



Full wwPDB X-ray Structure Validation Report i

Nov 22, 2023 – 10:47 PM JST

PDB ID : 7XWW
Title : Crystal structure of NTR in complex with BN-XB
Authors : Chen, X.; Chen, J.; Li, J.L.
Deposited on : 2022-05-27
Resolution : 2.80 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

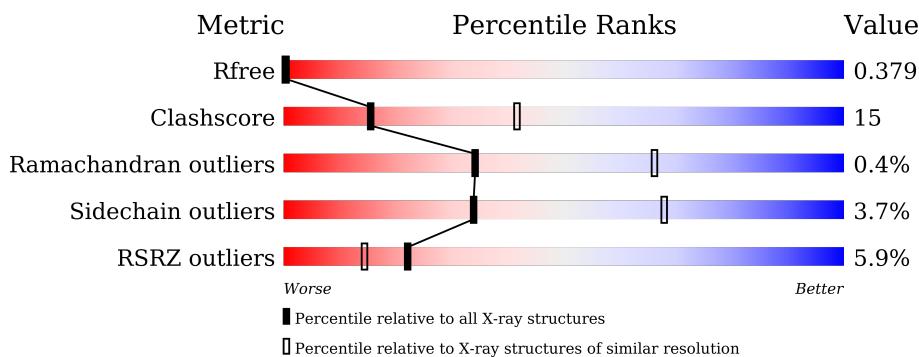
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

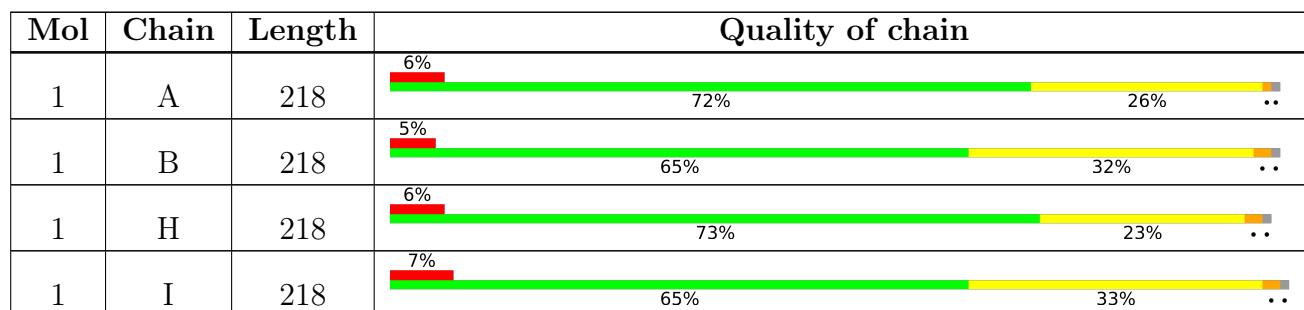
The reported resolution of this entry is 2.80 Å.

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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.



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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	I5O	A	301	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6850 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.

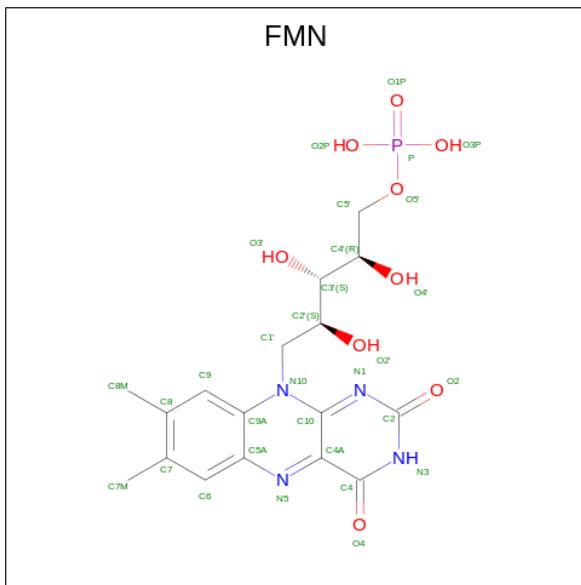
- Molecule 1 is a protein called Dihydropteridine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	216	Total 1676	C 1065	N 287	O 319	S 5	0	0	0
1	A	216	Total 1676	C 1065	N 287	O 319	S 5	0	0	0
1	H	216	Total 1670	C 1059	N 287	O 319	S 5	0	0	0
1	I	216	Total 1670	C 1062	N 284	O 319	S 5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

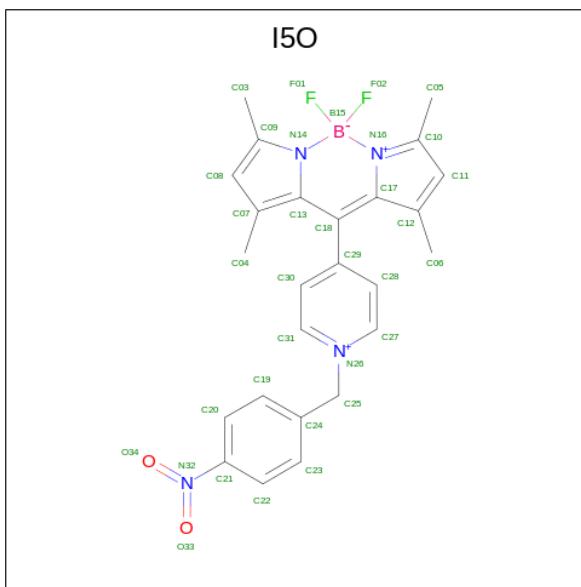
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP A0A094VLP5
A	0	SER	-	expression tag	UNP A0A094VLP5
H	0	SER	-	expression tag	UNP A0A094VLP5
I	0	SER	-	expression tag	UNP A0A094VLP5

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 2,2-bis(fluoranyl)-4,6,10,12-tetramethyl-8-[1-[(4-nitrophenyl)methyl]pyridin-1-i um-4-yl]-3-aza-1-azonia-2-boranuidatricyclo[7.3.0.0^{\{3,7\}}]dodeca-1(12),4,6,8,10-pentae ne (three-letter code: I5O) (formula: C₂₅H₂₄BF₂N₄O₂) (labeled as "Ligand of Interest" by depositor).

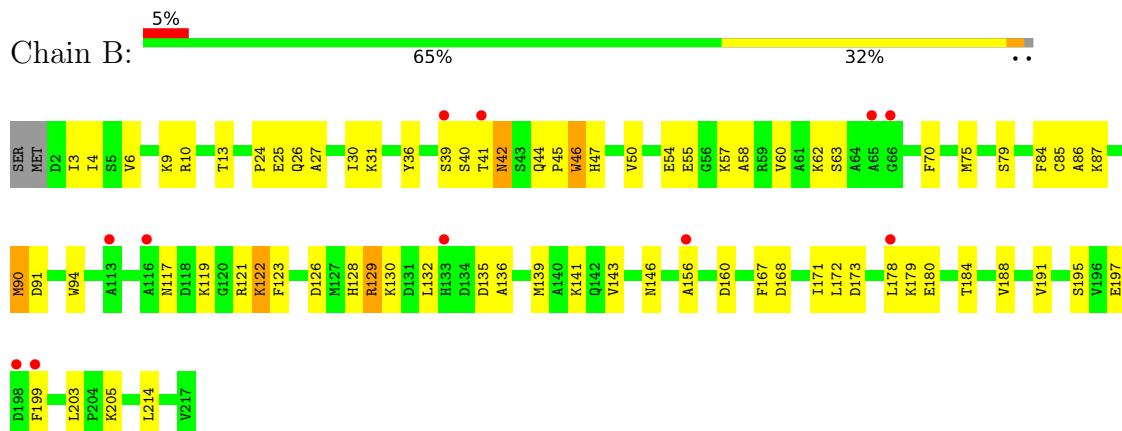


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	B	C	F	N	O		
3	A	1	34	1	25	2	4	2	0	0

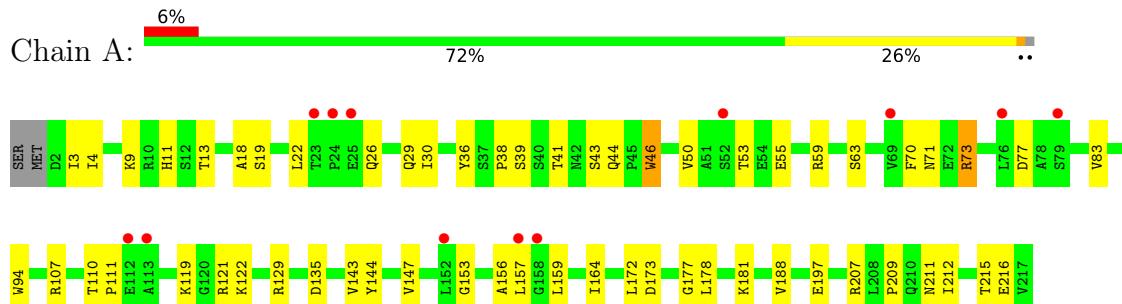
3 Residue-property plots

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.

