Full wwPDB X-ray Structure Validation Report (i)

Aug 18, 2026 – 11:07 am BST

PDB ID	:	6FRM / pdb_00006frm
Title	:	Crystal Structure of coenzyme F420H2 oxidase (FprA) co-crystallized with 10 mM Tb-Xo4
Authors	:	Engilberge, S.; Riobe, F.; Wagner, T.; Di Pietro, S.; Shima, S.; Girard, E.; Dumont, E.; Maury, O.
Deposited on	:	2018-02-16
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

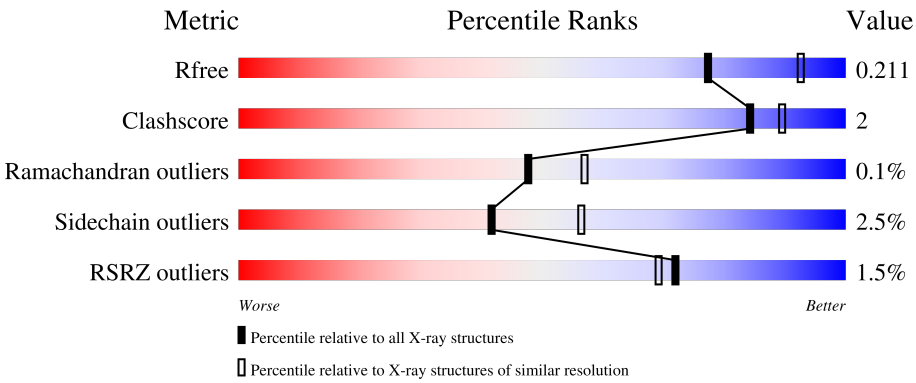
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	410	2% 89% 8% • •
1	B	410	% 86% 11% •
1	C	410	% 92% 7%
1	D	410	2% 89% 9% •

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Mol	Chain	Length	Quality of chain
1	E	410	89% 8%
1	F	410	88% 8%
1	G	410	89% 10%
1	H	410	91% 8%

2 Entry composition (i)

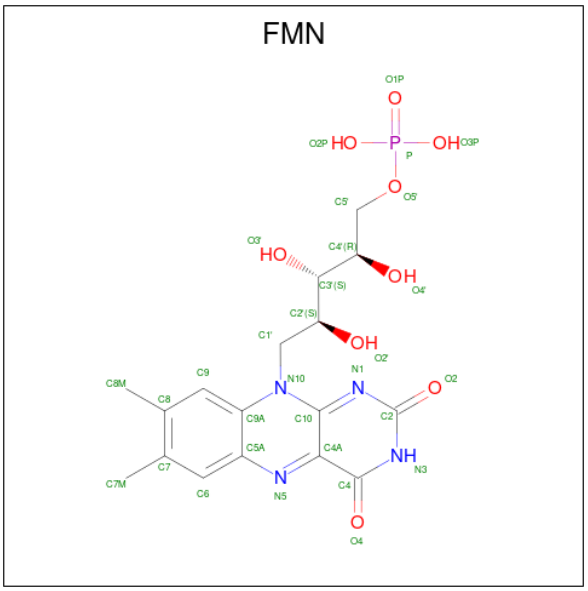
There are 7 unique types of molecules in this entry. The entry contains 27500 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Coenzyme F420H2 oxidase (FprA).

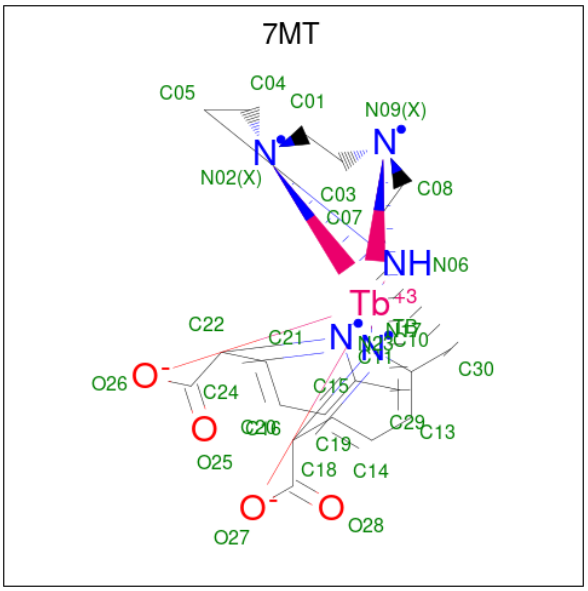
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3185	2060	513	592	20	0	1	0
1	B	400	3177	2056	512	589	20	0	1	0
1	C	408	3244	2101	523	600	20	0	2	0
1	D	403	3192	2063	514	595	20	0	1	0
1	E	397	3154	2039	509	586	20	0	2	0
1	F	395	3139	2029	508	582	20	0	2	0
1	G	408	3239	2098	522	599	20	0	1	0
1	H	409	3246	2102	523	601	20	0	1	0

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	17	4	9	1	0	0
2	B	1	31	17	4	9	1	0	0
2	C	1	31	17	4	9	1	0	0
2	D	1	31	17	4	9	1	0	0
2	E	1	31	17	4	9	1	0	0
2	F	1	31	17	4	9	1	0	0
2	G	1	31	17	4	9	1	0	0
2	H	1	31	17	4	9	1	0	0

- Molecule 3 is Tb-Xo4 (CCD ID: 7MT) (formula: $C_{20}H_{23}N_5O_4Tb$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	Tb		
3	A	1	30	20	5	4	1	0	0
			Total	C	N	O	Tb		
3	F	1	30	20	5	4	1	0	0

- Molecule 4 is TERBIUM(III) ION (CCD ID: TB) (formula: Tb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Tb		
4	A	1	1	1	0	0
			Total	Tb		
4	B	1	1	1	0	0
			Total	Tb		
4	C	2	2	2	0	0
			Total	Tb		
4	D	3	3	3	0	0
			Total	Tb		
4	E	1	1	1	0	0
			Total	Tb		
4	F	1	1	1	0	0
			Total	Tb		
4	G	3	3	3	0	0
			Total	Tb		
4	H	2	2	2	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0
5	B	2	Total Cl 2 2	0	0
5	C	2	Total Cl 2 2	0	0
5	D	2	Total Cl 2 2	0	0
5	E	3	Total Cl 3 3	0	0
5	F	3	Total Cl 3 3	0	0
5	G	1	Total Cl 1 1	0	0
5	H	2	Total Cl 2 2	0	0

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Fe 1 1	0	0
6	D	1	Total Fe 1 1	0	0
6	G	1	Total Fe 1 1	0	0
6	H	1	Total Fe 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	175	Total O 175 175	0	0
7	B	206	Total O 206 206	0	0
7	C	190	Total O 190 190	0	0
7	D	157	Total O 157 157	0	0
7	E	192	Total O 192 192	0	0
7	F	232	Total O 232 232	0	0

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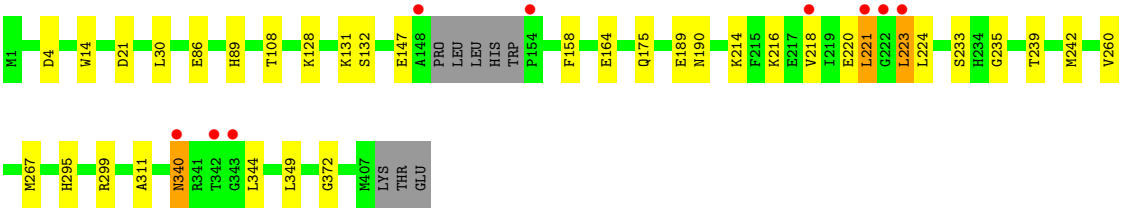
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	G	208	208	208	0	0
			Total	O		
7	H	221	221	221	0	0

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.

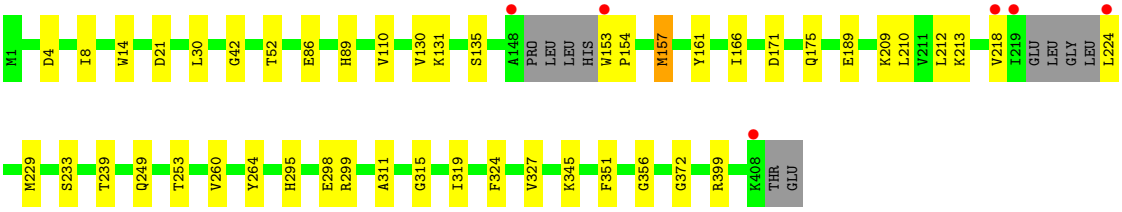
• Molecule 1: Coenzyme F420H2 oxidase (FprA)

Chain A:



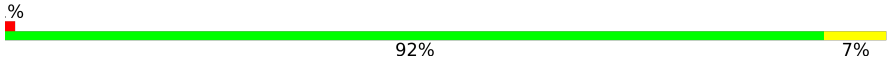
• Molecule 1: Coenzyme F420H2 oxidase (FprA)

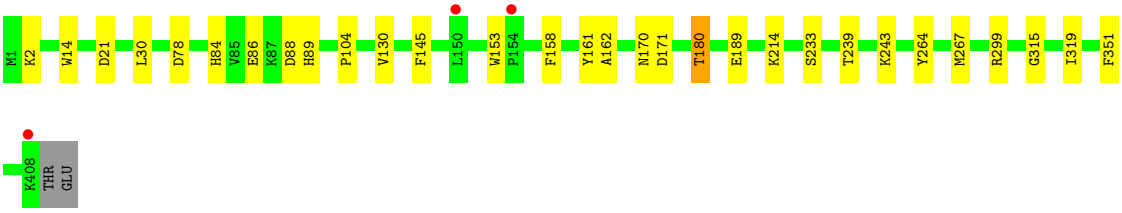
Chain B:



• Molecule 1: Coenzyme F420H2 oxidase (FprA)

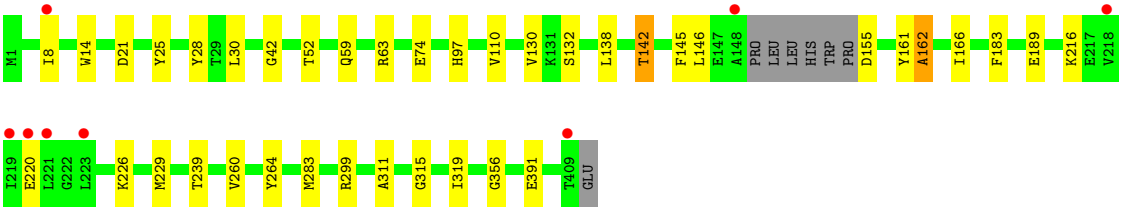
Chain C:





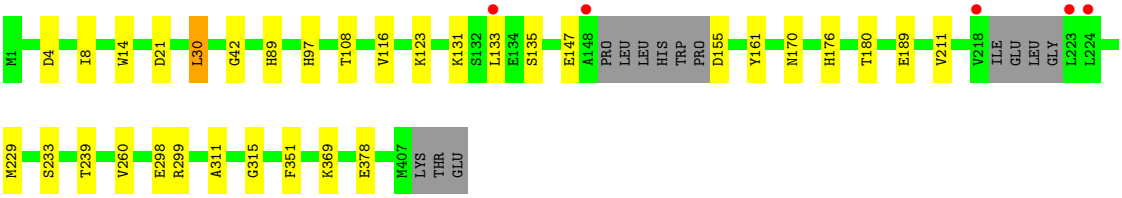
• Molecule 1: Coenzyme F420H2 oxidase (FprA)

Chain D:



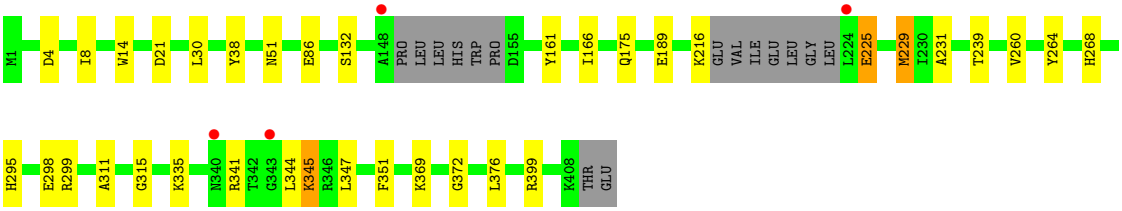
• Molecule 1: Coenzyme F420H2 oxidase (FprA)

Chain E:



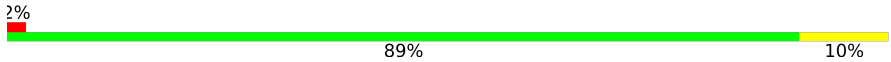
• Molecule 1: Coenzyme F420H2 oxidase (FprA)

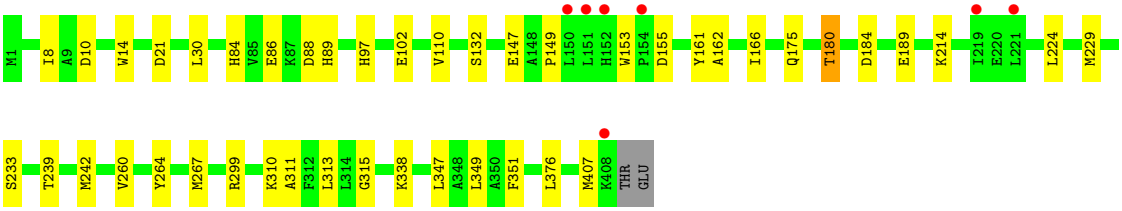
Chain F:



• Molecule 1: Coenzyme F420H2 oxidase (FprA)

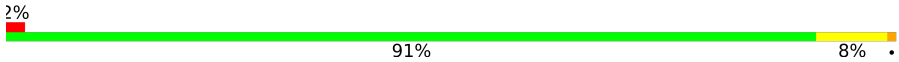
Chain G:

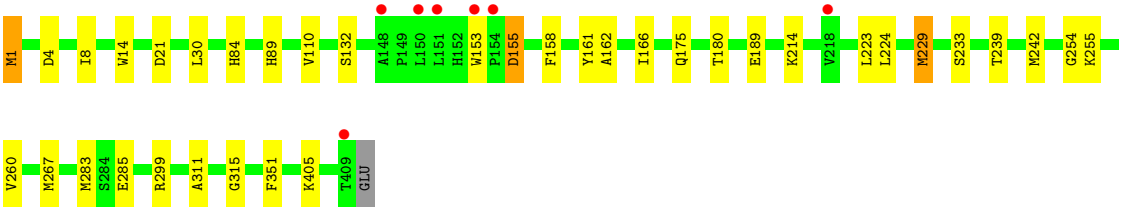




• Molecule 1: Coenzyme F420H2 oxidase (FprA)

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.17Å 147.88Å 146.06Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	48.69 – 2.20 48.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.69-2.20) 98.8 (48.69-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.177 , 0.209 0.179 , 0.211	Depositor DCC
R_{free} test set	8913 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,-l,-k 0.004 for -h,l,k 0.067 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	27500	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, CL, TB, FMN, 7MT

