



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:53 PM EDT

PDB ID : 7N2W
Title : The crystal structure of an FMN-dependent NADH-azoreductase, AzoA in complex with Red 40
Authors : Arcinas, A.J.; Fedorov, E.; Kelly, L.; Almo, S.C.; Ghosh, A.
Deposited on : 2021-05-30
Resolution : 2.65 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

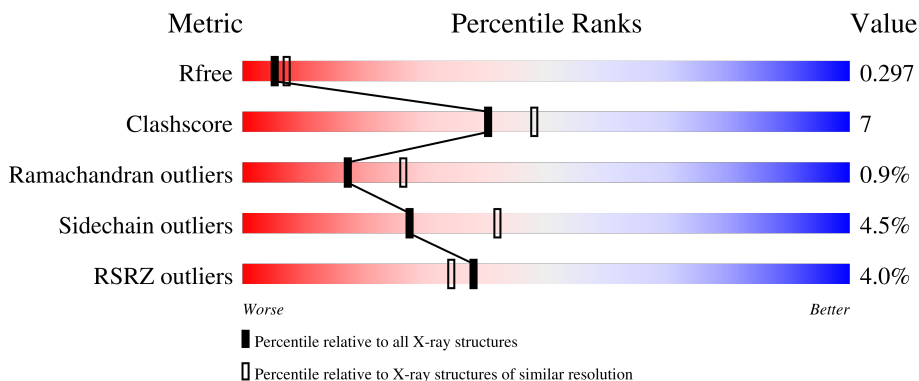
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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

Mol	Chain	Length	Quality of chain
1	A	223	 4% 68% 21% 10%
1	B	223	 3% 74% 15% 9%
1	C	223	 5% 67% 20% 10%
1	D	223	 3% 77% 13% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6291 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:quinone oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	1502	950	268	280	4	0	0	0
1	B	202	1514	957	269	284	4	0	0	0
1	C	200	1497	946	267	281	3	0	0	0
1	D	201	1490	940	265	281	4	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP A6TCS9
A	-20	HIS	-	expression tag	UNP A6TCS9
A	-19	HIS	-	expression tag	UNP A6TCS9
A	-18	HIS	-	expression tag	UNP A6TCS9
A	-17	HIS	-	expression tag	UNP A6TCS9
A	-16	HIS	-	expression tag	UNP A6TCS9
A	-15	HIS	-	expression tag	UNP A6TCS9
A	-14	SER	-	expression tag	UNP A6TCS9
A	-13	SER	-	expression tag	UNP A6TCS9
A	-12	GLY	-	expression tag	UNP A6TCS9
A	-11	VAL	-	expression tag	UNP A6TCS9
A	-10	ASP	-	expression tag	UNP A6TCS9
A	-9	LEU	-	expression tag	UNP A6TCS9
A	-8	GLY	-	expression tag	UNP A6TCS9
A	-7	THR	-	expression tag	UNP A6TCS9
A	-6	GLU	-	expression tag	UNP A6TCS9
A	-5	ASN	-	expression tag	UNP A6TCS9
A	-4	LEU	-	expression tag	UNP A6TCS9
A	-3	TYR	-	expression tag	UNP A6TCS9
A	-2	PHE	-	expression tag	UNP A6TCS9
A	-1	GLN	-	expression tag	UNP A6TCS9

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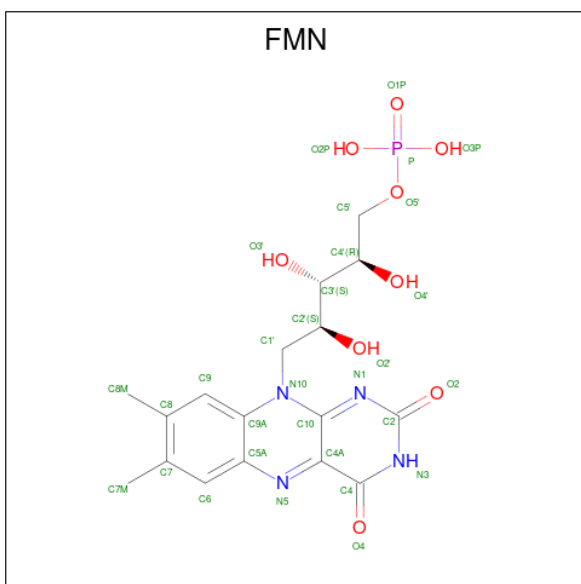
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A6TCS9
B	-21	MET	-	expression tag	UNP A6TCS9
B	-20	HIS	-	expression tag	UNP A6TCS9
B	-19	HIS	-	expression tag	UNP A6TCS9
B	-18	HIS	-	expression tag	UNP A6TCS9
B	-17	HIS	-	expression tag	UNP A6TCS9
B	-16	HIS	-	expression tag	UNP A6TCS9
B	-15	HIS	-	expression tag	UNP A6TCS9
B	-14	SER	-	expression tag	UNP A6TCS9
B	-13	SER	-	expression tag	UNP A6TCS9
B	-12	GLY	-	expression tag	UNP A6TCS9
B	-11	VAL	-	expression tag	UNP A6TCS9
B	-10	ASP	-	expression tag	UNP A6TCS9
B	-9	LEU	-	expression tag	UNP A6TCS9
B	-8	GLY	-	expression tag	UNP A6TCS9
B	-7	THR	-	expression tag	UNP A6TCS9
B	-6	GLU	-	expression tag	UNP A6TCS9
B	-5	ASN	-	expression tag	UNP A6TCS9
B	-4	LEU	-	expression tag	UNP A6TCS9
B	-3	TYR	-	expression tag	UNP A6TCS9
B	-2	PHE	-	expression tag	UNP A6TCS9
B	-1	GLN	-	expression tag	UNP A6TCS9
B	0	SER	-	expression tag	UNP A6TCS9
C	-21	MET	-	expression tag	UNP A6TCS9
C	-20	HIS	-	expression tag	UNP A6TCS9
C	-19	HIS	-	expression tag	UNP A6TCS9
C	-18	HIS	-	expression tag	UNP A6TCS9
C	-17	HIS	-	expression tag	UNP A6TCS9
C	-16	HIS	-	expression tag	UNP A6TCS9
C	-15	HIS	-	expression tag	UNP A6TCS9
C	-14	SER	-	expression tag	UNP A6TCS9
C	-13	SER	-	expression tag	UNP A6TCS9
C	-12	GLY	-	expression tag	UNP A6TCS9
C	-11	VAL	-	expression tag	UNP A6TCS9
C	-10	ASP	-	expression tag	UNP A6TCS9
C	-9	LEU	-	expression tag	UNP A6TCS9
C	-8	GLY	-	expression tag	UNP A6TCS9
C	-7	THR	-	expression tag	UNP A6TCS9
C	-6	GLU	-	expression tag	UNP A6TCS9
C	-5	ASN	-	expression tag	UNP A6TCS9
C	-4	LEU	-	expression tag	UNP A6TCS9
C	-3	TYR	-	expression tag	UNP A6TCS9

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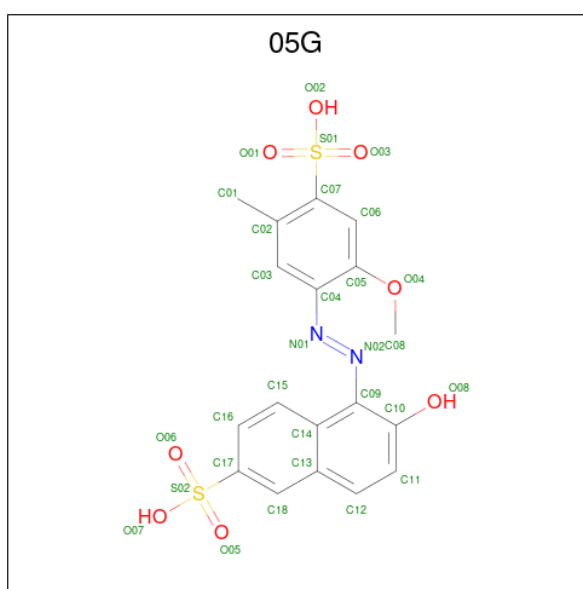
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	expression tag	UNP A6TCS9
C	-1	GLN	-	expression tag	UNP A6TCS9
C	0	SER	-	expression tag	UNP A6TCS9
D	-21	MET	-	expression tag	UNP A6TCS9
D	-20	HIS	-	expression tag	UNP A6TCS9
D	-19	HIS	-	expression tag	UNP A6TCS9
D	-18	HIS	-	expression tag	UNP A6TCS9
D	-17	HIS	-	expression tag	UNP A6TCS9
D	-16	HIS	-	expression tag	UNP A6TCS9
D	-15	HIS	-	expression tag	UNP A6TCS9
D	-14	SER	-	expression tag	UNP A6TCS9
D	-13	SER	-	expression tag	UNP A6TCS9
D	-12	GLY	-	expression tag	UNP A6TCS9
D	-11	VAL	-	expression tag	UNP A6TCS9
D	-10	ASP	-	expression tag	UNP A6TCS9
D	-9	LEU	-	expression tag	UNP A6TCS9
D	-8	GLY	-	expression tag	UNP A6TCS9
D	-7	THR	-	expression tag	UNP A6TCS9
D	-6	GLU	-	expression tag	UNP A6TCS9
D	-5	ASN	-	expression tag	UNP A6TCS9
D	-4	LEU	-	expression tag	UNP A6TCS9
D	-3	TYR	-	expression tag	UNP A6TCS9
D	-2	PHE	-	expression tag	UNP A6TCS9
D	-1	GLN	-	expression tag	UNP A6TCS9
D	0	SER	-	expression tag	UNP A6TCS9

