



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 04:11 am BST

PDB ID : 6H6V
Title : Structure of the UbiD-class enzyme HmfF from *Pelotomaculum thermopropionicum* in complex with FMN
Authors : Payne, K.A.P.; Leys, D.
Deposited on : 2018-07-30
Resolution : 2.66 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

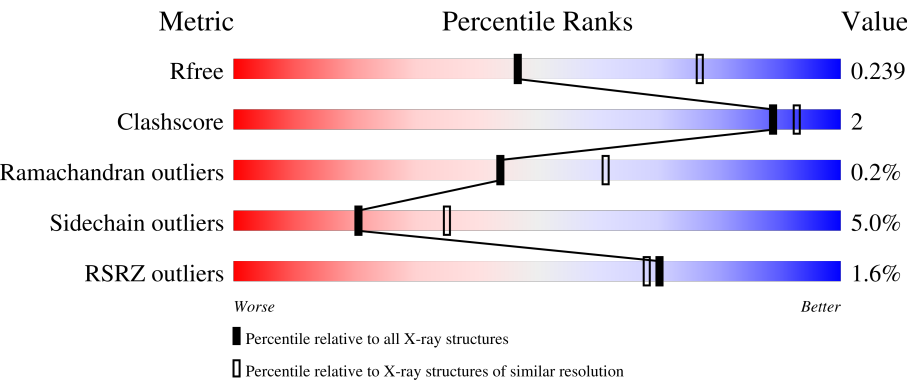
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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}	164625	1003 (2.66-2.66)
Clashscore	180529	1063 (2.66-2.66)
Ramachandran outliers	177936	1052 (2.66-2.66)
Sidechain outliers	177891	1052 (2.66-2.66)
RSRZ outliers	164620	1003 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	448	<div><div>%</div><div>92%7% ..</div></div>
1	B	448	<div><div>%</div><div>93%6% .</div></div>
1	C	448	<div><div>2%</div><div>92%6% .</div></div>
1	D	448	<div><div>%</div><div>92%7% .</div></div>
1	E	448	<div><div>%</div><div>91%8% ..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	448	<div><div></div><div>4%</div><div>93%</div><div>6%</div></div>

2 Entry composition [i](#)

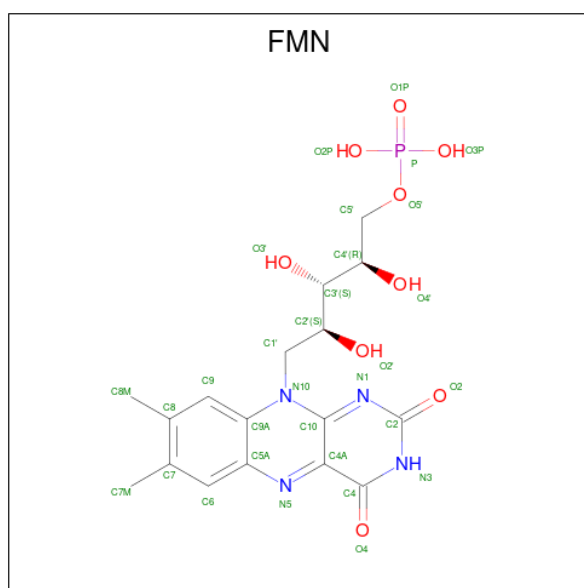
There are 6 unique types of molecules in this entry. The entry contains 20880 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-polyprenyl-4-hydroxybenzoate decarboxylase and related decarboxylases.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	Se	0	0	0
			3406	2173	605	617	6	5			
1	B	445	Total	C	N	O	S	Se	0	0	0
			3406	2173	605	617	6	5			
1	C	445	Total	C	N	O	S	Se	0	0	0
			3406	2173	605	617	6	5			
1	D	444	Total	C	N	O	S	Se	0	0	0
			3398	2167	604	616	6	5			
1	E	445	Total	C	N	O	S	Se	0	0	0
			3406	2173	605	617	6	5			
1	F	446	Total	C	N	O	S	Se	0	0	0
			3411	2176	606	618	6	5			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (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 POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		
3	F	1	Total	K	0	0
			1	1		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		
4	C	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		
4	E	1	Total	Mn	0	0
			1	1		
4	F	1	Total	Mn	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Ca 1	0	0
5	B	1	Total 1	Ca 1	0	0
5	C	1	Total 1	Ca 1	0	0
5	D	1	Total 1	Ca 1	0	0
5	E	1	Total 1	Ca 1	0	0
5	F	1	Total 1	Ca 1	0	0

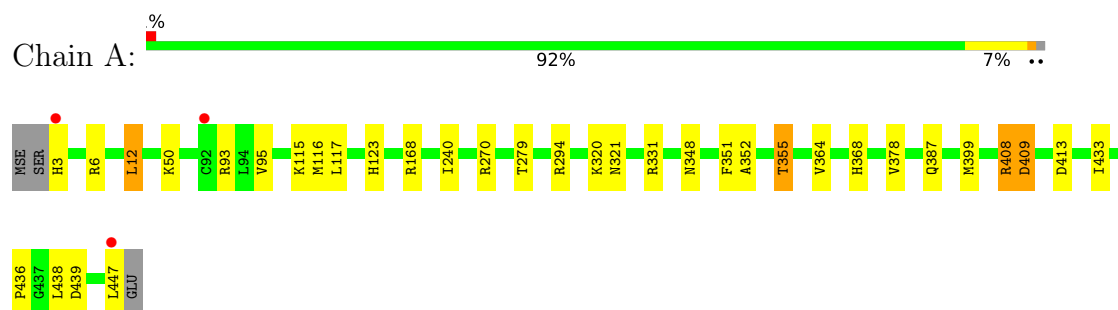
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	38	Total 38	O 38	0	0
6	B	54	Total 54	O 54	0	0
6	C	40	Total 40	O 40	0	0
6	D	44	Total 44	O 44	0	0
6	E	32	Total 32	O 32	0	0
6	F	35	Total 35	O 35	0	0

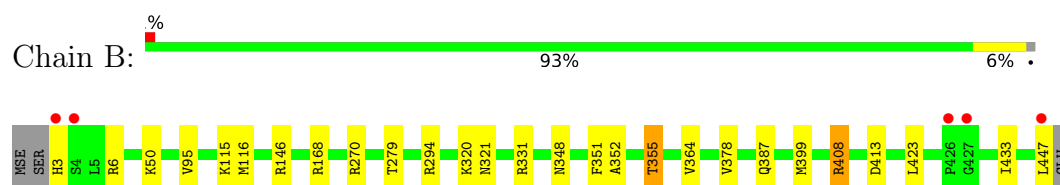
3 Residue-property plots [i](#)

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

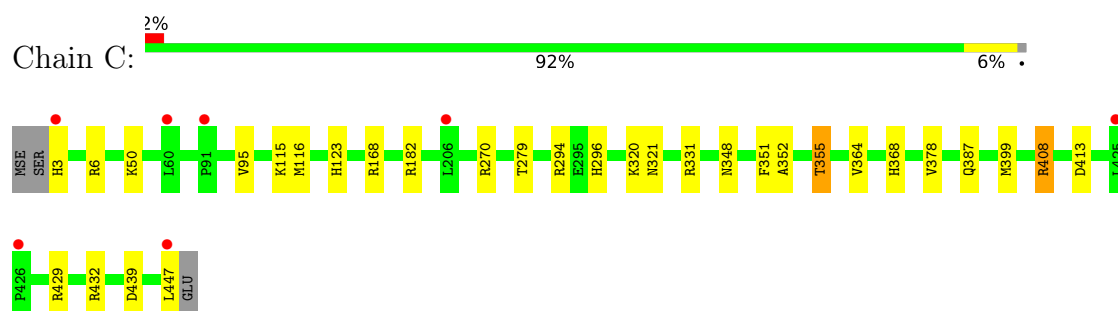
- Molecule 1: 3-polyprenyl-4-hydroxybenzoate decarboxylase and related decarboxylases



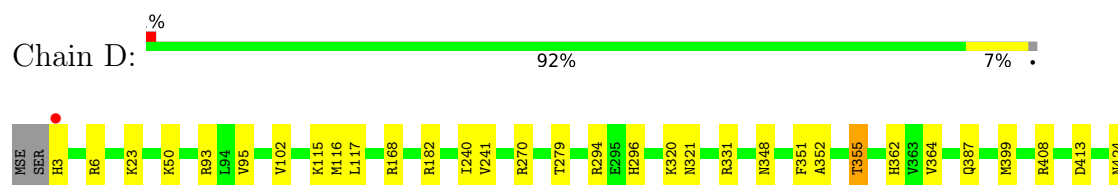
- Molecule 1: 3-polyprenyl-4-hydroxybenzoate decarboxylase and related decarboxylases

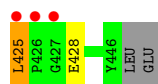


- Molecule 1: 3-polyprenyl-4-hydroxybenzoate decarboxylase and related decarboxylases