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	0.81	0/3261	1.30	14/4397 (0.3%)
1	B	0.84	1/3253 (0.0%)	1.27	14/4386 (0.3%)
1	C	0.82	0/3327	1.28	9/4491 (0.2%)
1	D	0.81	0/3266	1.28	10/4403 (0.2%)
1	E	0.83	0/3231	1.28	16/4355 (0.4%)
1	F	0.83	1/3216 (0.0%)	1.30	11/4333 (0.3%)
1	G	0.83	0/3319	1.29	13/4480 (0.3%)
1	H	0.85	1/3326 (0.0%)	1.28	12/4490 (0.3%)
All	All	0.83	3/26199 (0.0%)	1.28	99/35335 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	157	MET	SD-CE	-11.03	1.51	1.79
1	F	229	MET	SD-CE	-6.83	1.62	1.79
1	H	229	MET	SD-CE	-5.53	1.65	1.79

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	102	GLU	CB-CG-CD	6.63	123.87	112.60
1	F	225	GLU	N-CA-C	-6.60	104.81	112.92
1	A	21	ASP	N-CA-C	6.35	121.03	113.28
1	E	21	ASP	N-CA-C	6.27	120.93	113.28
1	A	340	ASN	CA-C-N	6.26	129.29	120.28
1	A	340	ASN	C-N-CA	6.26	129.29	120.28
1	B	21	ASP	N-CA-C	6.18	120.82	113.28
1	C	21	ASP	N-CA-C	6.10	120.73	113.28
1	G	299	ARG	N-CA-C	5.96	118.54	111.33
1	F	21	ASP	N-CA-C	5.95	120.54	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	4	ASP	CA-CB-CG	5.93	118.53	112.60
1	H	21	ASP	N-CA-C	5.89	120.46	113.28
1	C	299	ARG	N-CA-C	5.87	118.44	111.33
1	C	239	THR	N-CA-C	-5.85	106.15	113.28
1	G	21	ASP	N-CA-C	5.83	120.39	113.28
1	D	21	ASP	N-CA-C	5.81	120.37	113.28
1	A	158	PHE	CA-CB-CG	5.80	119.60	113.80
1	H	267	MET	N-CA-C	-5.79	106.26	113.55
1	E	239	THR	N-CA-C	-5.78	106.23	113.28
1	A	299	ARG	N-CA-C	5.75	118.29	111.33
1	F	299	ARG	N-CA-C	5.75	118.29	111.33
1	D	14	TRP	N-CA-C	-5.72	99.97	109.46
1	B	161	TYR	CA-C-N	5.66	128.18	120.54
1	B	161	TYR	C-N-CA	5.66	128.18	120.54
1	C	14	TRP	N-CA-C	-5.63	100.11	109.46
1	E	131	LYS	CA-C-N	5.63	132.29	121.54
1	E	131	LYS	C-N-CA	5.63	132.29	121.54
1	H	14	TRP	N-CA-C	-5.61	100.15	109.46
1	H	239	THR	N-CA-C	-5.61	106.44	113.28
1	A	14	TRP	N-CA-C	-5.59	100.18	109.46
1	B	239	THR	N-CA-C	-5.57	106.48	113.28
1	E	299	ARG	N-CA-C	5.57	118.07	111.33
1	D	299	ARG	N-CA-C	5.54	118.04	111.33
1	B	161	TYR	N-CA-C	-5.54	97.57	107.98
1	C	267	MET	N-CA-C	-5.53	106.58	113.55
1	H	299	ARG	N-CA-C	5.52	118.01	111.33
1	G	84	HIS	CA-CB-CG	5.52	119.32	113.80
1	B	52	THR	CA-C-N	5.48	128.00	120.39
1	B	52	THR	C-N-CA	5.48	128.00	120.39
1	B	298	GLU	CA-C-N	5.47	127.87	120.38
1	B	298	GLU	C-N-CA	5.47	127.87	120.38
1	F	239	THR	N-CA-C	-5.46	106.62	113.28
1	F	14	TRP	N-CA-C	-5.46	100.40	109.46
1	G	267	MET	N-CA-C	-5.43	105.71	112.93
1	F	161	TYR	N-CA-C	-5.42	97.78	107.98
1	E	161	TYR	N-CA-C	-5.41	97.80	107.98
1	E	14	TRP	N-CA-C	-5.41	100.48	109.46
1	A	131	LYS	N-CA-C	-5.40	102.46	110.46
1	B	299	ARG	N-CA-C	5.38	117.84	111.33
1	G	184	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	180	THR	N-CA-C	-5.38	105.58	111.82
1	F	161	TYR	CA-C-N	5.38	127.80	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	161	TYR	C-N-CA	5.38	127.80	120.54
1	E	161	TYR	CA-C-N	5.37	127.79	120.54
1	E	161	TYR	C-N-CA	5.37	127.79	120.54
1	B	14	TRP	N-CA-C	-5.37	100.42	108.96
1	E	211	VAL	CA-C-N	5.37	127.47	120.28
1	E	211	VAL	C-N-CA	5.37	127.47	120.28
1	A	239	THR	N-CA-C	-5.36	106.74	113.28
1	H	162	ALA	N-CA-C	5.35	117.53	111.11
1	E	4	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	42	GLY	N-CA-C	-5.28	104.55	112.89
1	H	158	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	235	GLY	CA-C-N	5.25	128.33	120.87
1	A	235	GLY	C-N-CA	5.25	128.33	120.87
1	D	239	THR	N-CA-C	-5.25	106.87	113.28
1	G	180	THR	N-CA-C	-5.24	105.74	111.82
1	G	161	TYR	N-CA-C	-5.23	98.15	107.98
1	E	298	GLU	CA-C-N	5.20	127.51	120.38
1	E	298	GLU	C-N-CA	5.20	127.51	120.38
1	C	162	ALA	N-CA-C	5.20	117.35	111.11
1	A	267	MET	N-CA-C	-5.19	106.03	112.93
1	G	239	THR	N-CA-C	-5.18	106.96	113.28
1	D	162	ALA	N-CA-C	5.17	117.31	111.11
1	G	14	TRP	N-CA-C	-5.17	100.89	109.46
1	C	161	TYR	N-CA-C	-5.13	98.33	107.98
1	F	4	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	161	TYR	N-CA-C	-5.12	98.36	107.98
1	D	52	THR	CA-C-N	5.11	127.50	120.39
1	D	52	THR	C-N-CA	5.11	127.50	120.39
1	H	180	THR	N-CA-C	-5.10	105.90	111.82
1	C	158	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	223	LEU	CA-C-N	5.08	127.35	120.38
1	A	223	LEU	C-N-CA	5.08	127.35	120.38
1	H	161	TYR	N-CA-C	-5.08	98.43	107.98
1	B	171	ASP	N-CA-C	5.07	117.54	111.71
1	G	161	TYR	CA-C-N	5.07	127.38	120.54
1	G	161	TYR	C-N-CA	5.07	127.38	120.54
1	B	4	ASP	CA-CB-CG	5.06	117.66	112.60
1	F	298	GLU	CA-C-N	5.05	127.30	120.38
1	F	298	GLU	C-N-CA	5.05	127.30	120.38
1	A	4	ASP	CA-CB-CG	5.04	117.64	112.60
1	E	42	GLY	N-CA-C	-5.03	104.95	112.89
1	H	161	TYR	CA-C-N	5.01	127.30	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	161	TYR	C-N-CA	5.01	127.30	120.54
1	E	180	THR	N-CA-C	-5.01	106.01	111.82
1	G	162	ALA	N-CA-C	5.00	117.12	111.11
1	D	161	TYR	CA-C-N	5.00	127.29	120.54
1	D	161	TYR	C-N-CA	5.00	127.29	120.54

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	3185	0	3179	7	0
1	B	3177	0	3168	16	0
1	C	3244	0	3243	19	0
1	D	3192	0	3190	19	0
1	E	3154	0	3145	11	0
1	F	3139	0	3132	12	0
1	G	3239	0	3237	19	0
1	H	3246	0	3244	19	0
2	A	31	0	19	0	0
2	B	31	0	19	4	0
2	C	31	0	19	1	0
2	D	31	0	19	2	0
2	E	31	0	19	1	0
2	F	31	0	19	2	0
2	G	31	0	19	0	0
2	H	31	0	19	0	0
3	A	30	0	0	0	0
3	F	30	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	3	0	0	0	0
4	H	2	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	1	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	F	3	0	0	1	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	175	0	0	0	0
7	B	206	0	0	1	0
7	C	190	0	0	0	0
7	D	157	0	0	1	0
7	E	192	0	0	3	0
7	F	232	0	0	3	0
7	G	208	0	0	1	0
7	H	221	0	0	2	0
All	All	27500	0	25690	118	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 (118) 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:340:ASN:HB3	1:A:372:GLY:HA3	1.53	0.88
1:C:86:GLU:HG2	1:C:88:ASP:OD1	1.82	0.80
1:B:212:LEU:HD21	1:B:253:THR:HG23	1.69	0.73
1:D:8:ILE:CG2	1:D:229:MET:HE1	2.20	0.72
1:C:130:VAL:HG21	1:C:145:PHE:CD2	2.25	0.71
1:D:142:THR:HG22	1:D:162:ALA:HB3	1.72	0.71
1:H:224:LEU:HG	1:H:242:MET:HE1	1.75	0.69
1:A:224:LEU:HG	1:A:242:MET:HE1	1.76	0.67
1:B:110:VAL:HG11	1:B:154:PRO:HB2	1.78	0.66
1:H:285:GLU:HB3	1:H:405:LYS:NZ	2.11	0.66
1:G:224:LEU:HG	1:G:242:MET:HE1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:HIS:CE1	1:C:233:SER:HB2	2.32	0.65
1:F:8:ILE:HD12	1:F:229:MET:HE1	1.80	0.64
1:C:189:GLU:HG3	1:C:243:LYS:HZ3	1.62	0.64
1:G:8:ILE:HD12	1:G:229:MET:HE1	1.79	0.64
1:B:399:ARG:NH1	5:B:503:CL:CL	2.69	0.63
1:H:84:HIS:HE1	1:H:153:TRP:HB2	1.64	0.62
1:B:8:ILE:HD12	1:B:229:MET:HE1	1.80	0.62
1:H:8:ILE:HD12	1:H:229:MET:HE1	1.83	0.60
1:D:8:ILE:HG22	1:D:229:MET:HE1	1.83	0.60
1:D:130:VAL:HG21	1:D:145:PHE:CD2	2.37	0.60
1:A:218:VAL:HA	1:A:221:LEU:HD23	1.84	0.60
1:G:89:HIS:CE1	1:G:233:SER:HB2	2.36	0.59
1:C:84:HIS:HE1	1:C:153:TRP:HB2	1.68	0.59
1:H:84:HIS:CE1	1:H:153:TRP:HB2	2.36	0.59
1:G:86:GLU:HG2	1:G:88:ASP:OD1	2.03	0.58
1:C:84:HIS:CE1	1:C:153:TRP:HB2	2.38	0.58
1:A:218:VAL:HG13	1:A:223:LEU:HB3	1.86	0.58
1:E:30:LEU:HD12	1:E:176:HIS:HB3	1.86	0.57
1:D:97:HIS:HD2	7:D:1503:HOH:O	1.86	0.57
1:G:310:LYS:HD3	1:G:407:MET:HG3	1.85	0.57
1:E:170:ASN:HB3	7:E:648:HOH:O	2.04	0.56
1:E:8:ILE:HD12	1:E:229:MET:HE1	1.87	0.56
1:H:110:VAL:HG12	7:H:748:HOH:O	2.05	0.55
1:C:189:GLU:HG3	1:C:243:LYS:NZ	2.20	0.55
1:B:130:VAL:HB	1:B:157:MET:HE1	1.87	0.55
1:B:212:LEU:HD21	1:B:253:THR:CG2	2.36	0.55
1:G:97:HIS:HD2	7:G:614:HOH:O	1.89	0.54
1:H:285:GLU:HB3	1:H:405:LYS:HZ1	1.71	0.54
2:B:501:FMN:H9	1:C:153:TRP:CZ2	2.43	0.54
1:F:345:LYS:HG3	1:F:372:GLY:O	2.10	0.52
1:D:110:VAL:HG13	1:D:155:ASP:HA	1.91	0.52
1:F:166:ILE:HG23	1:F:229:MET:HE2	1.91	0.52
1:A:89:HIS:CE1	1:A:233:SER:HB2	2.45	0.52
1:C:170:ASN:ND2	1:C:171:ASP:H	2.07	0.51
1:D:166:ILE:HG23	1:D:229:MET:HE2	1.92	0.50
1:H:254:GLY:HA2	7:H:613:HOH:O	2.11	0.49
2:B:501:FMN:H9	1:C:153:TRP:HZ2	1.77	0.49
1:G:166:ILE:HG23	1:G:229:MET:HE2	1.95	0.49
1:D:8:ILE:HD12	1:D:183:PHE:CZ	2.48	0.48
1:B:166:ILE:HG23	1:B:229:MET:HE2	1.94	0.48
1:A:260:VAL:HG22	1:A:311:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:HIS:HE1	1:G:86:GLU:OE2	1.96	0.48
1:D:216:LYS:O	1:D:220:GLU:HG2	2.13	0.48
1:F:399:ARG:NH1	5:F:504:CL:CL	2.84	0.48
1:F:260:VAL:HG22	1:F:311:ALA:HB3	1.95	0.48
7:F:611:HOH:O	1:G:338:LYS:HE3	2.14	0.47
1:E:260:VAL:HG22	1:E:311:ALA:HB3	1.95	0.47
1:H:260:VAL:HG22	1:H:311:ALA:HB3	1.96	0.46
1:G:260:VAL:HG22	1:G:311:ALA:HB3	1.97	0.46
1:H:166:ILE:HG23	1:H:229:MET:HE2	1.97	0.46
1:B:260:VAL:HG22	1:B:311:ALA:HB3	1.97	0.45
1:D:260:VAL:HG22	1:D:311:ALA:HB3	1.97	0.45
2:F:502:FMN:H9	1:G:153:TRP:CZ2	2.52	0.45
1:B:345:LYS:HD2	1:B:372:GLY:O	2.17	0.45
1:C:84:HIS:HE1	1:C:153:TRP:CG	2.35	0.45
1:D:42:GLY:HA3	1:D:138:LEU:HB3	1.98	0.44
1:H:84:HIS:HE1	1:H:153:TRP:CG	2.36	0.44
1:C:170:ASN:HD22	1:C:171:ASP:H	1.66	0.43
1:G:147:GLU:C	1:G:149:PRO:HD3	2.43	0.43
1:C:180:THR:HG22	1:D:283:MET:SD	2.59	0.43
1:H:110:VAL:HG13	1:H:155:ASP:HA	1.99	0.43
1:A:108:THR:HG22	1:A:147:GLU:HG2	2.00	0.43
1:H:84:HIS:HE1	1:H:153:TRP:CB	2.31	0.43
1:G:315:GLY:HA2	1:G:351:PHE:O	2.19	0.43
1:C:315:GLY:HA2	1:C:351:PHE:O	2.17	0.43
1:B:315:GLY:HA2	1:B:351:PHE:O	2.19	0.43
1:C:2:LYS:HD2	1:D:391:GLU:HG3	2.01	0.43
1:B:356:GLY:N	2:B:501:FMN:O2	2.50	0.43
1:E:97:HIS:HD2	7:E:602:HOH:O	2.02	0.43
1:H:285:GLU:HB3	1:H:405:LYS:HZ2	1.80	0.43
1:H:315:GLY:HA2	1:H:351:PHE:O	2.19	0.42
1:E:89:HIS:CE1	1:E:233:SER:HB2	2.54	0.42
2:F:502:FMN:H9	1:G:153:TRP:HZ2	1.84	0.42
1:C:78:ASP:O	1:C:104:PRO:HD2	2.18	0.42
1:H:89:HIS:CE1	1:H:233:SER:HB2	2.54	0.42
1:B:324:PHE:O	1:B:327:VAL:HG22	2.19	0.42
1:F:315:GLY:HA2	1:F:351:PHE:O	2.19	0.42
1:E:369:LYS:HG2	7:E:722:HOH:O	2.17	0.42
1:B:110:VAL:HG12	7:B:654:HOH:O	2.18	0.42
1:B:89:HIS:CE1	1:B:233:SER:HB2	2.55	0.41
1:C:319:ILE:HG13	2:C:501:FMN:C6	2.50	0.41
1:E:8:ILE:HD12	1:E:229:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ILE:HG13	2:D:501:FMN:C6	2.50	0.41
1:E:116:VAL:HG13	1:E:123:LYS:HG3	2.01	0.41
1:E:108:THR:HG22	1:E:147:GLU:HG3	2.01	0.41
1:B:319:ILE:HG13	2:B:501:FMN:C6	2.50	0.41
1:D:59:GLN:O	1:D:63:ARG:HG3	2.19	0.41
1:D:142:THR:CG2	1:D:162:ALA:HB3	2.43	0.41
1:G:110:VAL:HG13	1:G:155:ASP:HA	2.03	0.41
1:C:84:HIS:HE1	1:C:153:TRP:CB	2.33	0.41
1:D:356:GLY:N	2:D:501:FMN:O2	2.51	0.41
2:E:501:FMN:H9	1:H:153:TRP:CZ2	2.56	0.41
1:C:264:TYR:HA	1:C:315:GLY:O	2.19	0.41
1:F:38:TYR:CZ	1:F:231:ALA:HB1	2.56	0.41
1:F:335:LYS:HD2	7:F:806:HOH:O	2.20	0.41
1:G:264:TYR:CD1	1:G:264:TYR:C	2.98	0.41
1:B:264:TYR:HA	1:B:315:GLY:O	2.21	0.40
1:F:264:TYR:HA	1:F:315:GLY:O	2.21	0.40
1:G:313:LEU:HG	1:G:349:LEU:HB2	2.03	0.40
1:H:1:MET:HE2	1:H:1:MET:HB2	1.99	0.40
1:D:25:TYR:O	1:D:28:TYR:HB3	2.21	0.40
1:D:264:TYR:HA	1:D:315:GLY:O	2.21	0.40
1:E:315:GLY:HA2	1:E:351:PHE:O	2.20	0.40
1:F:347:LEU:HD13	1:F:376:LEU:HD11	2.04	0.40
1:G:180:THR:HG22	1:H:283:MET:SD	2.62	0.40
1:G:347:LEU:HD13	1:G:376:LEU:HD11	2.02	0.40
1:F:369:LYS:HG2	7:F:732:HOH:O	2.20	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	399/410 (97%)	390 (98%)	9 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	395/410 (96%)	385 (98%)	10 (2%)	0	100	100
1	C	408/410 (100%)	398 (98%)	10 (2%)	0	100	100
1	D	400/410 (98%)	391 (98%)	9 (2%)	0	100	100
1	E	393/410 (96%)	384 (98%)	9 (2%)	0	100	100
1	F	391/410 (95%)	381 (97%)	8 (2%)	2 (0%)	24	27
1	G	407/410 (99%)	396 (97%)	11 (3%)	0	100	100
1	H	408/410 (100%)	399 (98%)	9 (2%)	0	100	100
All	All	3201/3280 (98%)	3124 (98%)	75 (2%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	132	SER
1	F	51	ASN