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



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

- Molecule 3 is 6-hydroxy-5-[(E)-(2-methoxy-5-methyl-4-sulfohenyl)diazenyl]naphthalene-2-sulfonic acid (three-letter code: 05G) (formula: C₁₈H₁₆N₂O₈S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	18	2	8	2		
3	B	1	Total	C	N	O	S	0	0
			30	18	2	8	2		
3	C	1	Total	C	N	O	S	0	0
			30	18	2	8	2		
3	C	1	Total	C	N	O	S	0	0
			30	18	2	8	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	7	Total O 7 7	0	0
4	C	15	Total O 15 15	0	0
4	D	16	Total O 16 16	0	0

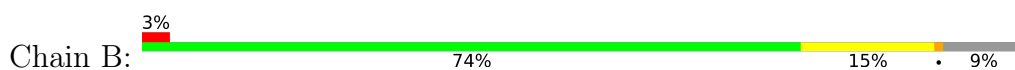
3 Residue-property plots [i](#)

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: FMN dependent NADH:quinone oxidoreductase



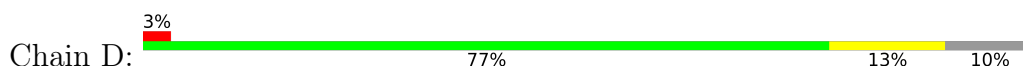
- Molecule 1: FMN dependent NADH:quinone oxidoreductase

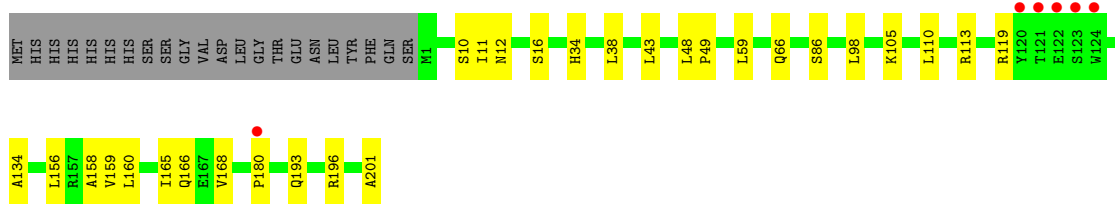


- Molecule 1: FMN dependent NADH:quinone oxidoreductase



- Molecule 1: FMN dependent NADH:quinone oxidoreductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.41Å 83.34Å 87.31Å 90.00° 100.26° 90.00°	Depositor
Resolution (Å)	19.96 – 2.65 19.96 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.2 (19.96-2.65) 96.3 (19.96-2.65)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.67Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.249 , 0.302 0.249 , 0.297	Depositor DCC
R_{free} test set	1205 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtrriage
Anisotropy	0.953	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6291	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 05G, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/1528	0.53	0/2079
1	B	0.29	0/1540	0.54	0/2096
1	C	0.28	0/1523	0.53	0/2074
1	D	0.32	0/1514	0.56	0/2061
All	All	0.29	0/6105	0.54	0/8310

There are no bond length outliers.

There are no bond angle outliers.

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	1502	0	1508	27	0
1	B	1514	0	1523	23	0
1	C	1497	0	1497	33	0
1	D	1490	0	1496	18	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	3	0
3	A	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	30	0	0	0	0
3	C	60	0	0	0	0
4	A	6	0	0	0	0
4	B	7	0	0	0	0
4	C	15	0	0	2	0
4	D	16	0	0	0	0
All	All	6291	0	6100	89	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:GLN:HG2	1:D:196:ARG:HH22	1.48	0.79
1:B:59:LEU:HB3	1:B:113:ARG:HD3	1.72	0.71
1:C:158:ALA:HB1	1:D:98:LEU:HD22	1.75	0.68
1:D:12:ASN:ND2	2:D:301:FMN:O3P	2.27	0.68
1:B:133:ARG:NH1	1:B:201:ALA:O	2.29	0.65
1:A:171:ILE:HD13	1:A:194:ILE:HD13	1.79	0.64
1:A:79:LEU:HD22	1:A:107:TRP:HE1	1.64	0.63
1:A:43:LEU:HD22	1:A:48:LEU:HD11	1.80	0.62
1:A:78:GLN:O	1:A:82:GLU:HG3	2.00	0.61
1:C:10:SER:O	1:C:44:SER:OG	2.20	0.59
1:D:166:GLN:H	1:D:166:GLN:CD	2.06	0.58
1:C:67:PRO:O	1:C:71:GLU:HG3	2.03	0.57
1:C:98:LEU:HD22	1:D:158:ALA:HB1	1.86	0.56
1:A:171:ILE:HG12	1:A:193:GLN:HB3	1.88	0.56
1:A:52:ASP:HA	1:B:11:ILE:HG21	1.89	0.55
1:D:49:PRO:HD2	1:D:110:LEU:HD11	1.88	0.55
1:A:38:LEU:HB2	1:D:38:LEU:HB2	1.90	0.54
1:D:59:LEU:HB3	1:D:113:ARG:HD3	1.90	0.54
1:B:178:ASN:HB3	1:B:182:GLY:HA3	1.90	0.54
1:C:166:GLN:N	4:C:404:HOH:O	2.38	0.53
1:A:157:ARG:NH2	1:A:168:VAL:O	2.41	0.53
1:A:53:ARG:HD2	1:B:11:ILE:O	2.08	0.53
1:B:29:ARG:NH2	1:B:201:ALA:OXT	2.41	0.53
1:B:29:ARG:NH1	1:B:36:ASP:OD1	2.41	0.52
1:C:29:ARG:NH2	1:C:201:ALA:OXT	2.42	0.52
1:C:56:PHE:CE2	2:D:301:FMN:HM82	2.44	0.52
1:C:178:ASN:HB2	1:C:182:GLY:HA3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:THR:HB	1:B:163:MET:HG2	1.92	0.51
1:A:192:ALA:O	1:A:196:ARG:HG3	2.10	0.51
1:D:10:SER:OG	2:D:301:FMN:O3P	2.28	0.49
1:A:178:ASN:HB2	1:A:182:GLY:HA3	1.94	0.49
1:A:108:PHE:HA	1:A:111:VAL:HG12	1.95	0.48
1:C:43:LEU:HA	1:C:46:MET:HG3	1.94	0.48
1:A:51:LEU:HD21	1:A:56:PHE:HB2	1.94	0.48
1:B:145:GLN:HB2	1:B:174:GLU:OE2	2.14	0.47
1:B:145:GLN:HG3	1:B:172:TYR:CE2	2.49	0.47
1:C:113:ARG:HB3	1:C:116:GLU:HB2	1.97	0.47
1:C:153:THR:HB	1:C:154:PRO:HD3	1.95	0.47
1:B:143:ILE:HG23	1:B:174:GLU:HB2	1.96	0.47
1:C:133:ARG:NH1	1:C:201:ALA:O	2.48	0.47
1:C:171:ILE:HD13	1:C:194:ILE:HG13	1.97	0.47
1:C:53:ARG:HD3	1:D:11:ILE:O	2.15	0.47
1:A:158:ALA:HB1	1:B:98:LEU:HD13	1.97	0.46
1:A:122:GLU:H	1:A:122:GLU:HG3	1.51	0.46
1:C:66:GLN:HG3	1:C:67:PRO:HD2	1.97	0.46
1:B:88:LEU:HD11	1:B:135:VAL:HG23	1.97	0.46
1:A:51:LEU:HD12	1:A:109:ASP:HB3	1.97	0.46
1:C:134:ALA:HB3	1:C:168:VAL:HG22	1.97	0.46
1:B:43:LEU:HD22	1:B:48:LEU:HD11	1.98	0.45
1:B:178:ASN:OD1	1:B:180:PRO:HD2	2.16	0.45
1:C:25:PHE:CE2	1:C:29:ARG:HD2	2.51	0.45
1:C:159:VAL:HA	1:D:98:LEU:HD13	1.99	0.45
1:A:99:ASN:HB2	1:B:155:TYR:CE1	2.52	0.45
1:C:190:ALA:O	1:C:193:GLN:N	2.49	0.45
1:A:199:VAL:O	1:A:201:ALA:N	2.49	0.45
1:C:183:ARG:NH1	4:C:403:HOH:O	2.34	0.45
1:B:84:LYS:NZ	1:B:116:GLU:O	2.43	0.44
1:D:193:GLN:HG2	1:D:196:ARG:NH2	2.24	0.44
1:C:124:TRP:HZ3	1:C:162:LEU:HA	1.82	0.44
1:C:120:TYR:HB2	1:C:125:PRO:HG3	2.00	0.44
1:C:124:TRP:CE3	1:C:125:PRO:HD2	2.53	0.44
1:A:66:GLN:HB3	1:A:69:ILE:HB	2.00	0.44
1:C:11:ILE:HG12	1:C:96:TYR:CE2	2.53	0.44
1:B:64:ASP:OD2	1:B:66:GLN:HB2	2.18	0.43
1:A:11:ILE:O	1:B:53:ARG:HB2	2.18	0.43
1:A:98:LEU:HD22	1:B:158:ALA:HB1	2.00	0.43
1:B:66:GLN:NE2	1:B:67:PRO:HD2	2.33	0.43
1:D:134:ALA:HB3	1:D:168:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:THR:HG22	1:A:106:LYS:HD2	2.01	0.43
1:A:144:HIS:N	1:A:174:GLU:OE2	2.49	0.43
1:C:48:LEU:O	1:C:106:LYS:HE2	2.19	0.43
1:A:180:PRO:HB2	1:A:181:HIS:H	1.70	0.42
1:C:183:ARG:O	1:C:187:ILE:HG13	2.19	0.42
1:D:34:HIS:CE1	1:D:201:ALA:HB2	2.54	0.42
1:A:153:THR:O	1:A:157:ARG:HG3	2.19	0.42
1:C:124:TRP:HA	1:C:125:PRO:HD3	1.87	0.42
1:D:156:LEU:HA	1:D:159:VAL:HG12	2.02	0.42
1:C:199:VAL:N	1:C:200:PRO:HD2	2.34	0.42
1:D:160:LEU:HB3	1:D:165:ILE:HB	2.02	0.42
1:A:100:VAL:HG12	1:A:152:VAL:HG13	2.02	0.42
1:C:100:VAL:HG12	1:C:152:VAL:HG22	2.00	0.42
1:C:77:ASP:OD1	1:C:113:ARG:NH1	2.53	0.41
1:C:180:PRO:HB2	1:C:181:HIS:H	1.77	0.41
1:C:199:VAL:H	1:C:200:PRO:HD2	1.86	0.41
1:C:99:ASN:HB3	1:D:105:LYS:HE2	2.01	0.41
1:A:95:MET:HG2	1:A:98:LEU:HA	2.03	0.41
1:D:43:LEU:HD22	1:D:48:LEU:HD11	2.02	0.40
1:B:181:HIS:CD2	1:B:181:HIS:H	2.39	0.40
1:B:69:ILE:O	1:B:73:VAL:HG23	2.21	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	199/223 (89%)	190 (96%)	6 (3%)	3 (2%)	10	15
1	B	200/223 (90%)	187 (94%)	12 (6%)	1 (0%)	29	43
1	C	198/223 (89%)	187 (94%)	9 (4%)	2 (1%)	15	23
1	D	199/223 (89%)	187 (94%)	11 (6%)	1 (0%)	29	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	796/892 (89%)	751 (94%)	38 (5%)	7 (1%)	17	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	PRO
1	C	200	PRO
1	A	123	SER
1	A	180	PRO
1	C	180	PRO
1	D	180	PRO
1	A	200	PRO

