



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2020 – 05:45 am BST

PDB ID : 6ODE
Title : Crystal Structure of Mycobacterium tuberculosis Proteasome in Complex with Phenylimidazole-based Inhibitor B6
Authors : Hsu, H.C.; Li, H.
Deposited on : 2019-03-26
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

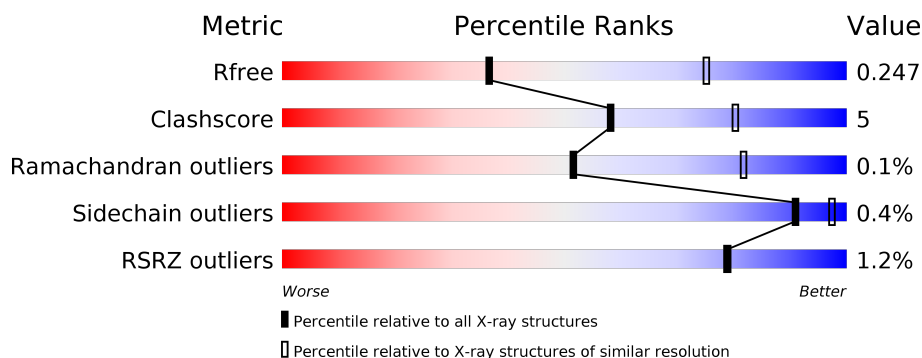
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	240	<div> <div></div> <div>73%18%9%</div> </div>
1	B	240	<div> <div>4%</div> <div>76%14%10%</div> </div>
1	C	240	<div> <div>5%</div> <div>66%23%10%</div> </div>
1	D	240	<div> <div>2%</div> <div>72%17%11%</div> </div>
1	E	240	<div> <div>%</div> <div>73%17%10%</div> </div>
1	F	240	<div> <div>%</div> <div>73%16%11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	240	
1	O	240	
1	P	240	
1	Q	240	
1	R	240	
1	S	240	
1	T	240	
1	U	240	
2	H	234	
2	I	234	
2	J	234	
2	K	234	
2	L	234	
2	M	234	
2	N	234	
2	V	234	
2	W	234	
2	X	234	
2	Y	234	
2	Z	234	
2	a	234	
2	b	234	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47311 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	B	215	Total	C	N	O	S	0	0	0
			1660	1041	303	312	4			
1	C	216	Total	C	N	O	S	0	0	0
			1664	1043	304	313	4			
1	D	214	Total	C	N	O	S	0	0	0
			1649	1032	302	311	4			
1	E	217	Total	C	N	O	S	0	0	0
			1671	1047	305	315	4			
1	F	214	Total	C	N	O	S	0	0	0
			1653	1036	302	311	4			
1	G	216	Total	C	N	O	S	0	0	0
			1662	1040	304	314	4			
1	O	216	Total	C	N	O	S	0	0	0
			1664	1042	304	314	4			
1	P	219	Total	C	N	O	S	0	0	0
			1685	1054	307	320	4			
1	Q	215	Total	C	N	O	S	0	0	0
			1660	1041	303	312	4			
1	R	215	Total	C	N	O	S	0	0	0
			1657	1038	303	312	4			
1	S	218	Total	C	N	O	S	0	0	0
			1678	1050	306	318	4			
1	T	217	Total	C	N	O	S	0	0	0
			1671	1047	305	315	4			
1	U	216	Total	C	N	O	S	0	0	0
			1664	1043	304	313	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP P9WHU1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	initiating methionine	UNP P9WHU1
C	9	MET	-	initiating methionine	UNP P9WHU1
D	9	MET	-	initiating methionine	UNP P9WHU1
E	9	MET	-	initiating methionine	UNP P9WHU1
F	9	MET	-	initiating methionine	UNP P9WHU1
G	9	MET	-	initiating methionine	UNP P9WHU1
O	9	MET	-	initiating methionine	UNP P9WHU1
P	9	MET	-	initiating methionine	UNP P9WHU1
Q	9	MET	-	initiating methionine	UNP P9WHU1
R	9	MET	-	initiating methionine	UNP P9WHU1
S	9	MET	-	initiating methionine	UNP P9WHU1
T	9	MET	-	initiating methionine	UNP P9WHU1
U	9	MET	-	initiating methionine	UNP P9WHU1

- Molecule 2 is a protein called Proteasome subunit beta.

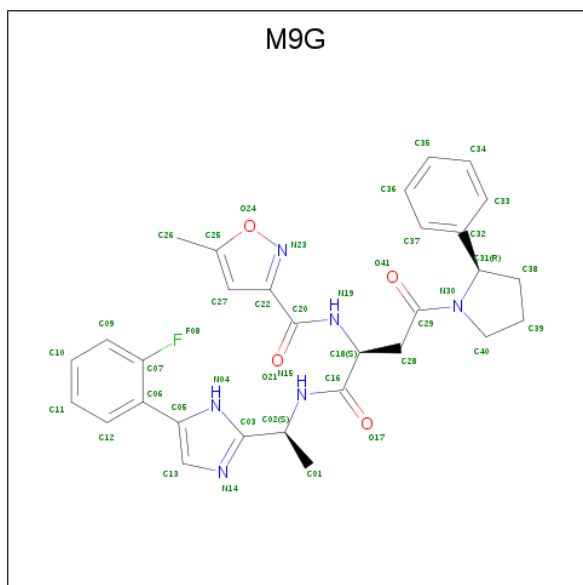
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	I	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	J	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	K	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	L	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	M	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	N	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	V	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	W	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	X	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	Y	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	Z	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	a	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	b	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			

- Molecule 3 is N-{(2S)-1-((1S)-1-[5-(2-fluorophenyl)-1H-imidazol-2-yl]ethyl)amino)-1,4-dioxo-4-[(2R)-2-phenylpyrrolidin-1-yl]butan-2-yl}-5-methyl-1,2-oxazole-3-carboxamide (three-letter code: M9G) (formula: C₃₀H₃₁FN₆O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	F	N	O	0	0
			41	30	1	6	4		
3	I	1	Total	C	F	N	O	0	0
			41	30	1	6	4		
3	J	1	Total	C	F	N	O	0	0
			41	30	1	6	4		
3	L	1	Total	C	F	N	O	0	0
			41	30	1	6	4		
3	L	1	Total	C	F	N	O	0	0
			41	30	1	6	4		
3	M	1	Total	C	F	N	O	0	0
			41	30	1	6	4		
3	N	1	Total	C	F	N	O	0	0
			41	30	1	6	4		
3	V	1	Total	C	F	N	O	0	0
			41	30	1	6	4		
3	W	1	Total	C	F	N	O	0	0
			41	30	1	6	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	X	1	Total 41	C 30	F 1	N 6	O 4	0	0
3	Y	1	Total 41	C 30	F 1	N 6	O 4	0	0
3	Z	1	Total 41	C 30	F 1	N 6	O 4	0	0
3	a	1	Total 41	C 30	F 1	N 6	O 4	0	0
3	b	1	Total 41	C 30	F 1	N 6	O 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total 15	O 15	0	0
4	B	11	Total 11	O 11	0	0
4	C	10	Total 10	O 10	0	0
4	D	6	Total 6	O 6	0	0
4	E	6	Total 6	O 6	0	0
4	F	9	Total 9	O 9	0	0
4	G	11	Total 11	O 11	0	0
4	H	14	Total 14	O 14	0	0
4	I	21	Total 21	O 21	0	0
4	J	28	Total 28	O 28	0	0
4	K	20	Total 20	O 20	0	0
4	L	24	Total 24	O 24	0	0
4	M	20	Total 20	O 20	0	0
4	N	22	Total 22	O 22	0	0

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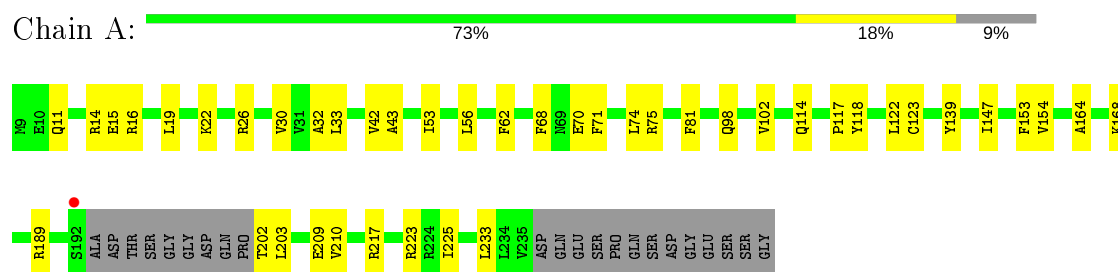
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	7	Total 7	O 7	0	0
4	P	11	Total 11	O 11	0	0
4	Q	15	Total 15	O 15	0	0
4	R	15	Total 15	O 15	0	0
4	S	10	Total 10	O 10	0	0
4	T	12	Total 12	O 12	0	0
4	U	11	Total 11	O 11	0	0
4	V	27	Total 27	O 27	0	0
4	W	21	Total 21	O 21	0	0
4	X	27	Total 27	O 27	0	0
4	Y	23	Total 23	O 23	0	0
4	Z	23	Total 23	O 23	0	0
4	a	16	Total 16	O 16	0	0
4	b	19	Total 19	O 19	0	0

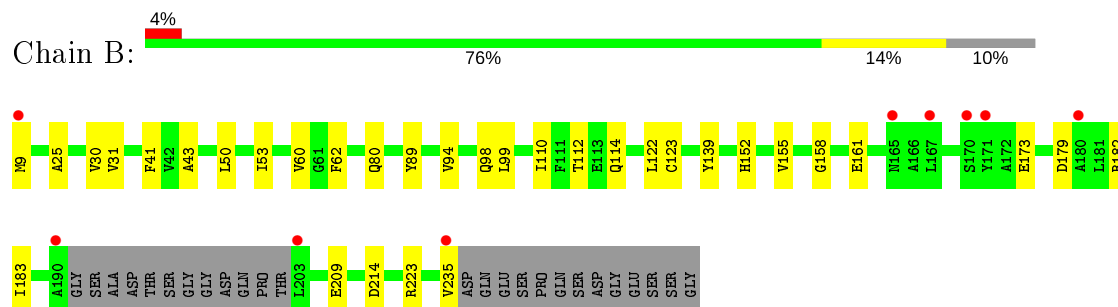
3 Residue-property plots [i](#)

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.