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	341/348 (98%)	325 (95%)	16 (5%)	23	31
1	B	340/348 (98%)	326 (96%)	14 (4%)	27	37
1	C	348/348 (100%)	346 (99%)	2 (1%)	78	89
1	D	342/348 (98%)	335 (98%)	7 (2%)	48	64
1	E	338/348 (97%)	332 (98%)	6 (2%)	51	68
1	F	336/348 (97%)	325 (97%)	11 (3%)	33	45
1	G	347/348 (100%)	341 (98%)	6 (2%)	53	69
1	H	348/348 (100%)	339 (97%)	9 (3%)	40	55
All	All	2740/2784 (98%)	2669 (97%)	71 (3%)	42	55

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	86	GLU
1	A	128	LYS
1	A	132	SER
1	A	164	GLU
1	A	175	GLN
1	A	189	GLU
1	A	190	ASN
1	A	214	LYS
1	A	216	LYS
1	A	220	GLU
1	A	221	LEU
1	A	295[A]	HIS
1	A	295[B]	HIS
1	A	344	LEU
1	A	349	LEU
1	B	30	LEU
1	B	86	GLU
1	B	131	LYS
1	B	135	SER
1	B	153	TRP
1	B	175	GLN
1	B	189	GLU
1	B	209	LYS
1	B	210	LEU
1	B	213	LYS
1	B	218	VAL
1	B	224	LEU
1	B	249	GLN
1	B	295	HIS
1	C	30	LEU
1	C	214	LYS
1	D	30	LEU
1	D	74	GLU
1	D	132	SER
1	D	142	THR
1	D	146	LEU
1	D	189	GLU
1	D	226	LYS
1	E	30	LEU
1	E	133	LEU
1	E	135	SER
1	E	155	ASP

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Mol	Chain	Res	Type
1	E	189	GLU
1	E	378	GLU
1	F	30	LEU
1	F	86	GLU
1	F	175	GLN
1	F	189	GLU
1	F	216	LYS
1	F	225	GLU
1	F	295[A]	HIS
1	F	295[B]	HIS
1	F	341	ARG
1	F	344	LEU
1	F	345	LYS
1	G	10	ASP
1	G	30	LEU
1	G	132	SER
1	G	175	GLN
1	G	189	GLU
1	G	214	LYS
1	H	1	MET
1	H	30	LEU
1	H	132	SER
1	H	155	ASP
1	H	175	GLN
1	H	189	GLU
1	H	214	LYS
1	H	223	LEU
1	H	255	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	196	ASN
1	B	84	HIS
1	B	196	ASN
1	B	249	GLN
1	C	84	HIS
1	C	89	HIS
1	C	118	HIS
1	C	170	ASN
1	C	196	ASN

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Mol	Chain	Res	Type
1	C	249	GLN
1	D	89	HIS
1	D	118	HIS
1	D	249	GLN
1	D	272	GLN
1	E	196	ASN
1	E	249	GLN
1	F	249	GLN
1	F	268	HIS
1	G	83	ASN
1	G	84	HIS
1	G	196	ASN
1	G	249	GLN
1	H	84	HIS
1	H	89	HIS
1	H	249	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 35 are monoatomic - leaving 10 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	C	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.21	6 (12%)
2	FMN	E	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.21	6 (12%)
2	FMN	A	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.21	6 (12%)
2	FMN	G	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.21	6 (12%)
2	FMN	D	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.21	6 (12%)
2	FMN	F	502	-	33,33,33	1.43	4 (12%)	48,50,50	1.21	6 (12%)
2	FMN	B	501	-	33,33,33	1.44	4 (12%)	48,50,50	1.21	6 (12%)
2	FMN	H	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.22	6 (12%)
3	7MT	A	502	1	31,38,38	2.25	7 (22%)	29,76,76	1.99	7 (24%)
3	7MT	F	501	1	31,38,38	1.84	7 (22%)	29,76,76	1.99	7 (24%)

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	C	501	-	-	4/18/18/18	0/3/3/3
2	FMN	E	501	-	-	5/18/18/18	0/3/3/3
2	FMN	A	501	-	-	3/18/18/18	0/3/3/3
2	FMN	G	501	-	-	2/18/18/18	0/3/3/3
2	FMN	D	501	-	-	4/18/18/18	0/3/3/3
2	FMN	F	502	-	-	6/18/18/18	0/3/3/3
2	FMN	B	501	-	-	6/18/18/18	0/3/3/3
2	FMN	H	501	-	-	5/18/18/18	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	7MT	TB-N17	9.24	2.63	2.50
3	F	501	7MT	TB-N17	5.79	2.58	2.50
2	E	501	FMN	C9A-C5A	5.08	1.49	1.41
2	D	501	FMN	C9A-C5A	5.06	1.49	1.41
2	B	501	FMN	C9A-C5A	5.06	1.49	1.41
2	A	501	FMN	C9A-C5A	5.05	1.49	1.41
2	F	502	FMN	C9A-C5A	5.05	1.49	1.41
2	G	501	FMN	C9A-C5A	5.04	1.49	1.41
2	C	501	FMN	C9A-C5A	5.03	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	FMN	C9A-C5A	5.00	1.49	1.41
3	A	502	7MT	C30-C10	3.56	1.55	1.49
3	F	501	7MT	C30-C10	3.54	1.55	1.49
3	A	502	7MT	C29-C11	3.38	1.55	1.49
3	F	501	7MT	C29-C11	3.33	1.55	1.49
2	G	501	FMN	C8-C7	3.33	1.49	1.40
2	H	501	FMN	C8-C7	3.33	1.49	1.40
2	D	501	FMN	C8-C7	3.32	1.49	1.40
2	C	501	FMN	C8-C7	3.31	1.49	1.40
2	B	501	FMN	C8-C7	3.31	1.49	1.40
2	A	501	FMN	C8-C7	3.31	1.49	1.40
2	F	502	FMN	C8-C7	3.29	1.49	1.40
2	E	501	FMN	C8-C7	3.29	1.49	1.40
3	A	502	7MT	C04-N02	-2.98	1.45	1.49
3	F	501	7MT	C04-N02	-2.95	1.45	1.49
2	E	501	FMN	C4A-N5	2.53	1.35	1.30
2	F	502	FMN	C4A-N5	2.53	1.35	1.30
2	C	501	FMN	C4A-N5	2.51	1.35	1.30
2	G	501	FMN	C4A-N5	2.50	1.35	1.30
2	A	501	FMN	C4A-N5	2.50	1.35	1.30
2	H	501	FMN	C4A-N5	2.49	1.35	1.30
2	B	501	FMN	C4A-N5	2.49	1.35	1.30
2	D	501	FMN	C4A-N5	2.48	1.35	1.30
2	B	501	FMN	C4-N3	-2.47	1.34	1.38
2	A	501	FMN	C4-N3	-2.45	1.34	1.38
2	G	501	FMN	C4-N3	-2.44	1.34	1.38
2	F	502	FMN	C4-N3	-2.44	1.34	1.38
2	D	501	FMN	C4-N3	-2.44	1.34	1.38
2	H	501	FMN	C4-N3	-2.44	1.34	1.38
2	C	501	FMN	C4-N3	-2.43	1.34	1.38
2	E	501	FMN	C4-N3	-2.42	1.34	1.38
3	F	501	7MT	O28-C18	2.29	1.26	1.21
3	A	502	7MT	O28-C18	2.28	1.26	1.21
3	A	502	7MT	O25-C24	2.22	1.26	1.21
3	F	501	7MT	O25-C24	2.19	1.26	1.21
3	F	501	7MT	C16-C18	2.09	1.53	1.49
3	A	502	7MT	C16-C18	2.04	1.53	1.49

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	501	7MT	C05-C04-N02	-4.74	109.12	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	7MT	C05-C04-N02	-4.72	109.14	112.86
3	F	501	7MT	C07-C08-N09	-4.41	109.38	112.86
3	A	502	7MT	C07-C08-N09	-4.38	109.40	112.86
3	A	502	7MT	C03-C01-N02	-4.19	109.55	112.86
3	F	501	7MT	C03-C01-N02	-4.13	109.60	112.86
3	A	502	7MT	C01-C03-N09	-4.02	109.68	112.86
3	F	501	7MT	C01-C03-N09	-4.01	109.69	112.86
3	F	501	7MT	O27-C18-O28	-2.95	119.97	125.24
3	A	502	7MT	O27-C18-O28	-2.94	120.00	125.24
3	A	502	7MT	O26-C24-O25	-2.94	120.00	125.24
3	F	501	7MT	O26-C24-O25	-2.91	120.06	125.24
2	B	501	FMN	C4-C4A-N5	2.75	122.14	118.23
2	H	501	FMN	C4-C4A-N5	2.73	122.12	118.23
2	D	501	FMN	C4-C4A-N5	2.73	122.12	118.23
2	E	501	FMN	C4-C4A-N5	2.73	122.11	118.23
2	C	501	FMN	C4-C4A-N5	2.72	122.10	118.23
2	G	501	FMN	C4-C4A-N5	2.70	122.08	118.23
2	F	502	FMN	C4-C4A-N5	2.70	122.07	118.23
2	A	501	FMN	C4-C4A-N5	2.69	122.06	118.23
2	E	501	FMN	C4A-C10-N1	-2.66	118.57	124.73
2	A	501	FMN	C4A-C10-N1	-2.65	118.57	124.73
2	F	502	FMN	C4A-C10-N1	-2.65	118.58	124.73
2	D	501	FMN	C4A-C10-N1	-2.64	118.60	124.73
2	G	501	FMN	C4A-C10-N1	-2.64	118.60	124.73
2	B	501	FMN	C4A-C10-N1	-2.64	118.61	124.73
2	C	501	FMN	C4A-C10-N1	-2.64	118.61	124.73
2	H	501	FMN	C4A-C10-N1	-2.63	118.62	124.73
3	F	501	7MT	C13-C10-N17	-2.27	120.52	124.20
3	A	502	7MT	C13-C10-N17	-2.26	120.54	124.20
2	E	501	FMN	C10-N1-C2	2.25	121.40	116.90
2	G	501	FMN	C10-N1-C2	2.24	121.39	116.90
2	B	501	FMN	C10-N1-C2	2.24	121.38	116.90
2	D	501	FMN	C10-N1-C2	2.24	121.38	116.90
2	A	501	FMN	C10-N1-C2	2.24	121.38	116.90
2	F	502	FMN	C10-N1-C2	2.23	121.37	116.90
2	C	501	FMN	C10-N1-C2	2.23	121.36	116.90
2	H	501	FMN	C10-N1-C2	2.22	121.34	116.90
2	B	501	FMN	O4-C4-C4A	-2.21	120.73	126.60
2	E	501	FMN	O4-C4-C4A	-2.20	120.77	126.60
2	D	501	FMN	O4-C4-C4A	-2.20	120.77	126.60
2	H	501	FMN	O4-C4-C4A	-2.19	120.78	126.60
2	F	502	FMN	O4-C4-C4A	-2.19	120.79	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	501	FMN	O4-C4-C4A	-2.19	120.80	126.60
2	A	501	FMN	O4-C4-C4A	-2.18	120.81	126.60
2	C	501	FMN	O4-C4-C4A	-2.18	120.82	126.60
2	D	501	FMN	C4A-C4-N3	2.08	118.47	113.19
2	H	501	FMN	C4A-C4-N3	2.08	118.47	113.19
2	B	501	FMN	C4A-C4-N3	2.07	118.44	113.19
2	E	501	FMN	C4A-C4-N3	2.06	118.43	113.19
2	F	502	FMN	C4A-C4-N3	2.06	118.43	113.19
2	B	501	FMN	C4A-C10-N10	2.06	119.49	116.48
2	G	501	FMN	C4A-C4-N3	2.06	118.42	113.19
2	G	501	FMN	C4A-C10-N10	2.06	119.49	116.48
2	H	501	FMN	C4A-C10-N10	2.05	119.48	116.48
2	A	501	FMN	C4A-C4-N3	2.05	118.41	113.19
2	C	501	FMN	C4A-C4-N3	2.05	118.40	113.19
2	E	501	FMN	C4A-C10-N10	2.05	119.47	116.48
2	F	502	FMN	C4A-C10-N10	2.05	119.47	116.48
2	A	501	FMN	C4A-C10-N10	2.04	119.46	116.48
2	C	501	FMN	C4A-C10-N10	2.04	119.46	116.48
2	D	501	FMN	C4A-C10-N10	2.00	119.41	116.48

