



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:28 pm BST

PDB ID : 2HFO
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 : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

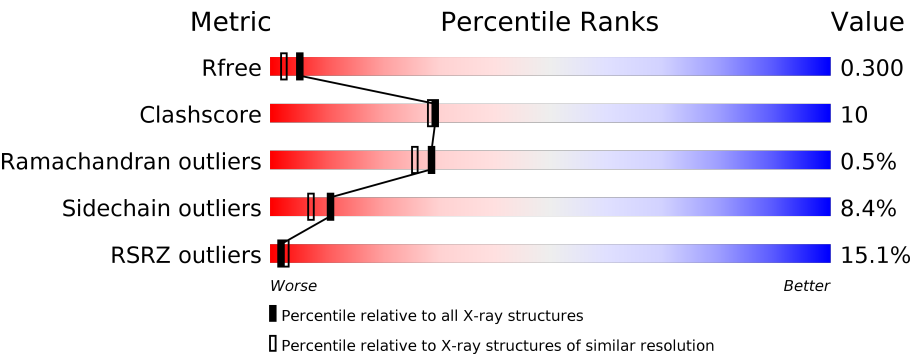
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div><div>11%</div><div><div></div><div>80%</div><div>15%</div><div>••</div></div></div>
1	B	153	<div><div>19%</div><div><div></div><div>71%</div><div>18%</div><div>••</div></div><div>8%</div></div>
1	C	153	<div><div>17%</div><div><div></div><div>66%</div><div>19%</div><div>•</div></div><div>11%</div></div>
1	D	153	<div><div>17%</div><div><div></div><div>69%</div><div>21%</div><div>5%</div></div><div>••</div></div>
1	E	153	<div><div>10%</div><div><div></div><div>76%</div><div>14%</div><div>•</div></div><div>8%</div></div>
1	F	153	<div><div>10%</div><div><div></div><div>75%</div><div>16%</div><div>•</div></div><div>8%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	153	<div><div></div><div>14%</div><div>75%</div><div>15%</div><div>•</div><div>9%</div></div>
1	H	153	<div><div></div><div>12%</div><div>74%</div><div>16%</div><div>•</div><div>8%</div></div>
1	I	153	<div><div></div><div>14%</div><div>74%</div><div>16%</div><div>•</div><div>7%</div></div>
1	J	153	<div><div></div><div>14%</div><div>72%</div><div>16%</div><div>••</div><div>9%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11646 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 Activator of photopigment and puc expression.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1205	762	205	230	8			
1	B	140	Total	C	N	O	S	0	0	0
			1109	702	193	206	8			
1	C	136	Total	C	N	O	S	0	0	0
			1067	675	186	198	8			
1	D	147	Total	C	N	O	S	0	0	0
			1167	737	201	221	8			
1	E	141	Total	C	N	O	S	0	0	0
			1107	700	190	209	8			
1	F	140	Total	C	N	O	S	0	0	0
			1115	704	194	209	8			
1	G	139	Total	C	N	O	S	0	0	0
			1099	693	192	206	8			
1	H	141	Total	C	N	O	S	0	0	0
			1121	708	195	210	8			
1	I	142	Total	C	N	O	S	0	0	0
			1117	707	193	209	8			
1	J	139	Total	C	N	O	S	0	0	0
			1100	692	190	210	8			

There are 30 discrepancies between the modelled and reference sequences:

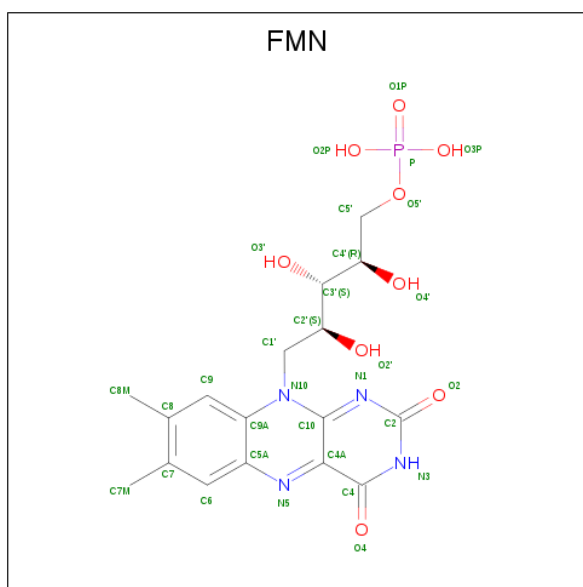
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	CLONING ARTIFACT	UNP P74295
A	2	GLY	-	CLONING ARTIFACT	UNP P74295
A	3	HIS	-	CLONING ARTIFACT	UNP P74295
B	1	ALA	-	CLONING ARTIFACT	UNP P74295
B	2	GLY	-	CLONING ARTIFACT	UNP P74295
B	3	HIS	-	CLONING ARTIFACT	UNP P74295
C	1	ALA	-	CLONING ARTIFACT	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 (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

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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		

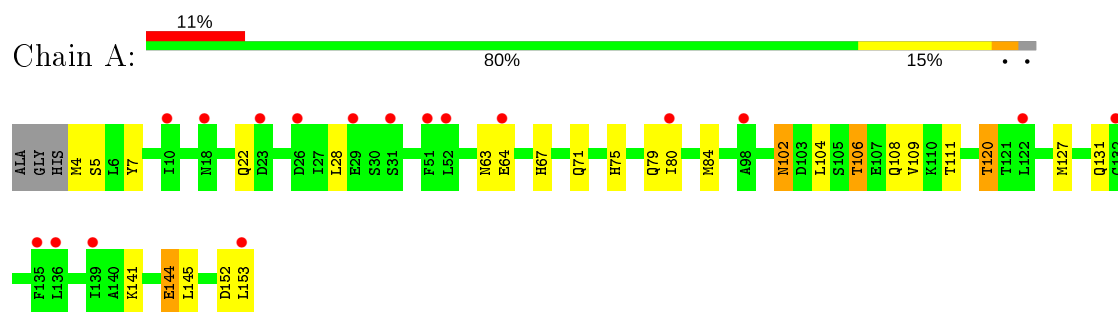
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	6	Total	O	0	0
			6	6		
3	C	12	Total	O	0	0
			12	12		
3	D	29	Total	O	0	0
			29	29		
3	E	12	Total	O	0	0
			12	12		
3	F	8	Total	O	0	0
			8	8		
3	G	13	Total	O	0	0
			13	13		
3	H	10	Total	O	0	0
			10	10		
3	I	9	Total	O	0	0
			9	9		
3	J	8	Total	O	0	0
			8	8		

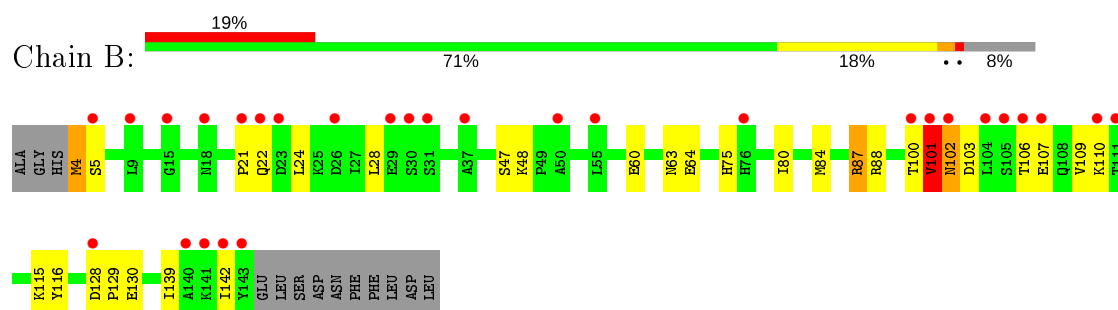
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

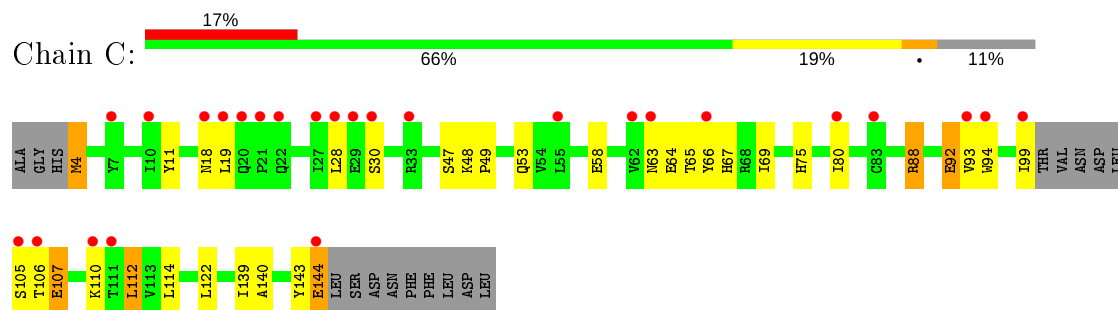
- Molecule 1: Activator of photopigment and puc expression



- Molecule 1: Activator of photopigment and puc expression

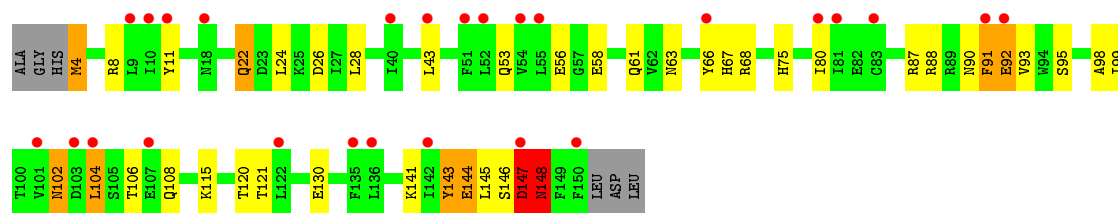


- Molecule 1: Activator of photopigment and puc expression

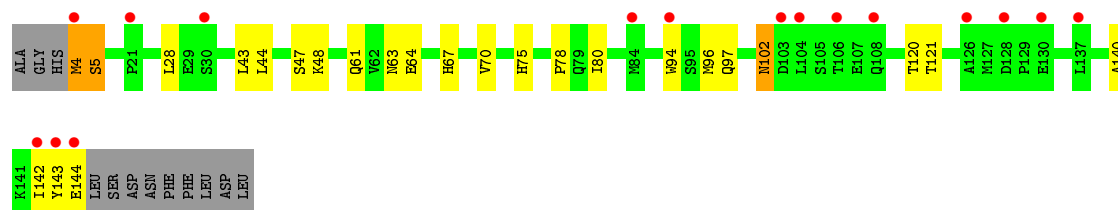


- Molecule 1: Activator of photopigment and puc expression

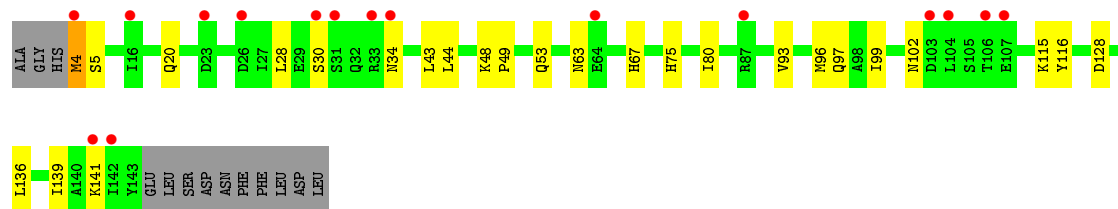
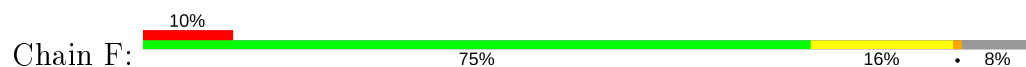




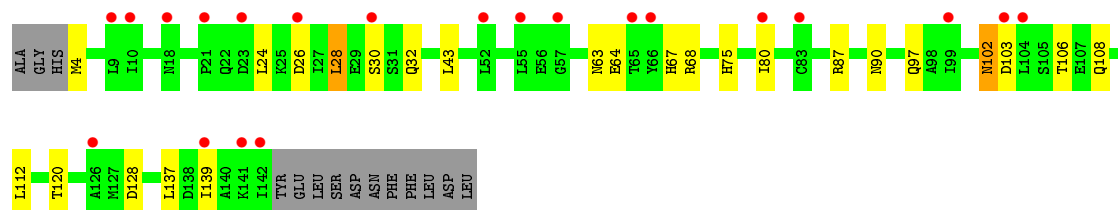
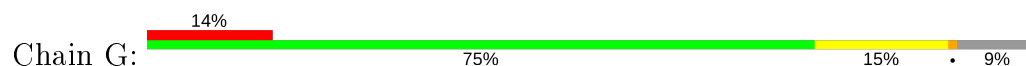
- Molecule 1: Activator of photopigment and puc expression



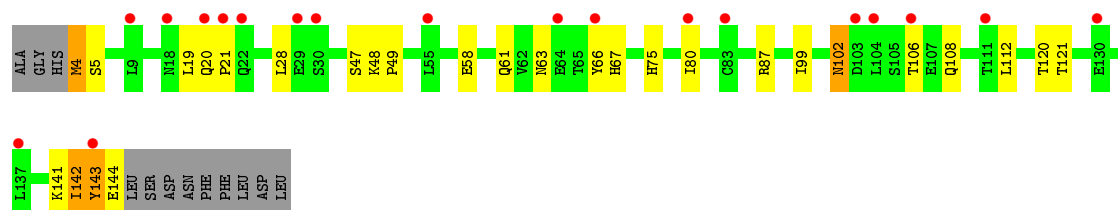
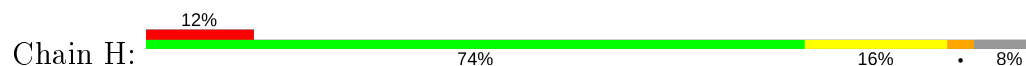
- Molecule 1: Activator of photopigment and puc expression




- Molecule 1: Activator of photopigment and puc expression

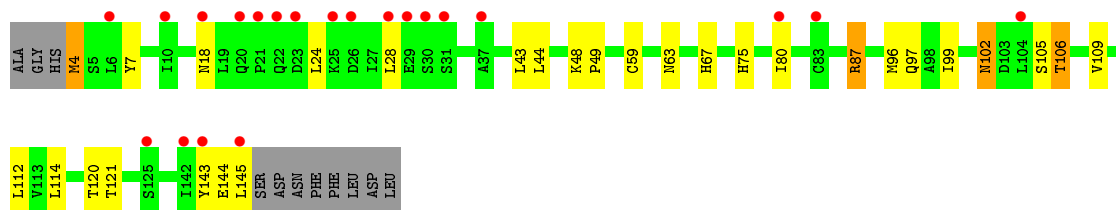


- Molecule 1: Activator of photopigment and puc expression



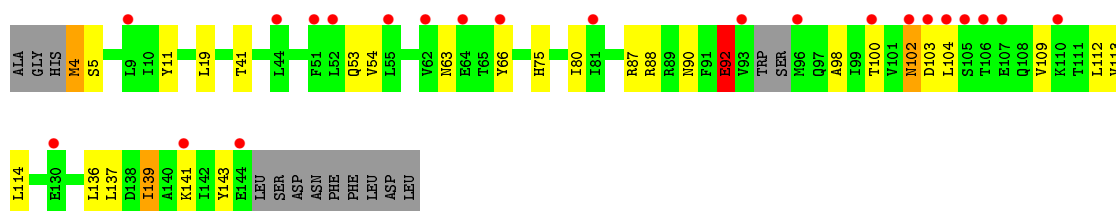
- Molecule 1: Activator of photopigment and puc expression