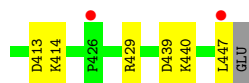
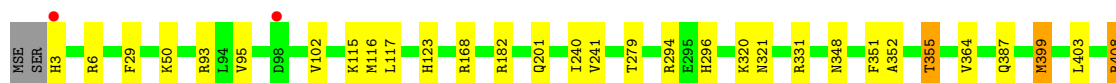
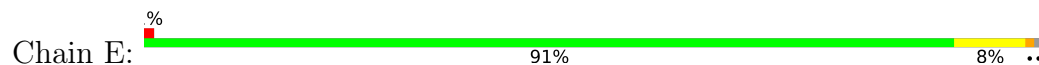


- Molecule 1: 3-polyprenyl-4-hydroxybenzoate decarboxylase and related decarboxylases

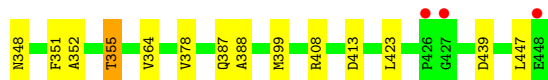
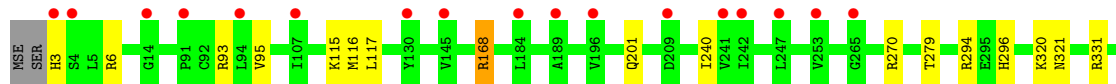




- Molecule 1: 3-polyprenyl-4-hydroxybenzoate decarboxylase and related decarboxylases



- Molecule 1: 3-polyprenyl-4-hydroxybenzoate decarboxylase and related decarboxylases



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.91Å 139.25Å 136.88Å 90.00° 93.74° 90.00°	Depositor
Resolution (Å)	74.20 – 2.66 74.20 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.20-2.66) 99.8 (74.20-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.199 , 0.236 0.205 , 0.239	Depositor DCC
R_{free} test set	4311 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20880	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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

5.1 Standard geometry

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

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	0.55	0/3474	0.79	4/4718 (0.1%)
1	B	0.55	0/3474	0.79	4/4718 (0.1%)
1	C	0.55	0/3474	0.78	4/4718 (0.1%)
1	D	0.55	0/3466	0.78	2/4707 (0.0%)
1	E	0.54	0/3474	0.77	0/4718
1	F	0.52	0/3479	0.78	2/4725 (0.0%)
All	All	0.54	0/20841	0.78	16/28304 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	439	ASP	CB-CG-OD1	7.75	125.27	118.30
1	A	409	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	A	12	LEU	CA-CB-CG	5.83	128.72	115.30
1	C	432	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	270	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	270	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	439	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	270	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	168	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	F	270	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	425	LEU	CB-CG-CD1	5.34	120.08	111.00
1	B	270	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	270	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	F	168	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	C	270	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	146	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	3406	0	3496	17	0
1	B	3406	0	3496	13	0
1	C	3406	0	3496	15	0
1	D	3398	0	3485	17	0
1	E	3406	0	3496	24	0
1	F	3411	0	3498	22	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	1	0
2	D	31	0	19	1	0
2	E	31	0	19	3	0
2	F	31	0	19	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	38	0	0	2	0
6	B	54	0	0	0	0
6	C	40	0	0	2	0
6	D	44	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	32	0	0	1	0
6	F	35	0	0	1	0
All	All	20880	0	21081	74	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 2.

All (74) 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:D:413:ASP:H	1:F:387:GLN:HE22	1.19	0.90
1:E:348:ASN:HD21	1:F:399:MSE:H	1.24	0.85
1:D:387:GLN:HE22	1:F:413:ASP:H	1.24	0.84
1:A:387:GLN:HE22	1:E:413:ASP:H	1.27	0.82
1:B:387:GLN:HE22	1:C:413:ASP:H	1.29	0.81
1:A:413:ASP:H	1:E:387:GLN:HE22	1.30	0.78
1:E:399:MSE:H	1:F:348:ASN:HD21	1.30	0.77
1:B:348:ASN:HD21	1:D:399:MSE:H	1.36	0.72
1:C:368:HIS:NE2	6:C:601:HOH:O	2.07	0.71
1:D:387:GLN:NE2	1:F:413:ASP:H	1.88	0.70
1:B:413:ASP:H	1:C:387:GLN:HE22	1.41	0.69
1:A:368:HIS:NE2	6:A:601:HOH:O	2.26	0.67
1:D:413:ASP:H	1:F:387:GLN:NE2	1.91	0.66
1:B:387:GLN:NE2	1:C:413:ASP:H	1.94	0.64
1:A:387:GLN:NE2	1:E:413:ASP:H	1.96	0.64
1:A:399:MSE:H	1:C:348:ASN:HD21	1.44	0.64
1:B:399:MSE:H	1:D:348:ASN:HD21	1.45	0.62
1:A:413:ASP:H	1:E:387:GLN:NE2	1.99	0.61
1:A:348:ASN:HD21	1:C:399:MSE:H	1.49	0.60
1:F:351:PHE:O	1:F:355:THR:HG23	2.02	0.59
1:C:351:PHE:O	1:C:355:THR:HG23	2.03	0.59
1:E:351:PHE:O	1:E:355:THR:HG23	2.03	0.59
1:A:351:PHE:O	1:A:355:THR:HG23	2.04	0.58
1:D:351:PHE:O	1:D:355:THR:HG23	2.04	0.58
1:B:351:PHE:O	1:B:355:THR:HG23	2.03	0.57
6:D:601:HOH:O	1:F:388:ALA:HB2	2.05	0.56
1:B:413:ASP:H	1:C:387:GLN:NE2	2.03	0.55
1:E:355:THR:HG21	1:F:352:ALA:HA	1.91	0.52
1:E:352:ALA:HA	1:F:355:THR:HG21	1.92	0.52
1:E:348:ASN:ND2	1:F:399:MSE:H	2.02	0.52
1:C:368:HIS:CE1	6:C:601:HOH:O	2.61	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:LYS:HE3	6:F:610:HOH:O	2.12	0.49
1:D:387:GLN:HE22	1:F:413:ASP:N	2.02	0.49
1:E:201:GLN:HE22	2:E:501:FMN:H9	1.77	0.49
1:F:117:LEU:HD22	1:F:240:ILE:HD13	1.95	0.48
1:D:362:HIS:NE2	6:D:601:HOH:O	2.35	0.48
1:D:117:LEU:HD22	1:D:240:ILE:HD13	1.95	0.47
1:A:433:ILE:HD12	1:E:123:HIS:CE1	2.51	0.46
1:B:423:LEU:HD23	1:B:423:LEU:HA	1.82	0.46
1:F:201:GLN:HE22	2:F:501:FMN:H3'	1.81	0.45
1:B:433:ILE:HD12	1:C:123:HIS:CE1	2.52	0.45
1:D:413:ASP:N	1:F:387:GLN:HE22	2.00	0.45
1:B:352:ALA:HA	1:D:355:THR:HG21	1.98	0.45
1:E:201:GLN:NE2	2:E:501:FMN:H9	2.31	0.45
1:F:348:ASN:HD22	1:F:348:ASN:H	1.64	0.44
1:A:117:LEU:HD22	1:A:240:ILE:HD13	2.00	0.43
1:A:387:GLN:HE22	1:E:413:ASP:N	2.06	0.43
1:A:352:ALA:HA	1:C:355:THR:HG21	2.01	0.42
1:C:296:HIS:CD2	2:C:501:FMN:HM73	2.54	0.42
1:E:117:LEU:HD22	1:E:240:ILE:HD13	2.01	0.42
1:F:201:GLN:NE2	2:F:501:FMN:H3'	2.34	0.42
1:B:355:THR:HG21	1:D:352:ALA:HA	2.01	0.42
1:A:355:THR:HG21	1:C:352:ALA:HA	2.02	0.42
1:E:355:THR:HG21	1:F:355:THR:CG2	2.49	0.42
1:B:348:ASN:HD22	1:B:348:ASN:H	1.66	0.42
1:E:408:ARG:HG2	1:E:408:ARG:HH11	1.84	0.42
1:A:348:ASN:HD22	1:A:348:ASN:H	1.68	0.42
1:E:355:THR:CG2	1:F:355:THR:HG21	2.50	0.42
1:F:296:HIS:CD2	2:F:501:FMN:HM73	2.55	0.42
1:A:408:ARG:HG2	1:A:408:ARG:HH11	1.85	0.41
1:E:102:VAL:HG21	1:E:241:VAL:HG23	2.03	0.41
1:E:440:LYS:HB2	6:E:631:HOH:O	2.19	0.41
1:A:123:HIS:HE1	6:A:638:HOH:O	2.03	0.41
1:C:408:ARG:HG2	1:C:408:ARG:HH11	1.85	0.41
1:D:296:HIS:CD2	2:D:501:FMN:HM73	2.55	0.41
1:D:424:ASN:O	1:D:425:LEU:HD12	2.20	0.41
1:D:102:VAL:HG21	1:D:241:VAL:HG23	2.02	0.41
1:E:296:HIS:CD2	2:E:501:FMN:HM73	2.56	0.41
1:B:408:ARG:HH11	1:B:408:ARG:HG2	1.85	0.41
1:D:348:ASN:HD22	1:D:348:ASN:H	1.69	0.41
1:E:399:MSE:H	1:F:348:ASN:ND2	2.08	0.40
1:F:423:LEU:HD12	1:F:423:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ASN:H	1:C:348:ASN:HD22	1.67	0.40
1:A:436:PRO:HG2	1:E:29:PHE:CD2	2.56	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	443/448 (99%)	430 (97%)	12 (3%)	1 (0%)	44	61
1	B	443/448 (99%)	429 (97%)	13 (3%)	1 (0%)	44	61
1	C	443/448 (99%)	429 (97%)	13 (3%)	1 (0%)	44	61
1	D	442/448 (99%)	427 (97%)	14 (3%)	1 (0%)	44	61
1	E	443/448 (99%)	429 (97%)	13 (3%)	1 (0%)	44	61
1	F	444/448 (99%)	431 (97%)	12 (3%)	1 (0%)	44	61
All	All	2658/2688 (99%)	2575 (97%)	77 (3%)	6 (0%)	44	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	ARG
1	B	331	ARG
1	C	331	ARG
1	D	331	ARG
1	E	331	ARG
1	F	331	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/360 (101%)	343 (94%)	20 (6%)	18	31
1	B	363/360 (101%)	348 (96%)	15 (4%)	26	43
1	C	363/360 (101%)	345 (95%)	18 (5%)	20	35
1	D	362/360 (101%)	344 (95%)	18 (5%)	20	35
1	E	363/360 (101%)	342 (94%)	21 (6%)	17	29
1	F	363/360 (101%)	346 (95%)	17 (5%)	22	37
All	All	2177/2160 (101%)	2068 (95%)	109 (5%)	20	35