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	FMN	C5'-O5'-P-O1P
2	C	501	FMN	C5'-O5'-P-O1P
2	E	501	FMN	C5'-O5'-P-O1P
2	F	502	FMN	C5'-O5'-P-O1P
2	H	501	FMN	C5'-O5'-P-O1P
2	B	501	FMN	C2'-C3'-C4'-O4'
2	F	502	FMN	C2'-C3'-C4'-O4'
2	B	501	FMN	O3'-C3'-C4'-O4'
2	D	501	FMN	C2'-C3'-C4'-O4'
2	E	501	FMN	C2'-C3'-C4'-O4'
2	A	501	FMN	C2'-C3'-C4'-O4'
2	H	501	FMN	C2'-C3'-C4'-O4'
2	B	501	FMN	C2'-C3'-C4'-C5'
2	D	501	FMN	C2'-C3'-C4'-C5'
2	E	501	FMN	C2'-C3'-C4'-C5'
2	F	502	FMN	C2'-C3'-C4'-C5'
2	F	502	FMN	O3'-C3'-C4'-O4'
2	A	501	FMN	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
2	H	501	FMN	C2'-C3'-C4'-C5'
2	B	501	FMN	C5'-O5'-P-O2P
2	D	501	FMN	O3'-C3'-C4'-O4'
2	C	501	FMN	C2'-C3'-C4'-O4'
2	A	501	FMN	O3'-C3'-C4'-O4'
2	E	501	FMN	O3'-C3'-C4'-O4'
2	H	501	FMN	O3'-C3'-C4'-O4'
2	G	501	FMN	C2'-C3'-C4'-O4'
2	B	501	FMN	O3'-C3'-C4'-C5'
2	C	501	FMN	O3'-C3'-C4'-O4'
2	C	501	FMN	C5'-O5'-P-O2P
2	E	501	FMN	C5'-O5'-P-O2P
2	F	502	FMN	C5'-O5'-P-O2P
2	H	501	FMN	C5'-O5'-P-O2P
2	F	502	FMN	O3'-C3'-C4'-C5'
2	G	501	FMN	O3'-C3'-C4'-O4'
2	D	501	FMN	O3'-C3'-C4'-C5'

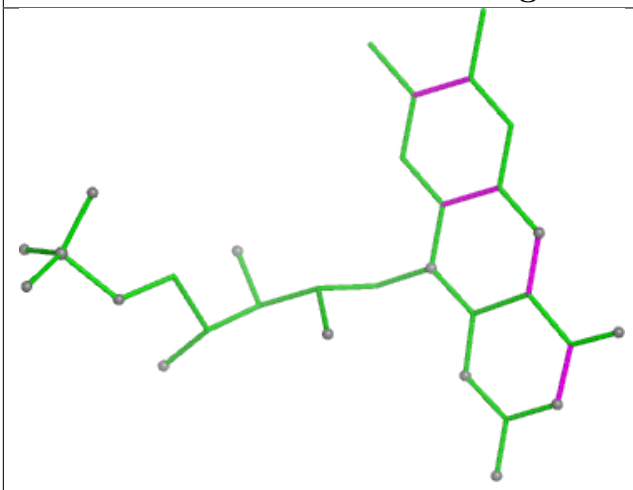
There are no ring outliers.

5 monomers are involved in 10 short contacts:

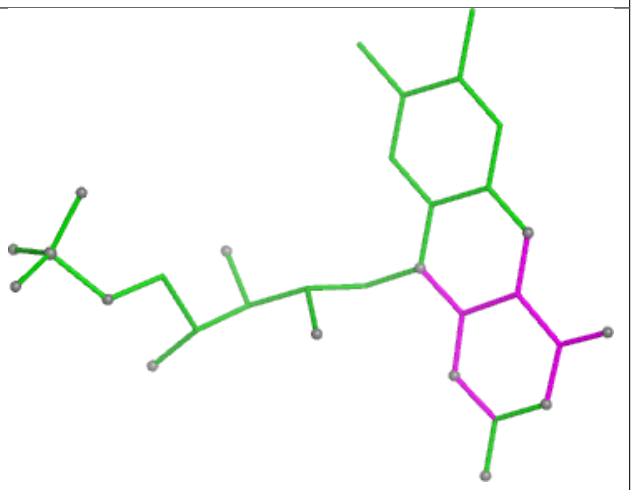
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	FMN	1	0
2	E	501	FMN	1	0
2	D	501	FMN	2	0
2	F	502	FMN	2	0
2	B	501	FMN	4	0

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.