Chain I: 



- Molecule 1: Activator of photopigment and puc expression

Chain J: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.42Å 147.68Å 96.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.10 47.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.8 (48.00-2.10) 90.8 (47.96-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.237 , 0.286 0.265 , 0.300	Depositor DCC
R_{free} test set	4490 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11646	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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	0.70	0/1229	0.74	0/1667
1	B	0.73	1/1131 (0.1%)	0.72	0/1536
1	C	0.68	0/1088	0.73	0/1478
1	D	0.70	0/1190	0.90	5/1616 (0.3%)
1	E	0.55	0/1129	0.70	0/1536
1	F	0.80	1/1137 (0.1%)	0.71	1/1544 (0.1%)
1	G	0.55	0/1120	0.73	0/1521
1	H	0.58	0/1143	0.66	0/1552
1	I	0.55	0/1139	0.69	1/1549 (0.1%)
1	J	0.60	0/1119	0.73	1/1518 (0.1%)
All	All	0.65	2/11425 (0.0%)	0.74	8/15517 (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	B	0	2
1	D	0	2
1	H	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	20	GLN	CD-OE1	17.50	1.62	1.24
1	B	22	GLN	CD-NE2	10.33	1.58	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	ASN	N-CA-C	-6.91	92.34	111.00
1	F	20	GLN	CG-CD-OE1	-6.27	109.06	121.60
1	D	91	PHE	C-N-CA	6.17	137.12	121.70
1	D	144	GLU	N-CA-C	-6.05	94.68	111.00
1	I	114	LEU	CA-CB-CG	5.97	129.03	115.30
1	D	43	LEU	CA-CB-CG	5.47	127.88	115.30
1	D	143	TYR	N-CA-C	5.47	125.76	111.00
1	J	114	LEU	CA-CB-CG	5.30	127.50	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	101	VAL	Peptide
1	B	102	ASN	Peptide
1	D	143	TYR	Peptide
1	D	147	ASP	Peptide
1	H	142	ILE	Peptide

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	1205	0	1182	20	0
1	B	1109	0	1096	18	0
1	C	1067	0	1036	34	0
1	D	1167	0	1141	44	0
1	E	1107	0	1078	26	0
1	F	1115	0	1102	22	0
1	G	1099	0	1087	19	0
1	H	1121	0	1106	21	0
1	I	1117	0	1094	30	0
1	J	1100	0	1079	20	0
2	A	31	0	19	0	0
2	B	31	0	19	1	0
2	C	31	0	19	1	0
2	D	31	0	19	1	0
2	E	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	31	0	19	2	0
2	G	31	0	19	1	0
2	H	31	0	19	0	0
2	I	31	0	19	0	0
2	J	31	0	19	0	0
3	A	22	0	0	3	0
3	B	6	0	0	0	0
3	C	12	0	0	0	0
3	D	29	0	0	5	0
3	E	12	0	0	1	0
3	F	8	0	0	1	0
3	G	13	0	0	1	0
3	H	10	0	0	1	0
3	I	9	0	0	2	0
3	J	8	0	0	1	0
All	All	11646	0	11191	216	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 (216) 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:59:CYS:HB3	3:I:160:HOH:O	1.26	1.27
1:D:93:VAL:HB	3:D:176:HOH:O	1.43	1.18
1:F:44:LEU:HB2	1:F:96:MET:CE	1.91	1.01
1:E:43:LEU:C	1:E:96:MET:HE1	1.81	1.00
1:A:84:MET:HB3	3:A:173:HOH:O	1.64	0.97
1:G:106:THR:HG22	1:G:108:GLN:H	1.30	0.97
1:I:44:LEU:N	1:I:96:MET:HE1	1.80	0.95
1:E:44:LEU:N	1:E:96:MET:HE1	1.82	0.94
1:I:96:MET:HE2	1:I:97:GLN:O	1.68	0.92
1:C:88:ARG:HH11	1:C:88:ARG:HG3	1.33	0.92
1:A:144:GLU:OE2	1:A:145:LEU:N	2.02	0.92
1:E:96:MET:HE2	1:E:97:GLN:O	1.70	0.91
1:G:128:ASP:OD1	1:I:87:ARG:NH1	2.02	0.91
1:C:143:TYR:HB2	1:C:144:GLU:HB2	1.54	0.88
1:E:43:LEU:CA	1:E:96:MET:HE1	2.05	0.86
3:A:173:HOH:O	1:B:84:MET:HE3	1.80	0.81
1:C:88:ARG:HG3	1:C:88:ARG:NH1	1.93	0.81
1:E:43:LEU:HA	1:E:96:MET:CE	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:43:LEU:C	1:I:96:MET:HE1	2.00	0.80
1:F:44:LEU:HB2	1:F:96:MET:HE3	1.64	0.80
1:I:96:MET:HE3	1:I:97:GLN:H	1.46	0.80
1:H:106:THR:HG21	3:H:163:HOH:O	1.83	0.79
1:A:152:ASP:O	1:A:153:LEU:HB2	1.82	0.78
1:F:44:LEU:CB	1:F:96:MET:HE3	2.15	0.76
1:I:96:MET:CE	1:I:97:GLN:H	1.99	0.75
1:E:43:LEU:CA	1:E:96:MET:CE	2.65	0.74
1:I:96:MET:CE	1:I:97:GLN:O	2.34	0.74
1:D:141:LYS:HD3	1:D:147:ASP:HB2	1.70	0.74
1:F:63:ASN:O	1:F:67:HIS:HD2	1.71	0.74
1:B:107:GLU:H	1:B:110:LYS:HB2	1.52	0.74
1:E:96:MET:CE	1:E:97:GLN:O	2.36	0.73
1:J:4:MET:HG2	1:J:5:SER:N	2.04	0.73
1:B:87:ARG:HG3	1:D:130:GLU:OE1	1.90	0.72
1:A:80:ILE:H	1:B:63:ASN:ND2	1.89	0.71
1:D:92:GLU:CB	1:D:146:SER:OG	2.38	0.71
1:E:43:LEU:HA	1:E:96:MET:HE3	1.71	0.71
1:C:53:GLN:HE21	1:C:94:TRP:HZ3	1.38	0.71
1:E:96:MET:HE3	1:E:97:GLN:H	1.53	0.71
1:E:63:ASN:ND2	1:F:80:ILE:H	1.88	0.70
1:C:140:ALA:O	1:C:144:GLU:HB3	1.90	0.69
1:G:43:LEU:HD13	1:G:97:GLN:HE21	1.58	0.69
1:A:80:ILE:H	1:B:63:ASN:HD21	1.39	0.69
1:H:142:ILE:O	1:H:143:TYR:HB2	1.92	0.69
1:A:111:THR:HG23	1:C:92:GLU:CG	2.24	0.68
1:I:43:LEU:CA	1:I:96:MET:HE1	2.23	0.68
1:D:4:MET:HG3	3:D:183:HOH:O	1.94	0.68
1:H:20:GLN:HB3	1:H:21:PRO:HD2	1.76	0.67
1:I:80:ILE:H	1:J:63:ASN:ND2	1.92	0.67
1:C:80:ILE:H	1:D:63:ASN:HD21	1.43	0.67
1:D:102:ASN:ND2	1:D:104:LEU:H	1.92	0.67
3:G:166:HOH:O	1:H:4:MET:HE1	1.94	0.66
1:I:43:LEU:HA	1:I:96:MET:CE	2.25	0.66
1:I:106:THR:HG22	1:I:109:VAL:H	1.59	0.66
1:G:63:ASN:ND2	1:H:80:ILE:H	1.95	0.65
1:A:111:THR:CG2	1:C:92:GLU:HG2	2.27	0.64
1:G:80:ILE:H	1:H:63:ASN:ND2	1.95	0.64
1:F:44:LEU:HB2	1:F:96:MET:HE1	1.79	0.64
1:A:111:THR:HG23	1:C:92:GLU:HG2	1.79	0.64
1:C:143:TYR:HB2	1:C:144:GLU:CB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ILE:H	1:D:63:ASN:ND2	1.95	0.64
1:D:141:LYS:NZ	3:D:174:HOH:O	2.32	0.63
1:E:80:ILE:H	1:F:63:ASN:ND2	1.97	0.63
1:D:141:LYS:HD3	1:D:147:ASP:CB	2.28	0.62
1:B:100:THR:O	1:B:102:ASN:N	2.32	0.62
1:I:80:ILE:H	1:J:63:ASN:HD21	1.48	0.62
1:E:63:ASN:HD21	1:F:80:ILE:H	1.46	0.62
1:J:98:ALA:CB	3:J:209:HOH:O	2.47	0.62
1:I:43:LEU:HA	1:I:96:MET:HE3	1.82	0.62
1:D:102:ASN:HD22	1:D:104:LEU:H	1.47	0.61
1:I:43:LEU:CA	1:I:96:MET:CE	2.79	0.61
1:D:68:ARG:NH1	2:D:154:FMN:O4'	2.33	0.61
1:E:80:ILE:H	1:F:63:ASN:HD21	1.49	0.60
1:A:106:THR:HG22	1:A:109:VAL:H	1.66	0.60
1:A:63:ASN:O	1:A:67:HIS:HD2	1.85	0.59
1:C:53:GLN:NE2	1:C:94:TRP:CZ3	2.71	0.59
1:A:127:MET:HE2	1:A:131:GLN:HB3	1.85	0.58
1:F:63:ASN:O	1:F:67:HIS:CD2	2.55	0.58
1:D:102:ASN:HD22	1:D:102:ASN:C	2.07	0.58
1:C:63:ASN:ND2	1:D:80:ILE:H	2.01	0.58
1:C:93:VAL:HG12	1:C:94:TRP:N	2.19	0.57
1:A:102:ASN:HD22	1:A:102:ASN:C	2.07	0.57
1:E:63:ASN:O	1:E:67:HIS:HD2	1.88	0.57
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.02	0.56
1:E:44:LEU:N	1:E:96:MET:CE	2.65	0.56
1:F:44:LEU:CB	1:F:96:MET:CE	2.71	0.56
1:J:41:THR:HG21	1:J:92:GLU:HA	1.87	0.56
1:F:4:MET:SD	1:F:4:MET:N	2.77	0.56
1:J:90:ASN:HB3	1:J:137:LEU:HD21	1.88	0.56
1:D:91:PHE:HA	1:D:92:GLU:HB2	1.86	0.56
1:A:63:ASN:ND2	1:B:80:ILE:H	2.04	0.55
1:H:58:GLU:HB3	1:H:61:GLN:HG2	1.88	0.55
1:C:67:HIS:HE1	1:D:66:TYR:OH	1.90	0.55
1:I:63:ASN:O	1:I:67:HIS:HD2	1.88	0.55
1:A:102:ASN:ND2	1:A:104:LEU:H	2.04	0.55
1:F:93:VAL:HG22	3:F:159:HOH:O	2.07	0.55
1:B:4:MET:N	1:B:4:MET:SD	2.79	0.55
1:C:66:TYR:OH	1:D:67:HIS:HE1	1.88	0.55
1:A:111:THR:HG23	1:C:92:GLU:HG3	1.89	0.54
1:C:63:ASN:HD21	1:D:80:ILE:H	1.54	0.54
1:A:144:GLU:OE2	1:A:144:GLU:CA	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:PRO:HA	1:B:24:LEU:HD12	1.90	0.53
1:C:93:VAL:HG12	1:C:94:TRP:H	1.73	0.53
1:B:88:ARG:HD2	1:D:115:LYS:HE3	1.91	0.53
1:H:20:GLN:HB3	1:H:21:PRO:CD	2.38	0.53
1:G:63:ASN:HD21	1:H:80:ILE:H	1.56	0.52
1:F:43:LEU:HD23	1:F:136:LEU:HD22	1.91	0.52
1:D:90:ASN:HD22	1:D:148:ASN:HD21	1.57	0.52
3:A:173:HOH:O	1:B:84:MET:CE	2.50	0.52
1:G:80:ILE:H	1:H:63:ASN:HD21	1.56	0.52
1:E:102:ASN:HD22	1:E:102:ASN:C	2.13	0.51
1:B:115:LYS:HD3	1:B:116:TYR:CE1	2.46	0.51
1:D:22:GLN:HB2	3:D:168:HOH:O	2.10	0.51
1:C:47:SER:OG	1:C:122:LEU:HB3	2.10	0.51
1:D:56:GLU:OE2	1:D:91:PHE:O	2.28	0.51
1:G:28:LEU:O	1:G:32:GLN:HG3	2.10	0.51
1:H:4:MET:N	1:H:4:MET:SD	2.84	0.51
1:I:44:LEU:H	1:I:96:MET:HE1	1.71	0.51
1:D:8:ARG:HD3	3:D:165:HOH:O	2.10	0.50
1:G:43:LEU:HD13	1:G:97:GLN:NE2	2.25	0.50
1:C:112:LEU:HD13	1:C:139:ILE:HD12	1.94	0.50
1:D:63:ASN:O	1:D:67:HIS:HD2	1.95	0.50
1:F:30:SER:HB3	2:F:154:FMN:H4'	1.93	0.50
1:C:67:HIS:CE1	1:D:66:TYR:OH	2.65	0.50
1:A:106:THR:CG2	1:A:108:GLN:HB3	2.42	0.49
1:H:142:ILE:O	1:H:143:TYR:CB	2.60	0.49
1:C:88:ARG:CG	1:C:88:ARG:HH11	2.10	0.49
1:G:63:ASN:O	1:G:67:HIS:HD2	1.96	0.49
1:B:128:ASP:HB2	1:B:129:PRO:HD2	1.94	0.49
1:F:115:LYS:HD3	1:F:116:TYR:CE1	2.48	0.49
1:I:63:ASN:ND2	1:J:80:ILE:H	2.11	0.49
1:D:92:GLU:CG	1:D:146:SER:OG	2.61	0.48
1:H:106:THR:HG22	1:H:108:GLN:N	2.27	0.48
1:E:143:TYR:N	1:E:144:GLU:HA	2.28	0.48
1:E:70:VAL:HG22	1:E:78:PRO:HG3	1.96	0.48
1:D:88:ARG:NH2	1:D:148:ASN:ND2	2.60	0.48
1:I:43:LEU:HD11	1:I:99:ILE:HG12	1.95	0.47
1:D:22:GLN:HE22	1:D:26:ASP:CG	2.18	0.47
1:I:99:ILE:HD12	1:I:143:TYR:CD2	2.49	0.47
1:C:66:TYR:OH	1:D:67:HIS:CE1	2.67	0.47
1:F:43:LEU:HD11	1:F:99:ILE:HG12	1.97	0.47
1:C:53:GLN:NE2	1:C:94:TRP:CH2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ASN:O	1:C:67:HIS:HD2	1.97	0.47
1:E:61:GLN:NE2	3:E:159:HOH:O	2.48	0.47
1:G:87:ARG:HA	1:G:87:ARG:NE	2.30	0.47
1:J:54:VAL:HG12	1:J:136:LEU:HD13	1.97	0.47
1:B:130:GLU:OE1	1:J:87:ARG:HD3	2.15	0.47
1:J:11:TYR:CE1	1:J:53:GLN:HB3	2.50	0.46
1:E:96:MET:CE	1:E:97:GLN:H	2.22	0.46
1:J:102:ASN:HD22	1:J:104:LEU:H	1.63	0.46
1:J:139:ILE:O	1:J:143:TYR:HD1	1.98	0.46
1:C:107:GLU:HA	1:C:110:LYS:HB2	1.98	0.46
1:C:4:MET:O	1:C:58:GLU:HG3	2.15	0.46
1:I:4:MET:N	3:I:160:HOH:O	2.49	0.46
1:E:43:LEU:HD22	1:E:140:ALA:HB2	1.97	0.46
1:H:63:ASN:O	1:H:67:HIS:HD2	1.99	0.46
1:I:67:HIS:HE1	1:J:66:TYR:OH	1.99	0.46
1:G:67:HIS:HE1	1:H:66:TYR:OH	1.98	0.45
1:A:79:GLN:HE22	1:B:60:GLU:HA	1.81	0.45
1:D:106:THR:HG22	1:D:108:GLN:H	1.81	0.45
1:G:106:THR:HG22	1:G:108:GLN:N	2.13	0.45
1:D:22:GLN:O	1:D:22:GLN:NE2	2.50	0.45
1:G:68:ARG:HH11	1:G:68:ARG:HG2	1.82	0.45
2:B:154:FMN:H1'1	2:B:154:FMN:H9	1.69	0.45
1:E:63:ASN:O	1:E:67:HIS:CD2	2.70	0.45
1:J:109:VAL:O	1:J:113:VAL:HG23	2.17	0.45
1:I:63:ASN:HD21	1:J:80:ILE:H	1.65	0.45
1:D:58:GLU:OE2	1:D:61:GLN:HG2	2.16	0.45
1:I:102:ASN:O	1:I:105:SER:HB2	2.17	0.45
1:E:47:SER:O	1:E:48:LYS:C	2.55	0.44
1:I:63:ASN:O	1:I:67:HIS:CD2	2.69	0.44
1:C:47:SER:HB3	1:C:99:ILE:HB	2.00	0.44
1:C:65:THR:O	1:C:69:ILE:HG13	2.18	0.44
1:F:48:LYS:HA	1:F:49:PRO:HA	1.78	0.44
1:D:99:ILE:HD11	1:D:145:LEU:HD11	1.99	0.44
1:I:80:ILE:HD13	1:J:80:ILE:HD13	2.00	0.44
1:C:11:TYR:CE1	1:C:53:GLN:HB3	2.53	0.43
1:B:87:ARG:CG	1:D:130:GLU:OE1	2.63	0.43
1:G:67:HIS:CE1	1:H:66:TYR:OH	2.71	0.43
1:D:28:LEU:HD11	1:D:98:ALA:HB2	1.99	0.43
1:I:144:GLU:HA	1:I:145:LEU:HA	1.85	0.43
1:H:47:SER:O	1:H:48:LYS:C	2.57	0.43
1:D:92:GLU:HG2	1:D:146:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:CG2	1:A:120:THR:O	2.67	0.43
1:C:48:LYS:HA	1:C:49:PRO:HA	1.74	0.43
1:G:30:SER:HB3	2:G:154:FMN:H4'	2.00	0.43
1:C:30:SER:HB3	2:C:154:FMN:H4'	1.99	0.43
1:B:103:ASP:HA	1:B:109:VAL:HG11	2.00	0.42
1:E:94:TRP:HZ3	1:E:140:ALA:HB1	1.84	0.42
1:D:92:GLU:HB2	1:D:146:SER:OG	2.17	0.42
1:D:92:GLU:HB3	1:D:146:SER:OG	2.16	0.42
1:F:53:GLN:NE2	1:F:96:MET:CE	2.82	0.42
1:H:102:ASN:HD22	1:H:102:ASN:C	2.23	0.42
1:H:106:THR:HG22	1:H:108:GLN:H	1.84	0.42
1:I:48:LYS:HA	1:I:49:PRO:HA	1.85	0.42
1:J:4:MET:HG2	1:J:5:SER:H	1.81	0.42
1:G:90:ASN:HB3	1:G:137:LEU:HD21	2.02	0.42
1:J:88:ARG:HG2	1:J:88:ARG:HH11	1.84	0.42
1:B:47:SER:O	1:B:48:LYS:C	2.57	0.42
1:D:28:LEU:HD21	1:D:98:ALA:HB2	2.01	0.42
1:H:48:LYS:HA	1:H:49:PRO:HA	1.90	0.41
1:I:67:HIS:CE1	1:J:66:TYR:OH	2.73	0.41
1:D:91:PHE:HA	1:D:92:GLU:CB	2.51	0.41
1:F:44:LEU:HB3	1:F:96:MET:HE3	2.00	0.41
1:I:87:ARG:CZ	1:I:87:ARG:HA	2.51	0.41
1:D:11:TYR:CE1	1:D:53:GLN:HB3	2.55	0.41
1:D:87:ARG:NH1	1:F:128:ASP:OD1	2.51	0.41
1:C:143:TYR:N	1:C:143:TYR:CD1	2.88	0.41
1:D:141:LYS:HD3	1:D:147:ASP:CG	2.40	0.41
1:H:99:ILE:CD1	1:H:144:GLU:H	2.34	0.41
1:D:95:SER:OG	1:D:145:LEU:HD13	2.21	0.41
1:E:94:TRP:CZ3	1:E:140:ALA:HB1	2.56	0.41
1:E:4:MET:HB2	1:E:5:SER:H	1.67	0.41
1:J:136:LEU:HA	1:J:139:ILE:HG22	2.03	0.41
1:G:102:ASN:C	1:G:102:ASN:HD22	2.24	0.40
1:G:63:ASN:O	1:G:67:HIS:CD2	2.74	0.40
1:F:34:ASN:HB2	2:F:154:FMN:O2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	148/153 (97%)	145 (98%)	3 (2%)	0	100	100
1	B	138/153 (90%)	131 (95%)	5 (4%)	2 (1%)	11	6
1	C	132/153 (86%)	128 (97%)	3 (2%)	1 (1%)	19	15
1	D	145/153 (95%)	140 (97%)	3 (2%)	2 (1%)	11	6
1	E	139/153 (91%)	137 (99%)	2 (1%)	0	100	100
1	F	138/153 (90%)	134 (97%)	4 (3%)	0	100	100
1	G	137/153 (90%)	132 (96%)	5 (4%)	0	100	100
1	H	139/153 (91%)	135 (97%)	3 (2%)	1 (1%)	22	18
1	I	140/153 (92%)	139 (99%)	1 (1%)	0	100	100
1	J	135/153 (88%)	129 (96%)	5 (4%)	1 (1%)	22	18
All	All	1391/1530 (91%)	1350 (97%)	34 (2%)	7 (0%)	29	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	VAL
1	C	107	GLU
1	D	92	GLU
1	H	143	TYR
1	J	92	GLU
1	D	147	ASP
1	B	142	ILE

