Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 05:42 PM EDT

PDB ID	:	6MVF
Title	:	Crystal structure of FMN-binding beta-glucuronidase from Facaelibacterium prausnitzii L2-6
Authors	:	Pellock, S.J.; Redinbo, M.R.
Deposited on	:	2018-10-25
Resolution	:	2.55 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:

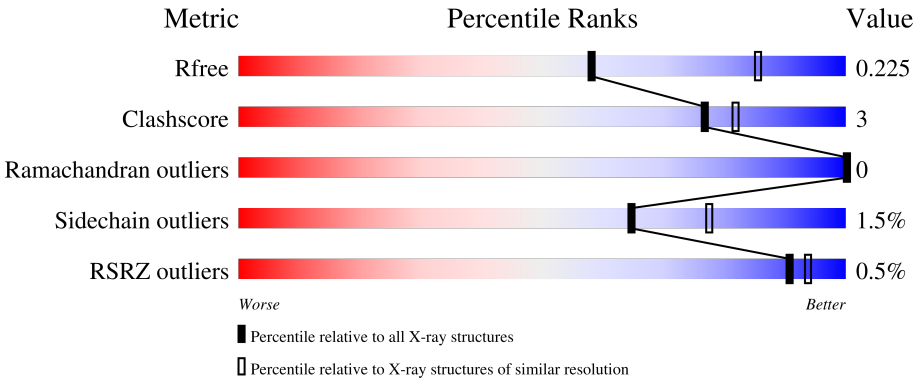
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	769	77% 6% 16%
1	B	769	% 78% 5% 16%
1	C	769	76% 8% 16%
1	D	769	% 75% 8% 16%
1	E	769	75% 8% 16%

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Mol	Chain	Length	Quality of chain
1	F	769	76% 7% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 32076 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/beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	643	Total	C	N	O	S	0	1	0
			5082	3211	860	987	24			
1	B	643	Total	C	N	O	S	0	1	0
			5082	3211	860	987	24			
1	C	643	Total	C	N	O	S	0	1	0
			5082	3211	860	987	24			
1	D	643	Total	C	N	O	S	0	1	0
			5082	3211	860	987	24			
1	E	643	Total	C	N	O	S	0	1	0
			5082	3211	860	987	24			
1	F	643	Total	C	N	O	S	0	1	0
			5082	3211	860	987	24			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	HIS	-	expression tag	UNP D4K3H3
A	-21	HIS	-	expression tag	UNP D4K3H3
A	-20	HIS	-	expression tag	UNP D4K3H3
A	-19	HIS	-	expression tag	UNP D4K3H3
A	-18	HIS	-	expression tag	UNP D4K3H3
A	-17	HIS	-	expression tag	UNP D4K3H3
A	-16	SER	-	expression tag	UNP D4K3H3
A	-15	SER	-	expression tag	UNP D4K3H3
A	-14	GLY	-	expression tag	UNP D4K3H3
A	-13	VAL	-	expression tag	UNP D4K3H3
A	-12	ASP	-	expression tag	UNP D4K3H3
A	-11	LEU	-	expression tag	UNP D4K3H3
A	-10	GLY	-	expression tag	UNP D4K3H3
A	-9	THR	-	expression tag	UNP D4K3H3
A	-8	GLU	-	expression tag	UNP D4K3H3
A	-7	ASN	-	expression tag	UNP D4K3H3
A	-6	LEU	-	expression tag	UNP D4K3H3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	TYR	-	expression tag	UNP D4K3H3
A	-4	PHE	-	expression tag	UNP D4K3H3
A	-3	GLN	-	expression tag	UNP D4K3H3
A	-2	SER	-	expression tag	UNP D4K3H3
A	-1	ASN	-	expression tag	UNP D4K3H3
A	0	ALA	-	expression tag	UNP D4K3H3
B	-22	HIS	-	expression tag	UNP D4K3H3
B	-21	HIS	-	expression tag	UNP D4K3H3
B	-20	HIS	-	expression tag	UNP D4K3H3
B	-19	HIS	-	expression tag	UNP D4K3H3
B	-18	HIS	-	expression tag	UNP D4K3H3
B	-17	HIS	-	expression tag	UNP D4K3H3
B	-16	SER	-	expression tag	UNP D4K3H3
B	-15	SER	-	expression tag	UNP D4K3H3
B	-14	GLY	-	expression tag	UNP D4K3H3
B	-13	VAL	-	expression tag	UNP D4K3H3
B	-12	ASP	-	expression tag	UNP D4K3H3
B	-11	LEU	-	expression tag	UNP D4K3H3
B	-10	GLY	-	expression tag	UNP D4K3H3
B	-9	THR	-	expression tag	UNP D4K3H3
B	-8	GLU	-	expression tag	UNP D4K3H3
B	-7	ASN	-	expression tag	UNP D4K3H3
B	-6	LEU	-	expression tag	UNP D4K3H3
B	-5	TYR	-	expression tag	UNP D4K3H3
B	-4	PHE	-	expression tag	UNP D4K3H3
B	-3	GLN	-	expression tag	UNP D4K3H3
B	-2	SER	-	expression tag	UNP D4K3H3
B	-1	ASN	-	expression tag	UNP D4K3H3
B	0	ALA	-	expression tag	UNP D4K3H3
C	-22	HIS	-	expression tag	UNP D4K3H3
C	-21	HIS	-	expression tag	UNP D4K3H3
C	-20	HIS	-	expression tag	UNP D4K3H3
C	-19	HIS	-	expression tag	UNP D4K3H3
C	-18	HIS	-	expression tag	UNP D4K3H3
C	-17	HIS	-	expression tag	UNP D4K3H3
C	-16	SER	-	expression tag	UNP D4K3H3
C	-15	SER	-	expression tag	UNP D4K3H3
C	-14	GLY	-	expression tag	UNP D4K3H3
C	-13	VAL	-	expression tag	UNP D4K3H3
C	-12	ASP	-	expression tag	UNP D4K3H3
C	-11	LEU	-	expression tag	UNP D4K3H3
C	-10	GLY	-	expression tag	UNP D4K3H3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	THR	-	expression tag	UNP D4K3H3
C	-8	GLU	-	expression tag	UNP D4K3H3
C	-7	ASN	-	expression tag	UNP D4K3H3
C	-6	LEU	-	expression tag	UNP D4K3H3
C	-5	TYR	-	expression tag	UNP D4K3H3
C	-4	PHE	-	expression tag	UNP D4K3H3
C	-3	GLN	-	expression tag	UNP D4K3H3
C	-2	SER	-	expression tag	UNP D4K3H3
C	-1	ASN	-	expression tag	UNP D4K3H3
C	0	ALA	-	expression tag	UNP D4K3H3
D	-22	HIS	-	expression tag	UNP D4K3H3
D	-21	HIS	-	expression tag	UNP D4K3H3
D	-20	HIS	-	expression tag	UNP D4K3H3
D	-19	HIS	-	expression tag	UNP D4K3H3
D	-18	HIS	-	expression tag	UNP D4K3H3
D	-17	HIS	-	expression tag	UNP D4K3H3
D	-16	SER	-	expression tag	UNP D4K3H3
D	-15	SER	-	expression tag	UNP D4K3H3
D	-14	GLY	-	expression tag	UNP D4K3H3
D	-13	VAL	-	expression tag	UNP D4K3H3
D	-12	ASP	-	expression tag	UNP D4K3H3
D	-11	LEU	-	expression tag	UNP D4K3H3
D	-10	GLY	-	expression tag	UNP D4K3H3
D	-9	THR	-	expression tag	UNP D4K3H3
D	-8	GLU	-	expression tag	UNP D4K3H3
D	-7	ASN	-	expression tag	UNP D4K3H3
D	-6	LEU	-	expression tag	UNP D4K3H3
D	-5	TYR	-	expression tag	UNP D4K3H3
D	-4	PHE	-	expression tag	UNP D4K3H3
D	-3	GLN	-	expression tag	UNP D4K3H3
D	-2	SER	-	expression tag	UNP D4K3H3
D	-1	ASN	-	expression tag	UNP D4K3H3
D	0	ALA	-	expression tag	UNP D4K3H3
E	-22	HIS	-	expression tag	UNP D4K3H3
E	-21	HIS	-	expression tag	UNP D4K3H3
E	-20	HIS	-	expression tag	UNP D4K3H3
E	-19	HIS	-	expression tag	UNP D4K3H3
E	-18	HIS	-	expression tag	UNP D4K3H3
E	-17	HIS	-	expression tag	UNP D4K3H3
E	-16	SER	-	expression tag	UNP D4K3H3
E	-15	SER	-	expression tag	UNP D4K3H3
E	-14	GLY	-	expression tag	UNP D4K3H3

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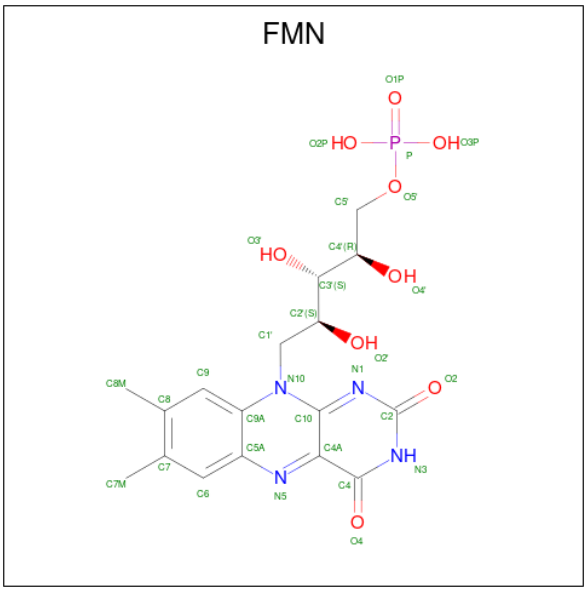
Chain	Residue	Modelled	Actual	Comment	Reference
E	-13	VAL	-	expression tag	UNP D4K3H3
E	-12	ASP	-	expression tag	UNP D4K3H3
E	-11	LEU	-	expression tag	UNP D4K3H3
E	-10	GLY	-	expression tag	UNP D4K3H3
E	-9	THR	-	expression tag	UNP D4K3H3
E	-8	GLU	-	expression tag	UNP D4K3H3
E	-7	ASN	-	expression tag	UNP D4K3H3
E	-6	LEU	-	expression tag	UNP D4K3H3
E	-5	TYR	-	expression tag	UNP D4K3H3
E	-4	PHE	-	expression tag	UNP D4K3H3
E	-3	GLN	-	expression tag	UNP D4K3H3
E	-2	SER	-	expression tag	UNP D4K3H3
E	-1	ASN	-	expression tag	UNP D4K3H3
E	0	ALA	-	expression tag	UNP D4K3H3
F	-22	HIS	-	expression tag	UNP D4K3H3
F	-21	HIS	-	expression tag	UNP D4K3H3
F	-20	HIS	-	expression tag	UNP D4K3H3
F	-19	HIS	-	expression tag	UNP D4K3H3
F	-18	HIS	-	expression tag	UNP D4K3H3
F	-17	HIS	-	expression tag	UNP D4K3H3
F	-16	SER	-	expression tag	UNP D4K3H3
F	-15	SER	-	expression tag	UNP D4K3H3
F	-14	GLY	-	expression tag	UNP D4K3H3
F	-13	VAL	-	expression tag	UNP D4K3H3
F	-12	ASP	-	expression tag	UNP D4K3H3
F	-11	LEU	-	expression tag	UNP D4K3H3
F	-10	GLY	-	expression tag	UNP D4K3H3
F	-9	THR	-	expression tag	UNP D4K3H3
F	-8	GLU	-	expression tag	UNP D4K3H3
F	-7	ASN	-	expression tag	UNP D4K3H3
F	-6	LEU	-	expression tag	UNP D4K3H3
F	-5	TYR	-	expression tag	UNP D4K3H3
F	-4	PHE	-	expression tag	UNP D4K3H3
F	-3	GLN	-	expression tag	UNP D4K3H3
F	-2	SER	-	expression tag	UNP D4K3H3
F	-1	ASN	-	expression tag	UNP D4K3H3
F	0	ALA	-	expression tag	UNP D4K3H3

- 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		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.