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	150/177 (85%)	141 (94%)	9 (6%)	19	30
1	B	153/177 (86%)	146 (95%)	7 (5%)	27	41
1	C	150/177 (85%)	143 (95%)	7 (5%)	26	40
1	D	150/177 (85%)	146 (97%)	4 (3%)	44	63
All	All	603/708 (85%)	576 (96%)	27 (4%)	27	42

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	26	LEU
1	A	53	ARG
1	A	86	SER
1	A	119	ARG
1	A	122	GLU
1	A	139	SER
1	A	157	ARG

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Mol	Chain	Res	Type
1	A	189	SER
1	B	44	SER
1	B	53	ARG
1	B	60	ARG
1	B	119	ARG
1	B	140	ARG
1	B	145	GLN
1	B	177	ASP
1	C	37	ARG
1	C	46	MET
1	C	53	ARG
1	C	124	TRP
1	C	145	GLN
1	C	181	HIS
1	C	189	SER
1	D	16	SER
1	D	66	GLN
1	D	86	SER
1	D	119	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	B	66	GLN
1	B	181	HIS
1	D	30	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 monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	C	301	-	33,33,33	1.08	2 (6%)	48,50,50	1.18	6 (12%)
3	05G	C	303	-	31,32,32	3.28	8 (25%)	46,49,49	2.06	12 (26%)
3	05G	C	302	-	31,32,32	3.36	11 (35%)	46,49,49	1.94	10 (21%)
3	05G	A	302	-	31,32,32	3.42	11 (35%)	46,49,49	1.86	11 (23%)
2	FMN	A	301	-	33,33,33	1.08	2 (6%)	48,50,50	1.18	7 (14%)
2	FMN	D	301	-	33,33,33	1.09	2 (6%)	48,50,50	1.24	8 (16%)
3	05G	B	301	-	31,32,32	3.37	11 (35%)	46,49,49	2.09	14 (30%)
2	FMN	B	302	-	33,33,33	1.07	2 (6%)	48,50,50	1.20	7 (14%)

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	301	-	-	0/18/18/18	0/3/3/3
3	05G	C	303	-	-	5/19/19/19	0/3/3/3
3	05G	C	302	-	-	12/19/19/19	0/3/3/3
3	05G	A	302	-	-	4/19/19/19	0/3/3/3
2	FMN	A	301	-	-	3/18/18/18	0/3/3/3
2	FMN	D	301	-	-	4/18/18/18	0/3/3/3
3	05G	B	301	-	-	6/19/19/19	0/3/3/3
2	FMN	B	302	-	-	0/18/18/18	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	05G	C06-C07	9.44	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	05G	C06-C07	9.37	1.53	1.39
3	B	301	05G	C03-C02	9.35	1.53	1.39
3	C	302	05G	C06-C07	9.29	1.53	1.39
3	C	302	05G	C03-C02	9.12	1.52	1.39
3	A	302	05G	C03-C02	8.99	1.52	1.39
3	C	303	05G	C06-C07	8.21	1.51	1.39
3	C	303	05G	C03-C02	8.20	1.51	1.39
3	C	303	05G	C02-C07	-7.75	1.31	1.40
3	A	302	05G	C02-C07	-7.12	1.32	1.40
3	A	302	05G	C05-C04	6.92	1.52	1.40
3	C	302	05G	C05-C04	6.82	1.52	1.40
3	B	301	05G	C05-C04	6.59	1.52	1.40
3	C	303	05G	C05-C04	6.21	1.51	1.40
3	C	303	05G	C03-C04	-6.14	1.30	1.40
3	C	302	05G	C02-C07	-6.13	1.33	1.40
3	B	301	05G	C02-C07	-6.07	1.33	1.40
3	A	302	05G	C03-C04	-5.47	1.31	1.40
3	C	302	05G	C03-C04	-5.20	1.31	1.40
3	B	301	05G	C03-C04	-5.15	1.31	1.40
3	C	303	05G	C06-C05	-4.15	1.31	1.38
2	C	301	FMN	C4A-N5	3.92	1.38	1.30
2	A	301	FMN	C4A-N5	3.92	1.38	1.30
2	B	302	FMN	C4A-N5	3.91	1.38	1.30
2	D	301	FMN	C4A-N5	3.88	1.38	1.30
3	C	302	05G	N02-N01	3.69	1.41	1.24
3	B	301	05G	N02-N01	3.68	1.41	1.24
3	C	302	05G	C06-C05	-3.68	1.32	1.38
3	A	302	05G	N02-N01	3.68	1.41	1.24
3	B	301	05G	C06-C05	-3.50	1.32	1.38
3	C	303	05G	N02-N01	3.45	1.40	1.24
3	A	302	05G	C06-C05	-3.39	1.32	1.38
2	A	301	FMN	C10-N1	2.68	1.38	1.33
2	C	301	FMN	C10-N1	2.60	1.38	1.33
2	D	301	FMN	C10-N1	2.56	1.38	1.33
2	B	302	FMN	C10-N1	2.52	1.38	1.33
3	B	301	05G	C09-C14	-2.34	1.39	1.43
3	C	302	05G	C17-S02	2.30	1.82	1.77
3	A	302	05G	C17-S02	2.28	1.81	1.77
3	C	303	05G	C17-S02	2.26	1.81	1.77
3	C	302	05G	C09-C14	-2.23	1.39	1.43
3	A	302	05G	C09-C14	-2.23	1.39	1.43
3	B	301	05G	O08-C10	2.17	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	05G	O04-C05	2.17	1.40	1.37
3	C	302	05G	O04-C05	2.16	1.40	1.37
3	C	302	05G	O08-C10	2.15	1.40	1.36
3	B	301	05G	C17-S02	2.09	1.81	1.77
3	A	302	05G	O08-C10	2.06	1.40	1.36
3	A	302	05G	O04-C05	2.03	1.40	1.37