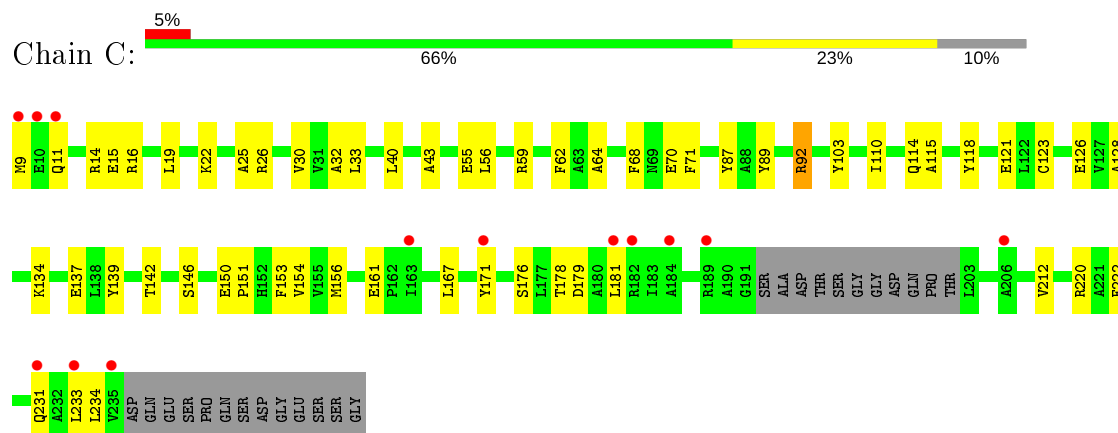
- Molecule 1: Proteasome subunit alpha



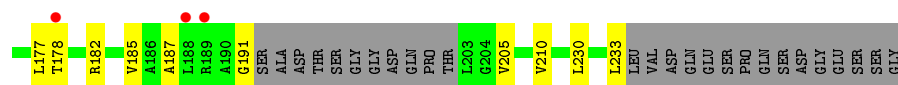
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



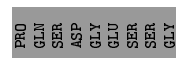
- Chain E:
-
- | Category | Percentage |
|----------|------------|
| M9 | 73% |
| E10 | 73% |
| Q11 | 73% |
| E15 | 73% |
| L33 | 73% |
| V42 | 73% |
| S54 | 73% |
| E55 | 73% |
| L56 | 73% |
| Y57 | 73% |
| D68 | 73% |
| R59 | 73% |
| V60 | 73% |
| F68 | 73% |
| F71 | 73% |
| D72 | 73% |
| M73 | 73% |
| L74 | 73% |
| R75 | 73% |
| R76 | 73% |
| D83 | 73% |
| Y89 | 73% |
| D90 | 73% |
| R91 | 73% |
| R92 | 73% |
| E121 | 73% |
| L122 | 73% |
| C123 | 73% |
| Y139 | 73% |
| E150 | 73% |
| F153 | 73% |
| V154 | 73% |
| M155 | 73% |
| A164 | 73% |
| L167 | 73% |
| K168 | 73% |
| E169 | 17% |
| S170 | 17% |
| D179 | 17% |
| I183 | 17% |
| A184 | 17% |
| L188 | 17% |

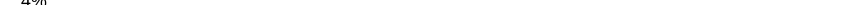


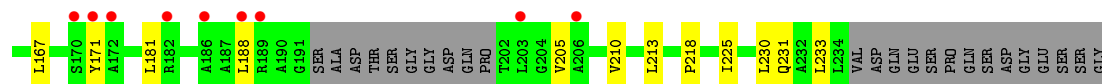
- Chain F:
-
- | Category | Percentage |
|----------|------------|
| Green | 73% |
| Yellow | 16% |
| Grey | 11% |
- Legend: %
- Labels: E9, E15, R16, S17, E18, R21, V31, A32, L33, I53, L56, F68, M69, E70, F71, L74, R91, R97, Q98, L99, I110, Q114, A115, K116, P117, L122, C123, Y139, E150, V154, V155, E161, P162, I163, A164, N165, A166, L167, K168, A172, S176



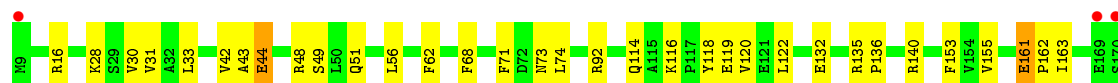
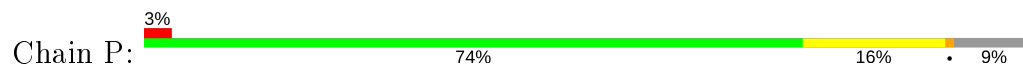
- Chain G:
-
- | Amino Acid | Percentage |
|------------|------------|
| M9 | ~1% |
| V30 | ~1% |
| L33 | ~1% |
| A43 | ~1% |
| I56 | ~1% |
| F62 | ~1% |
| F68 | ~1% |
| F71 | ~1% |
| Y89 | ~1% |
| R92 | ~1% |
| K134 | ~1% |
| E137 | ~1% |
| R140 | ~1% |
| F153 | ~1% |
| V154 | ~1% |
| L181 | ~1% |
| V185 | ~1% |
| S192 | ~1% |
| A194 | ~1% |
| ASP | ~1% |
| THR | ~1% |
| SER | ~1% |
| GLY | ~1% |
| GLY | ~1% |
| ASP | ~1% |
| ASP | ~1% |
| GLN | ~1% |
| PRO | ~1% |
| THR | ~1% |
| THR | ~1% |
| LEU | ~1% |
| L204 | ~1% |
| V205 | ~1% |
| R217 | ~1% |
| L230 | ~1% |
| Q231 | ~1% |
| Q232 | ~1% |
| L233 | ~1% |
| L234 | ~1% |
| V235 | ~1% |
| ASP | ~1% |
| GLN | ~1% |
| GLU | ~1% |
| SER | ~1% |



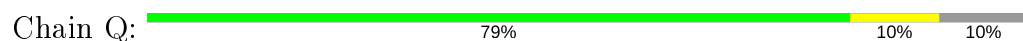
- Chain O: 



- Molecule 1: Proteasome subunit alpha



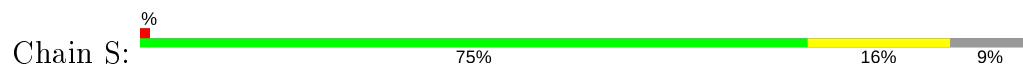
- Molecule 1: Proteasome subunit alpha



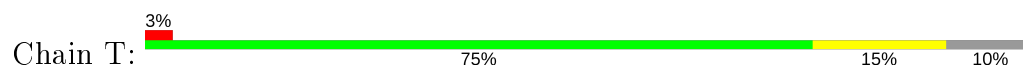
- Molecule 1: Proteasome subunit alpha

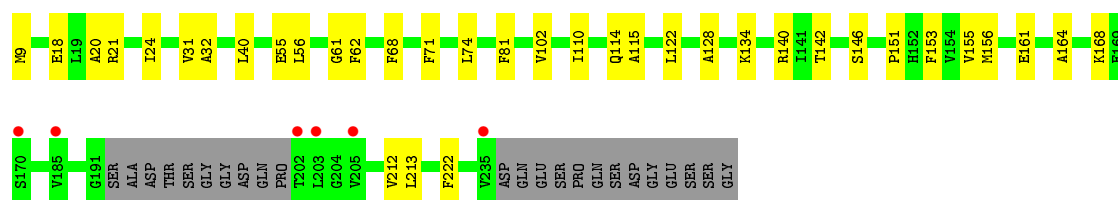


- Molecule 1: Proteasome subunit alpha

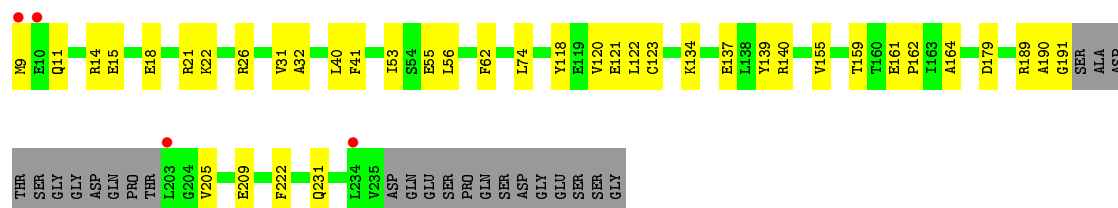
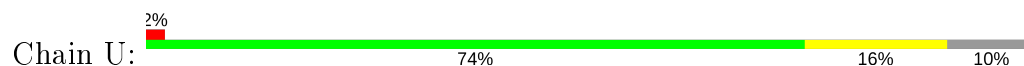


- Molecule 1: Proteasome subunit alpha

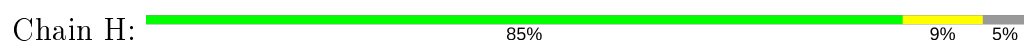




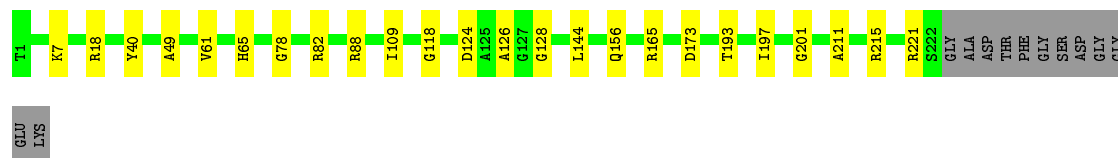
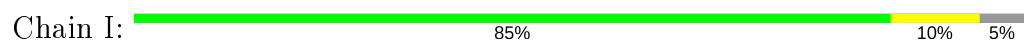
- Molecule 1: Proteasome subunit alpha



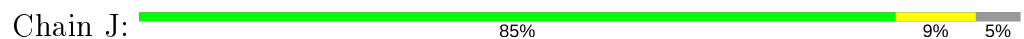
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta




- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta




- Molecule 2: Proteasome subunit beta

Chain L:  89% 6% 5%



- Molecule 2: Proteasome subunit beta

Chain M:  88% 7% 5%



- Molecule 2: Proteasome subunit beta

Chain N:  89% 6% 5%



- Molecule 2: Proteasome subunit beta

Chain V:  90% 6% 5%




- Molecule 2: Proteasome subunit beta

Chain W:  92% 5% 5%




- Molecule 2: Proteasome subunit beta

Chain X:  86% 9% 5%




- Molecule 2: Proteasome subunit beta

Chain Y:  88% 8% 5%



- Molecule 2: Proteasome subunit beta

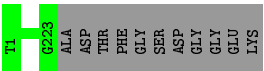
Chain Z:  90% 5% 5%



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.60Å 198.38Å 166.51Å 90.00° 103.10° 90.00°	Depositor
Resolution (Å)	53.97 – 2.90 53.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (53.97-2.90) 99.9 (53.97-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.197 , 0.247 0.197 , 0.247	Depositor DCC
R_{free} test set	8403 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	47311	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: M9G

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	0.26	0/1701	0.45	0/2297
1	B	0.25	0/1684	0.44	0/2274
1	C	0.26	0/1688	0.46	0/2279
1	D	0.25	0/1673	0.46	0/2258
1	E	0.25	0/1695	0.45	0/2289
1	F	0.33	0/1677	0.49	0/2264
1	G	0.25	0/1686	0.44	0/2276
1	O	0.27	0/1688	0.45	0/2279
1	P	0.28	0/1709	0.46	0/2308
1	Q	0.26	0/1684	0.44	0/2274
1	R	0.36	0/1681	0.47	0/2269
1	S	0.25	0/1702	0.45	0/2298
1	T	0.25	0/1695	0.45	0/2289
1	U	0.25	0/1688	0.44	0/2279
2	H	0.26	0/1662	0.47	0/2254
2	I	0.26	0/1662	0.47	0/2254
2	J	0.25	0/1662	0.45	0/2254
2	K	0.26	0/1666	0.46	0/2259
2	L	0.26	0/1666	0.46	0/2259
2	M	0.25	0/1662	0.45	0/2254
2	N	0.26	0/1666	0.46	0/2259
2	V	0.26	0/1666	0.46	0/2259
2	W	0.25	0/1666	0.47	0/2259
2	X	0.25	0/1662	0.46	0/2254
2	Y	0.26	0/1666	0.46	0/2259
2	Z	0.25	0/1666	0.46	0/2259
2	a	0.26	0/1666	0.47	0/2259
2	b	0.26	0/1666	0.46	0/2259
All	All	0.26	0/46955	0.46	0/63534

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1677	0	1680	26	0
1	B	1660	0	1665	23	0
1	C	1664	0	1668	41	0
1	D	1649	0	1648	30	0
1	E	1671	0	1675	28	0
1	F	1653	0	1656	23	0
1	G	1662	0	1662	12	0
1	O	1664	0	1666	31	0
1	P	1685	0	1684	27	0
1	Q	1660	0	1665	16	0
1	R	1657	0	1659	25	0
1	S	1678	0	1677	23	0
1	T	1671	0	1675	20	0
1	U	1664	0	1668	19	0
2	H	1638	0	1633	13	0
2	I	1638	0	1633	13	0
2	J	1638	0	1633	16	0
2	K	1642	0	1636	10	0
2	L	1642	0	1636	10	0
2	M	1638	0	1633	12	0
2	N	1642	0	1636	8	0
2	V	1642	0	1636	8	0
2	W	1642	0	1636	4	0
2	X	1638	0	1633	12	0
2	Y	1642	0	1636	11	0
2	Z	1642	0	1636	6	0
2	a	1642	0	1636	0	0
2	b	1642	0	1636	0	0
3	H	41	0	0	0	0
3	I	41	0	0	1	0
3	J	41	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	82	0	0	0	0
3	M	41	0	0	1	0
3	N	41	0	0	1	0
3	V	41	0	0	0	0
3	W	41	0	0	0	0
3	X	41	0	0	0	0
3	Y	41	0	0	0	0
3	Z	41	0	0	0	0
3	a	41	0	0	0	0
3	b	41	0	0	0	0
4	A	15	0	0	0	0
4	B	11	0	0	1	0
4	C	10	0	0	0	0
4	D	6	0	0	0	0
4	E	6	0	0	0	0
4	F	9	0	0	0	0
4	G	11	0	0	0	0
4	H	14	0	0	0	0
4	I	21	0	0	0	0
4	J	28	0	0	1	0
4	K	20	0	0	0	0
4	L	24	0	0	0	0
4	M	20	0	0	0	0
4	N	22	0	0	0	0
4	O	7	0	0	0	0
4	P	11	0	0	1	0
4	Q	15	0	0	0	0
4	R	15	0	0	1	0
4	S	10	0	0	1	0
4	T	12	0	0	0	0
4	U	11	0	0	0	0
4	V	27	0	0	0	0
4	W	21	0	0	0	0
4	X	27	0	0	0	0
4	Y	23	0	0	0	0
4	Z	23	0	0	0	0
4	a	16	0	0	0	0
4	b	19	0	0	0	0
All	All	47311	0	46237	424	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 5.