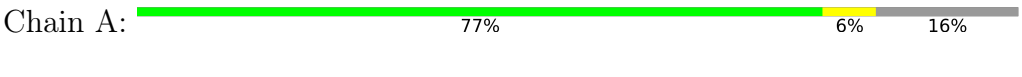
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	230	Total	O	0	0
			230	230		
3	B	242	Total	O	0	0
			242	242		
3	C	235	Total	O	0	0
			235	235		
3	D	244	Total	O	0	0
			244	244		
3	E	227	Total	O	0	0
			227	227		
3	F	220	Total	O	0	0
			220	220		

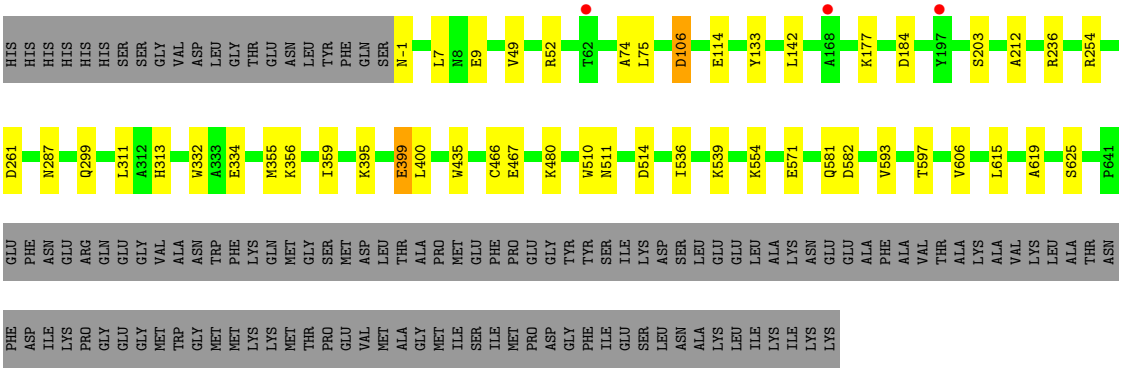
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Beta-galactosidase/beta-glucuronidase

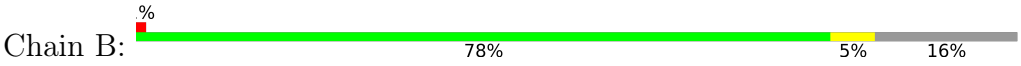
Chain A:

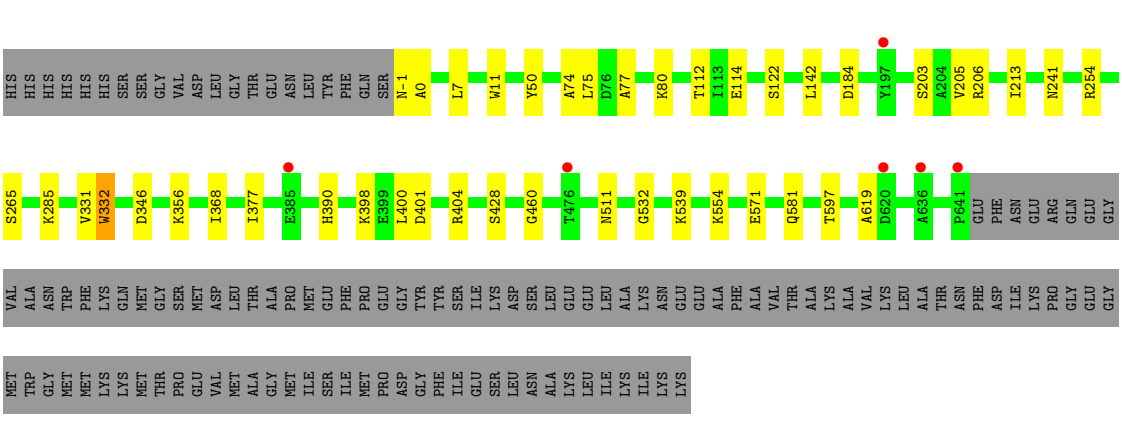




• Molecule 1: Beta-galactosidase/beta-glucuronidase

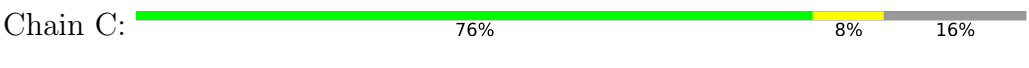
Chain B:

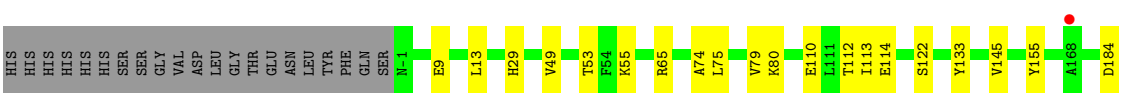


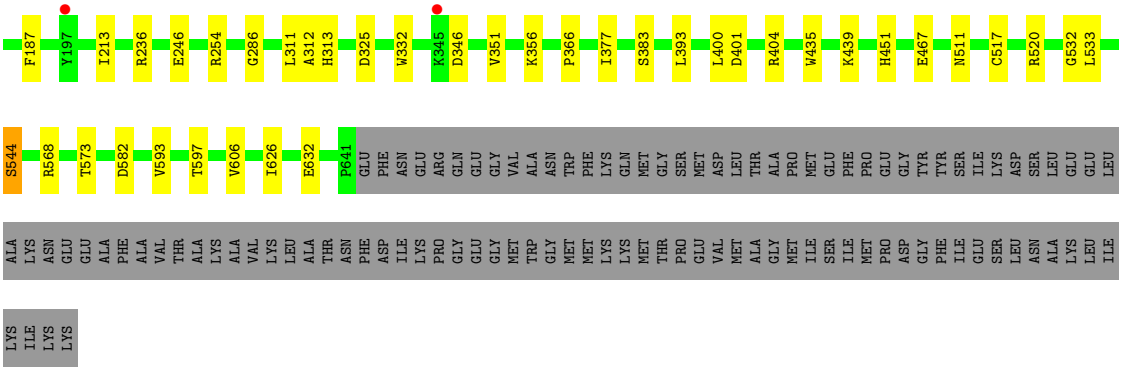


• Molecule 1: Beta-galactosidase/beta-glucuronidase

Chain C:

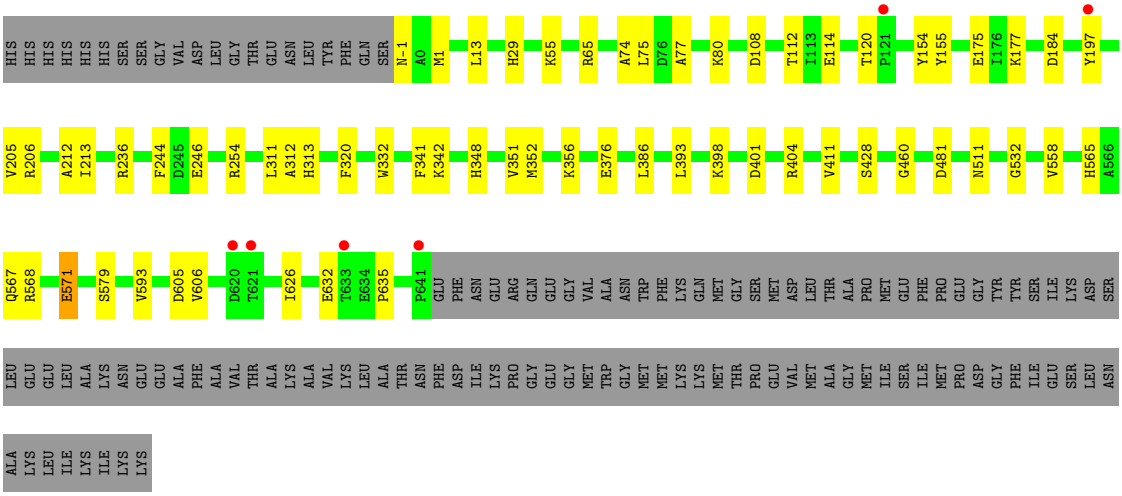






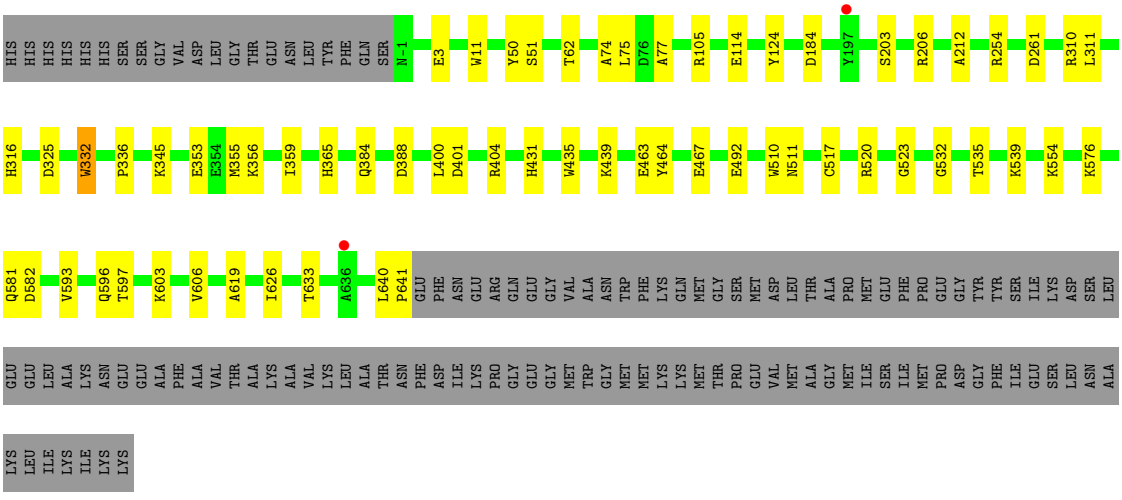
• Molecule 1: Beta-galactosidase/beta-glucuronidase

Chain D:



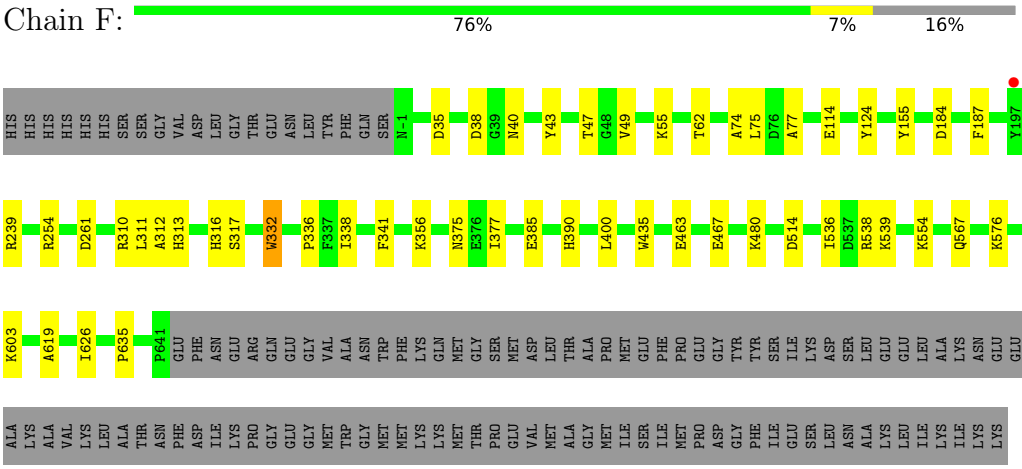
• Molecule 1: Beta-galactosidase/beta-glucuronidase

Chain E:



• Molecule 1: Beta-galactosidase/beta-glucuronidase

Chain F:


76%
7%
16%
HIS HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER N-1 D35 D38 G39 N40 Y43 T47 G48 V49 K55 T62 A74 L75 D76 A77 E114 Y124 Y155 D184 F187 Y197 S203 E227
R239 R254 D261 R310 L311 A312 H313 H316 S317 W332 P336 F337 I338 F341 K356 N375 E376 I377 E385 H390 L400 W435 E463 E467 K480 D514 I536 D537 R538 K539 K554 Q567 K576 Q581 D582 T597
K603 A619 I626 P635 P641 GLU PHE ASN GLU ARG GLN GLU GLY VAL ALA ASN TRP PHE LYS GLN MET GLY SER MET ASP LEU THR ALA PRO MET GLU PHE PRO GLU GLY TYR TYR SER ILE LYS ASP SER LEU GLU GLU LEU ALA LYS ASN GLU GLU ALA PHE ALA VAL THR
ALA LYS ALA VAL LYS LEU ALA THR ASN PHE ASP ILE LYS PRO GLY GLU GLY MET TRP GLY MET MET LYS LYS MET THR PRO GLU VAL MET ALA GLY MET ILE SER ILE MET PRO ASP GLY PHE ILE GLU SER LEU ASN ALA LYS LEU ILE LYS ILE LYS LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	129.56Å 106.81Å 183.82Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	29.52 – 2.55 29.52 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.52-2.55) 99.7 (29.52-2.55)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.167 , 0.226 0.167 , 0.225	Depositor DCC
R_{free} test set	2002 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32076	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8477e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.46	1/5216 (0.0%)	0.61	0/7101
1	B	0.45	0/5216	0.60	0/7101
1	C	0.45	0/5216	0.61	0/7101
1	D	0.46	0/5216	0.61	1/7101 (0.0%)
1	E	0.45	0/5216	0.61	0/7101
1	F	0.45	0/5216	0.62	0/7101
All	All	0.45	1/31296 (0.0%)	0.61	1/42606 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	CYS	CB-SG	-5.36	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	481	ASP	CB-CG-OD1	5.40	123.16	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5082	0	4819	29	0
1	B	5082	0	4819	26	0
1	C	5082	0	4819	34	0
1	D	5082	0	4819	34	0
1	E	5082	0	4819	32	0
1	F	5082	0	4819	32	0
2	A	31	0	19	1	0
2	B	31	0	19	1	0
2	C	31	0	19	1	0
2	D	31	0	19	3	0
2	E	31	0	19	0	0
2	F	31	0	19	1	0
3	A	230	0	0	3	0
3	B	242	0	0	2	0
3	C	235	0	0	2	0
3	D	244	0	0	3	0
3	E	227	0	0	0	0
3	F	220	0	0	3	0
All	All	32076	0	29028	181	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 3.