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	05G	O01-S01-C07	6.82	118.04	106.51
3	B	301	05G	O01-S01-C07	6.60	117.67	106.51
3	C	303	05G	C03-C02-C07	5.90	121.07	116.94
3	C	303	05G	O03-S01-C07	5.56	115.92	106.51
3	A	302	05G	O01-S01-C07	4.98	114.93	106.51
3	C	303	05G	C10-C09-N02	-4.41	119.88	124.20
3	B	301	05G	O03-S01-C07	4.14	113.51	106.51
3	A	302	05G	O03-S01-C07	4.08	113.41	106.51
3	A	302	05G	C10-C09-N02	-3.98	120.29	124.20
3	B	301	05G	C03-C02-C07	3.98	119.72	116.94
3	C	302	05G	C03-C02-C07	3.67	119.51	116.94
3	B	301	05G	O06-S02-C17	3.66	115.08	106.65
3	B	301	05G	O05-S02-C17	3.65	115.05	106.65
3	C	302	05G	O03-S01-C07	3.54	112.49	106.51
3	A	302	05G	C03-C02-C07	3.43	119.34	116.94
3	C	303	05G	O06-S02-C17	3.39	114.45	106.65
3	C	302	05G	C10-C09-N02	-3.30	120.97	124.20
3	A	302	05G	O05-S02-C17	3.26	114.15	106.65
3	B	301	05G	C15-C14-C09	-3.23	118.10	123.74
3	C	303	05G	C04-N01-N02	3.23	122.01	114.56
3	C	303	05G	O05-S02-C17	3.19	113.98	106.65
3	A	302	05G	O06-S02-C17	3.15	113.89	106.65
3	C	302	05G	O06-S02-C17	3.13	113.85	106.65
2	B	302	FMN	C4-N3-C2	-3.11	119.90	125.64
2	D	301	FMN	C4-N3-C2	-3.00	120.09	125.64
3	C	302	05G	O05-S02-C17	2.98	113.51	106.65
2	C	301	FMN	C4-N3-C2	-2.98	120.14	125.64
3	A	302	05G	C01-C02-C07	-2.97	121.25	124.16
3	C	302	05G	O07-S02-C17	2.96	114.34	106.69
2	A	301	FMN	C4-N3-C2	-2.96	120.18	125.64
3	C	303	05G	O07-S02-C17	2.88	114.13	106.69
3	A	302	05G	O07-S02-C17	2.84	114.02	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	05G	C08-O04-C05	-2.82	113.27	117.53
2	B	302	FMN	C4A-C4-N3	2.68	119.99	113.19
2	A	301	FMN	C4A-C4-N3	2.67	119.98	113.19
2	C	301	FMN	C4A-C4-N3	2.64	119.89	113.19
2	D	301	FMN	C4A-C4-N3	2.61	119.81	113.19
3	C	302	05G	C15-C14-C09	-2.54	119.31	123.74
2	C	301	FMN	O4-C4-C4A	-2.53	119.89	126.60
3	B	301	05G	C09-N02-N01	2.53	123.07	117.04
2	B	302	FMN	C4A-C10-N10	2.52	120.17	116.48
2	B	302	FMN	C10-C4A-N5	-2.49	119.56	124.86
3	B	301	05G	C16-C17-S02	-2.47	116.43	119.79
2	D	301	FMN	C10-C4A-N5	-2.46	119.64	124.86
2	D	301	FMN	C9A-C5A-N5	-2.45	119.76	122.43
2	A	301	FMN	O4-C4-C4A	-2.45	120.10	126.60
2	A	301	FMN	C4A-C10-N10	2.42	120.02	116.48
3	B	301	05G	C18-C17-S02	2.42	124.06	119.89
2	D	301	FMN	C4A-C10-N10	2.40	119.99	116.48
3	B	301	05G	C12-C11-C10	2.37	122.66	120.32
2	B	302	FMN	O4-C4-C4A	-2.33	120.43	126.60
3	C	302	05G	O04-C05-C04	2.32	119.88	115.66
2	C	301	FMN	C4A-C10-N10	2.30	119.84	116.48
2	C	301	FMN	C10-C4A-N5	-2.30	119.98	124.86
2	D	301	FMN	C4'-C3'-C2'	-2.30	108.59	113.36
2	A	301	FMN	C10-C4A-N5	-2.29	119.99	124.86
2	D	301	FMN	O4-C4-C4A	-2.28	120.55	126.60
2	B	302	FMN	C4A-C10-N1	-2.28	119.45	124.73
3	C	302	05G	C09-N02-N01	2.24	122.38	117.04
3	C	303	05G	C01-C02-C07	-2.21	122.00	124.16
2	C	301	FMN	C9A-C5A-N5	-2.20	120.04	122.43
3	A	302	05G	O04-C05-C04	2.18	119.63	115.66
3	C	303	05G	O04-C05-C06	-2.18	120.37	124.12
2	A	301	FMN	C9A-C5A-N5	-2.17	120.08	122.43
2	A	301	FMN	C4A-C10-N1	-2.17	119.70	124.73
3	C	303	05G	C14-C09-N02	2.17	120.86	115.81
3	A	302	05G	C15-C14-C09	-2.16	119.98	123.74
3	B	301	05G	C09-C14-C13	2.16	121.83	118.84
2	B	302	FMN	C9A-C5A-N5	-2.15	120.09	122.43
3	B	301	05G	C15-C16-C17	2.14	122.69	119.74
3	C	303	05G	O03-S01-O01	-2.12	101.84	112.86
3	B	301	05G	C16-C15-C14	-2.11	118.20	121.13
2	D	301	FMN	C4A-C10-N1	-2.11	119.84	124.73
3	B	301	05G	C04-N01-N02	2.03	119.25	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	05G	C08-O04-C05	-2.00	114.50	117.53

There are no chirality outliers.

All (34) torsion outliers are listed below:

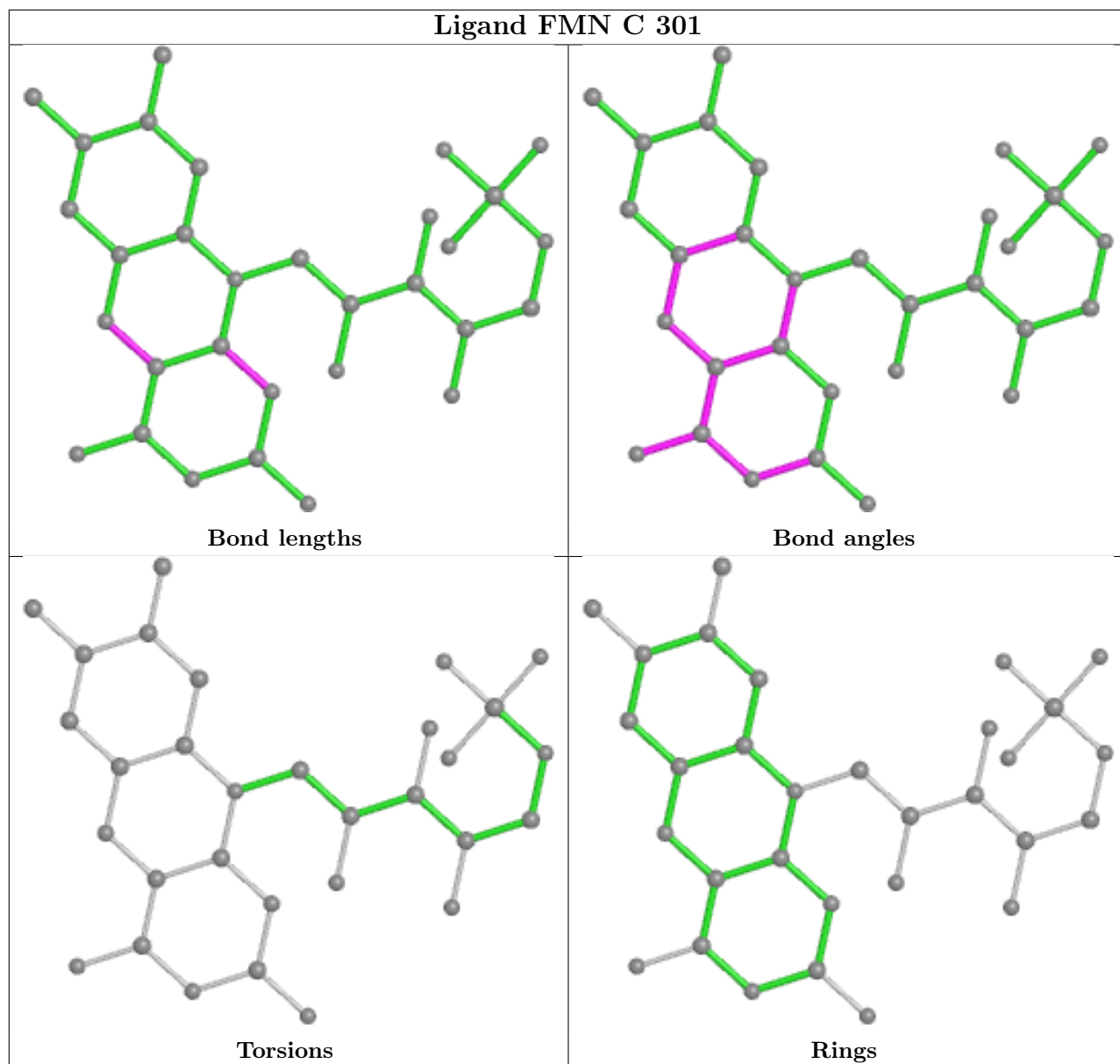
Mol	Chain	Res	Type	Atoms
2	A	301	FMN	C5'-O5'-P-O1P
3	A	302	05G	C14-C09-N02-N01
3	B	301	05G	C06-C07-S01-O01
3	B	301	05G	C06-C07-S01-O03
3	C	302	05G	C02-C07-S01-O01
3	C	302	05G	C02-C07-S01-O03
3	C	302	05G	C06-C07-S01-O01
3	C	302	05G	C06-C07-S01-O02
3	C	302	05G	C06-C07-S01-O03
3	C	303	05G	C03-C04-N01-N02
3	C	302	05G	C03-C04-N01-N02
3	A	302	05G	C03-C04-N01-N02
3	A	302	05G	C05-C04-N01-N02
2	D	301	FMN	O3'-C3'-C4'-O4'
3	B	301	05G	C02-C07-S01-O01
3	C	303	05G	C05-C04-N01-N02
2	D	301	FMN	C2'-C3'-C4'-O4'
3	C	302	05G	C05-C04-N01-N02
3	B	301	05G	C02-C07-S01-O03
2	D	301	FMN	C2'-C3'-C4'-C5'
2	D	301	FMN	O3'-C3'-C4'-C5'
3	C	303	05G	C04-C05-O04-C08
3	C	302	05G	C04-C05-O04-C08
3	C	303	05G	C06-C05-O04-C08
3	B	301	05G	C02-C07-S01-O02
3	B	301	05G	C06-C07-S01-O02
3	C	302	05G	C02-C07-S01-O02
3	C	302	05G	C06-C05-O04-C08
3	C	302	05G	C04-N01-N02-C09
2	A	301	FMN	C5'-O5'-P-O2P
3	A	302	05G	C10-C09-N02-N01
3	C	302	05G	C10-C09-N02-N01
3	C	303	05G	C14-C09-N02-N01
2	A	301	FMN	O4'-C4'-C5'-O5'

