



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 02:57 AM BST

PDB ID : 6JXN
Title : Crystal Structure of Indigo reductase from *Bacillus smithii* type strain DSM 4216
Authors : Yoneda, K.; Sakuraba, H.; Ohshima, T.
Deposited on : 2019-04-24
Resolution : 1.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

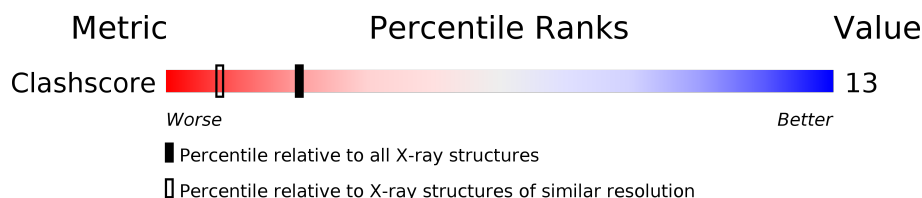
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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))
Clashscore	141614	1014 (1.98-1.98)

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	231	 74% 15% • 9%
1	B	231	 79% 13% 8%
1	C	231	 76% 13% • 10%
1	D	231	 78% 13% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PE8	A	302	-	-	X	-
3	PE8	C	302	-	-	X	-
4	NHE	B	302	-	-	X	-
4	NHE	B	303	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NHE	D	302	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7273 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 FMN-dependent NADH-azoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1649	1062	266	313	8			
1	B	212	Total	C	N	O	S	0	0	0
			1658	1067	268	315	8			
1	C	208	Total	C	N	O	S	0	0	0
			1629	1051	263	307	8			
1	D	212	Total	C	N	O	S	0	0	0
			1658	1067	268	315	8			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP G9QLG5
A	-18	GLY	-	expression tag	UNP G9QLG5
A	-17	SER	-	expression tag	UNP G9QLG5
A	-16	SER	-	expression tag	UNP G9QLG5
A	-15	HIS	-	expression tag	UNP G9QLG5
A	-14	HIS	-	expression tag	UNP G9QLG5
A	-13	HIS	-	expression tag	UNP G9QLG5
A	-12	HIS	-	expression tag	UNP G9QLG5
A	-11	HIS	-	expression tag	UNP G9QLG5
A	-10	HIS	-	expression tag	UNP G9QLG5
A	-9	SER	-	expression tag	UNP G9QLG5
A	-8	SER	-	expression tag	UNP G9QLG5
A	-7	GLY	-	expression tag	UNP G9QLG5
A	-6	LEU	-	expression tag	UNP G9QLG5
A	-5	VAL	-	expression tag	UNP G9QLG5
A	-4	PRO	-	expression tag	UNP G9QLG5
A	-3	ARG	-	expression tag	UNP G9QLG5
A	-2	GLY	-	expression tag	UNP G9QLG5
A	-1	SER	-	expression tag	UNP G9QLG5
A	0	HIS	-	expression tag	UNP G9QLG5
B	-19	MET	-	expression tag	UNP G9QLG5

Continued on next page...

Continued from previous page...

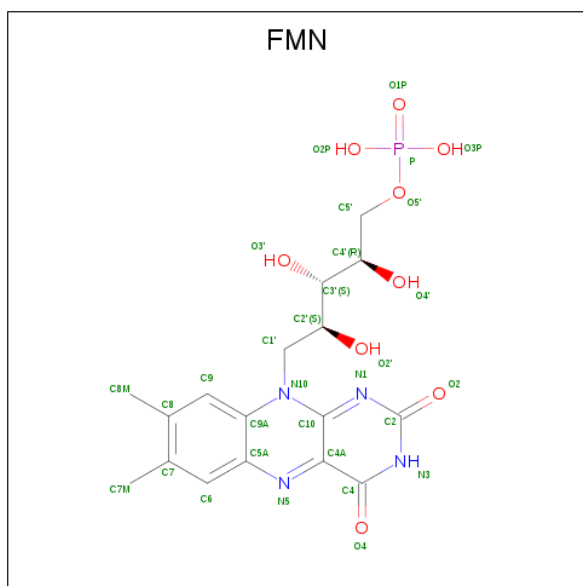
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP G9QLG5
B	-17	SER	-	expression tag	UNP G9QLG5
B	-16	SER	-	expression tag	UNP G9QLG5
B	-15	HIS	-	expression tag	UNP G9QLG5
B	-14	HIS	-	expression tag	UNP G9QLG5
B	-13	HIS	-	expression tag	UNP G9QLG5
B	-12	HIS	-	expression tag	UNP G9QLG5
B	-11	HIS	-	expression tag	UNP G9QLG5
B	-10	HIS	-	expression tag	UNP G9QLG5
B	-9	SER	-	expression tag	UNP G9QLG5
B	-8	SER	-	expression tag	UNP G9QLG5
B	-7	GLY	-	expression tag	UNP G9QLG5
B	-6	LEU	-	expression tag	UNP G9QLG5
B	-5	VAL	-	expression tag	UNP G9QLG5
B	-4	PRO	-	expression tag	UNP G9QLG5
B	-3	ARG	-	expression tag	UNP G9QLG5
B	-2	GLY	-	expression tag	UNP G9QLG5
B	-1	SER	-	expression tag	UNP G9QLG5
B	0	HIS	-	expression tag	UNP G9QLG5
C	-19	MET	-	expression tag	UNP G9QLG5
C	-18	GLY	-	expression tag	UNP G9QLG5
C	-17	SER	-	expression tag	UNP G9QLG5
C	-16	SER	-	expression tag	UNP G9QLG5
C	-15	HIS	-	expression tag	UNP G9QLG5
C	-14	HIS	-	expression tag	UNP G9QLG5
C	-13	HIS	-	expression tag	UNP G9QLG5
C	-12	HIS	-	expression tag	UNP G9QLG5
C	-11	HIS	-	expression tag	UNP G9QLG5
C	-10	HIS	-	expression tag	UNP G9QLG5
C	-9	SER	-	expression tag	UNP G9QLG5
C	-8	SER	-	expression tag	UNP G9QLG5
C	-7	GLY	-	expression tag	UNP G9QLG5
C	-6	LEU	-	expression tag	UNP G9QLG5
C	-5	VAL	-	expression tag	UNP G9QLG5
C	-4	PRO	-	expression tag	UNP G9QLG5
C	-3	ARG	-	expression tag	UNP G9QLG5
C	-2	GLY	-	expression tag	UNP G9QLG5
C	-1	SER	-	expression tag	UNP G9QLG5
C	0	HIS	-	expression tag	UNP G9QLG5
D	-19	MET	-	expression tag	UNP G9QLG5
D	-18	GLY	-	expression tag	UNP G9QLG5
D	-17	SER	-	expression tag	UNP G9QLG5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP G9QLG5
D	-15	HIS	-	expression tag	UNP G9QLG5
D	-14	HIS	-	expression tag	UNP G9QLG5
D	-13	HIS	-	expression tag	UNP G9QLG5
D	-12	HIS	-	expression tag	UNP G9QLG5
D	-11	HIS	-	expression tag	UNP G9QLG5
D	-10	HIS	-	expression tag	UNP G9QLG5
D	-9	SER	-	expression tag	UNP G9QLG5
D	-8	SER	-	expression tag	UNP G9QLG5
D	-7	GLY	-	expression tag	UNP G9QLG5
D	-6	LEU	-	expression tag	UNP G9QLG5
D	-5	VAL	-	expression tag	UNP G9QLG5
D	-4	PRO	-	expression tag	UNP G9QLG5
D	-3	ARG	-	expression tag	UNP G9QLG5
D	-2	GLY	-	expression tag	UNP G9QLG5
D	-1	SER	-	expression tag	UNP G9QLG5
D	0	HIS	-	expression tag	UNP G9QLG5

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by author).



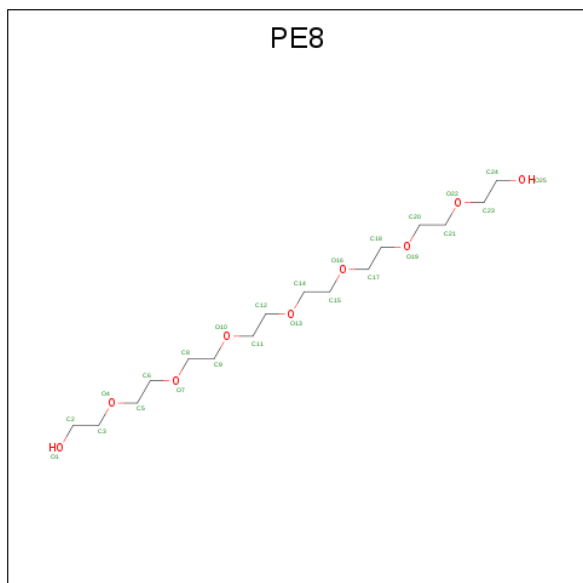
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

Continued on next page...

Continued from previous page...

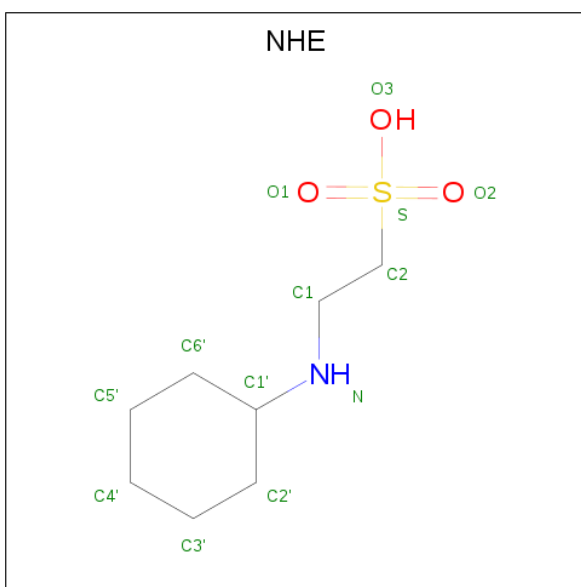
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: $C_{16}H_{34}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	16	9		
3	C	1	Total	C	O	0	0
			25	16	9		

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	D	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 5 is water.