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	137/141 (97%)	124 (90%)	13 (10%)	8	5
1	B	124/141 (88%)	115 (93%)	9 (7%)	14	11
1	C	117/141 (83%)	104 (89%)	13 (11%)	6	3
1	D	131/141 (93%)	121 (92%)	10 (8%)	13	10
1	E	123/141 (87%)	114 (93%)	9 (7%)	14	11
1	F	126/141 (89%)	118 (94%)	8 (6%)	18	15
1	G	124/141 (88%)	113 (91%)	11 (9%)	9	6
1	H	126/141 (89%)	115 (91%)	11 (9%)	10	7
1	I	124/141 (88%)	112 (90%)	12 (10%)	8	5
1	J	124/141 (88%)	114 (92%)	10 (8%)	11	8
All	All	1256/1410 (89%)	1150 (92%)	106 (8%)	11	7

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	5	SER
1	A	7	TYR
1	A	22	GLN
1	A	28	LEU
1	A	64	GLU
1	A	71	GLN
1	A	75	HIS
1	A	102	ASN
1	A	106	THR
1	A	120	THR
1	A	141	LYS
1	A	144	GLU
1	B	4	MET
1	B	5	SER
1	B	28	LEU
1	B	64	GLU
1	B	75	HIS
1	B	87	ARG
1	B	101	VAL
1	B	106	THR
1	B	139	ILE
1	C	4	MET

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Mol	Chain	Res	Type
1	C	18	ASN
1	C	19	LEU
1	C	28	LEU
1	C	64	GLU
1	C	75	HIS
1	C	88	ARG
1	C	92	GLU
1	C	105	SER
1	C	106	THR
1	C	112	LEU
1	C	114	LEU
1	C	144	GLU
1	D	4	MET
1	D	22	GLN
1	D	24	LEU
1	D	75	HIS
1	D	102	ASN
1	D	104	LEU
1	D	120	THR
1	D	121	THR
1	D	144	GLU
1	D	148	ASN
1	E	4	MET
1	E	5	SER
1	E	28	LEU
1	E	64	GLU
1	E	75	HIS
1	E	102	ASN
1	E	120	THR
1	E	121	THR
1	E	142	ILE
1	F	4	MET
1	F	5	SER
1	F	28	LEU
1	F	75	HIS
1	F	97	GLN
1	F	102	ASN
1	F	139	ILE
1	F	141	LYS
1	G	4	MET
1	G	24	LEU
1	G	26	ASP

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Mol	Chain	Res	Type
1	G	28	LEU
1	G	64	GLU
1	G	75	HIS
1	G	102	ASN
1	G	103	ASP
1	G	112	LEU
1	G	120	THR
1	G	139	ILE
1	H	4	MET
1	H	5	SER
1	H	19	LEU
1	H	28	LEU
1	H	75	HIS
1	H	87	ARG
1	H	102	ASN
1	H	112	LEU
1	H	120	THR
1	H	121	THR
1	H	141	LYS
1	I	4	MET
1	I	7	TYR
1	I	18	ASN
1	I	24	LEU
1	I	28	LEU
1	I	75	HIS
1	I	87	ARG
1	I	102	ASN
1	I	106	THR
1	I	112	LEU
1	I	120	THR
1	I	121	THR
1	J	4	MET
1	J	19	LEU
1	J	75	HIS
1	J	92	GLU
1	J	100	THR
1	J	102	ASN
1	J	103	ASP
1	J	112	LEU
1	J	139	ILE
1	J	141	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	22	GLN
1	A	32	GLN
1	A	34	ASN
1	A	53	GLN
1	A	61	GLN
1	A	63	ASN
1	A	67	HIS
1	A	79	GLN
1	A	102	ASN
1	B	32	GLN
1	B	34	ASN
1	B	63	ASN
1	B	67	HIS
1	C	22	GLN
1	C	61	GLN
1	C	63	ASN
1	C	67	HIS
1	C	71	GLN
1	D	22	GLN
1	D	32	GLN
1	D	61	GLN
1	D	63	ASN
1	D	67	HIS
1	D	97	GLN
1	D	102	ASN
1	D	148	ASN
1	E	32	GLN
1	E	63	ASN
1	E	67	HIS
1	E	102	ASN
1	F	32	GLN
1	F	53	GLN
1	F	61	GLN
1	F	63	ASN
1	F	67	HIS
1	F	102	ASN
1	G	32	GLN
1	G	61	GLN
1	G	63	ASN
1	G	67	HIS
1	G	97	GLN

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Mol	Chain	Res	Type
1	G	102	ASN
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	61	GLN
1	I	63	ASN
1	I	67	HIS
1	I	102	ASN
1	J	32	GLN
1	J	61	GLN
1	J	63	ASN
1	J	67	HIS
1	J	71	GLN
1	J	102	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	F	154	-	31,33,33	1.56	5 (16%)	40,50,50	1.59	6 (15%)
2	FMN	G	154	-	31,33,33	1.46	5 (16%)	40,50,50	1.72	7 (17%)
2	FMN	D	154	-	31,33,33	1.66	7 (22%)	40,50,50	1.56	7 (17%)
2	FMN	E	154	-	31,33,33	1.60	5 (16%)	40,50,50	1.97	8 (20%)
2	FMN	B	154	-	31,33,33	1.61	5 (16%)	40,50,50	1.67	6 (15%)
2	FMN	C	154	-	31,33,33	1.29	4 (12%)	40,50,50	1.58	7 (17%)
2	FMN	A	154	-	31,33,33	1.52	5 (16%)	40,50,50	1.48	7 (17%)
2	FMN	J	201	-	31,33,33	1.70	5 (16%)	40,50,50	1.72	10 (25%)
2	FMN	H	154	-	31,33,33	1.42	6 (19%)	40,50,50	1.87	8 (20%)
2	FMN	I	154	-	31,33,33	1.48	5 (16%)	40,50,50	1.69	9 (22%)