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	6	ARG
1	A	12	LEU
1	A	50	LYS
1	A	93	ARG
1	A	95	VAL
1	A	115	LYS
1	A	116	MSE
1	A	168	ARG
1	A	279	THR
1	A	294	ARG
1	A	320	LYS
1	A	321	ASN
1	A	355	THR
1	A	364	VAL
1	A	378	VAL
1	A	408	ARG
1	A	409	ASP
1	A	438	LEU
1	A	447	LEU
1	B	3	HIS
1	B	6	ARG

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Mol	Chain	Res	Type
1	B	50	LYS
1	B	95	VAL
1	B	115	LYS
1	B	116	MSE
1	B	279	THR
1	B	294	ARG
1	B	320	LYS
1	B	321	ASN
1	B	355	THR
1	B	364	VAL
1	B	378	VAL
1	B	408	ARG
1	B	447	LEU
1	C	3	HIS
1	C	6	ARG
1	C	50	LYS
1	C	95	VAL
1	C	115	LYS
1	C	116	MSE
1	C	168	ARG
1	C	182	ARG
1	C	279	THR
1	C	294	ARG
1	C	320	LYS
1	C	321	ASN
1	C	355	THR
1	C	364	VAL
1	C	378	VAL
1	C	408	ARG
1	C	429	ARG
1	C	447	LEU
1	D	3	HIS
1	D	6	ARG
1	D	23	LYS
1	D	50	LYS
1	D	93	ARG
1	D	95	VAL
1	D	115	LYS
1	D	116	MSE
1	D	168	ARG
1	D	182	ARG
1	D	279	THR

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Mol	Chain	Res	Type
1	D	294	ARG
1	D	320	LYS
1	D	321	ASN
1	D	355	THR
1	D	364	VAL
1	D	408	ARG
1	D	428	GLU
1	E	3	HIS
1	E	6	ARG
1	E	50	LYS
1	E	93	ARG
1	E	95	VAL
1	E	115	LYS
1	E	116	MSE
1	E	168	ARG
1	E	182	ARG
1	E	279	THR
1	E	294	ARG
1	E	320	LYS
1	E	321	ASN
1	E	355	THR
1	E	364	VAL
1	E	399	MSE
1	E	403	LEU
1	E	408	ARG
1	E	429	ARG
1	E	439	ASP
1	E	447	LEU
1	F	3	HIS
1	F	6	ARG
1	F	93	ARG
1	F	95	VAL
1	F	115	LYS
1	F	116	MSE
1	F	168	ARG
1	F	279	THR
1	F	294	ARG
1	F	320	LYS
1	F	321	ASN
1	F	355	THR
1	F	364	VAL
1	F	378	VAL

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Mol	Chain	Res	Type
1	F	408	ARG
1	F	439	ASP
1	F	447	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	201	GLN
1	A	314	GLN
1	A	348	ASN
1	A	387	GLN
1	B	123	HIS
1	B	201	GLN
1	B	314	GLN
1	B	348	ASN
1	B	387	GLN
1	C	123	HIS
1	C	201	GLN
1	C	314	GLN
1	C	348	ASN
1	C	387	GLN
1	D	201	GLN
1	D	314	GLN
1	D	348	ASN
1	D	387	GLN
1	E	123	HIS
1	E	201	GLN
1	E	314	GLN
1	E	348	ASN
1	E	387	GLN
1	F	201	GLN
1	F	314	GLN
1	F	348	ASN
1	F	387	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 18 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FMN	D	501	3,4	33,33,33	1.68	7 (21%)	48,50,50	1.62	10 (20%)
2	FMN	F	501	3,4	33,33,33	1.65	5 (15%)	48,50,50	1.77	13 (27%)
2	FMN	B	501	3,4	33,33,33	1.63	6 (18%)	48,50,50	1.50	11 (22%)
2	FMN	E	501	3,4	33,33,33	1.58	5 (15%)	48,50,50	1.74	12 (25%)
2	FMN	C	501	3,4	33,33,33	1.60	6 (18%)	48,50,50	1.58	11 (22%)
2	FMN	A	501	3,4	33,33,33	1.55	5 (15%)	48,50,50	1.52	9 (18%)

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	D	501	3,4	-	4/18/18/18	0/3/3/3
2	FMN	F	501	3,4	-	2/18/18/18	0/3/3/3
2	FMN	B	501	3,4	-	0/18/18/18	0/3/3/3
2	FMN	E	501	3,4	-	0/18/18/18	0/3/3/3
2	FMN	C	501	3,4	-	0/18/18/18	0/3/3/3
2	FMN	A	501	3,4	-	0/18/18/18	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FMN	C9A-C5A	5.78	1.50	1.41
2	E	501	FMN	C9A-C5A	5.31	1.50	1.41
2	C	501	FMN	C9A-C5A	5.23	1.49	1.41
2	A	501	FMN	C9A-C5A	5.15	1.49	1.41
2	F	501	FMN	C9A-C5A	5.10	1.49	1.41
2	D	501	FMN	C9A-C5A	5.09	1.49	1.41
2	F	501	FMN	C8-C7	4.46	1.52	1.40
2	D	501	FMN	C8-C7	4.29	1.51	1.40
2	E	501	FMN	C8-C7	3.73	1.50	1.40
2	E	501	FMN	C1'-C2'	-3.61	1.47	1.52
2	B	501	FMN	C8-C7	3.25	1.49	1.40
2	F	501	FMN	C5A-N5	-3.21	1.33	1.39
2	A	501	FMN	C8-C7	3.18	1.48	1.40
2	A	501	FMN	C4-N3	-3.09	1.33	1.38
2	C	501	FMN	C4-N3	-3.02	1.33	1.38
2	C	501	FMN	C5A-N5	-2.85	1.34	1.39
2	D	501	FMN	C5A-N5	-2.68	1.34	1.39
2	D	501	FMN	C4-N3	-2.62	1.34	1.38
2	C	501	FMN	C5'-C4'	2.61	1.55	1.51
2	B	501	FMN	C5A-N5	-2.60	1.34	1.39
2	A	501	FMN	C1'-C2'	-2.56	1.49	1.52
2	F	501	FMN	C5'-C4'	2.47	1.55	1.51
2	C	501	FMN	C8-C7	2.46	1.47	1.40
2	C	501	FMN	C4A-N5	2.44	1.35	1.30
2	B	501	FMN	C4A-N5	2.43	1.35	1.30
2	F	501	FMN	C4-N3	-2.33	1.34	1.38
2	E	501	FMN	C5A-N5	-2.30	1.35	1.39
2	B	501	FMN	C4-N3	-2.24	1.34	1.38
2	D	501	FMN	C1'-C2'	-2.22	1.49	1.52
2	D	501	FMN	C4A-N5	2.17	1.35	1.30
2	E	501	FMN	C4'-C3'	-2.16	1.49	1.53
2	D	501	FMN	C6-C5A	-2.12	1.36	1.40
2	B	501	FMN	C2-N3	-2.07	1.34	1.39
2	A	501	FMN	C2-N3	-2.01	1.34	1.39