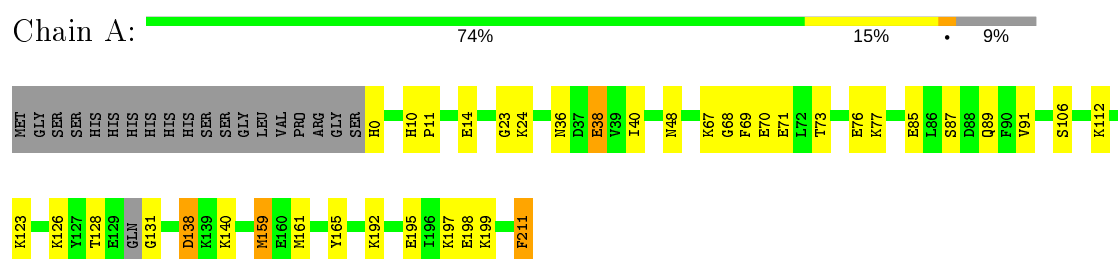
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total	O	0	0
			105	105		
5	B	119	Total	O	0	0
			119	119		
5	C	119	Total	O	0	0
			119	119		
5	D	123	Total	O	0	0
			123	123		

3 Residue-property plots [i](#)

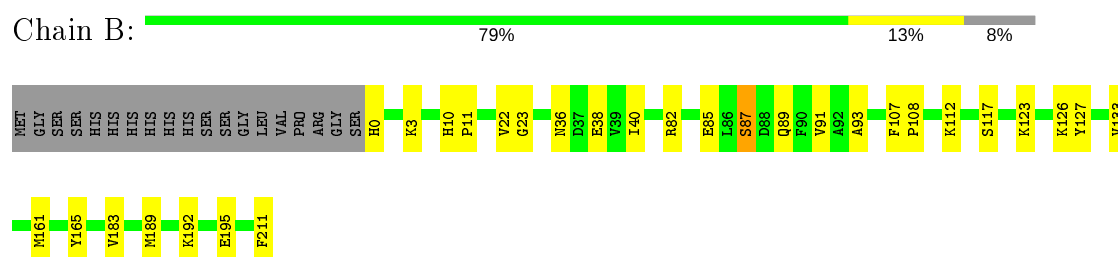
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

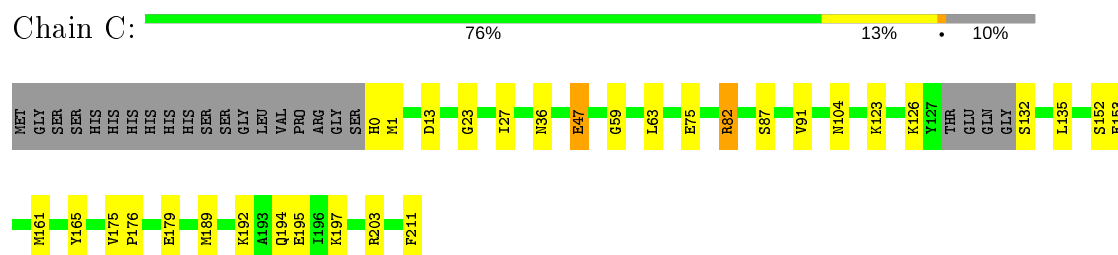
- Molecule 1: FMN-dependent NADH-azoreductase



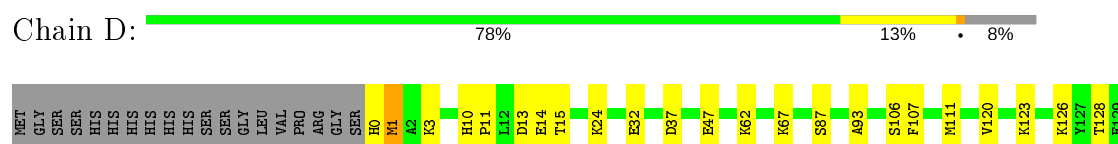
- Molecule 1: FMN-dependent NADH-azoreductase



- Molecule 1: FMN-dependent NADH-azoreductase



- Molecule 1: FMN-dependent NADH-azoreductase





4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.48 Å 105.14 Å 87.78 Å 90.00° 92.49° 90.00°	Depositor
Resolution (Å)	35.62 – 1.97	Depositor
% Data completeness (in resolution range)	99.9 (35.62-1.97)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.16 (at 1.97 Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.178 , 0.186	Depositor
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.072	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
Total number of atoms	7273	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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, NHE, PE8

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	1.40	6/1688 (0.4%)	0.87	1/2277 (0.0%)
1	B	1.37	5/1698 (0.3%)	0.83	0/2292
1	C	1.40	7/1668 (0.4%)	0.85	2/2250 (0.1%)
1	D	1.43	5/1698 (0.3%)	0.84	3/2292 (0.1%)
All	All	1.40	23/6752 (0.3%)	0.85	6/9111 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	211	PHE	C-OXT	-10.33	1.03	1.23
1	A	211	PHE	C-OXT	-10.28	1.03	1.23
1	C	179	GLU	CD-OE1	-6.79	1.18	1.25
1	C	47	GLU	CD-OE2	-6.71	1.18	1.25
1	B	85	GLU	CD-OE2	-6.56	1.18	1.25
1	C	179	GLU	CD-OE2	-6.48	1.18	1.25
1	D	179	GLU	CG-CD	6.40	1.61	1.51
1	B	87	SER	CB-OG	-6.30	1.34	1.42
1	D	32	GLU	CD-OE2	-6.01	1.19	1.25
1	A	106	SER	CB-OG	-5.82	1.34	1.42
1	B	117	SER	CB-OG	-5.81	1.34	1.42
1	D	47	GLU	CD-OE2	-5.79	1.19	1.25
1	D	179	GLU	CD-OE1	5.79	1.32	1.25
1	C	87	SER	CB-OG	-5.71	1.34	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211	PHE	C-OXT	-5.60	1.12	1.23
1	A	23	GLY	C-O	-5.48	1.14	1.23
1	C	195	GLU	CD-OE2	-5.46	1.19	1.25
1	A	85	GLU	CD-OE2	-5.37	1.19	1.25
1	C	211	PHE	C-OXT	-5.28	1.13	1.23
1	C	23	GLY	C-O	-5.26	1.15	1.23
1	A	138	ASP	CB-CG	-5.11	1.41	1.51
1	B	23	GLY	C-O	-5.10	1.15	1.23
1	A	38	GLU	CD-OE2	-5.09	1.20	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	159	MET	CG-SD-CE	-5.79	90.94	100.20
1	D	138	ASP	CB-CG-OD2	5.60	123.34	118.30
1	D	1	MET	CB-CG-SD	-5.51	95.87	112.40
1	D	0	HIS	CB-CA-C	5.10	120.60	110.40
1	C	13	ASP	CB-CG-OD1	5.09	122.89	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	153	GLU	Peptide

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	1649	0	1615	69	0
1	B	1658	0	1624	45	0
1	C	1629	0	1599	36	0
1	D	1658	0	1624	22	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	31	0	19	0	0
3	A	25	0	34	19	0
3	C	25	0	34	13	0
4	B	26	0	32	22	0
4	D	13	0	16	9	0
5	A	105	0	0	4	0
5	B	119	0	0	2	0
5	C	119	0	0	4	0
5	D	123	0	0	5	0
All	All	7273	0	6654	169	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 13.