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	F	154	-	-	4/18/18/18	0/3/3/3
2	FMN	G	154	-	-	0/18/18/18	0/3/3/3
2	FMN	D	154	-	-	2/18/18/18	0/3/3/3
2	FMN	E	154	-	-	2/18/18/18	0/3/3/3
2	FMN	B	154	-	-	7/18/18/18	0/3/3/3
2	FMN	C	154	-	-	0/18/18/18	0/3/3/3
2	FMN	A	154	-	-	3/18/18/18	0/3/3/3
2	FMN	J	201	-	-	4/18/18/18	0/3/3/3
2	FMN	H	154	-	-	0/18/18/18	0/3/3/3
2	FMN	I	154	-	-	1/18/18/18	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	201	FMN	C4A-N5	4.80	1.40	1.33
2	B	154	FMN	C10-N1	4.45	1.39	1.33
2	E	154	FMN	C10-N1	4.25	1.38	1.33
2	F	154	FMN	C10-N1	4.20	1.38	1.33
2	B	154	FMN	C1'-N10	4.08	1.52	1.48
2	E	154	FMN	C4A-N5	4.06	1.39	1.33
2	A	154	FMN	C4A-N5	3.96	1.39	1.33
2	I	154	FMN	C4A-N5	3.91	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	154	FMN	C1'-N10	3.90	1.52	1.48
2	J	201	FMN	C10-N1	3.87	1.38	1.33
2	G	154	FMN	C4A-N5	3.75	1.38	1.33
2	D	154	FMN	C4A-N5	3.74	1.38	1.33
2	I	154	FMN	C10-N1	3.70	1.38	1.33
2	A	154	FMN	C10-N1	3.69	1.38	1.33
2	A	154	FMN	C1'-N10	3.64	1.52	1.48
2	E	154	FMN	C4-N3	3.59	1.39	1.33
2	J	201	FMN	C4-N3	3.54	1.39	1.33
2	G	154	FMN	C10-N1	3.53	1.37	1.33
2	I	154	FMN	C4-N3	3.41	1.39	1.33
2	B	154	FMN	C4A-N5	3.40	1.38	1.33
2	H	154	FMN	C4A-N5	3.35	1.38	1.33
2	F	154	FMN	C4A-N5	3.33	1.38	1.33
2	F	154	FMN	C4-N3	3.33	1.38	1.33
2	J	201	FMN	C1'-N10	3.28	1.51	1.48
2	G	154	FMN	C1'-N10	3.26	1.51	1.48
2	E	154	FMN	C1'-N10	3.24	1.51	1.48
2	F	154	FMN	C1'-N10	3.22	1.51	1.48
2	G	154	FMN	C4-N3	3.17	1.38	1.33
2	J	201	FMN	C5A-N5	3.14	1.40	1.35
2	A	154	FMN	C4-N3	3.05	1.38	1.33
2	H	154	FMN	C10-N1	3.05	1.37	1.33
2	B	154	FMN	C4-N3	3.04	1.38	1.33
2	C	154	FMN	C1'-N10	3.04	1.51	1.48
2	D	154	FMN	C10-N1	3.01	1.37	1.33
2	H	154	FMN	C1'-N10	2.93	1.51	1.48
2	A	154	FMN	C5A-N5	2.91	1.40	1.35
2	D	154	FMN	C5A-N5	2.85	1.40	1.35
2	C	154	FMN	C4A-N5	2.80	1.37	1.33
2	C	154	FMN	C4-N3	2.76	1.37	1.33
2	H	154	FMN	C5A-N5	2.61	1.39	1.35
2	H	154	FMN	C4-N3	2.59	1.37	1.33
2	D	154	FMN	C4-C4A	-2.59	1.36	1.41
2	F	154	FMN	C5A-N5	2.57	1.39	1.35
2	E	154	FMN	C5A-N5	2.55	1.39	1.35
2	I	154	FMN	C1'-N10	2.51	1.50	1.48
2	D	154	FMN	C4-N3	2.50	1.37	1.33
2	C	154	FMN	C10-N1	2.45	1.36	1.33
2	B	154	FMN	C5A-N5	2.45	1.39	1.35
2	H	154	FMN	C9A-C5A	-2.23	1.38	1.42
2	D	154	FMN	C4A-C10	-2.14	1.36	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	154	FMN	C5A-N5	2.03	1.38	1.35
2	I	154	FMN	C6-C5A	-2.01	1.38	1.41

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	154	FMN	C4-N3-C2	7.79	121.72	115.14
2	I	154	FMN	C4-N3-C2	6.23	120.40	115.14
2	F	154	FMN	C4-N3-C2	6.14	120.33	115.14
2	H	154	FMN	C4-N3-C2	6.04	120.24	115.14
2	D	154	FMN	C4-N3-C2	5.59	119.86	115.14
2	B	154	FMN	C4-N3-C2	5.58	119.85	115.14
2	J	201	FMN	C4-N3-C2	5.20	119.53	115.14
2	G	154	FMN	C4-N3-C2	5.16	119.50	115.14
2	C	154	FMN	C4-N3-C2	5.05	119.41	115.14
2	B	154	FMN	C5A-C9A-N10	5.05	121.37	117.72
2	A	154	FMN	C4-N3-C2	4.46	118.91	115.14
2	H	154	FMN	C10-C4A-N5	-4.32	118.27	121.26
2	J	201	FMN	C5A-C9A-N10	4.28	120.82	117.72
2	G	154	FMN	C10-C4A-N5	-3.98	118.50	121.26
2	G	154	FMN	C4A-N5-C5A	3.88	120.64	116.77
2	H	154	FMN	C1'-N10-C9A	3.86	121.33	118.29
2	H	154	FMN	C4A-N5-C5A	3.72	120.49	116.77
2	A	154	FMN	C10-C4A-N5	-3.71	118.69	121.26
2	E	154	FMN	C10-C4A-N5	-3.58	118.78	121.26
2	F	154	FMN	C10-C4A-N5	-3.53	118.82	121.26
2	C	154	FMN	C10-C4A-N5	-3.46	118.86	121.26
2	E	154	FMN	C4-C4A-N5	3.44	122.53	118.60
2	H	154	FMN	C4-C4A-N5	3.42	122.51	118.60
2	G	154	FMN	C1'-N10-C9A	3.37	120.95	118.29
2	J	201	FMN	C4-C4A-N5	3.36	122.44	118.60
2	F	154	FMN	C4A-C4-N3	-3.36	118.84	123.43
2	B	154	FMN	C1'-N10-C10	3.35	121.41	118.41
2	C	154	FMN	C4-C4A-N5	3.35	122.42	118.60
2	I	154	FMN	C5A-C9A-N10	3.30	120.11	117.72
2	E	154	FMN	C5A-C9A-N10	3.29	120.10	117.72
2	A	154	FMN	C4A-N5-C5A	3.21	119.98	116.77
2	G	154	FMN	C4-C4A-N5	3.21	122.26	118.60
2	E	154	FMN	C4A-N5-C5A	3.19	119.96	116.77
2	H	154	FMN	C4A-C4-N3	-3.12	119.16	123.43
2	D	154	FMN	C1'-N10-C9A	3.06	120.70	118.29
2	J	201	FMN	C10-C4A-N5	-3.06	119.14	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	154	FMN	C4A-N5-C5A	3.01	119.78	116.77
2	G	154	FMN	C1'-N10-C10	-2.99	115.73	118.41
2	D	154	FMN	O4'-C4'-C5'	-2.92	103.35	109.92
2	E	154	FMN	C4A-C4-N3	-2.89	119.48	123.43
2	I	154	FMN	C4A-C4-N3	-2.89	119.48	123.43
2	C	154	FMN	C4A-N5-C5A	2.80	119.57	116.77
2	G	154	FMN	C4A-C4-N3	-2.75	119.67	123.43
2	I	154	FMN	C1'-N10-C9A	2.72	120.44	118.29
2	C	154	FMN	C1'-N10-C9A	2.72	120.43	118.29
2	B	154	FMN	C4A-C4-N3	-2.70	119.73	123.43
2	I	154	FMN	C10-C4A-N5	-2.69	119.40	121.26
2	A	154	FMN	C4-C4A-N5	2.66	121.64	118.60
2	H	154	FMN	C1'-N10-C10	-2.59	116.09	118.41
2	J	201	FMN	C6-C5A-N5	2.54	121.85	119.05
2	A	154	FMN	C4A-C4-N3	-2.53	119.97	123.43
2	I	154	FMN	C4A-N5-C5A	2.49	119.26	116.77
2	I	154	FMN	C4-C4A-N5	2.46	121.41	118.60
2	B	154	FMN	C9A-N10-C10	-2.43	118.73	121.91
2	A	154	FMN	C1'-N10-C9A	2.42	120.20	118.29
2	C	154	FMN	C4A-C4-N3	-2.42	120.13	123.43
2	I	154	FMN	C9A-N10-C10	-2.41	118.76	121.91
2	E	154	FMN	C9A-N10-C10	-2.38	118.79	121.91
2	J	201	FMN	C4A-N5-C5A	2.38	119.15	116.77
2	J	201	FMN	C9A-N10-C10	-2.36	118.82	121.91
2	J	201	FMN	C4-C4A-C10	-2.35	118.39	119.95
2	D	154	FMN	C4A-C4-N3	-2.34	120.24	123.43
2	J	201	FMN	C4A-C4-N3	-2.32	120.26	123.43
2	D	154	FMN	C4A-N5-C5A	2.25	119.02	116.77
2	J	201	FMN	O3'-C3'-C4'	-2.24	103.40	108.81
2	H	154	FMN	C5A-C9A-N10	2.19	119.30	117.72
2	D	154	FMN	C10-C4A-N5	-2.17	119.75	121.26
2	E	154	FMN	C1'-C2'-C3'	2.13	115.74	109.79
2	F	154	FMN	C5A-C9A-N10	2.09	119.23	117.72
2	C	154	FMN	C5A-C9A-N10	2.08	119.22	117.72
2	A	154	FMN	O4'-C4'-C3'	2.07	114.14	109.10
2	I	154	FMN	O2P-P-O5'	2.05	112.20	106.73
2	F	154	FMN	C9A-N10-C10	-2.05	119.23	121.91
2	D	154	FMN	C5A-C9A-N10	2.02	119.18	117.72
2	B	154	FMN	C4A-N5-C5A	2.01	118.78	116.77

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	154	FMN	C2'-C1'-N10-C9A
2	E	154	FMN	O4'-C4'-C5'-O5'
2	B	154	FMN	C2'-C1'-N10-C9A
2	A	154	FMN	C5'-O5'-P-O1P
2	A	154	FMN	C5'-O5'-P-O2P
2	A	154	FMN	C5'-O5'-P-O3P
2	J	201	FMN	C5'-O5'-P-O1P
2	J	201	FMN	C5'-O5'-P-O2P
2	J	201	FMN	C5'-O5'-P-O3P
2	B	154	FMN	O3'-C3'-C4'-O4'
2	B	154	FMN	C2'-C3'-C4'-O4'
2	B	154	FMN	O3'-C3'-C4'-C5'
2	B	154	FMN	C2'-C3'-C4'-C5'
2	F	154	FMN	C2'-C3'-C4'-O4'
2	E	154	FMN	C3'-C4'-C5'-O5'
2	I	154	FMN	O2'-C2'-C3'-C4'
2	F	154	FMN	O3'-C3'-C4'-O4'
2	D	154	FMN	O3'-C3'-C4'-O4'
2	D	154	FMN	C2'-C3'-C4'-O4'
2	B	154	FMN	C5'-O5'-P-O3P
2	F	154	FMN	O3'-C3'-C4'-C5'
2	J	201	FMN	O3'-C3'-C4'-O4'
2	B	154	FMN	N10-C1'-C2'-O2'

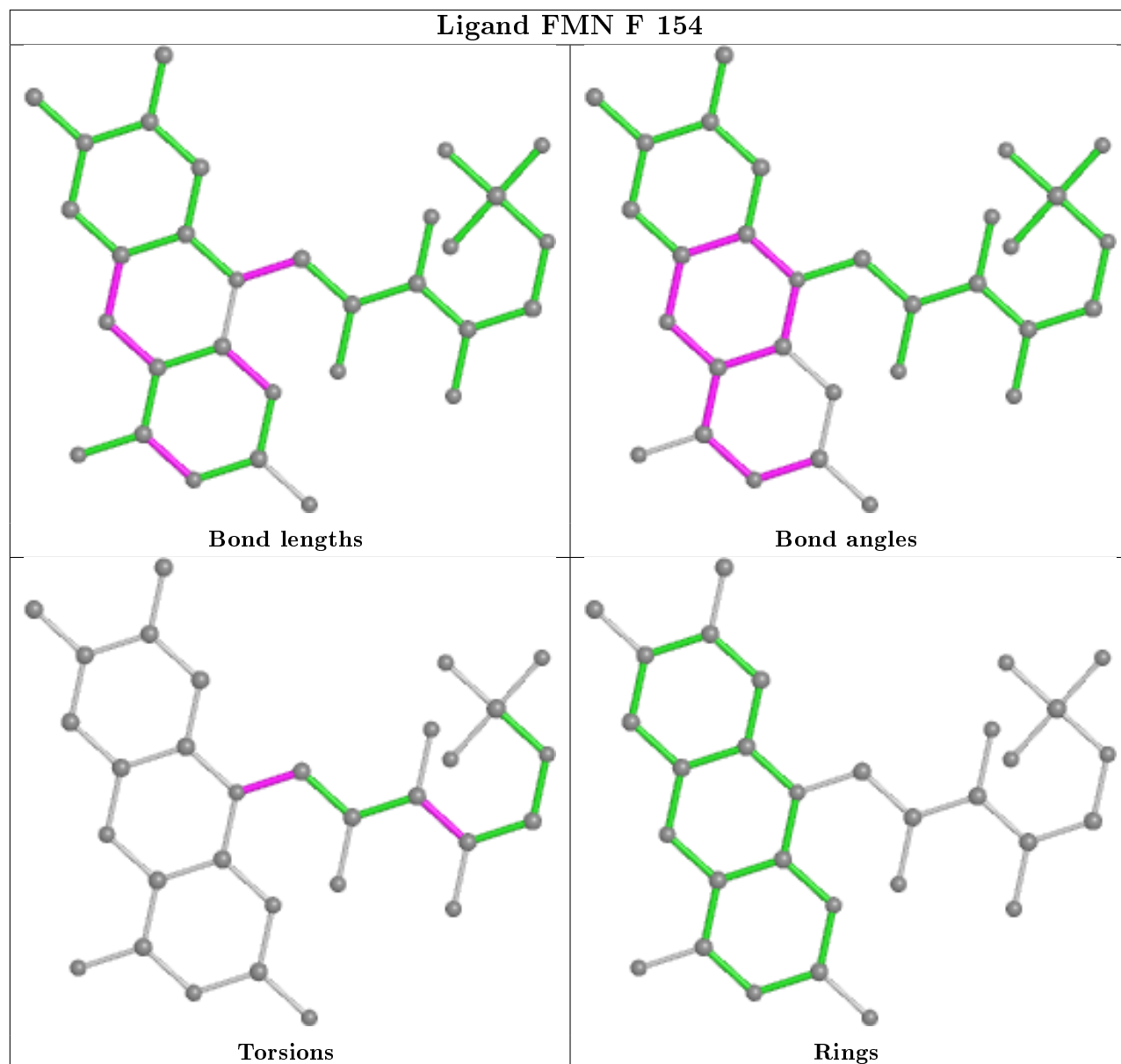
There are no ring outliers.