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	FMN	P-O5'-C5'	4.43	130.48	118.30
2	E	501	FMN	O4-C4-C4A	-4.04	115.89	126.60
2	E	501	FMN	O2-C2-N1	-3.92	115.33	121.83
2	E	501	FMN	O4-C4-N3	3.84	127.47	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	FMN	C7M-C7-C6	-3.66	112.72	119.49
2	A	501	FMN	C4-C4A-N5	3.32	122.96	118.23
2	D	501	FMN	C7M-C7-C6	-3.27	113.45	119.49
2	D	501	FMN	O5'-C5'-C4'	-3.22	100.76	109.36
2	C	501	FMN	O5'-P-O1P	-3.20	97.49	106.47
2	B	501	FMN	O4-C4-C4A	-3.11	118.35	126.60
2	C	501	FMN	C4-C4A-N5	3.02	122.53	118.23
2	C	501	FMN	C10-N1-C2	2.99	122.88	116.90
2	D	501	FMN	C4-C4A-N5	2.98	122.48	118.23
2	D	501	FMN	C1'-C2'-C3'	-2.92	101.64	109.79
2	C	501	FMN	C4A-C10-N10	2.91	120.73	116.48
2	A	501	FMN	C10-N1-C2	2.89	122.69	116.90
2	F	501	FMN	C4A-C10-N1	-2.87	118.07	124.73
2	A	501	FMN	C4A-C10-N1	-2.86	118.09	124.73
2	F	501	FMN	C7M-C7-C8	2.85	126.57	120.74
2	A	501	FMN	C4A-C4-N3	2.83	120.38	113.19
2	E	501	FMN	C4A-C10-N1	-2.83	118.17	124.73
2	B	501	FMN	O3P-P-O5'	-2.81	99.25	106.73
2	E	501	FMN	O3P-P-O2P	2.77	118.23	107.64
2	C	501	FMN	C4A-C10-N1	-2.75	118.35	124.73
2	A	501	FMN	C4A-C10-N10	2.74	120.49	116.48
2	F	501	FMN	C4A-C10-N10	2.74	120.48	116.48
2	D	501	FMN	O4-C4-C4A	-2.70	119.45	126.60
2	C	501	FMN	C4A-C4-N3	2.69	120.03	113.19
2	E	501	FMN	C4A-C10-N10	2.67	120.38	116.48
2	C	501	FMN	C1'-N10-C9A	2.62	124.88	120.51
2	B	501	FMN	O3P-P-O2P	2.58	117.48	107.64
2	D	501	FMN	C1'-N10-C9A	2.55	124.76	120.51
2	B	501	FMN	C1'-N10-C9A	2.52	124.71	120.51
2	D	501	FMN	P-O5'-C5'	2.49	125.16	118.30
2	C	501	FMN	O4-C4-C4A	-2.49	120.00	126.60
2	A	501	FMN	O5'-C5'-C4'	-2.46	102.81	109.36
2	F	501	FMN	O4-C4-C4A	-2.42	120.18	126.60
2	F	501	FMN	O2P-P-O1P	2.39	120.05	110.68
2	F	501	FMN	O2-C2-N1	-2.39	117.87	121.83
2	D	501	FMN	O2P-P-O1P	2.34	119.84	110.68
2	B	501	FMN	C4A-C10-N1	-2.33	119.33	124.73
2	F	501	FMN	C1'-C2'-C3'	-2.33	103.28	109.79
2	C	501	FMN	C9A-N10-C10	-2.32	117.15	120.77
2	D	501	FMN	O2-C2-N1	-2.30	118.02	121.83
2	B	501	FMN	O2-C2-N1	-2.29	118.03	121.83
2	E	501	FMN	C9A-N10-C10	-2.28	117.21	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FMN	C4-N3-C2	-2.26	121.46	125.64
2	C	501	FMN	C4-N3-C2	-2.26	121.46	125.64
2	E	501	FMN	C4-N3-C2	-2.26	121.47	125.64
2	E	501	FMN	C7M-C7-C6	-2.25	115.32	119.49
2	F	501	FMN	O4'-C4'-C5'	2.25	114.98	109.92
2	A	501	FMN	O2'-C2'-C3'	2.24	114.54	109.10
2	F	501	FMN	C10-N1-C2	2.22	121.35	116.90
2	F	501	FMN	O4'-C4'-C3'	-2.22	103.69	109.10
2	E	501	FMN	O3P-P-O5'	-2.20	100.88	106.73
2	B	501	FMN	C9A-N10-C10	-2.16	117.40	120.77
2	E	501	FMN	C7M-C7-C8	2.16	125.16	120.74
2	A	501	FMN	O4-C4-C4A	-2.15	120.89	126.60
2	B	501	FMN	C4A-C10-N10	2.14	119.61	116.48
2	C	501	FMN	O2-C2-N1	-2.14	118.29	121.83
2	B	501	FMN	C10-N1-C2	2.14	121.17	116.90
2	E	501	FMN	N3-C2-N1	2.13	123.56	119.38
2	B	501	FMN	C4A-C4-N3	2.10	118.53	113.19
2	B	501	FMN	O2'-C2'-C3'	2.04	114.06	109.10
2	F	501	FMN	O2'-C2'-C1'	2.04	114.73	109.80
2	D	501	FMN	C9-C8-C7	-2.02	116.78	119.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

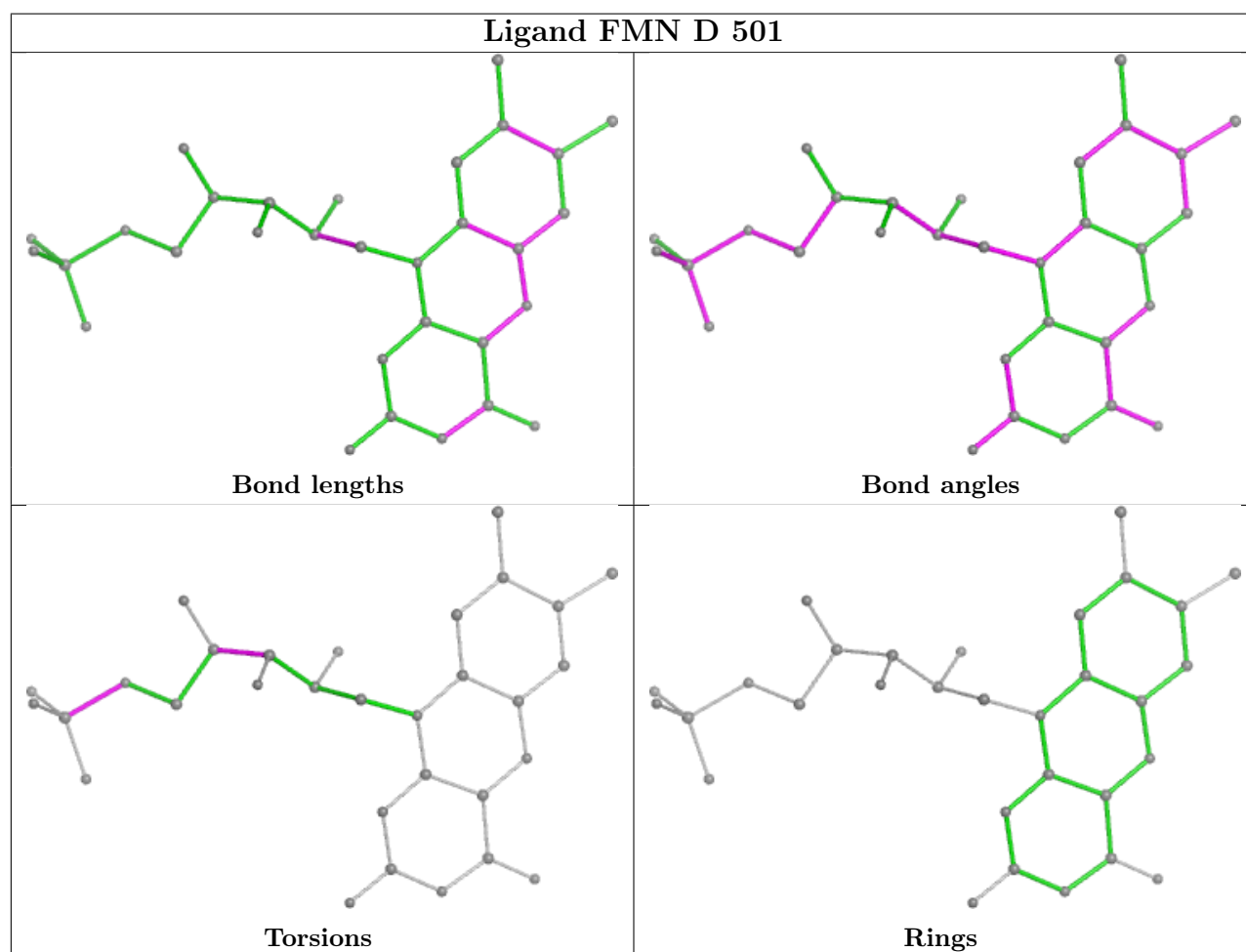
Mol	Chain	Res	Type	Atoms
2	F	501	FMN	O4'-C4'-C5'-O5'
2	D	501	FMN	C2'-C3'-C4'-O4'
2	F	501	FMN	C3'-C4'-C5'-O5'
2	D	501	FMN	C5'-O5'-P-O3P
2	D	501	FMN	C2'-C3'-C4'-C5'
2	D	501	FMN	O3'-C3'-C4'-O4'