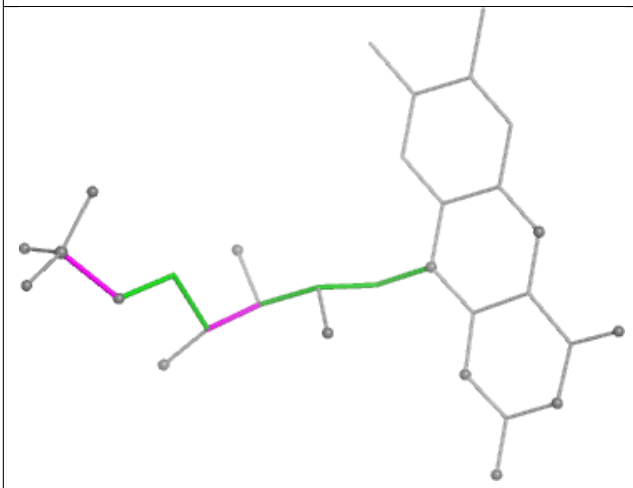
Ligand FMN C 501



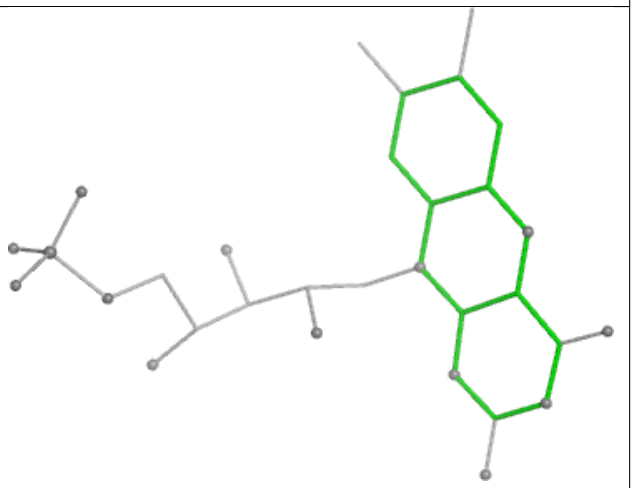
Bond lengths



Bond angles

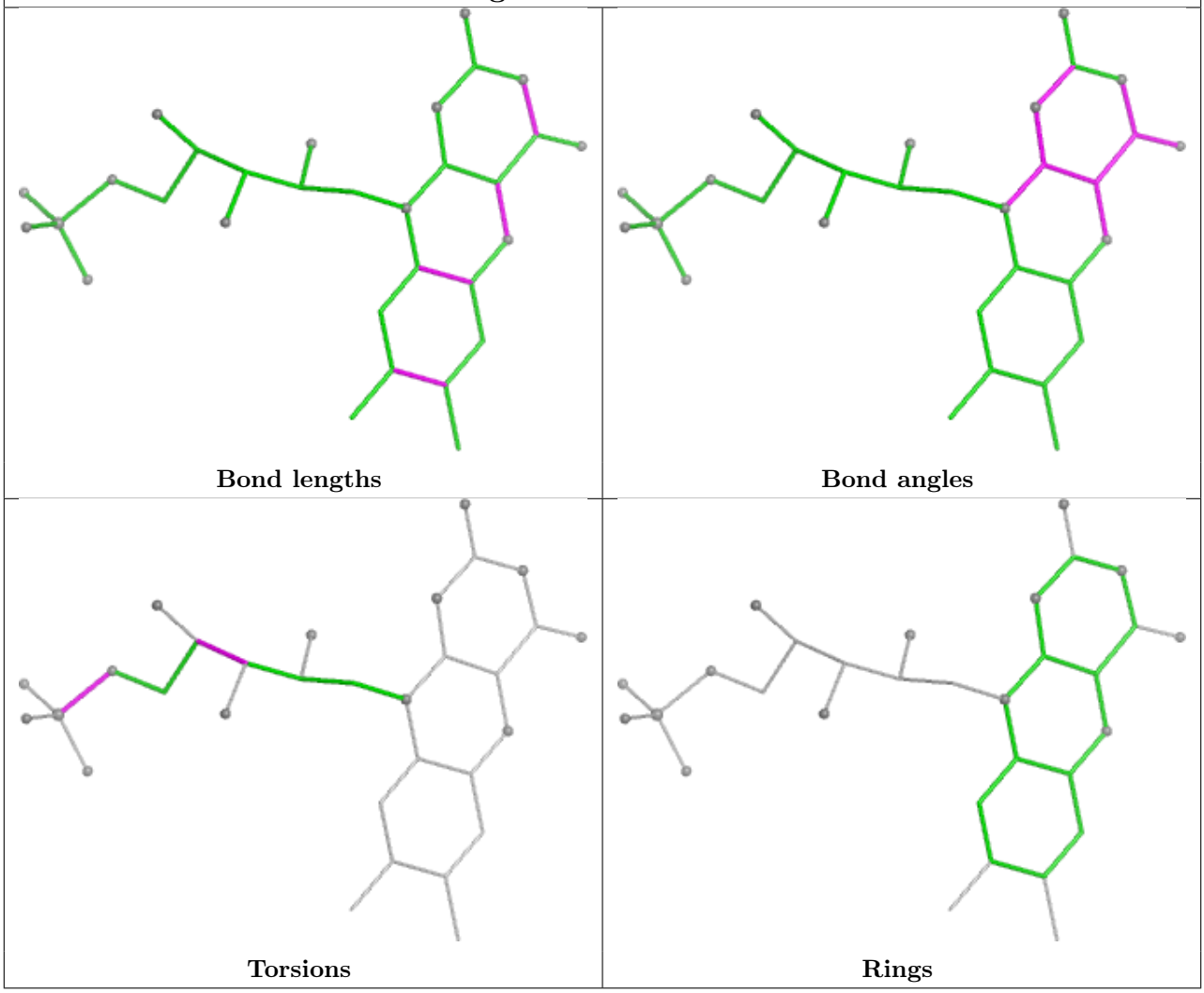


Torsions

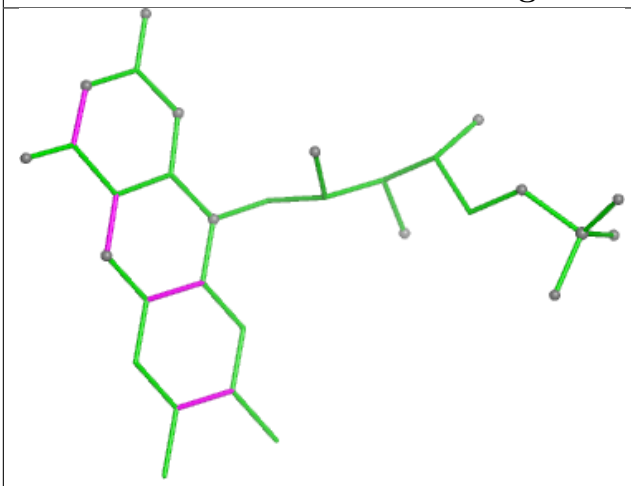


Rings

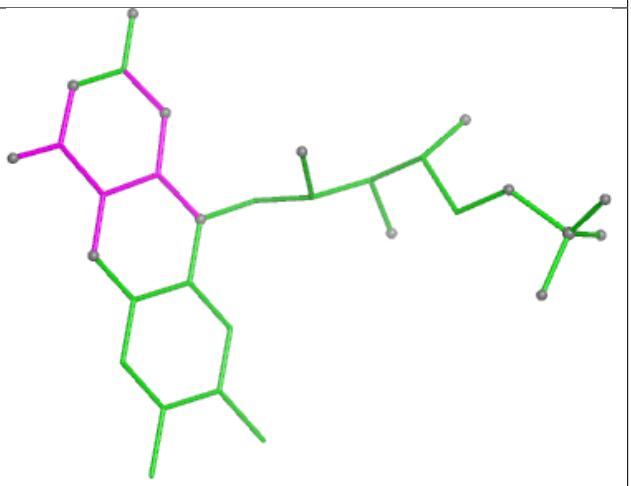
Ligand FMN E 501



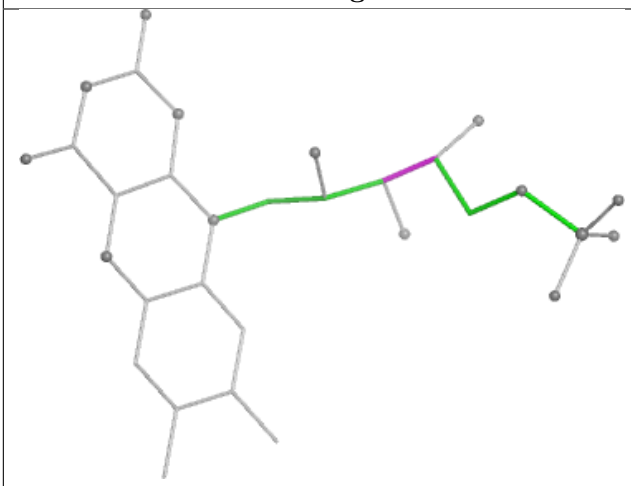
Ligand FMN A 501



Bond lengths



Bond angles



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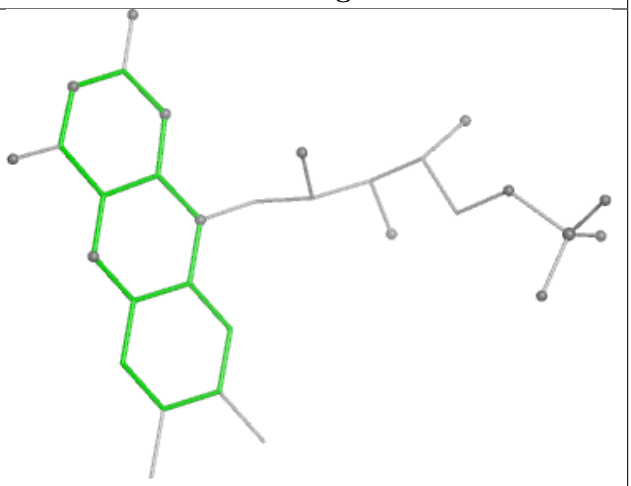
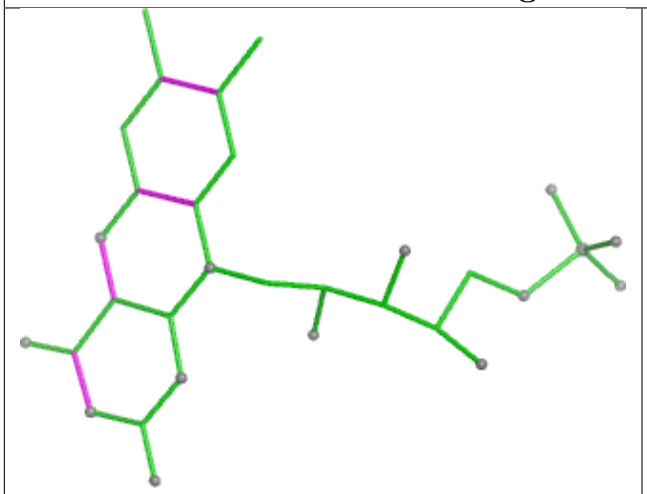
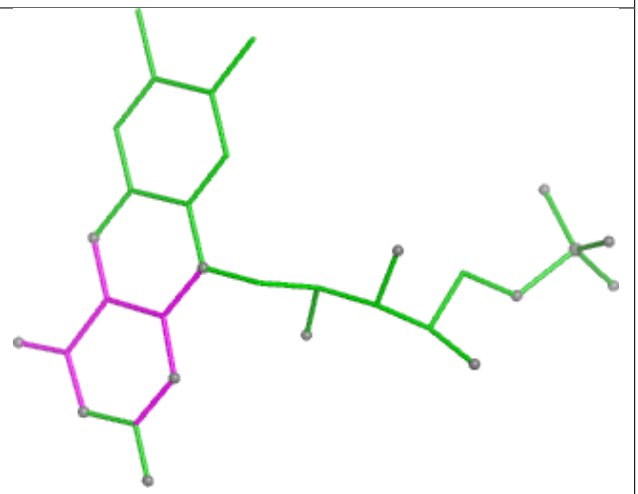


Rings

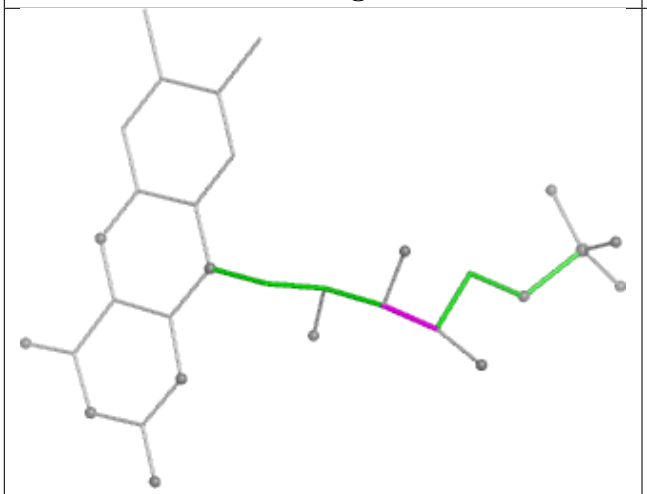
Ligand FMN G 501



Bond lengths



Bond angles



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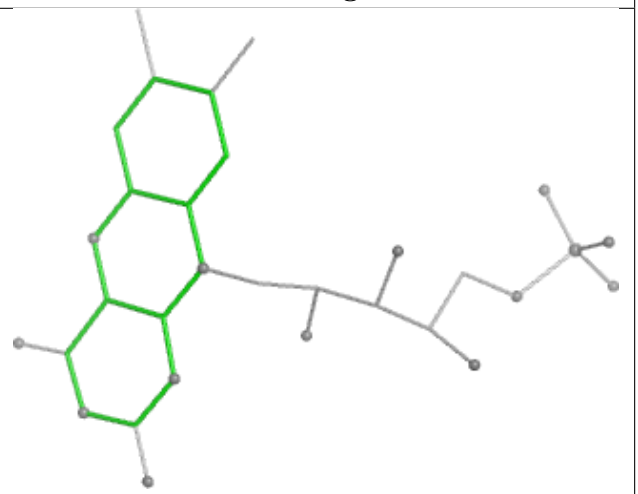
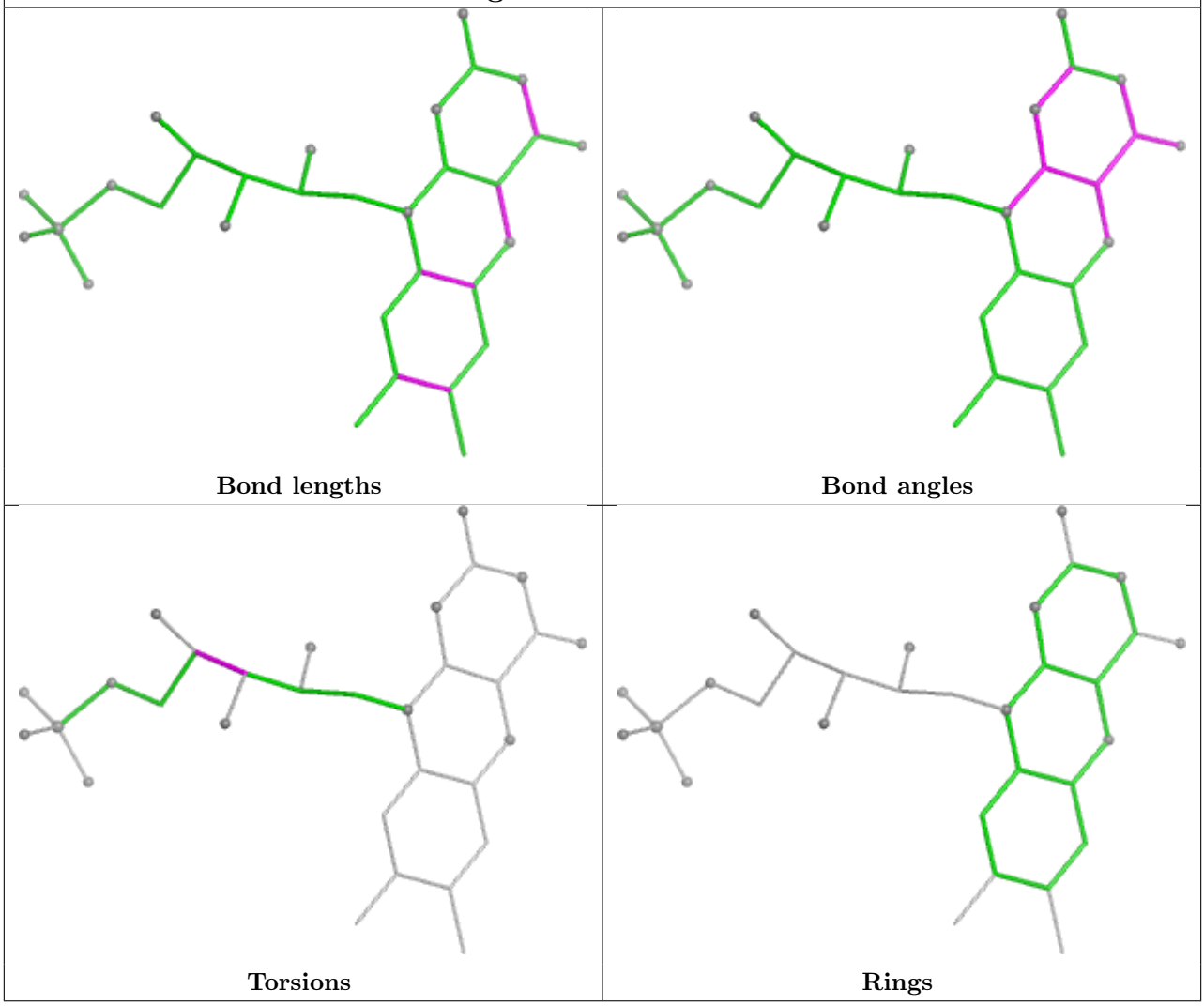
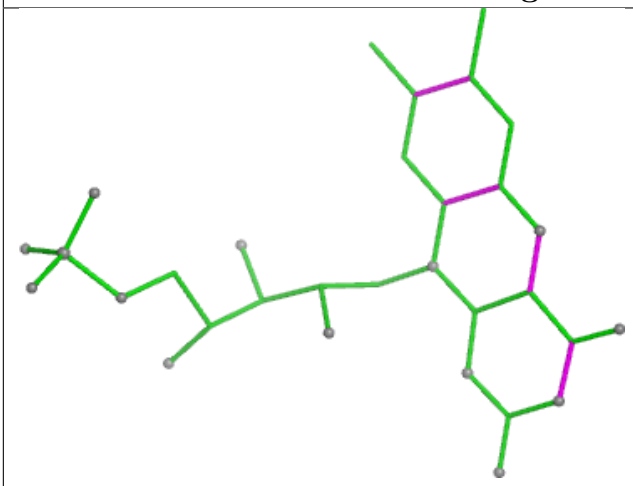


