



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:24 AM UTC

PDB ID : 2HFN / pdb_00002hfn
Title : Crystal Structures of the Synechocystis Photoreceptor Slr1694 Reveal Distinct Structural States Related to Signaling
Authors : Yuan, H.; Anderson, S.; Masuda, S.; Dragnea, V.; Moffat, K.; Bauer, C.E.
Deposited on : 2006-06-24
Resolution : 1.80 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 ⓘ 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:

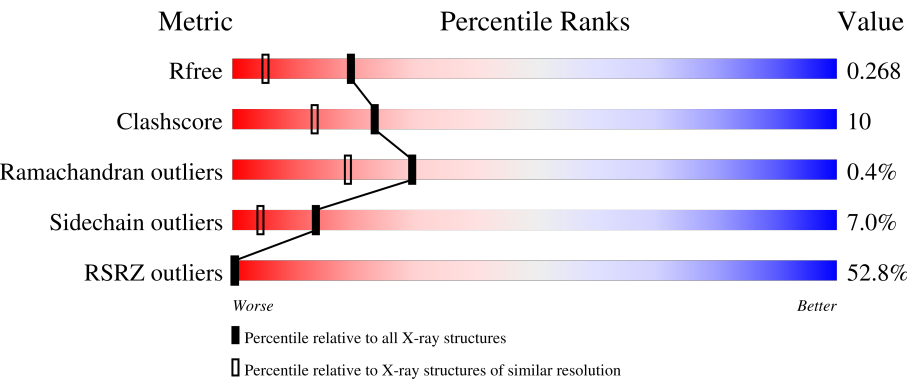
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	153	32% 72%21%... .
1	B	153	67% 75%15%8%
1	C	153	48% 75%15%8%
1	D	153	20% 73%18%5%
1	E	153	51% 78%10%9%

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Mol	Chain	Length	Quality of chain
1	F	153	39% 78% 10% • 9%
1	G	153	82% 75% 15% • 9%
1	H	153	80% 76% 12% • 9%
1	I	153	27% 71% 15% • • 9%
1	J	153	42% 69% 20% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11655 atoms, of which 2 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 Synechocystis Photoreceptor (Slr1694).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	149	Total	C	H	N	O	S	0	0	0
			1198	757	1	204	229	7			
1	B	140	Total	C	N	O	S		0	0	0
			1094	690	191	205	8				
1	C	140	Total	C	N	O	S		0	0	0
			1104	695	193	208	8				
1	D	146	Total	C	N	O	S		0	0	0
			1177	741	201	227	8				
1	E	139	Total	C	H	N	O	S	0	0	0
			1092	687	1	192	205	7			
1	F	139	Total	C	N	O	S		0	0	0
			1101	693	193	208	7				
1	G	139	Total	C	N	O	S		0	0	0
			1092	688	189	208	7				
1	H	139	Total	C	N	O	S		0	0	0
			1099	691	192	209	7				
1	I	139	Total	C	N	O	S		0	0	0
			1109	700	194	208	7				
1	J	142	Total	C	N	O	S		0	0	0
			1131	714	197	213	7				

There are 30 discrepancies between the modelled and reference sequences:

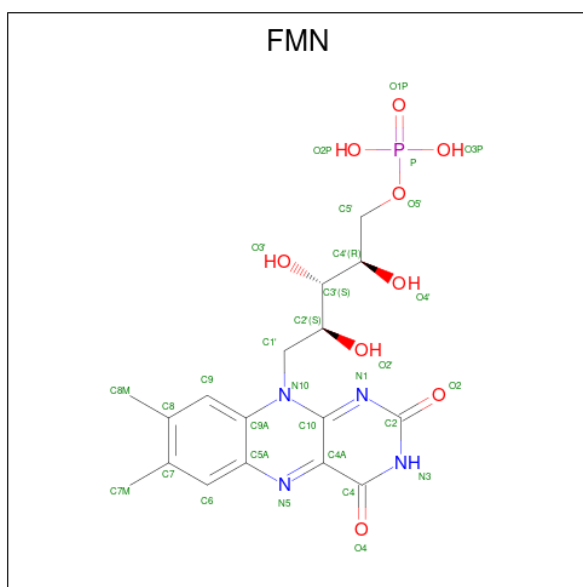
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	cloning artifact	UNP P74295
A	2	GLY	-	cloning artifact	UNP P74295
A	3	HIS	-	cloning artifact	UNP P74295
B	1	ALA	-	cloning artifact	UNP P74295
B	2	GLY	-	cloning artifact	UNP P74295
B	3	HIS	-	cloning artifact	UNP P74295
C	1	ALA	-	cloning artifact	UNP P74295
C	2	GLY	-	cloning artifact	UNP P74295
C	3	HIS	-	cloning artifact	UNP P74295

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	ALA	-	cloning artifact	UNP P74295
D	2	GLY	-	cloning artifact	UNP P74295
D	3	HIS	-	cloning artifact	UNP P74295
E	1	ALA	-	cloning artifact	UNP P74295
E	2	GLY	-	cloning artifact	UNP P74295
E	3	HIS	-	cloning artifact	UNP P74295
F	1	ALA	-	cloning artifact	UNP P74295
F	2	GLY	-	cloning artifact	UNP P74295
F	3	HIS	-	cloning artifact	UNP P74295
G	1	ALA	-	cloning artifact	UNP P74295
G	2	GLY	-	cloning artifact	UNP P74295
G	3	HIS	-	cloning artifact	UNP P74295
H	1	ALA	-	cloning artifact	UNP P74295
H	2	GLY	-	cloning artifact	UNP P74295
H	3	HIS	-	cloning artifact	UNP P74295
I	1	ALA	-	cloning artifact	UNP P74295
I	2	GLY	-	cloning artifact	UNP P74295
I	3	HIS	-	cloning artifact	UNP P74295
J	1	ALA	-	cloning artifact	UNP P74295
J	2	GLY	-	cloning artifact	UNP P74295
J	3	HIS	-	cloning artifact	UNP P74295

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



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

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

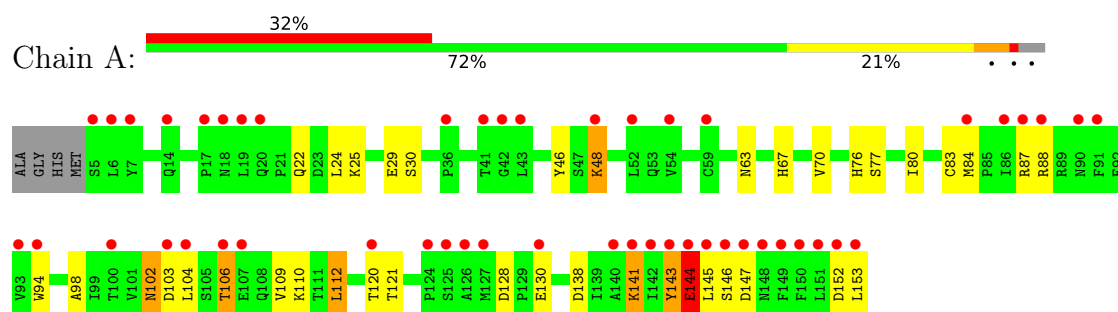
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	14	Total	O	0	0
			14	14		
3	C	15	Total	O	0	0
			15	15		
3	D	33	Total	O	0	0
			33	33		
3	E	4	Total	O	0	0
			4	4		
3	F	11	Total	O	0	0
			11	11		
3	G	2	Total	O	0	0
			2	2		
3	I	15	Total	O	0	0
			15	15		
3	J	12	Total	O	0	0
			12	12		

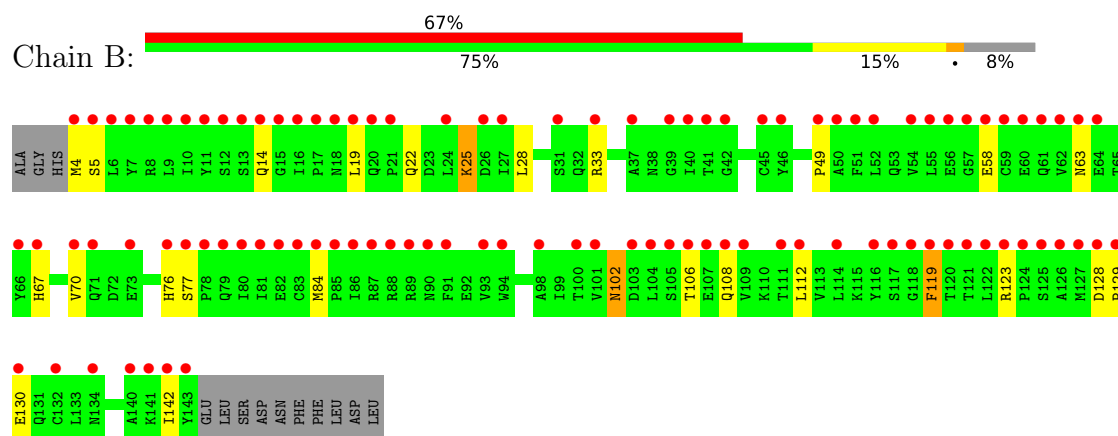
3 Residue-property plots [i](#)

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.

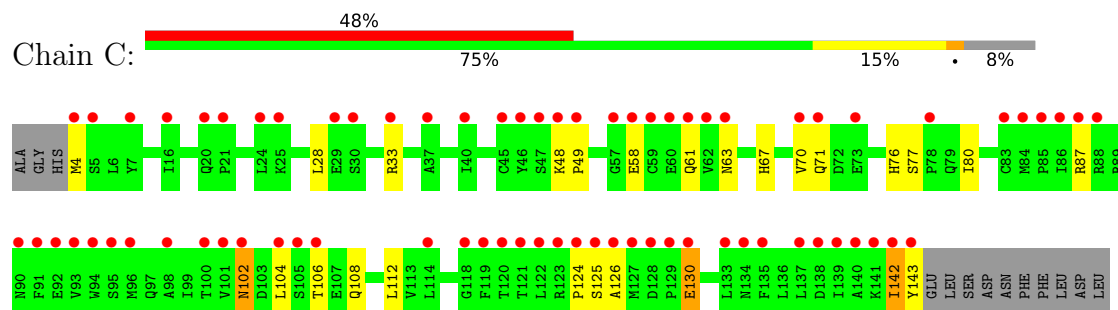
• Molecule 1: Synechocystis Photoreceptor (Slr1694)



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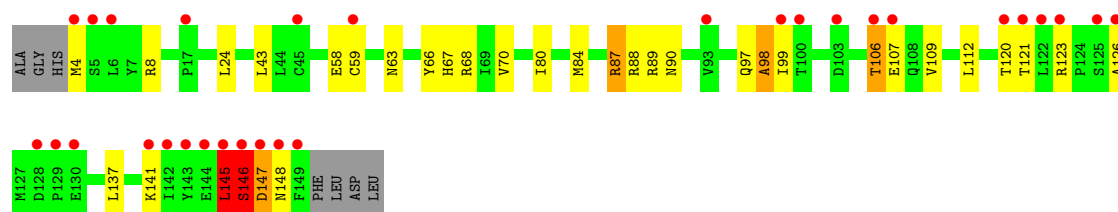


• Molecule 1: Synechocystis Photoreceptor (Slr1694)



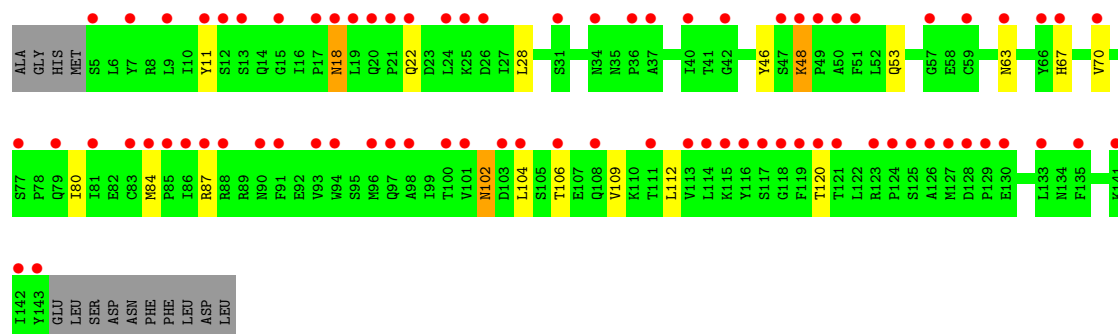
• Molecule 1: Synechocystis Photoreceptor (Slr1694)

Chain D: 



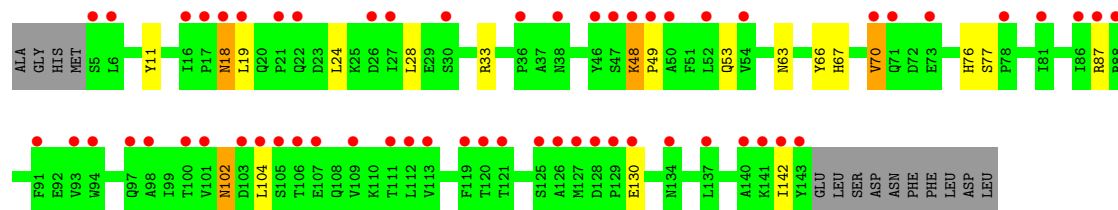
- Molecule 1: Synechocystis Photoreceptor (Slr1694)

Chain E: 



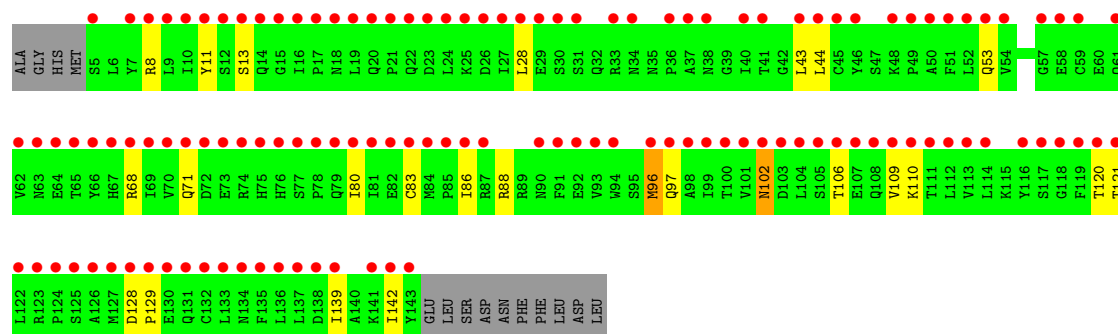
- Molecule 1: Synechocystis Photoreceptor (Slr1694)

Chain F: 



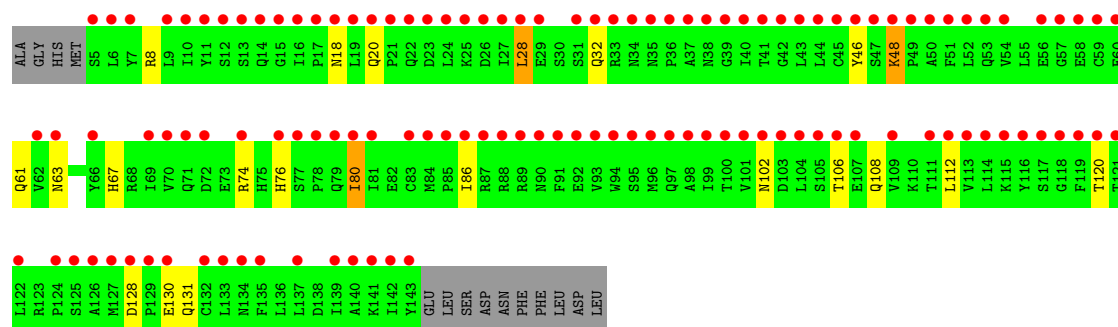
- Molecule 1: Synechocystis Photoreceptor (Slr1694)

Chain G: 



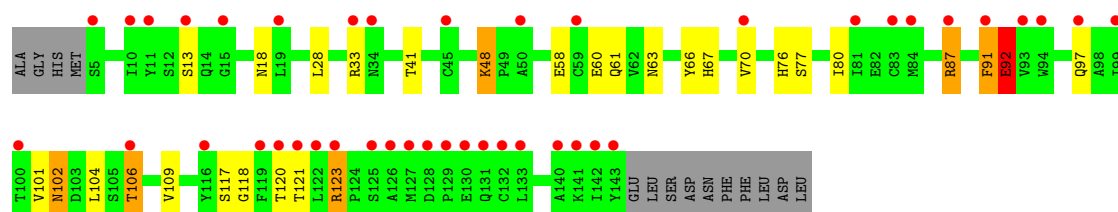
- Molecule 1: Synechocystis Photoreceptor (Slr1694)

Chain H: 



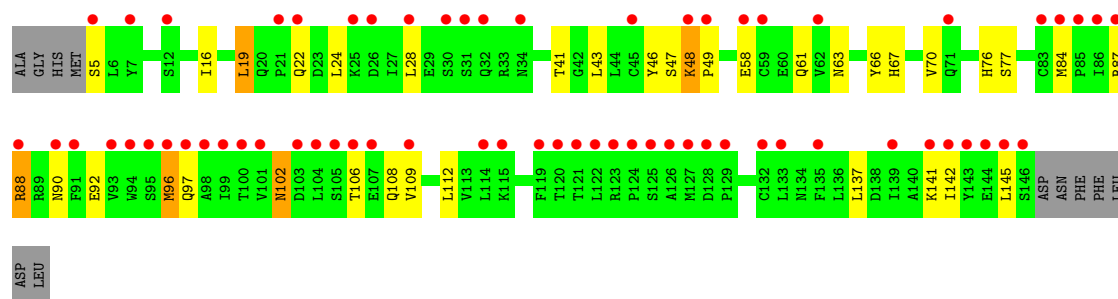
• Molecule 1: Synechocystis Photoreceptor (Slr1694)

Chain I: 



• Molecule 1: Synechocystis Photoreceptor (Slr1694)