The worst 5 of 424 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:O:31:VAL:HG12	1:O:155:VAL:HG22	1.64	0.78
1:P:161:GLU:HG2	1:P:162:PRO:HD3	1.65	0.78
1:F:161:GLU:O	1:F:165:ASN:ND2	2.19	0.76
1:C:231:GLN:HA	1:C:234:LEU:HD12	1.68	0.75
1:S:110:ILE:HG23	1:S:114:GLN:HG3	1.69	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/240 (89%)	207 (97%)	7 (3%)	0	100	100
1	B	211/240 (88%)	202 (96%)	9 (4%)	0	100	100
1	C	212/240 (88%)	202 (95%)	10 (5%)	0	100	100
1	D	210/240 (88%)	199 (95%)	11 (5%)	0	100	100
1	E	213/240 (89%)	207 (97%)	6 (3%)	0	100	100
1	F	210/240 (88%)	207 (99%)	3 (1%)	0	100	100
1	G	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
1	O	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
1	P	215/240 (90%)	207 (96%)	8 (4%)	0	100	100
1	Q	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
1	R	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
1	S	214/240 (89%)	206 (96%)	8 (4%)	0	100	100
1	T	213/240 (89%)	205 (96%)	7 (3%)	1 (0%)	29	61
1	U	212/240 (88%)	202 (95%)	9 (4%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	220/234 (94%)	213 (97%)	7 (3%)	0	100	100
2	I	220/234 (94%)	215 (98%)	5 (2%)	0	100	100
2	J	220/234 (94%)	212 (96%)	8 (4%)	0	100	100
2	K	221/234 (94%)	216 (98%)	5 (2%)	0	100	100
2	L	221/234 (94%)	215 (97%)	6 (3%)	0	100	100
2	M	220/234 (94%)	214 (97%)	6 (3%)	0	100	100
2	N	221/234 (94%)	215 (97%)	6 (3%)	0	100	100
2	V	221/234 (94%)	219 (99%)	2 (1%)	0	100	100
2	W	221/234 (94%)	217 (98%)	4 (2%)	0	100	100
2	X	220/234 (94%)	215 (98%)	4 (2%)	1 (0%)	29	61
2	Y	221/234 (94%)	214 (97%)	7 (3%)	0	100	100
2	Z	221/234 (94%)	215 (97%)	5 (2%)	1 (0%)	29	61
2	a	221/234 (94%)	217 (98%)	3 (1%)	1 (0%)	29	61
2	b	221/234 (94%)	215 (97%)	6 (3%)	0	100	100
All	All	6059/6636 (91%)	5876 (97%)	178 (3%)	5 (0%)	51	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	190	ALA
1	T	151	PRO
2	a	9	PRO
2	Z	9	PRO
2	X	9	PRO

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	167/184 (91%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	165/184 (90%)	165 (100%)	0	100	100
1	C	165/184 (90%)	163 (99%)	2 (1%)	71	91
1	D	163/184 (89%)	163 (100%)	0	100	100
1	E	166/184 (90%)	165 (99%)	1 (1%)	86	96
1	F	164/184 (89%)	162 (99%)	2 (1%)	71	91
1	G	165/184 (90%)	165 (100%)	0	100	100
1	O	165/184 (90%)	164 (99%)	1 (1%)	86	96
1	P	168/184 (91%)	165 (98%)	3 (2%)	59	85
1	Q	165/184 (90%)	164 (99%)	1 (1%)	86	96
1	R	164/184 (89%)	164 (100%)	0	100	100
1	S	167/184 (91%)	167 (100%)	0	100	100
1	T	166/184 (90%)	165 (99%)	1 (1%)	86	96
1	U	165/184 (90%)	162 (98%)	3 (2%)	59	85
2	H	165/172 (96%)	165 (100%)	0	100	100
2	I	165/172 (96%)	165 (100%)	0	100	100
2	J	165/172 (96%)	165 (100%)	0	100	100
2	K	165/172 (96%)	163 (99%)	2 (1%)	71	91
2	L	165/172 (96%)	165 (100%)	0	100	100
2	M	165/172 (96%)	164 (99%)	1 (1%)	86	96
2	N	165/172 (96%)	165 (100%)	0	100	100
2	V	165/172 (96%)	165 (100%)	0	100	100
2	W	165/172 (96%)	165 (100%)	0	100	100
2	X	165/172 (96%)	165 (100%)	0	100	100
2	Y	165/172 (96%)	165 (100%)	0	100	100
2	Z	165/172 (96%)	164 (99%)	1 (1%)	86	96
2	a	165/172 (96%)	163 (99%)	2 (1%)	71	91
2	b	165/172 (96%)	165 (100%)	0	100	100
All	All	4625/4984 (93%)	4605 (100%)	20 (0%)	91	97

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	44	GLU

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Mol	Chain	Res	Type
1	P	161	GLU
1	U	179	ASP
2	M	37	THR
1	O	163	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	129	HIS
2	b	22	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 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
3	M9G	J	301	-	41,45,45	3.28	16 (39%)	49,63,63	1.78	10 (20%)
3	M9G	M	301	-	41,45,45	3.30	16 (39%)	49,63,63	1.50	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	M9G	H	301	-	41,45,45	3.30	16 (39%)	49,63,63	1.56	7 (14%)
3	M9G	V	301	-	41,45,45	3.29	16 (39%)	49,63,63	1.67	11 (22%)
3	M9G	I	301	-	41,45,45	3.28	17 (41%)	49,63,63	1.61	10 (20%)
3	M9G	W	301	-	41,45,45	3.27	16 (39%)	49,63,63	1.63	9 (18%)
3	M9G	Z	301	-	41,45,45	3.30	16 (39%)	49,63,63	1.45	7 (14%)
3	M9G	X	301	-	41,45,45	3.27	16 (39%)	49,63,63	1.83	11 (22%)
3	M9G	Y	301	-	41,45,45	3.28	16 (39%)	49,63,63	1.48	7 (14%)
3	M9G	L	302	-	41,45,45	3.33	15 (36%)	49,63,63	1.60	8 (16%)
3	M9G	b	301	-	41,45,45	3.31	16 (39%)	49,63,63	1.57	10 (20%)
3	M9G	N	301	-	41,45,45	3.25	16 (39%)	49,63,63	1.57	6 (12%)
3	M9G	a	301	-	41,45,45	3.29	16 (39%)	49,63,63	1.55	8 (16%)
3	M9G	L	301	-	41,45,45	3.30	16 (39%)	49,63,63	1.56	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
3	M9G	J	301	-	-	0/30/46/46	0/5/5/5
3	M9G	M	301	-	-	2/30/46/46	0/5/5/5
3	M9G	H	301	-	-	1/30/46/46	0/5/5/5
3	M9G	V	301	-	-	3/30/46/46	0/5/5/5
3	M9G	I	301	-	-	4/30/46/46	0/5/5/5
3	M9G	W	301	-	-	1/30/46/46	0/5/5/5
3	M9G	Z	301	-	-	0/30/46/46	0/5/5/5
3	M9G	X	301	-	-	2/30/46/46	0/5/5/5
3	M9G	Y	301	-	-	1/30/46/46	0/5/5/5
3	M9G	L	302	-	-	3/30/46/46	0/5/5/5
3	M9G	b	301	-	-	1/30/46/46	0/5/5/5
3	M9G	N	301	-	-	1/30/46/46	0/5/5/5
3	M9G	a	301	-	-	0/30/46/46	0/5/5/5
3	M9G	L	301	-	-	2/30/46/46	0/5/5/5

The worst 5 of 224 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	302	M9G	C38-C31	-9.21	1.30	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	301	M9G	C38-C31	-9.12	1.30	1.54
3	a	301	M9G	C38-C31	-9.12	1.30	1.54
3	N	301	M9G	C38-C31	-9.10	1.30	1.54
3	L	301	M9G	C38-C31	-9.06	1.30	1.54

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	301	M9G	C40-N30-C31	-5.39	105.57	111.83
3	X	301	M9G	C40-N30-C31	-5.23	105.76	111.83
3	M	301	M9G	C40-N30-C31	-5.15	105.85	111.83
3	J	301	M9G	C40-N30-C31	-5.12	105.88	111.83
3	L	301	M9G	C40-N30-C31	-5.09	105.92	111.83

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	V	301	M9G	O21-C20-C22-C27
3	X	301	M9G	O21-C20-C22-C27
3	I	301	M9G	C13-C05-C06-C07
3	L	302	M9G	C13-C05-C06-C12
3	L	302	M9G	N04-C05-C06-C12

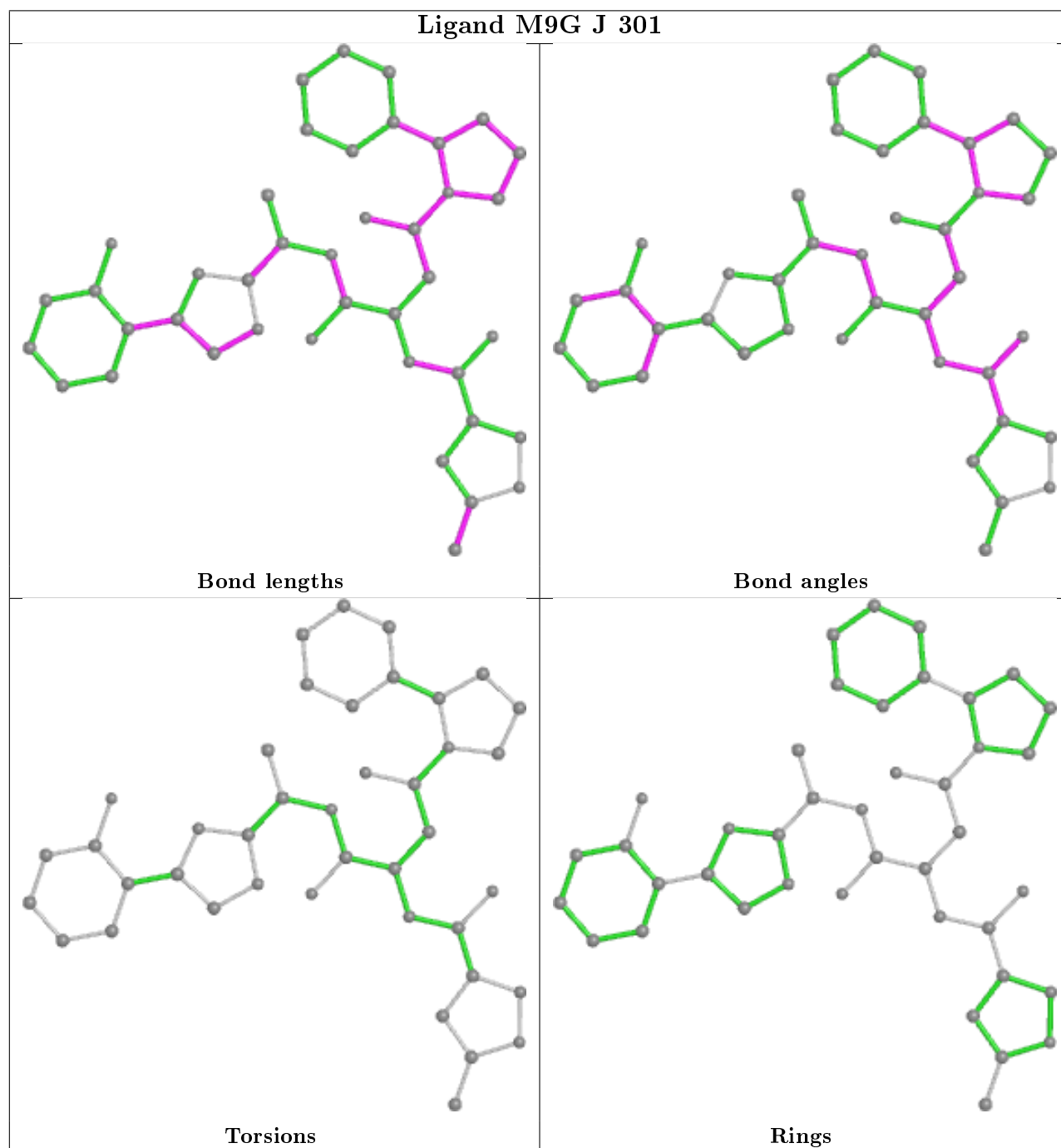
There are no ring outliers.