Rings

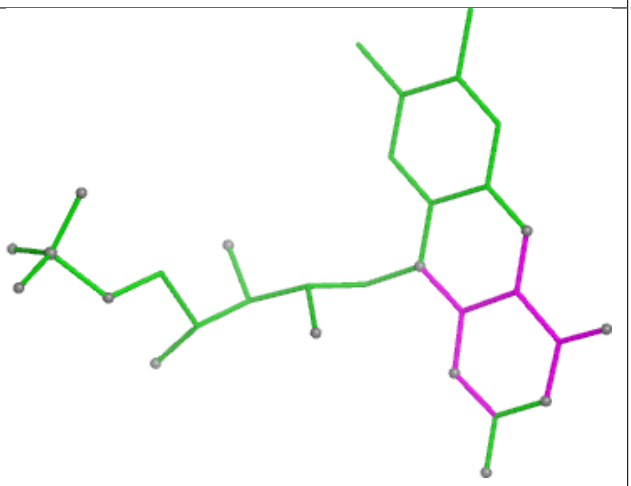
Ligand FMN D 501



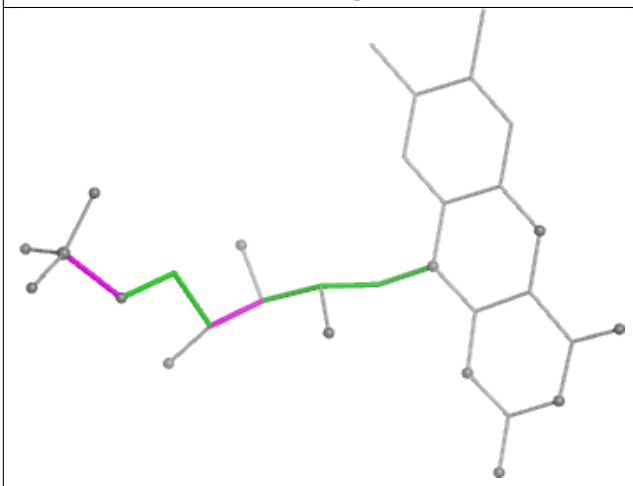
Ligand FMN F 502



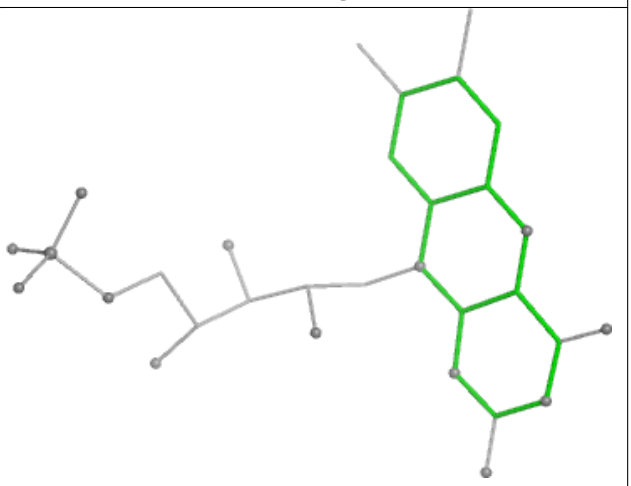
Bond lengths



Bond angles

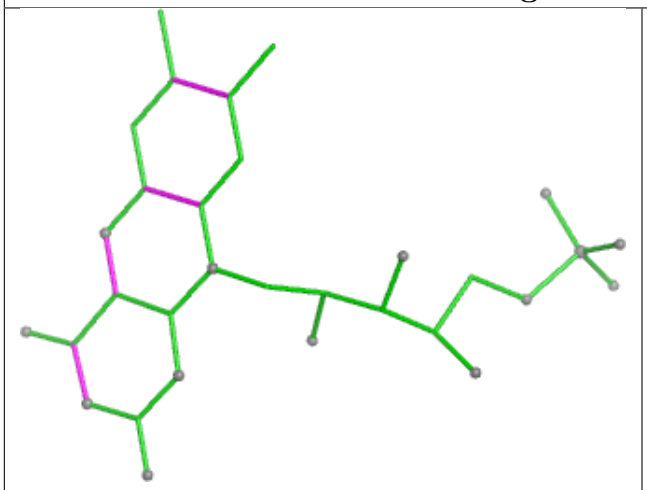


Torsions

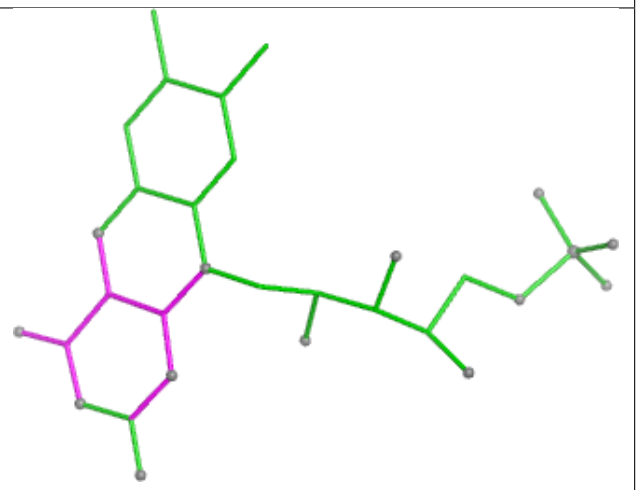


Rings

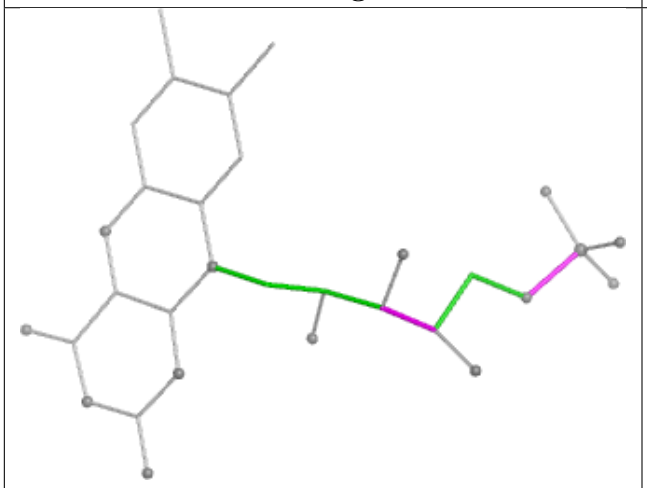
Ligand FMN B 501



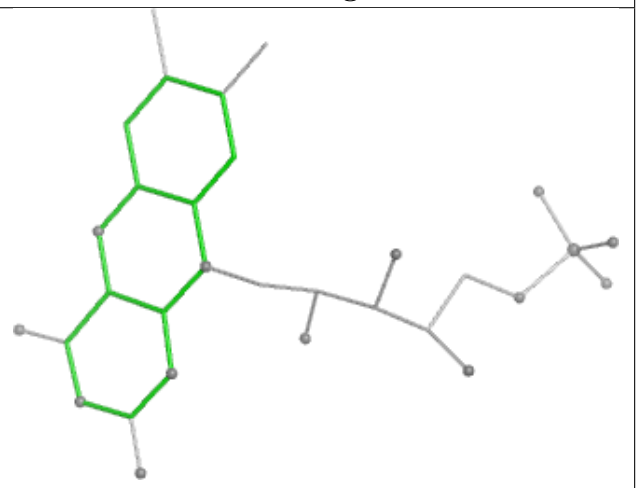
Bond lengths



Bond angles

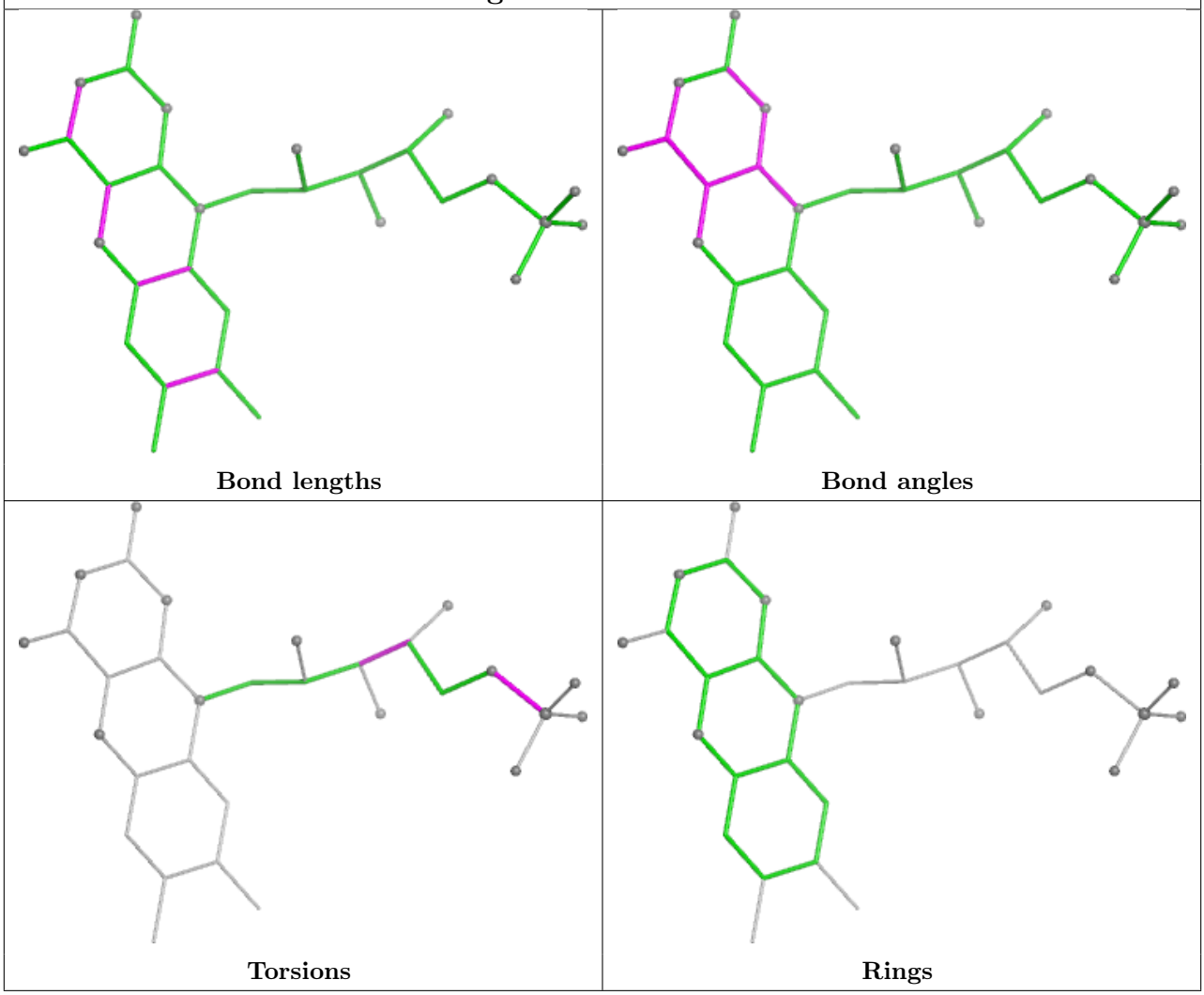


Torsions

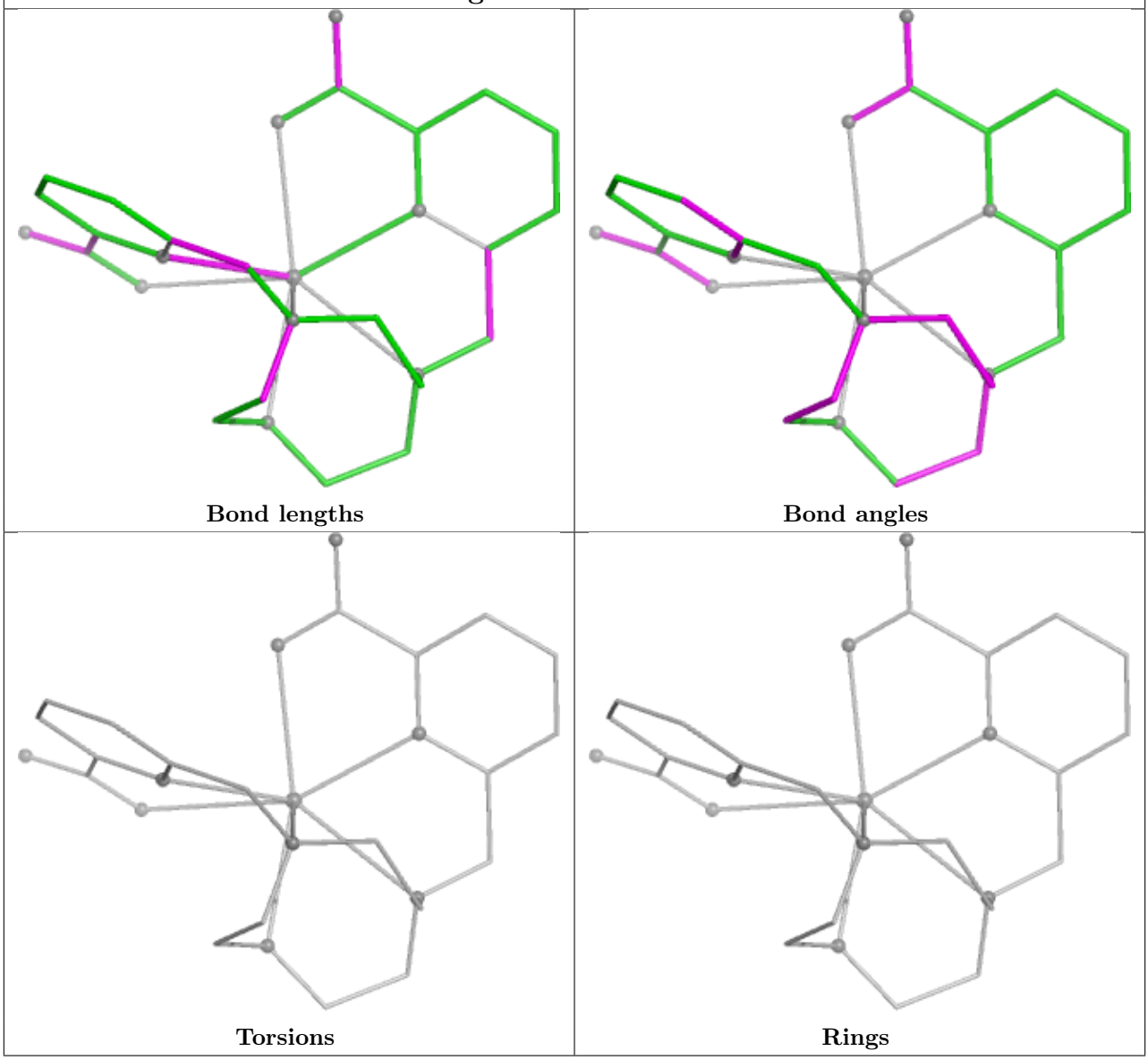


Rings

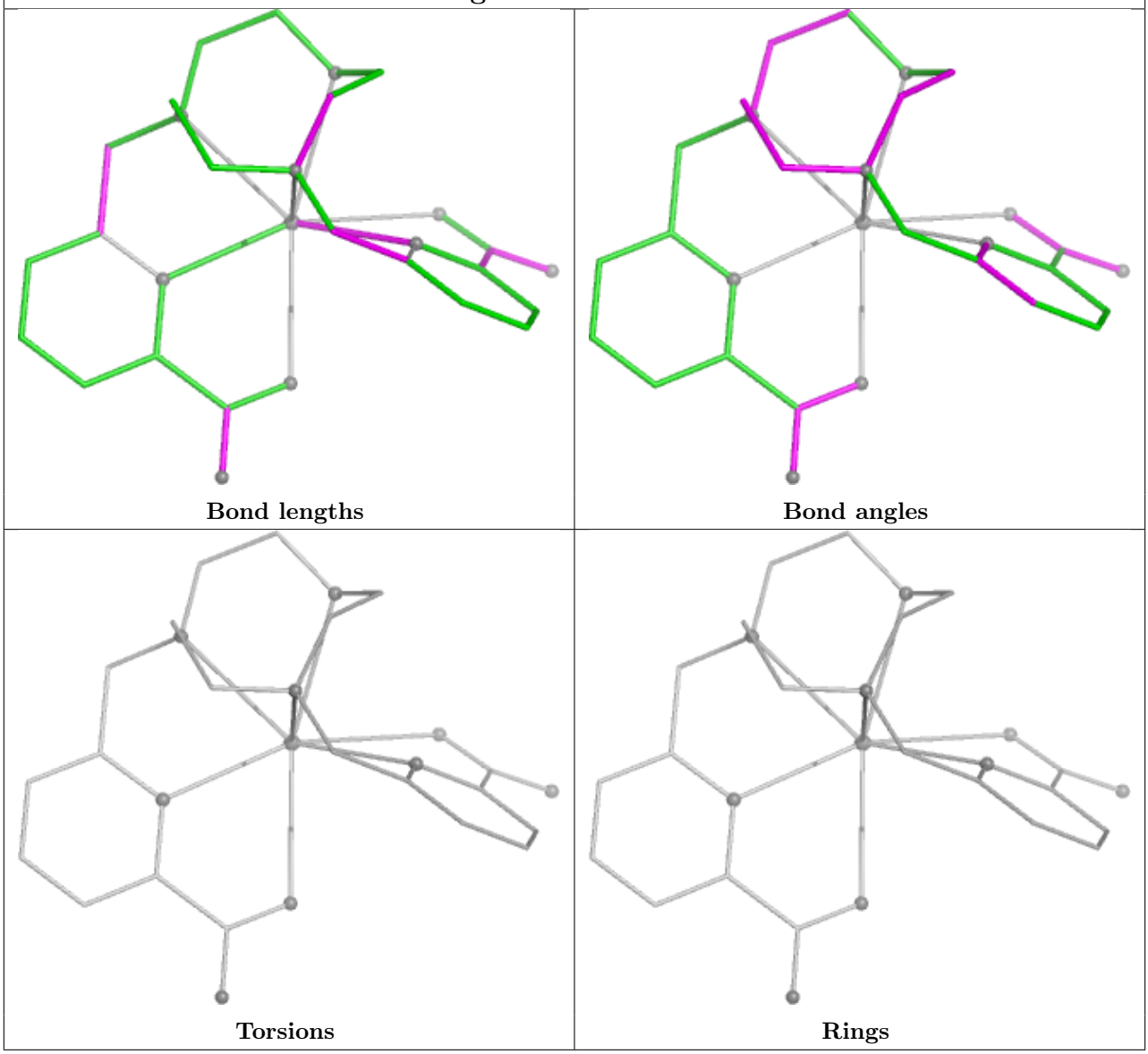
Ligand FMN H 501



Ligand 7MT A 502



Ligand 7MT F 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	402/410 (98%)	-0.08	9 (2%)	62	59	28, 51, 78, 119	1 (0%)
1	B	400/410 (97%)	-0.12	6 (1%)	72	69	35, 49, 76, 124	1 (0%)
1	C	408/410 (99%)	-0.07	3 (0%)	84	82	29, 49, 78, 114	2 (0%)
1	D	403/410 (98%)	0.03	8 (1%)	65	62	31, 53, 88, 126	1 (0%)
1	E	397/410 (96%)	-0.19	5 (1%)	75	73	25, 46, 72, 100	2 (0%)
1	F	395/410 (96%)	-0.17	4 (1%)	79	77	28, 45, 73, 111	2 (0%)
1	G	408/410 (99%)	-0.11	7 (1%)	69	66	29, 48, 83, 131	1 (0%)
1	H	409/410 (99%)	-0.16	7 (1%)	69	66	32, 44, 73, 121	1 (0%)
All	All	3222/3280 (98%)	-0.11	49 (1%)	72	69	25, 48, 79, 131	11 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	ALA	6.1
1	E	148	ALA	5.9
1	F	148	ALA	5.2
1	B	153	TRP	4.4
1	D	223	LEU	4.3
1	D	148	ALA	4.0
1	E	133	LEU	4.0
1	D	409	THR	4.0
1	F	224	LEU	4.0
1	H	409	THR	3.9
1	E	223	LEU	3.9
1	B	148	ALA	3.8
1	H	150	LEU	3.8
1	D	221	LEU	3.7
1	B	219	ILE	3.6
1	E	218	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	154	PRO	3.3
1	C	150	LEU	3.1
1	G	151	LEU	3.1
1	D	219	ILE	3.1
1	B	408	LYS	3.0
1	G	150	LEU	3.0
1	D	8	ILE	3.0
1	H	153	TRP	3.0
1	G	219	ILE	2.7
1	G	154	PRO	2.7
1	A	343	GLY	2.6
1	C	408	LYS	2.5
1	B	218	VAL	2.5
1	G	221	LEU	2.5
1	G	408	LYS	2.5
1	F	340	ASN	2.5
1	F	343	GLY	2.4
1	H	151	LEU	2.4
1	C	154	PRO	2.4
1	H	154	PRO	2.4
1	A	223	LEU	2.3
1	E	224	LEU	2.3
1	H	148	ALA	2.3
1	B	224	LEU	2.3
1	A	342	THR	2.3
1	A	218	VAL	2.3
1	G	152	HIS	2.2
1	A	222	GLY	2.2
1	D	220	GLU	2.2
1	A	340	ASN	2.1
1	H	218	VAL	2.1
1	D	218	VAL	2.1
1	A	221	LEU	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 oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TB	G	504	1/1	0.84	0.34	35,35,35,35	1
5	CL	D	506	1/1	0.87	0.12	89,89,89,89	0
5	CL	H	505	1/1	0.87	0.16	85,85,85,85	0
5	CL	E	503	1/1	0.89	0.16	94,94,94,94	0