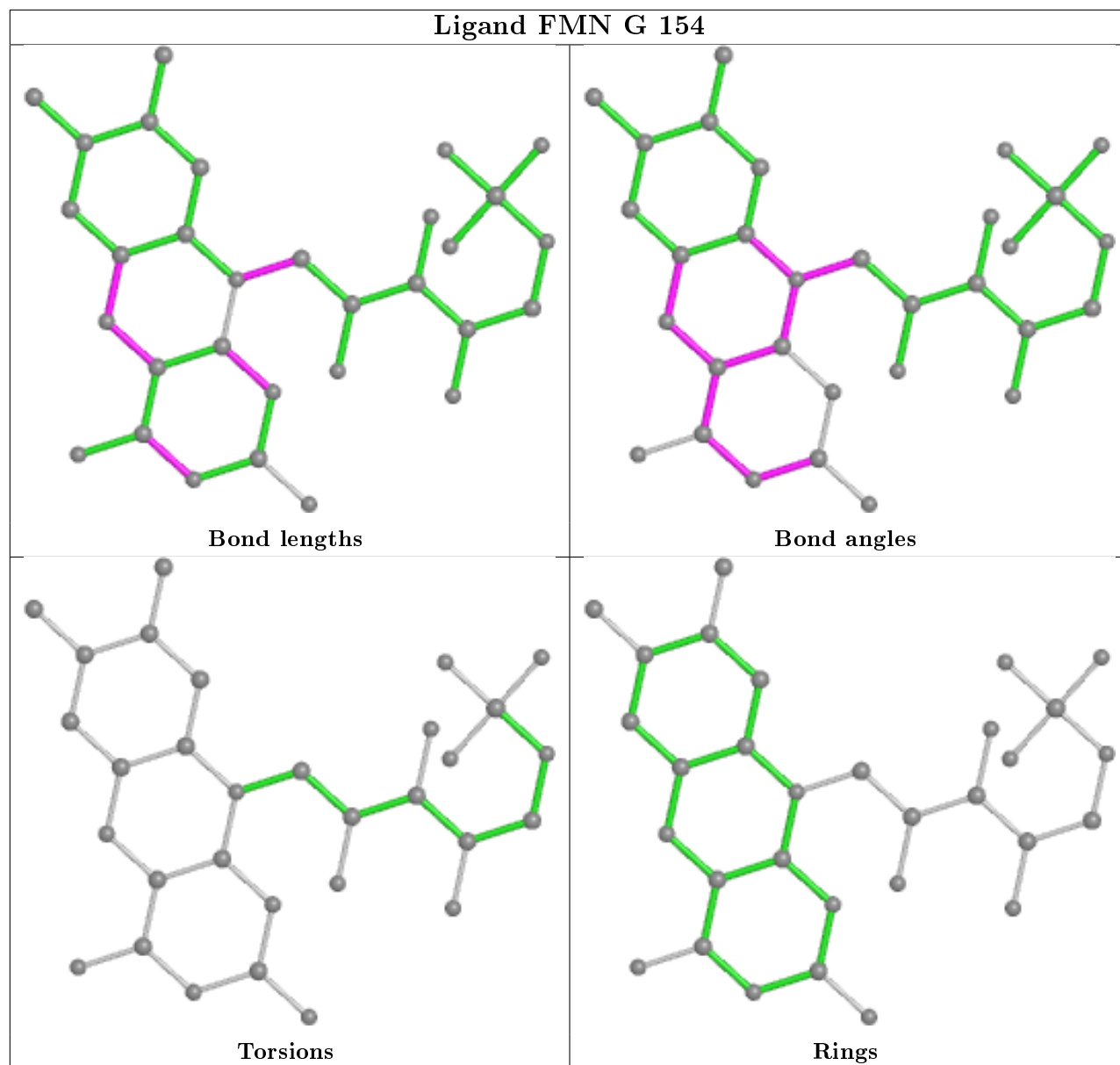
5 monomers are involved in 6 short contacts:

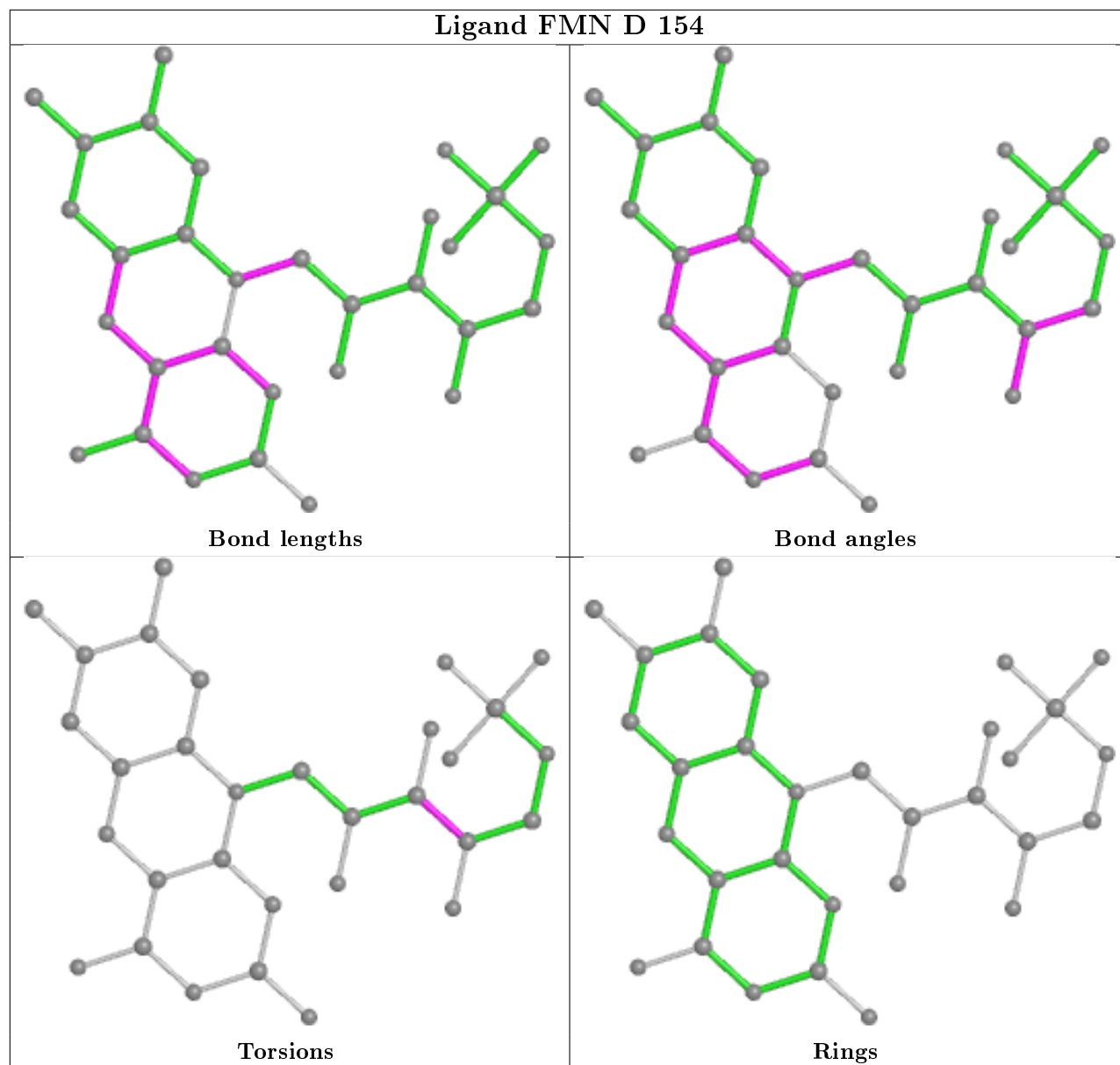
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	154	FMN	2	0
2	G	154	FMN	1	0
2	D	154	FMN	1	0
2	B	154	FMN	1	0
2	C	154	FMN	1	0

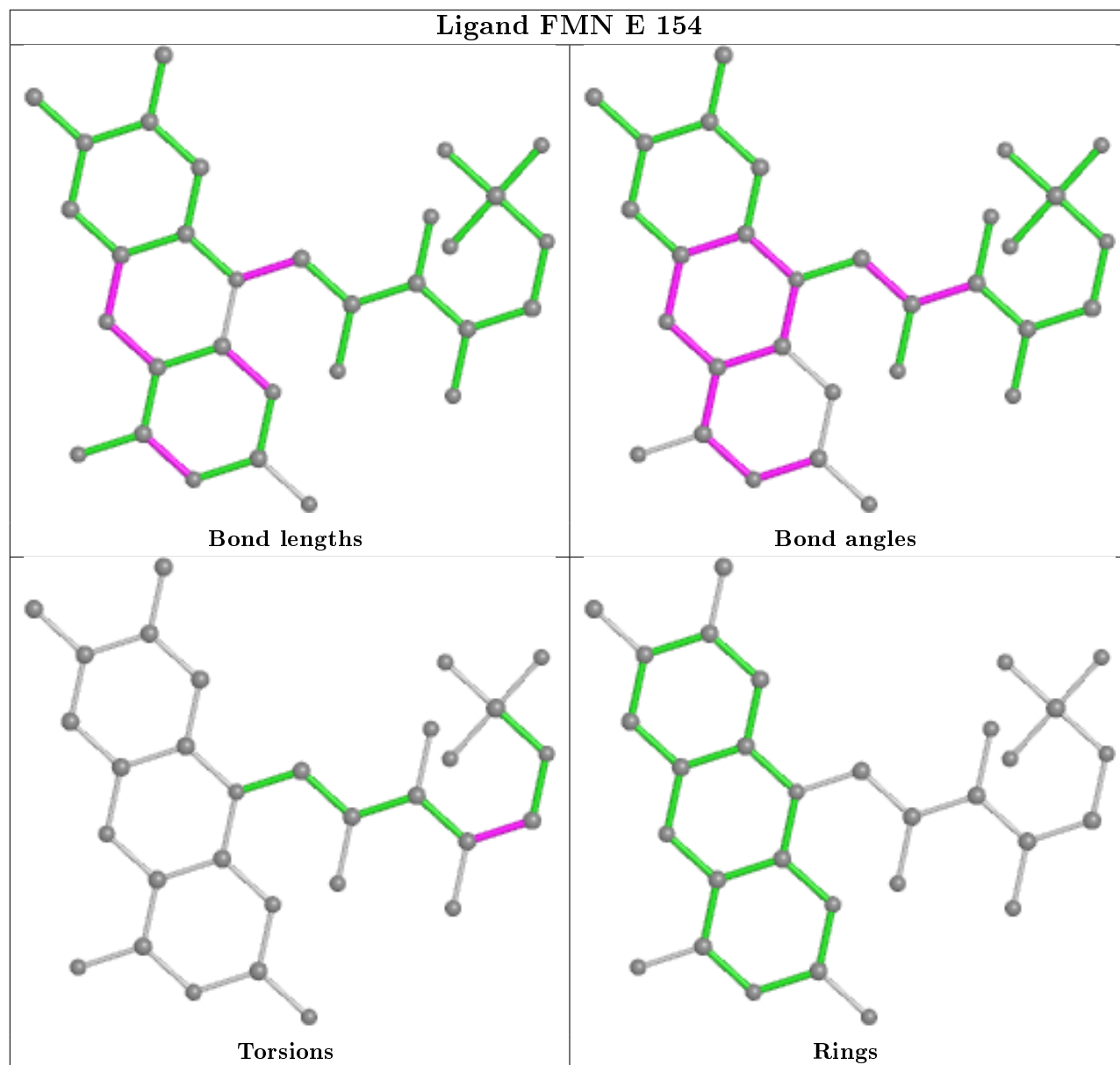
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

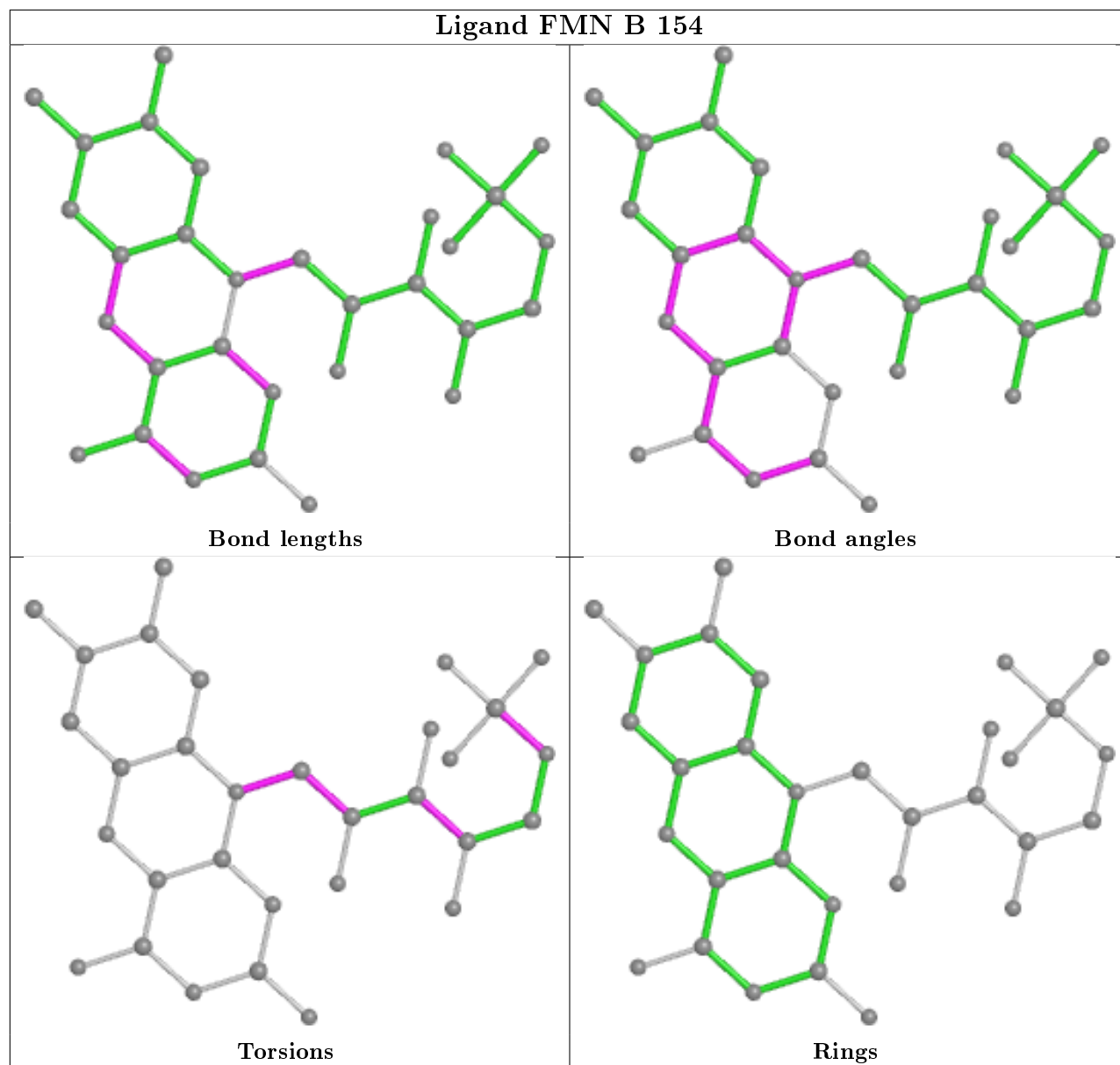
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