Chain J: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.93Å 118.11Å 97.10Å 90.00° 110.79° 90.00°	Depositor
Resolution (Å)	48.51 – 1.80 48.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.51-1.80) 97.3 (48.51-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.240 , 0.266 0.240 , 0.268	Depositor DCC
R_{free} test set	8644 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11655	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 3.69% 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

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	0.85	0/1221	1.01	2/1656 (0.1%)
1	B	0.70	0/1116	0.88	1/1516 (0.1%)
1	C	0.71	0/1126	0.85	0/1527
1	D	0.86	0/1200	1.14	6/1628 (0.4%)
1	E	0.64	0/1113	0.86	1/1512 (0.1%)
1	F	0.65	0/1122	0.85	1/1522 (0.1%)
1	G	0.62	0/1114	0.86	0/1511
1	H	0.90	7/1121 (0.6%)	0.89	2/1522 (0.1%)
1	I	0.70	0/1131	0.99	2/1535 (0.1%)
1	J	0.72	0/1153	0.89	1/1565 (0.1%)
All	All	0.74	7/11417 (0.1%)	0.93	16/15494 (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	A	0	1
1	D	1	3
All	All	1	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	74	ARG	CZ-NH1	14.88	1.53	1.32
1	H	74	ARG	CZ-NH2	8.47	1.44	1.33
1	H	74	ARG	CD-NE	8.00	1.57	1.46
1	H	76	HIS	CE1-NE2	7.88	1.40	1.32
1	H	20	GLN	CD-NE2	6.86	1.47	1.33
1	H	20	GLN	CD-OE1	6.68	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	76	HIS	CG-CD2	5.04	1.41	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	146	SER	N-CA-C	14.85	142.44	110.80
1	I	91	PHE	N-CA-C	-11.15	99.64	108.78
1	D	147	ASP	N-CA-C	7.39	122.45	111.81
1	A	144	GLU	CA-C-O	7.29	130.94	120.51
1	A	144	GLU	CB-CA-C	-6.49	97.52	110.42
1	H	74	ARG	NE-CZ-NH2	-6.36	113.48	119.20
1	F	19	LEU	N-CA-C	6.22	119.38	110.10
1	I	117	SER	N-CA-C	6.07	116.57	108.38
1	D	98	ALA	N-CA-C	5.60	122.73	110.80
1	E	84	MET	CB-CA-C	-5.38	101.11	109.55
1	J	84	MET	N-CA-C	5.36	113.04	108.22
1	D	84	MET	N-CA-C	5.35	113.03	108.22
1	H	20	GLN	OE1-CD-NE2	5.35	127.95	122.60
1	B	119	PHE	N-CA-C	5.22	116.22	108.86
1	D	145	LEU	CA-C-N	5.00	131.10	121.54
1	D	145	LEU	C-N-CA	5.00	131.10	121.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	146	SER	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	TYR	Peptide
1	D	145	LEU	Peptide
1	D	146	SER	Peptide
1	D	97	GLN	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	1197	1	1174	30	0
1	B	1094	0	1065	24	0
1	C	1104	0	1079	26	0
1	D	1177	0	1155	32	0
1	E	1091	1	1063	19	0
1	F	1101	0	1087	24	0
1	G	1092	0	1065	21	0
1	H	1099	0	1068	13	0
1	I	1109	0	1097	36	0
1	J	1131	0	1116	43	0
2	A	31	0	19	1	0
2	B	31	0	19	1	0
2	C	31	0	19	2	0
2	D	31	0	19	1	0
2	E	31	0	19	1	0
2	F	31	0	19	1	0
2	G	31	0	19	0	0
2	H	31	0	19	0	0
2	I	31	0	19	0	0
2	J	31	0	19	0	0
3	A	42	0	0	2	0
3	B	14	0	0	1	0
3	C	15	0	0	1	0
3	D	33	0	0	1	0
3	E	4	0	0	0	0
3	F	11	0	0	0	0
3	G	2	0	0	0	0
3	I	15	0	0	1	0
3	J	12	0	0	2	0
All	All	11653	2	11159	230	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 10.

All (230) 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:J:43:LEU:HA	1:J:96:MET:HE1	1.25	1.16
1:E:48:LYS:HD2	1:E:48:LYS:N	1.62	1.11
1:J:96:MET:HE3	1:J:97:GLN:H	1.08	1.10
1:J:43:LEU:CA	1:J:96:MET:HE1	1.82	1.07
1:J:48:LYS:H	1:J:48:LYS:HD3	0.93	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:LYS:H	1:E:48:LYS:CD	1.66	1.05
1:I:48:LYS:CD	1:I:48:LYS:H	1.64	1.05
1:I:48:LYS:H	1:I:48:LYS:HD3	1.21	1.00
1:J:48:LYS:HD3	1:J:48:LYS:N	1.74	1.00
1:J:48:LYS:H	1:J:48:LYS:CD	1.67	0.96
1:A:46:TYR:CE2	1:A:48:LYS:HD3	2.01	0.95
1:J:96:MET:HE3	1:J:97:GLN:N	1.82	0.95
1:E:48:LYS:HD2	1:E:48:LYS:H	0.77	0.93
1:G:96:MET:HE3	1:G:97:GLN:H	1.34	0.93
1:J:96:MET:HE2	1:J:97:GLN:O	1.69	0.92
1:I:87:ARG:HE	1:I:87:ARG:HA	1.37	0.90
1:J:5:SER:HA	3:J:1113:HOH:O	1.71	0.90
1:D:4:MET:HE3	1:D:59:CYS:HB3	1.54	0.88
1:J:96:MET:CE	1:J:97:GLN:H	1.88	0.87
1:A:143:TYR:CA	1:A:144:GLU:HB2	2.05	0.86
1:E:102:ASN:HD22	1:E:104:LEU:H	1.22	0.83
1:F:87:ARG:HE	1:F:87:ARG:HA	1.43	0.83
1:A:143:TYR:HA	1:A:144:GLU:HB2	1.61	0.82
1:D:43:LEU:HD11	1:D:99:ILE:HG12	1.60	0.82
1:F:33:ARG:NH1	2:F:201:FMN:O3P	2.13	0.81
1:B:128:ASP:OD1	1:J:87:ARG:NH2	2.13	0.81
1:G:96:MET:HE3	1:G:97:GLN:N	1.95	0.81
1:G:44:LEU:N	1:G:96:MET:HE1	1.97	0.80
1:G:128:ASP:OD1	1:I:87:ARG:NH2	2.16	0.79
1:J:43:LEU:HA	1:J:96:MET:CE	2.11	0.78
1:F:48:LYS:H	1:F:48:LYS:HD2	1.48	0.78
1:J:88:ARG:HH11	1:J:88:ARG:HG2	1.52	0.75
1:G:68:ARG:O	1:G:71:GLN:HG2	1.88	0.74
1:D:8:ARG:HD3	3:D:1036:HOH:O	1.89	0.72
1:J:58:GLU:OE2	1:J:61:GLN:HG2	1.89	0.72
1:J:46:TYR:CE2	1:J:48:LYS:HD2	2.24	0.72
1:F:87:ARG:HH12	1:H:130:GLU:HB3	1.54	0.72
1:F:48:LYS:H	1:F:48:LYS:CD	2.00	0.72
1:B:14:GLN:HE22	1:B:49:PRO:HG2	1.53	0.72
1:B:119:PHE:HD2	1:B:123:ARG:HH12	1.36	0.72
1:I:80:ILE:H	1:J:63:ASN:HD21	1.37	0.71
1:A:80:ILE:H	1:B:63:ASN:HD21	1.38	0.71
1:I:91:PHE:O	1:I:92:GLU:OE1	2.08	0.71
1:I:58:GLU:OE2	1:I:61:GLN:HG2	1.92	0.70
1:D:87:ARG:HH22	1:F:130:GLU:CD	2.00	0.70
1:I:41:THR:HG21	1:I:92:GLU:HA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLU:HB3	1:C:61:GLN:HE21	1.58	0.68
1:G:139:ILE:O	1:G:142:ILE:HG12	1.94	0.68
1:I:91:PHE:O	1:I:92:GLU:CB	2.35	0.68
1:E:63:ASN:O	1:E:67:HIS:HD2	1.76	0.68
1:I:80:ILE:H	1:J:63:ASN:ND2	1.92	0.68
1:A:80:ILE:H	1:B:63:ASN:ND2	1.91	0.68
1:D:106:THR:HG22	1:D:109:VAL:H	1.58	0.68
1:G:43:LEU:C	1:G:96:MET:HE1	2.19	0.67
1:F:48:LYS:HD2	1:F:48:LYS:N	2.09	0.67
1:B:119:PHE:HD2	1:B:123:ARG:NH1	1.93	0.67
1:I:48:LYS:CD	1:I:48:LYS:N	2.46	0.67
1:A:130:GLU:OE1	1:C:87:ARG:HD3	1.95	0.66
1:G:80:ILE:H	1:H:63:ASN:HD21	1.44	0.66
1:J:48:LYS:HE3	1:J:102:ASN:HB3	1.77	0.65
1:I:48:LYS:HD3	1:I:48:LYS:N	2.04	0.65
1:D:4:MET:HE3	1:D:59:CYS:CB	2.24	0.65
1:E:102:ASN:ND2	1:E:104:LEU:H	1.91	0.65
1:G:80:ILE:H	1:H:63:ASN:ND2	1.95	0.65
1:A:110:LYS:HB3	1:A:120:THR:OG1	1.97	0.64
1:A:144:GLU:HG3	1:A:145:LEU:HG	1.79	0.64
1:G:128:ASP:CG	1:I:87:ARG:HH22	2.06	0.64
1:G:43:LEU:CA	1:G:96:MET:HE1	2.28	0.64
1:B:67:HIS:O	1:B:70:VAL:HG22	1.98	0.64
1:C:106:THR:HG22	1:C:108:GLN:H	1.63	0.63
1:D:87:ARG:NH2	1:F:130:GLU:CD	2.57	0.63
1:F:87:ARG:HA	1:F:87:ARG:NE	2.14	0.62
1:I:91:PHE:O	1:I:92:GLU:HB3	1.99	0.62
1:B:76:HIS:HD2	1:B:77:SER:OG	1.81	0.62
1:H:106:THR:HG22	1:H:108:GLN:H	1.63	0.62
1:J:43:LEU:C	1:J:96:MET:HE1	2.23	0.62
1:B:106:THR:HG22	1:B:108:GLN:H	1.66	0.61
1:A:46:TYR:HE2	1:A:48:LYS:HD3	1.58	0.61
1:E:102:ASN:HD22	1:E:104:LEU:N	1.95	0.61
1:I:87:ARG:HE	1:I:87:ARG:CA	2.10	0.60
1:J:96:MET:CE	1:J:97:GLN:O	2.46	0.60
1:D:4:MET:N	1:D:58:GLU:OE2	2.34	0.60
1:C:80:ILE:H	1:D:63:ASN:HD21	1.51	0.59
1:F:87:ARG:NH1	1:H:130:GLU:HB3	2.17	0.59
1:J:5:SER:CA	3:J:1113:HOH:O	2.42	0.58
1:A:106:THR:HG22	1:A:109:VAL:H	1.68	0.58
1:C:63:ASN:ND2	1:D:80:ILE:H	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ASN:HD22	1:B:102:ASN:C	2.12	0.58
1:J:96:MET:CE	1:J:97:GLN:N	2.58	0.57
1:J:88:ARG:HH11	1:J:88:ARG:CG	2.16	0.57
1:G:43:LEU:HA	1:G:96:MET:HE1	1.86	0.57
1:C:87:ARG:HA	1:C:87:ARG:CZ	2.34	0.57
1:I:123:ARG:HB2	1:I:123:ARG:CZ	2.35	0.57
1:I:91:PHE:O	1:I:92:GLU:CD	2.47	0.57
1:C:63:ASN:HD21	1:D:80:ILE:H	1.53	0.57
1:A:102:ASN:C	1:A:102:ASN:HD22	2.14	0.56
1:C:48:LYS:HD2	1:C:49:PRO:CA	2.36	0.56
1:C:48:LYS:HD2	1:C:49:PRO:HA	1.88	0.56
1:B:4:MET:N	3:B:1063:HOH:O	2.39	0.55
1:I:48:LYS:HE3	1:I:102:ASN:HB3	1.88	0.55
1:J:106:THR:HG22	1:J:108:GLN:H	1.71	0.55
1:A:48:LYS:HG2	3:A:1003:HOH:O	2.07	0.55
1:C:63:ASN:O	1:C:67:HIS:HD2	1.90	0.55
1:J:102:ASN:C	1:J:102:ASN:HD22	2.14	0.55
1:I:102:ASN:C	1:I:102:ASN:HD22	2.15	0.55
1:B:119:PHE:CD2	1:B:123:ARG:NH1	2.75	0.55
1:I:63:ASN:O	1:I:67:HIS:HD2	1.90	0.55
1:B:14:GLN:HE22	1:B:49:PRO:CG	2.18	0.54
1:I:106:THR:HG22	1:I:109:VAL:H	1.72	0.54
1:G:102:ASN:HD22	1:G:102:ASN:C	2.15	0.54
1:I:102:ASN:ND2	1:I:104:LEU:H	2.06	0.54
1:J:63:ASN:O	1:J:67:HIS:HD2	1.90	0.54
1:C:33:ARG:NH1	2:C:201:FMN:O3P	2.41	0.54
1:C:80:ILE:H	1:D:63:ASN:ND2	2.06	0.54
1:A:152:ASP:CG	1:A:153:LEU:H	2.16	0.54
1:F:87:ARG:NH1	1:H:128:ASP:OD2	2.42	0.53
1:J:41:THR:HG21	1:J:92:GLU:HA	1.89	0.53
1:C:102:ASN:HD22	1:C:104:LEU:H	1.55	0.53
1:J:67:HIS:O	1:J:70:VAL:HG22	2.09	0.53
1:E:63:ASN:O	1:E:67:HIS:CD2	2.60	0.53
1:I:76:HIS:HD2	1:I:77:SER:OG	1.91	0.53
1:G:106:THR:HG23	1:G:109:VAL:H	1.74	0.53
1:A:84:MET:HE2	1:B:84:MET:HB3	1.91	0.53
1:I:66:TYR:OH	1:J:67:HIS:HE1	1.93	0.52
1:A:112:LEU:HD21	1:A:138:ASP:CB	2.39	0.52
1:D:4:MET:HE3	1:D:59:CYS:SG	2.50	0.52
1:A:76:HIS:HD2	1:A:77:SER:OG	1.92	0.52
1:G:110:LYS:HB3	1:G:120:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:MET:O	1:B:58:GLU:HG3	2.11	0.51
1:C:76:HIS:HD2	1:C:77:SER:OG	1.93	0.51
1:C:102:ASN:ND2	1:C:104:LEU:H	2.09	0.51
1:C:130:GLU:HB3	1:E:87:ARG:HH11	1.76	0.51
1:F:76:HIS:HD2	1:F:77:SER:OG	1.94	0.51
1:G:96:MET:CE	1:G:97:GLN:O	2.59	0.51
1:J:48:LYS:N	1:J:48:LYS:CD	2.46	0.50
1:E:80:ILE:H	1:F:63:ASN:ND2	2.08	0.50
1:I:101:VAL:HG12	3:I:1124:HOH:O	2.11	0.50
1:I:102:ASN:HD22	1:I:104:LEU:H	1.58	0.50
1:A:87:ARG:HG2	1:A:87:ARG:HH21	1.78	0.49
1:J:96:MET:HE3	1:J:96:MET:HA	1.94	0.49
1:H:46:TYR:CE2	1:H:48:LYS:HG3	2.48	0.49
1:A:25:LYS:O	1:A:29:GLU:HG3	2.13	0.48
1:C:70:VAL:CG2	3:C:1111:HOH:O	2.60	0.48
1:B:4:MET:HA	1:B:58:GLU:CG	2.43	0.48
1:C:4:MET:O	1:C:58:GLU:HG3	2.12	0.48
1:I:67:HIS:HE1	1:J:66:TYR:OH	1.96	0.48
1:J:88:ARG:CG	1:J:88:ARG:NH1	2.76	0.47
1:H:8:ARG:HB2	1:H:86:ILE:HD13	1.97	0.47
1:D:87:ARG:HH21	1:D:87:ARG:CG	2.28	0.47
1:B:4:MET:HA	1:B:58:GLU:HG2	1.96	0.47
1:G:8:ARG:HB2	1:G:86:ILE:HD13	1.97	0.47
1:D:87:ARG:NH2	1:F:130:GLU:OE1	2.48	0.47
1:E:67:HIS:O	1:E:70:VAL:HG22	2.15	0.46
1:E:106:THR:HG22	1:E:109:VAL:HG23	1.96	0.46
1:D:87:ARG:NH2	1:D:87:ARG:HB3	2.31	0.46
1:G:83:CYS:SG	1:H:80:ILE:HG12	2.54	0.46
1:J:109:VAL:HG22	1:J:142:ILE:HD11	1.96	0.46
1:I:48:LYS:H	1:I:48:LYS:HD2	1.67	0.46
1:C:67:HIS:HE1	1:D:66:TYR:OH	1.99	0.46
1:D:68:ARG:NH1	2:D:201:FMN:O4'	2.48	0.46
1:F:102:ASN:HD22	1:F:104:LEU:H	1.63	0.46
1:B:4:MET:HB3	1:D:126:ALA:CB	2.46	0.46
1:I:67:HIS:CE1	1:J:66:TYR:OH	2.69	0.46
1:D:146:SER:OG	1:D:147:ASP:HA	2.16	0.45
1:E:48:LYS:HD3	1:E:102:ASN:HB3	1.98	0.45
1:I:66:TYR:OH	1:J:67:HIS:CE1	2.69	0.45
1:E:18:ASN:N	1:E:18:ASN:OD1	2.49	0.45
1:E:46:TYR:CD2	1:E:48:LYS:HE2	2.52	0.45
1:F:87:ARG:HH11	1:H:131:GLN:HG3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ARG:HH12	1:F:130:GLU:HB3	1.81	0.44
1:A:83:CYS:O	1:A:84:MET:HG3	2.17	0.44
1:B:63:ASN:HD22	1:B:67:HIS:HE1	1.64	0.44
1:B:128:ASP:HB2	1:B:129:PRO:CD	2.48	0.44
1:C:124:PRO:C	1:C:126:ALA:H	2.25	0.44
1:F:48:LYS:HA	1:F:49:PRO:HA	1.79	0.44
1:B:22:GLN:HE22	1:B:25:LYS:NZ	2.16	0.44
1:B:4:MET:HB3	1:D:126:ALA:HB1	1.99	0.44
1:E:48:LYS:N	1:E:48:LYS:CD	2.46	0.44
1:I:118:GLY:H	1:I:123:ARG:HH12	1.66	0.44
1:A:128:ASP:OD1	1:C:87:ARG:NH2	2.50	0.44
1:D:67:HIS:HA	1:D:70:VAL:HG22	2.00	0.44
1:A:48:LYS:HG2	1:A:48:LYS:H	1.55	0.43
1:D:4:MET:N	1:D:58:GLU:CG	2.81	0.43
1:E:11:TYR:CE1	1:E:53:GLN:HB3	2.53	0.43
1:A:48:LYS:HE2	3:A:1003:HOH:O	2.18	0.43
1:D:88:ARG:NH1	1:D:89:ARG:O	2.52	0.43
1:A:102:ASN:ND2	1:A:104:LEU:H	2.16	0.43
1:I:58:GLU:OE2	1:I:60:GLU:HB3	2.19	0.43
1:A:112:LEU:HD21	1:A:138:ASP:HB3	2.00	0.43
1:D:90:ASN:HB3	1:D:137:LEU:HD21	2.00	0.42
1:B:33:ARG:NH1	2:B:201:FMN:O3P	2.52	0.42
1:E:67:HIS:HE1	1:F:66:TYR:OH	2.02	0.42
1:E:80:ILE:H	1:F:63:ASN:HD21	1.66	0.42
1:A:98:ALA:O	1:A:147:ASP:HA	2.19	0.42
1:C:63:ASN:O	1:C:67:HIS:CD2	2.71	0.42
1:A:143:TYR:CB	1:A:144:GLU:HB2	2.49	0.42
1:H:63:ASN:O	1:H:67:HIS:HD2	2.03	0.42
1:A:30:SER:HB3	2:A:201:FMN:H4'	2.01	0.42
1:H:28:LEU:O	1:H:32:GLN:HG3	2.20	0.42
1:I:87:ARG:HA	1:I:87:ARG:NE	2.17	0.42
1:J:47:SER:O	1:J:48:LYS:C	2.62	0.42
1:D:88:ARG:NH2	1:D:148:ASN:OD1	2.52	0.41
2:E:201:FMN:H9	2:E:201:FMN:H1'1	1.84	0.41
1:I:63:ASN:O	1:I:67:HIS:CD2	2.71	0.41
1:I:91:PHE:O	1:I:92:GLU:CG	2.68	0.41
1:J:48:LYS:HA	1:J:49:PRO:HA	1.89	0.41
1:A:63:ASN:O	1:A:67:HIS:HD2	2.03	0.41
1:F:11:TYR:CE1	1:F:53:GLN:HB3	2.56	0.41
1:F:18:ASN:OD1	1:F:18:ASN:N	2.52	0.41
1:C:4:MET:C	1:C:58:GLU:HG3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:HIS:CE1	1:D:66:TYR:OH	2.73	0.41
1:G:11:TYR:CE1	1:G:53:GLN:HB3	2.55	0.41
1:J:16:ILE:O	1:J:19:LEU:HB2	2.21	0.41
1:B:130:GLU:OE1	1:J:87:ARG:NH1	2.49	0.41
1:D:99:ILE:HD11	1:D:145:LEU:HD11	2.03	0.41
1:F:67:HIS:HA	1:F:70:VAL:HG12	2.03	0.41
1:G:128:ASP:HB2	1:G:129:PRO:CD	2.50	0.41
1:J:43:LEU:N	1:J:96:MET:HE1	2.34	0.41
1:D:146:SER:HB3	1:D:147:ASP:HB2	2.03	0.41
1:F:87:ARG:CZ	1:H:130:GLU:OE1	2.69	0.41
1:C:33:ARG:HH12	2:C:201:FMN:P	2.44	0.41
1:D:87:ARG:NE	1:D:87:ARG:HA	2.36	0.41
1:A:141:LYS:HB2	1:A:141:LYS:HE2	1.67	0.40
1:D:87:ARG:HH21	1:D:87:ARG:HG3	1.85	0.40
1:G:44:LEU:H	1:G:96:MET:HE1	1.84	0.40
1:J:90:ASN:HB3	1:J:137:LEU:HD21	2.04	0.40
1:J:76:HIS:HD2	1:J:77:SER:OG	2.05	0.40
1:A:94:TRP:CZ3	1:A:146:SER:HB3	2.57	0.40
1:C:142:ILE:HG13	1:C:143:TYR:N	2.36	0.40
1:I:87:ARG:CA	1:I:87:ARG:NE	2.81	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	147/153 (96%)	145 (99%)	1 (1%)	1 (1%)	18	8
1	B	138/153 (90%)	138 (100%)	0	0	100	100
1	C	138/153 (90%)	134 (97%)	4 (3%)	0	100	100
1	D	144/153 (94%)	142 (99%)	0	2 (1%)	9	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	F	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	G	137/153 (90%)	133 (97%)	4 (3%)	0	100	100
1	H	137/153 (90%)	136 (99%)	1 (1%)	0	100	100
1	I	137/153 (90%)	132 (96%)	4 (3%)	1 (1%)	18	8
1	J	140/153 (92%)	134 (96%)	5 (4%)	1 (1%)	18	8
All	All	1392/1530 (91%)	1364 (98%)	23 (2%)	5 (0%)	30	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLU
1	D	98	ALA
1	I	92	GLU
1	J	145	LEU
1	D	146	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/141 (96%)	124 (91%)	12 (9%)	9	2
1	B	121/141 (86%)	114 (94%)	7 (6%)	18	7
1	C	123/141 (87%)	116 (94%)	7 (6%)	18	8
1	D	135/141 (96%)	125 (93%)	10 (7%)	13	4
1	E	121/141 (86%)	114 (94%)	7 (6%)	18	7
1	F	124/141 (88%)	117 (94%)	7 (6%)	19	8
1	G	122/141 (86%)	116 (95%)	6 (5%)	22	10
1	H	123/141 (87%)	115 (94%)	8 (6%)	15	5
1	I	125/141 (89%)	111 (89%)	14 (11%)	6	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	127/141 (90%)	117 (92%)	10 (8%)	11	3
All	All	1257/1410 (89%)	1169 (93%)	88 (7%)	14	4