All (169) 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:0:HIS:HB2	1:A:36:ASN:O	1.54	1.08
1:A:40:ILE:HD11	1:B:40:ILE:HD11	1.37	1.03
1:A:89:GLN:HE22	1:B:0:HIS:CE1	1.77	1.02
1:A:197:LYS:HZ2	3:A:302:PE8:H121	1.28	0.98
1:A:197:LYS:HZ1	3:A:302:PE8:H182	1.29	0.97
1:A:192:LYS:O	1:A:195:GLU:HG2	1.68	0.94
1:D:123:LYS:HE3	5:D:403:HOH:O	1.68	0.93
1:A:165:TYR:HB2	4:D:302:NHE:HC12	1.51	0.92
1:B:192:LYS:O	1:B:195:GLU:HG2	1.70	0.90
1:A:197:LYS:NZ	3:A:302:PE8:H182	1.88	0.89
1:A:89:GLN:NE2	1:B:0:HIS:ND1	2.22	0.88
1:B:107:PHE:CE1	4:B:303:NHE:H3'1	2.09	0.86
1:A:0:HIS:HB3	1:B:82:ARG:HH12	1.43	0.84
1:A:0:HIS:CB	1:A:36:ASN:O	2.26	0.83
1:A:67:LYS:HB3	1:A:71:GLU:HG3	1.61	0.83
1:B:3:LYS:HE3	1:B:93:ALA:HB2	1.61	0.81
1:A:197:LYS:NZ	3:A:302:PE8:H121	1.96	0.80
1:B:0:HIS:HB2	1:B:38:GLU:HG3	1.62	0.80
1:A:161:MET:HB3	4:D:302:NHE:O2	1.81	0.80
1:D:106:SER:OG	4:D:302:NHE:H5'1	1.81	0.79
1:C:197:LYS:HZ2	3:C:302:PE8:C20	1.97	0.78
1:A:197:LYS:HZ2	3:A:302:PE8:C15	1.98	0.77
1:A:0:HIS:CG	1:A:36:ASN:O	2.40	0.75
1:D:107:PHE:CE1	4:D:302:NHE:H4'2	2.22	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LYS:NZ	3:C:302:PE8:H172	2.01	0.74
1:C:152:SER:O	1:C:153:GLU:HG3	1.88	0.73
1:D:24:LYS:NZ	5:D:401:HOH:O	2.21	0.73
1:A:68:GLY:H	1:A:71:GLU:HG3	1.54	0.72
4:B:303:NHE:O1	1:C:161:MET:HB3	1.89	0.72
1:B:165:TYR:HB2	4:B:303:NHE:HC12	1.69	0.72
1:B:0:HIS:CB	1:B:38:GLU:HG3	2.19	0.72
1:A:40:ILE:CD1	1:B:40:ILE:HD11	2.15	0.72
1:A:0:HIS:CD2	1:A:36:ASN:O	2.43	0.72
1:D:161:MET:HB3	4:D:302:NHE:S	2.30	0.71
1:B:161:MET:SD	4:B:303:NHE:O3	2.48	0.71
4:B:302:NHE:H6'1	4:B:302:NHE:HC22	1.74	0.70
1:B:0:HIS:CD2	1:B:38:GLU:HG2	2.28	0.69
1:A:197:LYS:HZ2	3:A:302:PE8:H152	1.57	0.69
1:C:197:LYS:HZ2	3:C:302:PE8:H201	1.57	0.68
1:A:68:GLY:O	1:A:71:GLU:HG2	1.94	0.68
1:A:14:GLU:HG3	1:A:24:LYS:HE2	1.75	0.67
1:A:89:GLN:HE22	1:B:0:HIS:CG	2.10	0.67
1:B:127:TYR:HE1	4:B:302:NHE:H5'1	1.59	0.66
1:A:197:LYS:HZ2	3:A:302:PE8:C12	2.06	0.66
1:C:197:LYS:HZ2	3:C:302:PE8:C17	2.08	0.65
1:B:112:LYS:HB2	4:B:303:NHE:H4'1	1.78	0.65
1:D:10:HIS:ND1	1:D:11:PRO:HD2	2.12	0.65
1:C:126:LYS:O	1:C:132:SER:HA	1.96	0.65
1:C:197:LYS:HZ2	3:C:302:PE8:H172	1.62	0.64
1:D:62:LYS:O	1:D:67:LYS:HD2	1.97	0.64
1:C:197:LYS:NZ	3:C:302:PE8:H232	2.12	0.64
1:C:197:LYS:NZ	3:C:302:PE8:C17	2.61	0.63
1:C:197:LYS:HZ2	3:C:302:PE8:H202	1.63	0.63
1:A:10:HIS:ND1	1:A:11:PRO:HD2	2.13	0.63
4:B:303:NHE:HC22	1:C:165:TYR:HB2	1.79	0.62
1:B:161:MET:O	4:B:303:NHE:HC11	2.00	0.61
1:A:48:ASN:HD22	1:B:36:ASN:HD21	1.49	0.60
1:A:68:GLY:H	1:A:71:GLU:CG	2.15	0.60
1:A:197:LYS:HZ2	3:A:302:PE8:H151	1.66	0.59
4:B:303:NHE:O1	1:C:161:MET:CB	2.51	0.59
1:B:107:PHE:CE1	4:B:303:NHE:C3'	2.82	0.59
4:B:302:NHE:C2	4:B:302:NHE:H6'1	2.32	0.58
1:D:106:SER:CB	4:D:302:NHE:H5'1	2.33	0.58
1:A:70:GLU:HG3	1:A:71:GLU:N	2.17	0.58
4:B:303:NHE:O1	1:C:161:MET:O	2.21	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:VAL:HG11	1:D:123:LYS:HD2	1.86	0.56
1:A:0:HIS:HB3	1:B:82:ARG:NH1	2.16	0.56
1:A:198:GLU:OE2	3:A:302:PE8:O25	2.23	0.56
1:C:197:LYS:HZ1	3:C:302:PE8:H232	1.70	0.56
1:A:68:GLY:O	1:A:70:GLU:N	2.38	0.56
1:A:89:GLN:NE2	1:B:0:HIS:CE1	2.61	0.55
1:B:3:LYS:HE3	1:B:93:ALA:CB	2.34	0.55
1:C:0:HIS:CE1	1:C:36:ASN:OD1	2.59	0.55
1:A:165:TYR:CB	4:D:302:NHE:HC12	2.30	0.55
1:A:89:GLN:NE2	1:B:0:HIS:CG	2.72	0.55
4:B:302:NHE:H6'2	2:C:301:FMN:C4A	2.37	0.55
4:B:303:NHE:O1	1:C:161:MET:CA	2.55	0.54
1:C:47:GLU:OE1	1:C:82:ARG:NH2	2.38	0.54
1:A:138:ASP:O	1:A:138:ASP:OD1	2.26	0.54
1:A:0:HIS:CD2	1:B:89:GLN:HE22	2.26	0.54
1:C:194:GLN:HG3	3:C:302:PE8:H112	1.90	0.54
1:A:128:THR:N	1:A:131:GLY:O	2.32	0.53
1:B:87:SER:HB2	5:B:481:HOH:O	2.09	0.53
1:A:112:LYS:HG2	4:D:302:NHE:H4'1	1.92	0.52
1:A:197:LYS:NZ	3:A:302:PE8:H152	2.24	0.52
3:A:302:PE8:H211	3:A:302:PE8:H51	1.92	0.51
4:B:303:NHE:C2	1:C:165:TYR:HB2	2.40	0.51
4:B:302:NHE:HC21	2:C:301:FMN:C5A	2.40	0.51
1:A:0:HIS:CE1	1:B:89:GLN:OE1	2.63	0.51
1:A:68:GLY:O	1:A:71:GLU:N	2.33	0.51
1:C:91:VAL:HG21	1:C:123:LYS:HB3	1.93	0.50
1:B:22:VAL:HG21	1:B:183:VAL:HG21	1.94	0.50
1:D:126:LYS:HG2	1:D:133:VAL:CG1	2.42	0.50
1:A:77:LYS:HB2	5:A:407:HOH:O	2.10	0.50
1:B:189:MET:CE	1:B:192:LYS:NZ	2.75	0.49
1:B:10:HIS:ND1	1:B:11:PRO:HD2	2.28	0.49
1:C:152:SER:C	1:C:153:GLU:HG3	2.33	0.49
1:A:0:HIS:CE1	1:B:89:GLN:HE22	2.31	0.49
1:C:189:MET:HG3	1:C:192:LYS:HD2	1.93	0.49
1:A:197:LYS:NZ	3:A:302:PE8:C12	2.69	0.49
1:A:14:GLU:CG	1:A:24:LYS:HE2	2.43	0.49
1:A:91:VAL:HG11	1:A:123:LYS:HB3	1.95	0.49
1:D:120:VAL:CG1	1:D:123:LYS:HD2	2.42	0.49
1:B:0:HIS:CG	1:B:36:ASN:O	2.66	0.48
1:B:189:MET:HE1	1:B:192:LYS:HZ1	1.78	0.48
1:A:68:GLY:N	1:A:71:GLU:HG3	2.26	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:TYR:HB2	4:B:303:NHE:C1	2.43	0.47
1:D:107:PHE:CD1	1:D:111:MET:HB3	2.49	0.47
1:A:73:THR:HG23	1:A:76:GLU:OE1	2.15	0.47
1:A:77:LYS:HE2	5:A:407:HOH:O	2.15	0.47
1:B:91:VAL:HG11	1:B:123:LYS:HB3	1.97	0.46
1:A:87:SER:OG	1:A:123:LYS:HD2	2.15	0.46
1:C:75:GLU:CG	5:C:411:HOH:O	2.62	0.46
1:C:203:ARG:HH11	1:C:203:ARG:HG3	1.79	0.46
1:C:1:MET:HE1	5:C:517:HOH:O	2.16	0.46
1:B:0:HIS:CG	1:B:38:GLU:HG2	2.51	0.45
1:A:126:LYS:HE2	5:A:430:HOH:O	2.17	0.45
1:C:197:LYS:HZ3	3:C:302:PE8:H172	1.77	0.45
1:A:197:LYS:HZ3	3:A:302:PE8:H91	1.82	0.45
1:B:0:HIS:CD2	1:B:36:ASN:O	2.70	0.45
1:B:189:MET:HE1	1:B:192:LYS:NZ	2.32	0.44
1:B:0:HIS:CD2	1:B:38:GLU:CG	2.99	0.44
1:D:14:GLU:H	1:D:14:GLU:HG3	1.67	0.44
1:A:159:MET:HE2	1:A:159:MET:HB2	1.61	0.43
1:C:59:GLY:O	1:C:63:LEU:HD23	2.18	0.43
1:B:189:MET:HE2	1:B:192:LYS:NZ	2.33	0.43
1:C:175:VAL:HA	1:C:176:PRO:HD3	1.90	0.43
1:A:68:GLY:O	1:A:69:PHE:C	2.55	0.43
1:B:0:HIS:CG	1:B:38:GLU:CG	3.02	0.43
1:C:126:LYS:HD3	1:C:135:LEU:HD21	2.01	0.43
1:A:197:LYS:HZ1	3:A:302:PE8:C18	2.15	0.43
1:B:126:LYS:HE2	1:B:133:VAL:HG11	2.00	0.43
1:D:179:GLU:HG3	5:D:440:HOH:O	2.19	0.43
1:D:3:LYS:HE3	1:D:93:ALA:HB2	1.99	0.43
1:A:197:LYS:NZ	3:A:302:PE8:C15	2.77	0.43
1:A:77:LYS:HB2	1:A:77:LYS:HE2	1.70	0.43
1:B:192:LYS:HA	1:B:195:GLU:CD	2.40	0.43
1:A:14:GLU:HG3	1:A:24:LYS:CE	2.47	0.42
1:C:197:LYS:HZ2	3:C:302:PE8:H171	1.81	0.42
1:D:126:LYS:HG2	1:D:133:VAL:HG12	2.01	0.42
1:D:13:ASP:OD1	1:D:15:THR:OG1	2.33	0.42
4:B:302:NHE:O2	5:B:401:HOH:O	2.21	0.42
1:D:1:MET:HB3	1:D:37:ASP:OD1	2.20	0.42
1:A:68:GLY:C	1:A:70:GLU:N	2.69	0.42
1:D:128:THR:C	1:D:130:GLN:N	2.70	0.42
1:A:197:LYS:HZ3	3:A:302:PE8:C9	2.32	0.42
3:A:302:PE8:H122	3:A:302:PE8:H91	1.65	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:MET:HE2	1:B:192:LYS:HE2	2.01	0.42
1:A:192:LYS:HA	1:A:195:GLU:CD	2.40	0.42
1:A:192:LYS:C	1:A:195:GLU:HG2	2.37	0.41
1:C:75:GLU:HG3	5:C:411:HOH:O	2.18	0.41
1:A:199:LYS:HG2	5:A:495:HOH:O	2.20	0.41
4:B:302:NHE:C6'	4:B:302:NHE:C2	2.96	0.41
1:D:87:SER:OG	1:D:123:LYS:HE3	2.21	0.41
1:A:197:LYS:CD	3:A:302:PE8:H151	2.50	0.41
1:C:27:ILE:HD12	1:C:27:ILE:HA	1.96	0.41
1:A:0:HIS:H3	1:A:38:GLU:HG3	1.86	0.41
1:B:107:PHE:HB2	1:B:108:PRO:HD2	2.03	0.41
4:B:302:NHE:H5'2	5:C:496:HOH:O	2.20	0.41
1:A:71:GLU:HG2	1:A:71:GLU:H	1.59	0.41
1:A:140:LYS:HE3	1:A:211:PHE:OXT	2.21	0.41
1:A:197:LYS:HD2	3:A:302:PE8:H151	2.03	0.41
4:D:302:NHE:HC22	4:D:302:NHE:HC'1	1.73	0.41
1:C:197:LYS:CD	3:C:302:PE8:H201	2.51	0.40
4:B:302:NHE:HC12	1:C:104:ASN:OD1	2.22	0.40
1:B:189:MET:HE2	1:B:192:LYS:CE	2.52	0.40
1:C:126:LYS:CD	1:C:135:LEU:HD21	2.52	0.40
1:D:191:ASP:HB3	5:D:508:HOH:O	2.22	0.40
1:D:67:LYS:CE	5:D:413:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NHE	B	302	-	13,13,13	2.91	3 (23%)	16,17,17	2.38	6 (37%)
4	NHE	D	302	-	13,13,13	3.45	4 (30%)	16,17,17	8.08	7 (43%)
3	PE8	A	302	-	24,24,24	0.44	0	23,23,23	0.59	0
2	FMN	C	301	-	31,33,33	2.46	11 (35%)	40,50,50	2.74	10 (25%)
2	FMN	A	301	-	31,33,33	2.42	7 (22%)	40,50,50	2.73	12 (30%)
2	FMN	D	301	-	31,33,33	2.63	7 (22%)	40,50,50	2.35	7 (17%)
2	FMN	B	301	-	31,33,33	2.55	10 (32%)	40,50,50	2.68	10 (25%)
4	NHE	B	303	-	13,13,13	3.07	2 (15%)	16,17,17	1.90	4 (25%)
3	PE8	C	302	-	24,24,24	0.45	0	23,23,23	0.82	0