All (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LYS:NZ	2:A:801:FMN:O3P	1.93	1.01
1:C:80:LYS:HB2	1:C:112:THR:HG22	1.61	0.81
1:B:206:ARG:HD3	1:B:213:ILE:HD13	1.63	0.81
1:C:593:VAL:HG11	1:C:606:VAL:HG22	1.66	0.77
1:A:49:VAL:HG22	1:A:114:GLU:HG2	1.69	0.74
1:C:79:VAL:HG22	1:C:113:ILE:HG12	1.68	0.73
1:D:351:VAL:HG22	1:D:393:LEU:HD21	1.72	0.71
1:D:206:ARG:HD3	1:D:213:ILE:HD13	1.73	0.71
1:D:356:LYS:NZ	3:D:902:HOH:O	2.24	0.70
1:A:236:ARG:NH1	3:A:901:HOH:O	2.25	0.69
1:F:356:LYS:HG3	1:F:400:LEU:HD11	1.75	0.69
1:D:593:VAL:HG11	1:D:606:VAL:HG22	1.78	0.65
1:F:47:THR:OG1	3:F:901:HOH:O	2.15	0.63
1:C:184:ASP:HB3	1:C:187:PHE:HD2	1.62	0.63
1:B:206:ARG:NH2	3:B:901:HOH:O	2.31	0.62
2:D:801:FMN:N1	2:D:801:FMN:O2'	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-1:ASN:N	3:D:905:HOH:O	2.33	0.61
1:A:356:LYS:HG3	1:A:400:LEU:HD11	1.83	0.60
1:C:451:HIS:NE2	3:C:902:HOH:O	2.30	0.60
1:C:122:SER:OG	1:C:346:ASP:HB3	2.01	0.59
1:C:53:THR:HG22	1:C:110:GLU:OE2	2.01	0.59
1:D:398:LYS:NZ	3:D:906:HOH:O	2.35	0.59
1:D:155:TYR:CZ	1:D:356:LYS:HD2	2.39	0.58
1:C:80:LYS:HB2	1:C:112:THR:CG2	2.31	0.58
1:A:581:GLN:HG3	1:A:619:ALA:HB1	1.86	0.57
1:C:155:TYR:CZ	1:C:356:LYS:HD3	2.39	0.57
1:C:49:VAL:HG22	1:C:114:GLU:HG2	1.86	0.57
1:B:7:LEU:HD11	1:B:142:LEU:HD13	1.87	0.56
1:E:310:ARG:HH12	1:E:463:GLU:HG3	1.72	0.55
2:D:801:FMN:O2'	2:D:801:FMN:O4'	2.18	0.55
1:B:539:LYS:HD3	1:D:236:ARG:HE	1.71	0.55
1:C:632:GLU:OE2	1:C:632:GLU:HA	2.06	0.55
1:D:511:ASN:O	1:D:532:GLY:HA2	2.05	0.55
1:E:401:ASP:OD2	1:E:404:ARG:HD2	2.07	0.55
1:E:593:VAL:HG11	1:E:606:VAL:HG22	1.88	0.55
1:F:35:ASP:OD2	1:F:43:TYR:HA	2.08	0.54
1:A:593:VAL:HG11	1:A:606:VAL:HG22	1.90	0.54
1:D:154:TYR:OH	2:D:801:FMN:O1P	2.21	0.53
1:F:49:VAL:HG22	1:F:114:GLU:HG2	1.90	0.53
1:E:356:LYS:HG3	1:E:400:LEU:HD11	1.90	0.52
1:D:401:ASP:OD2	1:D:404:ARG:HD2	2.09	0.52
1:A:313:HIS:HA	1:A:334:GLU:OE2	2.10	0.52
1:A:539:LYS:HD3	1:C:236:ARG:HE	1.74	0.52
1:B:581:GLN:HG3	1:B:619:ALA:HB1	1.92	0.52
1:A:435:TRP:CZ2	1:A:467:GLU:HG3	2.44	0.52
1:F:581:GLN:HG3	1:F:619:ALA:HB1	1.92	0.51
1:F:435:TRP:CZ2	1:F:467:GLU:HG3	2.45	0.51
1:C:356:LYS:HG3	1:C:400:LEU:HD11	1.92	0.51
1:E:517[B]:CYS:HB2	1:E:520:ARG:HG3	1.93	0.51
1:A:106:ASP:N	1:A:106:ASP:OD1	2.43	0.50
1:D:558:VAL:HG23	1:D:579:SER:HB2	1.93	0.50
1:A:177:LYS:HD2	1:A:212:ALA:HB2	1.94	0.50
1:C:517[B]:CYS:HB2	1:C:520:ARG:HG3	1.94	0.50
1:E:492:GLU:OE2	1:E:576:LYS:NZ	2.32	0.49
1:B:241:ASN:HB3	1:E:535:THR:HG22	1.94	0.49
1:F:38:ASP:OD1	1:F:40:ASN:ND2	2.43	0.49
1:D:626:ILE:HA	1:E:203:SER:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:ILE:HG13	1:F:375:ASN:HD22	1.78	0.49
1:C:626:ILE:HA	1:F:203:SER:O	2.13	0.48
1:F:567:GLN:OE1	1:F:635:PRO:HG3	2.12	0.48
1:C:597:THR:HG22	1:E:597:THR:HG22	1.95	0.48
1:D:571:GLU:HA	1:D:571:GLU:OE2	2.14	0.48
2:B:801:FMN:H9	2:B:801:FMN:O2'	2.14	0.48
1:A:355:MET:HE2	1:A:359:ILE:HD11	1.96	0.48
1:D:376:GLU:HG2	1:D:411:VAL:HA	1.95	0.48
1:F:582:ASP:O	1:F:597:THR:HA	2.13	0.47
1:C:511:ASN:O	1:C:532:GLY:HA2	2.15	0.47
1:D:311:LEU:HD21	1:D:320:PHE:CE2	2.49	0.47
1:B:77:ALA:HA	1:B:114:GLU:O	2.15	0.47
1:E:523:GLY:HA2	1:E:640:LEU:HD11	1.96	0.47
1:B:74:ALA:HA	1:B:75:LEU:HA	1.70	0.47
1:C:582:ASP:O	1:C:597:THR:HA	2.15	0.47
1:A:435:TRP:O	1:A:480:LYS:NZ	2.48	0.47
1:A:597:THR:HG22	1:B:597:THR:HG22	1.96	0.47
1:C:401:ASP:OD2	1:C:404:ARG:HD2	2.15	0.47
1:D:205:VAL:O	1:D:206:ARG:HD2	2.15	0.47
1:E:582:ASP:O	1:E:597:THR:HA	2.14	0.47
1:B:554:LYS:HE2	3:B:1110:HOH:O	2.14	0.47
1:E:355:MET:HE2	1:E:359:ILE:HD11	1.97	0.47
2:F:801:FMN:H9	2:F:801:FMN:H1'1	1.57	0.46
1:D:74:ALA:HA	1:D:75:LEU:HA	1.64	0.46
1:C:311:LEU:HD23	1:C:311:LEU:HA	1.79	0.46
1:B:356:LYS:HG3	1:B:400:LEU:HD11	1.97	0.46
1:D:565:HIS:CD2	1:D:568:ARG:HD3	2.50	0.46
1:D:177:LYS:HD2	1:D:212:ALA:HB2	1.98	0.46
1:F:124:TYR:HB3	1:F:336:PRO:O	2.15	0.46
1:F:155:TYR:CZ	1:F:356:LYS:HD3	2.51	0.46
1:C:236:ARG:NE	1:C:246:GLU:OE1	2.49	0.46
1:C:312:ALA:HB1	1:C:313:HIS:ND1	2.31	0.45
1:D:341:PHE:HB2	1:D:386:LEU:HD12	1.97	0.45
1:D:567:GLN:OE1	1:D:635:PRO:HG3	2.17	0.45
1:F:312:ALA:HB1	1:F:313:HIS:ND1	2.32	0.45
1:F:576:LYS:HG3	1:F:603:LYS:HG2	1.98	0.45
2:C:801:FMN:H9	2:C:801:FMN:H1'1	1.59	0.45
1:F:74:ALA:HA	1:F:75:LEU:HA	1.62	0.45
1:F:239:ARG:NH2	3:F:906:HOH:O	2.42	0.45
1:B:401:ASP:OD2	1:B:404:ARG:HD2	2.17	0.45
1:E:439:LYS:HB2	1:E:439:LYS:HE2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:ASN:O	1:B:532:GLY:HA2	2.17	0.45
1:E:581:GLN:HG3	1:E:619:ALA:HB1	1.98	0.45
1:D:1:MET:HE3	1:D:244:PHE:HA	1.99	0.44
1:F:77:ALA:HA	1:F:114:GLU:O	2.18	0.44
1:A:615:LEU:O	1:A:625:SER:HA	2.18	0.44
1:E:511:ASN:O	1:E:532:GLY:HA2	2.17	0.44
1:B:11:TRP:CE3	1:B:50:TYR:HB3	2.53	0.44
1:F:311:LEU:HB3	1:F:316:HIS:CD2	2.53	0.44
1:E:596:GLN:NE2	1:E:603:LYS:O	2.43	0.44
1:D:428:SER:HA	1:D:460:GLY:O	2.18	0.43
1:E:325:ASP:OD2	1:E:365:HIS:ND1	2.52	0.43
1:B:203:SER:O	1:E:626:ILE:HA	2.19	0.43
1:D:348:HIS:O	1:D:352:MET:HG2	2.18	0.43
1:B:0:ALA:H	1:E:539:LYS:HE3	1.84	0.43
1:B:122:SER:HB3	1:B:346:ASP:HB3	1.99	0.43
1:F:435:TRP:O	1:F:480:LYS:NZ	2.51	0.43
1:A:74:ALA:HA	1:A:75:LEU:HA	1.71	0.43
1:C:74:ALA:HA	1:C:75:LEU:HA	1.67	0.43
1:A:236:ARG:HE	1:F:539:LYS:HD3	1.84	0.43
1:B:332:TRP:CD1	1:B:332:TRP:C	2.92	0.43
1:D:632:GLU:HA	1:D:632:GLU:OE2	2.18	0.43
1:E:11:TRP:CE3	1:E:50:TYR:HB3	2.53	0.43
1:B:206:ARG:HA	1:B:206:ARG:HD2	1.80	0.43
1:C:122:SER:HG	1:C:346:ASP:HB3	1.82	0.43
1:C:213:ILE:HD12	1:C:213:ILE:HA	1.86	0.43
1:E:77:ALA:HA	1:E:114:GLU:O	2.19	0.43
1:E:124:TYR:HB3	1:E:336:PRO:O	2.18	0.43
1:B:377:ILE:HG21	1:B:390:HIS:CE1	2.54	0.43
1:D:55:LYS:HE3	1:D:108:ASP:OD1	2.19	0.43
1:A:9:GLU:O	1:A:52:ARG:NH1	2.52	0.42
1:C:377:ILE:HD12	1:C:377:ILE:HA	1.88	0.42
1:A:203:SER:O	1:F:626:ILE:HA	2.19	0.42
1:B:398:LYS:HD3	1:B:398:LYS:HA	1.87	0.42
1:F:184:ASP:HB3	1:F:187:PHE:HD2	1.85	0.42
1:D:236:ARG:NE	1:D:246:GLU:OE1	2.52	0.42
1:F:55:LYS:HE2	1:F:55:LYS:HB3	1.74	0.42
1:E:431:HIS:O	1:E:464:TYR:HA	2.20	0.42
1:D:120:THR:O	1:D:342:LYS:NZ	2.53	0.42
1:F:554:LYS:HD3	1:F:554:LYS:HA	1.76	0.42
1:A:7:LEU:HD11	1:A:142:LEU:HD13	2.02	0.41
1:F:341:PHE:HZ	1:F:385:GLU:HG2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:ARG:HD2	1:C:573:THR:OG1	2.19	0.41
1:F:377:ILE:HG21	1:F:390:HIS:CE1	2.55	0.41
1:A:582:ASP:O	1:A:597:THR:HA	2.21	0.41
1:A:-1:ASN:N	3:A:916:HOH:O	2.54	0.41
1:B:554:LYS:HA	1:B:554:LYS:HD3	1.76	0.41
1:C:451:HIS:HA	3:C:955:HOH:O	2.20	0.41
1:E:206:ARG:HD2	1:E:212:ALA:O	2.20	0.41
1:E:384:GLN:NE2	1:E:388:ASP:OD1	2.53	0.41
1:E:435:TRP:CZ2	1:E:467:GLU:HG3	2.55	0.41
1:A:133:TYR:HB2	1:A:287:ASN:ND2	2.36	0.41
1:A:554:LYS:HD3	1:A:554:LYS:HA	1.84	0.41
1:C:325:ASP:CG	1:C:366:PRO:HD2	2.41	0.41
1:D:312:ALA:HB1	1:D:313:HIS:ND1	2.36	0.41
1:A:261:ASP:HB2	3:A:1001:HOH:O	2.19	0.41
1:C:533:LEU:CD2	1:C:544:SER:HB3	2.51	0.41
1:E:554:LYS:HA	1:E:554:LYS:HD3	1.90	0.41
1:A:311:LEU:HA	1:A:311:LEU:HD23	1.67	0.41
1:A:395:LYS:HE2	1:A:399:GLU:OE2	2.20	0.41
1:B:428:SER:HA	1:B:460:GLY:O	2.21	0.41
1:C:13:LEU:HD22	1:C:29:HIS:CE1	2.56	0.41
1:E:332:TRP:CD1	1:E:332:TRP:C	2.94	0.41
1:F:310:ARG:HH12	1:F:463:GLU:HG3	1.85	0.41
1:A:510:TRP:HA	1:A:511:ASN:HA	1.91	0.41
1:C:133:TYR:CE1	1:C:286:GLY:HA2	2.56	0.41
1:C:435:TRP:CZ2	1:C:467:GLU:HG3	2.56	0.41
1:E:640:LEU:HD23	1:E:641:PRO:HD2	2.02	0.41
1:C:351:VAL:HG12	1:C:393:LEU:HD21	2.02	0.40
1:D:77:ALA:HA	1:D:114:GLU:O	2.22	0.40
1:D:80:LYS:HB2	1:D:112:THR:OG1	2.22	0.40
1:E:74:ALA:HA	1:E:75:LEU:HA	1.62	0.40
1:E:311:LEU:HB3	1:E:316:HIS:CD2	2.57	0.40
1:B:80:LYS:HB2	1:B:112:THR:OG1	2.20	0.40
1:B:205:VAL:O	1:B:206:ARG:HD2	2.21	0.40
1:B:331:VAL:HB	1:B:368:ILE:HA	2.03	0.40
1:D:13:LEU:HD22	1:D:29:HIS:CE1	2.56	0.40
1:F:514:ASP:HB2	1:F:536:ILE:HB	2.03	0.40
1:A:514:ASP:HB2	1:A:536:ILE:HB	2.03	0.40
1:D:398:LYS:HD3	1:D:398:LYS:HA	1.84	0.40
1:F:332:TRP:CD1	1:F:332:TRP:C	2.95	0.40
1:F:341:PHE:CZ	1:F:385:GLU:HG2	2.56	0.40
1:F:538:ARG:HG2	3:F:909:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:510:TRP:HA	1:E:511:ASN:HA	1.89	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	642/769 (84%)	620 (97%)	22 (3%)	0	100	100
1	B	642/769 (84%)	623 (97%)	19 (3%)	0	100	100
1	C	642/769 (84%)	617 (96%)	25 (4%)	0	100	100
1	D	642/769 (84%)	617 (96%)	25 (4%)	0	100	100
1	E	642/769 (84%)	622 (97%)	20 (3%)	0	100	100
1	F	642/769 (84%)	618 (96%)	24 (4%)	0	100	100
All	All	3852/4614 (84%)	3717 (96%)	135 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	544/649 (84%)	537 (99%)	7 (1%)	69	80
1	B	544/649 (84%)	537 (99%)	7 (1%)	69	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	544/649 (84%)	535 (98%)	9 (2%)	60 75
1	D	544/649 (84%)	536 (98%)	8 (2%)	65 77
1	E	544/649 (84%)	533 (98%)	11 (2%)	55 70
1	F	544/649 (84%)	538 (99%)	6 (1%)	73 83
All	All	3264/3894 (84%)	3216 (98%)	48 (2%)	65 77