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	24	LEU
1	A	48	LYS
1	A	70	VAL
1	A	88	ARG
1	A	102	ASN
1	A	103	ASP
1	A	106	THR
1	A	112	LEU
1	A	121	THR
1	A	141	LYS
1	A	144	GLU
1	B	5	SER
1	B	19	LEU
1	B	25	LYS
1	B	28	LEU
1	B	102	ASN
1	B	112	LEU
1	B	142	ILE
1	C	28	LEU
1	C	71	GLN
1	C	102	ASN
1	C	112	LEU
1	C	125	SER
1	C	130	GLU
1	C	142	ILE
1	D	24	LEU
1	D	87	ARG
1	D	106	THR
1	D	107	GLU
1	D	112	LEU
1	D	120	THR
1	D	121	THR
1	D	123	ARG
1	D	141	LYS
1	D	146	SER

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Mol	Chain	Res	Type
1	E	18	ASN
1	E	22	GLN
1	E	28	LEU
1	E	48	LYS
1	E	102	ASN
1	E	112	LEU
1	E	120	THR
1	F	18	ASN
1	F	24	LEU
1	F	28	LEU
1	F	48	LYS
1	F	70	VAL
1	F	102	ASN
1	F	142	ILE
1	G	13	SER
1	G	28	LEU
1	G	88	ARG
1	G	96	MET
1	G	102	ASN
1	G	121	THR
1	H	18	ASN
1	H	28	LEU
1	H	48	LYS
1	H	61	GLN
1	H	80	ILE
1	H	102	ASN
1	H	112	LEU
1	H	120	THR
1	I	13	SER
1	I	18	ASN
1	I	28	LEU
1	I	33	ARG
1	I	48	LYS
1	I	70	VAL
1	I	87	ARG
1	I	92	GLU
1	I	97	GLN
1	I	102	ASN
1	I	106	THR
1	I	120	THR
1	I	121	THR
1	I	123	ARG

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Mol	Chain	Res	Type
1	J	19	LEU
1	J	22	GLN
1	J	24	LEU
1	J	28	LEU
1	J	48	LYS
1	J	88	ARG
1	J	96	MET
1	J	102	ASN
1	J	112	LEU
1	J	141	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	32	GLN
1	A	67	HIS
1	A	76	HIS
1	A	97	GLN
1	A	102	ASN
1	B	14	GLN
1	B	22	GLN
1	B	32	GLN
1	B	63	ASN
1	B	76	HIS
1	B	102	ASN
1	C	32	GLN
1	C	61	GLN
1	C	63	ASN
1	C	67	HIS
1	C	76	HIS
1	C	102	ASN
1	D	18	ASN
1	D	53	GLN
1	D	61	GLN
1	D	63	ASN
1	D	97	GLN
1	E	32	GLN
1	E	61	GLN
1	E	67	HIS
1	E	71	GLN
1	E	76	HIS

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Mol	Chain	Res	Type
1	E	102	ASN
1	F	32	GLN
1	F	63	ASN
1	F	67	HIS
1	F	76	HIS
1	G	32	GLN
1	G	61	GLN
1	G	67	HIS
1	G	102	ASN
1	G	108	GLN
1	H	61	GLN
1	H	63	ASN
1	H	67	HIS
1	H	90	ASN
1	H	102	ASN
1	I	32	GLN
1	I	67	HIS
1	I	76	HIS
1	I	97	GLN
1	J	20	GLN
1	J	22	GLN
1	J	32	GLN
1	J	61	GLN
1	J	63	ASN
1	J	67	HIS
1	J	76	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

10 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	G	201	-	33,33,33	1.05	2 (6%)	48,50,50	1.31	7 (14%)
2	FMN	E	201	-	33,33,33	1.08	2 (6%)	48,50,50	1.39	7 (14%)
2	FMN	H	201	-	33,33,33	1.01	2 (6%)	48,50,50	1.25	6 (12%)
2	FMN	J	201	-	33,33,33	1.05	3 (9%)	48,50,50	1.40	11 (22%)
2	FMN	D	201	-	33,33,33	1.18	3 (9%)	48,50,50	1.16	6 (12%)
2	FMN	B	201	-	33,33,33	1.04	2 (6%)	48,50,50	1.28	7 (14%)
2	FMN	C	201	-	33,33,33	1.05	1 (3%)	48,50,50	1.45	9 (18%)
2	FMN	I	201	-	33,33,33	1.14	2 (6%)	48,50,50	1.45	10 (20%)
2	FMN	A	201	-	33,33,33	1.14	2 (6%)	48,50,50	1.25	6 (12%)
2	FMN	F	201	-	33,33,33	1.07	2 (6%)	48,50,50	1.39	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	G	201	-	-	4/18/18/18	0/3/3/3
2	FMN	E	201	-	-	0/18/18/18	0/3/3/3
2	FMN	H	201	-	-	9/18/18/18	0/3/3/3
2	FMN	J	201	-	-	7/18/18/18	0/3/3/3
2	FMN	D	201	-	-	0/18/18/18	0/3/3/3
2	FMN	B	201	-	-	7/18/18/18	0/3/3/3
2	FMN	C	201	-	-	4/18/18/18	0/3/3/3
2	FMN	I	201	-	-	0/18/18/18	0/3/3/3
2	FMN	A	201	-	-	0/18/18/18	0/3/3/3
2	FMN	F	201	-	-	0/18/18/18	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	FMN	C4A-N5	3.88	1.39	1.30
2	E	201	FMN	C4A-N5	3.88	1.39	1.30
2	D	201	FMN	C4A-N5	3.71	1.38	1.30
2	F	201	FMN	C4A-N5	3.61	1.38	1.30
2	H	201	FMN	C4A-N5	3.60	1.38	1.30
2	G	201	FMN	C4A-N5	3.54	1.38	1.30
2	I	201	FMN	C4A-N5	3.51	1.38	1.30
2	B	201	FMN	C4A-N5	3.15	1.37	1.30
2	I	201	FMN	C10-N1	3.11	1.39	1.33
2	G	201	FMN	C10-N1	3.05	1.39	1.33
2	D	201	FMN	C10-N1	2.92	1.39	1.33
2	C	201	FMN	C4A-N5	2.81	1.36	1.30
2	J	201	FMN	C4A-N5	2.71	1.36	1.30
2	A	201	FMN	C10-N1	2.68	1.38	1.33
2	H	201	FMN	C10-N1	2.64	1.38	1.33
2	F	201	FMN	C10-N1	2.63	1.38	1.33
2	E	201	FMN	C10-N1	2.48	1.38	1.33
2	J	201	FMN	C10-N1	2.30	1.37	1.33
2	D	201	FMN	C1'-N10	2.15	1.53	1.47
2	J	201	FMN	C9A-N10	-2.13	1.37	1.41
2	B	201	FMN	C10-N1	2.11	1.37	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	FMN	C9A-C5A-N5	-3.71	118.52	122.45
2	A	201	FMN	C4A-C10-N10	3.36	121.29	116.48
2	I	201	FMN	C4-N3-C2	-3.33	119.73	125.64
2	I	201	FMN	C4-C4A-N5	3.21	122.65	118.21
2	E	201	FMN	C4-N3-C2	-3.19	119.97	125.64
2	F	201	FMN	C10-C4A-N5	-3.18	118.32	124.81
2	B	201	FMN	C4A-C10-N10	3.14	120.97	116.48
2	F	201	FMN	C4-N3-C2	-3.08	120.17	125.64
2	I	201	FMN	C10-C4A-N5	-3.08	118.51	124.81
2	F	201	FMN	C9A-C5A-N5	-3.06	119.21	122.45
2	A	201	FMN	C10-C4A-N5	-3.04	118.59	124.81
2	J	201	FMN	C4A-C10-N10	3.02	120.81	116.48
2	I	201	FMN	C4A-C4-N3	3.02	120.93	113.25
2	I	201	FMN	C9A-C5A-N5	-3.01	119.26	122.45
2	E	201	FMN	C10-C4A-N5	-2.98	118.72	124.81
2	D	201	FMN	C4A-C10-N10	2.93	120.68	116.48
2	D	201	FMN	C10-C4A-N5	-2.91	118.86	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	FMN	C10-C4A-N5	-2.87	118.94	124.81
2	B	201	FMN	C4-N3-C2	-2.87	120.54	125.64
2	H	201	FMN	C4A-C10-N10	2.87	120.59	116.48
2	I	201	FMN	C4A-C10-N10	2.87	120.58	116.48
2	B	201	FMN	C10-C4A-N5	-2.85	118.98	124.81
2	H	201	FMN	C4-N3-C2	-2.81	120.64	125.64
2	J	201	FMN	O2-C2-N1	-2.78	117.18	121.80
2	F	201	FMN	C4A-C10-N10	2.77	120.45	116.48
2	E	201	FMN	C9A-C5A-N5	-2.74	119.55	122.45
2	E	201	FMN	C4A-C10-N10	2.74	120.40	116.48
2	G	201	FMN	C4-N3-C2	-2.73	120.79	125.64
2	G	201	FMN	C4A-C10-N10	2.69	120.33	116.48
2	J	201	FMN	C10-C4A-N5	-2.68	119.34	124.81
2	H	201	FMN	C10-C4A-N5	-2.62	119.45	124.81
2	I	201	FMN	C10-N1-C2	2.61	122.50	116.85
2	C	201	FMN	O4-C4-C4A	-2.61	119.65	126.53
2	C	201	FMN	C10-C4A-N5	-2.60	119.50	124.81
2	C	201	FMN	C4A-C10-N10	2.58	120.17	116.48
2	E	201	FMN	C4A-C4-N3	2.57	119.80	113.25
2	J	201	FMN	O4-C4-C4A	-2.57	119.75	126.53
2	C	201	FMN	C4-N3-C2	-2.53	121.14	125.64
2	G	201	FMN	C9A-C5A-N5	-2.51	119.79	122.45
2	B	201	FMN	C9A-C5A-N5	-2.51	119.80	122.45
2	H	201	FMN	C4'-C3'-C2'	-2.49	109.43	113.57
2	E	201	FMN	C4-C4A-N5	2.46	121.61	118.21
2	A	201	FMN	C4-C4A-N5	2.45	121.58	118.21
2	I	201	FMN	C5A-N5-C4A	2.41	121.99	118.09
2	F	201	FMN	C5A-N5-C4A	2.39	121.95	118.09
2	A	201	FMN	C4-N3-C2	-2.38	121.41	125.64
2	J	201	FMN	O2-C2-N3	2.37	123.12	118.58
2	H	201	FMN	C4A-C4-N3	2.36	119.27	113.25
2	G	201	FMN	C4A-C4-N3	2.35	119.24	113.25
2	F	201	FMN	C4-C4A-N5	2.35	121.45	118.21
2	J	201	FMN	C9A-C5A-N5	-2.34	119.97	122.45
2	I	201	FMN	C4A-C10-N1	-2.31	118.92	124.59
2	C	201	FMN	C4A-C4-N3	2.30	119.11	113.25
2	C	201	FMN	C5A-N5-C4A	2.27	121.76	118.09
2	F	201	FMN	C4A-C4-N3	2.25	118.97	113.25
2	J	201	FMN	O3'-C3'-C4'	2.23	114.01	108.93
2	G	201	FMN	O4-C4-C4A	-2.22	120.68	126.53
2	E	201	FMN	O4-C4-C4A	-2.22	120.68	126.53
2	J	201	FMN	C4-C4A-C10	2.21	120.72	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	FMN	C4-C4A-N5	2.21	121.26	118.21
2	D	201	FMN	C4-N3-C2	-2.20	121.74	125.64
2	C	201	FMN	C5A-C9A-N10	2.17	119.93	117.97
2	H	201	FMN	C4A-C10-N1	-2.17	119.28	124.59
2	D	201	FMN	C4A-C10-N1	-2.16	119.29	124.59
2	B	201	FMN	C4-C4A-C10	2.16	120.64	116.93
2	I	201	FMN	O2P-P-O5'	2.15	112.28	106.67
2	J	201	FMN	C4-N3-C2	-2.13	121.85	125.64
2	D	201	FMN	C4A-C4-N3	2.13	118.67	113.25
2	J	201	FMN	C1'-C2'-C3'	2.12	115.41	109.66
2	B	201	FMN	C4A-C4-N3	2.12	118.66	113.25
2	C	201	FMN	C10-N1-C2	2.10	121.40	116.85
2	A	201	FMN	C9A-C5A-N5	-2.09	120.24	122.45
2	D	201	FMN	C4-C4A-N5	2.08	121.08	118.21
2	F	201	FMN	O4-C4-C4A	-2.08	121.06	126.53
2	A	201	FMN	O2P-P-O5'	2.03	111.97	106.67
2	J	201	FMN	C5A-C9A-N10	2.03	119.80	117.97
2	B	201	FMN	C4A-C10-N1	-2.03	119.62	124.59
2	F	201	FMN	C4A-C10-N1	-2.01	119.67	124.59