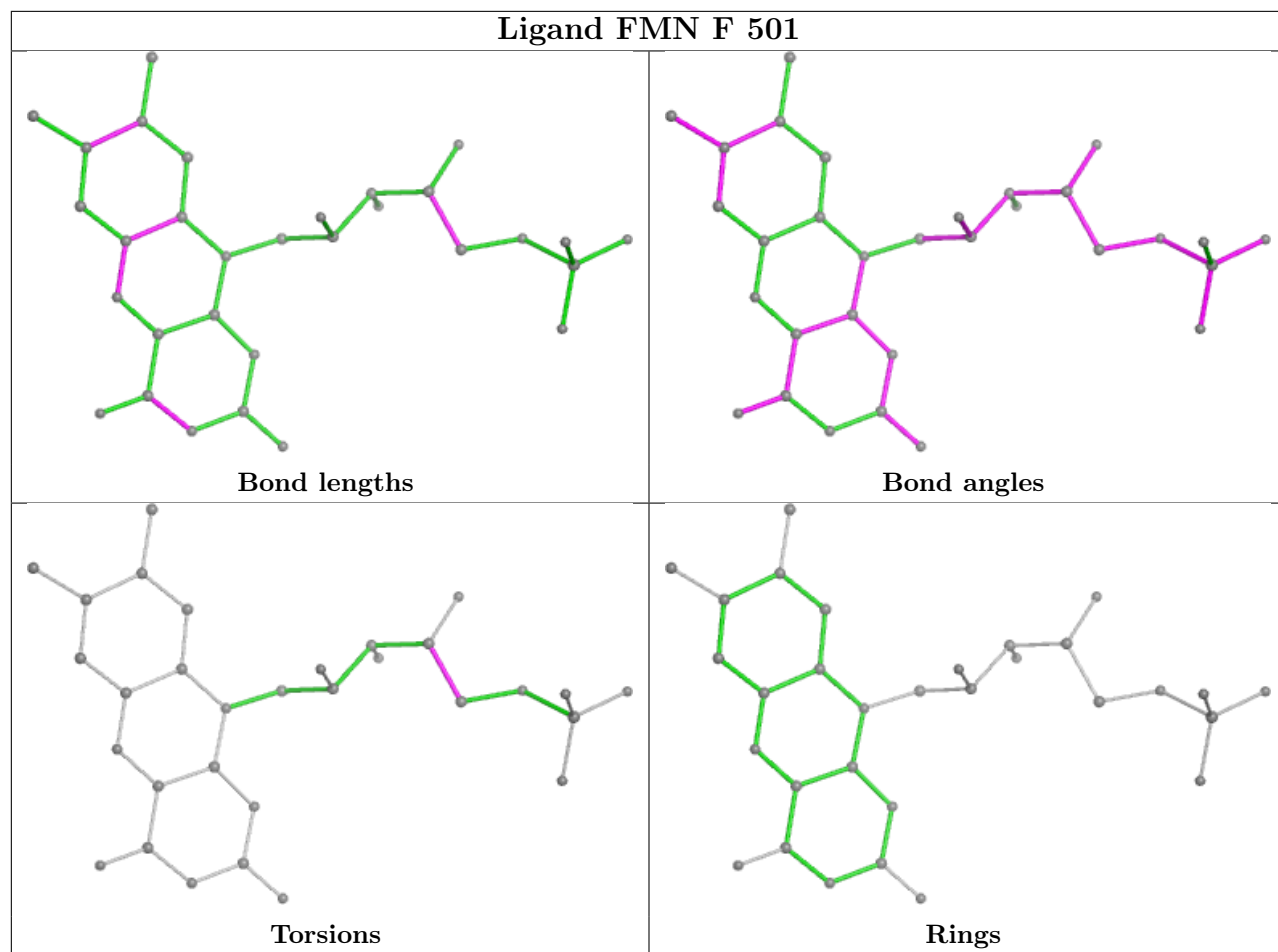
There are no ring outliers.

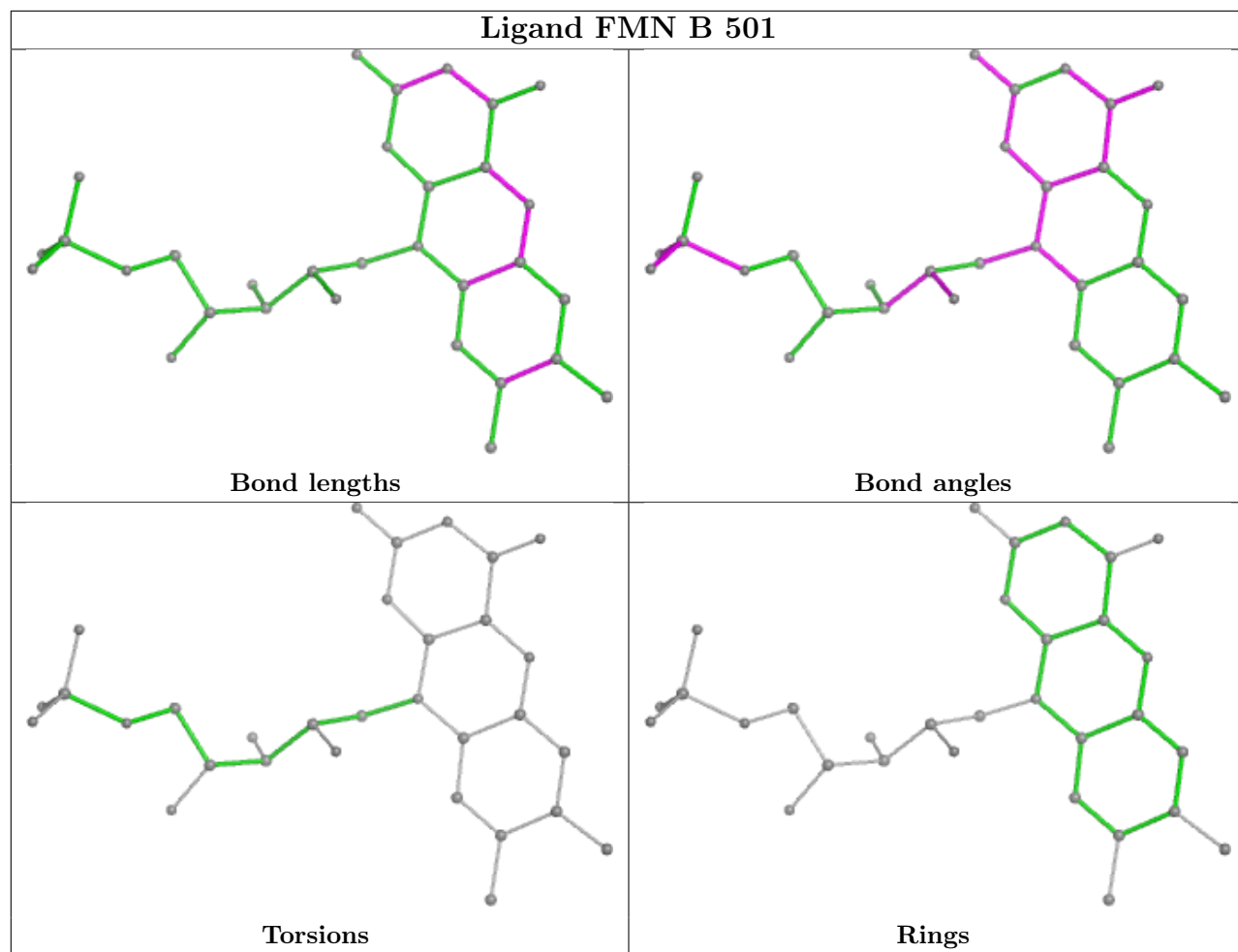
4 monomers are involved in 8 short contacts:

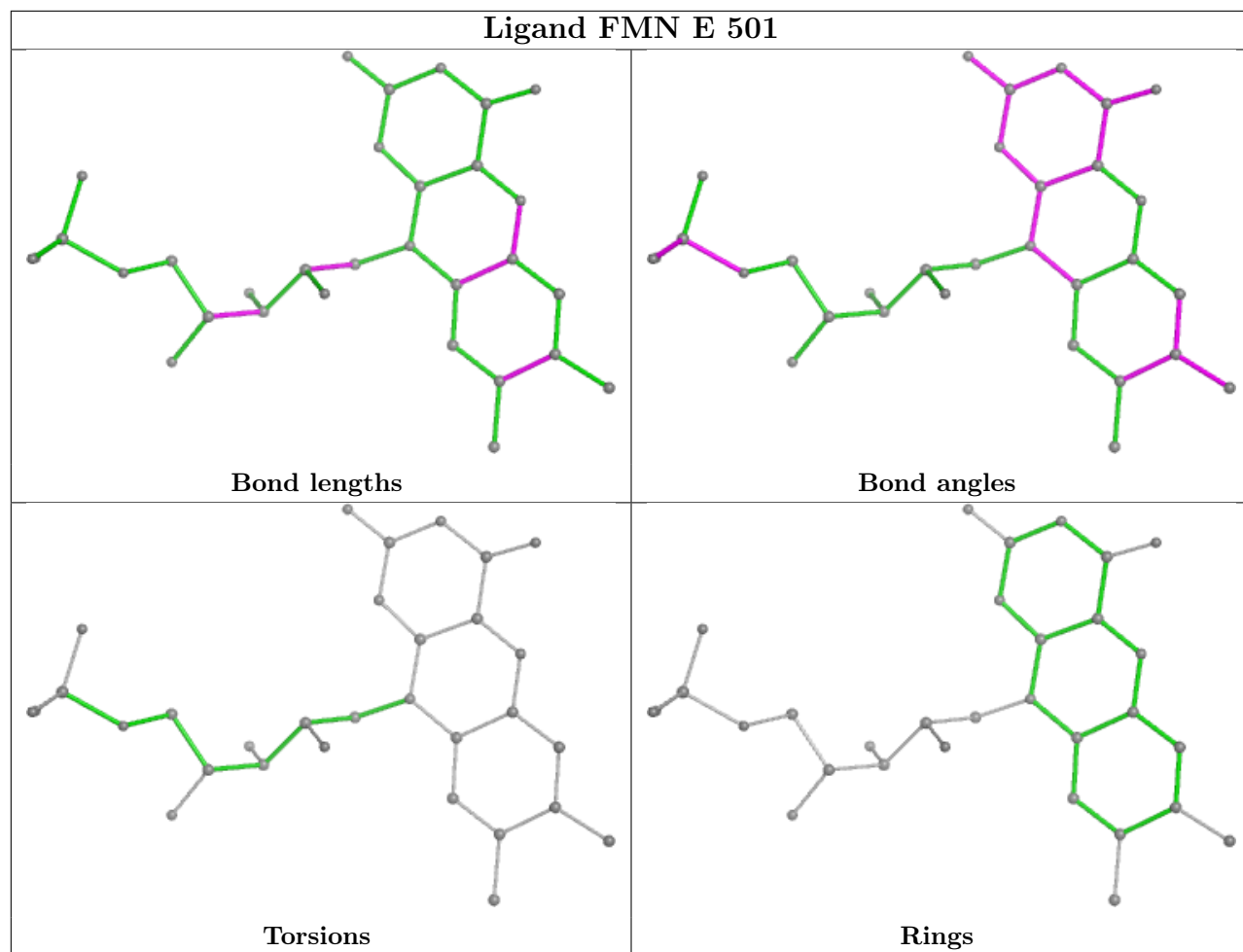
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	FMN	1	0
2	F	501	FMN	3	0
2	E	501	FMN	3	0
2	C	501	FMN	1	0

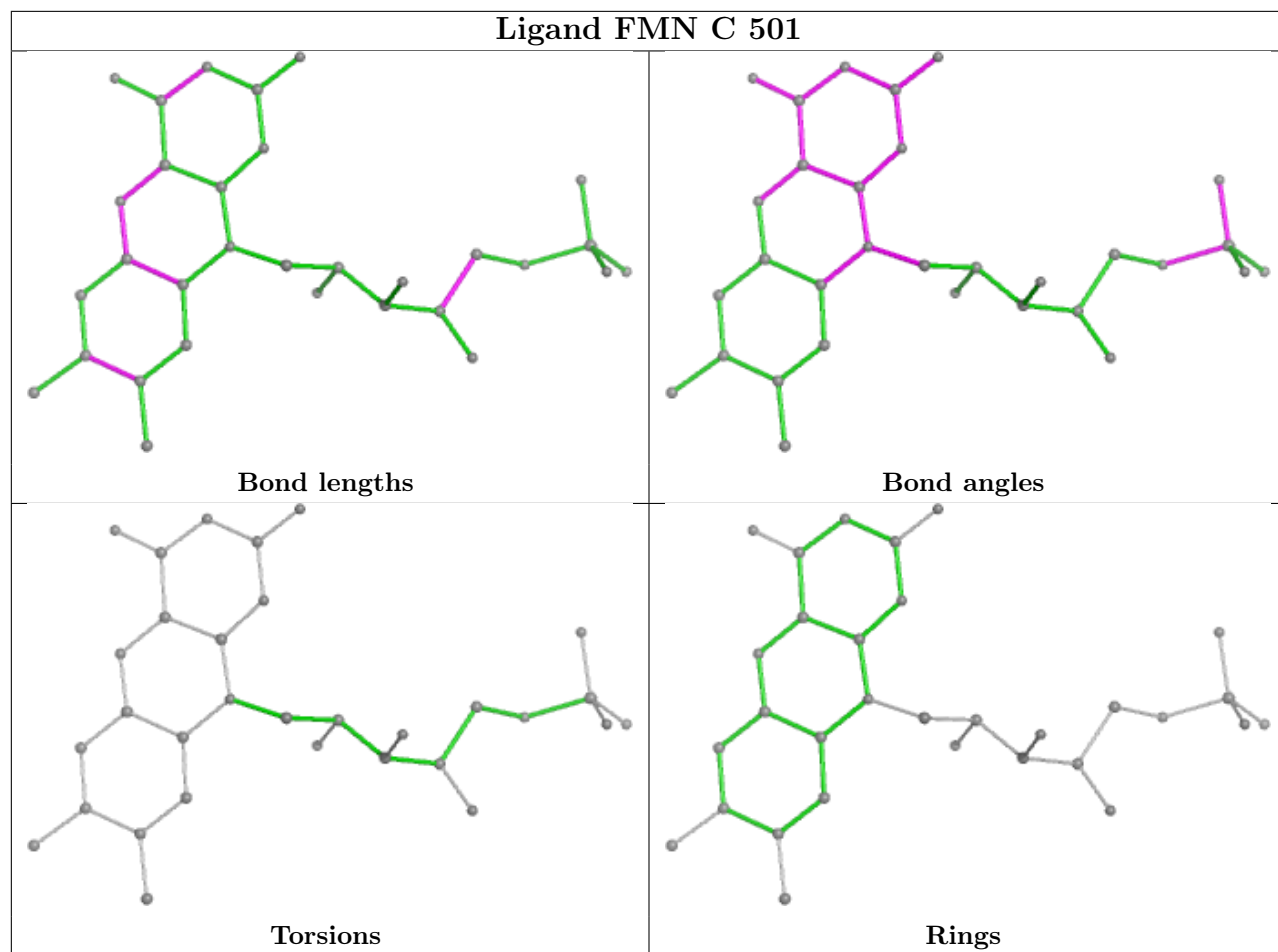
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