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
4	NHE	B	302	-	-	4/7/15/15	0/1/1/1
4	NHE	D	302	-	-	3/7/15/15	0/1/1/1
3	PE8	A	302	-	-	14/22/22/22	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	C	301	-	-	2/18/18/18	0/3/3/3
2	FMN	A	301	-	-	3/18/18/18	0/3/3/3
2	FMN	D	301	-	-	2/18/18/18	0/3/3/3
2	FMN	B	301	-	-	2/18/18/18	0/3/3/3
4	NHE	B	303	-	-	4/7/15/15	0/1/1/1
3	PE8	C	302	-	-	10/22/22/22	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	FMN	C4A-C10	11.17	1.50	1.38
2	B	301	FMN	C4A-C10	10.45	1.49	1.38
2	A	301	FMN	C4A-C10	9.96	1.48	1.38
4	D	302	NHE	C2-S	-9.82	1.63	1.77
2	C	301	FMN	C4A-C10	9.78	1.48	1.38
4	B	303	NHE	C2-S	-8.65	1.65	1.77
4	B	302	NHE	C2-S	-8.35	1.65	1.77
4	D	302	NHE	O2-S	6.49	1.64	1.45
4	B	303	NHE	O2-S	6.27	1.63	1.45
4	B	302	NHE	O2-S	5.26	1.60	1.45
2	A	301	FMN	C4-C4A	4.55	1.49	1.41
2	D	301	FMN	C4-C4A	4.47	1.49	1.41
2	B	301	FMN	C9A-C5A	4.19	1.51	1.42
2	D	301	FMN	C9A-C5A	4.03	1.50	1.42
2	C	301	FMN	C9A-C5A	3.91	1.50	1.42
2	C	301	FMN	C4-C4A	3.76	1.47	1.41
2	B	301	FMN	C4-C4A	3.70	1.47	1.41
2	A	301	FMN	C9A-C5A	3.23	1.49	1.42
2	D	301	FMN	C6-C5A	-3.11	1.37	1.41
2	C	301	FMN	C8-C7	3.05	1.48	1.40
2	B	301	FMN	C6-C5A	-2.84	1.37	1.41
2	D	301	FMN	C1'-N10	-2.82	1.45	1.48
2	D	301	FMN	P-O2P	-2.77	1.44	1.54
2	C	301	FMN	C1'-N10	-2.76	1.45	1.48
2	B	301	FMN	P-O2P	-2.75	1.44	1.54
2	A	301	FMN	P-O2P	-2.72	1.44	1.54
2	C	301	FMN	P-O2P	-2.69	1.44	1.54
2	B	301	FMN	C1'-N10	-2.69	1.45	1.48
2	A	301	FMN	C8-C7	2.64	1.47	1.40
2	C	301	FMN	C6-C5A	-2.57	1.37	1.41
4	D	302	NHE	C1'-N	-2.55	1.41	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	FMN	C8-C7	2.53	1.47	1.40
4	D	302	NHE	C1-N	-2.53	1.41	1.47
4	B	302	NHE	C1'-N	-2.47	1.41	1.48
2	C	301	FMN	C2-N1	-2.36	1.33	1.38
2	C	301	FMN	P-O3P	-2.35	1.45	1.54
2	B	301	FMN	P-O3P	-2.34	1.45	1.54
2	A	301	FMN	P-O3P	-2.34	1.45	1.54
2	A	301	FMN	C2-N3	-2.28	1.33	1.38
2	C	301	FMN	C9A-N10	2.21	1.41	1.38
2	C	301	FMN	C2-N3	-2.16	1.33	1.38
2	B	301	FMN	O4-C4	-2.16	1.19	1.24
2	B	301	FMN	C10-N1	2.14	1.36	1.33
2	D	301	FMN	C8-C7	2.06	1.46	1.40

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	302	NHE	O2-S-C2	-26.06	75.53	106.92
4	D	302	NHE	O1-S-C2	13.23	122.85	106.92
2	C	301	FMN	C4-N3-C2	10.65	124.14	115.14
2	B	301	FMN	C4-N3-C2	9.78	123.40	115.14
2	A	301	FMN	C4-N3-C2	9.67	123.31	115.14
2	D	301	FMN	C4-N3-C2	8.59	122.39	115.14
2	A	301	FMN	C4-C4A-C10	-8.24	114.50	119.95
4	D	302	NHE	O3-S-O2	-8.03	91.64	111.27
2	B	301	FMN	C4-C4A-C10	-7.65	114.88	119.95
4	D	302	NHE	O2-S-O1	-7.49	88.04	113.95
2	C	301	FMN	C4-C4A-C10	-7.36	115.08	119.95
4	D	302	NHE	O3-S-C2	7.13	117.30	105.77
2	C	301	FMN	C1'-N10-C9A	5.76	122.83	118.29
2	B	301	FMN	C4-C4A-N5	5.70	125.12	118.60
2	D	301	FMN	C4A-N5-C5A	5.52	122.28	116.77
2	D	301	FMN	C4-C4A-C10	-5.27	116.46	119.95
2	A	301	FMN	C4-C4A-N5	4.89	124.19	118.60
2	A	301	FMN	C4A-N5-C5A	4.82	121.58	116.77
2	C	301	FMN	C4-C4A-N5	4.78	124.06	118.60
2	C	301	FMN	C4A-N5-C5A	4.77	121.54	116.77
2	D	301	FMN	C4-C4A-N5	4.77	124.05	118.60
4	B	303	NHE	O3-S-C2	4.68	113.33	105.77
2	A	301	FMN	C1'-N10-C9A	4.62	121.93	118.29
4	B	302	NHE	C3'-C2'-C1'	-4.58	102.49	111.11
2	B	301	FMN	C4A-N5-C5A	4.49	121.26	116.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	FMN	C4A-C4-N3	-4.13	117.79	123.43
4	B	302	NHE	O2-S-C2	4.10	111.85	106.92
4	B	302	NHE	O3-S-C2	3.94	112.14	105.77
2	D	301	FMN	C4A-C4-N3	-3.93	118.06	123.43
4	B	302	NHE	O3-S-O2	-3.90	101.73	111.27
4	B	303	NHE	O2-S-C2	-3.60	102.58	106.92
2	B	301	FMN	C1'-N10-C9A	3.48	121.03	118.29
2	A	301	FMN	P-O5'-C5'	3.12	126.88	118.30
4	B	302	NHE	O1-S-C2	-3.05	103.24	106.92
2	D	301	FMN	C1'-N10-C9A	3.02	120.67	118.29
2	A	301	FMN	C4A-C4-N3	-2.98	119.36	123.43
2	A	301	FMN	O2P-P-O5'	-2.91	98.98	106.73
2	B	301	FMN	C4A-C4-N3	-2.86	119.53	123.43
2	B	301	FMN	P-O5'-C5'	2.69	125.71	118.30
4	D	302	NHE	O3-S-O1	2.56	117.52	111.27
2	D	301	FMN	C10-C4A-N5	-2.56	119.49	121.26
2	A	301	FMN	C9A-N10-C10	-2.45	118.69	121.91
4	B	303	NHE	C4'-C3'-C2'	-2.40	106.52	111.42
2	A	301	FMN	O3P-P-O2P	2.31	116.47	107.64
2	A	301	FMN	C5A-C9A-N10	2.27	119.36	117.72
2	B	301	FMN	C9A-N10-C10	-2.27	118.93	121.91
4	B	303	NHE	O3-S-O1	-2.26	105.74	111.27
2	B	301	FMN	O2'-C2'-C1'	2.24	114.99	109.59
2	C	301	FMN	O2'-C2'-C1'	2.21	114.90	109.59
2	B	301	FMN	O2P-P-O1P	2.18	119.21	110.68
4	B	302	NHE	C1-N-C1'	2.17	118.41	114.14
2	A	301	FMN	C6-C5A-N5	2.13	121.39	119.05
2	C	301	FMN	P-O5'-C5'	2.11	124.11	118.30
2	C	301	FMN	O5'-C5'-C4'	2.10	114.97	109.36
2	C	301	FMN	C9A-N10-C10	-2.04	119.23	121.91
4	D	302	NHE	C4'-C5'-C6'	-2.04	107.26	111.42

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	NHE	C1-C2-S-O2
4	B	302	NHE	C1-C2-S-O3
4	D	302	NHE	C2-C1-N-C1'
4	D	302	NHE	C1-C2-S-O1
4	D	302	NHE	C1-C2-S-O3
2	A	301	FMN	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

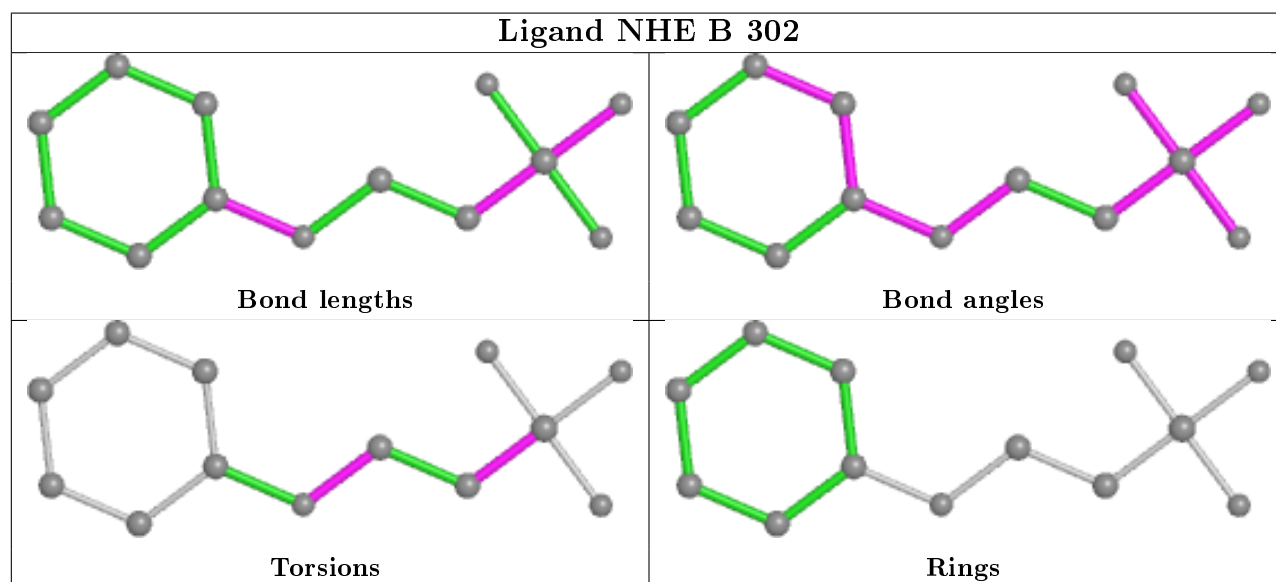
Mol	Chain	Res	Type	Atoms
4	B	303	NHE	C2-C1-N-C1'
4	B	303	NHE	C1-C2-S-O1
4	B	303	NHE	C1-C2-S-O2
4	B	303	NHE	C1-C2-S-O3
3	A	302	PE8	C15-C14-O13-C12
3	A	302	PE8	C18-C17-O16-C15
3	C	302	PE8	C17-C18-O19-C20
3	C	302	PE8	C20-C21-O22-C23
3	C	302	PE8	O7-C8-C9-O10
3	A	302	PE8	O7-C8-C9-O10
3	A	302	PE8	O19-C20-C21-O22
3	A	302	PE8	O22-C23-C24-O25
3	A	302	PE8	C12-C11-O10-C9
3	A	302	PE8	O4-C5-C6-O7
3	C	302	PE8	O16-C17-C18-O19
3	C	302	PE8	O10-C11-C12-O13
2	A	301	FMN	C4'-C5'-O5'-P
2	D	301	FMN	C4'-C5'-O5'-P
2	A	301	FMN	C2'-C3'-C4'-C5'
3	A	302	PE8	C24-C23-O22-C21
2	C	301	FMN	C4'-C5'-O5'-P
3	C	302	PE8	C12-C11-O10-C9
3	A	302	PE8	C6-C5-O4-C3
2	B	301	FMN	C2'-C3'-C4'-C5'
2	B	301	FMN	C4'-C5'-O5'-P
3	C	302	PE8	C14-C15-O16-C17
4	B	302	NHE	C1-C2-S-O1
3	C	302	PE8	O19-C20-C21-O22
3	A	302	PE8	C21-C20-O19-C18
3	A	302	PE8	C17-C18-O19-C20
2	D	301	FMN	C2'-C3'-C4'-C5'
4	B	302	NHE	C2-C1-N-C1'
2	C	301	FMN	O4'-C4'-C5'-O5'
3	C	302	PE8	C21-C20-O19-C18
3	C	302	PE8	C15-C14-O13-C12
3	A	302	PE8	O16-C17-C18-O19
3	A	302	PE8	O10-C11-C12-O13
3	A	302	PE8	O13-C14-C15-O16