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	FMN	C1'-C2'-C3'-C4'
2	C	201	FMN	C1'-C2'-C3'-C4'
2	G	201	FMN	C1'-C2'-C3'-C4'
2	H	201	FMN	C1'-C2'-C3'-O3'
2	H	201	FMN	C1'-C2'-C3'-C4'
2	H	201	FMN	O2'-C2'-C3'-O3'
2	H	201	FMN	O2'-C2'-C3'-C4'
2	H	201	FMN	C3'-C4'-C5'-O5'
2	H	201	FMN	O4'-C4'-C5'-O5'
2	H	201	FMN	C5'-O5'-P-O1P
2	H	201	FMN	C5'-O5'-P-O2P
2	H	201	FMN	C5'-O5'-P-O3P
2	J	201	FMN	C1'-C2'-C3'-C4'
2	J	201	FMN	O3'-C3'-C4'-O4'
2	J	201	FMN	O3'-C3'-C4'-C5'
2	J	201	FMN	C2'-C3'-C4'-O4'
2	B	201	FMN	O3'-C3'-C4'-O4'
2	B	201	FMN	C2'-C3'-C4'-O4'

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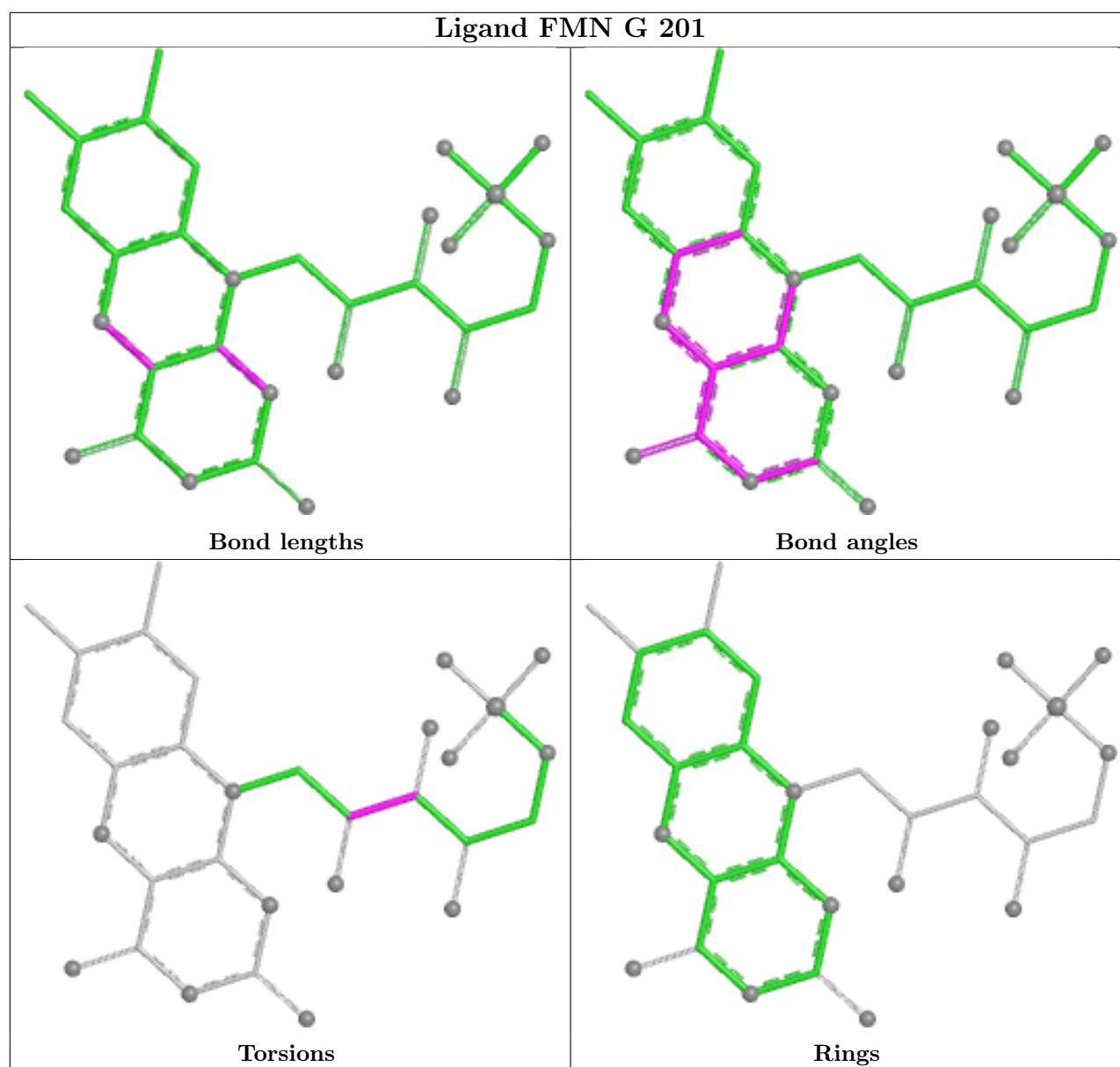
Mol	Chain	Res	Type	Atoms
2	B	201	FMN	O3'-C3'-C4'-C5'
2	B	201	FMN	C2'-C3'-C4'-C5'
2	J	201	FMN	C2'-C3'-C4'-C5'
2	G	201	FMN	O2'-C2'-C3'-C4'
2	G	201	FMN	O2'-C2'-C3'-O3'
2	C	201	FMN	O2'-C2'-C3'-C4'
2	J	201	FMN	O2'-C2'-C3'-C4'
2	B	201	FMN	O2'-C2'-C3'-C4'
2	C	201	FMN	O2'-C2'-C3'-O3'
2	C	201	FMN	O3'-C3'-C4'-O4'
2	B	201	FMN	O2'-C2'-C3'-O3'
2	G	201	FMN	C1'-C2'-C3'-O3'
2	J	201	FMN	O2'-C2'-C3'-O3'

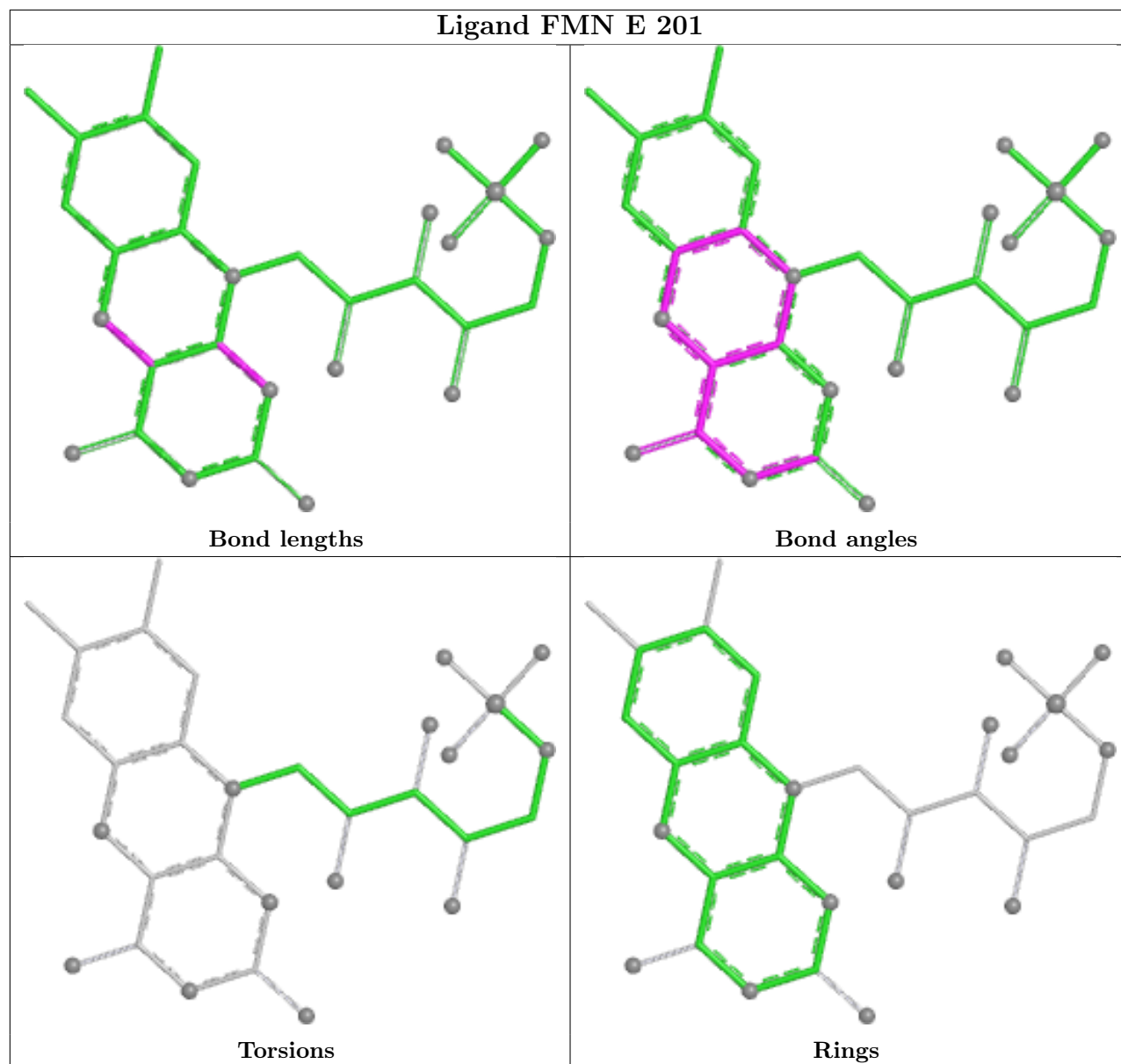
There are no ring outliers.

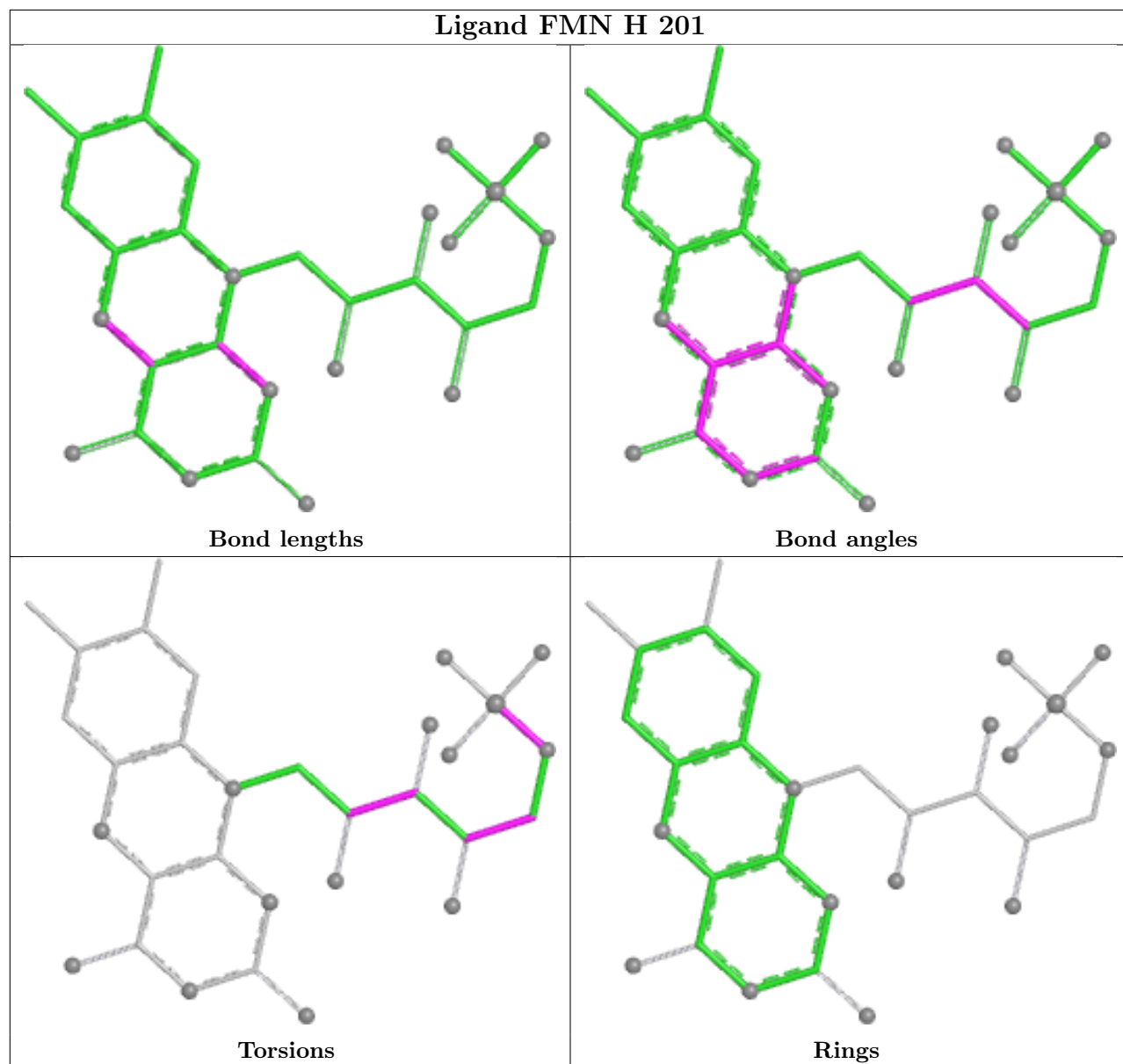
6 monomers are involved in 7 short contacts:

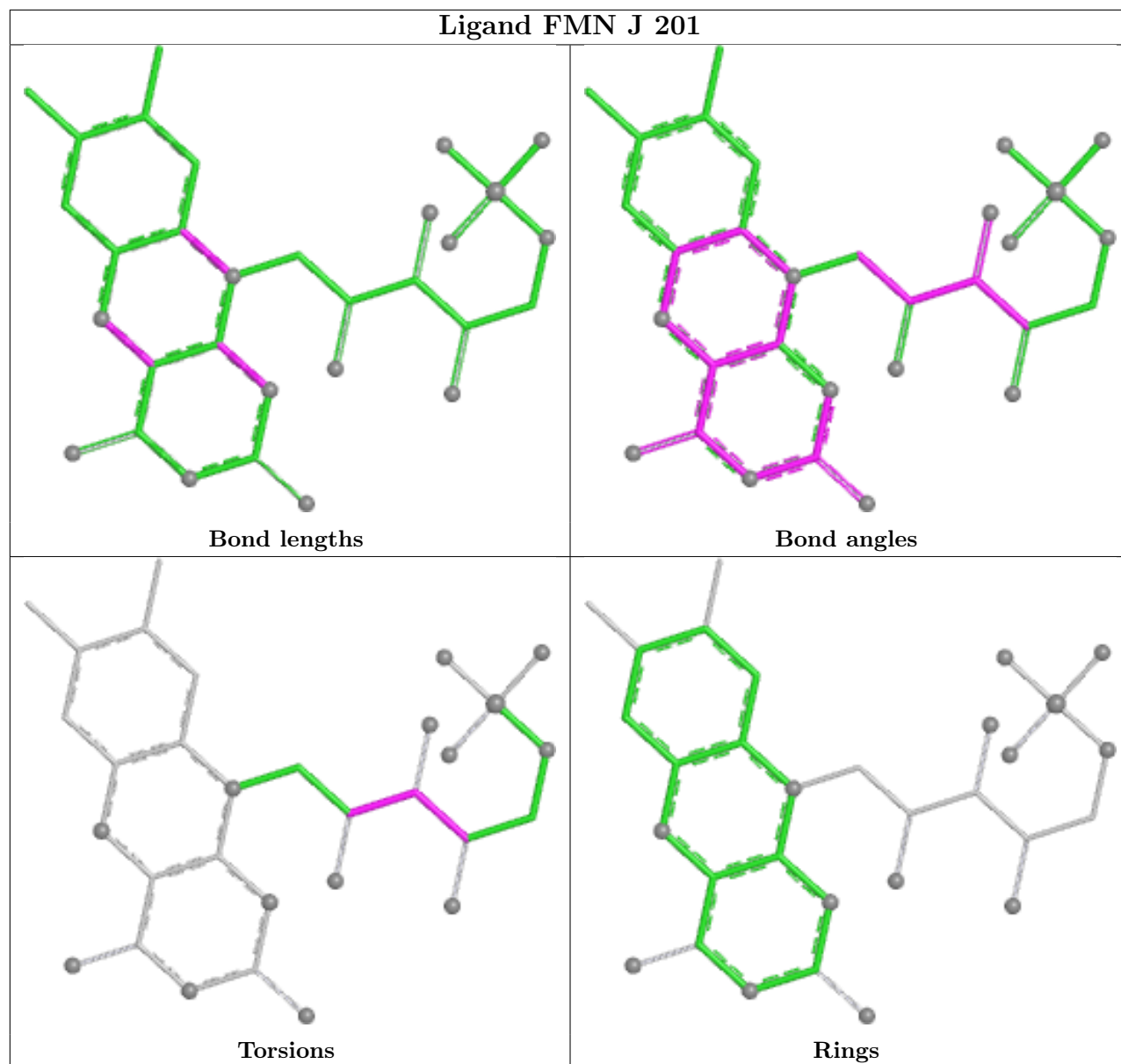
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201	FMN	1	0
2	D	201	FMN	1	0
2	B	201	FMN	1	0
2	C	201	FMN	2	0
2	A	201	FMN	1	0
2	F	201	FMN	1	0