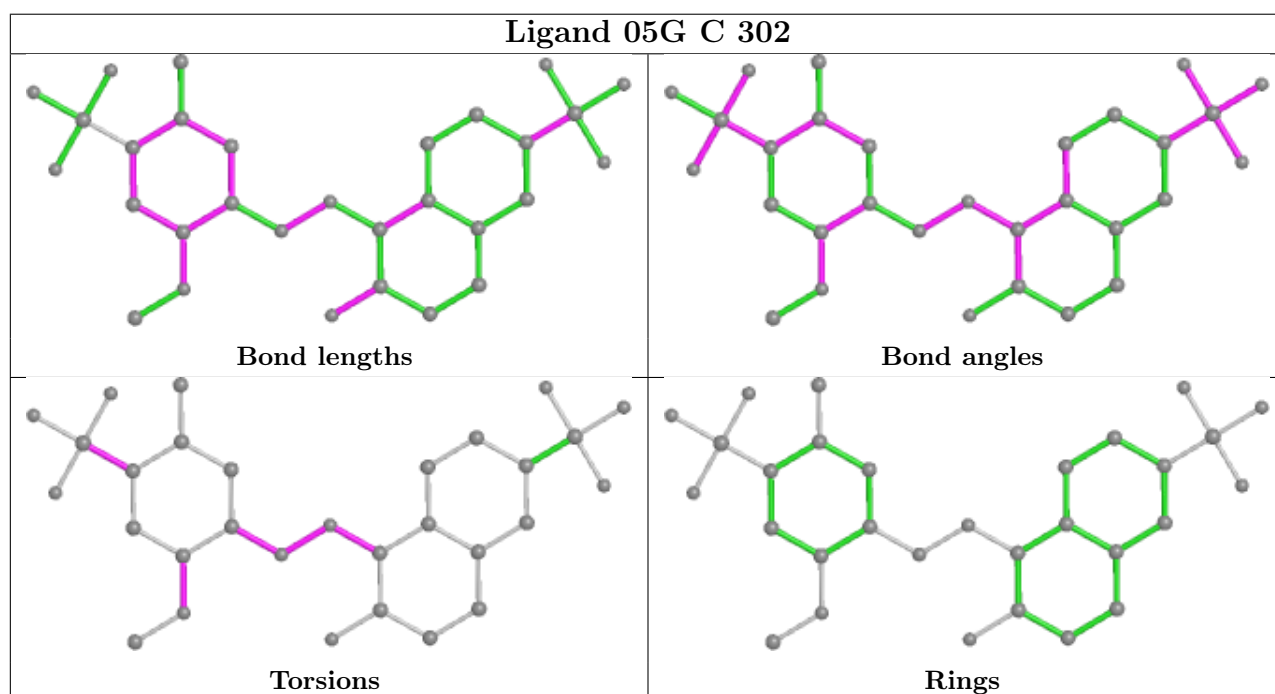
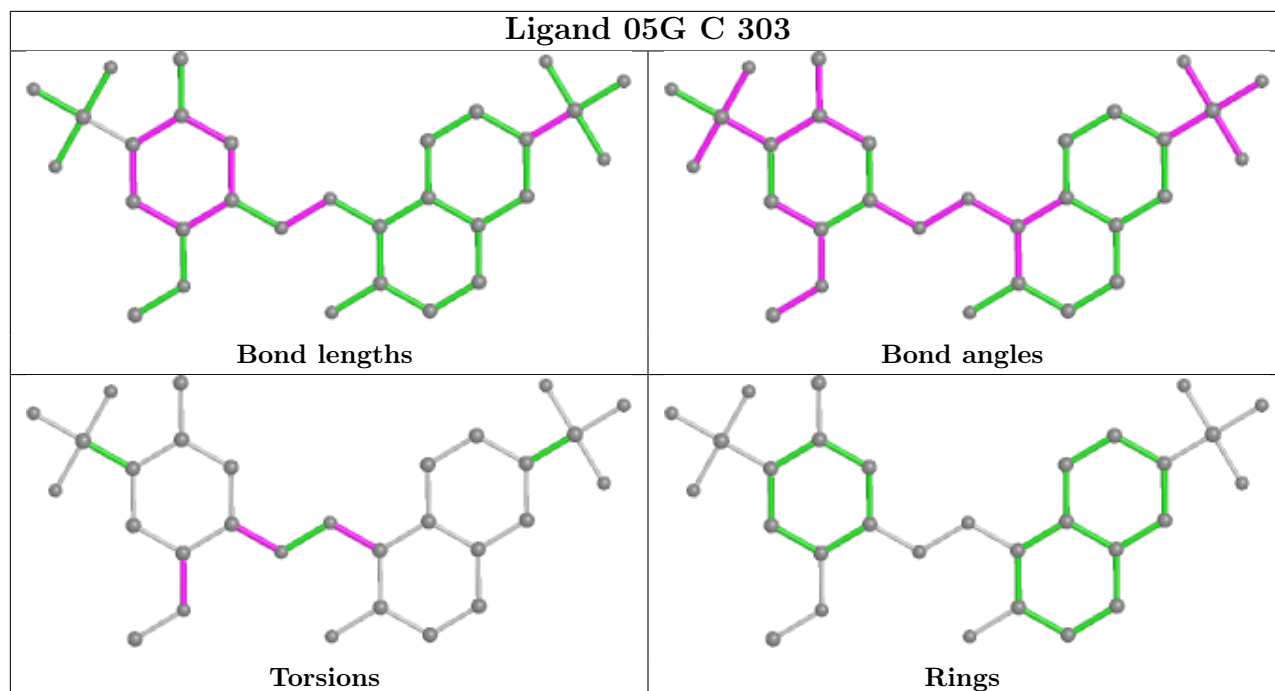
There are no ring outliers.

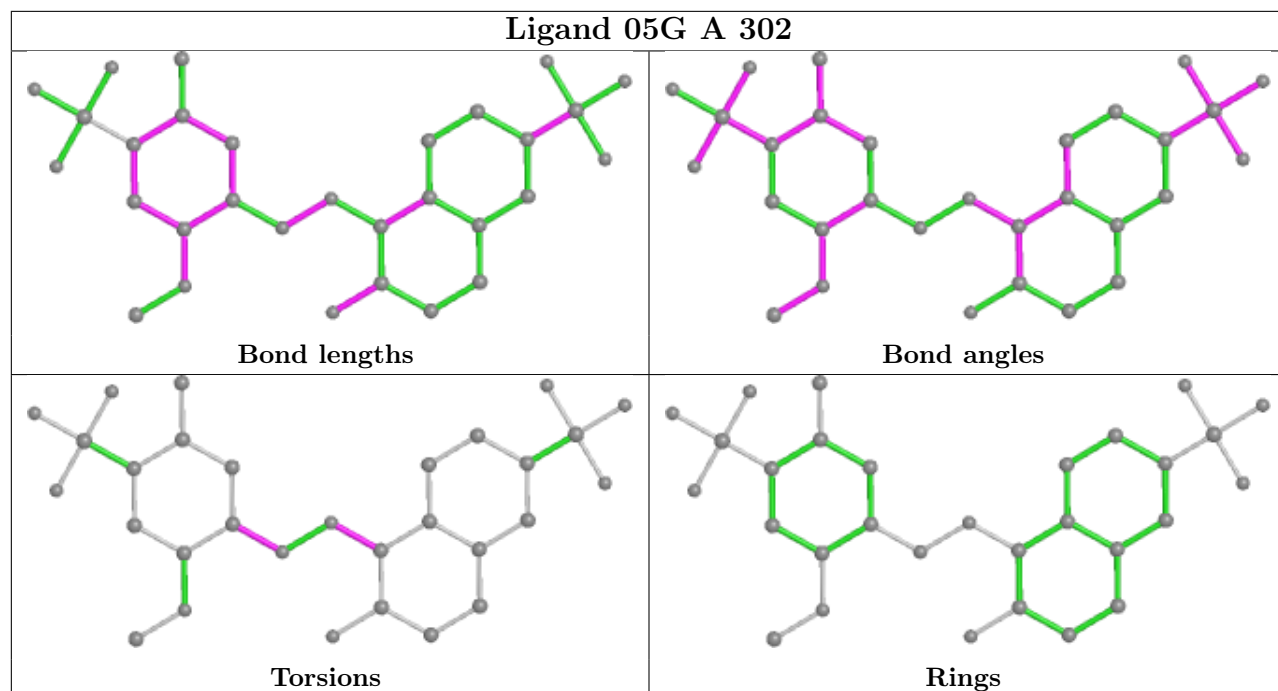
1 monomer is involved in 3 short contacts:

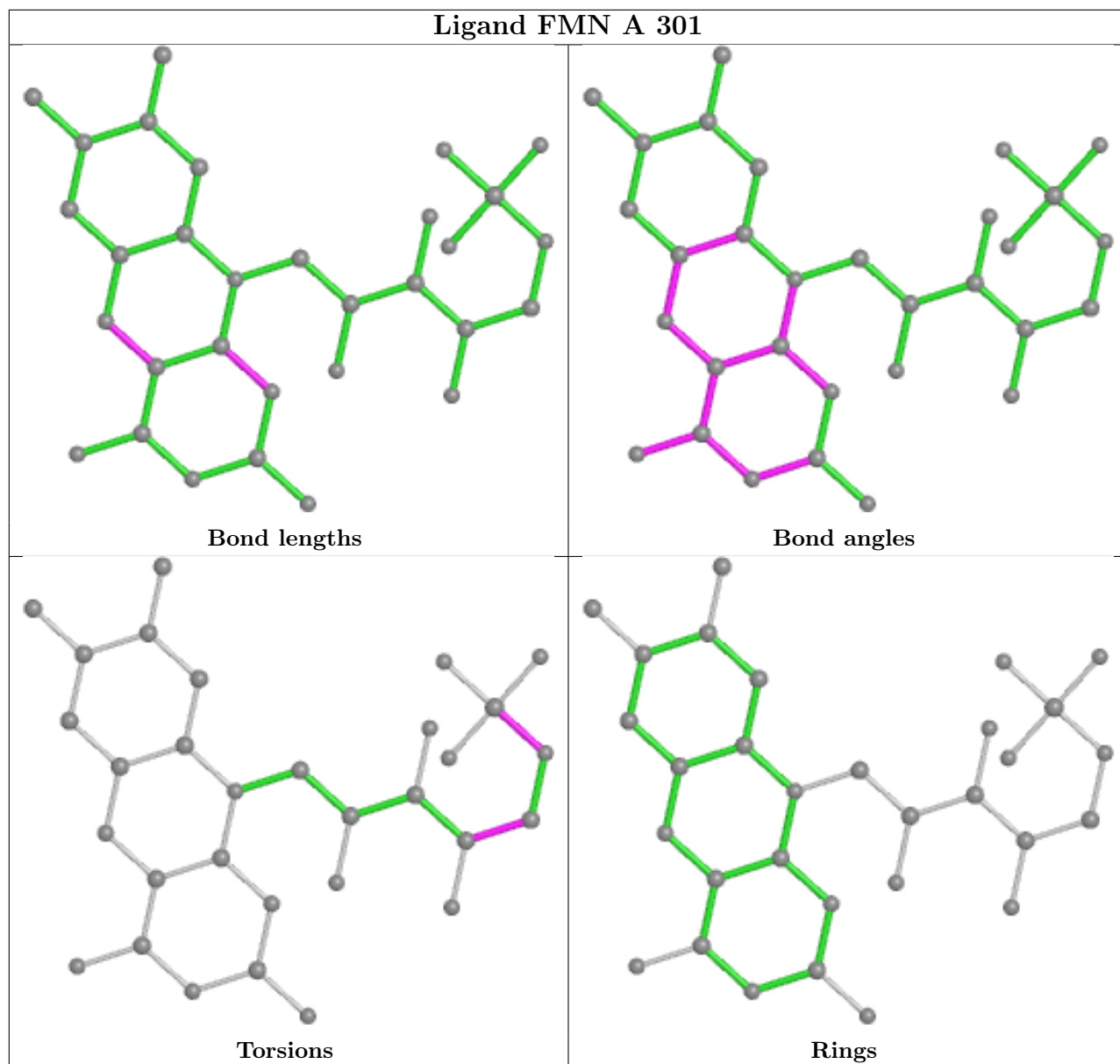
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	FMN	3	0