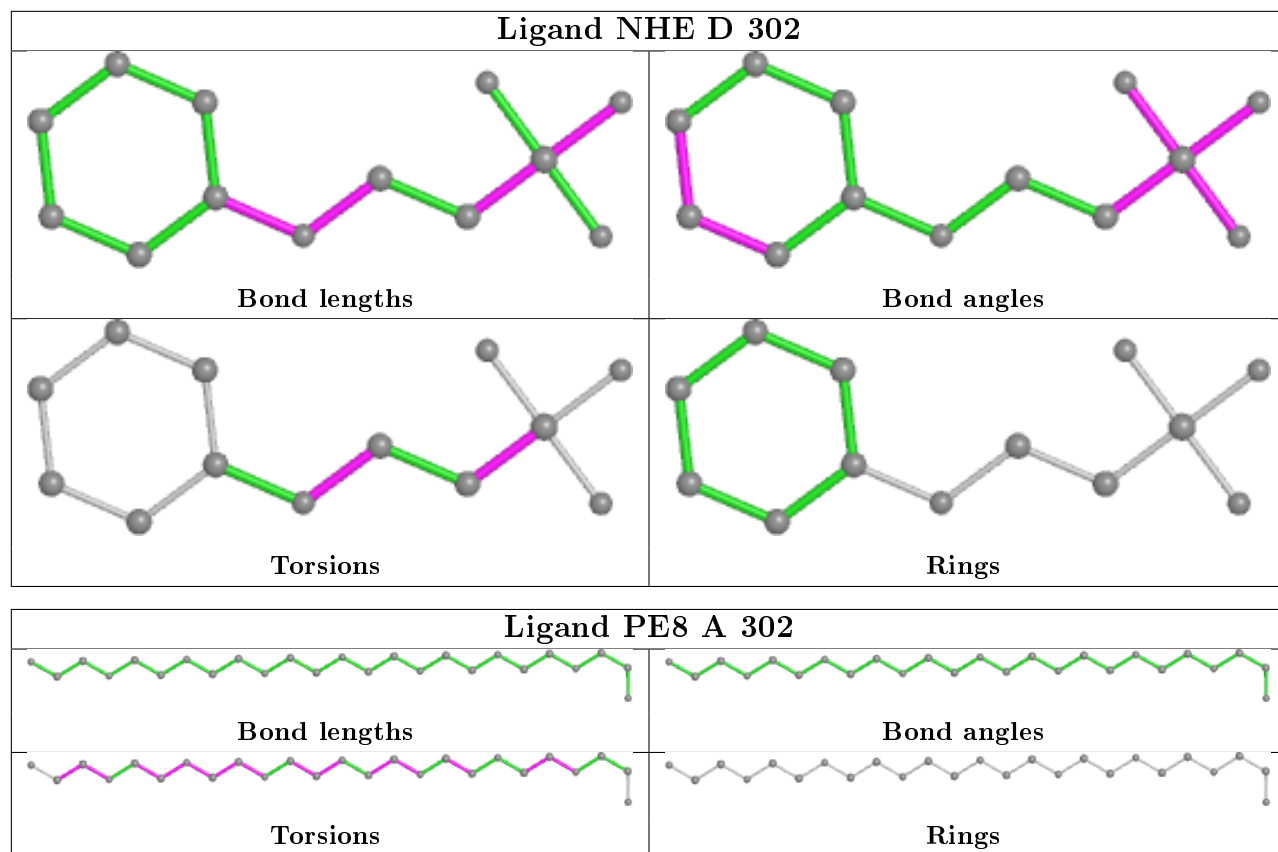
There are no ring outliers.

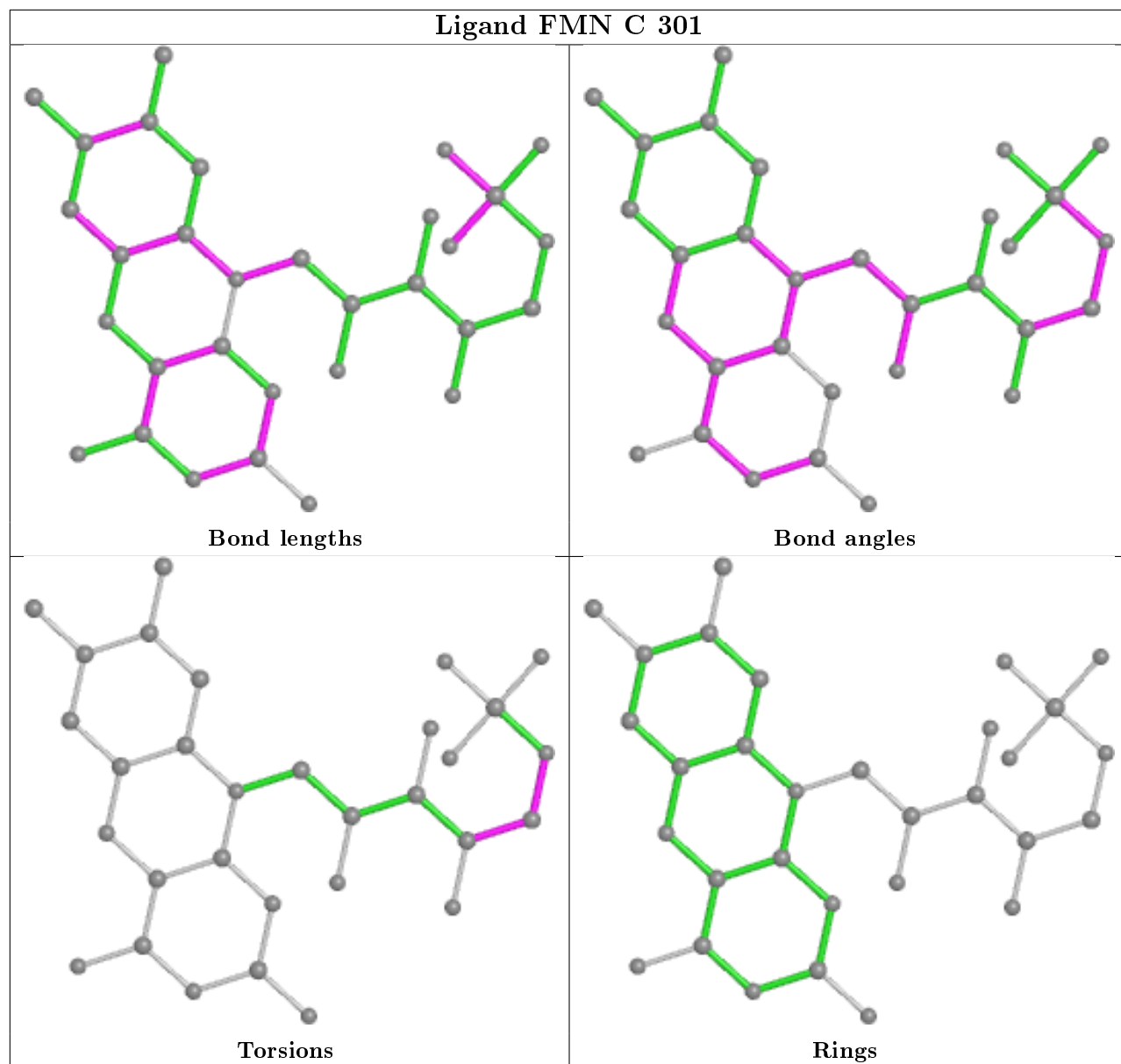
6 monomers are involved in 63 short contacts:

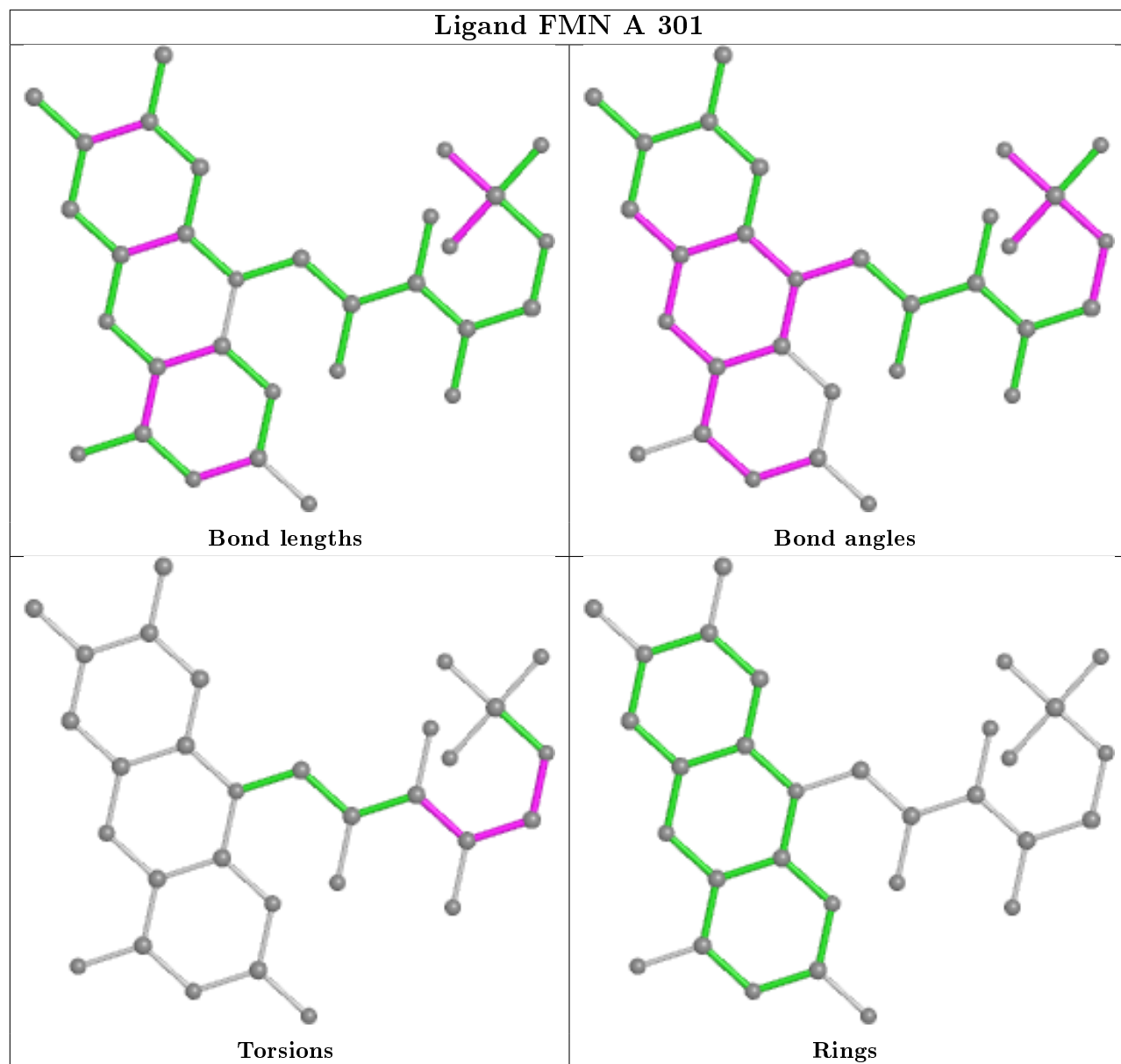
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	NHE	9	0
4	D	302	NHE	9	0
3	A	302	PE8	19	0
2	C	301	FMN	2	0
4	B	303	NHE	13	0
3	C	302	PE8	13	0

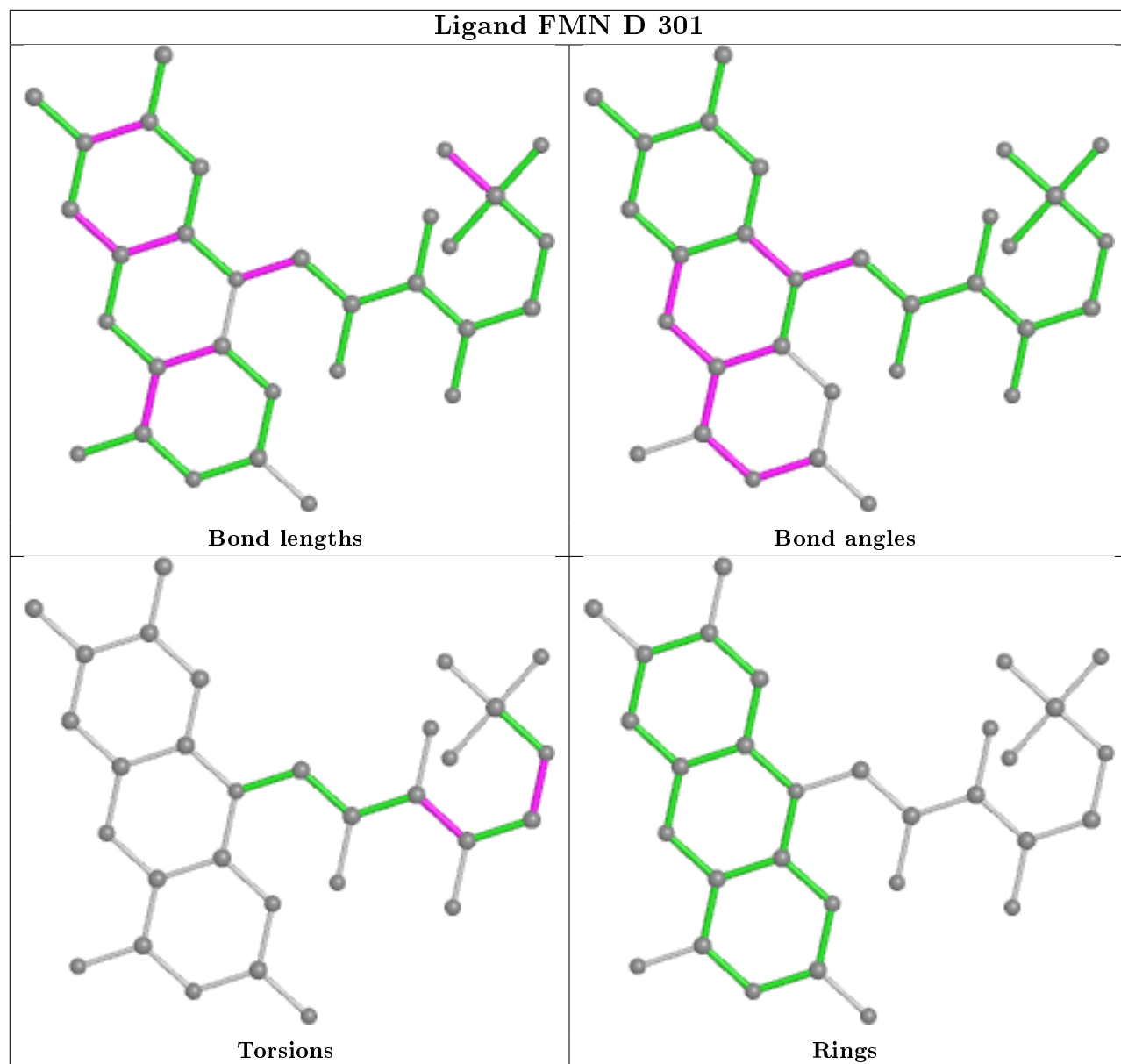
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

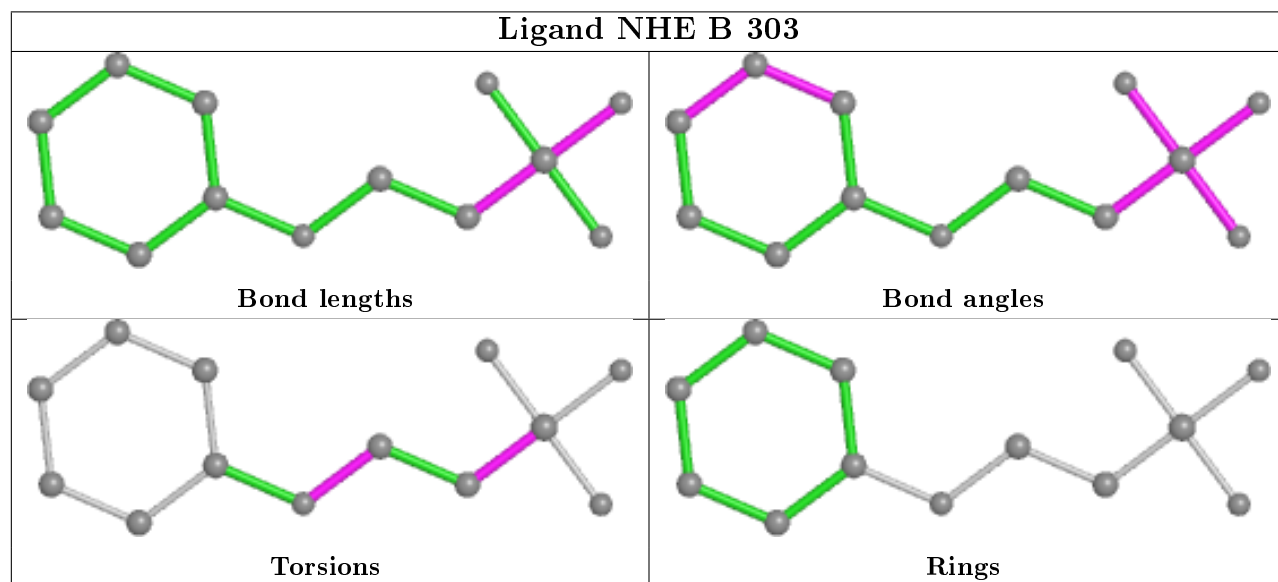
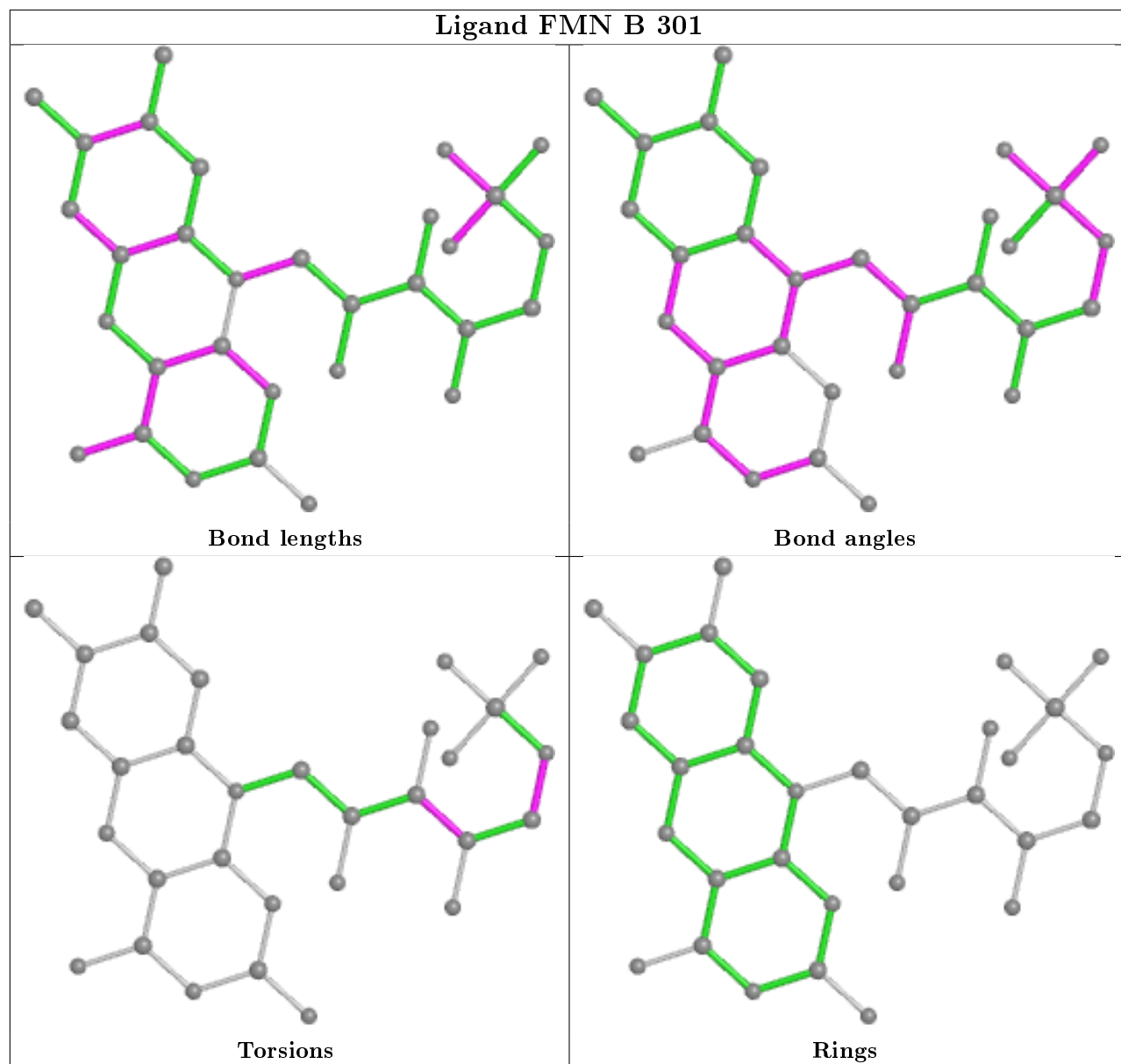