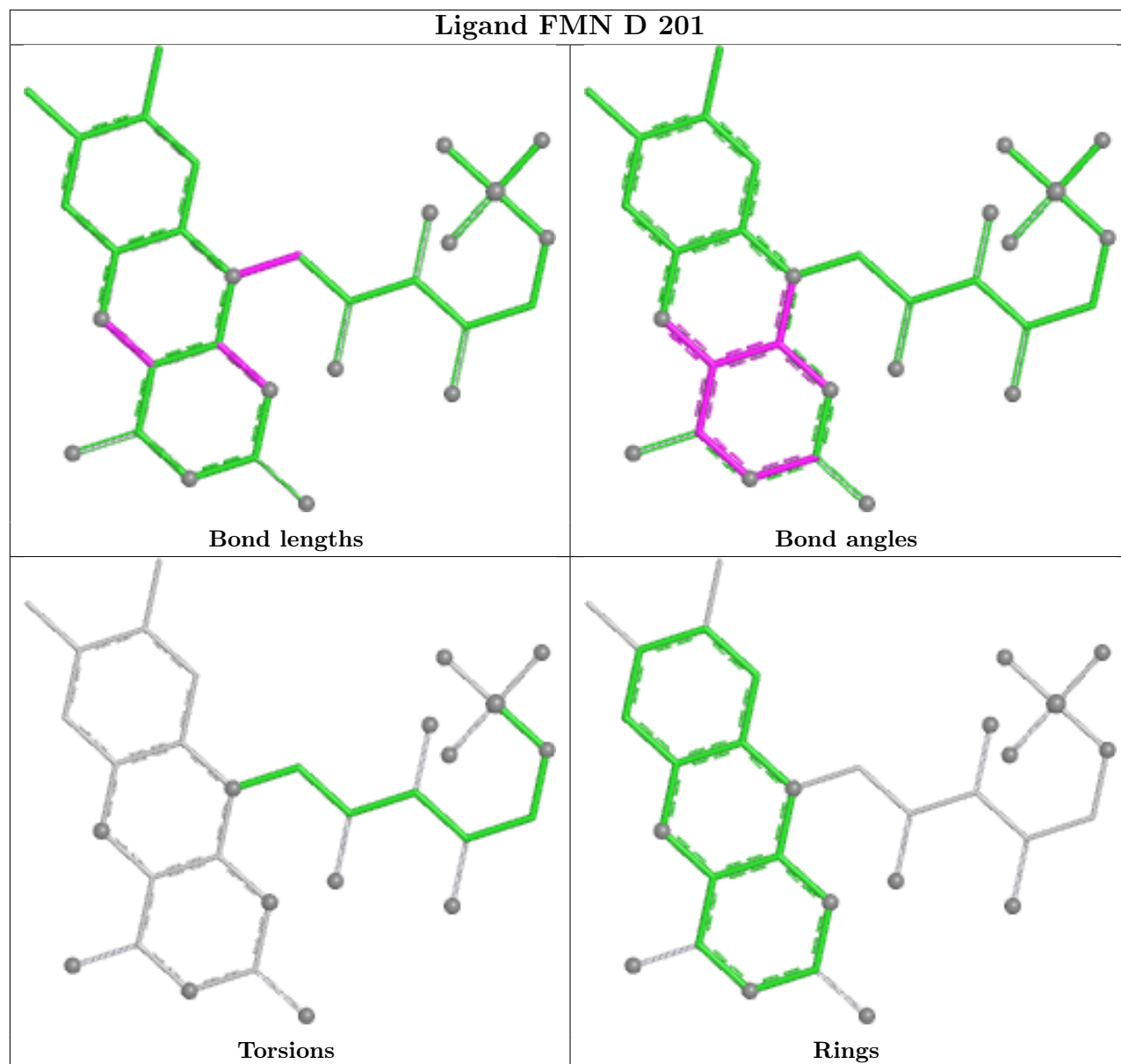
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