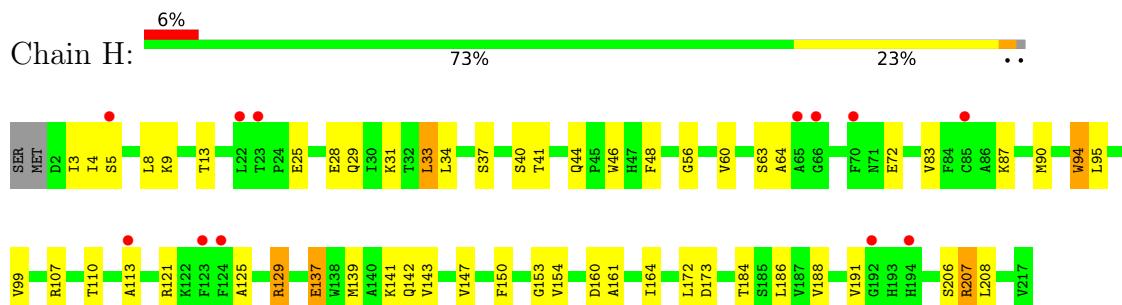
- Molecule 1: Dihydropteridine reductase



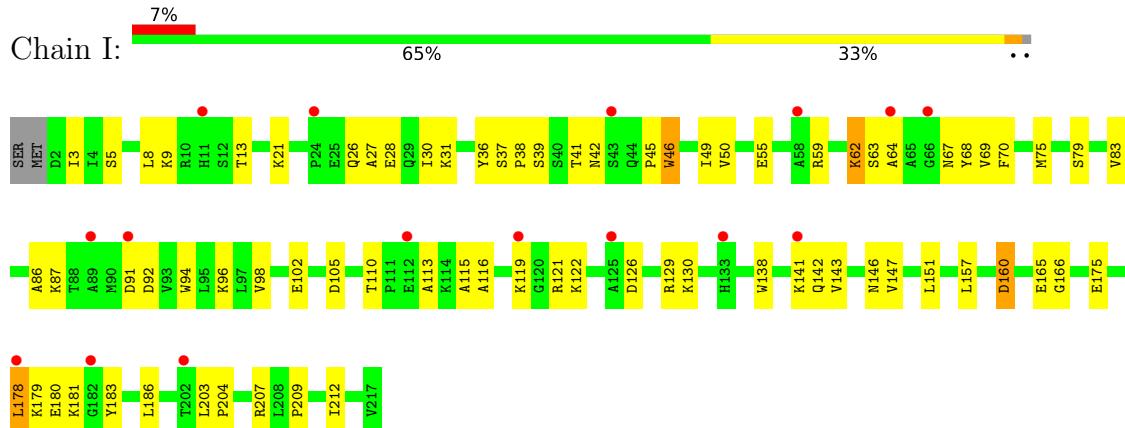
- Molecule 1: Dihydropteridine reductase



- Molecule 1: Dihydropteridine reductase



- Molecule 1: Dihydropteridine reductase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.87 Å 61.67 Å 88.33 Å 96.64° 100.83° 110.72°	Depositor
Resolution (Å)	35.26 – 2.80 35.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.3 (35.26-2.80) 75.3 (35.26-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	4.49 (at 2.81 Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R , R_{free}	0.286 , 0.379 0.288 , 0.379	Depositor DCC
R_{free} test set	972 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.833	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.1	EDS
L-test for twinning ²	$< L > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	6850	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: I5O, 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	0.33	0/1711	0.54	0/2318
1	B	0.31	0/1711	0.53	0/2318
1	H	0.31	0/1704	0.51	0/2309
1	I	0.32	0/1705	0.56	0/2311
All	All	0.32	0/6831	0.54	0/9256

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	1676	0	1661	55	0
1	B	1676	0	1661	62	0
1	H	1670	0	1654	44	0
1	I	1670	0	1650	68	0
2	A	31	0	19	3	0
2	B	31	0	19	1	0
2	H	31	0	19	0	0
2	I	31	0	19	1	0
3	A	34	0	0	2	0
All	All	6850	0	6702	201	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 15.