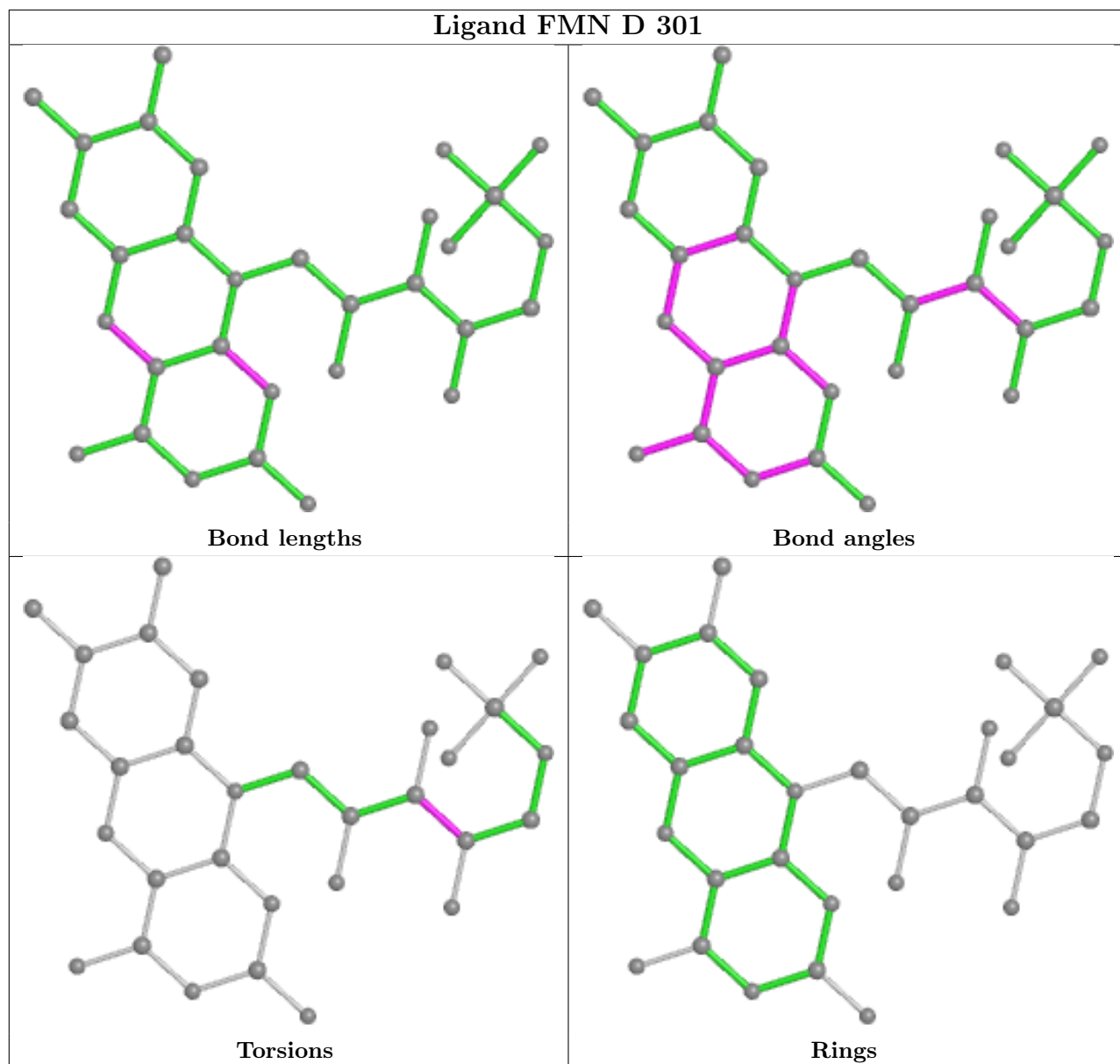
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