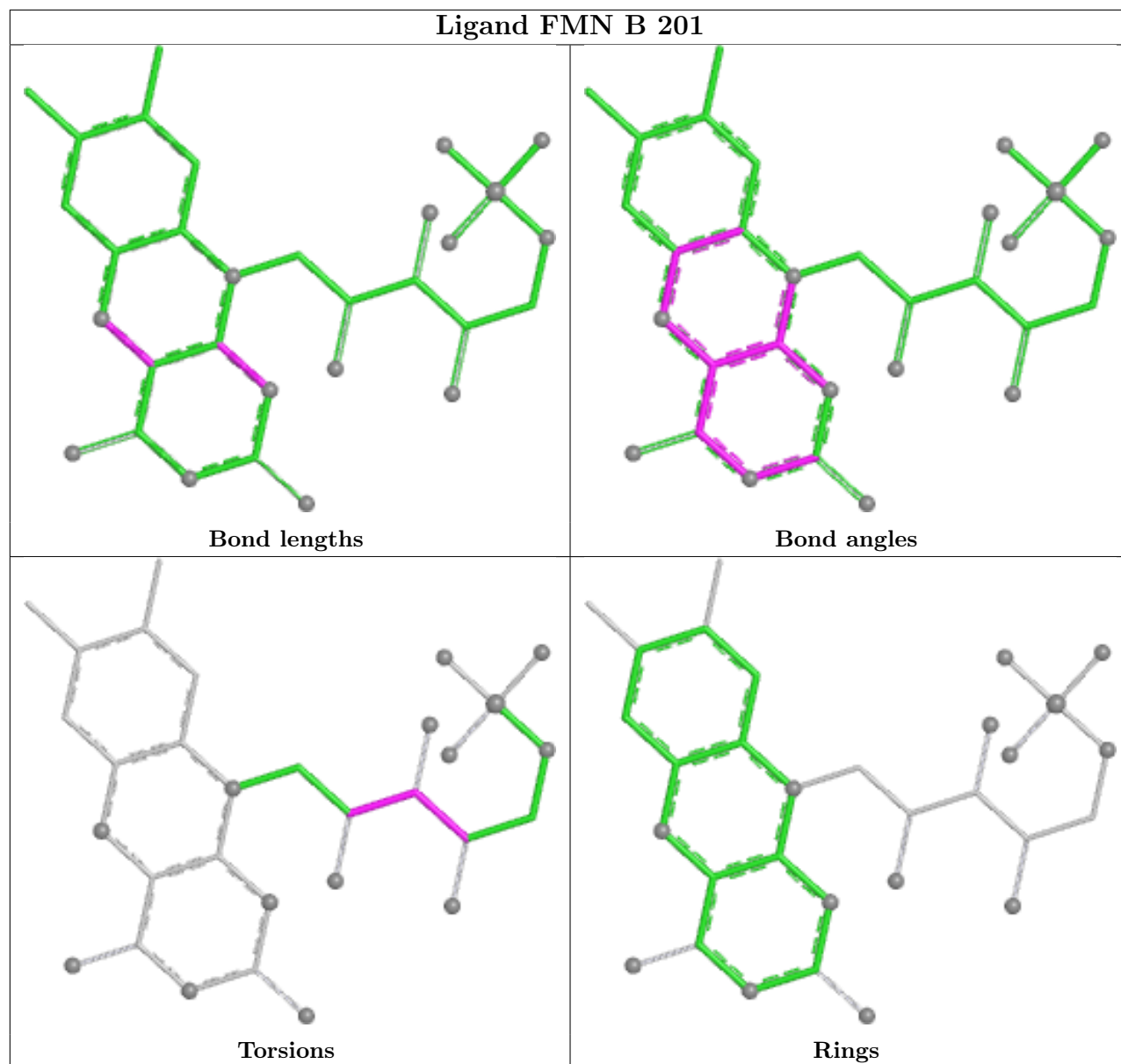


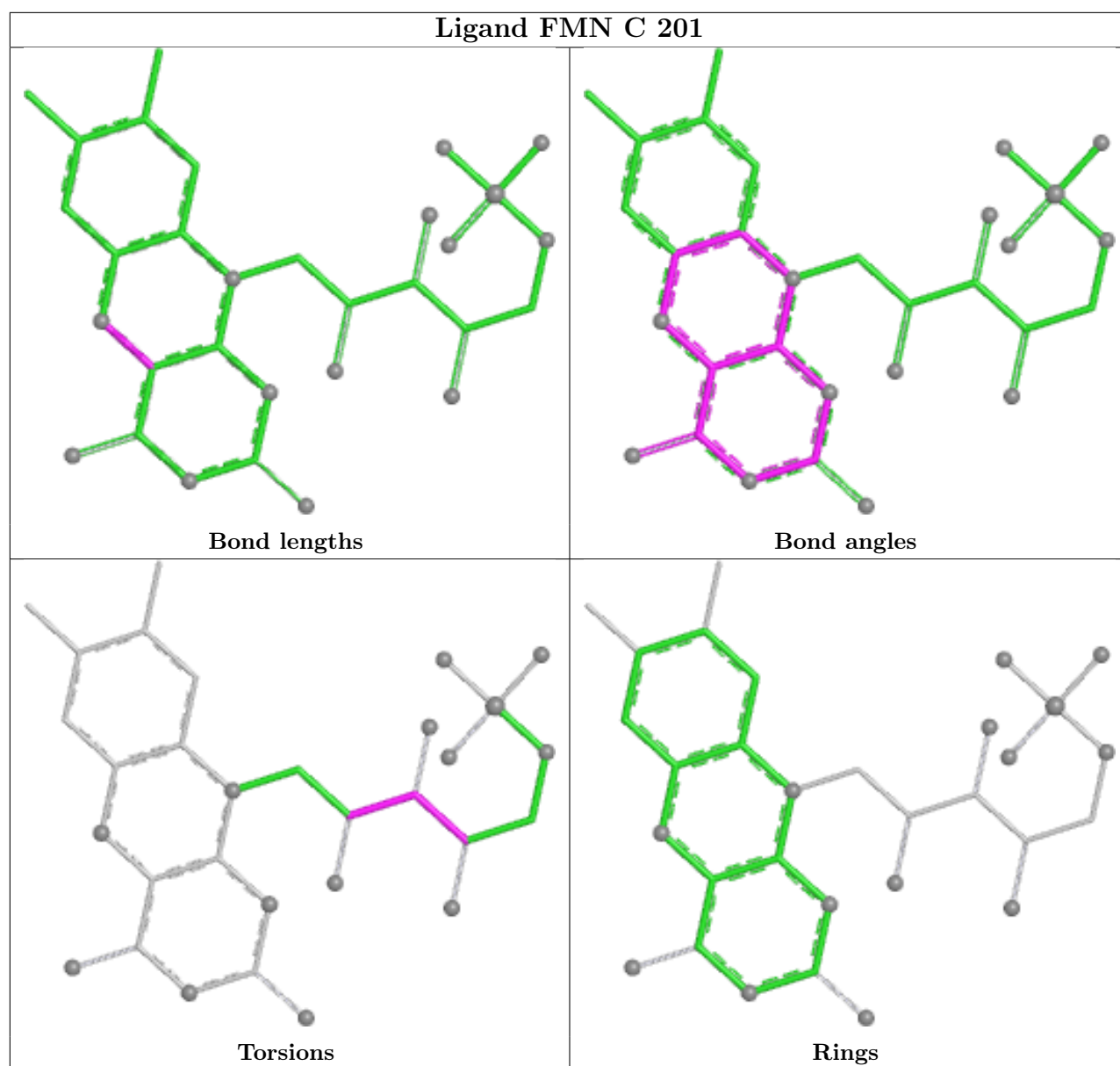




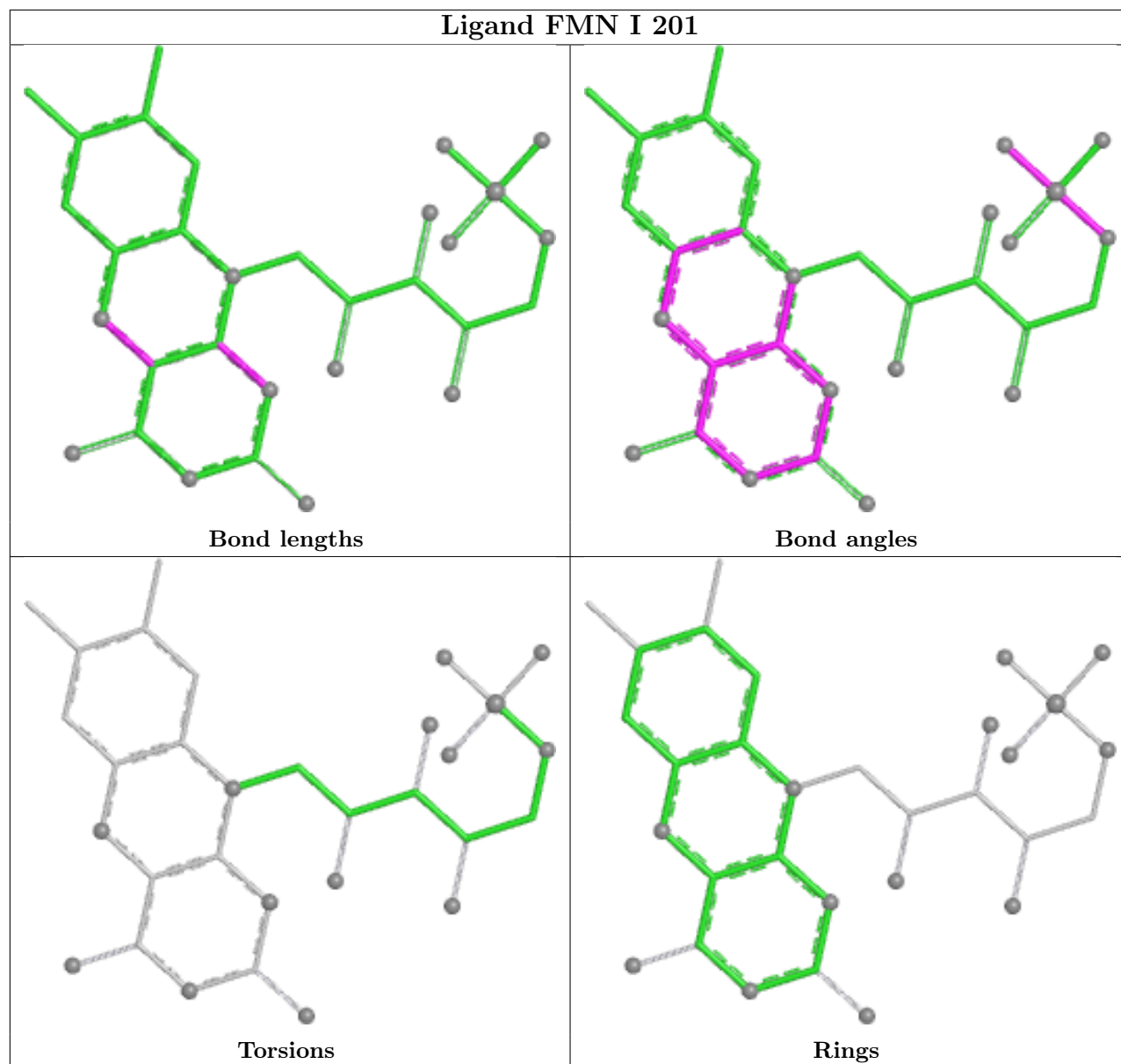


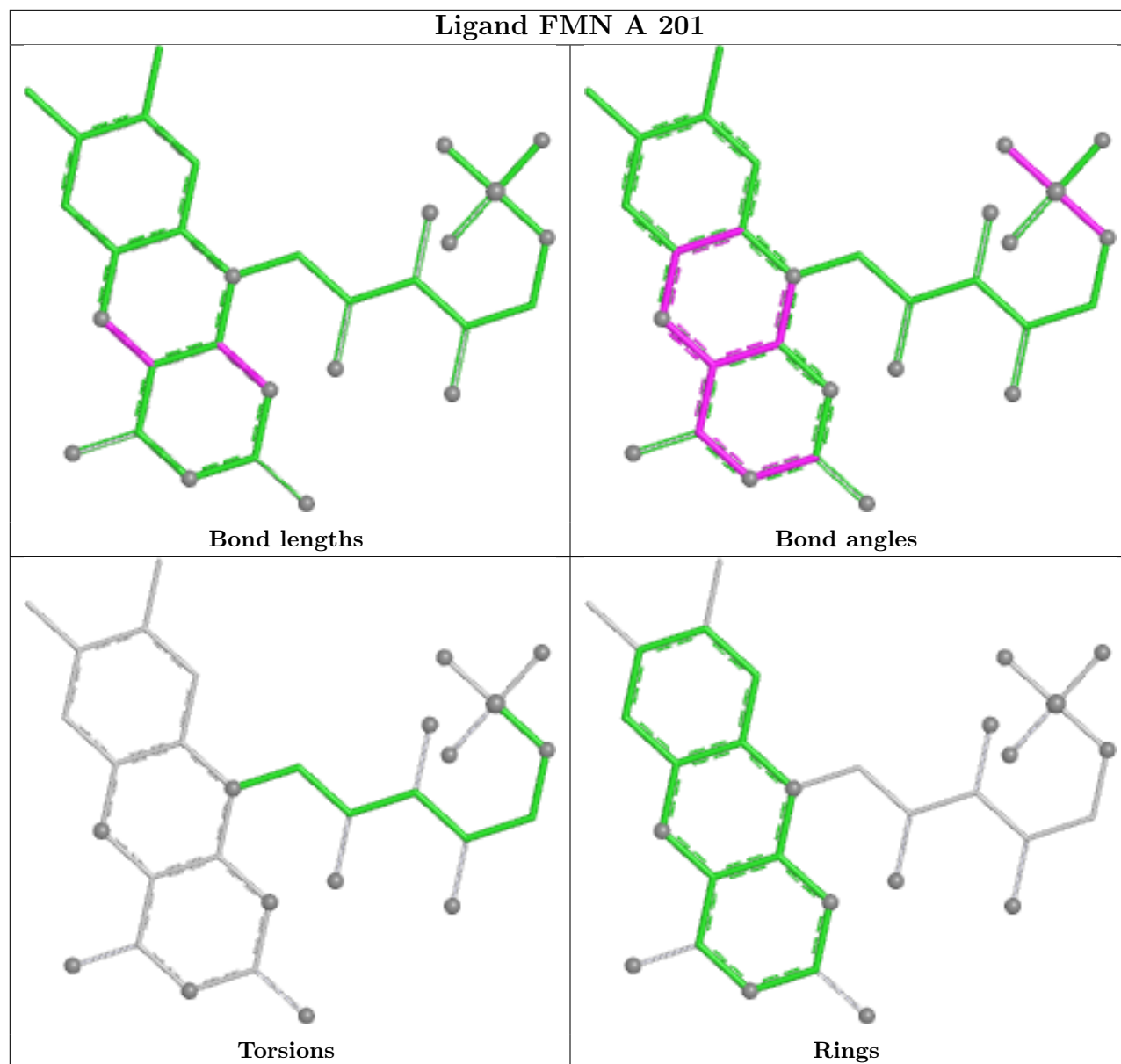


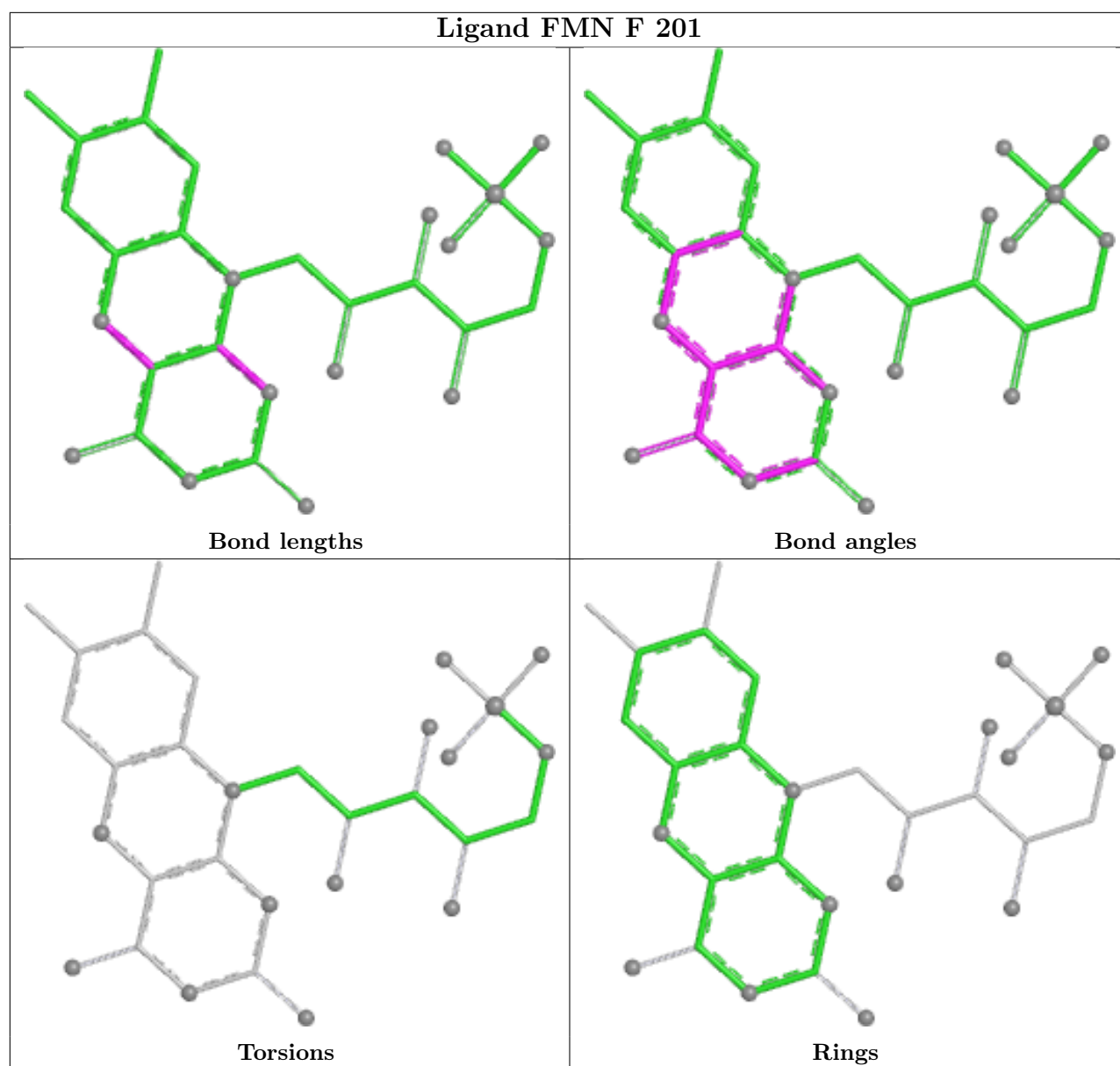




Ligand FMN I 201







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	149/153 (97%)	1.68	49 (32%) 1 1	17, 31, 38, 43	0
1	B	140/153 (91%)	2.70	102 (72%) 0 0	25, 36, 49, 56	0
1	C	140/153 (91%)	2.12	73 (52%) 0 0	23, 33, 50, 58	0
1	D	146/153 (95%)	1.35	30 (20%) 2 2	23, 28, 39, 43	0
1	E	139/153 (90%)	2.40	78 (56%) 0 0	19, 41, 49, 56	0
1	F	139/153 (90%)	2.00	59 (42%) 0 0	34, 39, 52, 57	0
1	G	139/153 (90%)	3.29	125 (89%) 0 0	42, 50, 60, 64	0
1	H	139/153 (90%)	3.09	122 (87%) 0 0	45, 51, 60, 64	0
1	I	139/153 (90%)	1.78	42 (30%) 1 1	32, 36, 47, 55	0
1	J	142/153 (92%)	2.21	65 (45%) 0 0	30, 36, 52, 64	0
All	All	1412/1530 (92%)	2.25	745 (52%) 0 0	17, 38, 54, 64	0