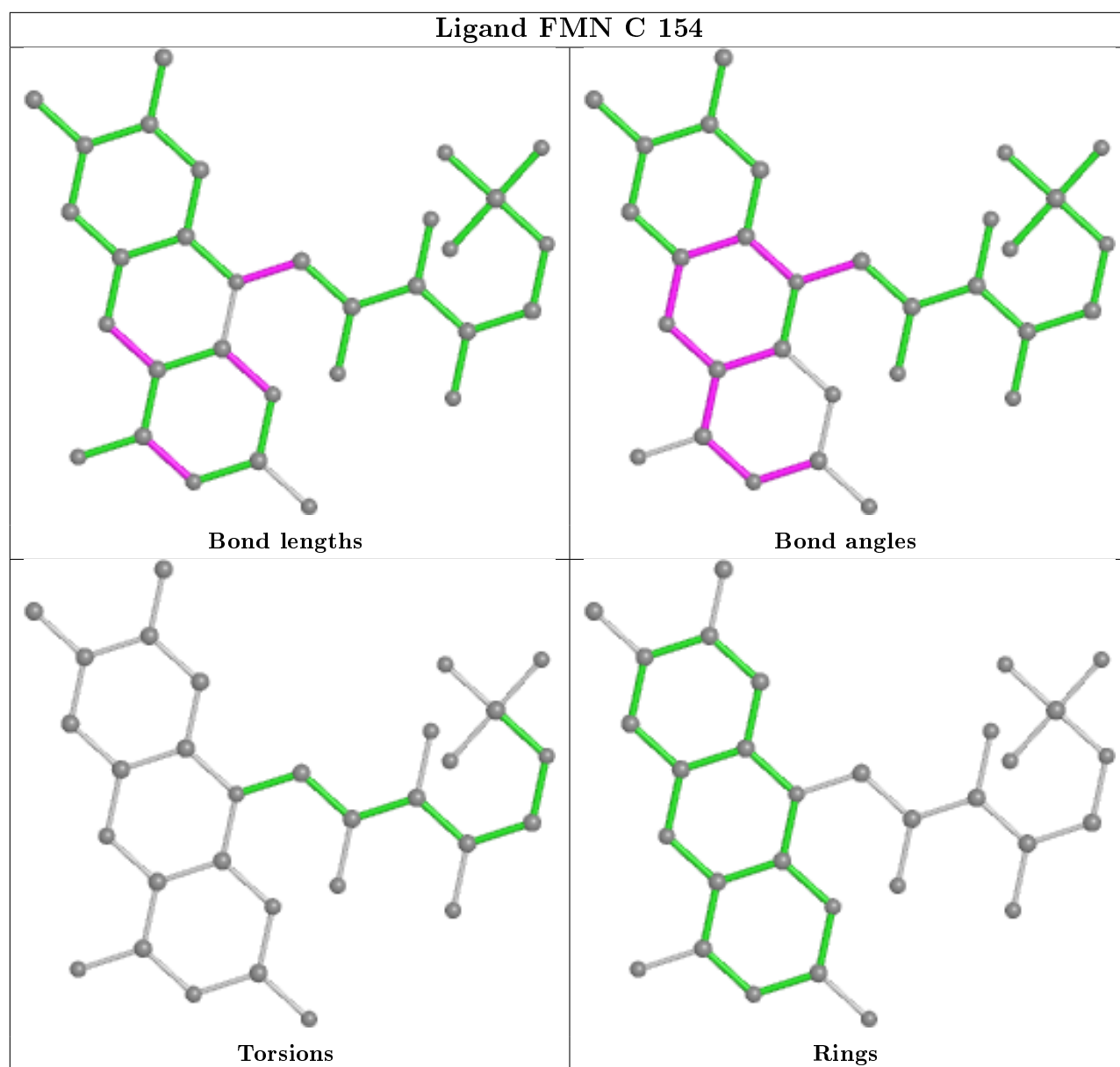


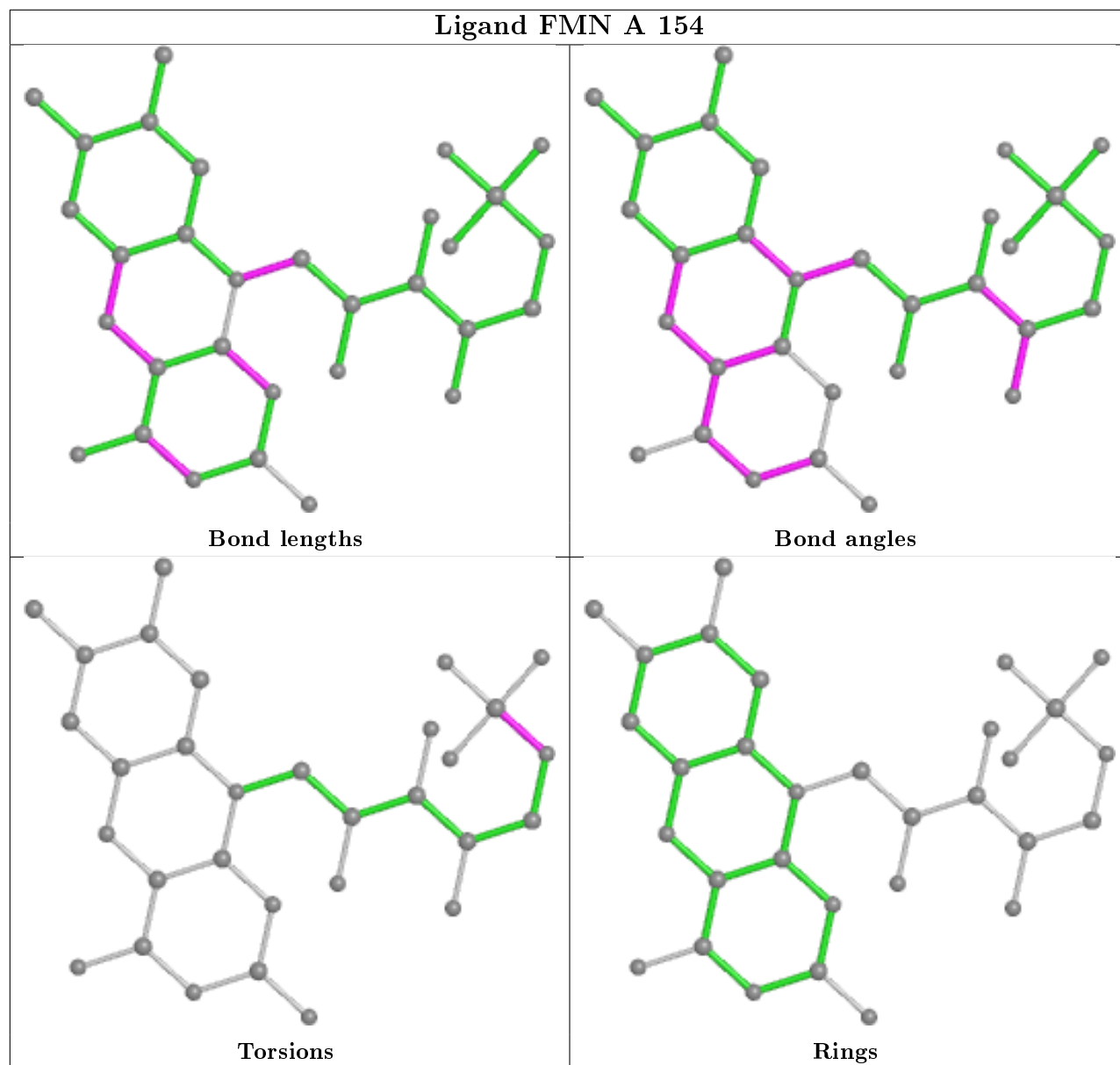


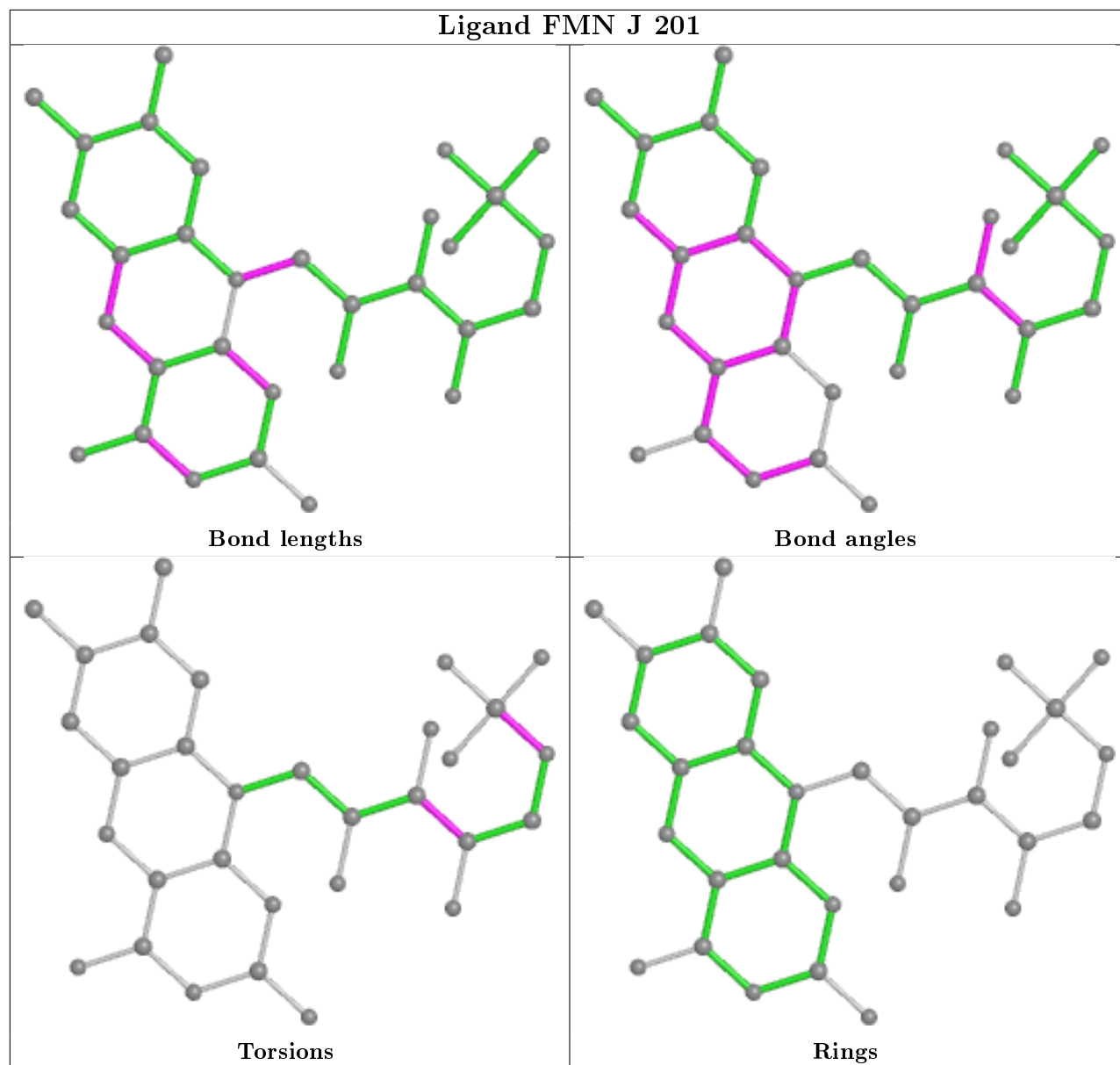


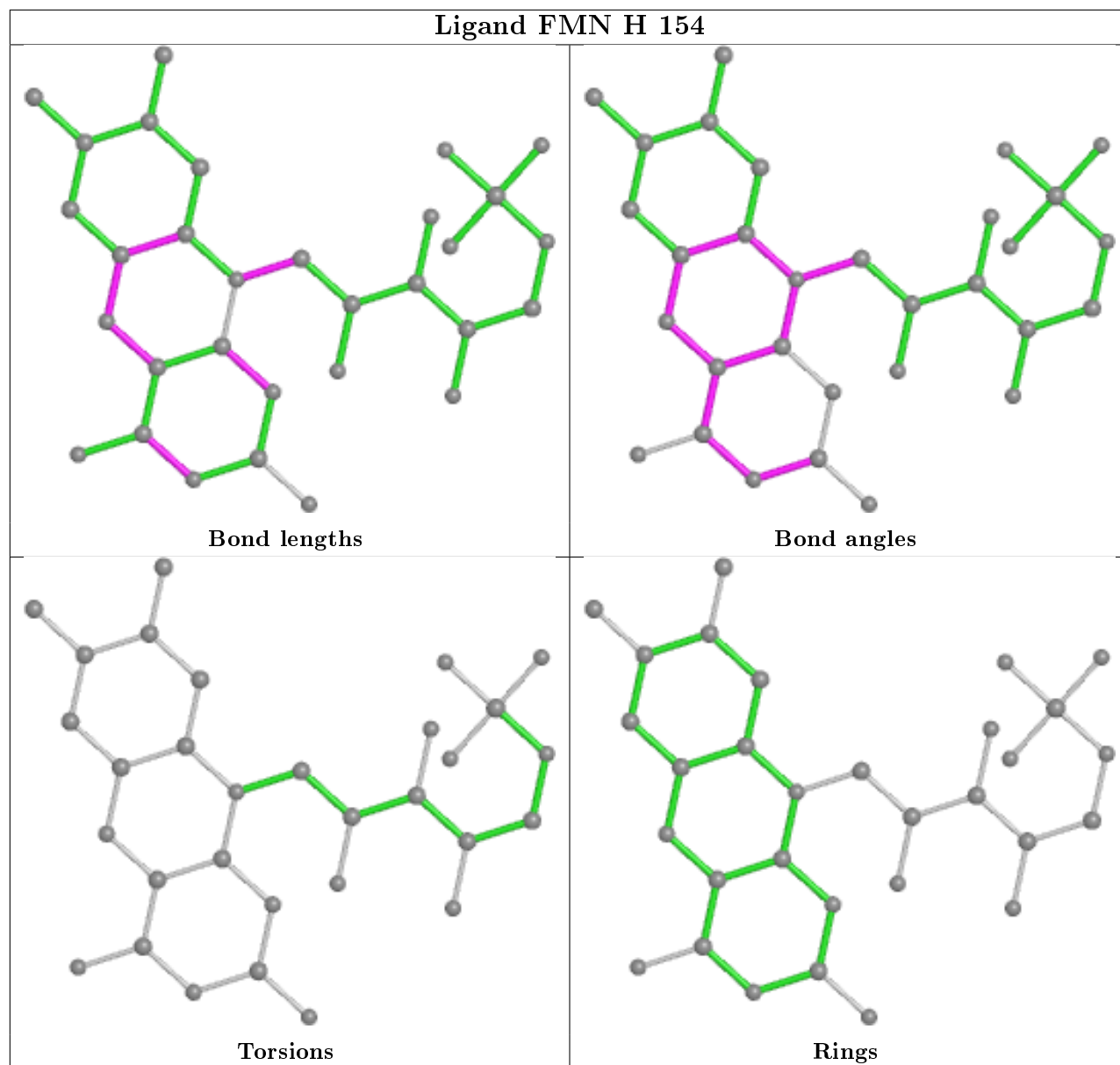


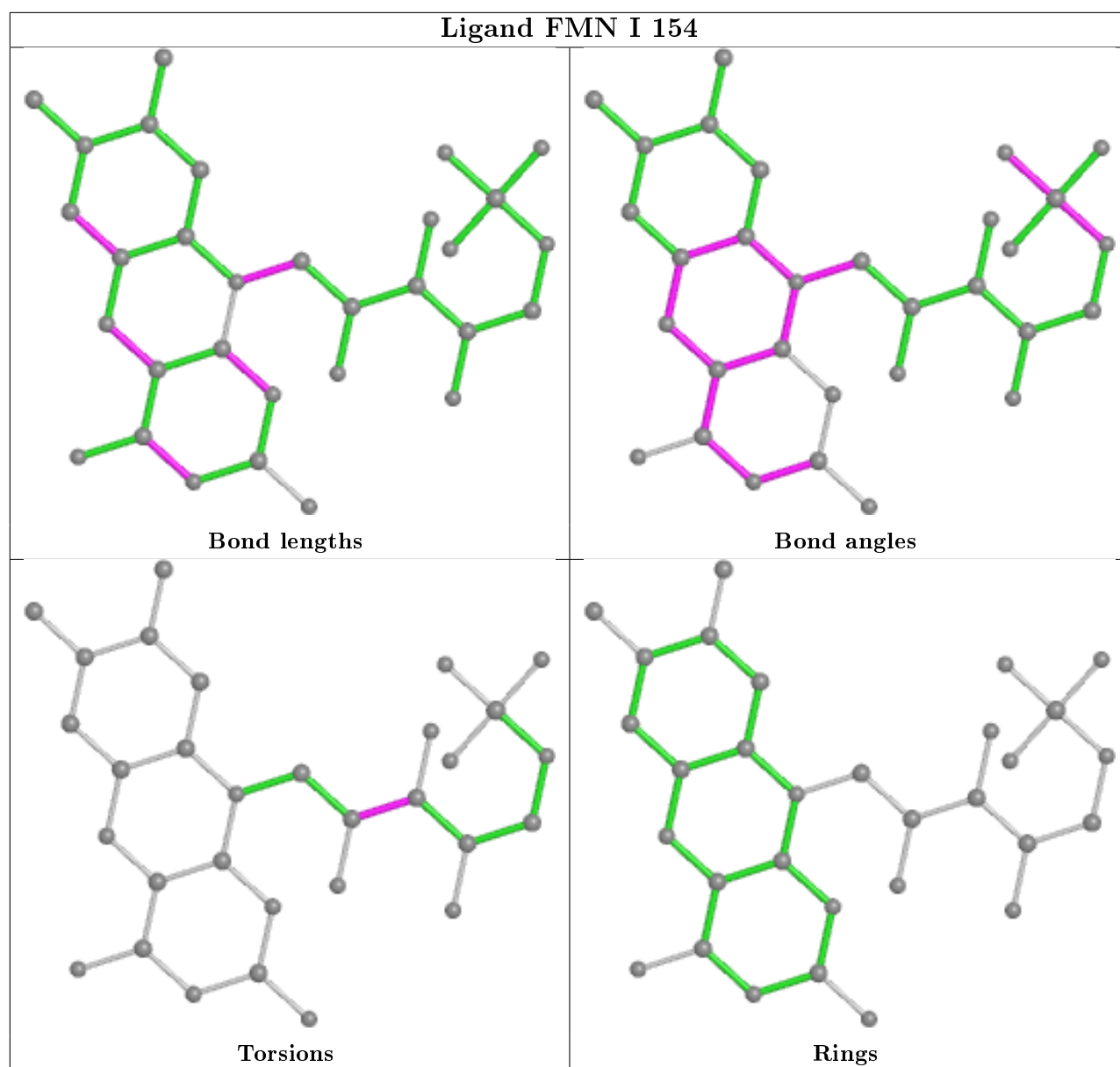












5.7 Other polymers [i](#)

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	150/153 (98%)	0.86	17 (11%) 5 6	32, 41, 47, 57	0
1	B	140/153 (91%)	1.30	29 (20%) 1 1	36, 42, 51, 64	0
1	C	136/153 (88%)	1.20	26 (19%) 1 1	35, 42, 50, 63	0
1	D	147/153 (96%)	1.26	26 (17%) 1 1	36, 42, 48, 55	0
1	E	141/153 (92%)	0.82	16 (11%) 5 6	35, 42, 48, 65	0
1	F	140/153 (91%)	1.03	16 (11%) 5 6	35, 41, 47, 68	0
1	G	139/153 (90%)	0.99	21 (15%) 2 3	37, 42, 47, 64	0
1	H	141/153 (92%)	1.06	19 (13%) 3 4	36, 42, 48, 64	0
1	I	142/153 (92%)	1.11	21 (14%) 2 3	36, 42, 50, 70	0
1	J	139/153 (90%)	1.16	22 (15%) 2 2	36, 42, 50, 66	0
All	All	1415/1530 (92%)	1.08	213 (15%) 2 3	32, 42, 49, 70	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	THR	9.7
1	F	104	LEU	7.5
1	F	103	ASP	7.1
1	B	101	VAL	7.0
1	H	21	PRO	5.8
1	B	18	ASN	5.6
1	B	140	ALA	5.5
1	J	104	LEU	5.5
1	H	104	LEU	5.4
1	F	30	SER	5.4
1	I	22	GLN	5.3
1	D	104	LEU	5.3
1	J	103	ASP	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	105	SER	5.2
1	C	22	GLN	5.0
1	I	145	LEU	4.9
1	J	106	THR	4.8
1	B	21	PRO	4.8
1	C	18	ASN	4.7
1	B	104	LEU	4.7
1	G	30	SER	4.6
1	F	106	THR	4.6
1	B	107	GLU	4.5
1	H	20	GLN	4.5
1	B	142	ILE	4.4
1	I	30	SER	4.4
1	F	26	ASP	4.1
1	J	102	ASN	4.1
1	J	105	SER	4.1
1	I	26	ASP	4.0
1	B	105	SER	4.0
1	E	103	ASP	4.0
1	D	52	LEU	4.0
1	B	22	GLN	4.0
1	E	128	ASP	4.0
1	H	106	THR	4.0
1	E	104	LEU	4.0
1	B	102	ASN	4.0
1	I	21	PRO	3.9
1	D	107	GLU	3.9
1	J	107	GLU	3.9
1	D	9	LEU	3.9
1	I	31	SER	3.8
1	F	142	ILE	3.8
1	A	52	LEU	3.8
1	G	18	ASN	3.7
1	I	18	ASN	3.6
1	F	107	GLU	3.6
1	E	21	PRO	3.6
1	I	23	ASP	3.6
1	F	31	SER	3.6
1	G	66	TYR	3.6
1	D	55	LEU	3.6
1	B	111	THR	3.5
1	E	4	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	50	ALA	3.5
1	G	103	ASP	3.5
1	H	18	ASN	3.5
1	D	81	ILE	3.4
1	A	18	ASN	3.4
1	E	94	TRP	3.4
1	C	21	PRO	3.3
1	H	103	ASP	3.3
1	G	9	LEU	3.3
1	H	30	SER	3.3
1	H	64	GLU	3.3
1	G	26	ASP	3.3
1	C	83	CYS	3.2
1	E	143	TYR	3.2
1	D	150	PHE	3.2
1	G	55	LEU	3.2
1	J	93	VAL	3.2
1	D	122	LEU	3.1
1	C	30	SER	3.1
1	F	141	LYS	3.1
1	B	143	TYR	3.1
1	D	10	ILE	3.1
1	D	91	PHE	3.1
1	G	141	LYS	3.1
1	D	43	LEU	3.0
1	J	141	LYS	3.0
1	F	23	ASP	3.0
1	E	84	MET	2.9
1	G	52	LEU	2.9
1	B	26	ASP	2.9
1	D	54	VAL	2.9
1	C	10	ILE	2.9
1	D	66	TYR	2.9
1	E	106	THR	2.9
1	J	9	LEU	2.9
1	I	20	GLN	2.9
1	D	83	CYS	2.9
1	D	80	ILE	2.8
1	E	142	ILE	2.8
1	H	66	TYR	2.8
1	J	100	THR	2.8
1	G	10	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	11	TYR	2.8