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ASP
1	A	184	ASP
1	A	254	ARG
1	A	299	GLN
1	A	332	TRP
1	A	399	GLU
1	A	571	GLU
1	B	-1	ASN
1	B	184	ASP
1	B	254	ARG
1	B	265	SER
1	B	285	LYS
1	B	332	TRP
1	B	571	GLU
1	C	9	GLU
1	C	55	LYS
1	C	65	ARG
1	C	145	VAL
1	C	254	ARG
1	C	332	TRP
1	C	383	SER
1	C	439	LYS
1	C	544	SER
1	D	65	ARG
1	D	175	GLU
1	D	184	ASP
1	D	197	TYR
1	D	254	ARG
1	D	332	TRP
1	D	571	GLU
1	D	605	ASP
1	E	3	GLU

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Mol	Chain	Res	Type
1	E	51	SER
1	E	62	THR
1	E	105	ARG
1	E	184	ASP
1	E	254	ARG
1	E	261	ASP
1	E	332	TRP
1	E	345	LYS
1	E	353	GLU
1	E	633	THR
1	F	62	THR
1	F	227	GLU
1	F	254	ARG
1	F	261	ASP
1	F	317	SER
1	F	332	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	413	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FMN	F	801	-	33,33,33	1.14	2 (6%)	48,50,50	1.46	11 (22%)
2	FMN	B	801	-	33,33,33	1.23	3 (9%)	48,50,50	1.64	13 (27%)
2	FMN	A	801	-	33,33,33	1.67	6 (18%)	48,50,50	1.48	9 (18%)
2	FMN	D	801	-	33,33,33	1.31	6 (18%)	48,50,50	1.60	11 (22%)
2	FMN	E	801	-	33,33,33	1.14	2 (6%)	48,50,50	1.32	9 (18%)
2	FMN	C	801	-	33,33,33	1.13	2 (6%)	48,50,50	1.37	11 (22%)

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	F	801	-	-	7/18/18/18	0/3/3/3
2	FMN	B	801	-	-	7/18/18/18	0/3/3/3
2	FMN	A	801	-	-	12/18/18/18	0/3/3/3
2	FMN	D	801	-	-	13/18/18/18	0/3/3/3
2	FMN	E	801	-	-	10/18/18/18	0/3/3/3
2	FMN	C	801	-	-	16/18/18/18	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FMN	C4-N3	-4.71	1.30	1.38
2	C	801	FMN	C4A-N5	4.46	1.39	1.30
2	F	801	FMN	C4A-N5	4.13	1.38	1.30
2	E	801	FMN	C4A-N5	4.06	1.38	1.30
2	D	801	FMN	C4A-N5	3.95	1.38	1.30
2	A	801	FMN	C5A-N5	-3.77	1.32	1.39
2	E	801	FMN	C10-N1	3.35	1.40	1.33
2	F	801	FMN	C10-N1	3.34	1.40	1.33
2	B	801	FMN	C4A-N5	3.24	1.37	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	FMN	C10-N1	3.16	1.39	1.33
2	A	801	FMN	C2-N3	-3.04	1.31	1.39
2	B	801	FMN	C10-N1	3.01	1.39	1.33
2	A	801	FMN	C9A-C5A	2.99	1.46	1.41
2	C	801	FMN	C10-N1	2.90	1.39	1.33
2	A	801	FMN	C6-C7	-2.89	1.35	1.39
2	D	801	FMN	C1'-N10	2.66	1.54	1.48
2	D	801	FMN	C10-N10	2.50	1.42	1.37
2	B	801	FMN	C1'-N10	2.45	1.54	1.48
2	A	801	FMN	C8-C7	2.12	1.46	1.40
2	D	801	FMN	C1'-C2'	2.06	1.55	1.52
2	D	801	FMN	C5'-C4'	2.02	1.54	1.51

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	FMN	C1'-N10-C9A	-3.56	114.58	120.51
2	D	801	FMN	C4A-C10-N1	-3.52	116.57	124.73
2	D	801	FMN	C5A-C9A-N10	3.45	121.52	117.95
2	A	801	FMN	O2'-C2'-C1'	-3.36	101.68	109.80
2	B	801	FMN	C4-C4A-C10	3.30	122.33	116.79
2	F	801	FMN	C4-N3-C2	-3.21	119.72	125.64
2	F	801	FMN	C9A-C5A-N5	-3.20	118.96	122.43
2	B	801	FMN	C4A-C10-N10	3.19	121.15	116.48
2	A	801	FMN	C4A-C10-N1	-3.16	117.39	124.73
2	D	801	FMN	C4A-C10-N10	3.01	120.89	116.48
2	F	801	FMN	C5A-C9A-N10	2.99	121.05	117.95
2	C	801	FMN	C9A-C5A-N5	-2.96	119.22	122.43
2	B	801	FMN	C1'-N10-C9A	2.96	125.44	120.51
2	B	801	FMN	C4A-C10-N1	-2.91	117.97	124.73
2	D	801	FMN	C4-N3-C2	-2.87	120.35	125.64
2	F	801	FMN	C4A-C4-N3	2.84	120.41	113.19
2	B	801	FMN	C1'-C2'-C3'	2.84	117.71	109.79
2	A	801	FMN	C5A-C9A-N10	2.82	120.87	117.95
2	B	801	FMN	C4'-C3'-C2'	2.79	119.16	113.36
2	D	801	FMN	C4-C4A-C10	2.78	121.45	116.79
2	C	801	FMN	C5A-C9A-N10	2.70	120.75	117.95
2	E	801	FMN	C5A-C9A-N10	2.67	120.72	117.95
2	D	801	FMN	C10-N1-C2	2.66	122.22	116.90
2	A	801	FMN	C9A-C5A-N5	-2.64	119.56	122.43
2	F	801	FMN	C4A-C10-N1	-2.64	118.62	124.73
2	E	801	FMN	C4A-C10-N1	-2.58	118.74	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	FMN	C6-C5A-C9A	2.56	122.56	118.94
2	E	801	FMN	C4-C4A-C10	2.53	121.04	116.79
2	C	801	FMN	C4A-C4-N3	2.53	119.61	113.19
2	B	801	FMN	C4-N3-C2	-2.51	121.00	125.64
2	C	801	FMN	O4-C4-C4A	-2.50	119.97	126.60
2	E	801	FMN	C4-N3-C2	-2.46	121.09	125.64
2	D	801	FMN	C9A-N10-C10	-2.46	116.93	120.77
2	E	801	FMN	C4A-C10-N10	2.46	120.08	116.48
2	E	801	FMN	C9A-C5A-N5	-2.44	119.78	122.43
2	A	801	FMN	O4-C4-C4A	-2.43	120.15	126.60
2	D	801	FMN	C4A-C4-N3	2.43	119.36	113.19
2	C	801	FMN	C4-N3-C2	-2.37	121.26	125.64
2	F	801	FMN	C10-C4A-N5	-2.35	119.87	124.86
2	A	801	FMN	C1'-N10-C9A	-2.33	116.63	120.51
2	A	801	FMN	N10-C10-N1	2.31	124.98	118.35
2	E	801	FMN	O4-C4-C4A	-2.29	120.53	126.60
2	B	801	FMN	C10-C4A-N5	-2.26	120.05	124.86
2	E	801	FMN	C4A-C4-N3	2.25	118.92	113.19
2	F	801	FMN	C1'-N10-C9A	-2.23	116.80	120.51
2	C	801	FMN	C4A-C10-N10	2.22	119.73	116.48
2	D	801	FMN	C10-C4A-N5	-2.20	120.19	124.86
2	C	801	FMN	C9-C9A-N10	-2.20	118.87	121.84
2	F	801	FMN	O4-C4-C4A	-2.18	120.83	126.60
2	B	801	FMN	C9-C9A-C5A	-2.15	116.04	120.11
2	C	801	FMN	C10-N1-C2	2.15	121.21	116.90
2	C	801	FMN	C4A-C10-N1	-2.15	119.73	124.73
2	C	801	FMN	C10-C4A-N5	-2.15	120.29	124.86
2	F	801	FMN	C4A-C10-N10	2.13	119.59	116.48
2	B	801	FMN	C9-C9A-N10	2.11	124.69	121.84
2	F	801	FMN	C10-N1-C2	2.09	121.09	116.90
2	A	801	FMN	C9A-N10-C10	-2.06	117.55	120.77
2	D	801	FMN	O3P-P-O5'	2.06	112.22	106.73
2	A	801	FMN	P-O5'-C5'	2.06	123.97	118.30
2	B	801	FMN	O4'-C4'-C3'	2.05	114.09	109.10
2	E	801	FMN	C10-C4A-N5	-2.03	120.54	124.86
2	B	801	FMN	C9A-N10-C10	-2.03	117.61	120.77
2	C	801	FMN	O2'-C2'-C3'	2.02	114.01	109.10
2	F	801	FMN	C4-C4A-C10	2.01	120.17	116.79