All (745) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	144	GLU	10.8
1	E	142	ILE	8.3
1	A	153	LEU	7.5
1	H	142	ILE	6.5
1	E	143	TYR	6.5
1	D	4	MET	6.2
1	B	142	ILE	6.1
1	B	86	ILE	6.0
1	H	50	ALA	5.9
1	H	119	PHE	5.9
1	J	98	ALA	5.9
1	B	7	TYR	5.8
1	H	106	THR	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	104	LEU	5.8
1	C	142	ILE	5.8
1	J	94	TRP	5.7
1	B	4	MET	5.6
1	G	66	TYR	5.6
1	F	143	TYR	5.5
1	G	129	PRO	5.5
1	A	144	GLU	5.5
1	J	146	SER	5.4
1	F	142	ILE	5.4
1	H	21	PRO	5.4
1	G	143	TYR	5.4
1	F	126	ALA	5.4
1	B	143	TYR	5.4
1	H	27	ILE	5.3
1	J	104	LEU	5.3
1	E	18	ASN	5.3
1	I	143	TYR	5.3
1	G	7	TYR	5.3
1	G	119	PHE	5.3
1	B	83	CYS	5.2
1	G	120	THR	5.2
1	G	83	CYS	5.2
1	E	19	LEU	5.2
1	E	106	THR	5.2
1	G	128	ASP	5.1
1	B	105	SER	5.1
1	D	146	SER	5.1
1	H	80	ILE	5.1
1	B	81	ILE	5.0
1	H	86	ILE	5.0
1	H	28	LEU	5.0
1	G	20	GLN	5.0
1	E	129	PRO	5.0
1	G	85	PRO	5.0
1	J	100	THR	5.0
1	G	81	ILE	5.0
1	F	125	SER	4.9
1	G	126	ALA	4.9
1	G	98	ALA	4.9
1	F	94	TRP	4.9
1	G	80	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	G	99	ILE	4.9
1	G	72	ASP	4.8
1	B	85	PRO	4.8
1	H	104	LEU	4.8
1	E	125	SER	4.8
1	C	129	PRO	4.8
1	E	17	PRO	4.6
1	D	142	ILE	4.6
1	C	94	TRP	4.6
1	G	118	GLY	4.6
1	H	18	ASN	4.6
1	J	93	VAL	4.6
1	E	141	LYS	4.5
1	I	123	ARG	4.5
1	C	143	TYR	4.5
1	C	120	THR	4.5
1	H	13	SER	4.5
1	A	103	ASP	4.5
1	F	141	LYS	4.5
1	C	125	SER	4.5
1	H	87	ARG	4.4
1	G	59	CYS	4.4
1	B	106	THR	4.4
1	A	18	ASN	4.4
1	G	45	CYS	4.4
1	G	18	ASN	4.4
1	G	12	SER	4.3
1	H	129	PRO	4.3
1	G	27	ILE	4.3
1	H	121	THR	4.3
1	J	142	ILE	4.3
1	E	85	PRO	4.3
1	H	44	LEU	4.3
1	G	132	CYS	4.3
1	H	45	CYS	4.3
1	G	86	ILE	4.2
1	G	142	ILE	4.2
1	B	126	ALA	4.2
1	A	84	MET	4.2
1	C	4	MET	4.2
1	H	143	TYR	4.2
1	J	126	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	J	97	GLN	4.2
1	G	124	PRO	4.2
1	G	30	SER	4.2
1	H	10	ILE	4.2
1	J	125	SER	4.2
1	J	120	THR	4.2
1	J	121	THR	4.2
1	J	145	LEU	4.2
1	F	18	ASN	4.1
1	G	19	LEU	4.1
1	B	101	VAL	4.1
1	I	126	ALA	4.1
1	H	46	TYR	4.1
1	G	17	PRO	4.1
1	B	93	VAL	4.1
1	G	113	VAL	4.1
1	H	113	VAL	4.1
1	B	129	PRO	4.1
1	G	77	SER	4.0
1	J	95	SER	4.0
1	B	19	LEU	4.0
1	G	62	VAL	4.0
1	F	120	THR	4.0
1	G	104	LEU	4.0
1	G	84	MET	4.0
1	G	96	MET	4.0
1	G	5	SER	4.0
1	B	103	ASP	4.0
1	G	9	LEU	4.0
1	B	90	ASN	4.0
1	G	69	ILE	4.0
1	G	101	VAL	4.0
1	H	93	VAL	4.0
1	C	100	THR	3.9
1	G	141	LYS	3.9
1	E	20	GLN	3.9
1	G	70	VAL	3.9
1	H	25	LYS	3.9
1	E	7	TYR	3.9
1	J	96	MET	3.9
1	C	106	THR	3.9
1	H	41	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	7	TYR	3.9
1	G	71	GLN	3.9
1	G	122	LEU	3.9
1	H	24	LEU	3.9
1	E	111	THR	3.9
1	E	49	PRO	3.8
1	G	21	PRO	3.8
1	H	17	PRO	3.8
1	F	106	THR	3.8
1	C	126	ALA	3.8
1	B	59	CYS	3.8
1	G	127	MET	3.8
1	E	86	ILE	3.8
1	G	125	SER	3.8
1	H	19	LEU	3.8
1	C	59	CYS	3.8
1	D	103	ASP	3.8
1	H	36	PRO	3.8
1	G	102	ASN	3.8
1	F	5	SER	3.8
1	G	13	SER	3.8
1	G	76	HIS	3.7
1	E	103	ASP	3.7
1	C	85	PRO	3.7
1	G	78	PRO	3.7
1	B	76	HIS	3.7
1	H	29	GLU	3.7
1	I	130	GLU	3.7
1	C	61	GLN	3.7
1	G	10	ILE	3.7
1	H	71	GLN	3.7
1	E	119	PHE	3.7
1	I	119	PHE	3.7
1	C	49	PRO	3.7
1	J	143	TYR	3.7
1	F	119	PHE	3.7
1	H	126	ALA	3.6
1	G	116	TYR	3.6
1	B	18	ASN	3.6
1	A	142	ILE	3.6
1	C	57	GLY	3.6
1	B	120	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	120	THR	3.6
1	G	130	GLU	3.6
1	D	125	SER	3.6
1	H	12	SER	3.6
1	B	104	LEU	3.6
1	G	24	LEU	3.6
1	F	48	LYS	3.6
1	H	90	ASN	3.6
1	G	54	VAL	3.6
1	H	95	SER	3.6
1	E	126	ALA	3.6
1	E	94	TRP	3.6
1	D	148	ASN	3.6
1	E	118	GLY	3.6
1	B	49	PRO	3.6
1	J	106	THR	3.6
1	J	103	ASP	3.6
1	B	141	LYS	3.6
1	C	121	THR	3.5
1	F	17	PRO	3.5
1	G	106	THR	3.5
1	H	49	PRO	3.5
1	G	11	TYR	3.5
1	E	97	GLN	3.5
1	H	51	PHE	3.5
1	H	91	PHE	3.5
1	H	9	LEU	3.5
1	B	15	GLY	3.5
1	B	31	SER	3.5
1	B	77	SER	3.5
1	I	13	SER	3.5
1	B	121	THR	3.5
1	G	100	THR	3.5
1	H	85	PRO	3.5
1	G	58	GLU	3.5
1	A	90	ASN	3.5
1	H	16	ILE	3.5
1	G	87	ARG	3.5
1	H	15	GLY	3.5
1	F	103	ASP	3.5
1	G	117	SER	3.4
1	G	29	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	107	GLU	3.4
1	B	46	TYR	3.4
1	B	27	ILE	3.4
1	E	123	ARG	3.4
1	H	109	VAL	3.4
1	J	91	PHE	3.4
1	G	133	LEU	3.4
1	G	53	GLN	3.4
1	G	63	ASN	3.4
1	E	120	THR	3.4
1	E	59	CYS	3.4
1	G	46	TYR	3.4
1	H	81	ILE	3.4
1	B	54	VAL	3.4
1	B	128	ASP	3.4
1	E	50	ALA	3.4
1	H	52	LEU	3.4
1	G	107	GLU	3.4
1	E	128	ASP	3.4
1	D	126	ALA	3.4
1	H	122	LEU	3.4
1	H	48	LYS	3.3
1	H	20	GLN	3.3
1	H	70	VAL	3.3
1	E	88	ARG	3.3
1	F	100	THR	3.3
1	H	100	THR	3.3
1	I	141	LYS	3.3
1	F	87	ARG	3.3
1	J	105	SER	3.3
1	A	126	ALA	3.3
1	H	114	LEU	3.3
1	B	111	THR	3.3
1	B	17	PRO	3.3
1	D	123	ARG	3.3
1	B	80	ILE	3.3
1	H	125	SER	3.3
1	J	5	SER	3.3
1	D	141	LYS	3.2
1	G	16	ILE	3.2
1	B	140	ALA	3.2
1	D	129	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	24	LEU	3.2
1	E	121	THR	3.2
1	H	112	LEU	3.2
1	H	34	ASN	3.2
1	E	5	SER	3.2
1	I	125	SER	3.2
1	G	131	GLN	3.2
1	B	8	ARG	3.2
1	B	16	ILE	3.2
1	B	88	ARG	3.2
1	H	40	ILE	3.2
1	J	99	ILE	3.2
1	C	124	PRO	3.2
1	G	31	SER	3.2
1	G	105	SER	3.2
1	H	84	MET	3.2
1	H	76	HIS	3.2
1	D	45	CYS	3.2
1	F	88	ARG	3.2
1	D	147	ASP	3.2
1	G	23	ASP	3.2
1	A	86	ILE	3.2
1	H	98	ALA	3.2
1	I	142	ILE	3.2
1	F	111	THR	3.2
1	A	54	VAL	3.2
1	B	24	LEU	3.2
1	C	24	LEU	3.2
1	G	103	ASP	3.2
1	H	26	ASP	3.2
1	H	59	CYS	3.2
1	C	37	ALA	3.1
1	I	120	THR	3.1
1	F	129	PRO	3.1
1	A	146	SER	3.1
1	D	5	SER	3.1
1	B	57	GLY	3.1
1	G	43	LEU	3.1
1	G	114	LEU	3.1
1	H	43	LEU	3.1
1	I	45	CYS	3.1
1	I	59	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	94	TRP	3.1
1	C	105	SER	3.1
1	B	42	GLY	3.1
1	B	66	TYR	3.1
1	B	122	LEU	3.1
1	E	133	LEU	3.1
1	H	128	ASP	3.1
1	G	91	PHE	3.1
1	H	14	GLN	3.1
1	B	84	MET	3.1
1	J	84	MET	3.1
1	J	90	ASN	3.1
1	E	83	CYS	3.1
1	J	59	CYS	3.1
1	H	120	THR	3.1
1	J	88	ARG	3.1
1	H	77	SER	3.1
1	C	86	ILE	3.1
1	D	130	GLU	3.1
1	H	7	TYR	3.1
1	I	83	CYS	3.1
1	G	65	THR	3.1
1	H	47	SER	3.1
1	B	73	GLU	3.1
1	B	124	PRO	3.1
1	E	98	ALA	3.1
1	G	50	ALA	3.1
1	J	86	ILE	3.0
1	F	71	GLN	3.0
1	G	94	TRP	3.0
1	I	94	TRP	3.0
1	C	134	ASN	3.0
1	H	89	ARG	3.0
1	B	100	THR	3.0
1	G	41	THR	3.0
1	G	79	GLN	3.0
1	J	141	LYS	3.0
1	B	10	ILE	3.0
1	H	69	ILE	3.0
1	F	104	LEU	3.0
1	G	112	LEU	3.0
1	G	109	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	116	TYR	3.0
1	B	82	GLU	3.0
1	E	114	LEU	3.0
1	D	143	TYR	3.0
1	H	11	TYR	3.0
1	A	150	PHE	3.0
1	G	48	LYS	3.0
1	G	33	ARG	3.0
1	H	83	CYS	3.0
1	F	73	GLU	3.0
1	H	107	GLU	3.0
1	B	9	LEU	2.9
1	G	52	LEU	2.9
1	E	66	TYR	2.9
1	B	61	GLN	2.9
1	G	22	GLN	2.9
1	C	118	GLY	2.9
1	I	100	THR	2.9
1	B	119	PHE	2.9
1	C	91	PHE	2.9
1	C	127	MET	2.9
1	E	84	MET	2.9
1	I	132	CYS	2.9
1	G	40	ILE	2.9
1	G	28	LEU	2.9
1	A	87	ARG	2.9
1	B	87	ARG	2.9
1	E	87	ARG	2.9
1	B	130	GLU	2.9
1	H	39	GLY	2.9
1	E	91	PHE	2.9
1	G	67	HIS	2.9
1	H	33	ARG	2.9
1	H	88	ARG	2.9
1	J	31	SER	2.9
1	G	44	LEU	2.9
1	C	58	GLU	2.9
1	F	127	MET	2.9
1	E	113	VAL	2.9
1	F	70	VAL	2.9
1	A	143	TYR	2.9
1	H	35	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	140	ALA	2.9
1	I	87	ARG	2.9
1	E	12	SER	2.9
1	F	30	SER	2.9
1	H	56	GLU	2.9
1	E	127	MET	2.9
1	F	19	LEU	2.9
1	B	39	GLY	2.9
1	D	106	THR	2.8
1	G	34	ASN	2.8
1	A	17	PRO	2.8
1	J	124	PRO	2.8
1	C	71	GLN	2.8
1	H	74	ARG	2.8
1	C	119	PHE	2.8
1	G	51	PHE	2.8
1	B	45	CYS	2.8
1	B	125	SER	2.8
1	H	94	TRP	2.8
1	I	133	LEU	2.8
1	H	97	GLN	2.8
1	C	87	ARG	2.8
1	F	107	GLU	2.8
1	B	13	SER	2.8
1	H	37	ALA	2.8
1	F	91	PHE	2.8
1	A	59	CYS	2.8
1	C	122	LEU	2.8
1	J	28	LEU	2.8
1	H	115	LYS	2.8
1	B	58	GLU	2.8
1	B	78	PRO	2.8
1	H	78	PRO	2.8
1	B	62	VAL	2.8
1	H	54	VAL	2.8
1	H	101	VAL	2.8
1	E	26	ASP	2.8
1	H	105	SER	2.8
1	C	98	ALA	2.8
1	I	131	GLN	2.8
1	E	48	LYS	2.8
1	A	43	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	137	LEU	2.8
1	H	92	GLU	2.8
1	A	36	PRO	2.8
1	C	84	MET	2.8
1	A	5	SER	2.7
1	I	5	SER	2.7
1	B	20	GLN	2.7
1	B	33	ARG	2.7
1	J	22	GLN	2.7
1	H	132	CYS	2.7
1	B	107	GLU	2.7
1	G	15	GLY	2.7
1	G	57	GLY	2.7
1	G	121	THR	2.7
1	G	136	LEU	2.7
1	G	139	ILE	2.7
1	B	21	PRO	2.7
1	B	89	ARG	2.7
1	C	93	VAL	2.7
1	I	97	GLN	2.7
1	J	109	VAL	2.7
1	B	132	CYS	2.7
1	J	119	PHE	2.7
1	F	121	THR	2.7
1	C	20	GLN	2.7
1	H	117	SER	2.7
1	B	109	VAL	2.7
1	I	140	ALA	2.7
1	H	66	TYR	2.7
1	J	7	TYR	2.7
1	D	59	CYS	2.7
1	D	128	ASP	2.7
1	F	26	ASP	2.7
1	H	96	MET	2.7
1	A	100	THR	2.7
1	H	111	THR	2.7
1	A	88	ARG	2.7
1	E	77	SER	2.7
1	H	6	LEU	2.7
1	B	60	GLU	2.7
1	H	63	ASN	2.7
1	J	48	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	93	VAL	2.7
1	E	37	ALA	2.6
1	F	140	ALA	2.6
1	I	50	ALA	2.6
1	J	127	MET	2.6
1	F	46	TYR	2.6
1	I	128	ASP	2.6
1	F	49	PRO	2.6
1	G	49	PRO	2.6
1	B	134	ASN	2.6
1	C	114	LEU	2.6
1	G	38	ASN	2.6
1	C	138	ASP	2.6
1	F	128	ASP	2.6
1	B	116	TYR	2.6
1	A	125	SER	2.6
1	E	101	VAL	2.6
1	E	130	GLU	2.6
1	H	58	GLU	2.6
1	G	37	ALA	2.6
1	H	141	LYS	2.6
1	G	90	ASN	2.6
1	C	45	CYS	2.6
1	D	149	PHE	2.6
1	I	127	MET	2.6
1	H	22	GLN	2.6
1	B	40	ILE	2.6
1	E	81	ILE	2.6
1	I	70	VAL	2.6
1	E	117	SER	2.6
1	J	123	ARG	2.5
1	G	97	GLN	2.5
1	I	19	LEU	2.5
1	A	141	LYS	2.5
1	A	140	ALA	2.5
1	G	75	HIS	2.5
1	I	106	THR	2.5
1	C	88	ARG	2.5
1	B	127	MET	2.5
1	C	96	MET	2.5
1	G	36	PRO	2.5
1	A	147	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	133	LEU	2.5
1	H	42	GLY	2.5
1	E	40	ILE	2.5
1	E	34	ASN	2.5
1	J	34	ASN	2.5
1	C	101	VAL	2.5
1	G	61	GLN	2.5
1	D	144	GLU	2.5
1	A	42	GLY	2.5
1	C	135	PHE	2.5
1	E	57	GLY	2.5
1	F	52	LEU	2.5
1	G	134	ASN	2.5
1	I	33	ARG	2.5
1	C	139	ILE	2.5
1	B	108	GLN	2.5
1	A	127	MET	2.5
1	A	152	ASP	2.5
1	E	70	VAL	2.5
1	G	26	ASP	2.5
1	J	129	PRO	2.5
1	H	57	GLY	2.4
1	H	118	GLY	2.4
1	E	116	TYR	2.4
1	B	52	LEU	2.4
1	B	55	LEU	2.4
1	F	130	GLU	2.4
1	C	40	ILE	2.4
1	F	16	ILE	2.4
1	B	37	ALA	2.4
1	B	50	ALA	2.4
1	J	115	LYS	2.4
1	C	21	PRO	2.4
1	I	129	PRO	2.4
1	J	87	ARG	2.4
1	B	118	GLY	2.4
1	F	38	ASN	2.4
1	C	29	GLU	2.4
1	E	108	GLN	2.4
1	I	116	TYR	2.4
1	J	133	LEU	2.4
1	I	81	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	98	ALA	2.4
1	D	17	PRO	2.4
1	C	70	VAL	2.4
1	C	73	GLU	2.4
1	C	130	GLU	2.4
1	G	92	GLU	2.4
1	H	38	ASN	2.4
1	E	15	GLY	2.4
1	A	104	LEU	2.4
1	C	48	LYS	2.4
1	D	145	LEU	2.4
1	H	133	LEU	2.4
1	G	135	PHE	2.4
1	H	139	ILE	2.4
1	I	10	ILE	2.4
1	C	140	ALA	2.4
1	F	50	ALA	2.4
1	A	107	GLU	2.4
1	G	64	GLU	2.4
1	E	90	ASN	2.4
1	D	93	VAL	2.4
1	J	101	VAL	2.4
1	H	127	MET	2.4
1	I	84	MET	2.4
1	B	26	ASP	2.3
1	C	128	ASP	2.3
1	A	145	LEU	2.3
1	D	6	LEU	2.3
1	A	7	TYR	2.3
1	C	92	GLU	2.3
1	H	53	GLN	2.3
1	I	99	ILE	2.3
1	F	21	PRO	2.3
1	H	124	PRO	2.3
1	E	93	VAL	2.3
1	F	101	VAL	2.3
1	H	5	SER	2.3
1	A	130	GLU	2.3
1	J	58	GLU	2.3
1	E	104	LEU	2.3
1	A	41	THR	2.3
1	B	41	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	121	THR	2.3
1	A	149	PHE	2.3
1	E	11	TYR	2.3
1	H	135	PHE	2.3
1	F	81	ILE	2.3
1	B	117	SER	2.3
1	H	32	GLN	2.3
1	J	71	GLN	2.3
1	A	94	TRP	2.3
1	F	134	ASN	2.3
1	G	110	LYS	2.3
1	C	33	ARG	2.3
1	E	47	SER	2.3
1	F	105	SER	2.3
1	H	72	ASP	2.3
1	J	128	ASP	2.3
1	B	71	GLN	2.3
1	F	97	GLN	2.3
1	C	62	VAL	2.3
1	H	134	ASN	2.3
1	J	132	CYS	2.3
1	A	48	LYS	2.3
1	A	120	THR	2.3
1	B	114	LEU	2.3
1	D	100	THR	2.3
1	E	115	LYS	2.3
1	I	122	LEU	2.3
1	B	11	TYR	2.2
1	B	91	PHE	2.2
1	E	135	PHE	2.2
1	I	15	GLY	2.2
1	C	47	SER	2.2
1	C	95	SER	2.2
1	E	31	SER	2.2
1	G	108	GLN	2.2
1	F	113	VAL	2.2
1	I	121	THR	2.2
1	A	6	LEU	2.2
1	B	56	GLU	2.2
1	J	21	PRO	2.2
1	J	26	ASP	2.2
1	B	63	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	67	HIS	2.2
1	C	25	LYS	2.2
1	E	63	ASN	2.2
1	F	54	VAL	2.2
1	A	106	THR	2.2
1	J	45	CYS	2.2
1	A	19	LEU	2.2
1	D	122	LEU	2.2
1	E	79	GLN	2.2
1	H	79	GLN	2.2
1	F	47	SER	2.2
1	H	103	ASP	2.2
1	J	12	SER	2.2
1	C	78	PRO	2.2
1	J	49	PRO	2.2
1	I	91	PHE	2.2
1	C	16	ILE	2.2
1	J	139	ILE	2.2
1	C	63	ASN	2.2
1	C	123	ARG	2.2
1	G	82	GLU	2.2
1	B	70	VAL	2.2
1	B	12	SER	2.2
1	C	5	SER	2.2
1	B	112	LEU	2.2
1	J	114	LEU	2.2
1	J	122	LEU	2.2
1	C	141	LYS	2.2
1	G	8	ARG	2.2
1	G	25	LYS	2.2
1	G	68	ARG	2.2
1	G	74	ARG	2.2
1	A	91	PHE	2.1
1	I	34	ASN	2.1
1	H	130	GLU	2.1
1	D	99	ILE	2.1
1	F	86	ILE	2.1
1	H	99	ILE	2.1
1	E	22	GLN	2.1
1	A	93	VAL	2.1
1	G	93	VAL	2.1
1	C	30	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	31	SER	2.1
1	J	30	SER	2.1
1	A	52	LEU	2.1
1	B	123	ARG	2.1
1	F	137	LEU	2.1
1	H	137	LEU	2.1
1	J	85	PRO	2.1
1	H	60	GLU	2.1
1	C	102	ASN	2.1
1	H	102	ASN	2.1
1	A	20	GLN	2.1
1	B	79	GLN	2.1
1	J	135	PHE	2.1
1	C	46	TYR	2.1
1	F	109	VAL	2.1
1	G	123	ARG	2.1
1	H	62	VAL	2.1
1	E	25	LYS	2.1
1	B	64	GLU	2.1
1	E	9	LEU	2.1
1	F	36	PRO	2.1
1	F	78	PRO	2.1
1	A	148	ASN	2.1
1	F	112	LEU	2.1
1	G	137	LEU	2.1
1	B	51	PHE	2.1
1	E	51	PHE	2.1
1	H	23	ASP	2.1
1	B	5	SER	2.1
1	E	13	SER	2.1
1	C	60	GLU	2.1
1	E	100	THR	2.1
1	G	73	GLU	2.1
1	C	90	ASN	2.1
1	J	62	VAL	2.1
1	E	36	PRO	2.1
1	E	124	PRO	2.1
1	J	32	GLN	2.1
1	A	151	LEU	2.1
1	C	83	CYS	2.1
1	G	138	ASP	2.1
1	D	107	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	25	LYS	2.0
1	E	96	MET	2.0
1	B	14	GLN	2.0
1	G	14	GLN	2.0
1	A	124	PRO	2.0
1	E	21	PRO	2.0
1	F	93	VAL	2.0
1	B	6	LEU	2.0
1	F	6	LEU	2.0
1	J	83	CYS	2.0
1	F	98	ALA	2.0
1	A	14	GLN	2.0
1	E	67	HIS	2.0
1	F	27	ILE	2.0
1	E	42	GLY	2.0
1	F	22	GLN	2.0
1	G	111	THR	2.0
1	I	11	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

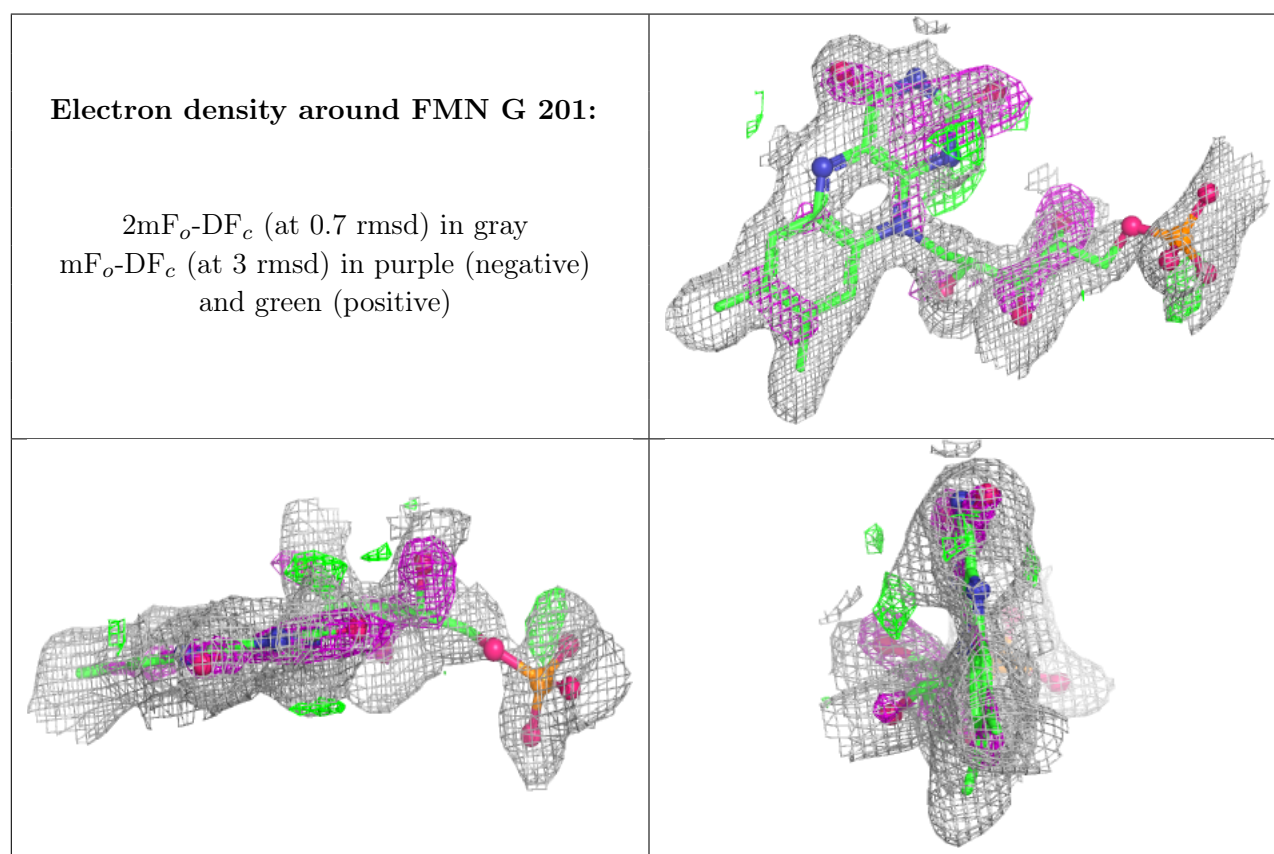
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	G	201	31/31	0.77	0.20	42,44,47,49	5
2	FMN	H	201	31/31	0.85	0.17	51,52,57,58	5
2	FMN	B	201	31/31	0.87	0.17	29,32,40,45	5
2	FMN	F	201	31/31	0.87	0.16	29,34,38,45	5
2	FMN	I	201	31/31	0.89	0.16	28,31,38,41	5