All (201) 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:I:178:LEU:HD22	1:I:183:TYR:HB2	1.43	1.00
1:H:64:ALA:HB3	1:H:72:GLU:HB3	1.42	0.99
1:I:178:LEU:CD2	1:I:183:TYR:HB2	1.93	0.97
1:H:64:ALA:CB	1:H:72:GLU:HB3	1.98	0.93
1:B:135:ASP:OD1	1:B:136:ALA:N	2.03	0.91
1:B:45:PRO:HB2	1:B:139:MET:HG2	1.51	0.90
1:A:3:ILE:HD12	1:A:4:ILE:N	1.88	0.86
1:I:178:LEU:HD22	1:I:183:TYR:CB	2.08	0.84
1:H:25:GLU:HG3	1:H:29:GLN:HE21	1.42	0.83
1:A:110:THR:OG1	1:A:111:PRO:CD	2.26	0.83
1:A:110:THR:OG1	1:A:111:PRO:HD2	1.79	0.83
1:B:13:THR:HG21	1:B:160:ASP:HB3	1.64	0.80
1:I:26:GLN:O	1:I:30:ILE:HG23	1.85	0.77
1:B:45:PRO:CB	1:B:139:MET:HG2	2.17	0.75
1:B:135:ASP:O	1:B:139:MET:HE2	1.88	0.73
1:H:40:SER:HB2	1:I:165:GLU:OE2	1.89	0.72
1:B:203:LEU:HD23	1:A:107:ARG:HG2	1.71	0.71
1:H:90:MET:HG3	1:H:95:LEU:HD11	1.72	0.71
1:I:27:ALA:HA	1:I:30:ILE:HG12	1.72	0.69
1:B:178:LEU:O	1:B:180:GLU:N	2.25	0.69
1:I:178:LEU:HD23	1:I:183:TYR:HB2	1.75	0.69
1:A:164:ILE:HG23	2:A:302:FMN:O4	1.93	0.68
1:B:173:ASP:HA	1:B:178:LEU:HD13	1.75	0.68
1:I:62:LYS:HE3	1:I:175:GLU:HG3	1.75	0.68
1:I:62:LYS:CE	1:I:175:GLU:HG3	2.25	0.67
1:I:178:LEU:CD2	1:I:183:TYR:CB	2.69	0.66
1:A:173:ASP:HA	1:A:178:LEU:HD23	1.77	0.66
1:B:3:ILE:HD13	1:A:153:GLY:HA2	1.78	0.66
1:B:36:TYR:HA	1:A:207:ARG:HE	1.61	0.65
1:A:119:LYS:HA	1:A:122:LYS:HB2	1.78	0.65
1:H:3:ILE:HD12	1:H:4:ILE:N	2.10	0.65
1:H:28:GLU:HG3	1:H:31:LYS:HE3	1.78	0.65
1:A:55:GLU:N	1:A:55:GLU:OE2	2.29	0.65
1:B:24:PRO:HA	1:B:27:ALA:HB3	1.77	0.65
1:I:86:ALA:HB2	1:I:186:LEU:HD11	1.78	0.65
1:H:5:SER:HB2	1:H:9:LYS:HE2	1.78	0.65
1:B:91:ASP:OD1	1:B:94:TRP:N	2.25	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:HD12	1:A:4:ILE:H	1.63	0.63
1:B:30:ILE:HG13	1:B:31:LYS:HG3	1.79	0.63
1:A:26:GLN:HA	1:A:29:GLN:HG2	1.81	0.63
1:B:4:ILE:HD11	1:A:157:LEU:HD21	1.79	0.63
1:I:165:GLU:HG2	2:I:301:FMN:H6	1.80	0.62
1:I:178:LEU:HD23	1:I:183:TYR:CD2	2.35	0.61
1:B:3:ILE:HD12	1:A:156:ALA:HB3	1.84	0.60
1:B:10:ARG:O	1:B:205:LYS:NZ	2.22	0.60
1:H:207:ARG:HD3	1:I:36:TYR:HA	1.83	0.59
1:A:22:LEU:CD2	1:A:30:ILE:HD12	2.32	0.59
1:A:129:ARG:HG2	1:A:129:ARG:O	2.02	0.59
1:B:87:LYS:NZ	1:B:91:ASP:OD2	2.36	0.59
1:I:63:SER:OG	1:I:75:MET:SD	2.59	0.58
1:H:141:LYS:HG2	1:I:141:LYS:HG2	1.86	0.58
1:I:5:SER:O	1:I:9:LYS:HG2	2.04	0.58
1:B:39:SER:OG	1:B:42:ASN:HA	2.04	0.58
1:B:117:ASN:OD1	1:B:121:ARG:NH2	2.36	0.58
1:H:164:ILE:HB	1:H:188:VAL:HG23	1.86	0.58
1:I:126:ASP:HA	1:I:129:ARG:HG2	1.85	0.58
1:B:50:VAL:HG13	1:A:216:GLU:HG2	1.86	0.57
1:H:13:THR:HG21	1:H:160:ASP:HB3	1.85	0.57
1:A:55:GLU:O	1:A:59:ARG:HG3	2.05	0.57
1:I:178:LEU:O	1:I:181:LYS:N	2.37	0.56
1:H:153:GLY:HA2	1:I:3:ILE:HD13	1.88	0.56
1:I:62:LYS:HE3	1:I:175:GLU:CG	2.35	0.56
1:A:71:ASN:OD1	1:A:164:ILE:HD13	2.04	0.56
1:H:83:VAL:HG22	1:H:188:VAL:HG12	1.88	0.55
1:I:110:THR:HG23	1:I:113:ALA:H	1.72	0.55
1:A:3:ILE:CD1	1:A:4:ILE:HG12	2.36	0.55
1:B:205:LYS:HD3	1:A:36:TYR:HD2	1.72	0.55
1:I:203:LEU:H	1:I:203:LEU:HD12	1.72	0.55
1:B:46:TRP:HB3	1:B:143:VAL:HG22	1.89	0.54
1:A:143:VAL:O	1:A:147:VAL:HG23	2.07	0.54
1:B:90:MET:CE	1:B:94:TRP:HD1	2.21	0.54
1:B:156:ALA:HB3	1:A:3:ILE:HG21	1.89	0.54
1:H:95:LEU:O	1:H:99:VAL:HG23	2.08	0.54
1:A:63:SER:HB2	1:A:172:LEU:HG	1.89	0.54
1:A:41:THR:HG22	1:A:121:ARG:NE	2.23	0.53
1:I:209:PRO:HD2	1:I:212:ILE:HG13	1.91	0.53
1:I:147:VAL:O	1:I:151:LEU:HG	2.08	0.53
1:I:116:ALA:O	1:I:119:LYS:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:PHE:HB2	3:A:301:I5O:C11	2.39	0.52
1:H:173:ASP:OD2	1:H:184:THR:HG23	2.08	0.52
1:H:44:GLN:O	1:H:94:TRP:HH2	1.92	0.52
1:H:137:GLU:O	1:H:141:LYS:HG3	2.09	0.52
1:A:41:THR:HG22	1:A:41:THR:O	2.10	0.52
1:B:90:MET:HE1	1:B:94:TRP:HD1	1.74	0.52
1:I:143:VAL:O	1:I:147:VAL:HG23	2.09	0.52
1:H:29:GLN:O	1:H:33:LEU:HD12	2.09	0.51
1:H:110:THR:HG23	1:H:113:ALA:H	1.75	0.51
1:A:22:LEU:HD23	1:A:30:ILE:HD12	1.93	0.51
1:H:25:GLU:O	1:H:29:GLN:HG3	2.10	0.51
1:B:55:GLU:HG3	1:I:70:PHE:CD2	2.46	0.50
1:B:30:ILE:HG13	1:B:31:LYS:N	2.26	0.50
1:B:55:GLU:HG3	1:I:70:PHE:HD2	1.76	0.50
1:B:173:ASP:OD1	1:B:178:LEU:HD22	2.11	0.50
1:H:5:SER:O	1:H:9:LYS:HG3	2.12	0.50
1:H:33:LEU:HD22	1:H:153:GLY:HA3	1.93	0.50
1:I:92:ASP:O	1:I:96:LYS:HG2	2.11	0.50
1:B:26:GLN:O	1:B:30:ILE:HG23	2.11	0.49
1:H:206:SER:OG	1:I:105:ASP:OD2	2.20	0.49
1:I:62:LYS:HE2	1:I:175:GLU:HG3	1.94	0.49
1:H:34:LEU:HD13	1:H:48:PHE:CD2	2.47	0.49
1:A:41:THR:HG21	1:A:121:ARG:HA	1.94	0.49
1:B:62:LYS:HE2	1:I:67:ASN:HA	1.94	0.49
1:H:139:MET:HA	1:H:142:GLN:HG2	1.95	0.49
1:B:85:CYS:HA	1:B:184:THR:O	2.12	0.49
1:B:50:VAL:CG1	1:A:216:GLU:HG2	2.43	0.49
1:A:18:ALA:HA	1:A:77:ASP:O	2.12	0.48
1:A:39:SER:HB3	1:A:46:TRP:CH2	2.47	0.48
1:A:53:THR:HB	1:A:55:GLU:OE2	2.13	0.48
1:B:63:SER:OG	1:B:167:PHE:HB2	2.13	0.48
1:H:41:THR:O	1:H:121:ARG:NE	2.43	0.48
1:I:59:ARG:HG2	1:I:62:LYS:HZ1	1.79	0.48
1:I:115:ALA:O	1:I:119:LYS:HG3	2.14	0.47
1:A:164:ILE:HA	2:A:302:FMN:N5	2.30	0.47
1:I:203:LEU:HD12	1:I:203:LEU:N	2.29	0.47
1:B:10:ARG:NH2	1:A:38:PRO:HD3	2.29	0.47
1:A:3:ILE:HD12	1:A:4:ILE:HG12	1.95	0.47
1:A:70:PHE:O	1:A:73:ARG:NH2	2.48	0.47
1:I:37:SER:HB3	1:I:146:ASN:ND2	2.30	0.47
1:B:57:LYS:NZ	1:B:79:SER:O	2.38	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:150:PHE:O	1:H:154:VAL:HG22	2.15	0.47
1:B:122:LYS:O	1:B:126:ASP:HB2	2.14	0.46
2:B:301:FMN:O2'	3:A:301:I5O:O34	2.27	0.46
1:I:39:SER:HB3	1:I:42:ASN:HA	1.96	0.46
1:B:86:ALA:HB1	1:B:139:MET:O	2.15	0.46
1:I:94:TRP:O	1:I:98:VAL:HG23	2.15	0.46
1:H:125:ALA:O	1:H:129:ARG:HB3	2.16	0.46
1:H:143:VAL:O	1:H:147:VAL:HG23	2.15	0.46
1:I:68:TYR:CD1	1:I:166:GLY:C	2.89	0.46
1:I:41:THR:HG21	1:I:121:ARG:HA	1.97	0.46
1:I:130:LYS:HD3	1:I:130:LYS:HA	1.76	0.46
1:I:91:ASP:OD1	1:I:94:TRP:HB2	2.16	0.46
1:I:46:TRP:HB3	1:I:143:VAL:HG22	1.98	0.46
1:H:60:VAL:HA	1:H:172:LEU:HD21	1.98	0.46
1:B:141:LYS:HB3	1:A:144:TYR:CD2	2.51	0.45
1:I:49:ILE:HB	1:I:83:VAL:HB	1.97	0.45
1:H:3:ILE:HD12	1:H:3:ILE:C	2.37	0.45
1:I:49:ILE:HD11	1:I:178:LEU:HD11	1.98	0.45
1:B:168:ASP:CG	1:B:171:ILE:HG12	2.37	0.45
1:B:214:LEU:HD21	1:A:50:VAL:HG12	1.98	0.45
1:I:45:PRO:O	1:I:87:LYS:HG3	2.17	0.45
1:A:3:ILE:HD12	1:A:3:ILE:C	2.36	0.45
1:B:30:ILE:HD12	1:B:50:VAL:HG21	1.98	0.45
1:A:3:ILE:CD1	1:A:4:ILE:N	2.73	0.45
1:A:43:SER:O	1:A:94:TRP:HZ3	2.00	0.45
1:H:5:SER:HA	1:H:8:LEU:HB2	1.99	0.45
1:H:161:ALA:HB2	1:H:191:VAL:HG12	1.98	0.45
1:I:41:THR:HG22	1:I:41:THR:O	2.17	0.45
1:B:90:MET:O	1:B:129:ARG:NH1	2.49	0.44
1:B:3:ILE:CD1	1:A:153:GLY:HA2	2.47	0.44
1:B:3:ILE:O	1:B:6:VAL:HB	2.16	0.44
1:I:138:TRP:O	1:I:142:GLN:HG2	2.17	0.44
1:B:41:THR:O	1:B:121:ARG:HD3	2.18	0.44
1:I:13:THR:OG1	1:I:160:ASP:HB3	2.17	0.44
1:B:84:PHE:HE2	1:B:146:ASN:ND2	2.15	0.44
1:H:107:ARG:HA	1:I:203:LEU:HD23	2.00	0.44
1:I:28:GLU:HA	1:I:31:LYS:HD2	2.00	0.44
1:H:208:LEU:HD11	1:I:98:VAL:HG22	1.99	0.44
1:H:63:SER:HB3	1:H:172:LEU:HG	1.98	0.44
1:H:87:LYS:HE3	1:H:87:LYS:HB3	1.83	0.44
1:H:207:ARG:HH21	1:I:38:PRO:HA	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:87:LYS:HE3	1:I:87:LYS:HB3	1.81	0.44
1:A:30:ILE:HD11	1:A:159:LEU:HD12	2.00	0.43
1:A:209:PRO:HG2	1:A:212:ILE:HG12	1.99	0.43
1:B:44:GLN:HB3	1:B:46:TRP:NE1	2.33	0.43
1:A:209:PRO:HB2	1:A:211:ASN:OD1	2.18	0.43
1:B:160:ASP:O	1:B:191:VAL:HG23	2.18	0.43
1:I:21:LYS:HD2	1:I:79:SER:OG	2.18	0.43
1:H:56:GLY:O	1:H:60:VAL:HG23	2.18	0.43
1:B:46:TRP:HE3	1:B:143:VAL:HG22	1.84	0.43
1:H:206:SER:HB3	1:I:102:GLU:HG2	2.00	0.43
1:B:128:HIS:HA	1:B:132:LEU:HB2	2.01	0.43
1:B:60:VAL:HA	1:B:172:LEU:CD1	2.49	0.43
1:B:119:LYS:O	1:B:123:PHE:N	2.51	0.43
1:A:119:LYS:HE2	1:A:119:LYS:HB2	1.84	0.43
1:H:207:ARG:CD	1:I:36:TYR:HA	2.49	0.42
1:B:54:GLU:HA	1:B:57:LYS:HG3	2.01	0.42
1:I:178:LEU:O	1:I:180:GLU:N	2.52	0.42
1:A:164:ILE:HG23	2:A:302:FMN:C4	2.50	0.42
1:I:30:ILE:CD1	1:I:50:VAL:HG11	2.50	0.42
1:B:75:MET:HE3	1:B:188:VAL:HG11	2.01	0.42
1:B:40:SER:O	1:B:41:THR:OG1	2.33	0.41
1:A:26:GLN:HA	1:A:29:GLN:CG	2.48	0.41
1:A:44:GLN:O	1:A:94:TRP:HH2	2.02	0.41
1:B:60:VAL:HA	1:B:172:LEU:HD11	2.02	0.41
1:A:177:GLY:O	1:A:181:LYS:HD2	2.19	0.41
1:I:5:SER:HA	1:I:8:LEU:HB2	2.02	0.41
1:B:58:ALA:HB1	1:I:69:VAL:CG2	2.51	0.41
1:I:203:LEU:HA	1:I:204:PRO:HD3	1.94	0.41
1:A:11:HIS:NE2	1:A:13:THR:HG22	2.35	0.41
1:H:37:SER:C	1:I:207:ARG:HH21	2.23	0.41
1:A:83:VAL:HG13	1:A:188:VAL:HG22	2.02	0.41
1:A:29:GLN:HE21	1:A:29:GLN:HB3	1.64	0.41
1:B:139:MET:HE2	1:B:139:MET:HB2	1.86	0.41
1:I:87:LYS:HG2	1:I:183:TYR:CE1	2.56	0.41
1:A:197:GLU:O	1:A:197:GLU:HG2	2.20	0.40
1:H:186:LEU:HA	1:H:186:LEU:HD23	1.77	0.40
1:I:129:ARG:HG3	1:I:130:LYS:HG2	2.03	0.40
1:I:157:LEU:HD23	1:I:157:LEU:HA	1.78	0.40
1:B:47:HIS:NE2	1:A:215:THR:OG1	2.39	0.40
1:B:9:LYS:HE2	1:B:9:LYS:HB2	1.85	0.40
1:I:122:LYS:H	1:I:122:LYS:HG2	1.72	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	214/218 (98%)	208 (97%)	6 (3%)	0	100 100
1	B	214/218 (98%)	205 (96%)	8 (4%)	1 (0%)	29 61
1	H	214/218 (98%)	209 (98%)	5 (2%)	0	100 100
1	I	214/218 (98%)	201 (94%)	11 (5%)	2 (1%)	17 46
All	All	856/872 (98%)	823 (96%)	30 (4%)	3 (0%)	34 66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	179	LYS
1	B	179	LYS
1	I	64	ALA