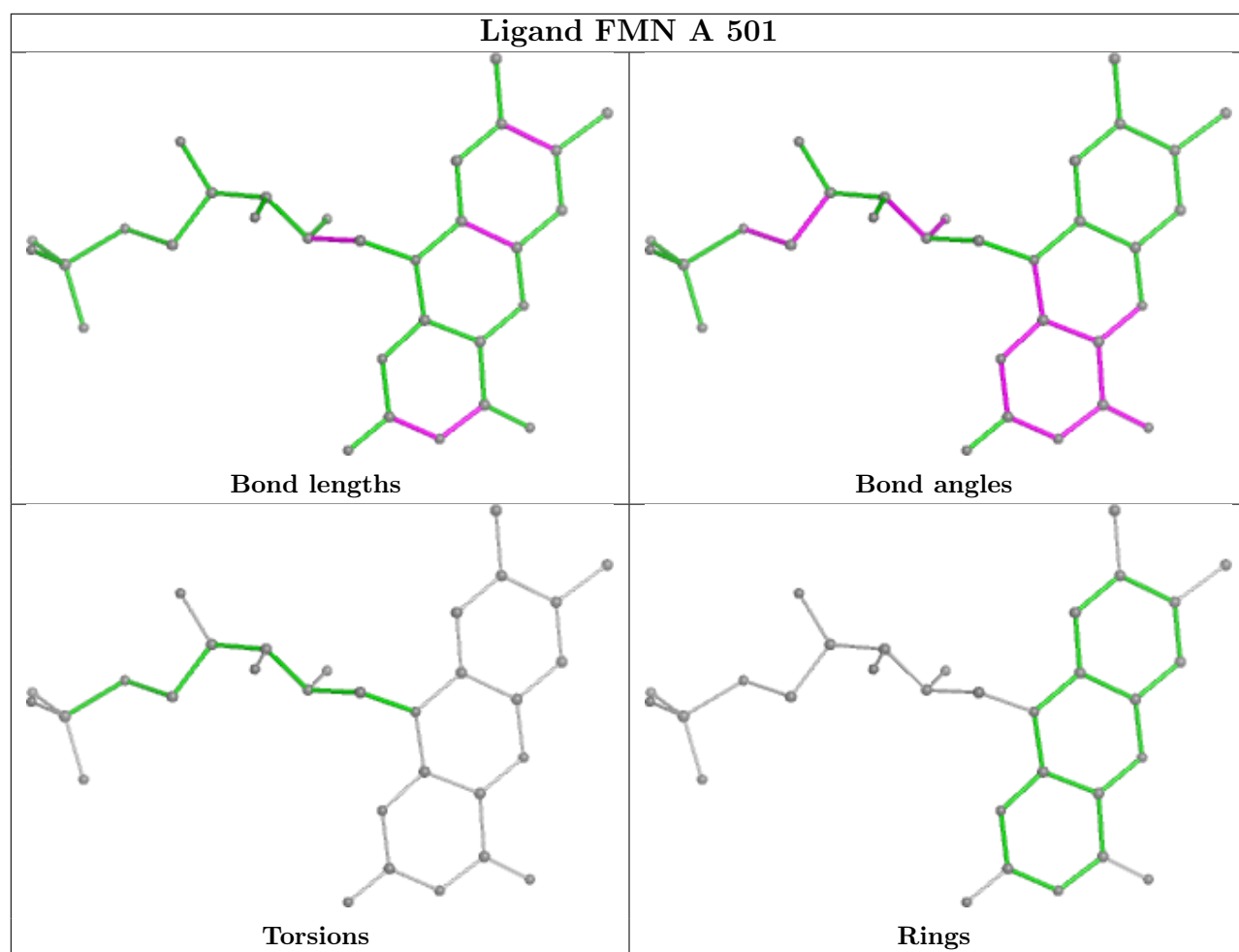












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	440/448 (98%)	-0.19	3 (0%)	84 82	27, 51, 82, 109	0
1	B	440/448 (98%)	-0.18	5 (1%)	77 75	27, 46, 76, 123	0
1	C	440/448 (98%)	-0.13	7 (1%)	70 68	29, 49, 83, 120	0
1	D	439/448 (97%)	-0.16	4 (0%)	81 79	28, 50, 84, 121	0
1	E	440/448 (98%)	0.02	4 (0%)	81 79	32, 53, 89, 136	0
1	F	441/448 (98%)	0.38	20 (4%)	39 36	33, 69, 109, 127	0
All	All	2640/2688 (98%)	-0.04	43 (1%)	70 68	27, 51, 93, 136	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	3	HIS	4.7
1	F	3	HIS	4.7
1	E	447	LEU	4.0
1	B	3	HIS	3.8
1	F	448	GLU	3.6
1	C	3	HIS	3.4
1	F	196	VAL	3.4
1	D	3	HIS	3.4
1	F	145	VAL	3.3
1	D	425	LEU	3.3
1	D	427	GLY	3.2
1	D	426	PRO	3.2
1	E	98	ASP	3.1
1	F	241	VAL	3.1
1	F	426	PRO	2.8
1	F	242	ILE	2.8
1	C	60	LEU	2.7
1	F	4	SER	2.7
1	A	3	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	427	GLY	2.6
1	B	426	PRO	2.5
1	F	107	ILE	2.5
1	A	447	LEU	2.5
1	C	425	LEU	2.5
1	C	447	LEU	2.4
1	F	247	LEU	2.4
1	B	447	LEU	2.4
1	F	253	VAL	2.3
1	E	426	PRO	2.3
1	A	92	CYS	2.3
1	F	94	LEU	2.3
1	F	184	LEU	2.3
1	F	189	ALA	2.2
1	F	91	PRO	2.2
1	C	206	LEU	2.2
1	F	265	GLY	2.2
1	F	130	TYR	2.1
1	F	427	GLY	2.1
1	F	209	ASP	2.1
1	B	4	SER	2.1
1	C	91	PRO	2.1
1	C	426	PRO	2.1
1	F	14	GLY	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 monosaccharides in this entry.

6.4 Ligands [i](#)

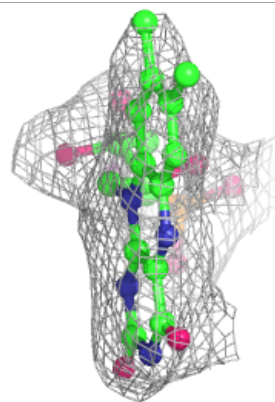
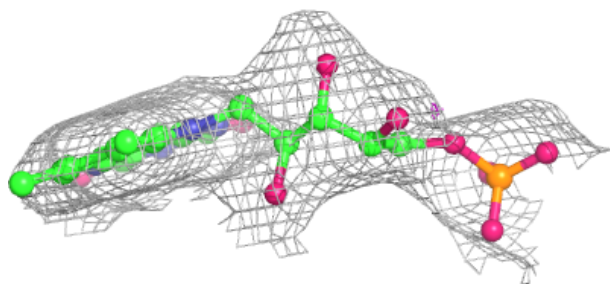
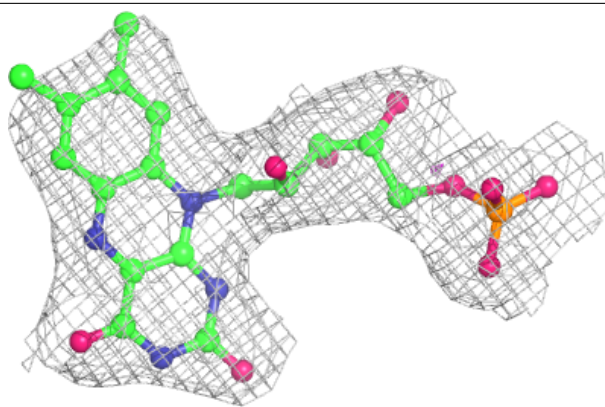
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	K	F	502	1/1	0.90	0.07	85,85,85,85	0
2	FMN	F	501	31/31	0.93	0.10	48,56,66,77	0
2	FMN	E	501	31/31	0.95	0.09	37,43,49,51	0
2	FMN	A	501	31/31	0.95	0.07	32,36,45,48	0
2	FMN	D	501	31/31	0.95	0.07	32,39,43,46	0
3	K	D	502	1/1	0.96	0.08	58,58,58,58	0
3	K	C	502	1/1	0.96	0.03	53,53,53,53	0
5	CA	A	504	1/1	0.96	0.05	56,56,56,56	0
2	FMN	C	501	31/31	0.97	0.06	34,42,45,48	0
2	FMN	B	501	31/31	0.97	0.06	31,35,41,43	0
3	K	A	502	1/1	0.97	0.04	56,56,56,56	0
3	K	B	502	1/1	0.97	0.04	44,44,44,44	0
5	CA	C	504	1/1	0.97	0.05	43,43,43,43	0
5	CA	D	504	1/1	0.97	0.05	64,64,64,64	0
3	K	E	502	1/1	0.98	0.06	46,46,46,46	0
5	CA	B	504	1/1	0.98	0.05	49,49,49,49	0
5	CA	E	504	1/1	0.98	0.05	44,44,44,44	0
5	CA	F	504	1/1	0.98	0.03	52,52,52,52	0
4	MN	C	503	1/1	0.99	0.02	42,42,42,42	0
4	MN	F	503	1/1	0.99	0.02	63,63,63,63	0
4	MN	E	503	1/1	1.00	0.01	47,47,47,47	0
4	MN	B	503	1/1	1.00	0.02	35,35,35,35	0
4	MN	A	503	1/1	1.00	0.01	45,45,45,45	0
4	MN	D	503	1/1	1.00	0.01	40,40,40,40	0