6	FE	C	504	1/1	0.90	0.07	53,53,53,53	1
6	FE	H	504	1/1	0.91	0.07	46,46,46,46	1
4	TB	C	502	1/1	0.92	0.14	62,62,62,62	1
6	FE	D	505	1/1	0.92	0.09	54,54,54,54	1
5	CL	D	507	1/1	0.92	0.25	74,74,74,74	0
5	CL	F	506	1/1	0.93	0.09	63,63,63,63	0
5	CL	E	504	1/1	0.94	0.18	65,65,65,65	0
5	CL	C	506	1/1	0.94	0.16	80,80,80,80	0
2	FMN	H	501	31/31	0.94	0.08	32,38,42,43	0
4	TB	D	503	1/1	0.95	0.09	63,63,63,63	1
4	TB	G	502	1/1	0.95	0.14	74,74,74,74	1
2	FMN	F	502	31/31	0.95	0.08	37,40,44,46	0
5	CL	F	504	1/1	0.95	0.14	71,71,71,71	0
5	CL	F	505	1/1	0.95	0.15	58,58,58,58	0
4	TB	H	502	1/1	0.95	0.13	52,52,52,52	1
5	CL	B	503	1/1	0.95	0.10	64,64,64,64	0
5	CL	H	506	1/1	0.95	0.17	63,63,63,63	0
5	CL	C	505	1/1	0.95	0.15	59,59,59,59	0
2	FMN	B	501	31/31	0.95	0.08	36,44,49,51	0
2	FMN	E	501	31/31	0.95	0.07	29,34,41,41	0
4	TB	D	502	1/1	0.96	0.10	71,71,71,71	1
2	FMN	C	501	31/31	0.96	0.07	35,39,45,48	0
2	FMN	G	501	31/31	0.96	0.07	34,41,45,47	0
5	CL	G	506	1/1	0.96	0.16	62,62,62,62	0
2	FMN	D	501	31/31	0.96	0.07	34,41,49,53	0
2	FMN	A	501	31/31	0.96	0.07	36,47,53,55	0
5	CL	A	504	1/1	0.96	0.17	68,68,68,68	0
5	CL	A	505	1/1	0.96	0.24	67,67,67,67	0
6	FE	G	505	1/1	0.96	0.04	52,52,52,52	1
5	CL	E	505	1/1	0.96	0.18	61,61,61,61	0
5	CL	B	504	1/1	0.97	0.19	59,59,59,59	0
4	TB	B	502	1/1	0.97	0.04	50,50,50,50	0
3	7MT	F	501	30/30	0.98	0.10	43,49,53,56	0

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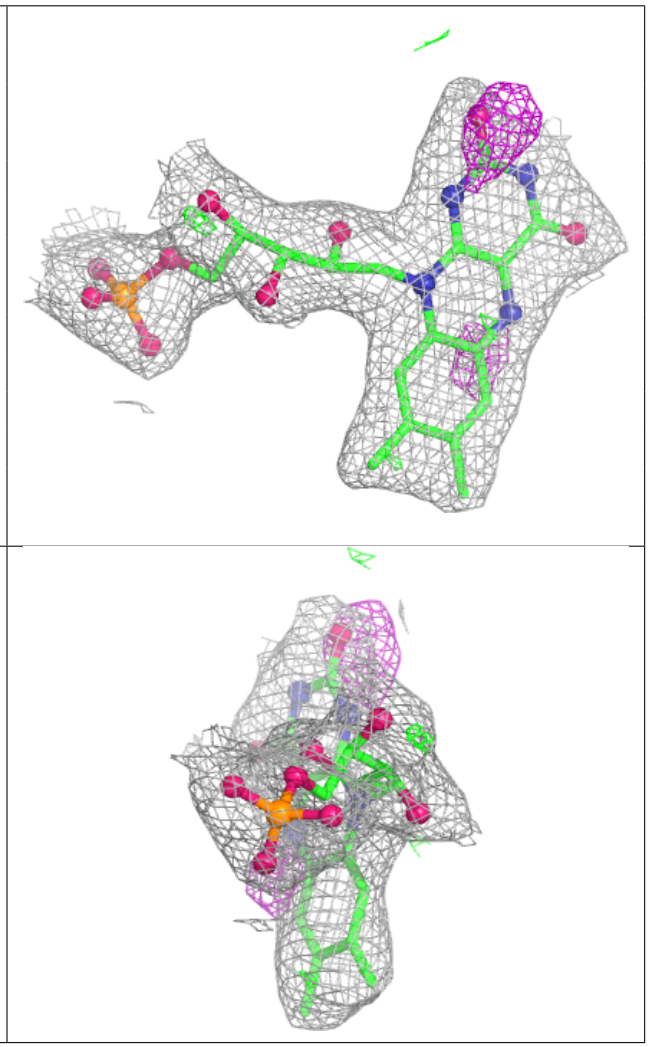
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TB	C	503	1/1	0.98	0.04	61,61,61,61	0
4	TB	A	503	1/1	0.98	0.04	52,52,52,52	0
3	7MT	A	502	30/30	0.98	0.10	37,47,53,57	0
4	TB	E	502	1/1	0.98	0.04	51,51,51,51	0
4	TB	F	503	1/1	0.98	0.04	48,48,48,48	0
4	TB	D	504	1/1	0.99	0.03	63,63,63,63	0
4	TB	G	503	1/1	0.99	0.03	60,60,60,60	0
4	TB	H	503	1/1	0.99	0.03	57,57,57,57	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.

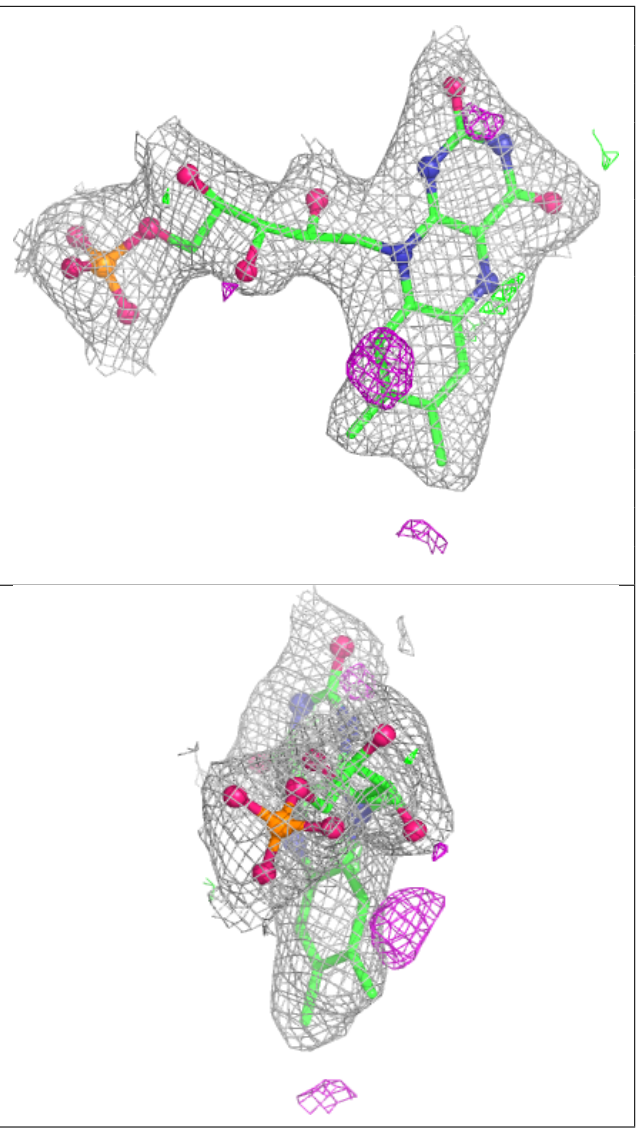
Electron density around FMN H 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



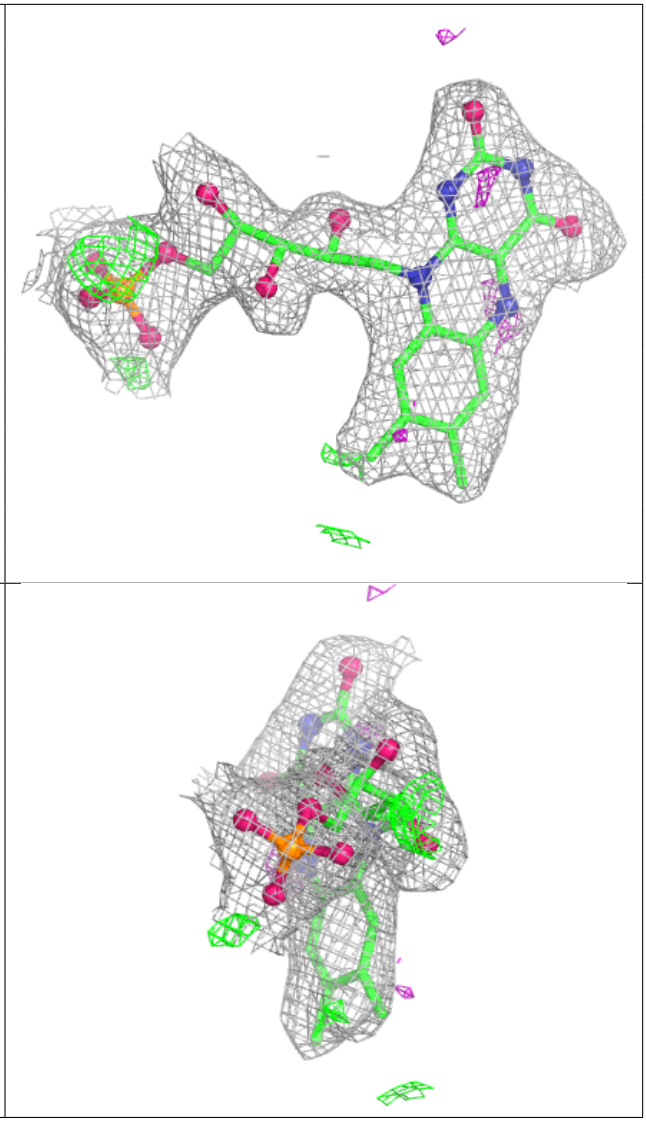
Electron density around FMN F 502:

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



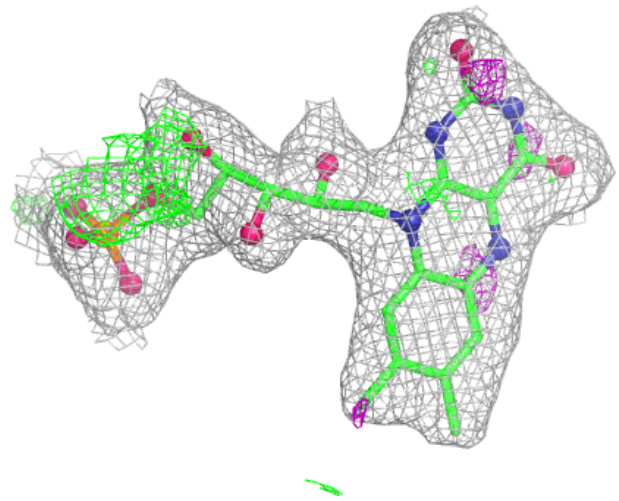
Electron density around FMN B 501:

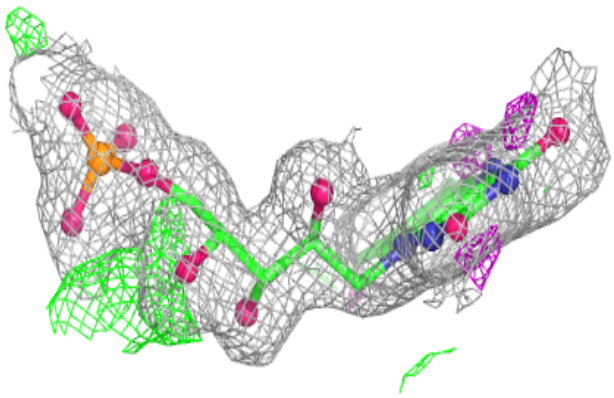
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

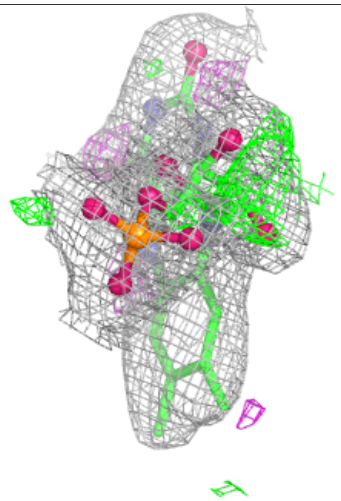


Electron density around FMN E 501:

$2mF_o$-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 C 501:

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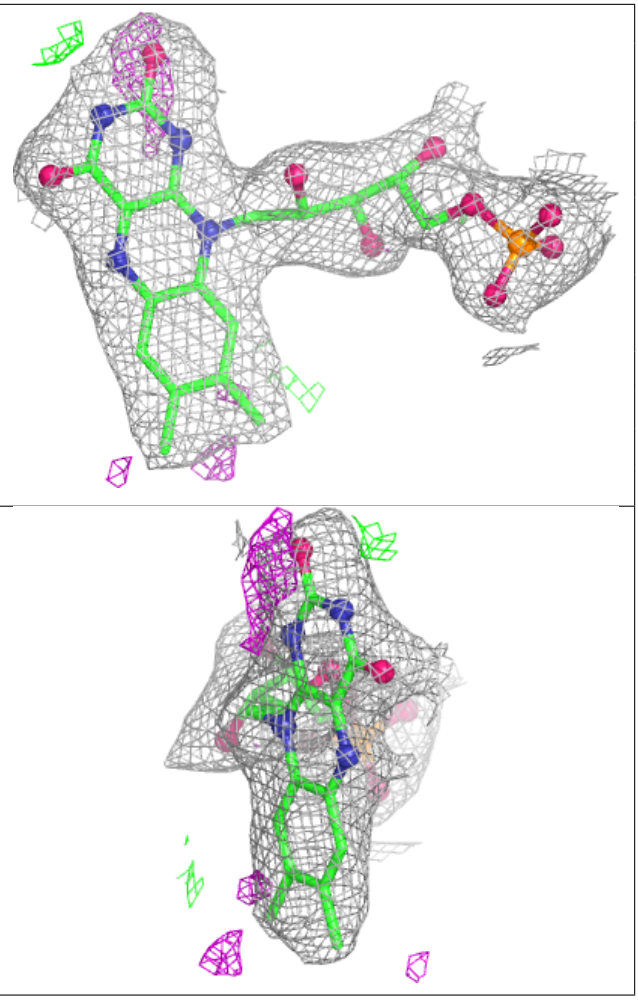
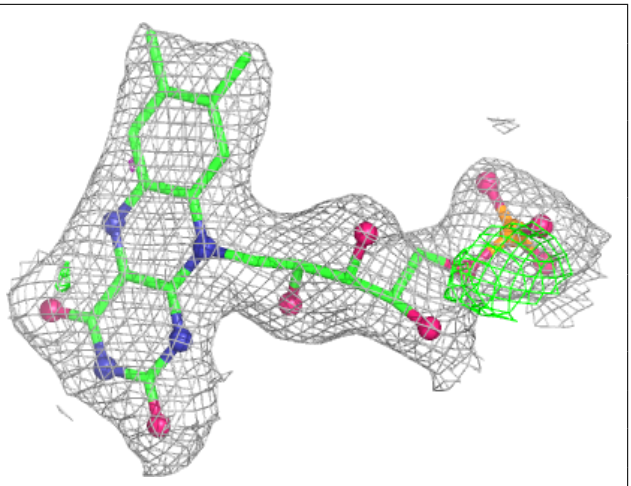
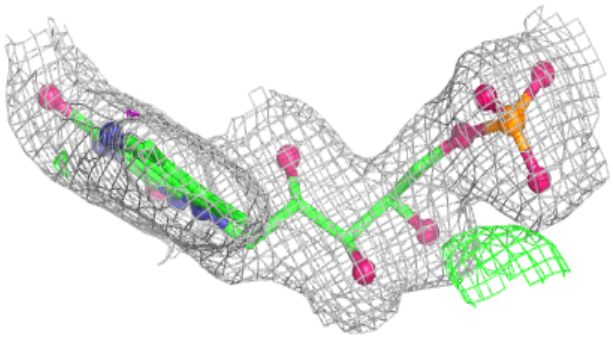
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN G 501:

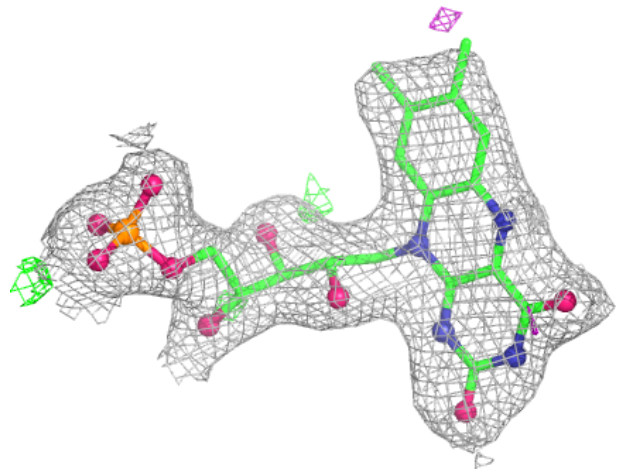
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

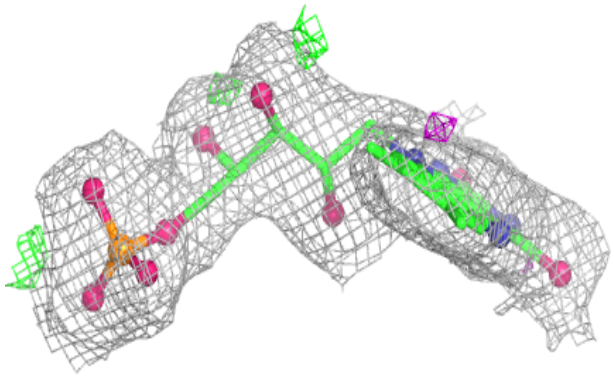


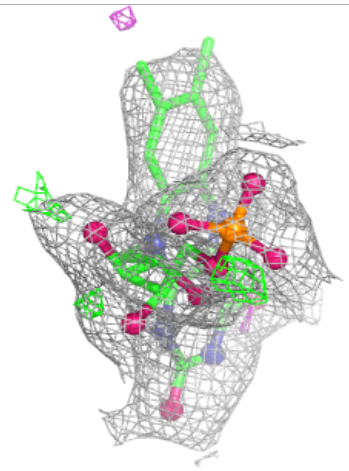


Electron density around FMN D 501:

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

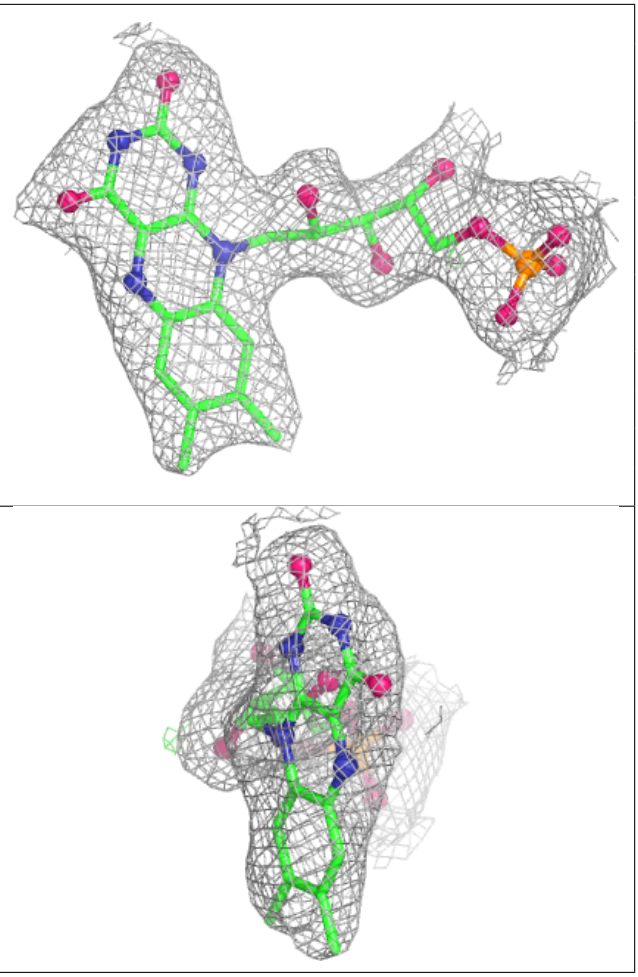






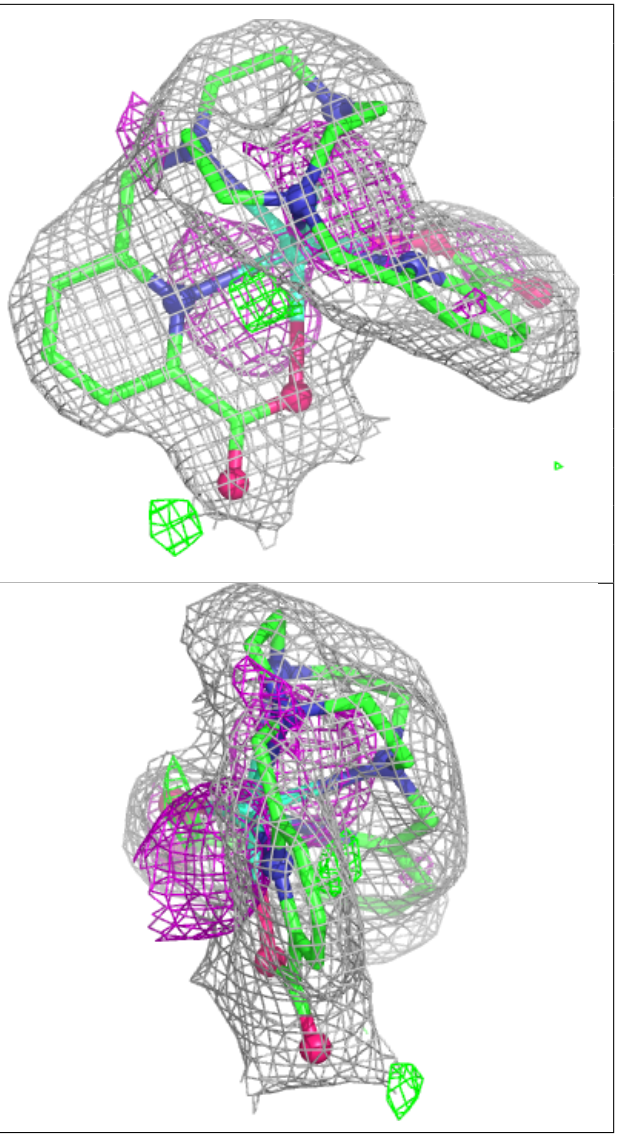
Electron density around FMN A 501:

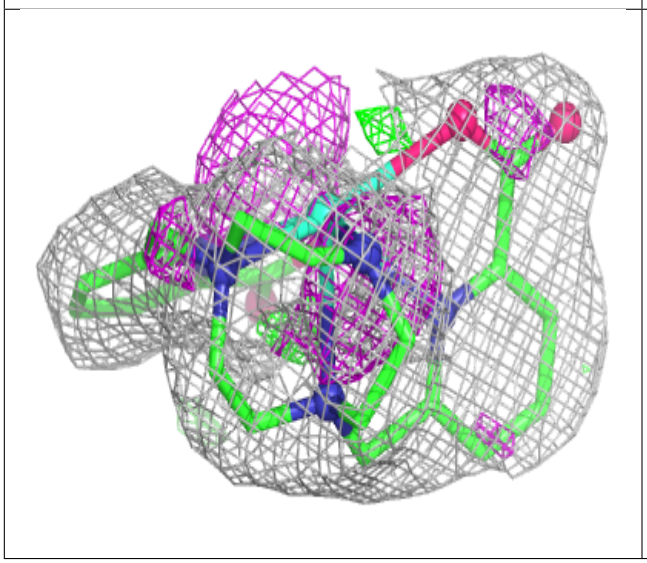
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 7MT F 501:

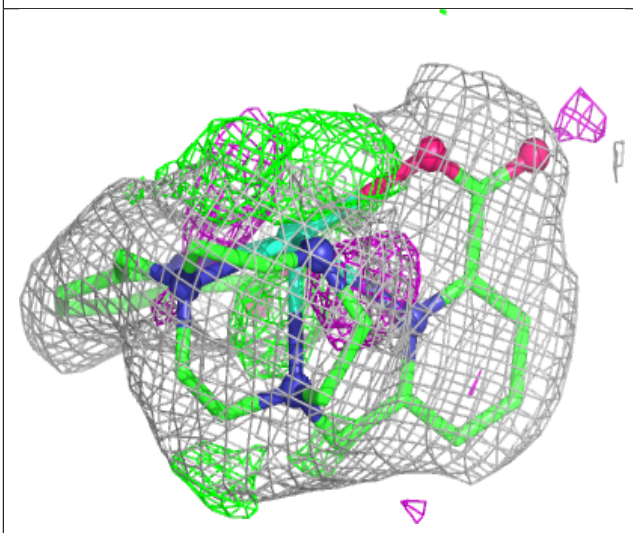
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

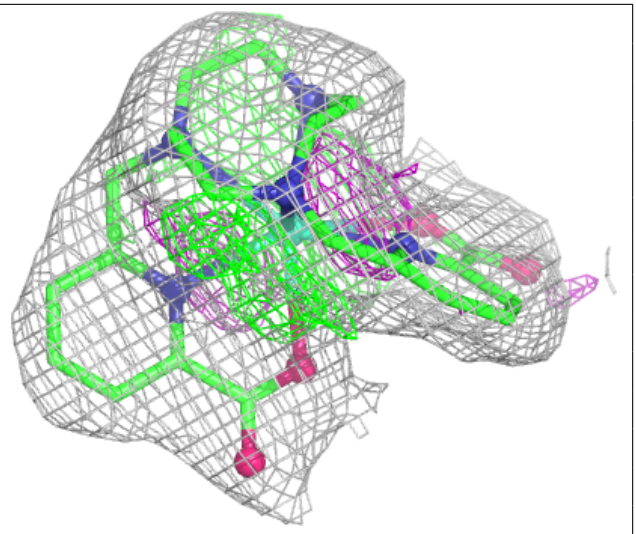


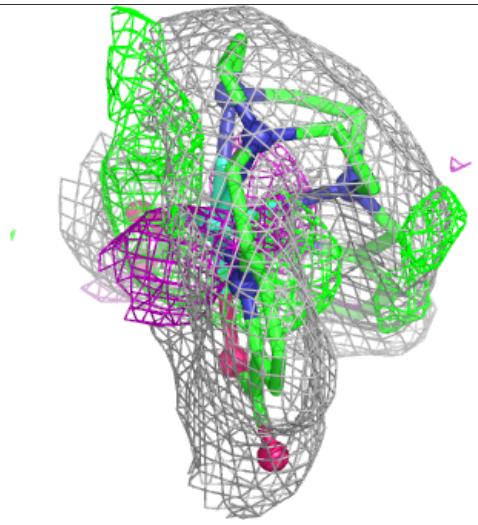


Electron density around 7MT A 502:

$2mF_o$-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.