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FMN	C1'-C2'-C3'-O3'
2	A	801	FMN	C1'-C2'-C3'-C4'
2	A	801	FMN	O2'-C2'-C3'-O3'
2	A	801	FMN	O2'-C2'-C3'-C4'
2	A	801	FMN	C3'-C4'-C5'-O5'
2	A	801	FMN	O4'-C4'-C5'-O5'
2	A	801	FMN	C5'-O5'-P-O3P
2	B	801	FMN	C2'-C3'-C4'-O4'
2	B	801	FMN	O3'-C3'-C4'-O4'
2	B	801	FMN	O3'-C3'-C4'-C5'
2	B	801	FMN	C3'-C4'-C5'-O5'
2	B	801	FMN	O4'-C4'-C5'-O5'
2	C	801	FMN	N10-C1'-C2'-O2'
2	C	801	FMN	N10-C1'-C2'-C3'
2	C	801	FMN	C1'-C2'-C3'-O3'
2	C	801	FMN	C1'-C2'-C3'-C4'
2	C	801	FMN	C3'-C4'-C5'-O5'
2	C	801	FMN	O4'-C4'-C5'-O5'
2	C	801	FMN	C5'-O5'-P-O2P
2	C	801	FMN	C5'-O5'-P-O3P
2	D	801	FMN	C2'-C1'-N10-C9A
2	D	801	FMN	C2'-C1'-N10-C10
2	D	801	FMN	N10-C1'-C2'-O2'
2	D	801	FMN	C2'-C3'-C4'-O4'
2	D	801	FMN	C2'-C3'-C4'-C5'
2	D	801	FMN	O3'-C3'-C4'-O4'
2	D	801	FMN	O3'-C3'-C4'-C5'
2	D	801	FMN	C3'-C4'-C5'-O5'
2	D	801	FMN	O4'-C4'-C5'-O5'
2	E	801	FMN	C1'-C2'-C3'-O3'
2	E	801	FMN	C1'-C2'-C3'-C4'
2	E	801	FMN	O2'-C2'-C3'-O3'
2	E	801	FMN	O2'-C2'-C3'-C4'
2	E	801	FMN	C3'-C4'-C5'-O5'
2	E	801	FMN	O4'-C4'-C5'-O5'
2	E	801	FMN	C5'-O5'-P-O1P
2	E	801	FMN	C5'-O5'-P-O2P
2	E	801	FMN	C5'-O5'-P-O3P
2	F	801	FMN	C2'-C1'-N10-C10
2	F	801	FMN	N10-C1'-C2'-O2'
2	F	801	FMN	N10-C1'-C2'-C3'
2	F	801	FMN	C1'-C2'-C3'-O3'
2	F	801	FMN	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
2	C	801	FMN	O2'-C2'-C3'-O3'
2	F	801	FMN	O2'-C2'-C3'-O3'
2	C	801	FMN	O2'-C2'-C3'-C4'
2	B	801	FMN	C2'-C3'-C4'-C5'
2	F	801	FMN	O2'-C2'-C3'-C4'
2	C	801	FMN	C2'-C3'-C4'-C5'
2	C	801	FMN	O3'-C3'-C4'-O4'
2	D	801	FMN	O2'-C2'-C3'-O3'
2	C	801	FMN	C2'-C3'-C4'-O4'
2	D	801	FMN	O2'-C2'-C3'-C4'
2	C	801	FMN	O3'-C3'-C4'-C5'
2	C	801	FMN	C2'-C1'-N10-C10
2	A	801	FMN	C2'-C3'-C4'-C5'
2	A	801	FMN	C5'-O5'-P-O2P
2	D	801	FMN	C1'-C2'-C3'-O3'
2	A	801	FMN	C5'-O5'-P-O1P
2	A	801	FMN	O3'-C3'-C4'-C5'
2	C	801	FMN	C5'-O5'-P-O1P
2	E	801	FMN	C2'-C3'-C4'-C5'
2	A	801	FMN	N10-C1'-C2'-O2'
2	D	801	FMN	N10-C1'-C2'-C3'
2	B	801	FMN	C2'-C1'-N10-C10

There are no ring outliers.

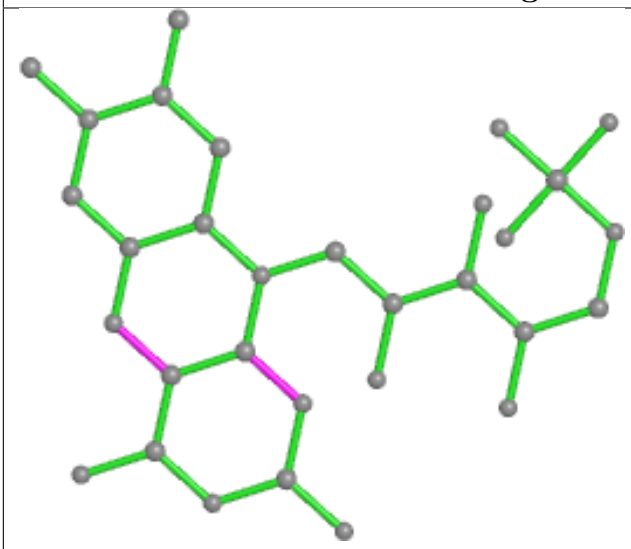
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	801	FMN	1	0
2	B	801	FMN	1	0
2	A	801	FMN	1	0
2	D	801	FMN	3	0
2	C	801	FMN	1	0

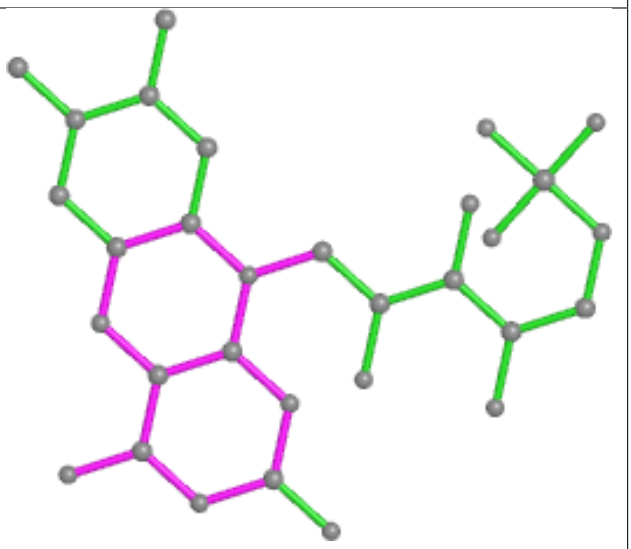
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

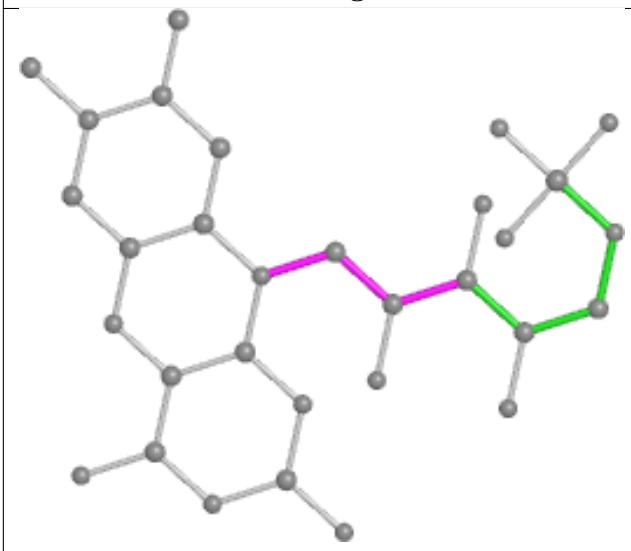
Ligand FMN F 801



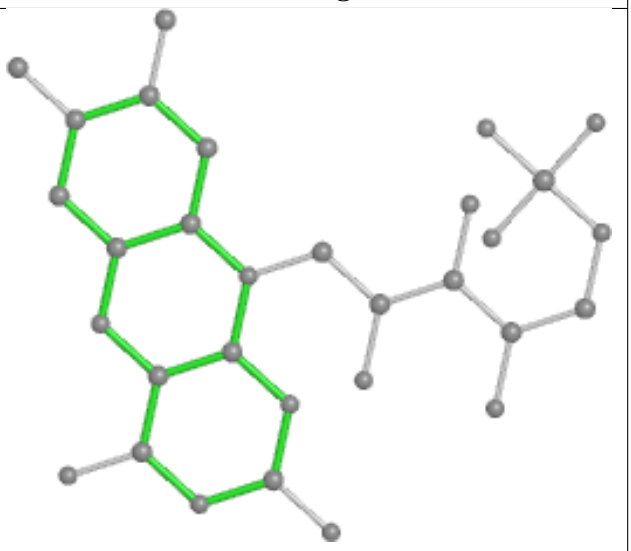
Bond lengths



Bond angles

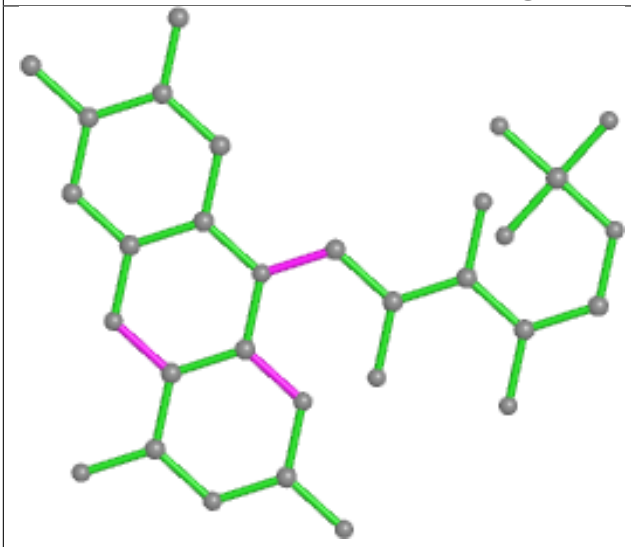


Torsions

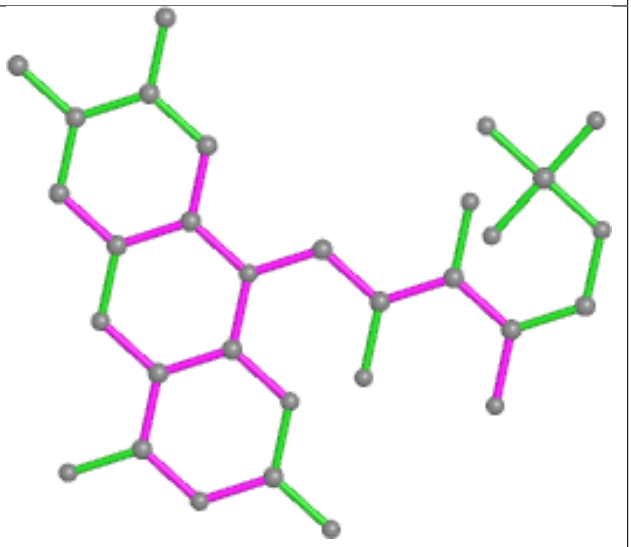


Rings

Ligand FMN B 801



Bond lengths



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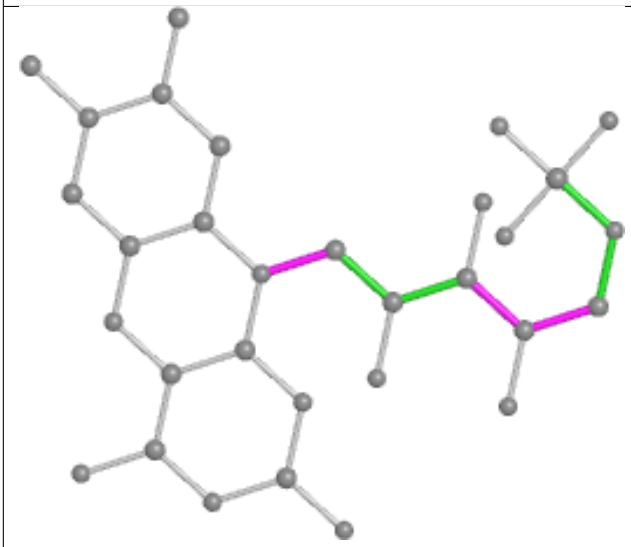