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	178/180 (99%)	173 (97%)	5 (3%)	43 77
1	B	178/180 (99%)	168 (94%)	10 (6%)	21 51
1	H	177/180 (98%)	171 (97%)	6 (3%)	37 71
1	I	177/180 (98%)	172 (97%)	5 (3%)	43 77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	710/720 (99%)	684 (96%)	26 (4%)	34 68

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	GLU
1	B	42	ASN
1	B	46	TRP
1	B	70	PHE
1	B	90	MET
1	B	122	LYS
1	B	129	ARG
1	B	130	LYS
1	B	195	SER
1	B	197	GLU
1	A	9	LYS
1	A	19	SER
1	A	46	TRP
1	A	73	ARG
1	A	135	ASP
1	H	33	LEU
1	H	46	TRP
1	H	94	TRP
1	H	129	ARG
1	H	137	GLU
1	H	207	ARG
1	I	46	TRP
1	I	55	GLU
1	I	62	LYS
1	I	160	ASP
1	I	178	LEU

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

Mol	Chain	Res	Type
1	B	42	ASN
1	A	29	GLN
1	H	29	GLN
1	I	101	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 [\(i\)](#)

5 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	H	301	-	33,33,33	1.11	2 (6%)	48,50,50	1.29	8 (16%)
3	I5O	A	301	-	36,38,38	4.82	8 (22%)	48,59,59	1.62	9 (18%)
2	FMN	B	301	-	33,33,33	1.08	2 (6%)	48,50,50	1.24	8 (16%)
2	FMN	I	301	-	33,33,33	1.18	2 (6%)	48,50,50	1.40	8 (16%)
2	FMN	A	302	-	33,33,33	1.04	2 (6%)	48,50,50	1.24	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	H	301	-	-	0/18/18/18	0/3/3/3
3	I5O	A	301	-	-	10/12/48/48	0/5/5/5
2	FMN	B	301	-	-	0/18/18/18	0/3/3/3
2	FMN	I	301	-	-	1/18/18/18	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	A	302	-	-	0/18/18/18	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	I5O	B15-F01	17.67	1.67	1.39
3	A	301	I5O	B15-F02	17.52	1.67	1.39
3	A	301	I5O	C18-C17	7.84	1.47	1.36
3	A	301	I5O	O34-N32	7.57	1.40	1.22
3	A	301	I5O	C17-N16	-5.83	1.32	1.40
3	A	301	I5O	C29-C18	4.37	1.57	1.49
2	I	301	FMN	C4A-N5	4.10	1.38	1.30
2	H	301	FMN	C4A-N5	4.08	1.38	1.30
2	B	301	FMN	C4A-N5	3.98	1.38	1.30
3	A	301	I5O	B15-N14	-3.78	1.50	1.57
2	A	302	FMN	C4A-N5	3.68	1.37	1.30
3	A	301	I5O	B15-N16	-2.97	1.50	1.54
2	H	301	FMN	C10-N1	2.63	1.38	1.33
2	I	301	FMN	C10-N1	2.63	1.38	1.33
2	B	301	FMN	C10-N1	2.60	1.38	1.33
2	A	302	FMN	C10-N1	2.44	1.38	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	I5O	B15-N16-C17	-4.08	120.92	125.21
3	A	301	I5O	C13-C18-C17	-3.82	116.35	125.46
3	A	301	I5O	C05-C10-N16	3.43	127.66	123.21
2	A	302	FMN	C4-N3-C2	-3.24	119.66	125.64
2	I	301	FMN	C4-N3-C2	-3.18	119.76	125.64
2	I	301	FMN	C10-C4A-N5	-3.18	118.11	124.86
3	A	301	I5O	F01-B15-N16	-3.04	105.83	110.03
2	B	301	FMN	C4-N3-C2	-3.02	120.05	125.64
2	H	301	FMN	C4-N3-C2	-3.01	120.07	125.64
2	I	301	FMN	C5'-C4'-C3'	-2.89	106.63	112.20
2	A	302	FMN	C4A-C10-N10	2.83	120.61	116.48
2	A	302	FMN	C4A-C4-N3	2.78	120.25	113.19
2	H	301	FMN	C9A-C5A-N5	-2.77	119.42	122.43
2	I	301	FMN	C4A-C10-N10	2.74	120.49	116.48
2	H	301	FMN	C4A-C4-N3	2.72	120.08	113.19
3	A	301	I5O	C17-N16-C10	2.71	110.55	108.17
3	A	301	I5O	C03-C09-C08	-2.70	123.78	128.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	FMN	O4-C4-C4A	-2.68	119.49	126.60
2	B	301	FMN	C4A-C4-N3	2.65	119.93	113.19
2	B	301	FMN	C5'-C4'-C3'	-2.64	107.10	112.20
3	A	301	I5O	C05-C10-C11	-2.61	123.56	128.17
2	I	301	FMN	C4A-C4-N3	2.60	119.78	113.19
2	B	301	FMN	O4-C4-C4A	-2.54	119.87	126.60
2	H	301	FMN	O4-C4-C4A	-2.51	119.95	126.60
2	H	301	FMN	C5A-C9A-N10	2.48	120.51	117.95
2	I	301	FMN	C4-C4A-N5	2.47	121.74	118.23
2	B	301	FMN	C4A-C10-N10	2.44	120.05	116.48
2	H	301	FMN	C4A-C10-N10	2.41	120.01	116.48
3	A	301	I5O	F01-B15-N14	-2.41	105.02	108.60
3	A	301	I5O	C29-C18-C17	-2.38	117.88	121.20
2	I	301	FMN	C4A-C10-N1	-2.37	119.24	124.73
2	H	301	FMN	C10-C4A-N5	-2.24	120.10	124.86
2	B	301	FMN	C10-C4A-N5	-2.24	120.11	124.86
2	A	302	FMN	C10-C4A-N5	-2.23	120.13	124.86
2	A	302	FMN	C4A-C10-N1	-2.17	119.69	124.73
2	B	301	FMN	C9A-C5A-N5	-2.11	120.13	122.43
2	I	301	FMN	C1'-C2'-C3'	-2.10	103.93	109.79
2	A	302	FMN	C5'-C4'-C3'	-2.08	108.18	112.20
2	B	301	FMN	C4A-C10-N1	-2.08	119.91	124.73
2	H	301	FMN	C4A-C10-N1	-2.06	119.96	124.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