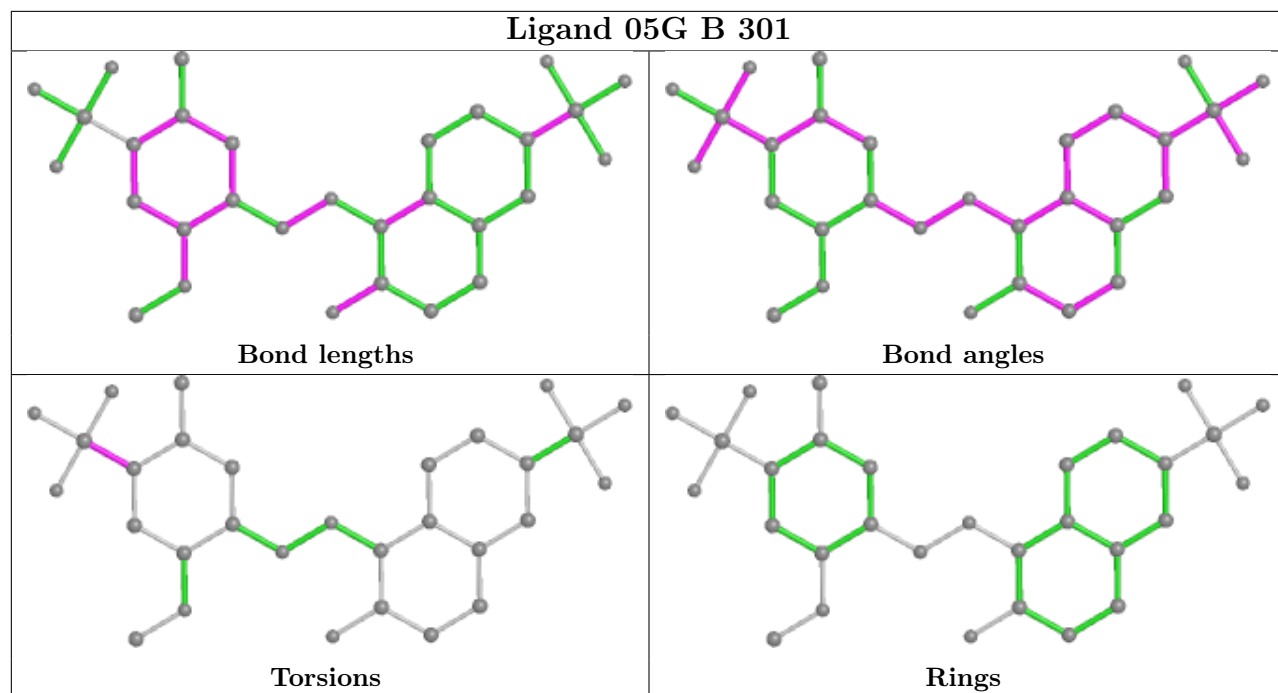


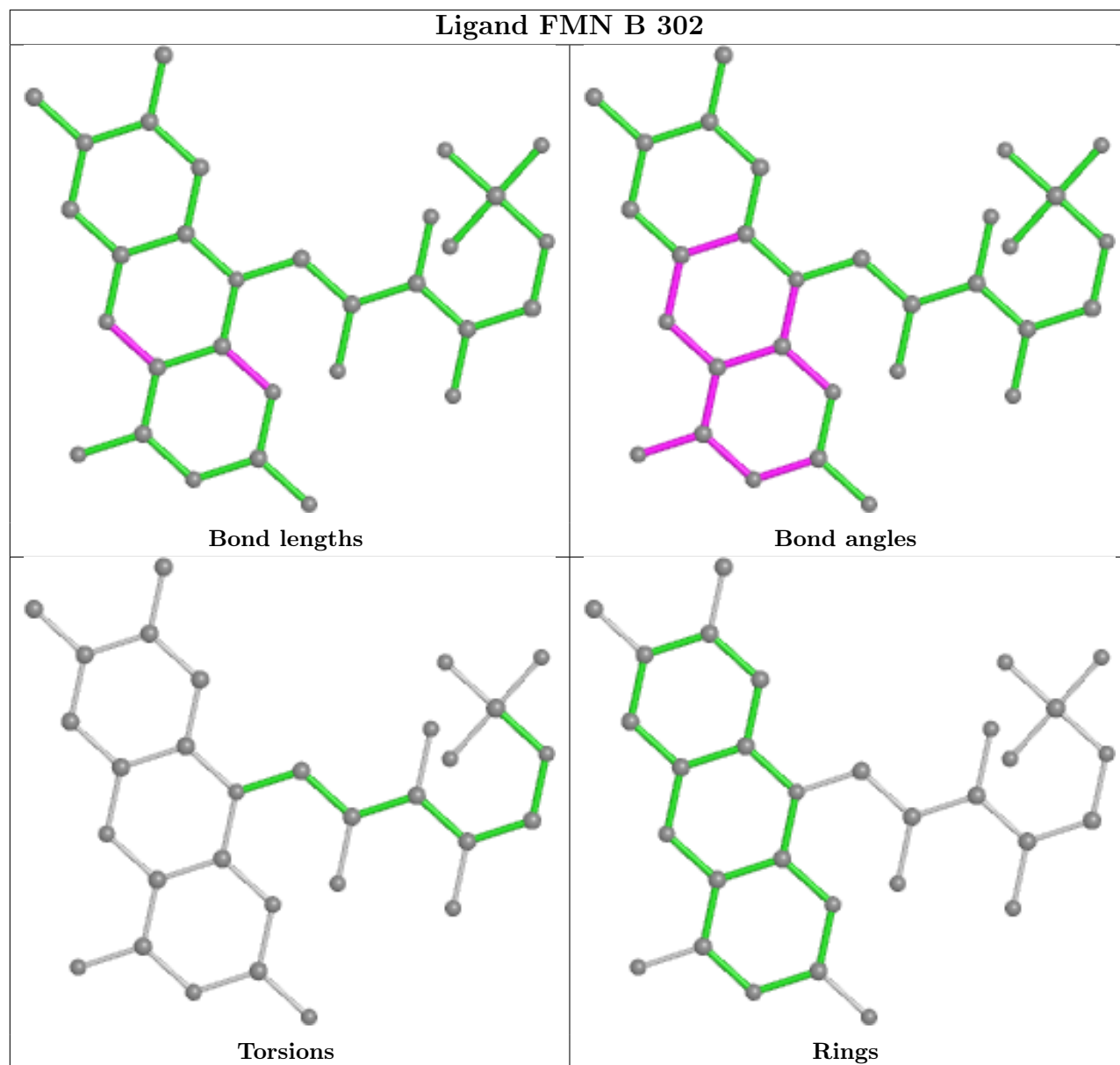












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	201/223 (90%)	0.17	8 (3%) 38 34	29, 39, 60, 79	0
1	B	202/223 (90%)	0.16	7 (3%) 44 40	29, 37, 57, 70	0
1	C	200/223 (89%)	0.26	11 (5%) 25 21	24, 35, 53, 82	0
1	D	201/223 (90%)	0.09	6 (2%) 50 47	25, 34, 53, 62	0
All	All	804/892 (90%)	0.17	32 (3%) 38 34	24, 36, 56, 82	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	SER	10.2
1	C	179	ARG	7.5
1	C	124	TRP	6.2
1	A	179	ARG	4.5
1	D	123	SER	4.5
1	C	120	TYR	4.2
1	A	180	PRO	4.2
1	C	148	THR	4.2
1	A	122	GLU	3.9
1	C	122	GLU	3.8
1	D	124	TRP	3.7
1	D	121	THR	3.7
1	B	122	GLU	3.2
1	A	181	HIS	3.2
1	D	122	GLU	3.2
1	D	120	TYR	3.2
1	C	121	THR	2.9
1	B	181	HIS	2.8
1	C	146	GLY	2.8
1	B	179	ARG	2.8
1	C	143	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	69	ILE	2.5
1	A	124	TRP	2.5
1	B	65	PRO	2.5
1	C	200	PRO	2.4
1	B	0	SER	2.3
1	D	180	PRO	2.2
1	B	33	GLY	2.2
1	A	65	PRO	2.1
1	C	65	PRO	2.0
1	A	126	GLN	2.0
1	B	63	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

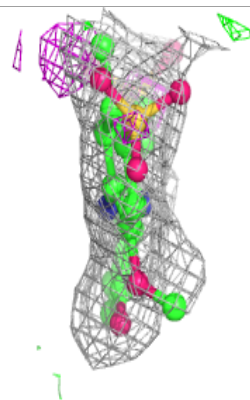
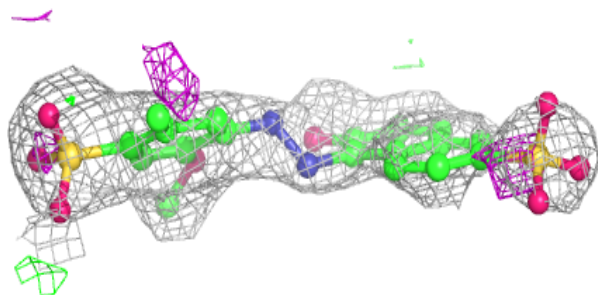
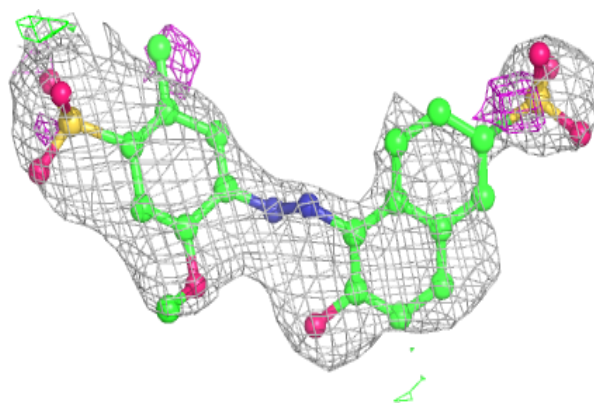
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	05G	C	303	30/30	0.74	0.33	43,53,58,60	0
3	05G	C	302	30/30	0.77	0.33	42,49,58,61	0
3	05G	A	302	30/30	0.81	0.33	47,54,62,65	0
3	05G	B	301	30/30	0.87	0.27	41,46,48,51	0
2	FMN	C	301	31/31	0.93	0.19	28,37,42,43	0
2	FMN	B	302	31/31	0.94	0.19	37,42,44,45	0
2	FMN	D	301	31/31	0.94	0.18	29,37,44,46	0
2	FMN	A	301	31/31	0.96	0.15	33,39,39,40	0

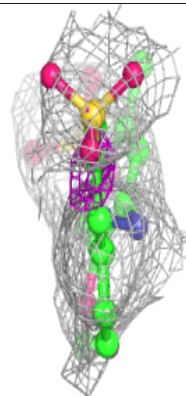
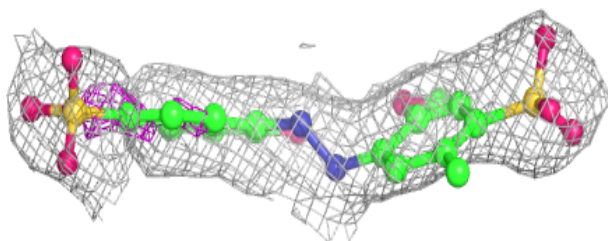
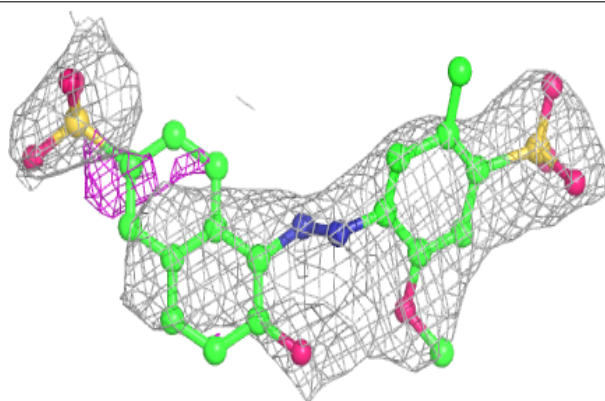
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 05G C 303:

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

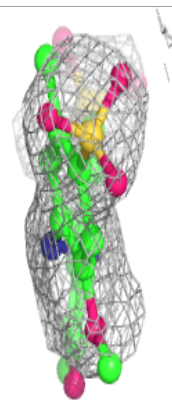
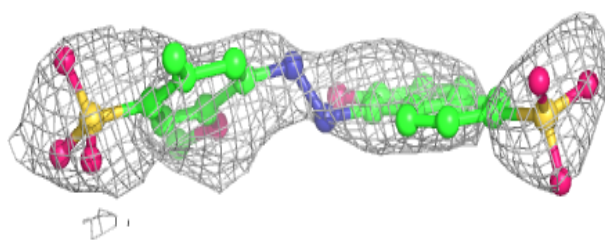
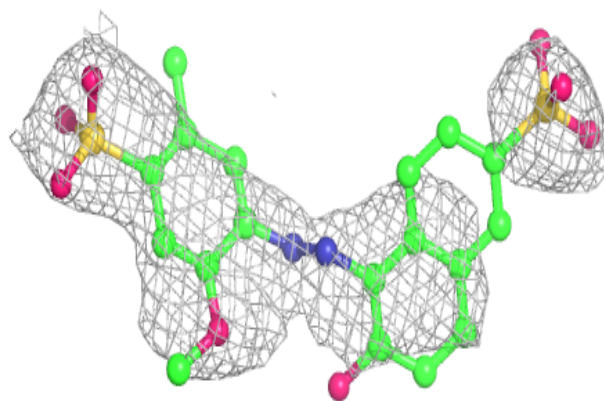
**Electron density around 05G C 302:**