1	C	33	ARG	2.8
1	B	31	SER	2.8
1	D	18	ASN	2.8
1	J	66	TYR	2.7
1	J	110	LYS	2.7
1	C	106	THR	2.7
1	D	103	ASP	2.7
1	D	142	ILE	2.7
1	I	142	ILE	2.7
1	J	62	VAL	2.7
1	D	51	PHE	2.7
1	A	23	ASP	2.6
1	D	135	PHE	2.6
1	H	130	GLU	2.6
1	G	23	ASP	2.6
1	H	9	LEU	2.6
1	C	62	VAL	2.6
1	C	80	ILE	2.5
1	G	142	ILE	2.5
1	A	26	ASP	2.5
1	F	64	GLU	2.5
1	A	135	PHE	2.5
1	C	93	VAL	2.5
1	J	144	GLU	2.5
1	B	141	LYS	2.5
1	G	57	GLY	2.5
1	B	5	SER	2.4
1	I	125	SER	2.4
1	A	153	LEU	2.4
1	C	29	GLU	2.4
1	E	144	GLU	2.4
1	F	16	ILE	2.4
1	B	23	ASP	2.4
1	B	76	HIS	2.4
1	B	55	LEU	2.4
1	I	28	LEU	2.4
1	C	94	TRP	2.4
1	A	31	SER	2.4
1	B	30	SER	2.4
1	C	111	THR	2.4
1	H	80	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	52	LEU	2.3
1	H	143	TYR	2.3
1	G	126	ALA	2.3
1	I	29	GLU	2.3
1	A	80	ILE	2.3
1	J	55	LEU	2.3
1	E	130	GLU	2.3
1	B	128	ASP	2.3
1	A	132	CYS	2.3
1	D	92	GLU	2.3
1	C	7	TYR	2.3
1	C	28	LEU	2.3
1	G	99	ILE	2.3
1	H	111	THR	2.3
1	B	15	GLY	2.3
1	F	34	ASN	2.3
1	H	29	GLU	2.3
1	I	143	TYR	2.2
1	I	10	ILE	2.2
1	H	55	LEU	2.2
1	C	144	GLU	2.2
1	G	21	PRO	2.2
1	C	99	ILE	2.2
1	J	130	GLU	2.2
1	A	98	ALA	2.2
1	A	51	PHE	2.2
1	J	64	GLU	2.2
1	C	20	GLN	2.2
1	B	110	LYS	2.2
1	C	27	ILE	2.2
1	D	136	LEU	2.2
1	D	101	VAL	2.2
1	J	51	PHE	2.2
1	A	64	GLU	2.2
1	A	122	LEU	2.2
1	A	136	LEU	2.2
1	G	104	LEU	2.2
1	I	104	LEU	2.2
1	C	63	ASN	2.2
1	F	4	MET	2.2
1	J	96	MET	2.2
1	H	22	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	19	LEU	2.1
1	B	29	GLU	2.1
1	C	110	LYS	2.1
1	B	9	LEU	2.1
1	H	83	CYS	2.1
1	E	30	SER	2.1
1	D	40	ILE	2.1
1	I	80	ILE	2.1
1	A	29	GLU	2.1
1	G	83	CYS	2.1
1	E	108	GLN	2.1
1	J	44	LEU	2.1
1	A	139	ILE	2.1
1	B	37	ALA	2.1
1	E	126	ALA	2.1
1	D	147	ASP	2.0
1	E	137	LEU	2.0
1	H	137	LEU	2.0
1	B	100	THR	2.0
1	I	25	LYS	2.0
1	I	37	ALA	2.0
1	C	66	TYR	2.0
1	A	10	ILE	2.0
1	I	83	CYS	2.0
1	C	55	LEU	2.0
1	I	6	LEU	2.0
1	J	81	ILE	2.0
1	G	65	THR	2.0
1	F	87	ARG	2.0
1	G	80	ILE	2.0
1	G	139	ILE	2.0
1	F	33	ARG	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 carbohydrates in this entry.

6.4 Ligands ⓘ

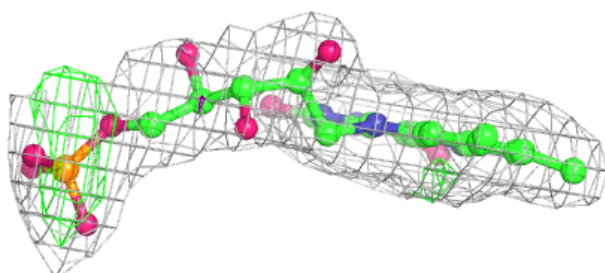
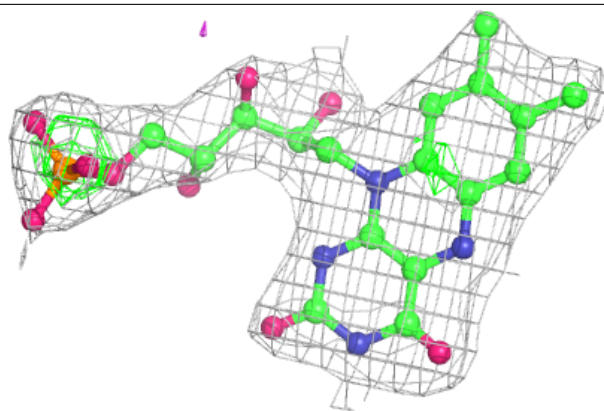
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMN	I	154	31/31	0.81	0.17	41,45,54,57	5
2	FMN	G	154	31/31	0.85	0.18	34,36,48,48	5
2	FMN	E	154	31/31	0.85	0.17	30,37,51,52	5
2	FMN	B	154	31/31	0.85	0.20	33,35,48,51	5
2	FMN	A	154	31/31	0.85	0.15	26,29,39,44	5
2	FMN	F	154	31/31	0.85	0.14	39,41,51,52	5
2	FMN	C	154	31/31	0.90	0.15	26,29,43,45	5
2	FMN	J	201	31/31	0.91	0.18	31,35,37,41	5
2	FMN	H	154	31/31	0.91	0.16	35,36,43,50	5
2	FMN	D	154	31/31	0.91	0.15	17,23,36,40	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.