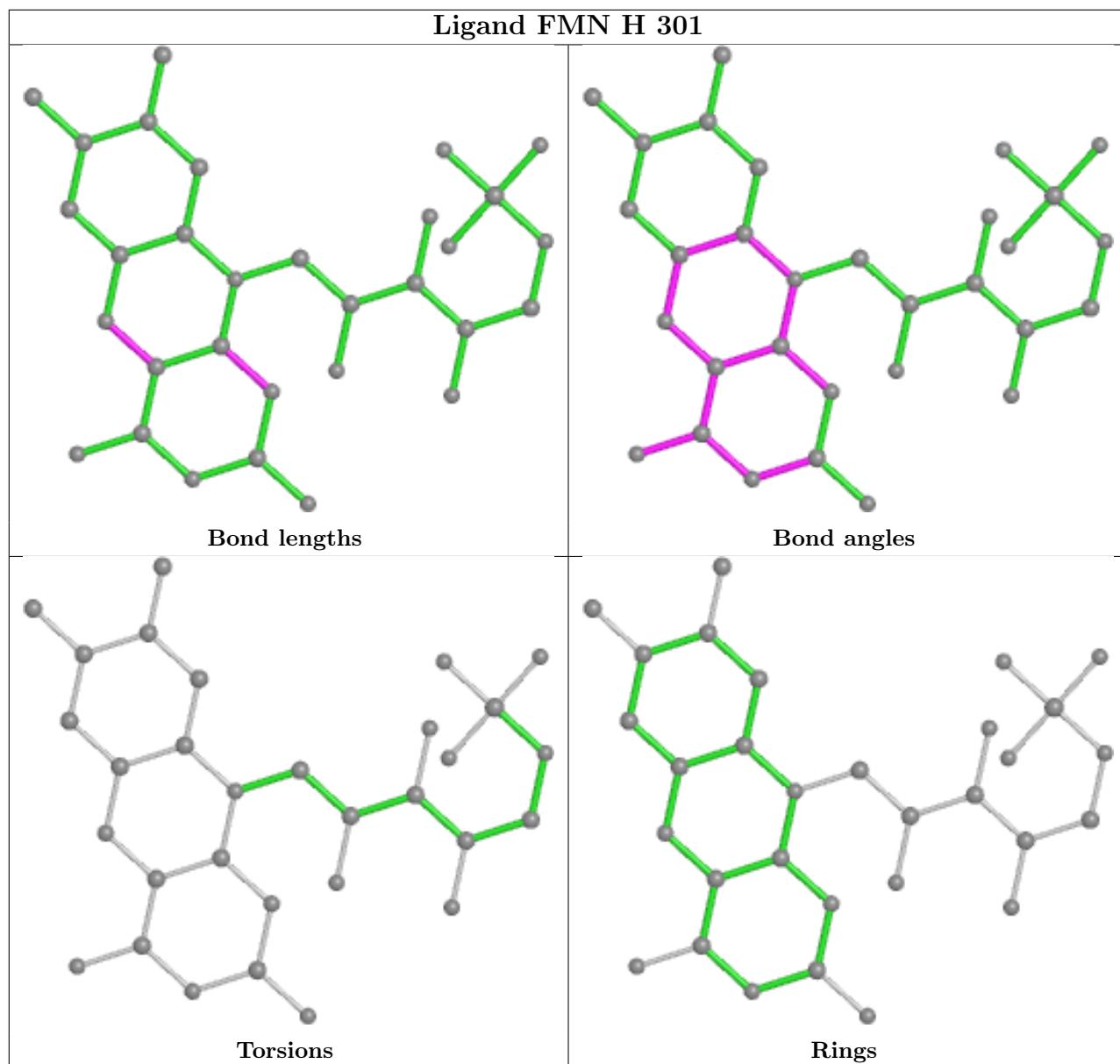
Mol	Chain	Res	Type	Atoms
3	A	301	I5O	C13-C18-C29-C28
3	A	301	I5O	C13-C18-C29-C30
3	A	301	I5O	C20-C21-N32-O33
3	A	301	I5O	C22-C21-N32-O34
3	A	301	I5O	C20-C21-N32-O34
3	A	301	I5O	C22-C21-N32-O33
3	A	301	I5O	C17-C18-C29-C28
3	A	301	I5O	C17-C18-C29-C30
3	A	301	I5O	C24-C25-N26-C31
3	A	301	I5O	C24-C25-N26-C27
2	I	301	FMN	N10-C1'-C2'-O2'

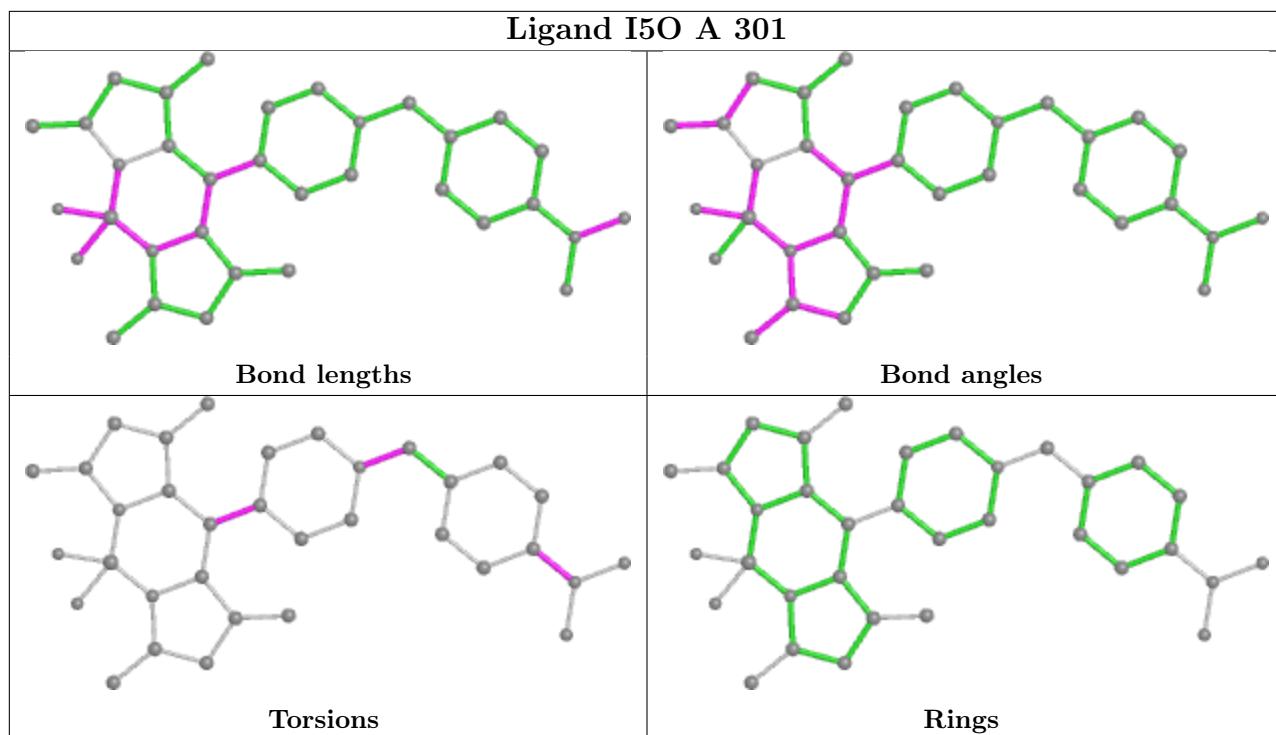
There are no ring outliers.

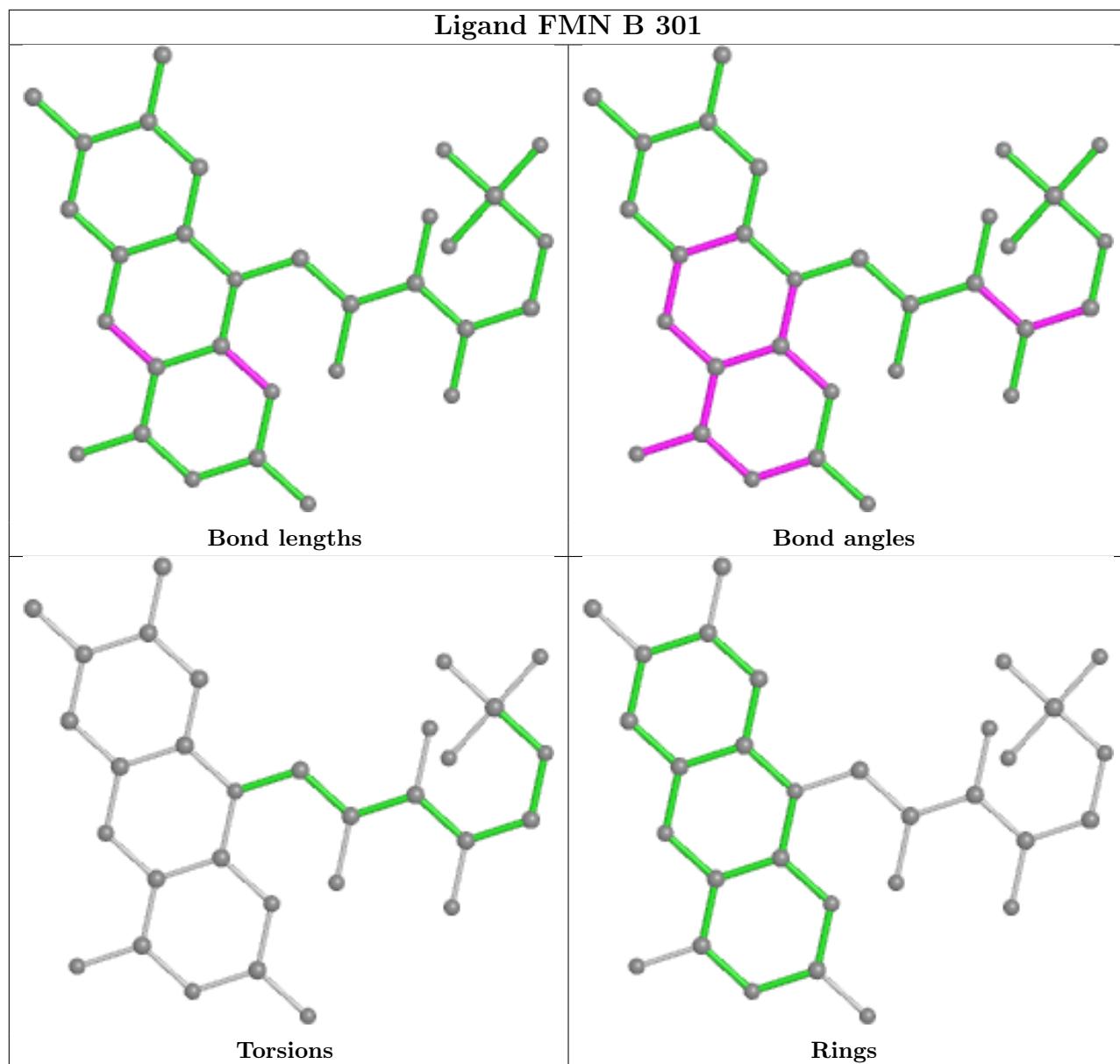
4 monomers are involved in 6 short contacts:

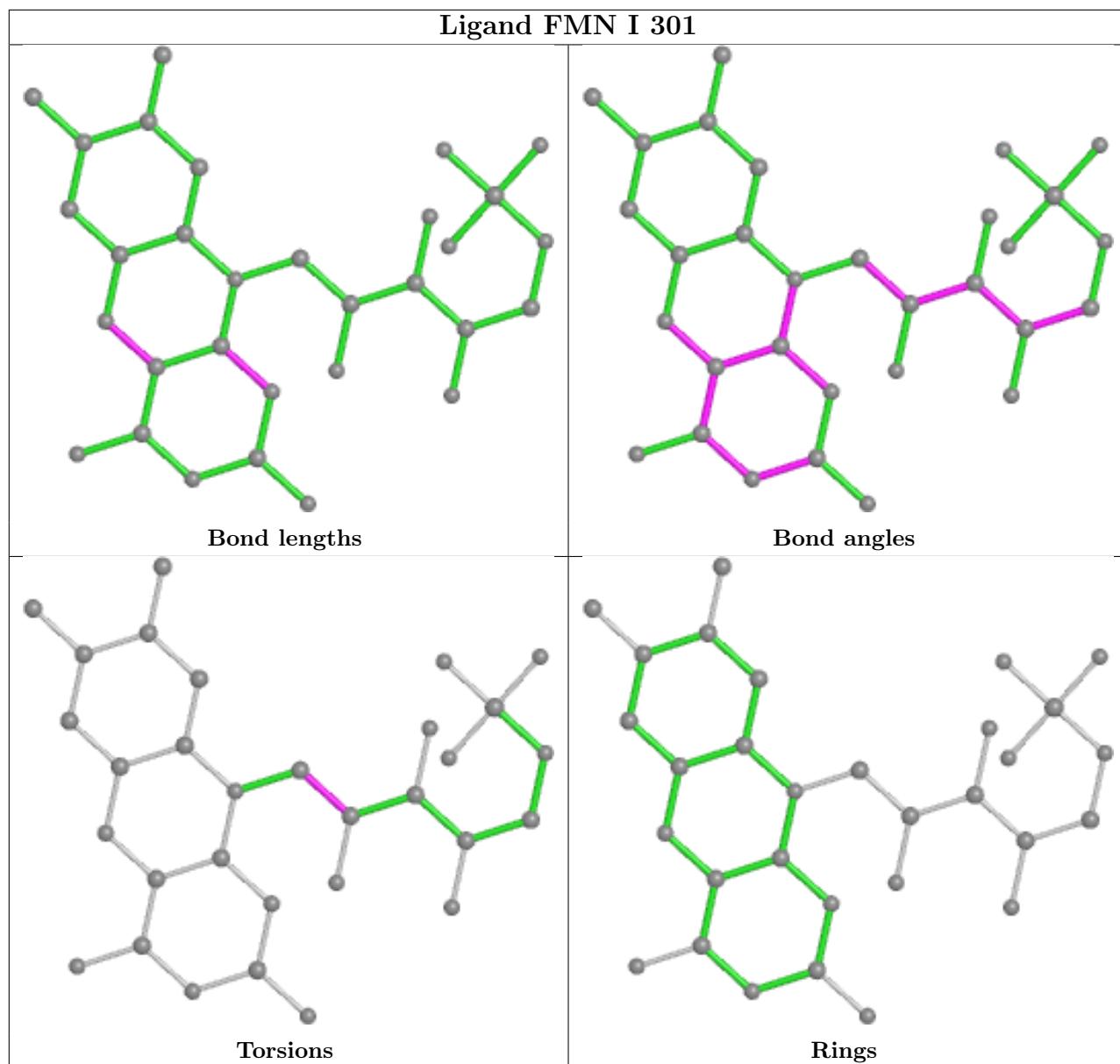
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	I5O	2	0
2	B	301	FMN	1	0
2	I	301	FMN	1	0
2	A	302	FMN	3	0

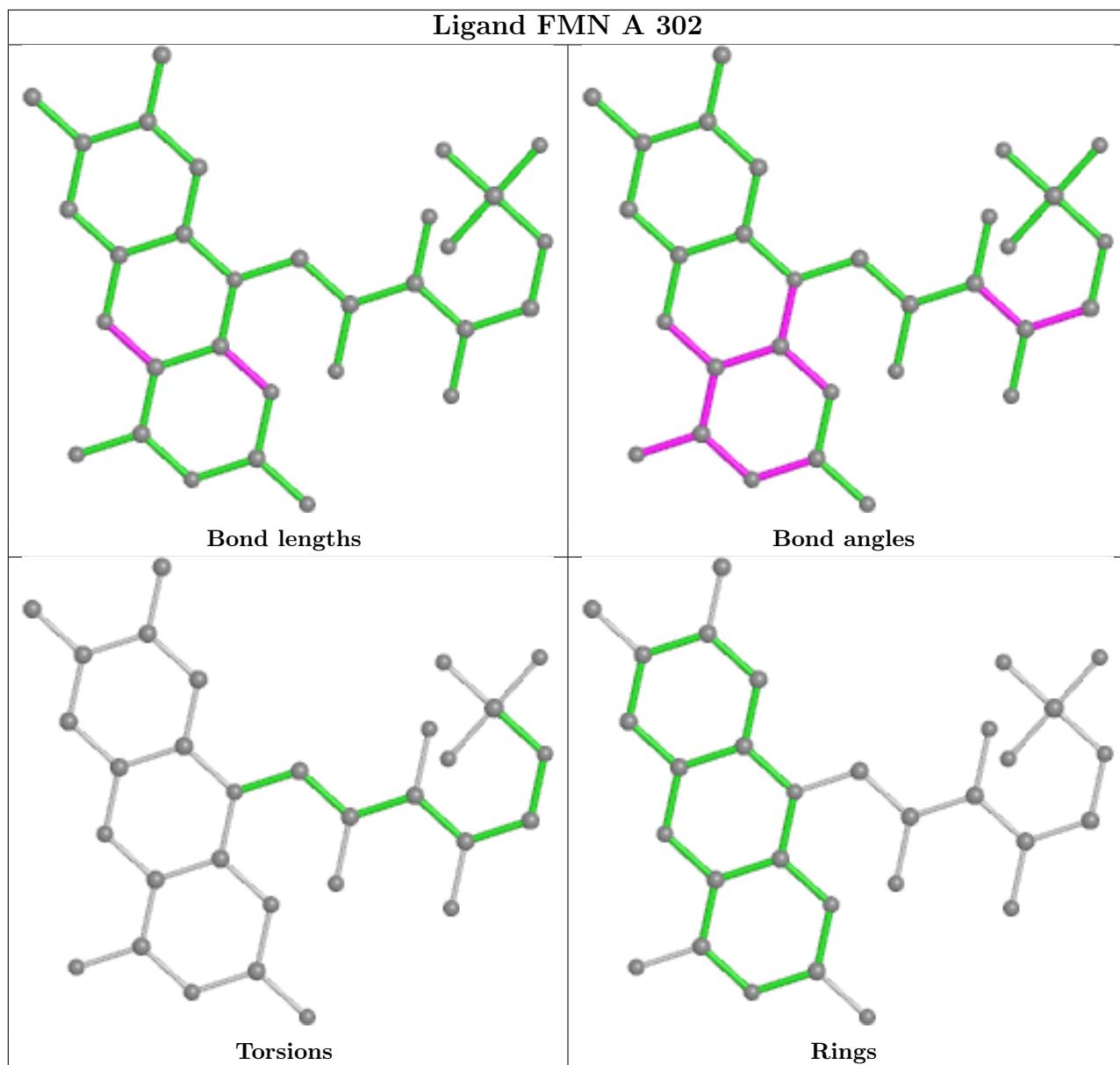
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 (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	216/218 (99%)	0.33	12 (5%) 24 16	9, 35, 70, 92	0
1	B	216/218 (99%)	0.34	11 (5%) 28 19	6, 37, 71, 100	0
1	H	216/218 (99%)	0.39	12 (5%) 24 16	11, 35, 72, 105	0
1	I	216/218 (99%)	0.39	16 (7%) 14 8	7, 38, 72, 86	0
All	All	864/872 (99%)	0.36	51 (5%) 22 14	6, 36, 72, 105	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	65	ALA	6.9
1	B	65	ALA	4.7
1	H	85	CYS	4.3
1	A	52	SER	3.8
1	I	112	GLU	3.6
1	I	64	ALA	3.5
1	H	23	THR	3.5
1	H	66	GLY	3.4
1	B	116	ALA	3.3
1	B	199	PHE	3.3
1	B	113	ALA	3.1
1	A	23	THR	3.1
1	H	123	PHE	3.1
1	A	25	GLU	3.1
1	B	66	GLY	3.0
1	H	113	ALA	2.8
1	H	5	SER	2.8
1	H	22	LEU	2.7
1	H	70	PHE	2.6
1	A	112	GLU	2.6
1	A	113	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	133	HIS	2.5
1	I	182	GLY	2.5
1	B	178	LEU	2.4
1	A	79	SER	2.4
1	A	152	LEU	2.4
1	B	41	THR	2.4
1	I	202	THR	2.4
1	I	91	ASP	2.4
1	B	156	ALA	2.4
1	H	124	PHE	2.4
1	B	39	SER	2.4
1	A	157	LEU	2.3
1	B	133	HIS	2.3
1	I	125	ALA	2.3
1	A	158	GLY	2.2
1	A	76	LEU	2.2
1	H	192	GLY	2.2
1	I	178	LEU	2.2
1	I	58	ALA	2.2
1	I	66	GLY	2.2
1	I	89	ALA	2.2
1	I	24	PRO	2.2
1	I	43	SER	2.2
1	A	24	PRO	2.1
1	H	194	HIS	2.1
1	B	198	ASP	2.1
1	I	141	LYS	2.1
1	I	119	LYS	2.0
1	A	69	VAL	2.0
1	I	11	HIS	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 [\(i\)](#)