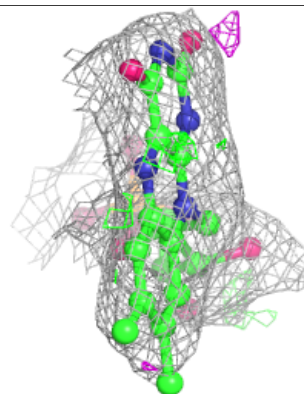
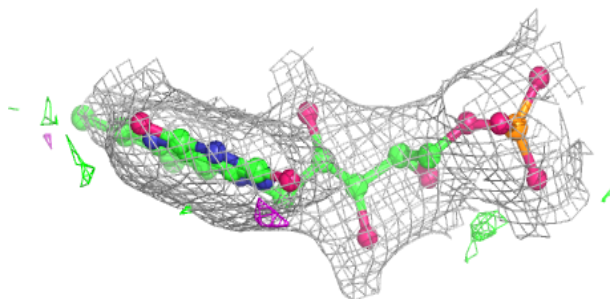
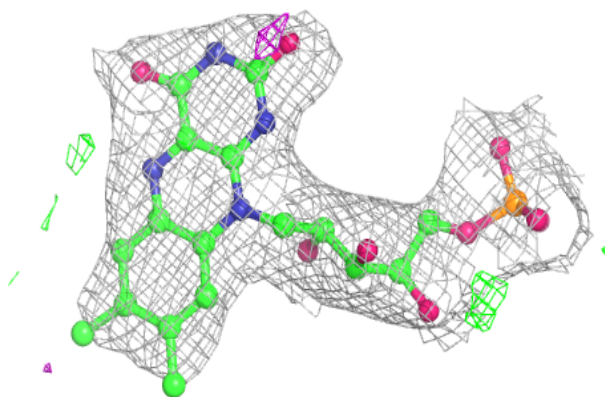
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN F 501:

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

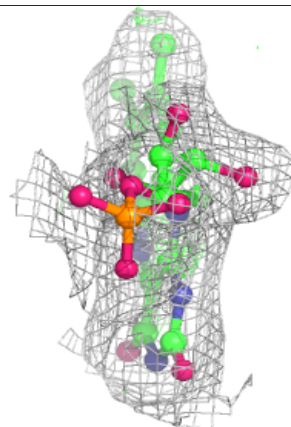
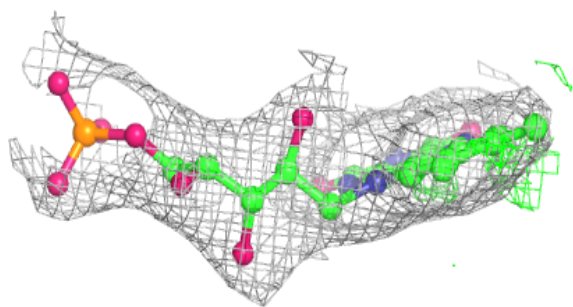
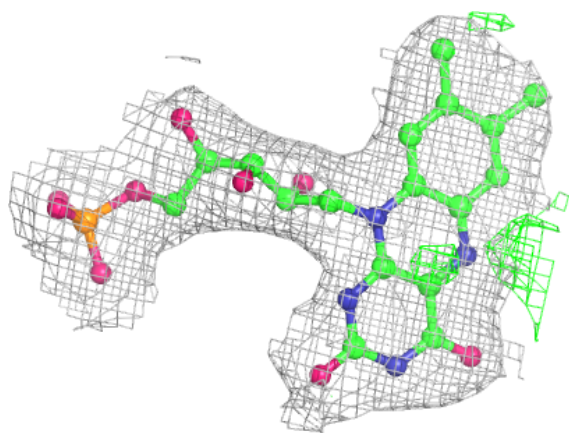
**Electron density around FMN E 501:**

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



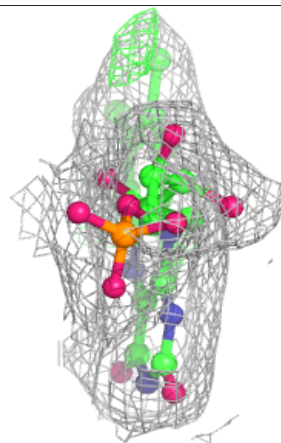
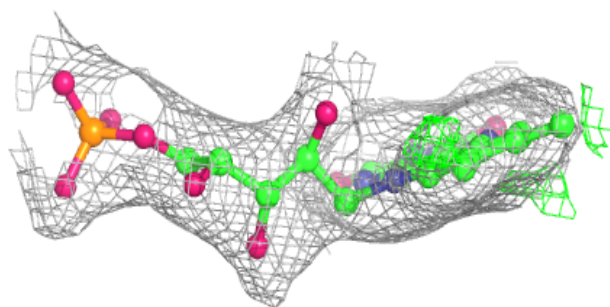
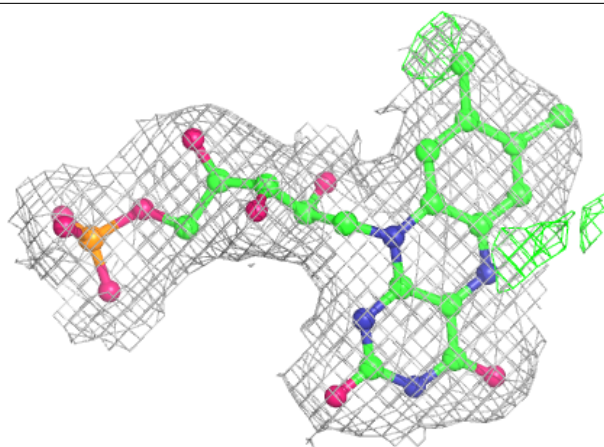
Electron density around FMN A 501:

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



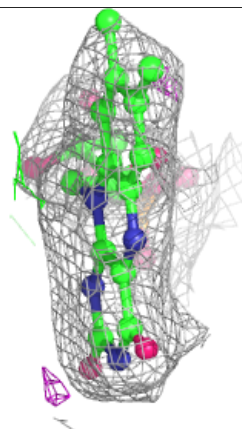
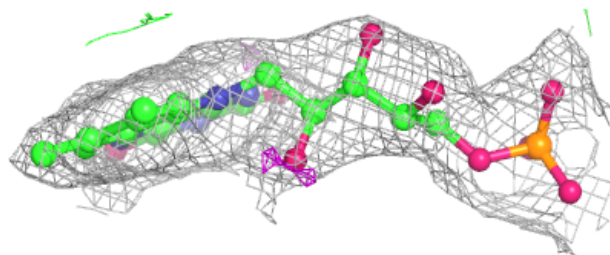
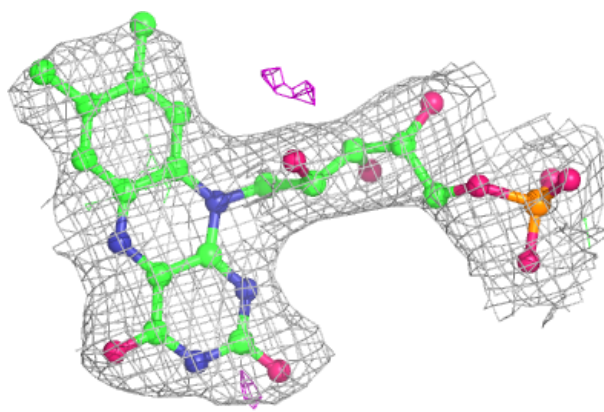
Electron density around FMN D 501:

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



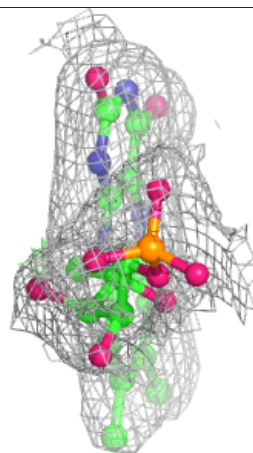
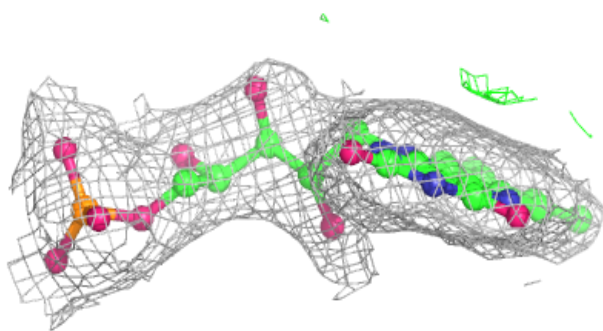
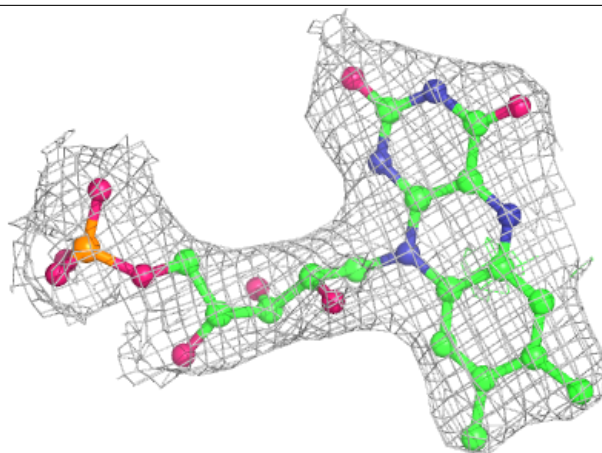
Electron density around FMN C 501:

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



Electron density around FMN B 501:

$2mF_o-DF_c$ (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.