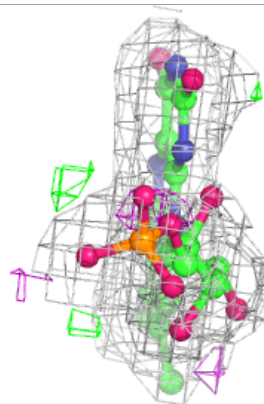
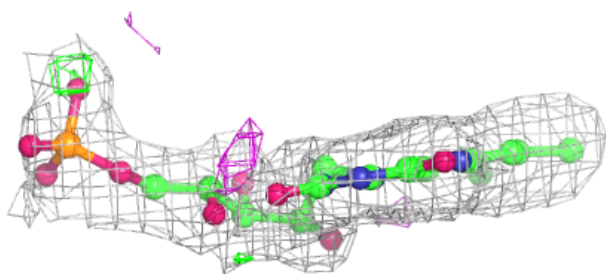
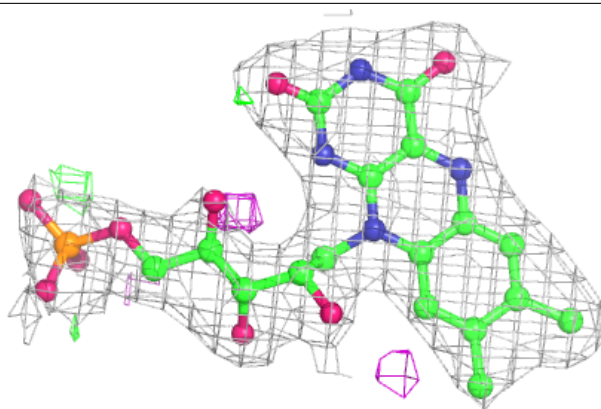
Electron density around FMN I 154:

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

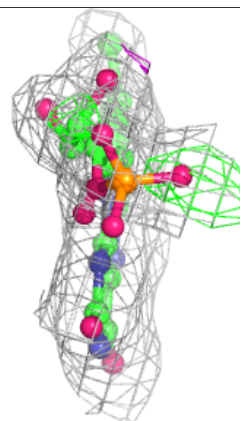
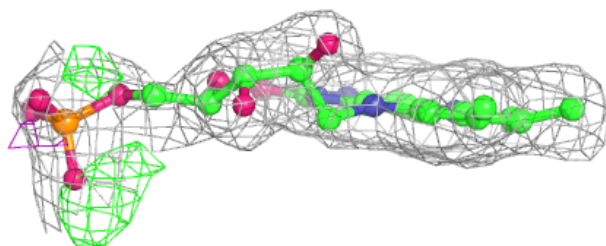
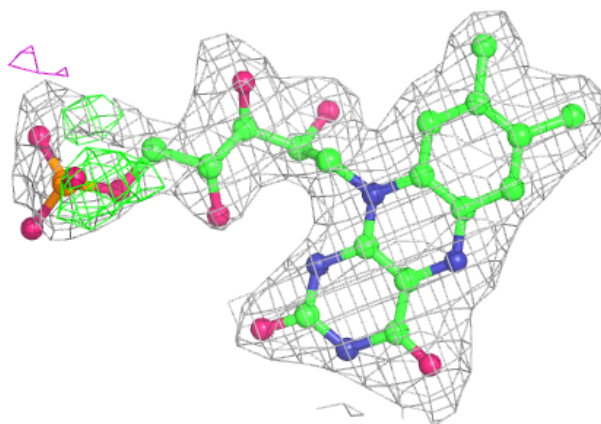


Electron density around FMN G 154:

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

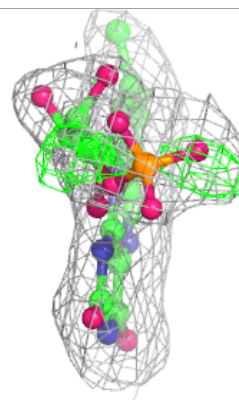
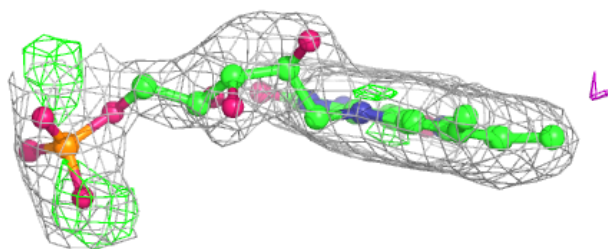
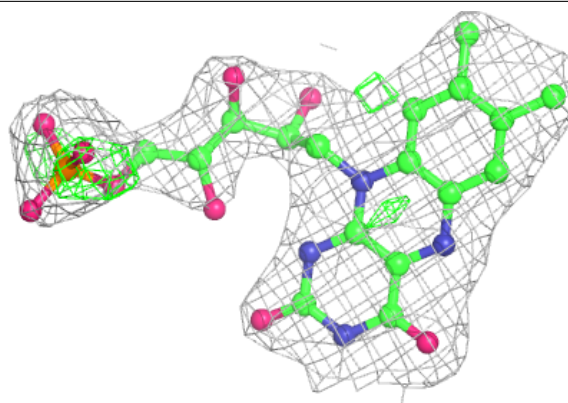
**Electron density around FMN E 154:**

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

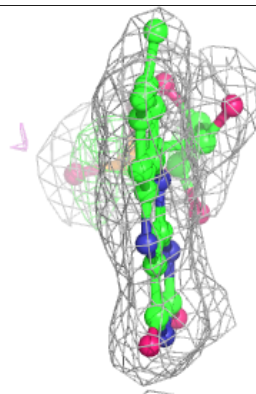
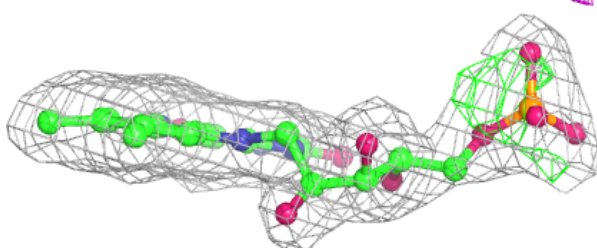
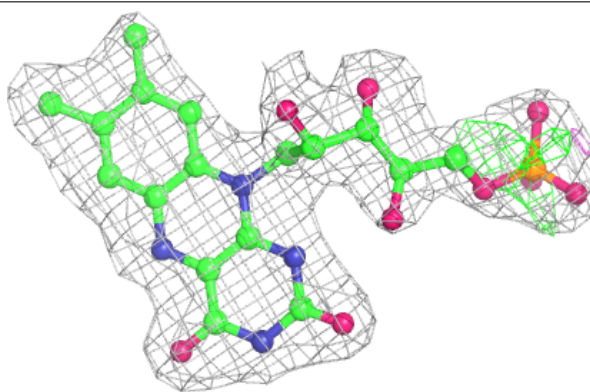


Electron density around FMN B 154:

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

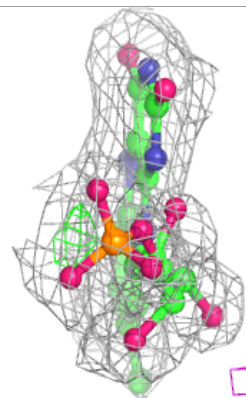
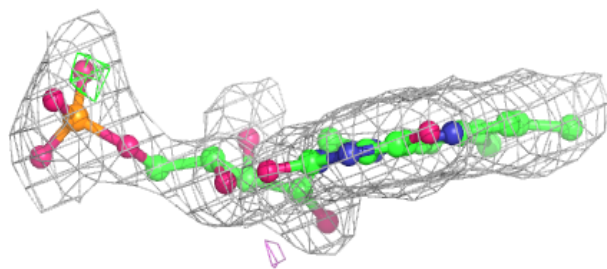
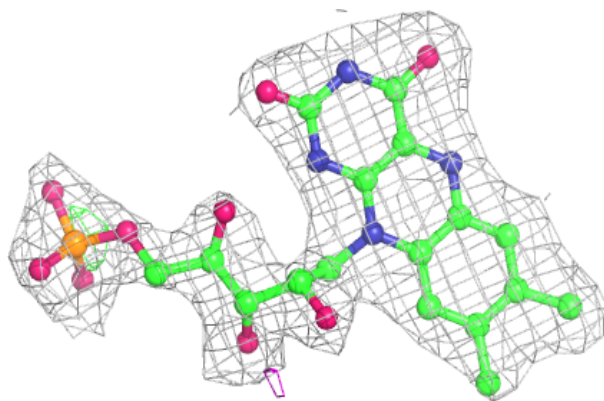
**Electron density around FMN A 154:**

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

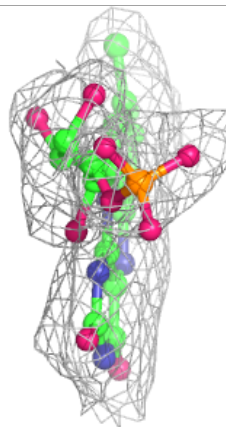
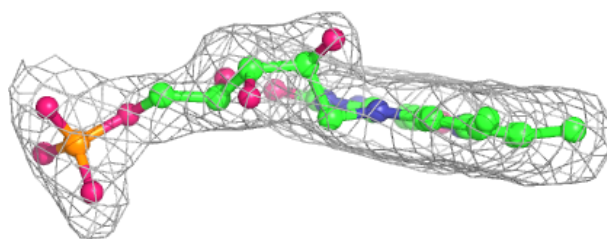
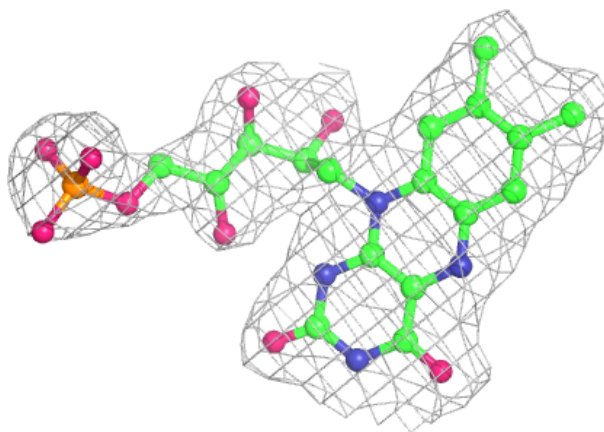


Electron density around FMN F 154:

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

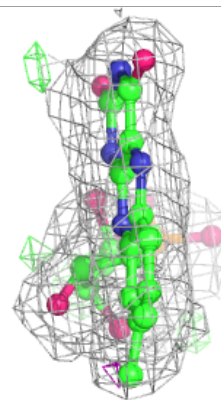
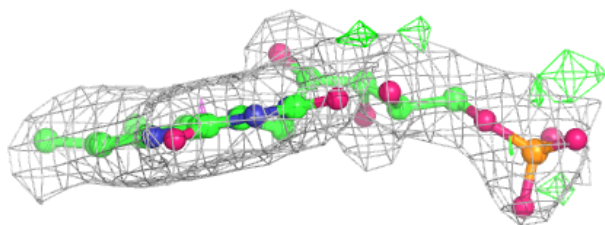
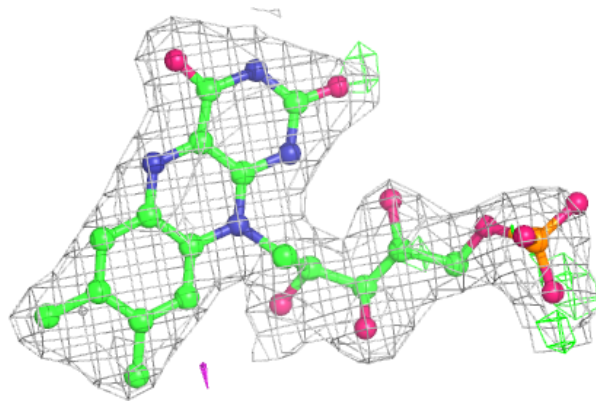
**Electron density around FMN C 154:**

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

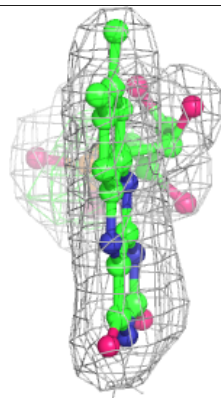
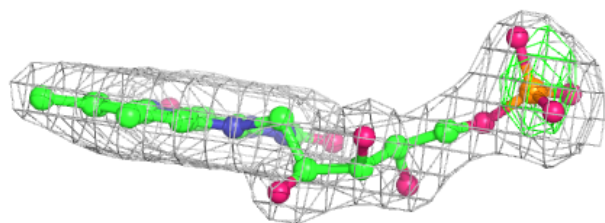
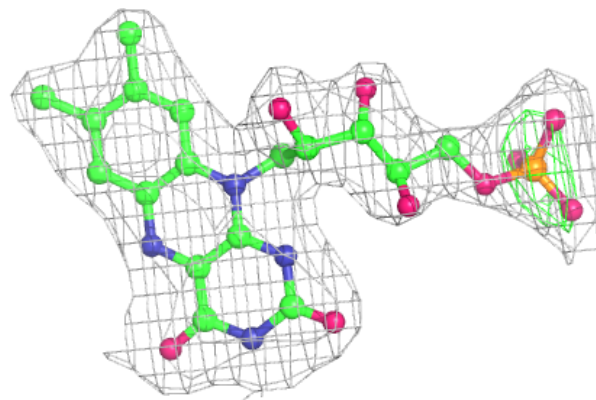


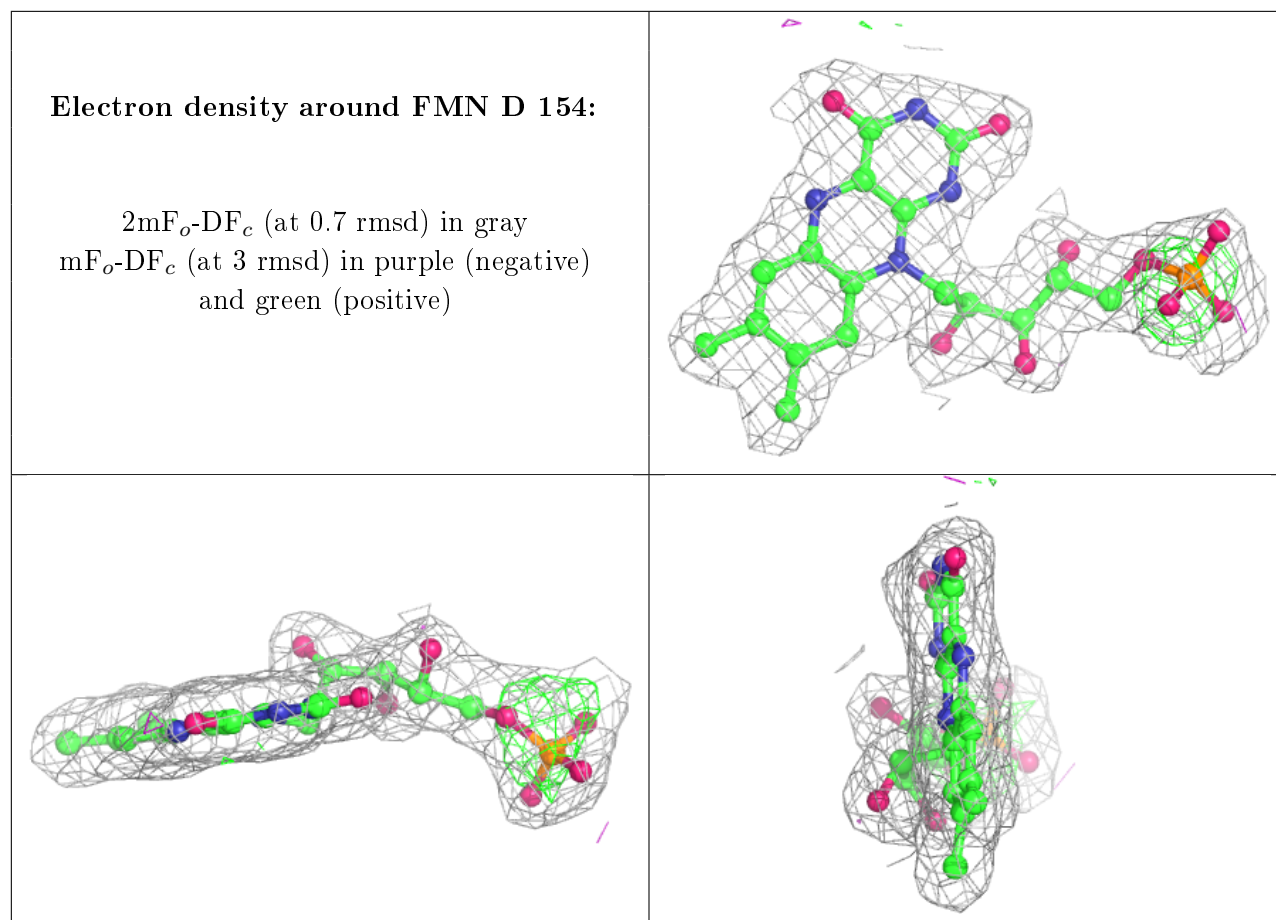
Electron density around FMN J 201:

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

**Electron density around FMN H 154:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.