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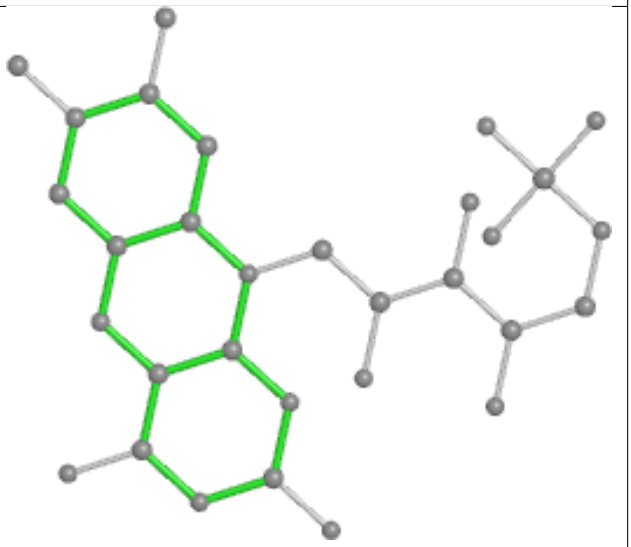
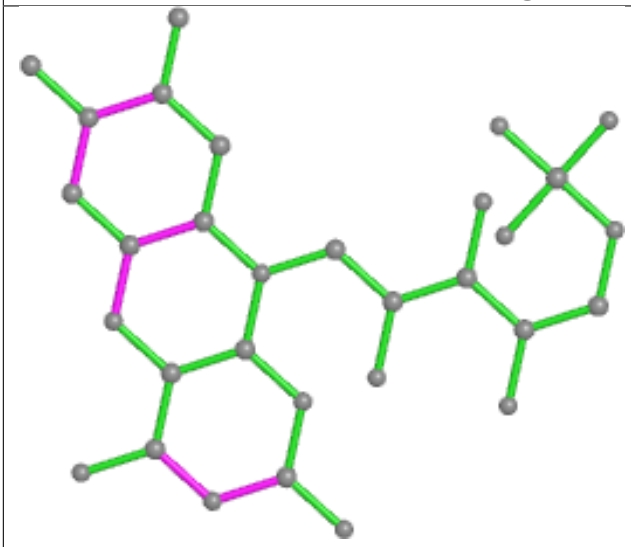
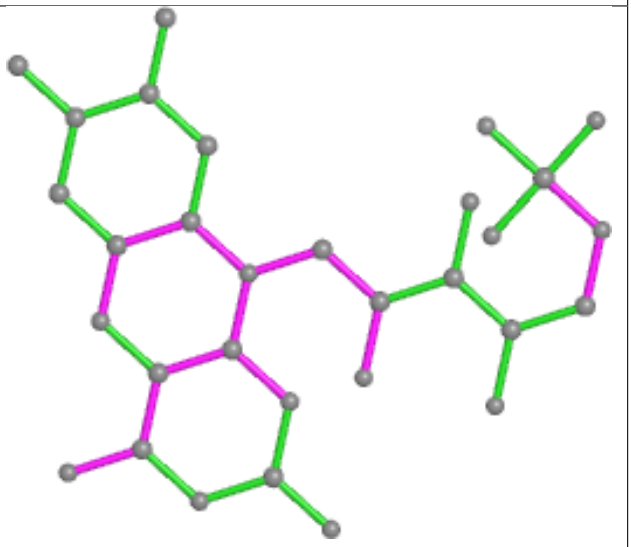