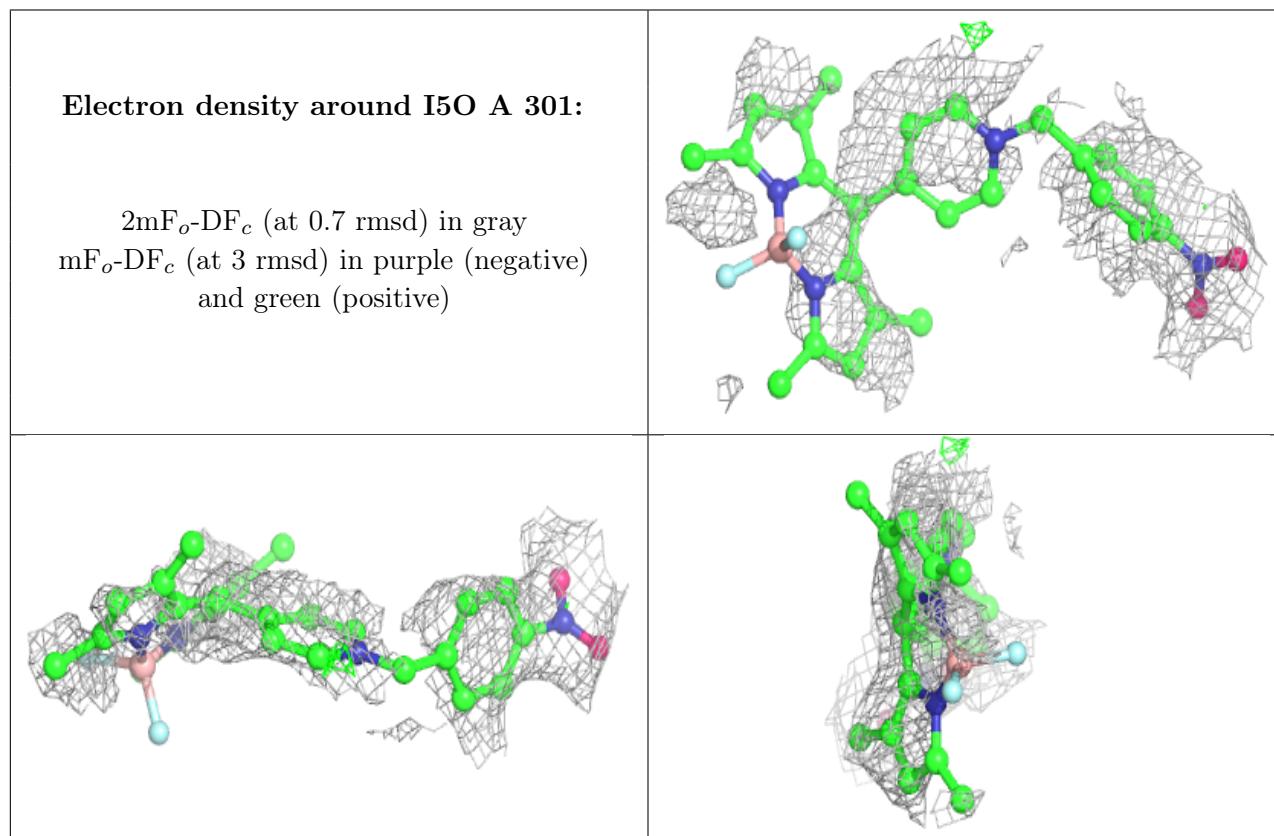
There are no monosaccharides in this entry.

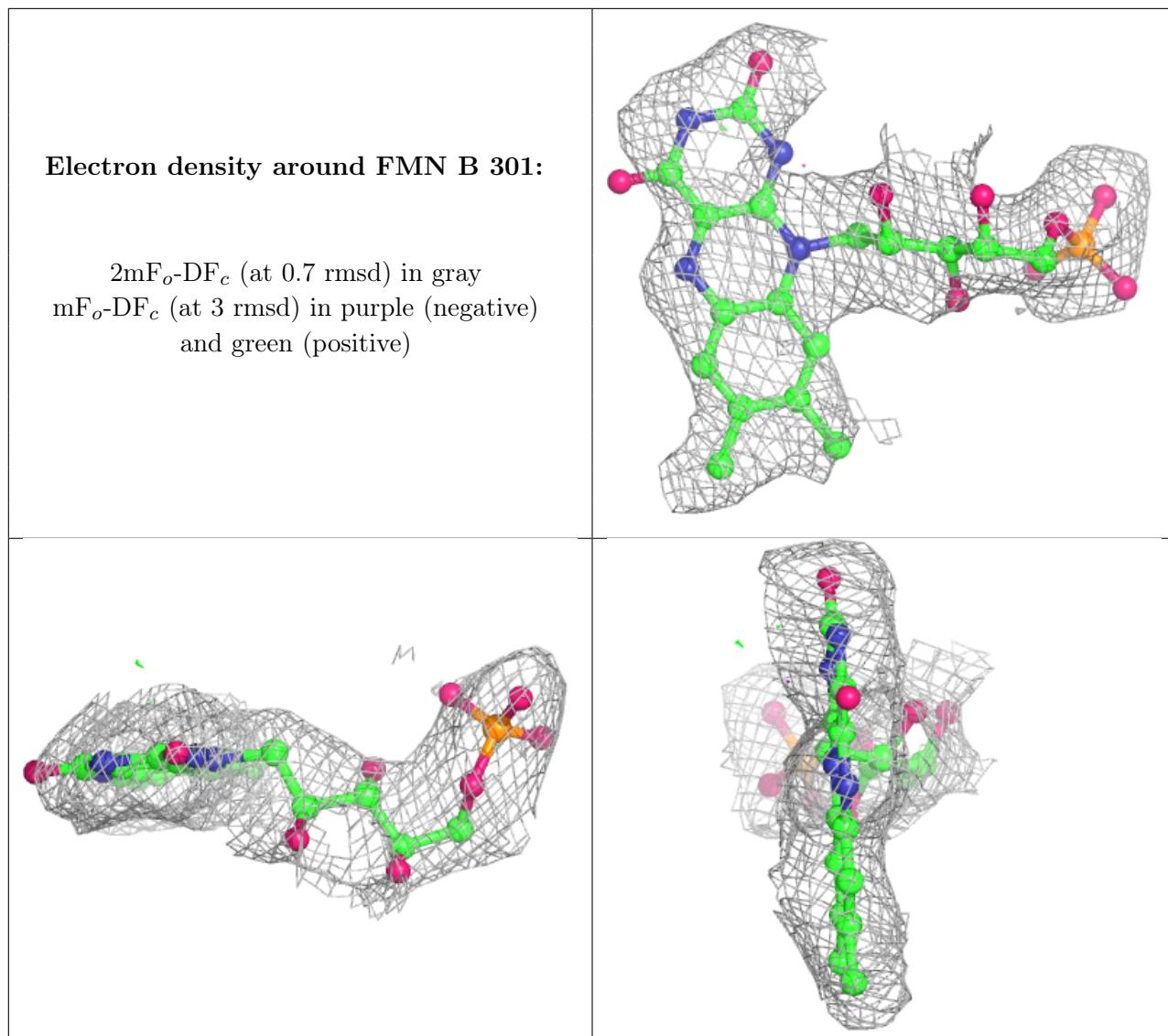
6.4 Ligands [\(i\)](#)

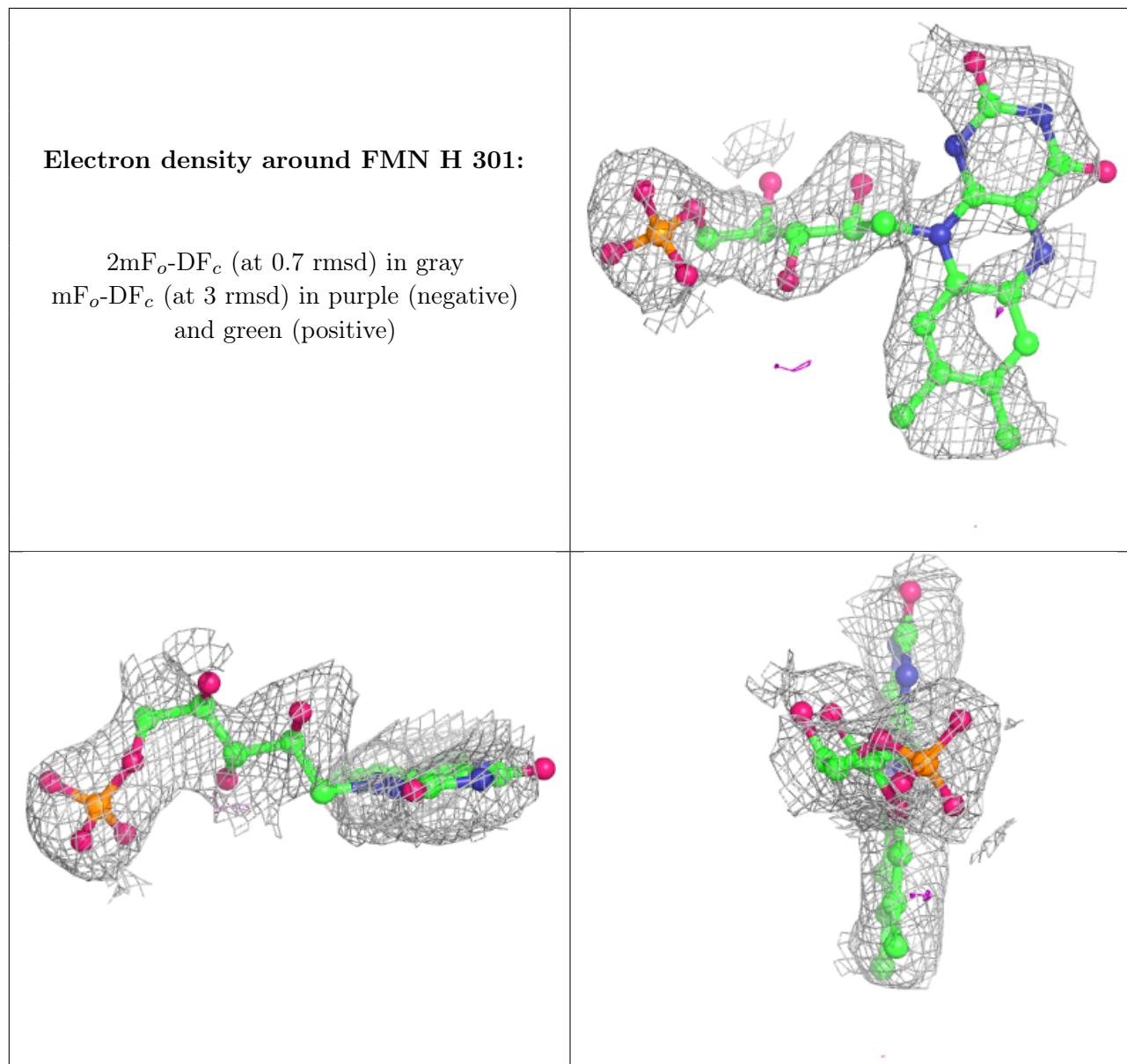
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