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

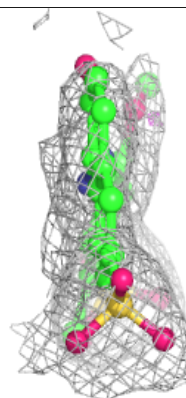
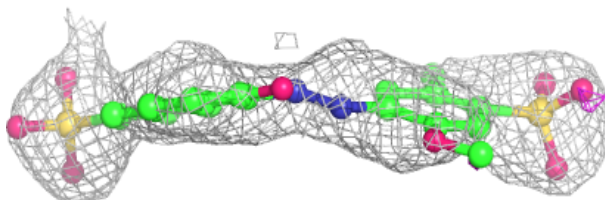
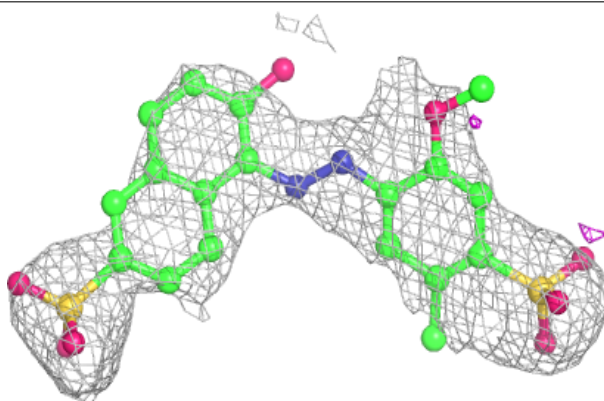


Electron density around 05G A 302:

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

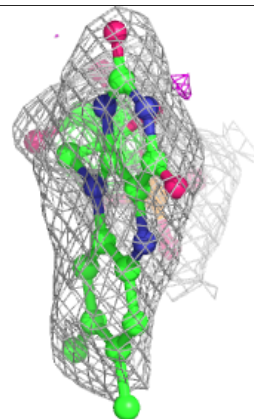
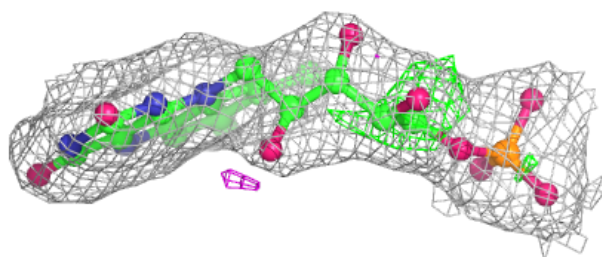
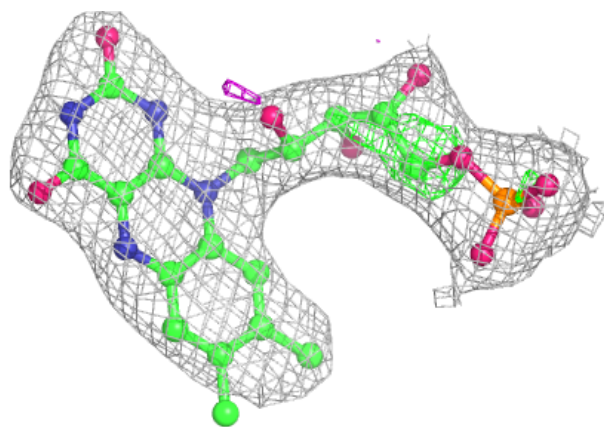
**Electron density around 05G B 301:**

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



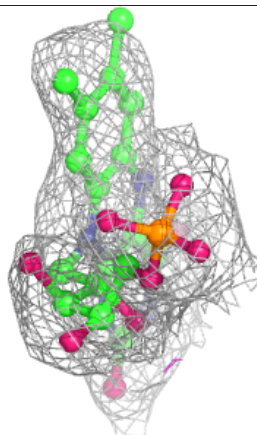
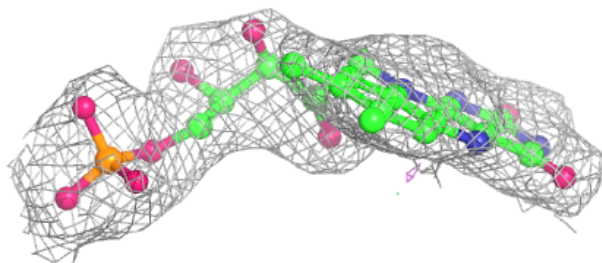
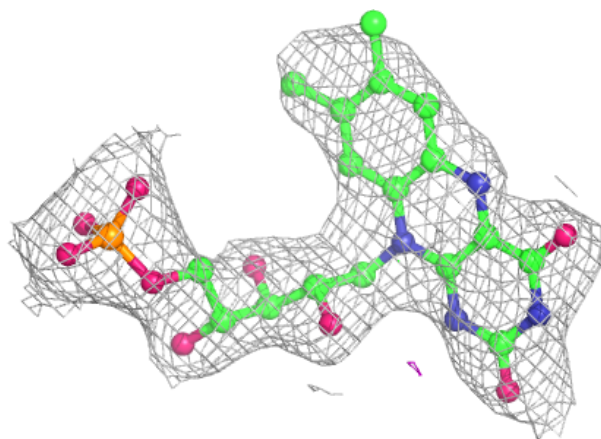
Electron density around FMN C 301:

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

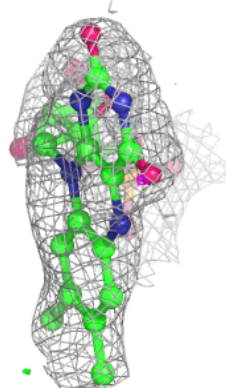
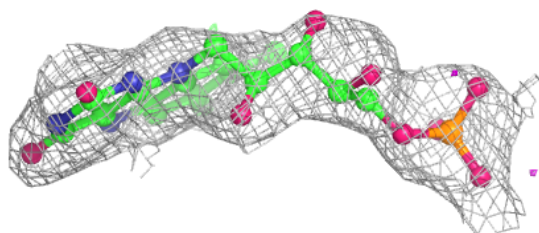
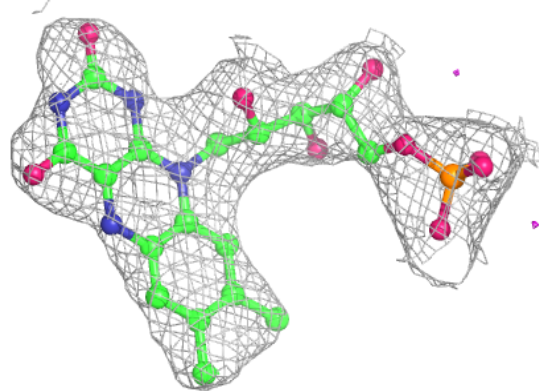


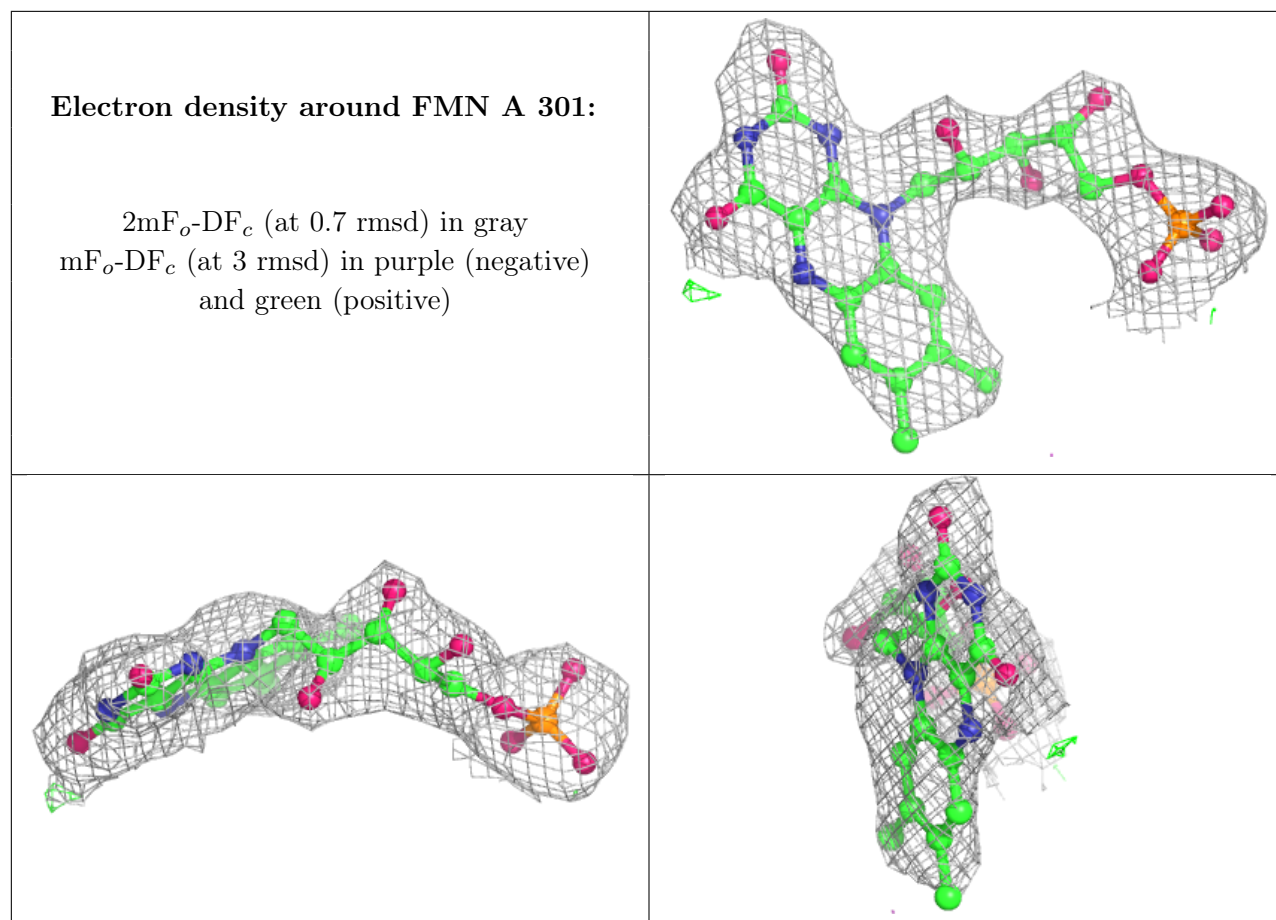
Electron density around FMN B 302:

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

**Electron density around FMN 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)





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.