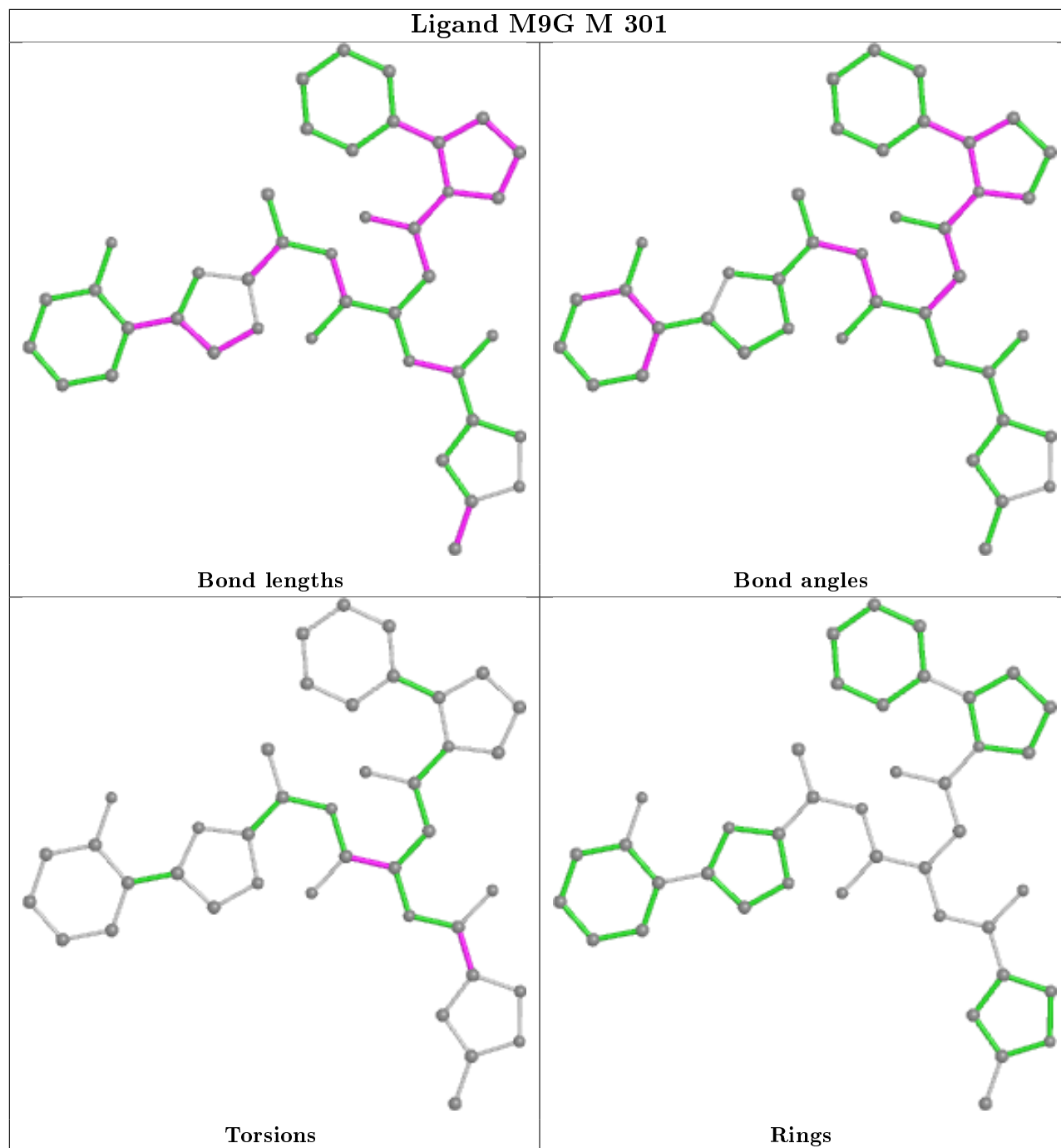
3 monomers are involved in 3 short contacts:

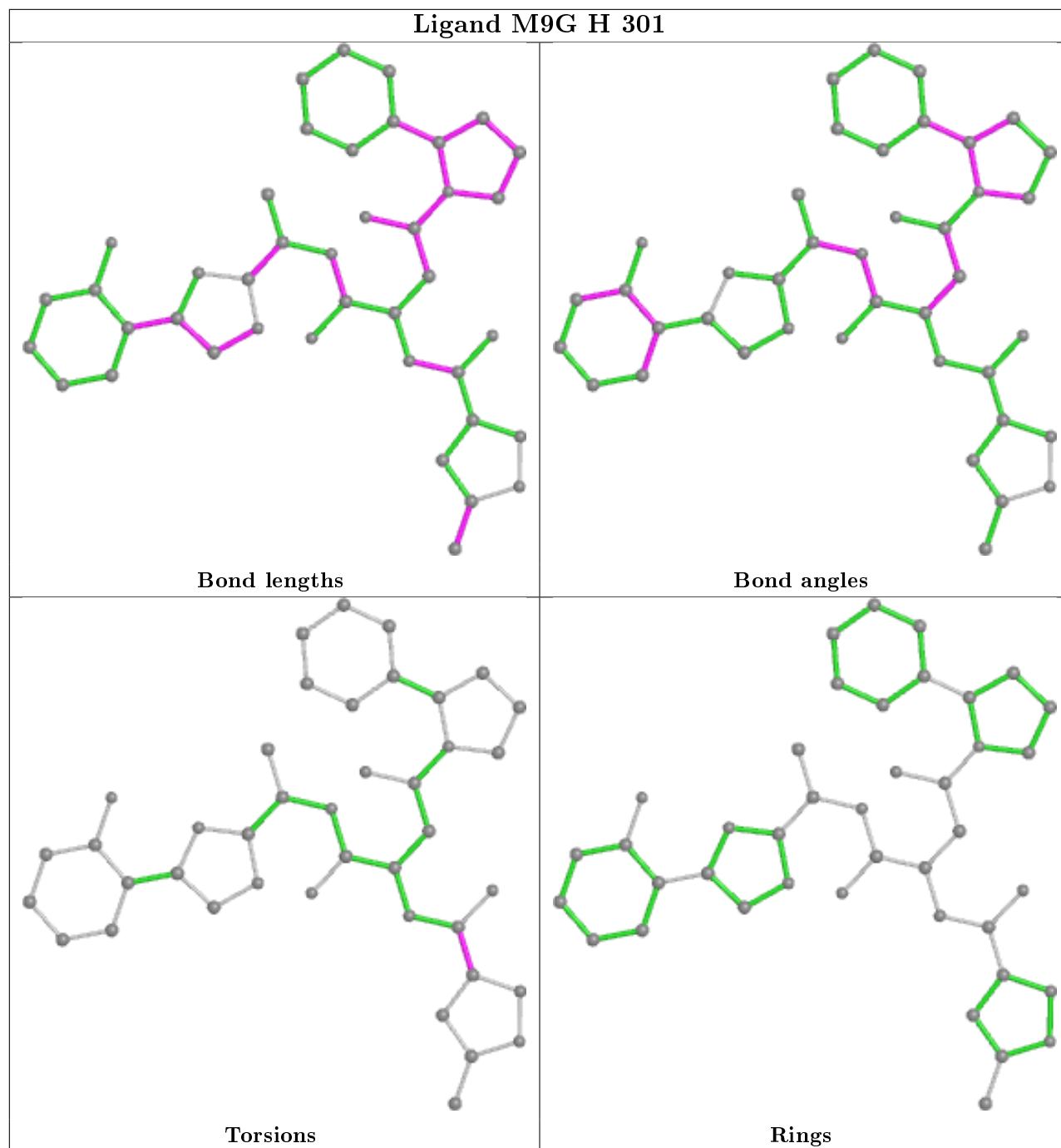
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	301	M9G	1	0
3	I	301	M9G	1	0
3	N	301	M9G	1	0

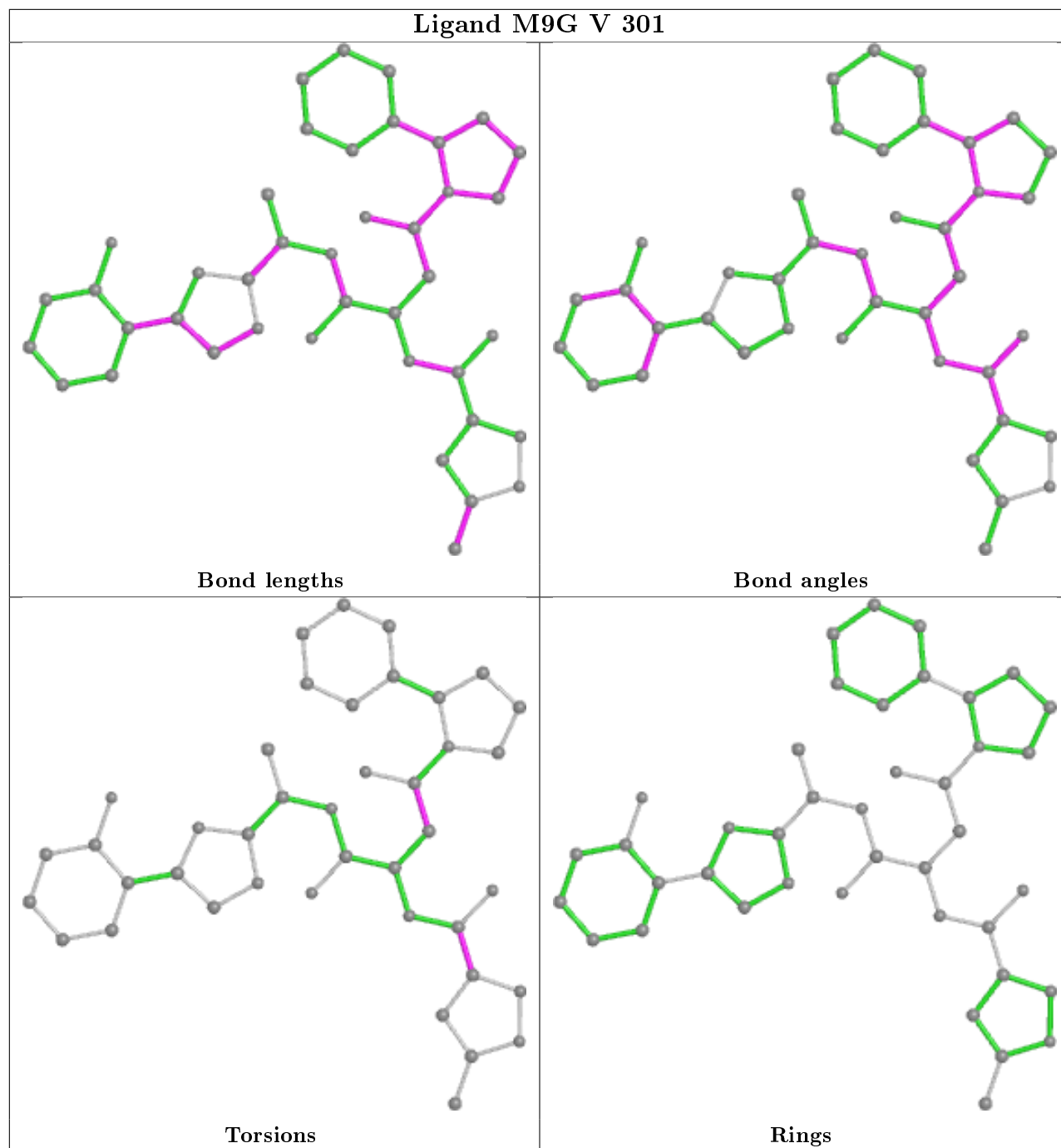
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

