	PRO	6.0
1	D	154	PHE	5.6
1	D	328	LEU	5.4
1	D	149	VAL	4.6
1	D	329	CYS	4.4
1	D	527	GLY	4.1
1	D	440	TYR	4.0
1	D	148	ALA	3.9
1	D	382	MET	3.8
1	D	155	ASP	3.8
1	D	526	GLY	3.6
1	B	636	THR	3.4
1	D	150	ASN	3.3
1	D	441	GLY	3.2
1	D	109	THR	3.2
1	D	536	LEU	3.2
1	D	85	VAL	3.1
1	A	17	THR	3.0
1	D	439	TRP	2.8
1	B	557	ASP	2.8
1	B	247	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	222	PRO	2.7
1	A	16	ALA	2.6
1	D	455	HIS	2.6
1	D	158	TYR	2.6
1	D	411	THR	2.6
1	C	174	ASP	2.6
1	B	189	ALA	2.6
1	D	454	PHE	2.6
1	D	442	GLY	2.6
1	C	557	ASP	2.6
1	D	161	GLY	2.6
1	B	67	ALA	2.6
1	A	639	GLU	2.6
1	C	441	GLY	2.5
1	D	102	VAL	2.5
1	D	108	LEU	2.5
1	D	152	SER	2.5
1	B	188	ALA	2.5
1	C	62	SER	2.5
1	A	512	VAL	2.5
1	C	511	HIS	2.5
1	B	600	GLN	2.4
1	D	303	ILE	2.4
1	D	112	GLU	2.4
1	D	427	ILE	2.3
1	A	593	GLY	2.3
1	C	173	ALA	2.2
1	D	156	LEU	2.2
1	A	382	MET	2.2
1	D	461	ILE	2.2
1	C	636	THR	2.2
1	B	559	PRO	2.2
1	C	281	VAL	2.2
1	D	106	LYS	2.2
1	A	248	ALA	2.2
1	D	524	ASN	2.2
1	D	462	PRO	2.2
1	D	22	GLU	2.2
1	B	316	LEU	2.1
1	C	282	SER	2.1
1	D	110	GLU	2.1
1	D	113	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	453	ASN	2.1
1	A	189	ALA	2.1
1	D	445	SER	2.1
1	B	337	TRP	2.1
1	A	62	SER	2.0
1	C	171	LYS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

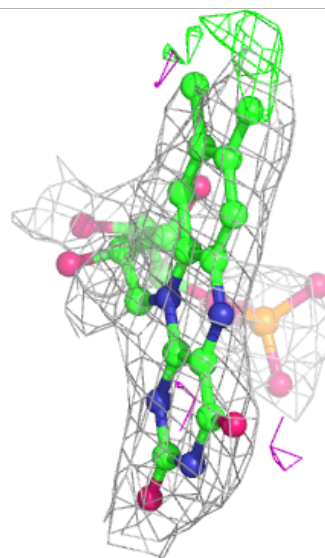
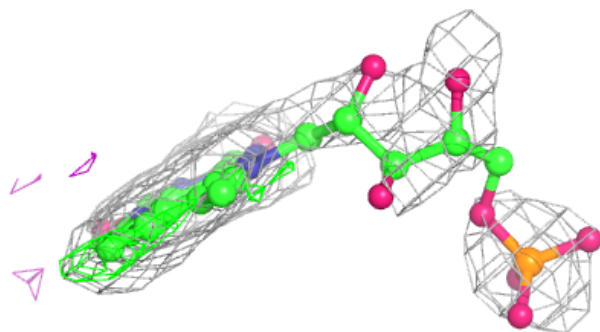
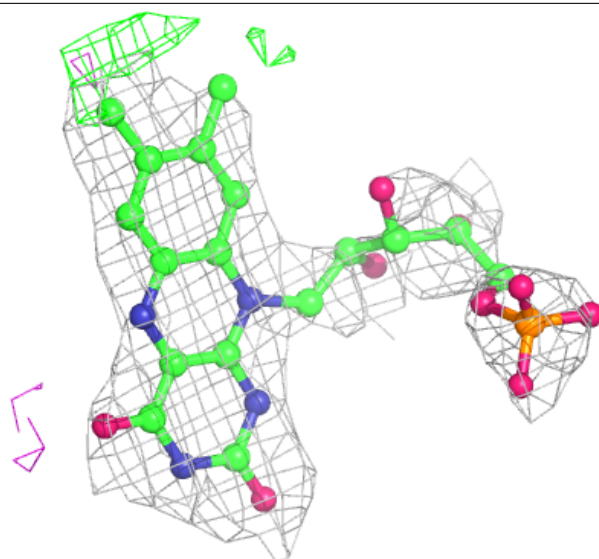
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FMN	D	802	31/31	0.76	0.35	42,61,85,90	0
3	FMN	A	802	31/31	0.77	0.31	29,41,67,88	0
3	FMN	B	802	31/31	0.81	0.26	36,43,86,88	0
3	FMN	C	802	31/31	0.83	0.28	39,49,76,100	0
2	CA	D	801	1/1	0.96	0.05	33,33,33,33	0
2	CA	A	801	1/1	0.96	0.06	26,26,26,26	0
2	CA	C	801	1/1	0.98	0.04	26,26,26,26	0
2	CA	B	801	1/1	1.00	0.06	23,23,23,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