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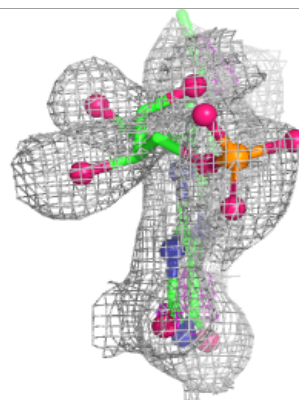
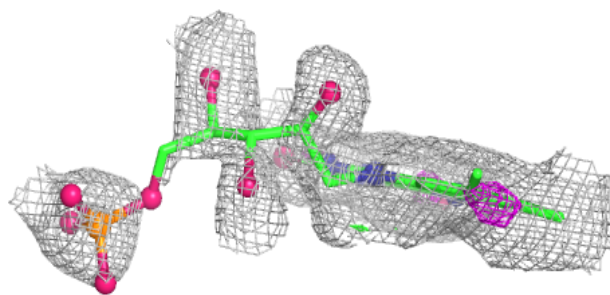
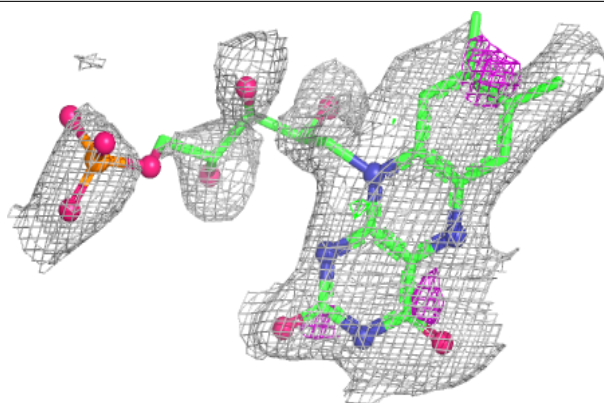
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	J	201	31/31	0.90	0.16	26,29,40,44	5
2	FMN	E	201	31/31	0.91	0.15	32,34,42,45	5
2	FMN	A	201	31/31	0.91	0.14	26,28,36,41	5
2	FMN	C	201	31/31	0.92	0.14	28,30,37,41	5
2	FMN	D	201	31/31	0.93	0.12	20,24,29,33	5

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

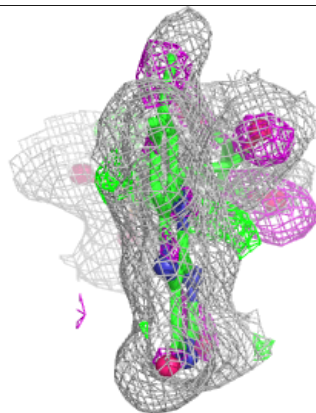
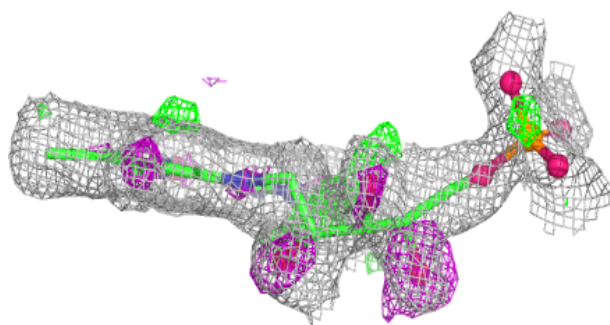
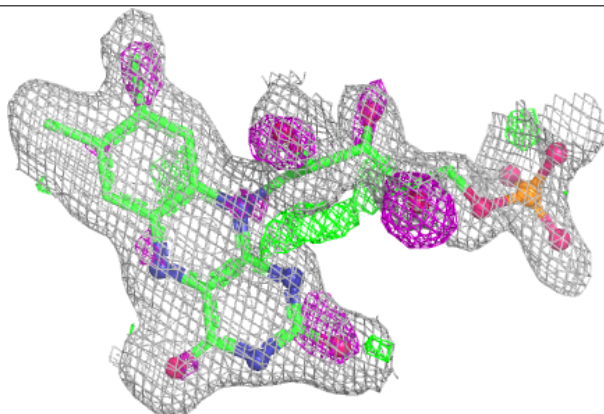


Electron density around FMN H 201:

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

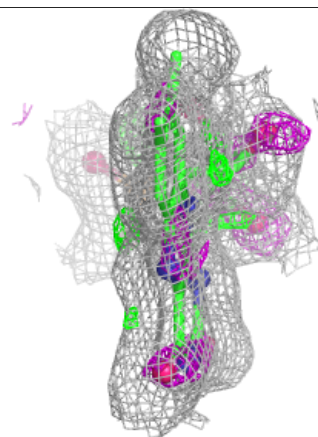
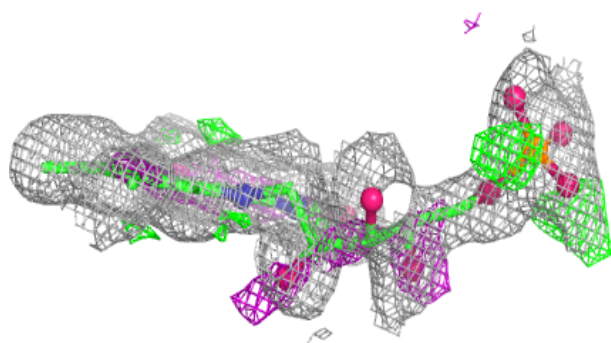
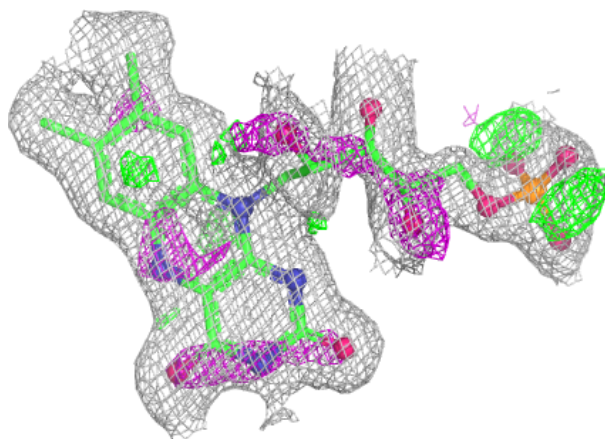
**Electron density around FMN B 201:**

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



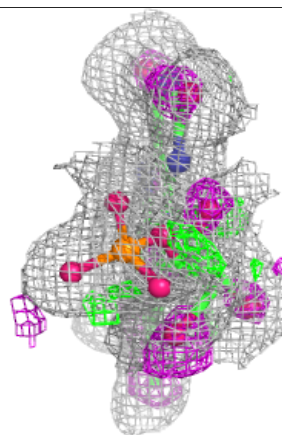
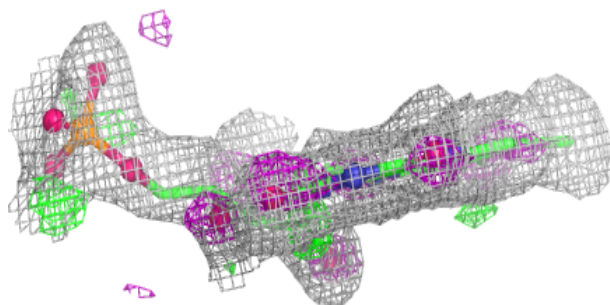
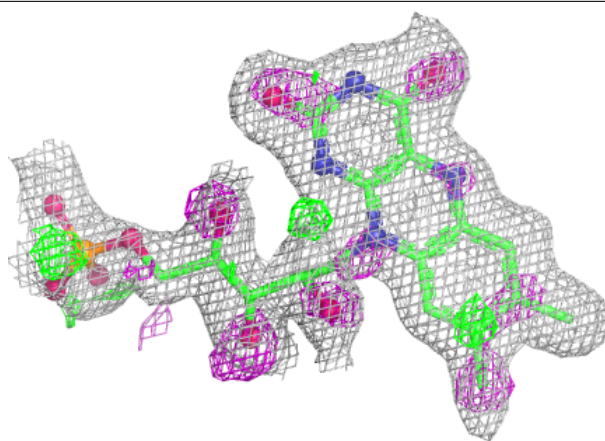
Electron density around FMN F 201:

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

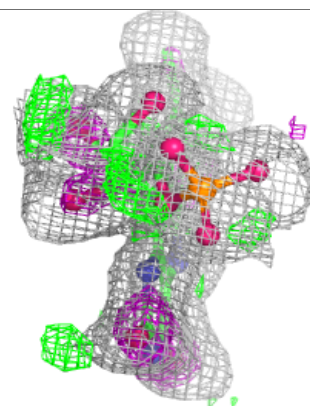
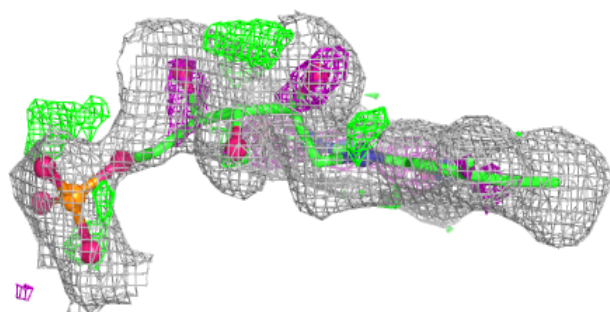
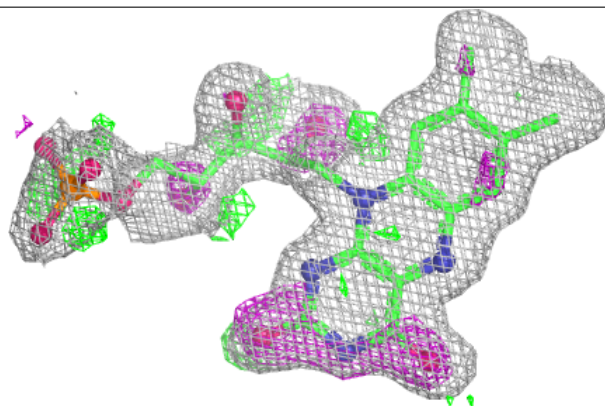


Electron density around FMN I 201:

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

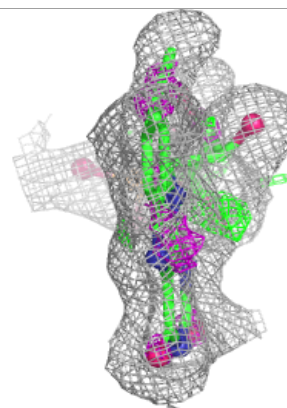
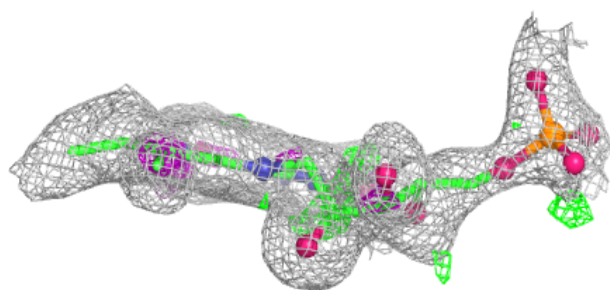
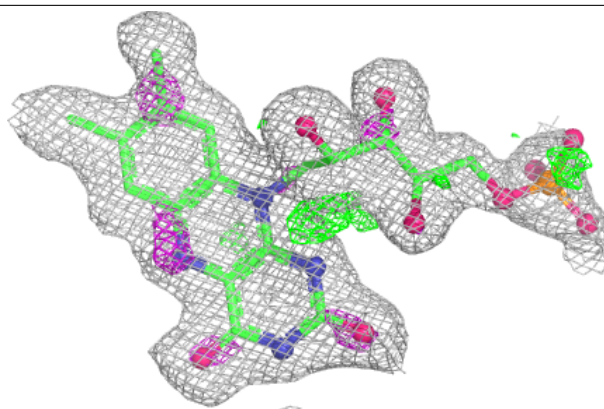
**Electron density around FMN J 201:**

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

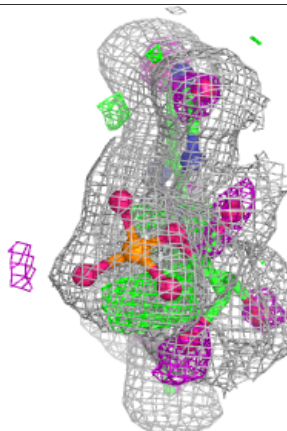
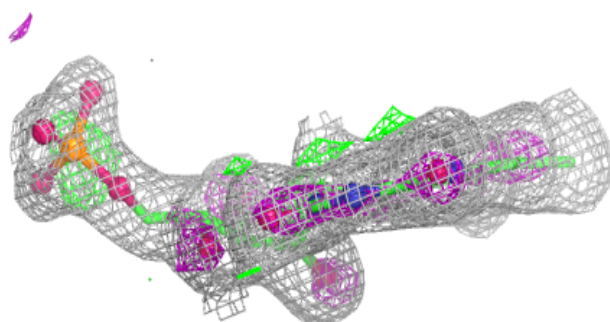
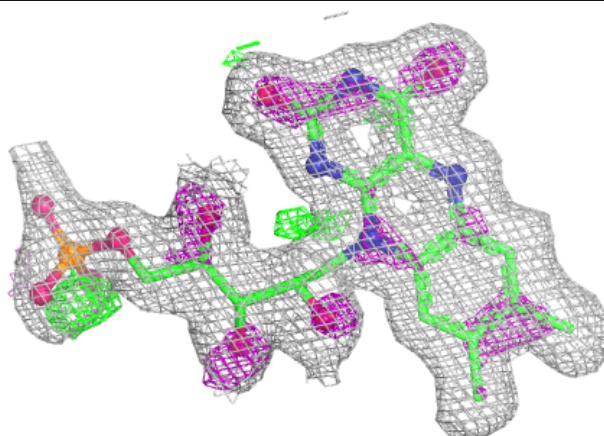


Electron density around FMN E 201:

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

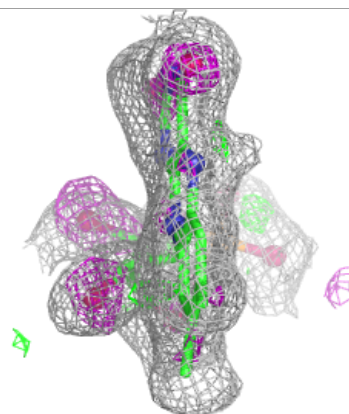
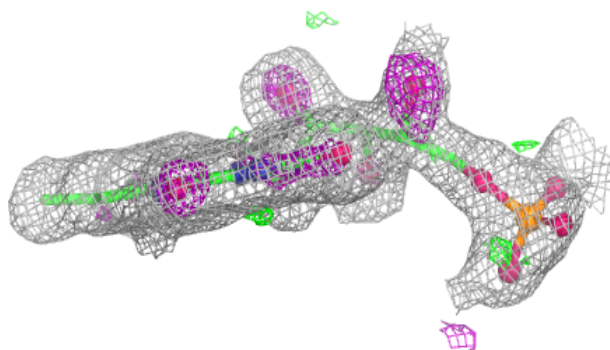
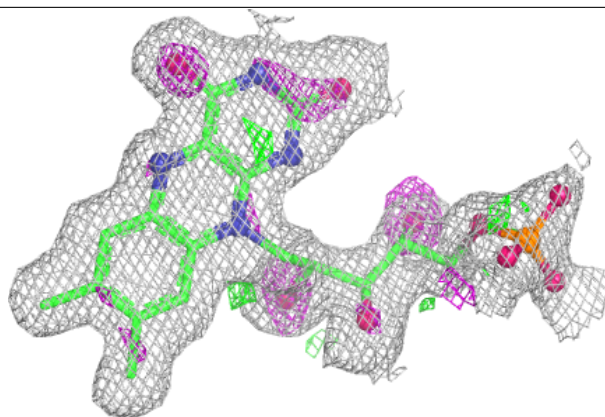
**Electron density around FMN A 201:**

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

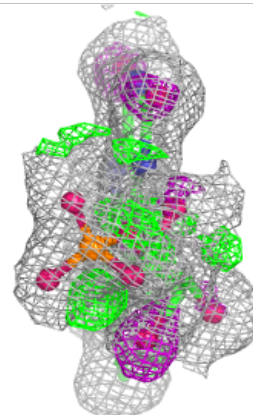
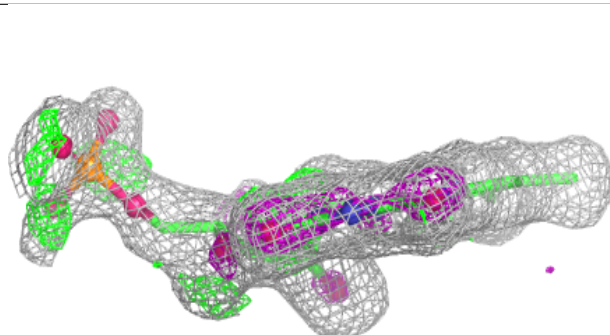
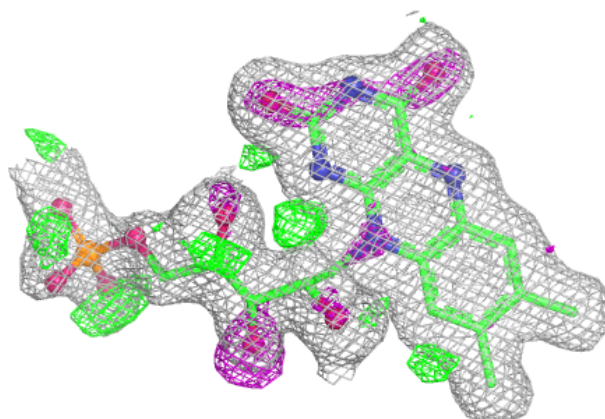


Electron density around FMN C 201:

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

**Electron density around FMN D 201:**

$2mF_o-DF_c$ (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.