Rings

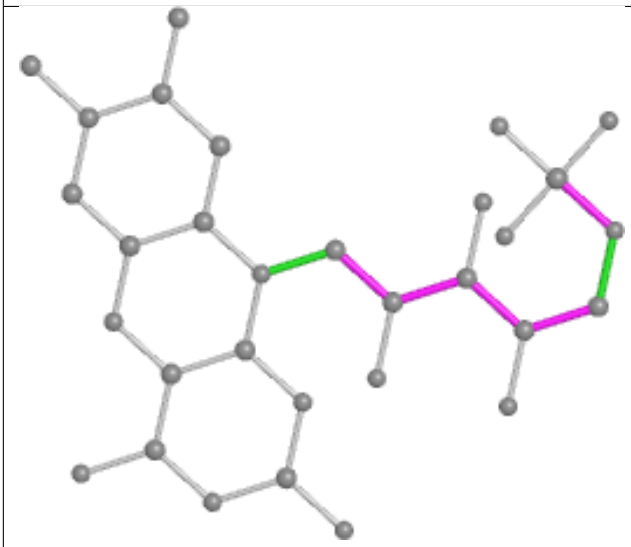
Ligand FMN A 801



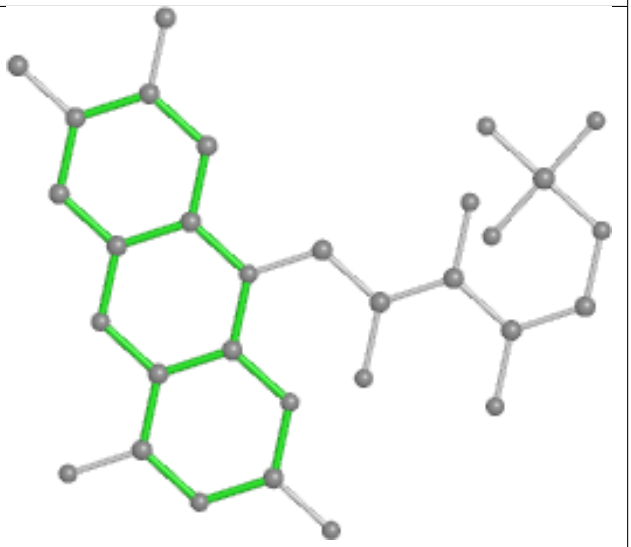
Bond lengths



Bond angles

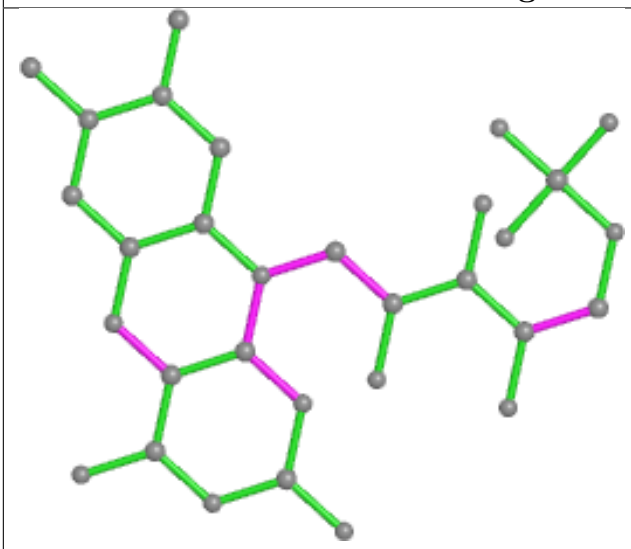


Torsions

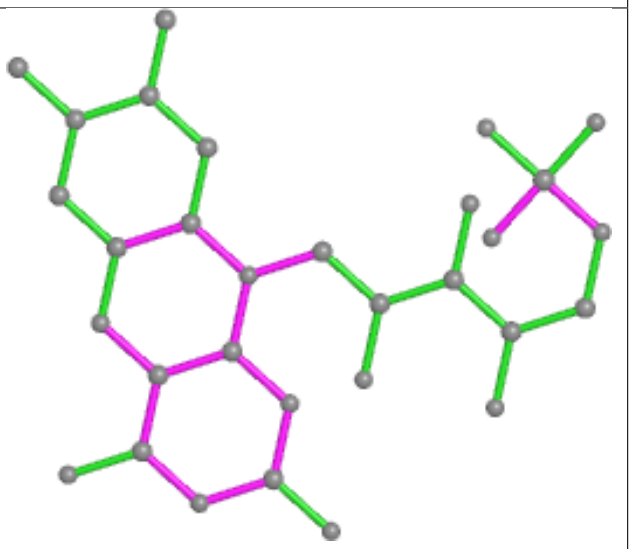


Rings

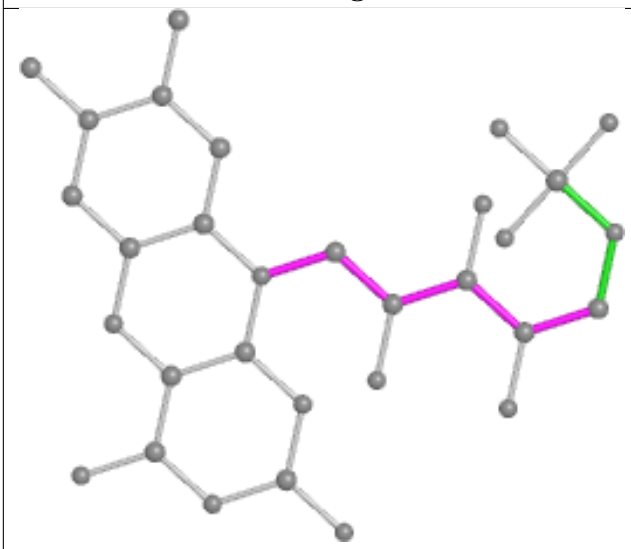
Ligand FMN D 801



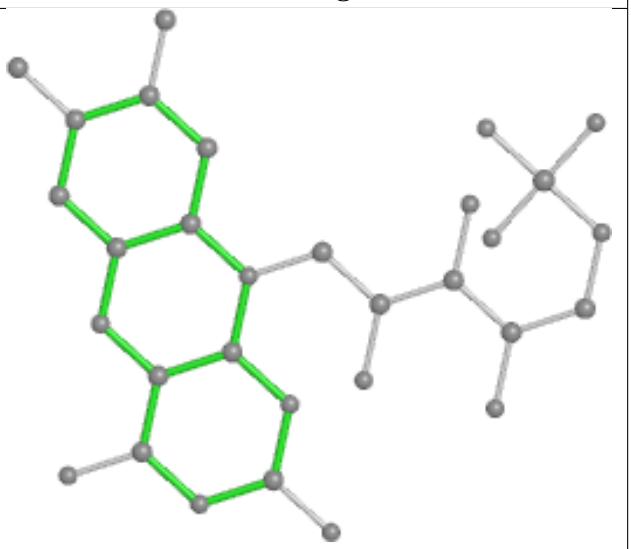
Bond lengths



Bond angles

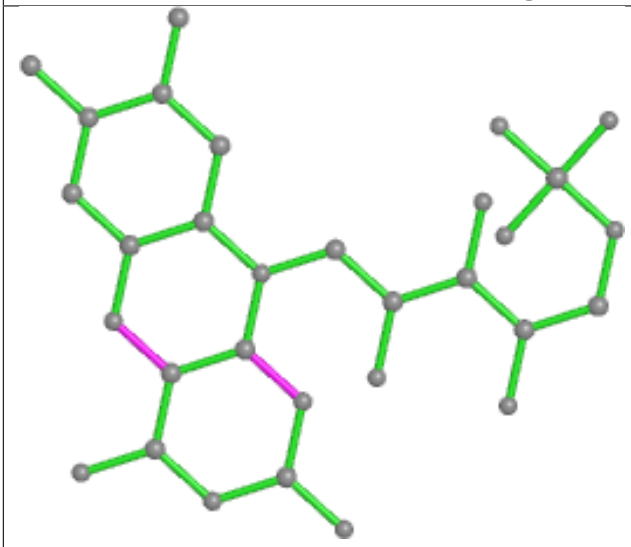


Torsions

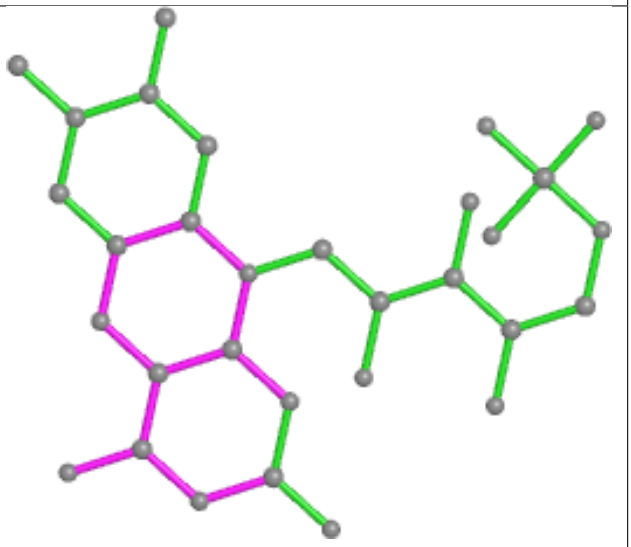


Rings

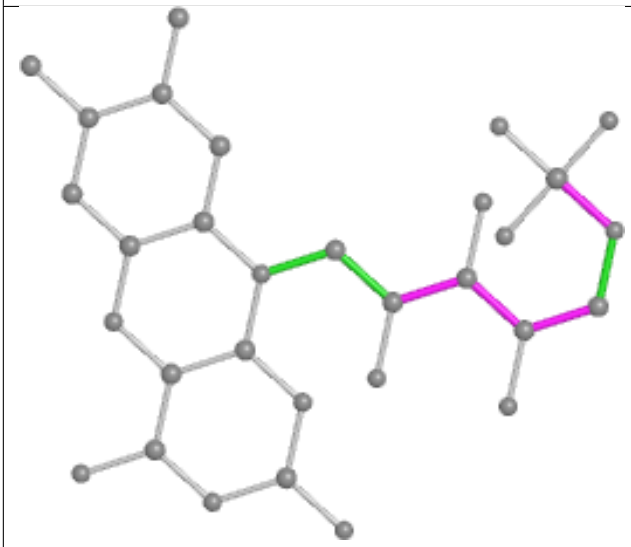
Ligand FMN E 801



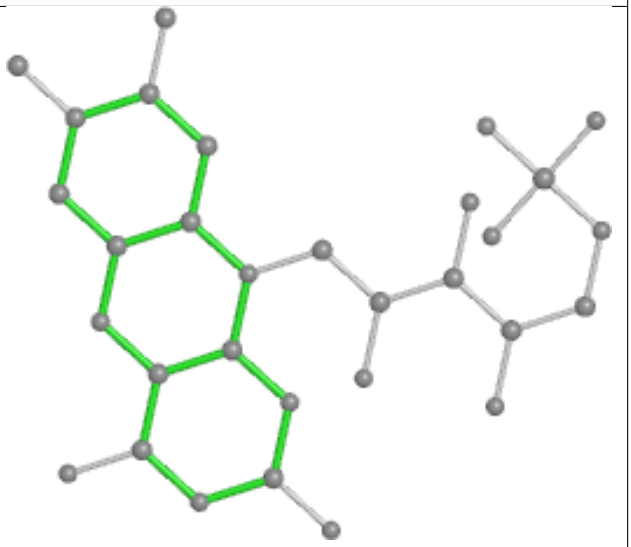
Bond lengths



Bond angles

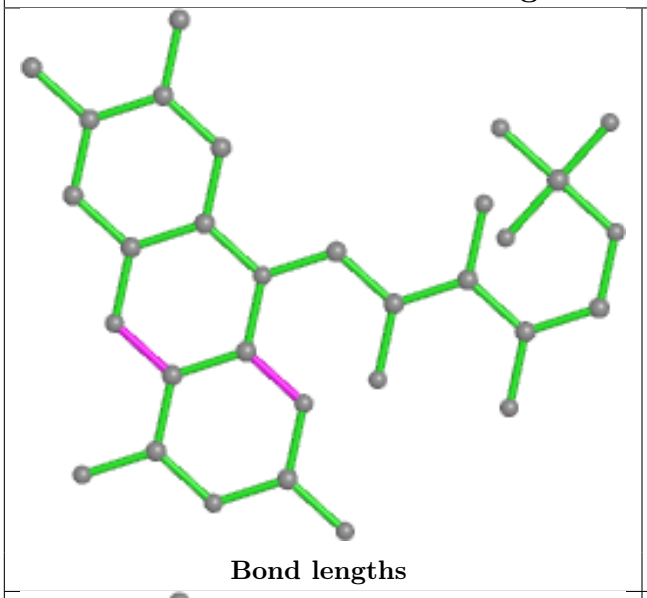


Torsions

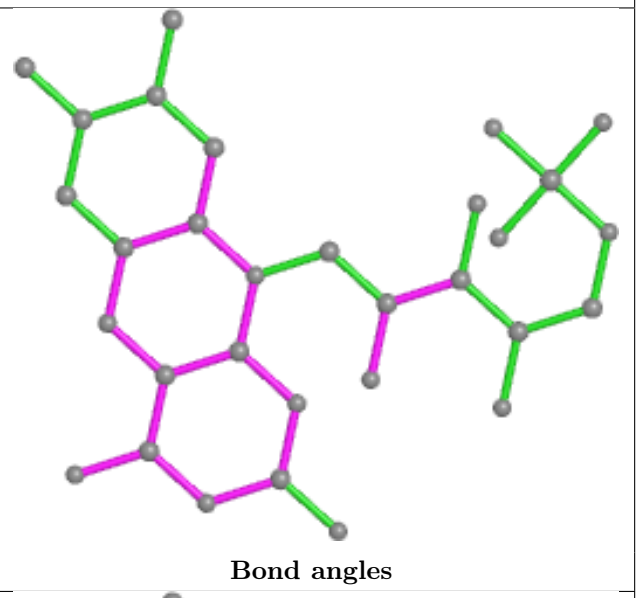


Rings

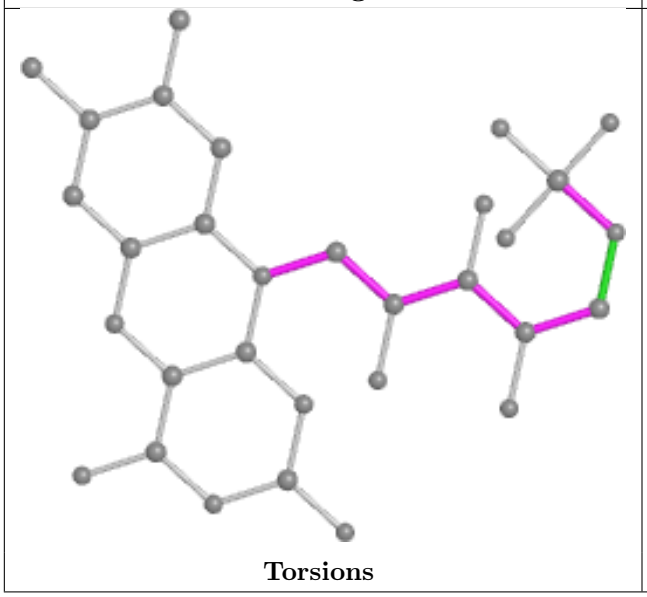
Ligand FMN C 801



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	643/769 (83%)	-0.37	3 (0%)	91	94	22, 33, 46, 58	0
1	B	643/769 (83%)	-0.37	6 (0%)	84	88	22, 32, 45, 61	0
1	C	643/769 (83%)	-0.37	3 (0%)	91	94	21, 33, 45, 61	0
1	D	643/769 (83%)	-0.33	6 (0%)	84	88	23, 33, 46, 58	0
1	E	643/769 (83%)	-0.36	2 (0%)	94	96	22, 32, 45, 58	0
1	F	643/769 (83%)	-0.32	1 (0%)	95	97	23, 34, 48, 59	0
All	All	3858/4614 (83%)	-0.35	21 (0%)	91	94	21, 33, 46, 61	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	197	TYR	4.5
1	A	197	TYR	3.4
1	E	197	TYR	3.3
1	C	197	TYR	3.3
1	D	621	THR	3.0
1	A	62	THR	2.8
1	B	641	PRO	2.8
1	D	197	TYR	2.8
1	B	620	ASP	2.6
1	B	476	THR	2.6
1	E	636	ALA	2.6
1	B	636	ALA	2.5
1	C	168	ALA	2.5
1	D	633	THR	2.5
1	B	197	TYR	2.5
1	B	385	GLU	2.4
1	D	641	PRO	2.4
1	D	620	ASP	2.3
1	A	168	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	345	LYS	2.2
1	D	121	PRO	2.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

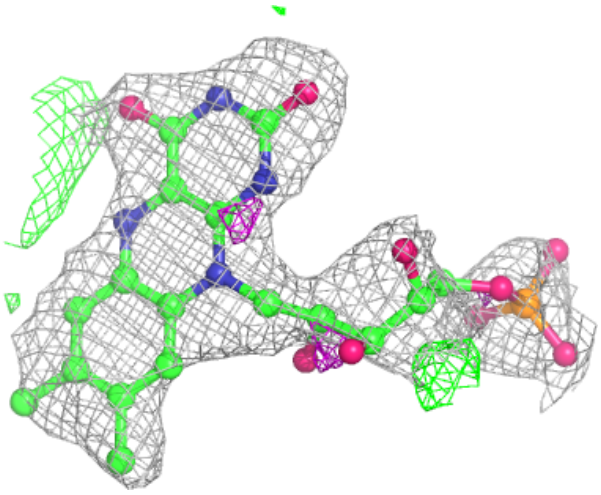
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

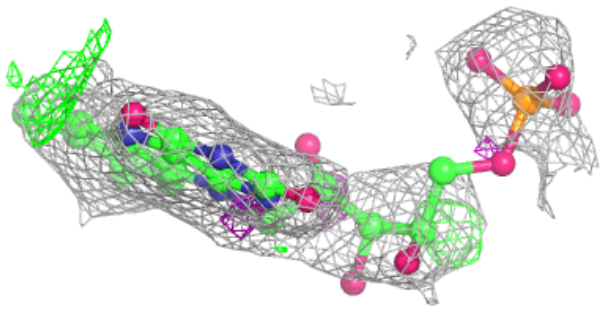
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FMN	E	801	31/31	0.84	0.34	40,54,103,115	0
2	FMN	F	801	31/31	0.84	0.41	41,55,110,118	0
2	FMN	D	801	31/31	0.85	0.31	41,56,94,101	0
2	FMN	B	801	31/31	0.86	0.29	37,53,89,98	0
2	FMN	A	801	31/31	0.87	0.35	44,55,94,107	0
2	FMN	C	801	31/31	0.89	0.34	38,51,98,106	0

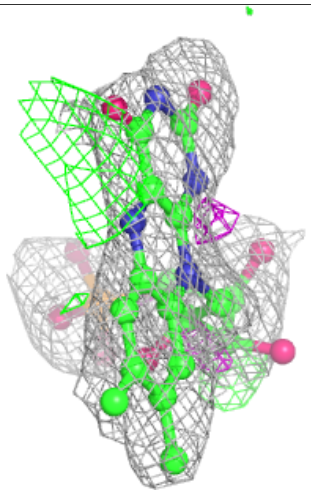
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN E 801:

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

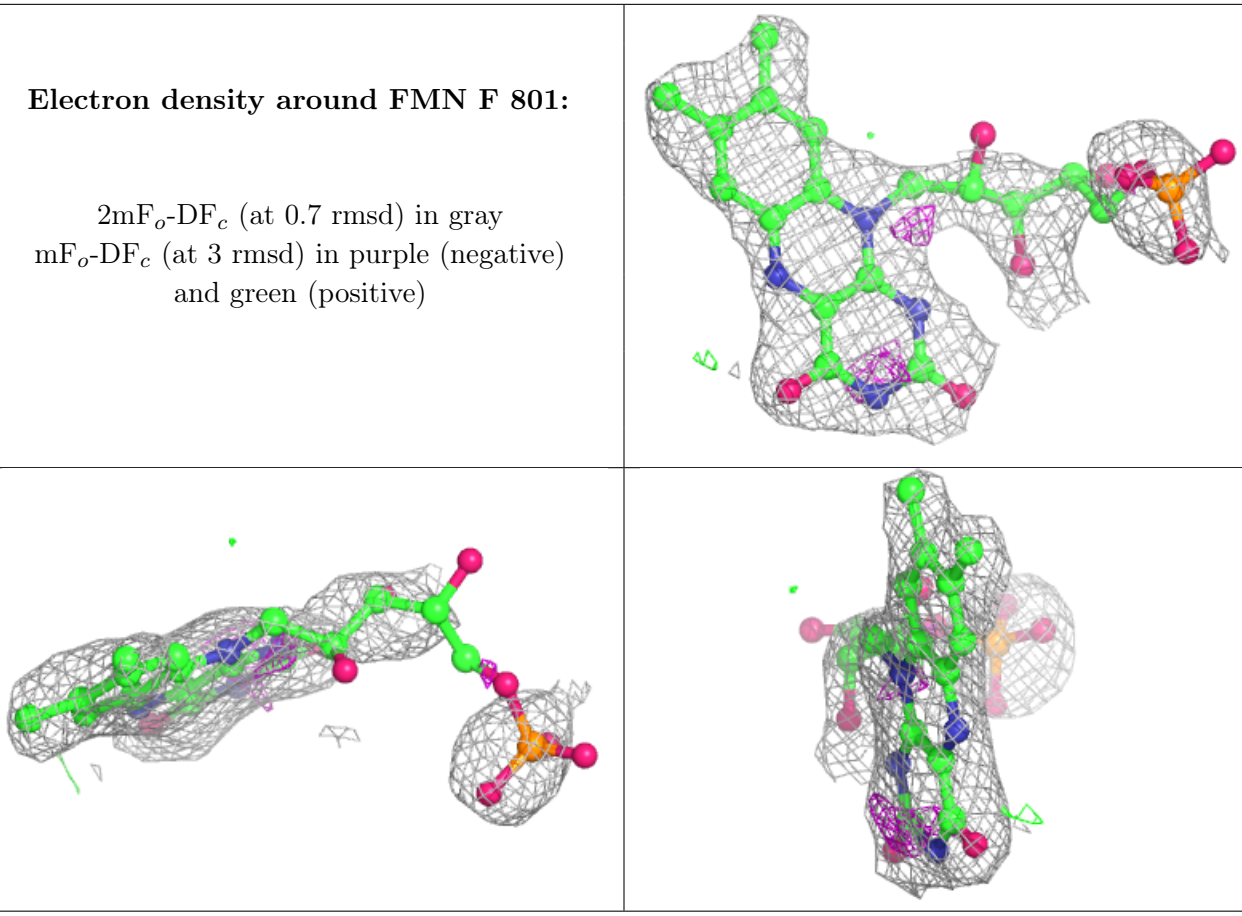






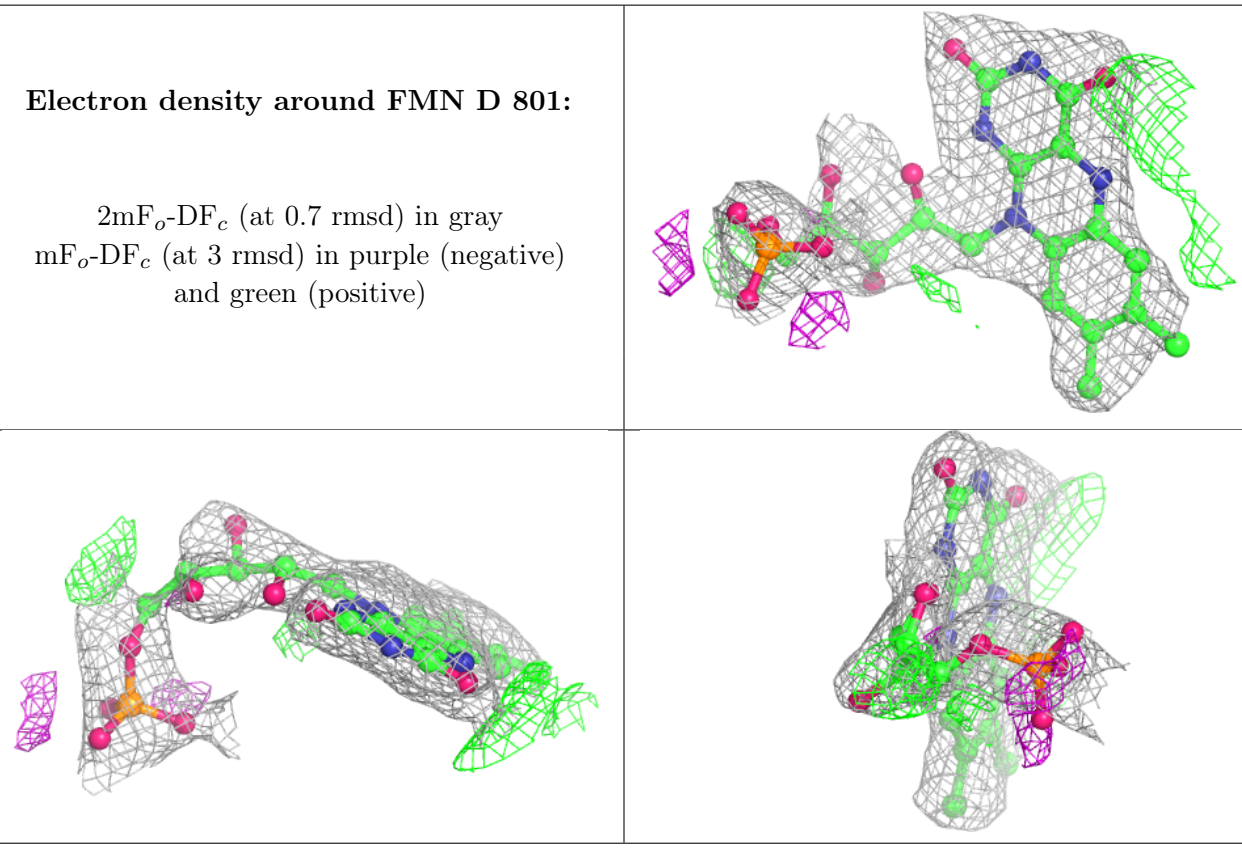
Electron density around FMN F 801:

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



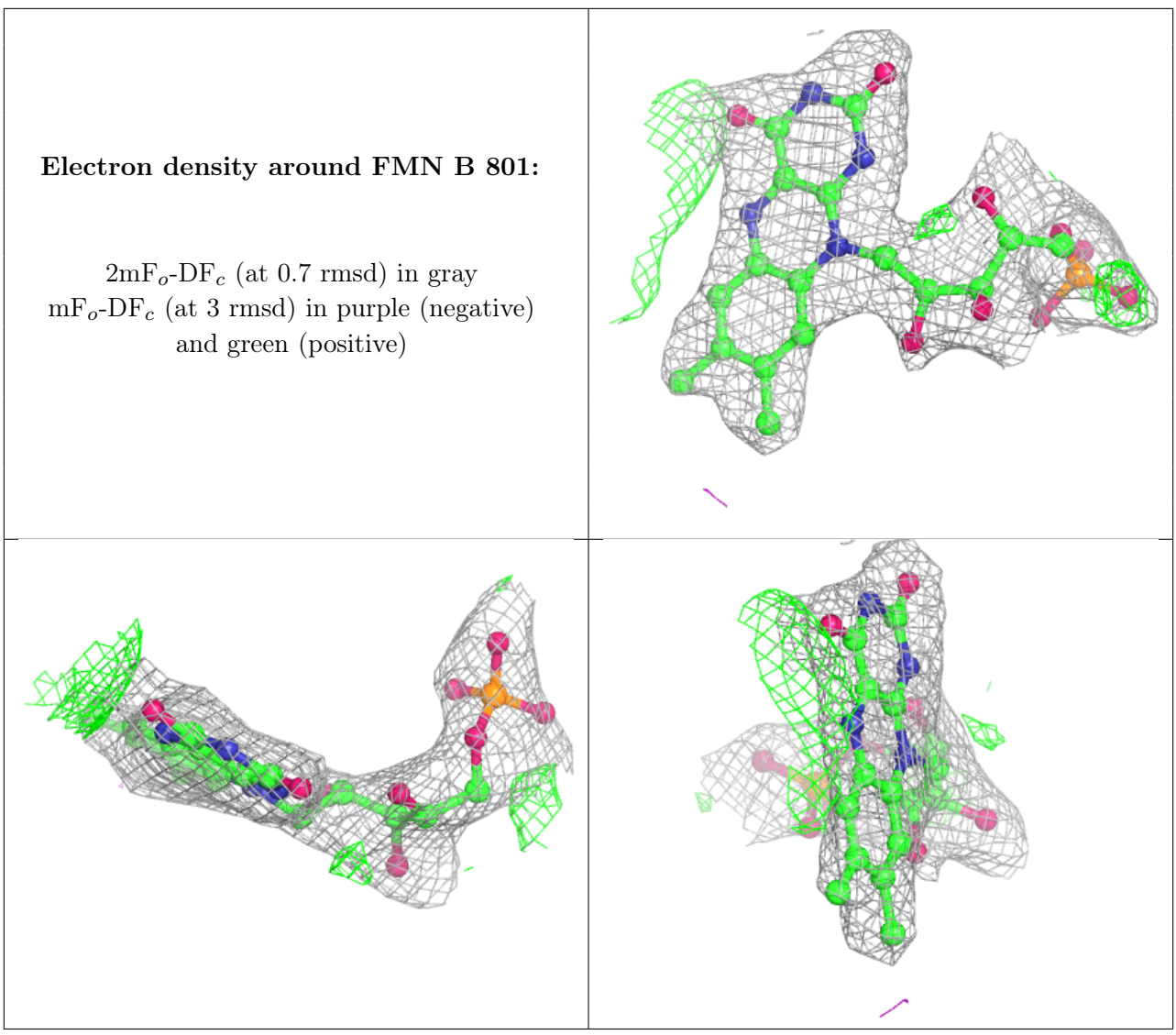
Electron density around FMN D 801:

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



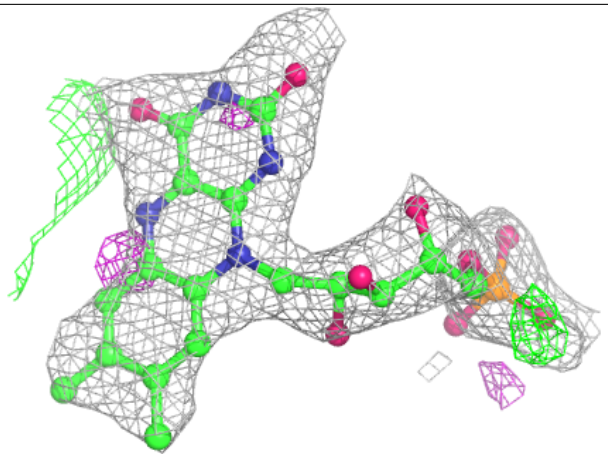
Electron density around FMN B 801:

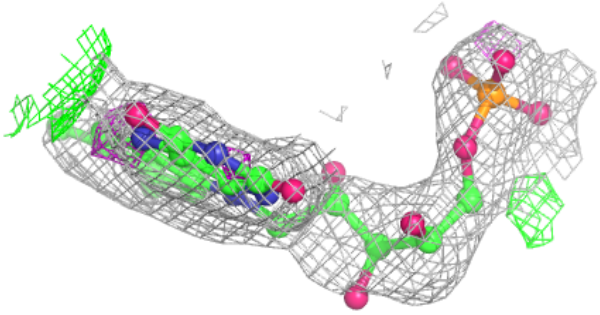
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

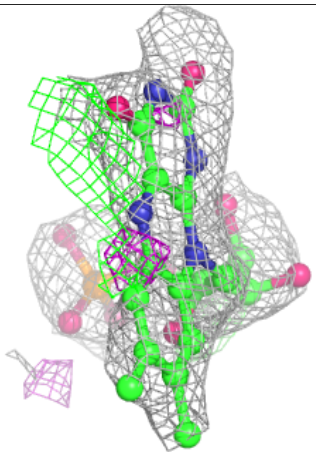


Electron density around FMN A 801:

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

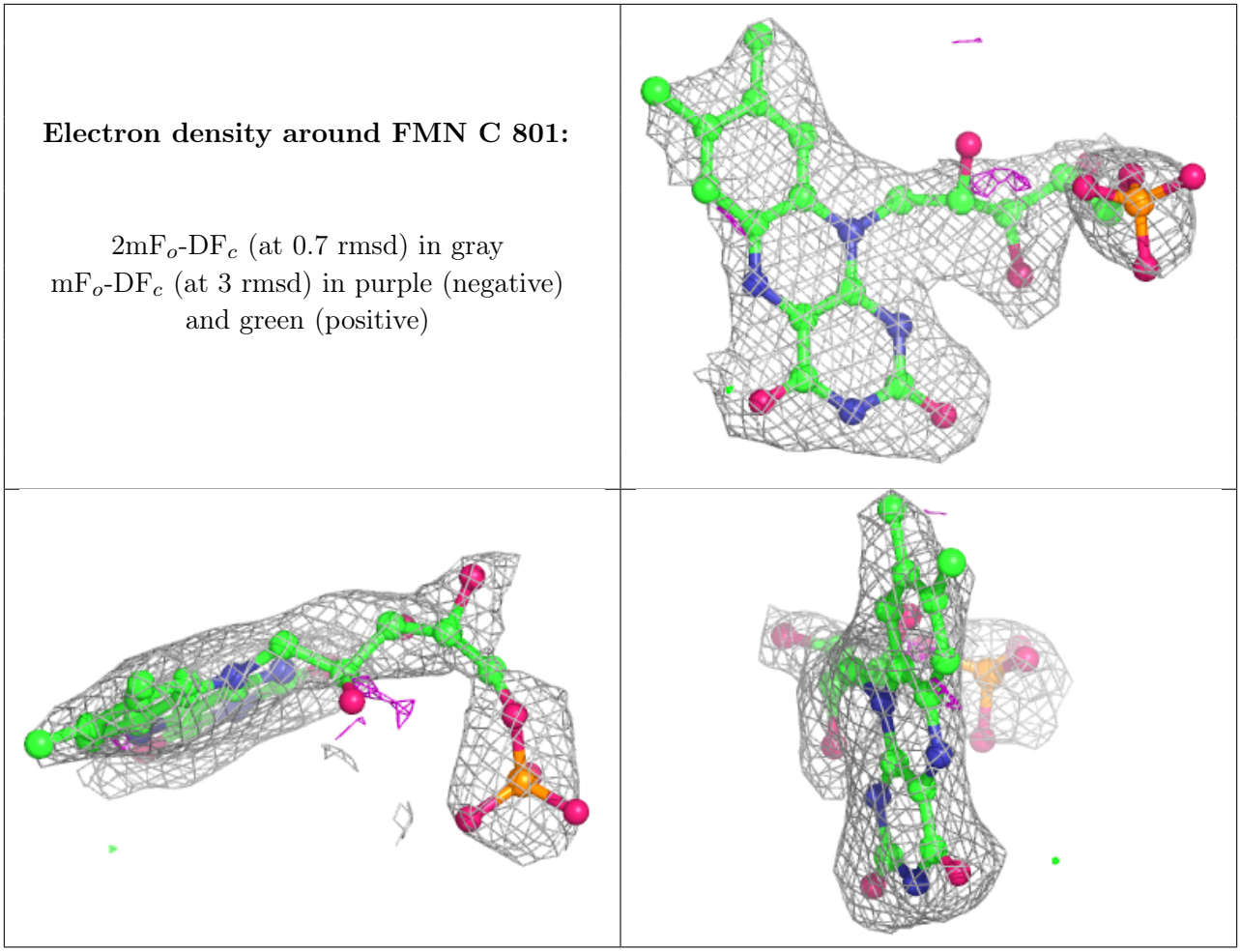






Electron density around FMN C 801:

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



6.5 Other polymers (i)

There are no such residues in this entry.