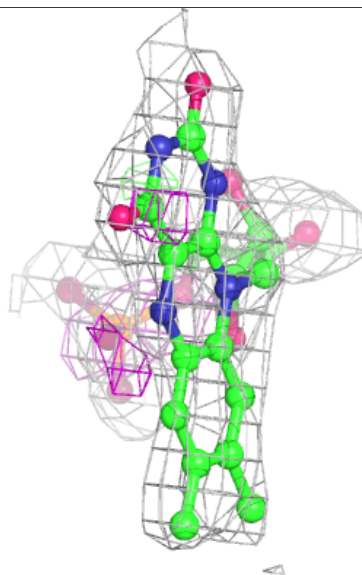
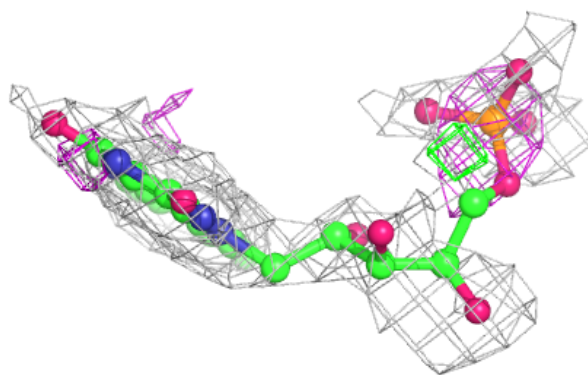
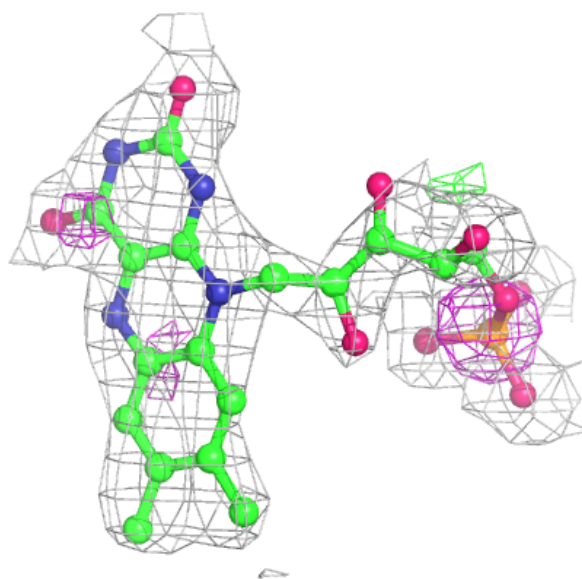
Electron density around FMN D 802:

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



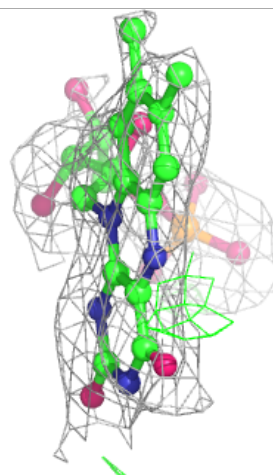
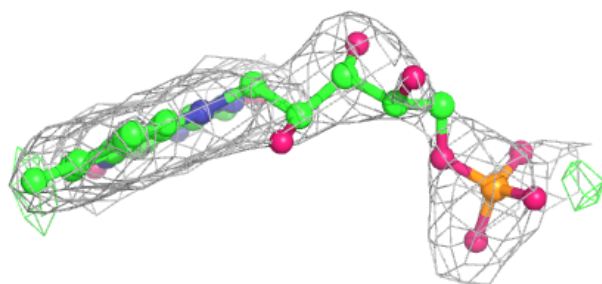
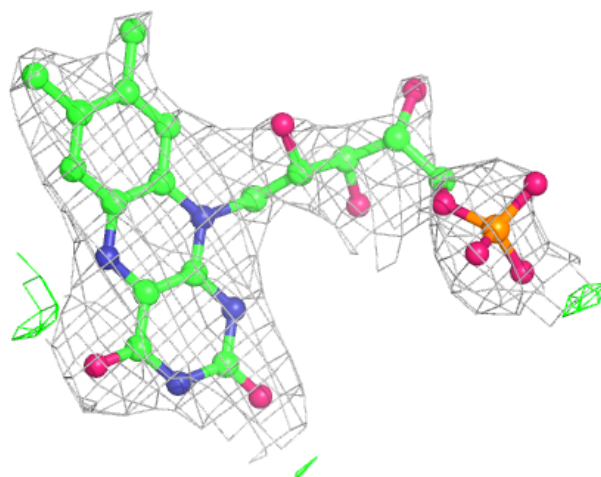
Electron density around FMN A 802:

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



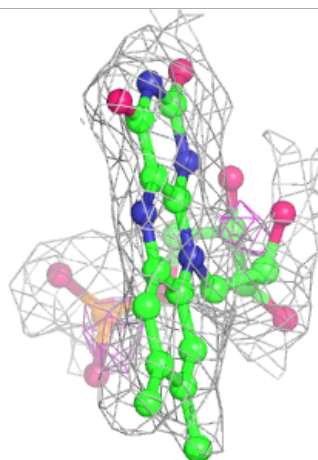
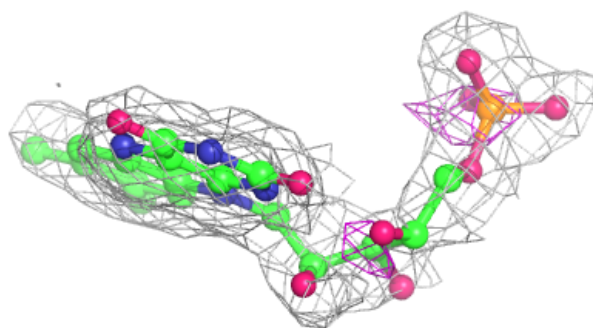
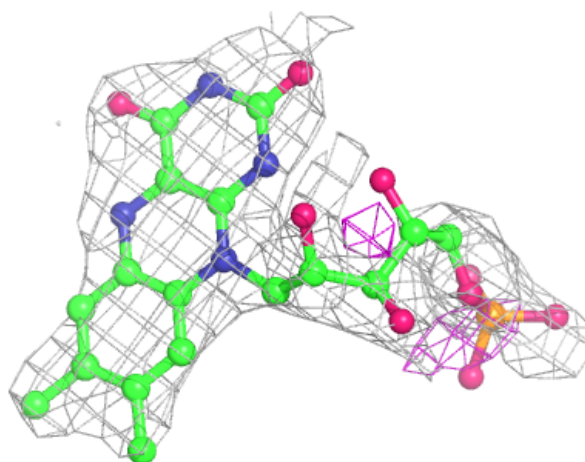
Electron density around FMN B 802:

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



Electron density around FMN C 802:

$2mF_o-DF_c$ (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.