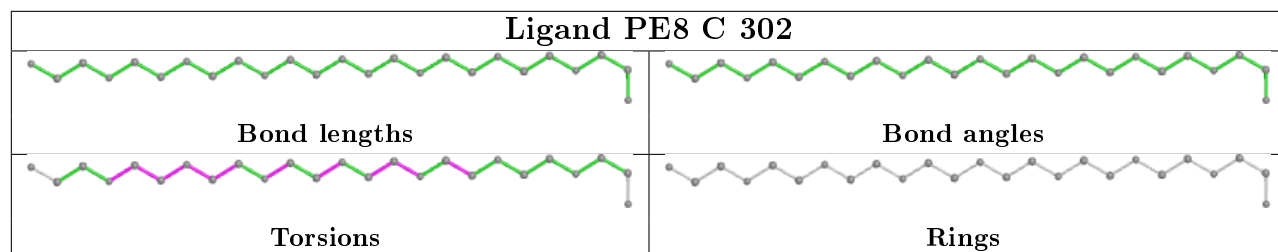












5.7 Other polymers [i](#)

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 ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

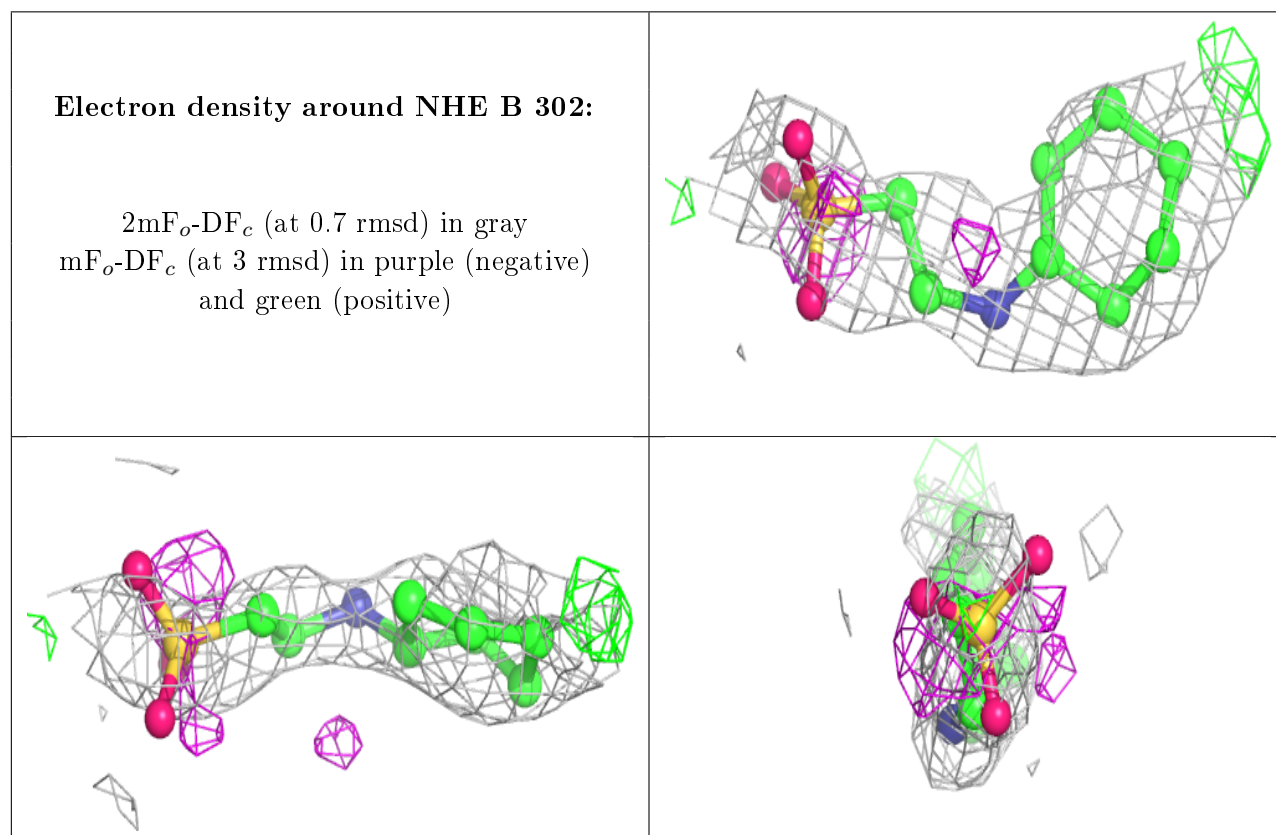
6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

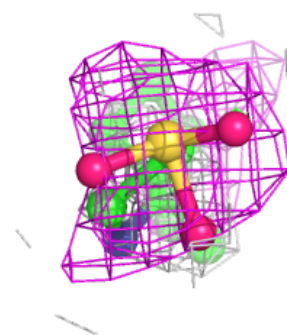
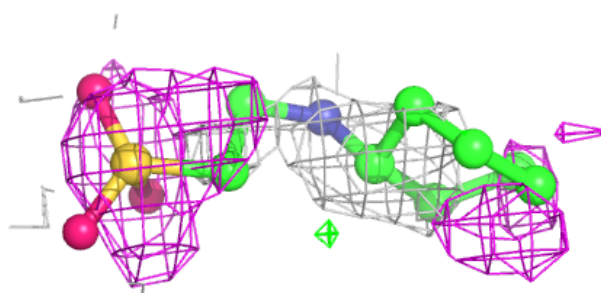
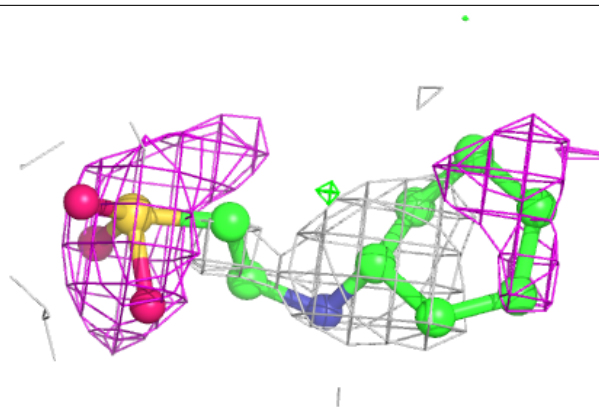
EDS failed to run properly - this section is therefore empty.

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.



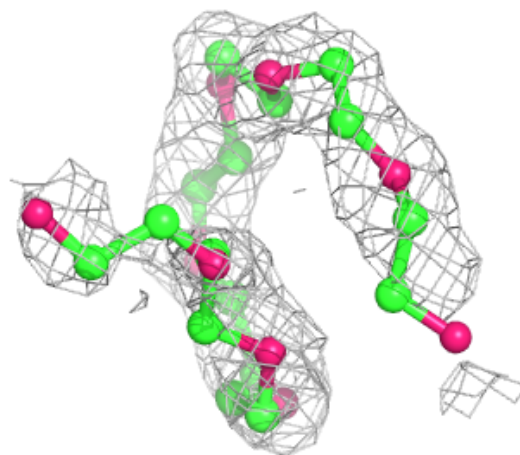
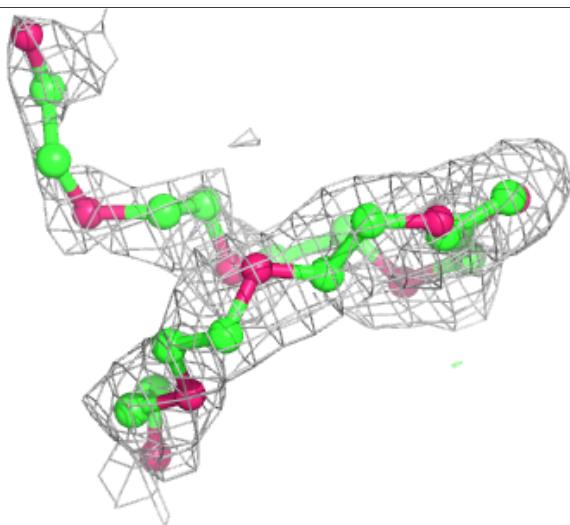
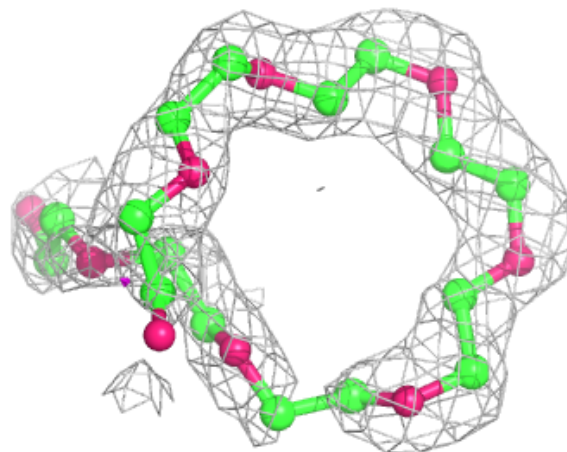
Electron density around NHE D 302:

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



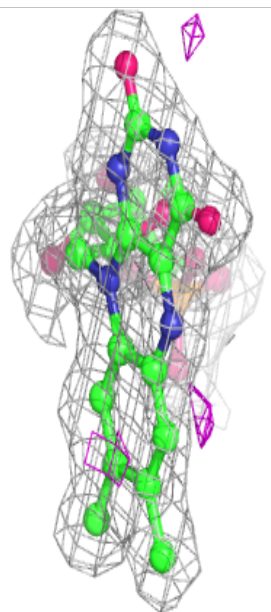
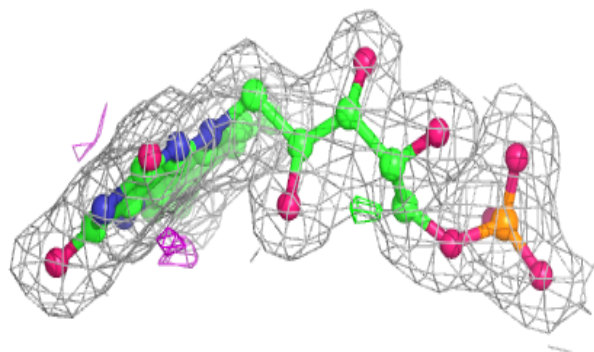
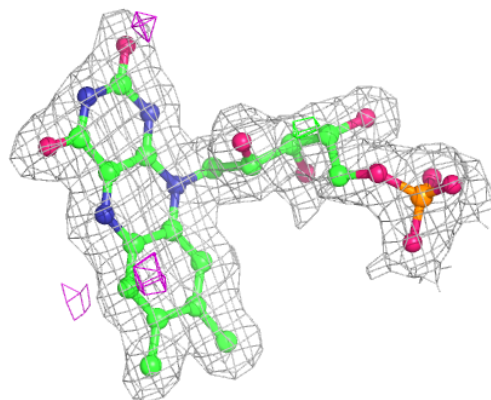
Electron density around PE8 A 302:

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



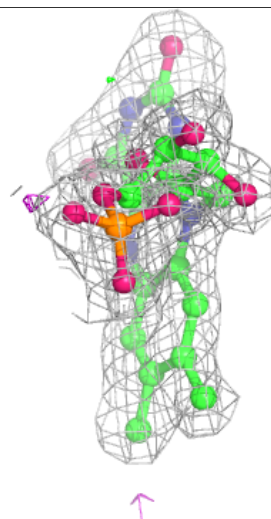
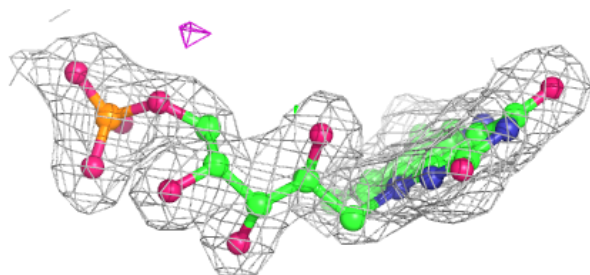
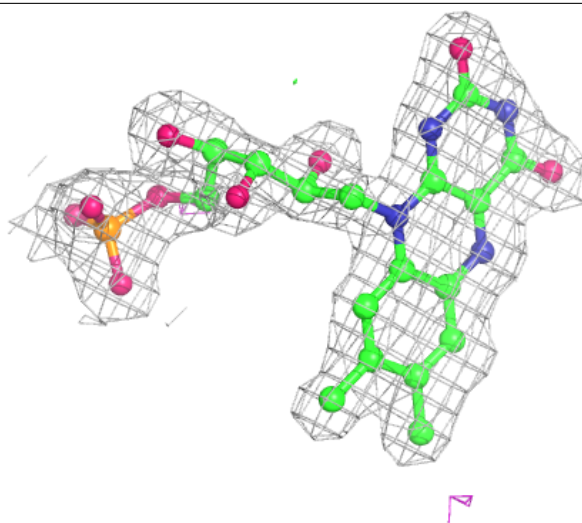
Electron density around FMN C 301:

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



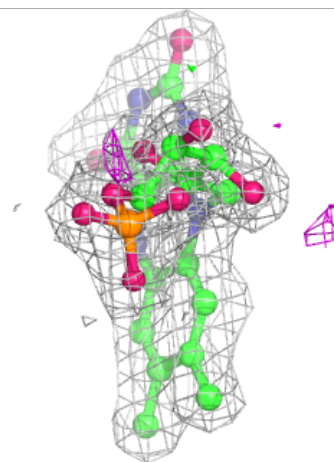
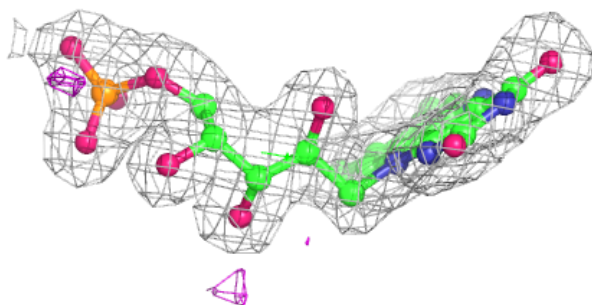
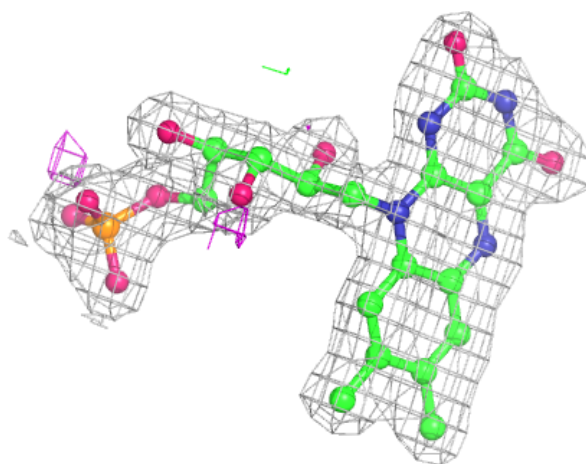
Electron density around FMN A 301:

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



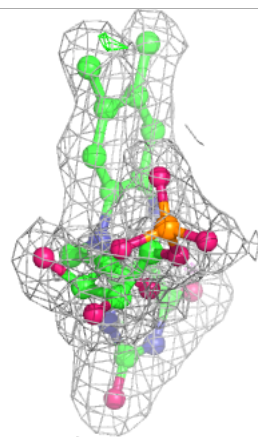
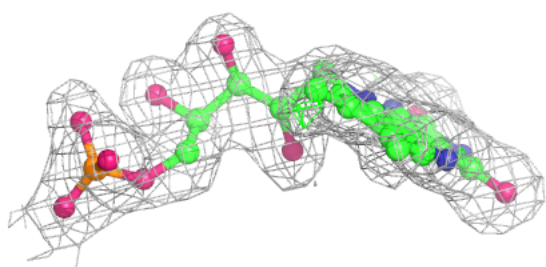
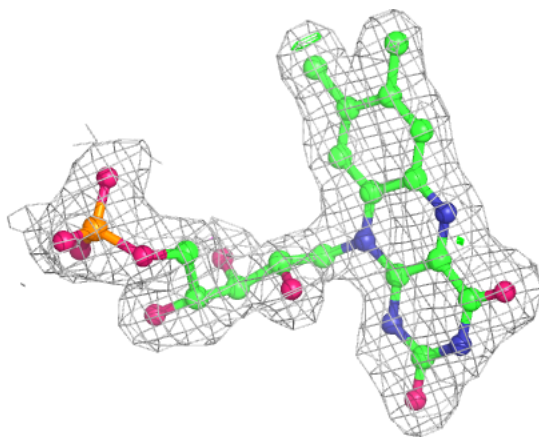
Electron density around FMN D 301:

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



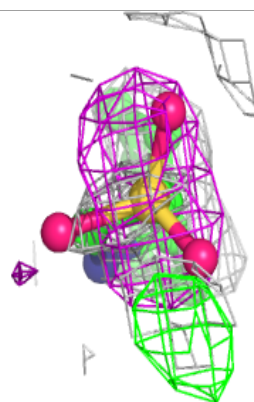
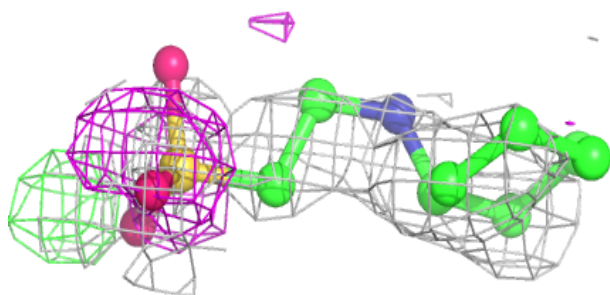
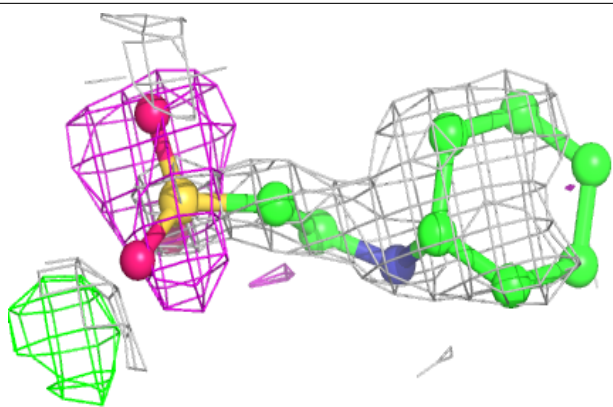
Electron density around FMN B 301:

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

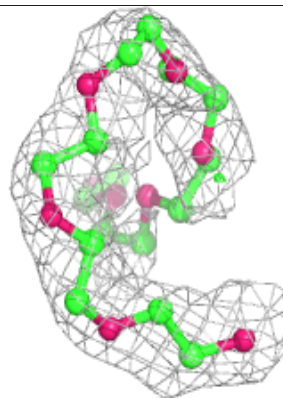
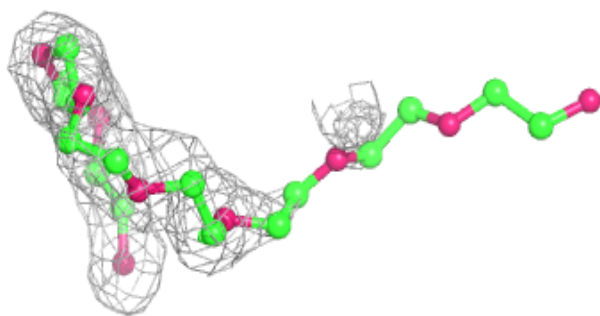
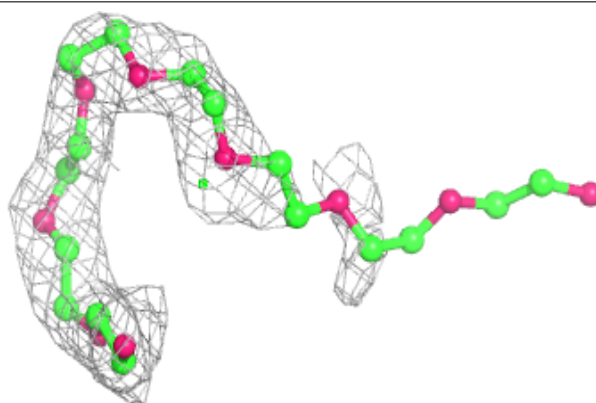


Electron density around NHE B 303:

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

**Electron density around PE8 C 302:**

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



6.5 Other polymers

EDS failed to run properly - this section is therefore empty.