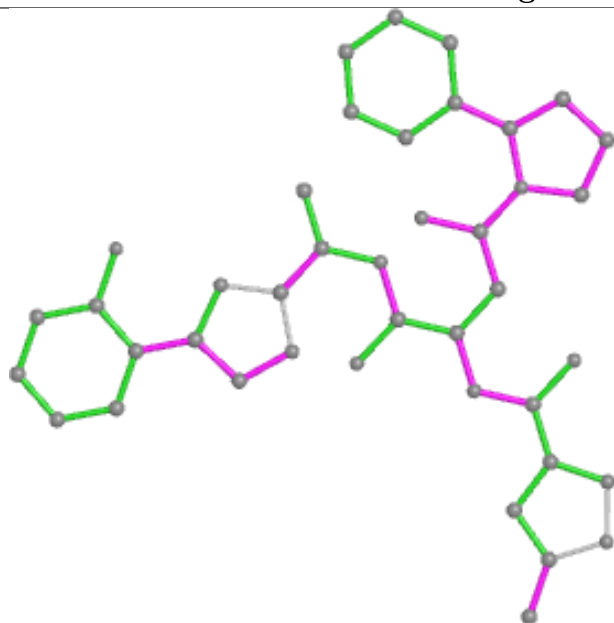




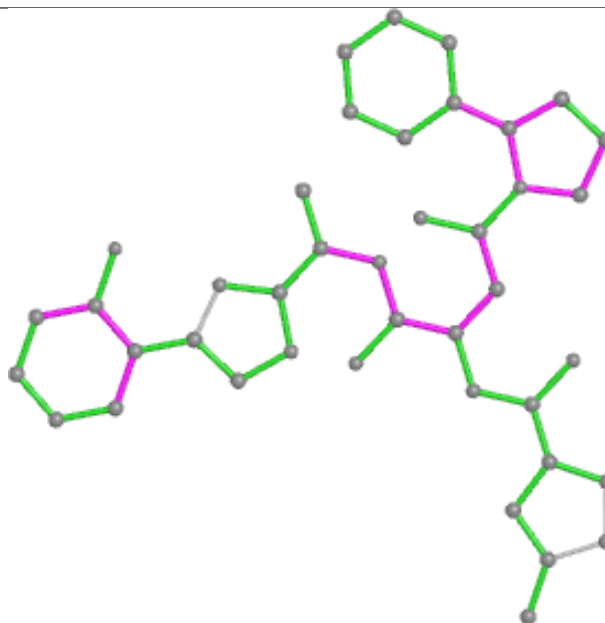




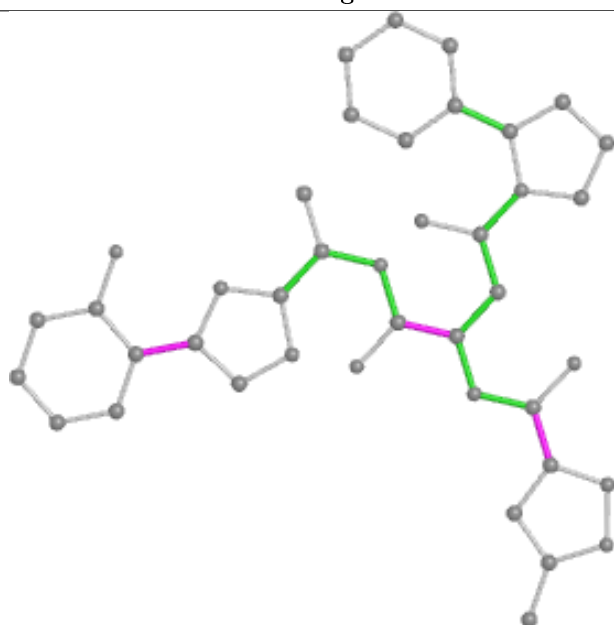
Ligand M9G I 301



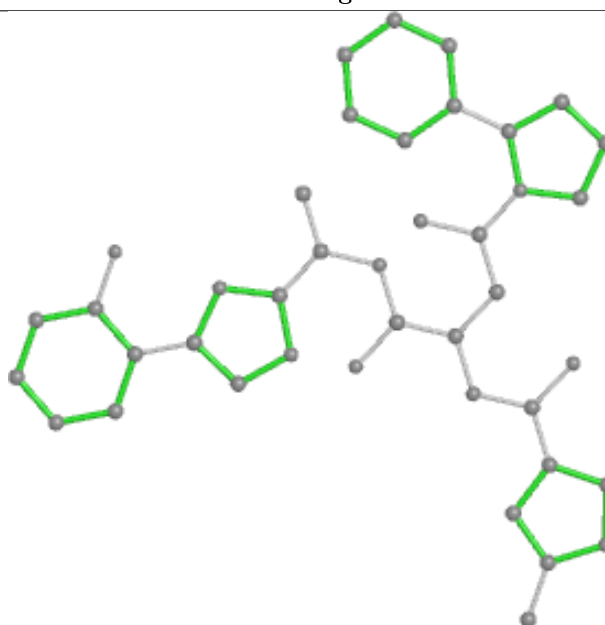
Bond lengths



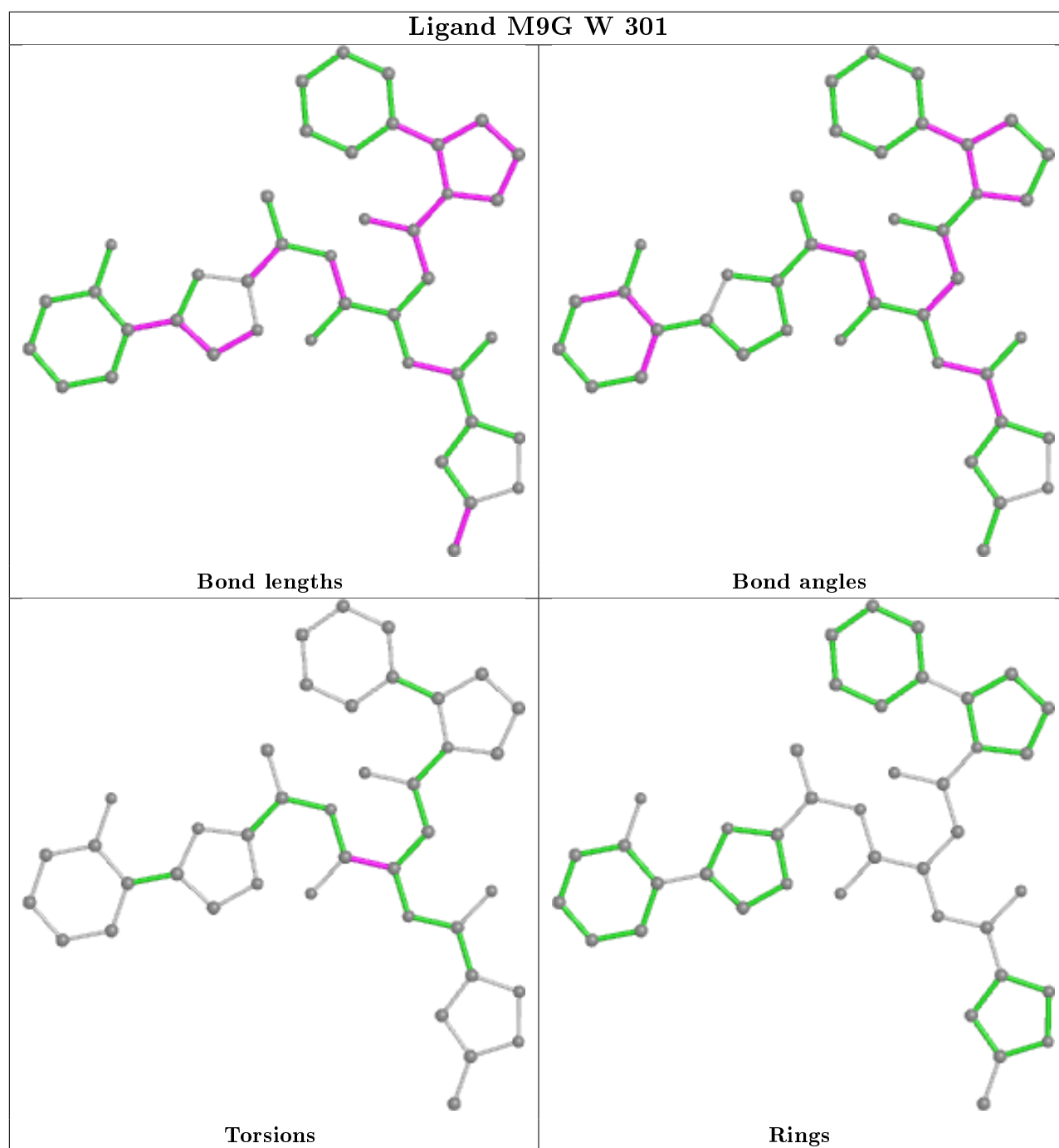
Bond angles



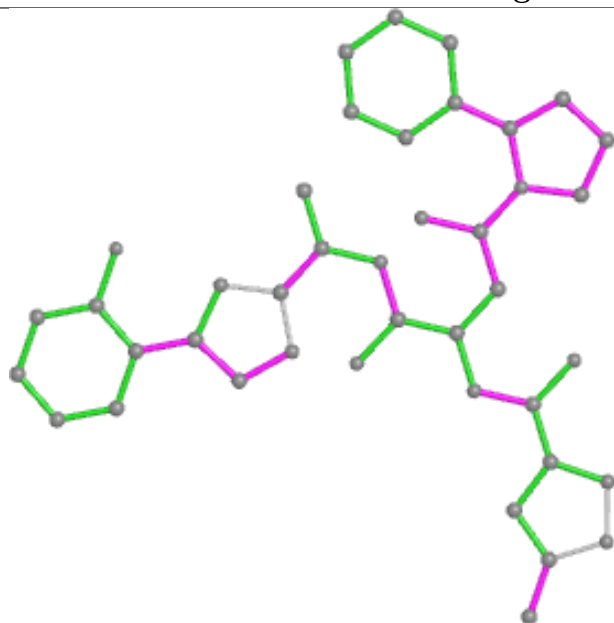
Torsions



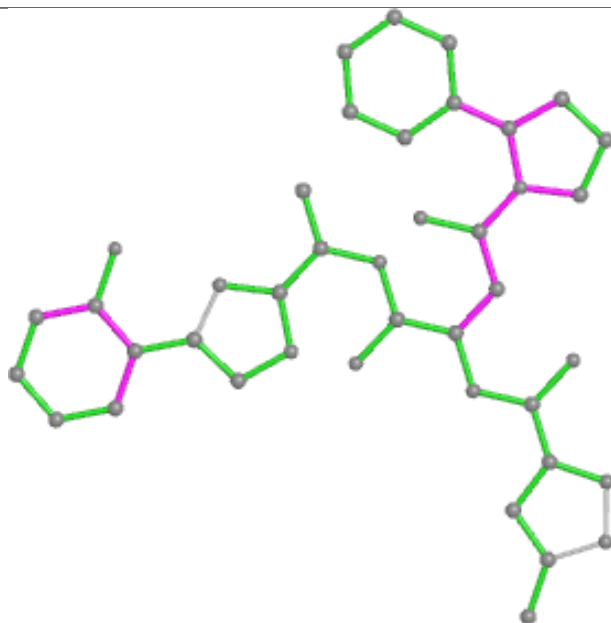
Rings



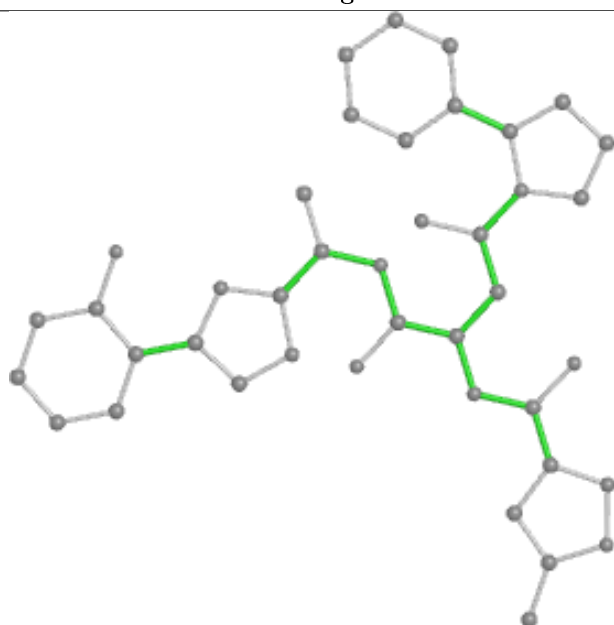
Ligand M9G Z 301



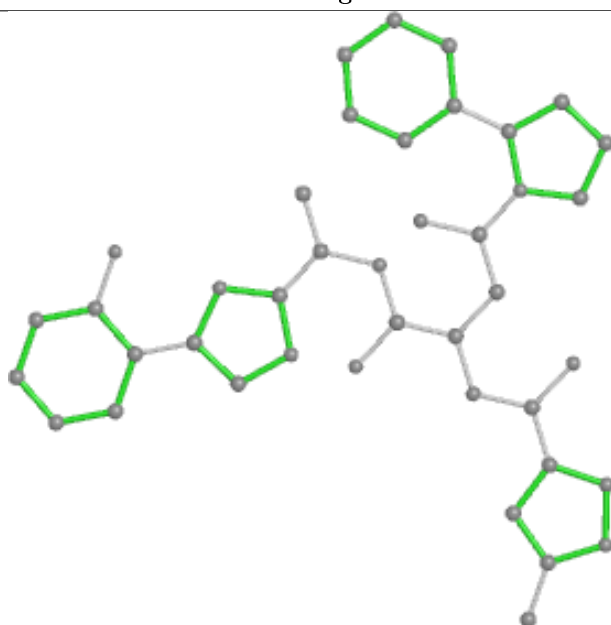
Bond lengths



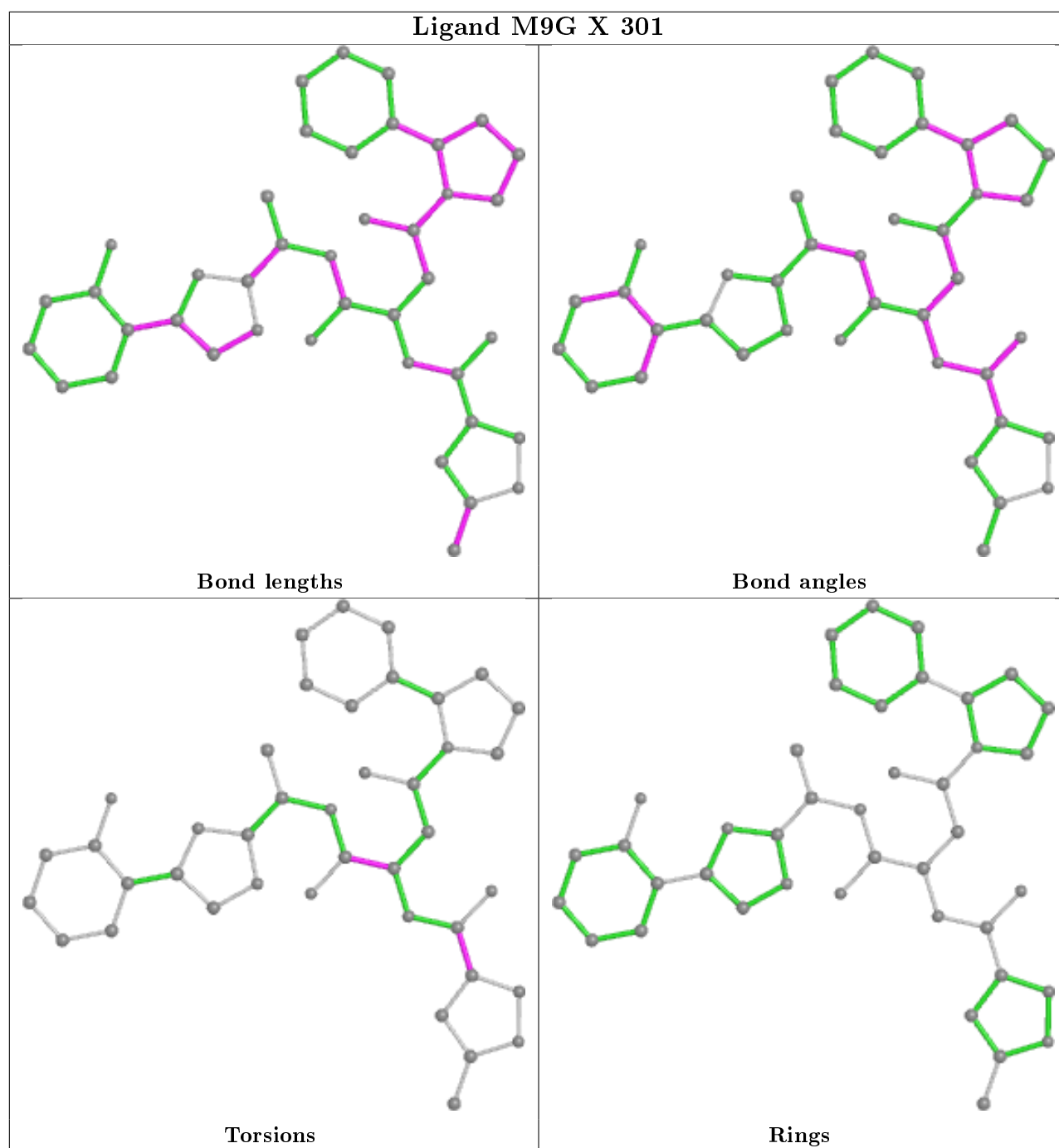
Bond angles

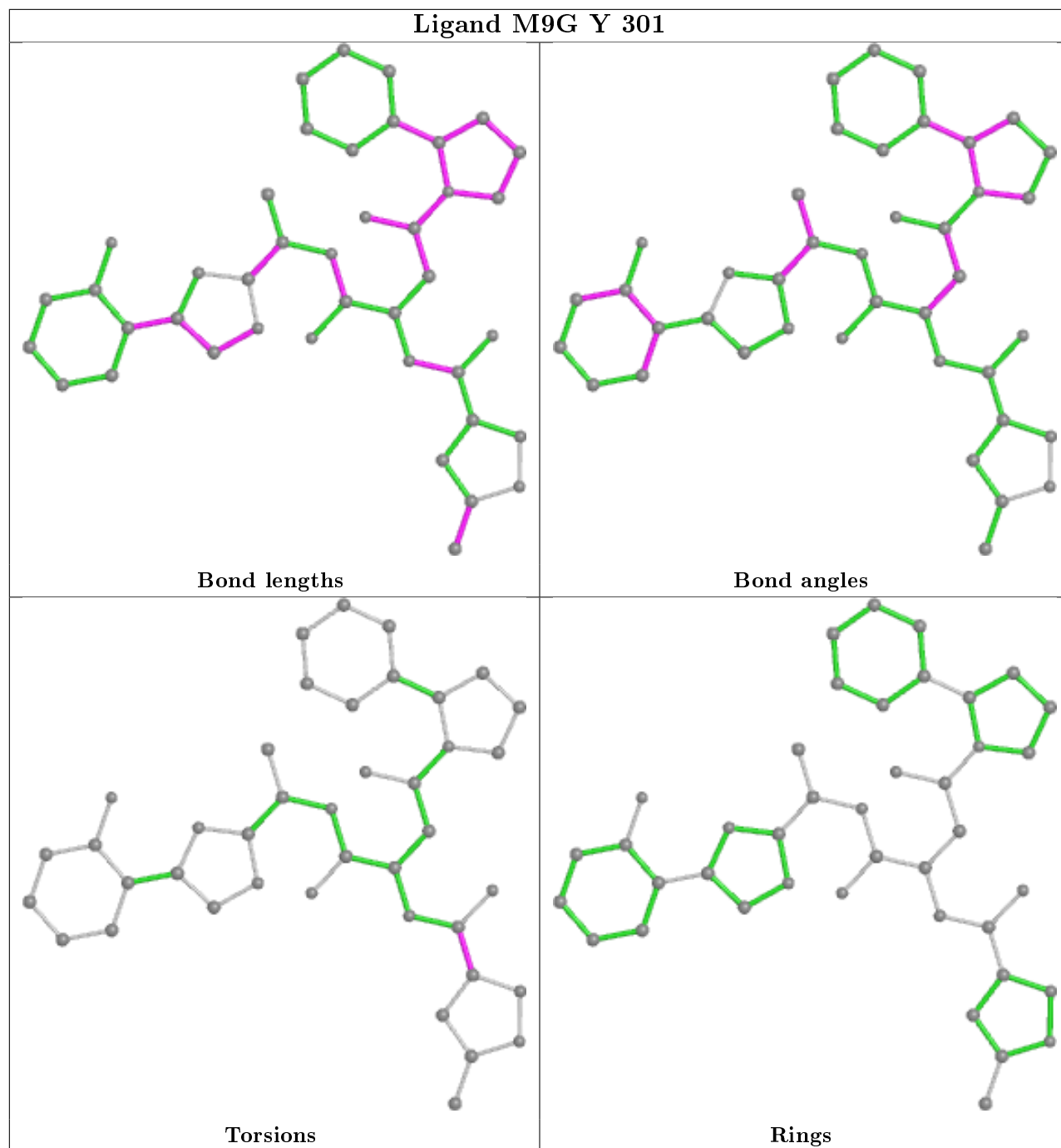


Torsions

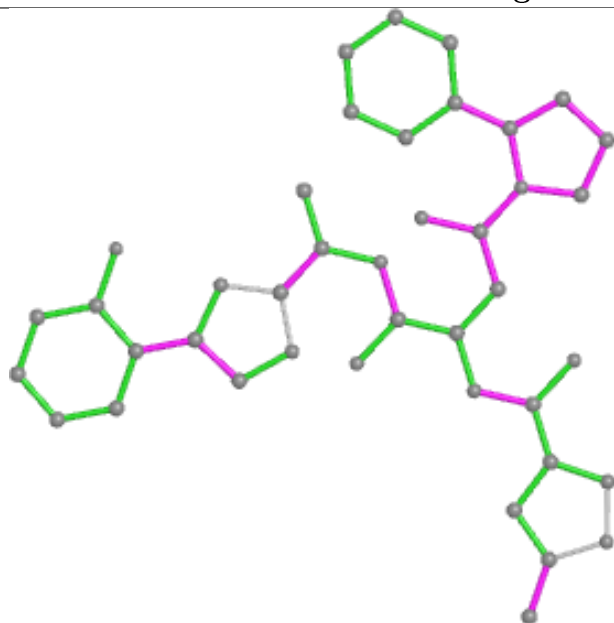


Rings

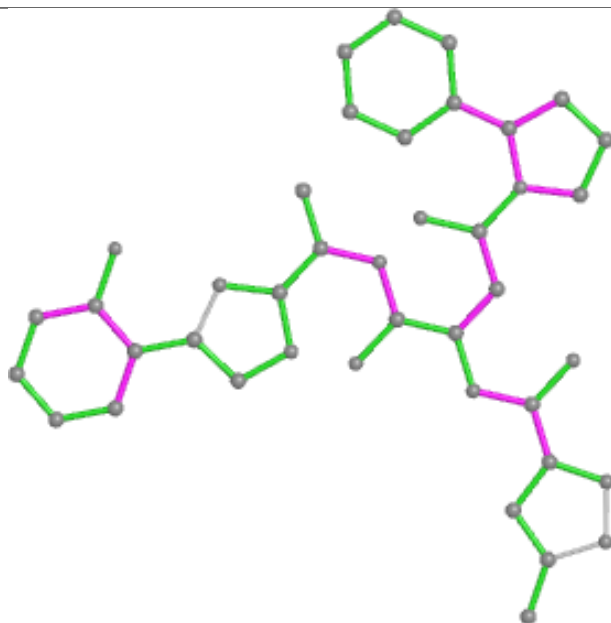




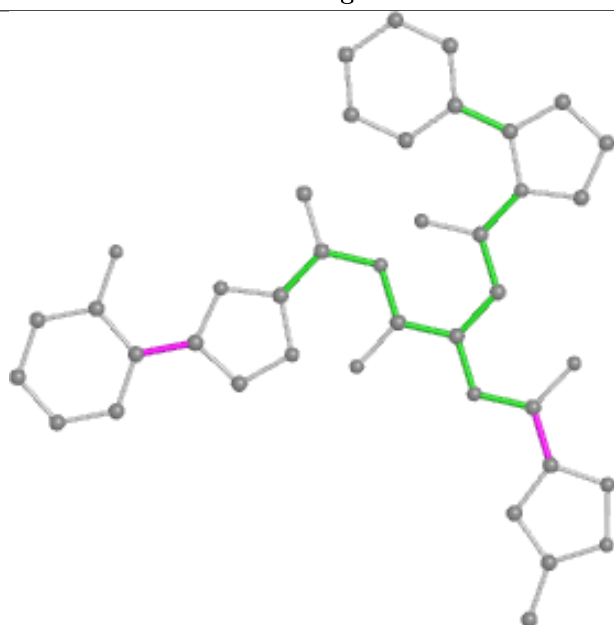
Ligand M9G L 302



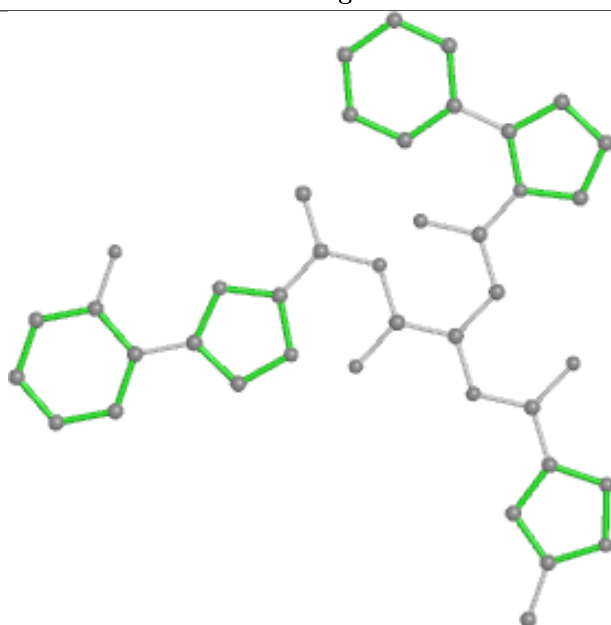
Bond lengths



Bond angles