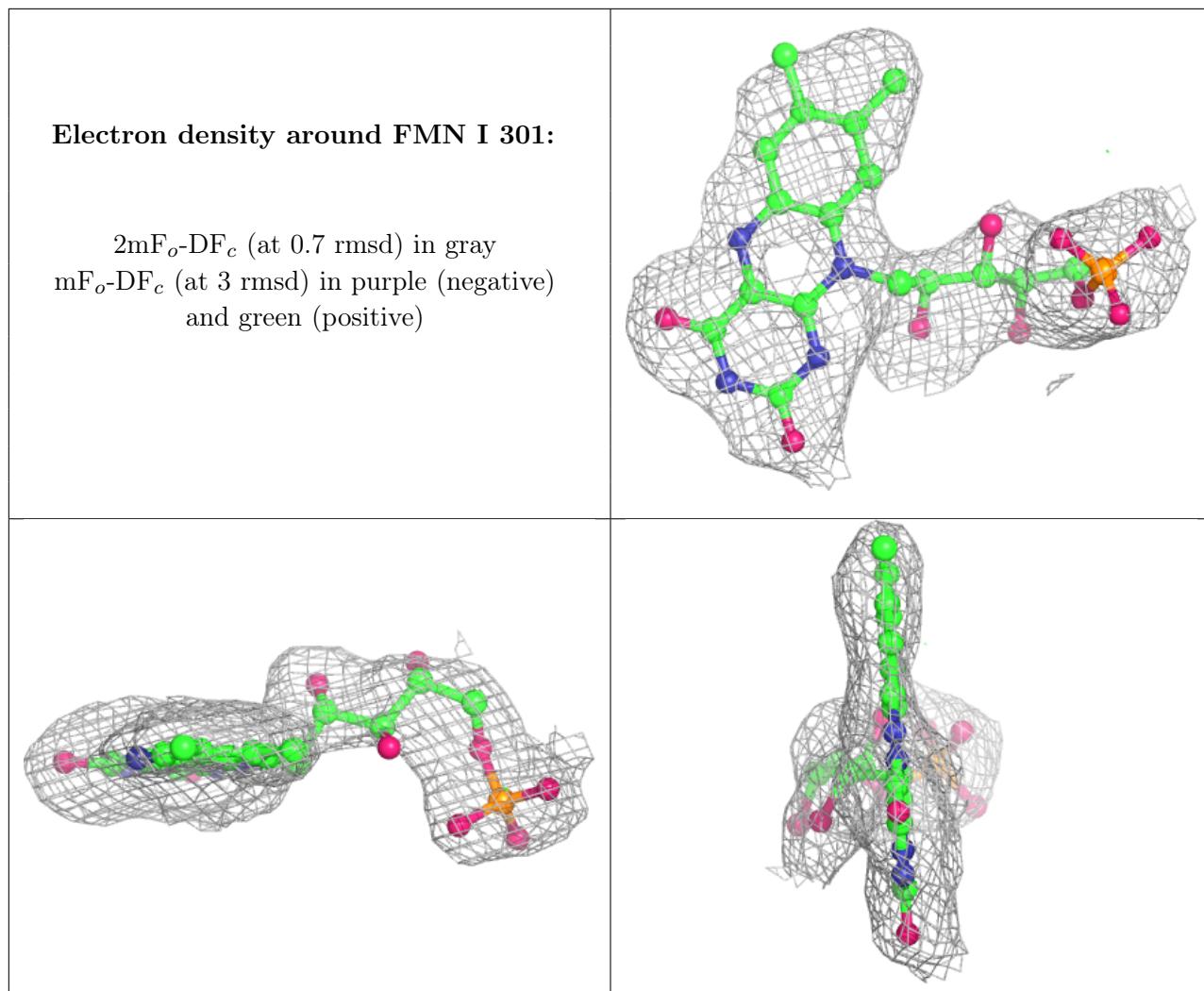
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	I5O	A	301	34/34	0.58	0.52	73,109,130,132	0
2	FMN	B	301	31/31	0.84	0.23	18,46,81,95	0
2	FMN	H	301	31/31	0.86	0.24	16,52,77,80	0
2	FMN	I	301	31/31	0.88	0.19	7,47,58,79	0
2	FMN	A	302	31/31	0.90	0.19	12,46,61,71	0

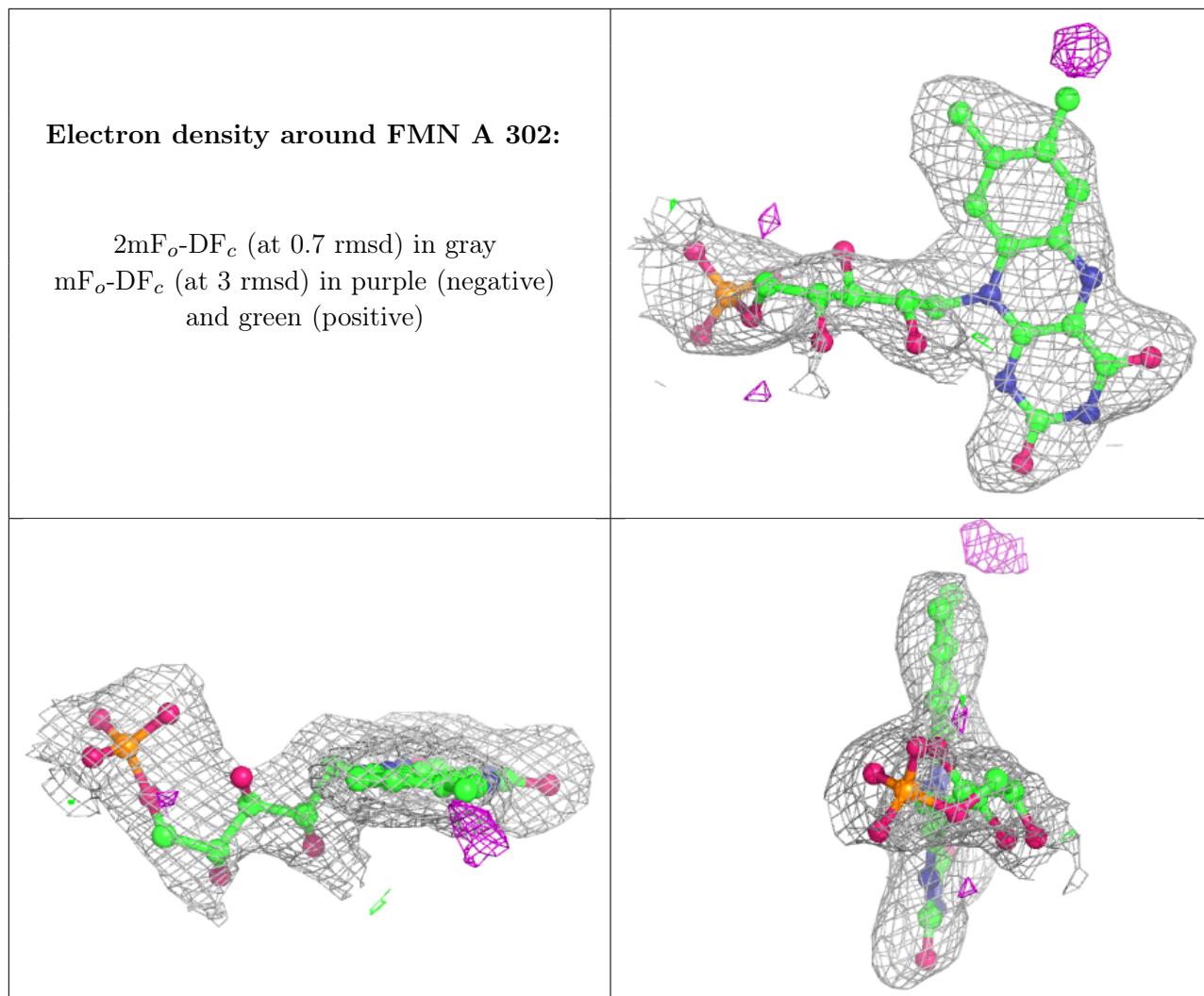
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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











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

There are no such residues in this entry.