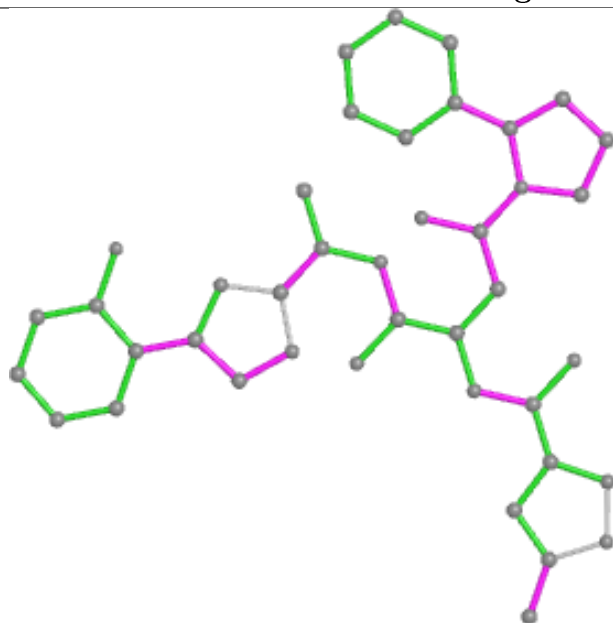


Torsions

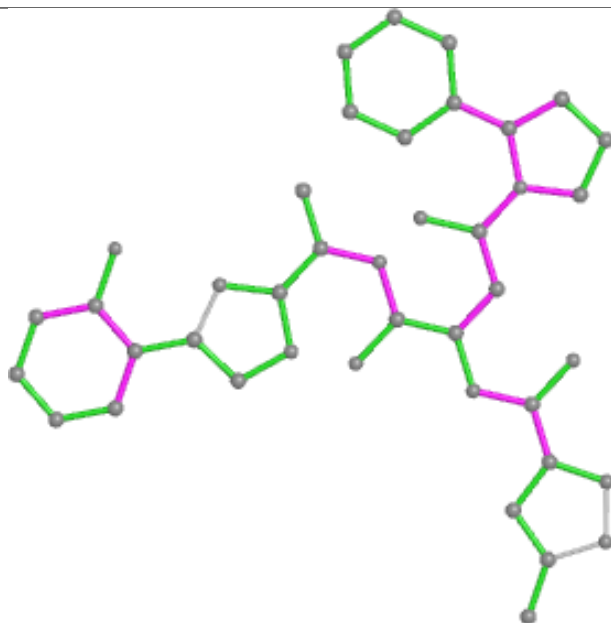


Rings

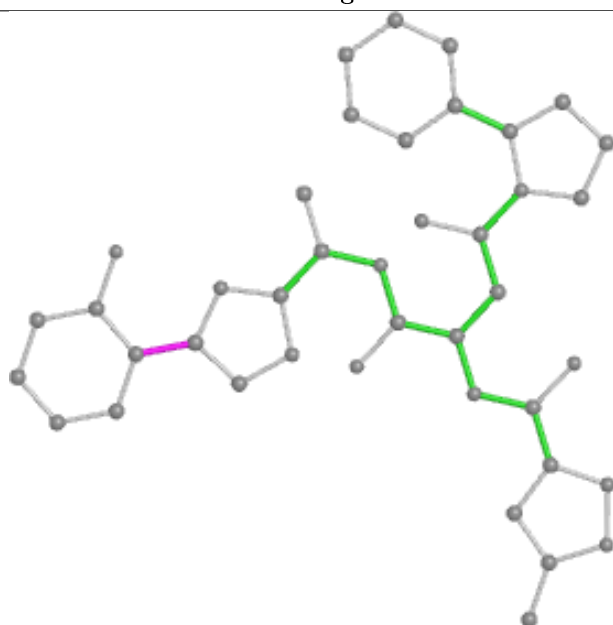
Ligand M9G b 301



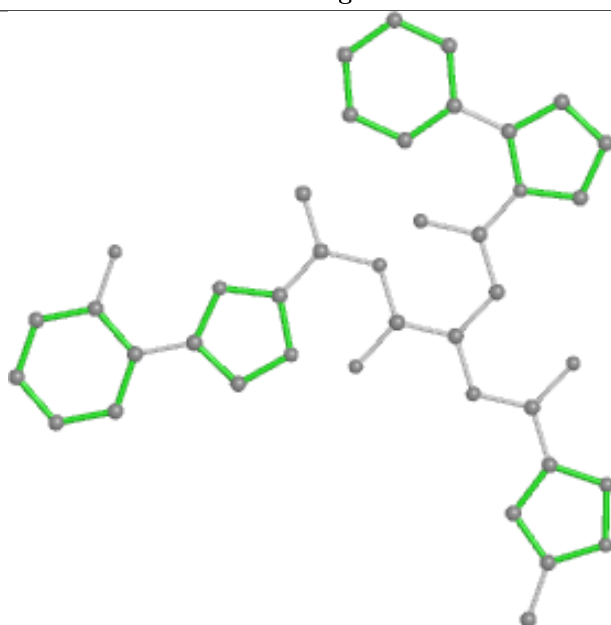
Bond lengths



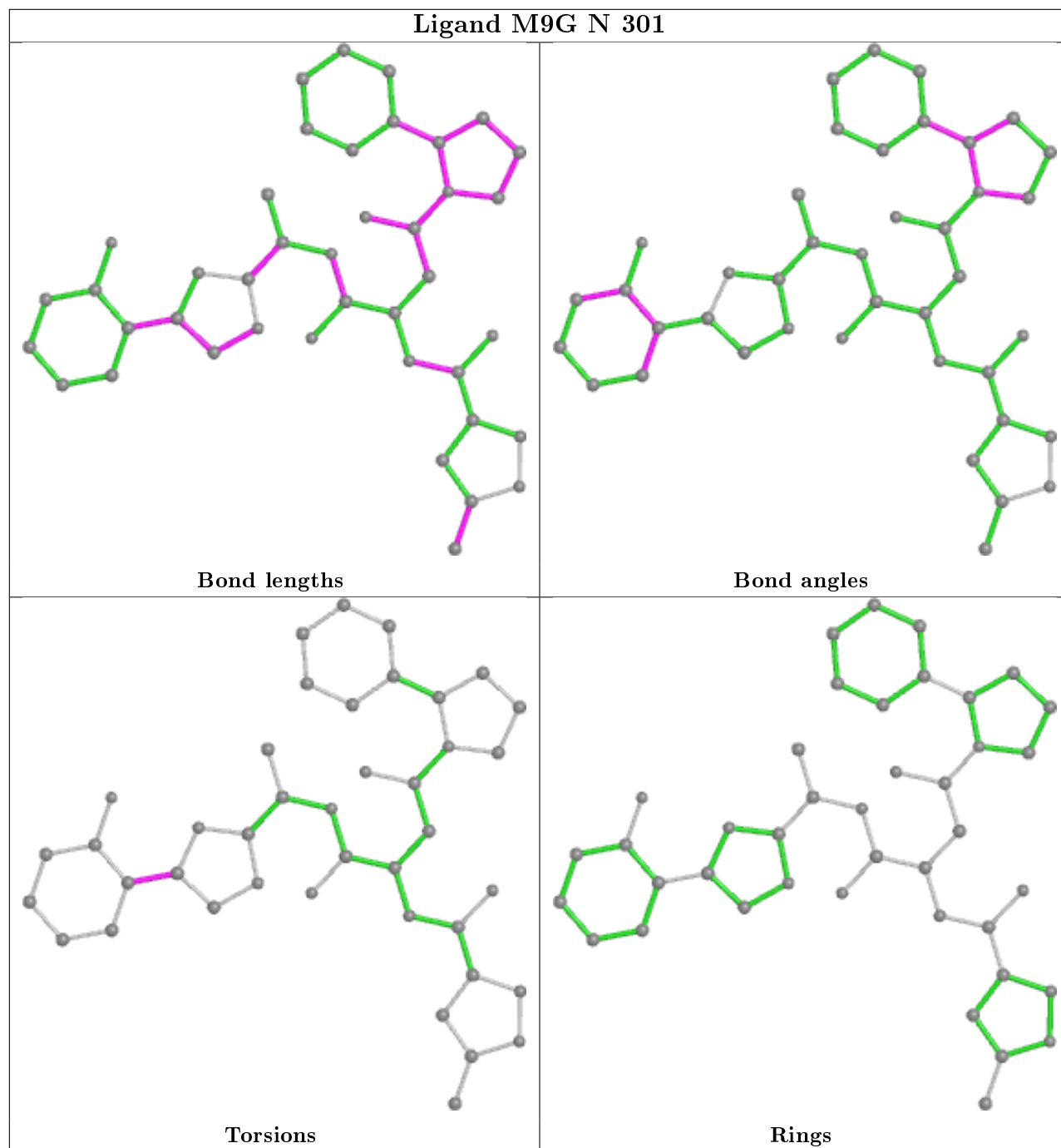
Bond angles



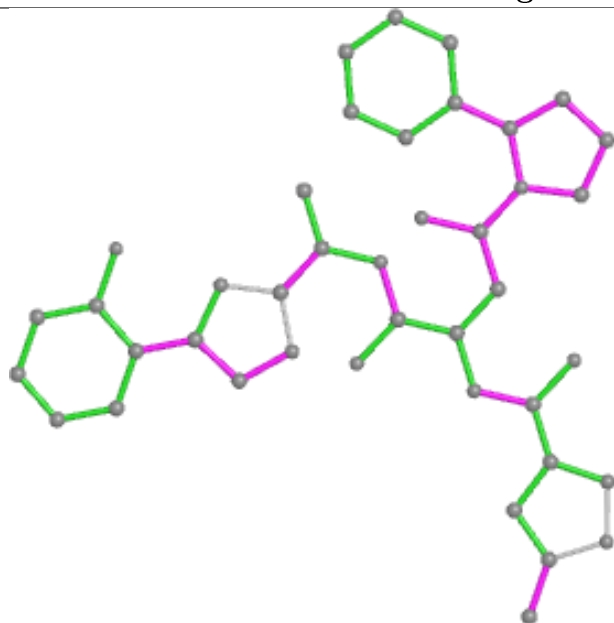
Torsions



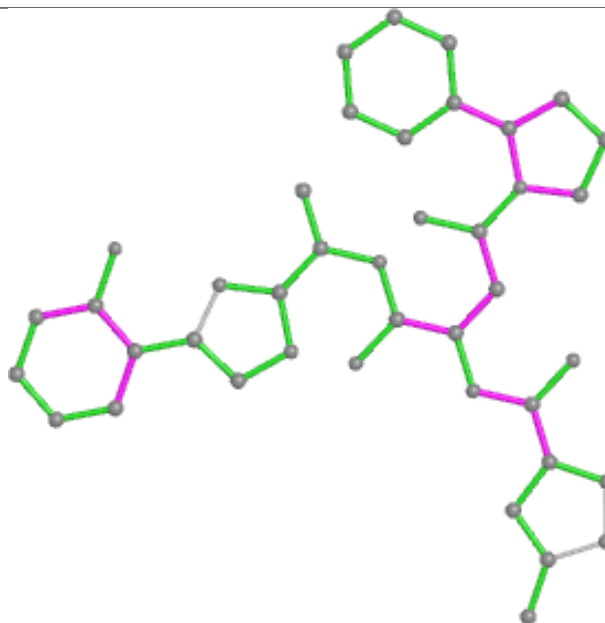
Rings



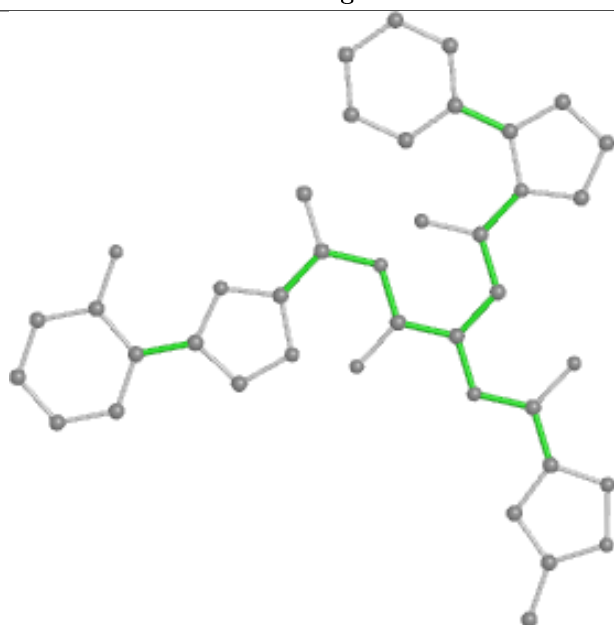
Ligand M9G a 301



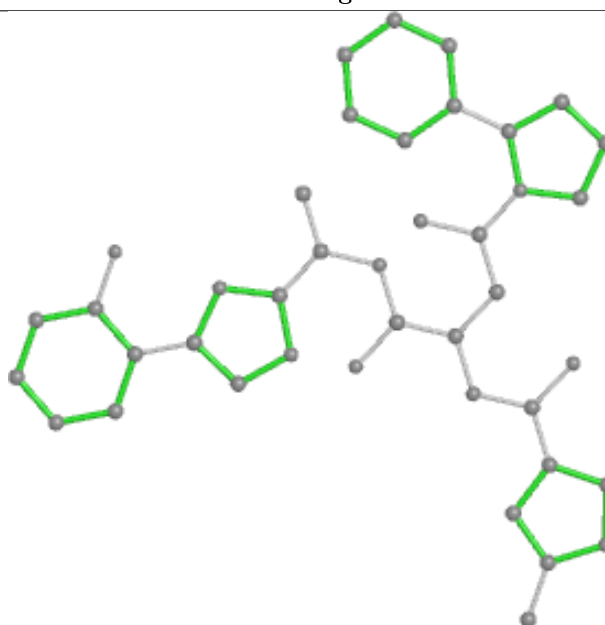
Bond lengths



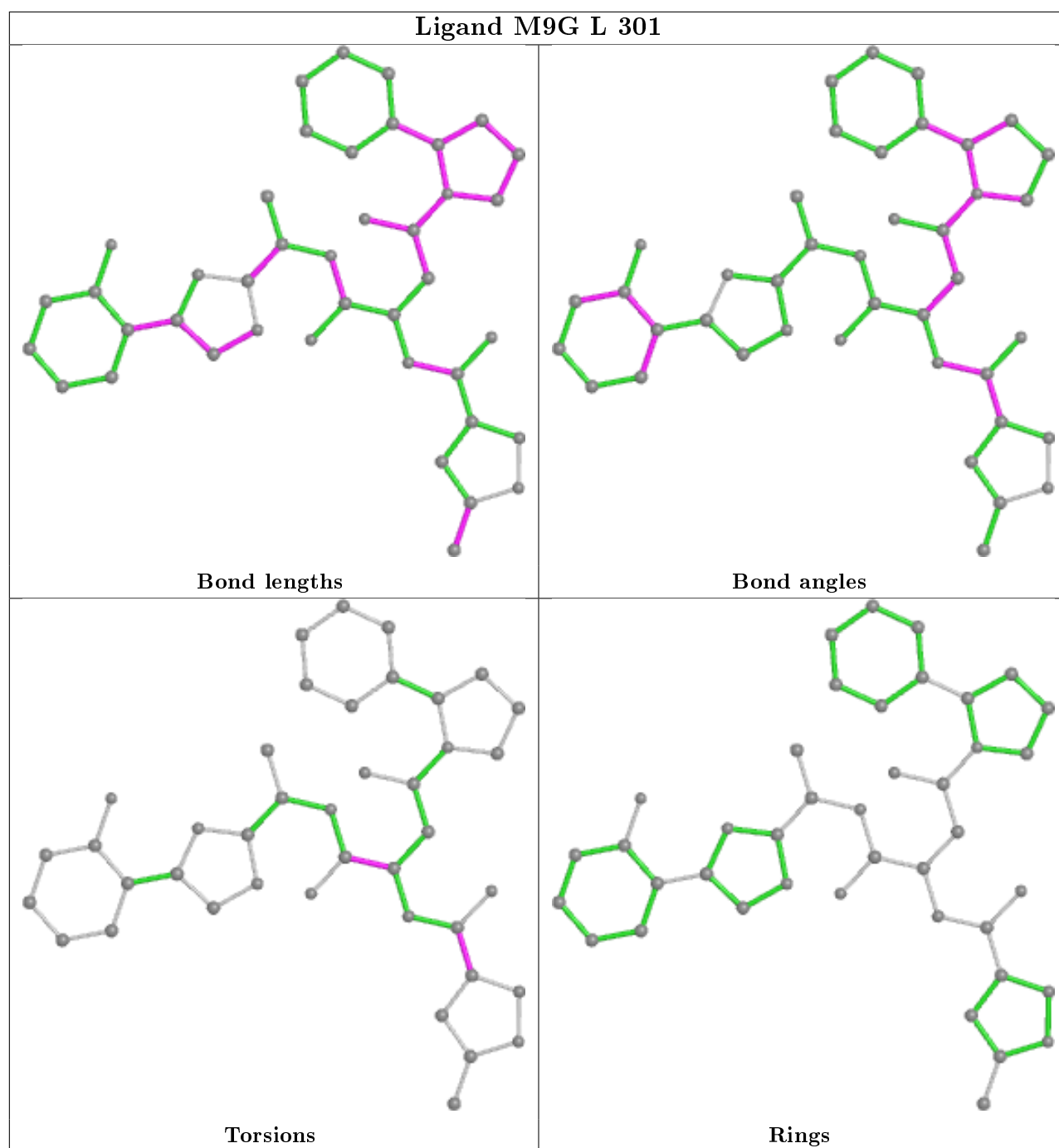
Bond angles



Torsions



Rings



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	218/240 (90%)	-0.16	1 (0%) 91 91	18, 33, 55, 81	0
1	B	215/240 (89%)	0.08	9 (4%) 36 32	20, 42, 71, 90	0
1	C	216/240 (90%)	0.31	13 (6%) 21 18	21, 46, 75, 89	0
1	D	214/240 (89%)	0.11	5 (2%) 60 58	23, 44, 68, 84	0
1	E	217/240 (90%)	-0.02	3 (1%) 75 75	21, 42, 68, 83	0
1	F	214/240 (89%)	0.07	2 (0%) 84 84	18, 44, 71, 81	0
1	G	216/240 (90%)	-0.22	4 (1%) 66 65	17, 36, 64, 78	0
1	O	216/240 (90%)	0.21	10 (4%) 32 29	22, 46, 74, 87	0
1	P	219/240 (91%)	-0.05	6 (2%) 54 50	19, 40, 67, 86	0
1	Q	215/240 (89%)	-0.12	1 (0%) 91 91	20, 39, 61, 75	0
1	R	215/240 (89%)	0.13	8 (3%) 41 37	17, 38, 58, 66	0
1	S	218/240 (90%)	-0.23	2 (0%) 84 84	18, 34, 59, 76	0
1	T	217/240 (90%)	0.21	6 (2%) 53 49	22, 45, 69, 100	0
1	U	216/240 (90%)	-0.07	4 (1%) 66 65	19, 38, 66, 84	0
2	H	222/234 (94%)	-0.39	0 100 100	15, 24, 42, 67	0
2	I	222/234 (94%)	-0.53	0 100 100	15, 23, 41, 61	0
2	J	222/234 (94%)	-0.45	0 100 100	15, 25, 42, 59	0
2	K	223/234 (95%)	-0.48	0 100 100	11, 23, 40, 54	0
2	L	223/234 (95%)	-0.45	0 100 100	16, 24, 41, 58	0
2	M	222/234 (94%)	-0.38	0 100 100	17, 27, 47, 63	0
2	N	223/234 (95%)	-0.38	0 100 100	16, 28, 49, 64	0
2	V	223/234 (95%)	-0.47	0 100 100	14, 24, 40, 54	0
2	W	223/234 (95%)	-0.46	0 100 100	16, 25, 42, 56	0
2	X	222/234 (94%)	-0.45	0 100 100	16, 25, 43, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	Y	223/234 (95%)	-0.43	1 (0%) 92 93	14, 24, 41, 66	0
2	Z	223/234 (95%)	-0.42	0 100 100	15, 26, 46, 60	0
2	a	223/234 (95%)	-0.37	0 100 100	19, 28, 48, 66	0
2	b	223/234 (95%)	-0.43	0 100 100	17, 27, 45, 64	0
All	All	6143/6636 (92%)	-0.21	75 (1%) 79 79	11, 31, 64, 100	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	202	THR	5.0
1	C	9	MET	3.8
1	P	170	SER	3.7
1	T	203	LEU	3.6
1	O	188	LEU	3.6

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 [i](#)

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

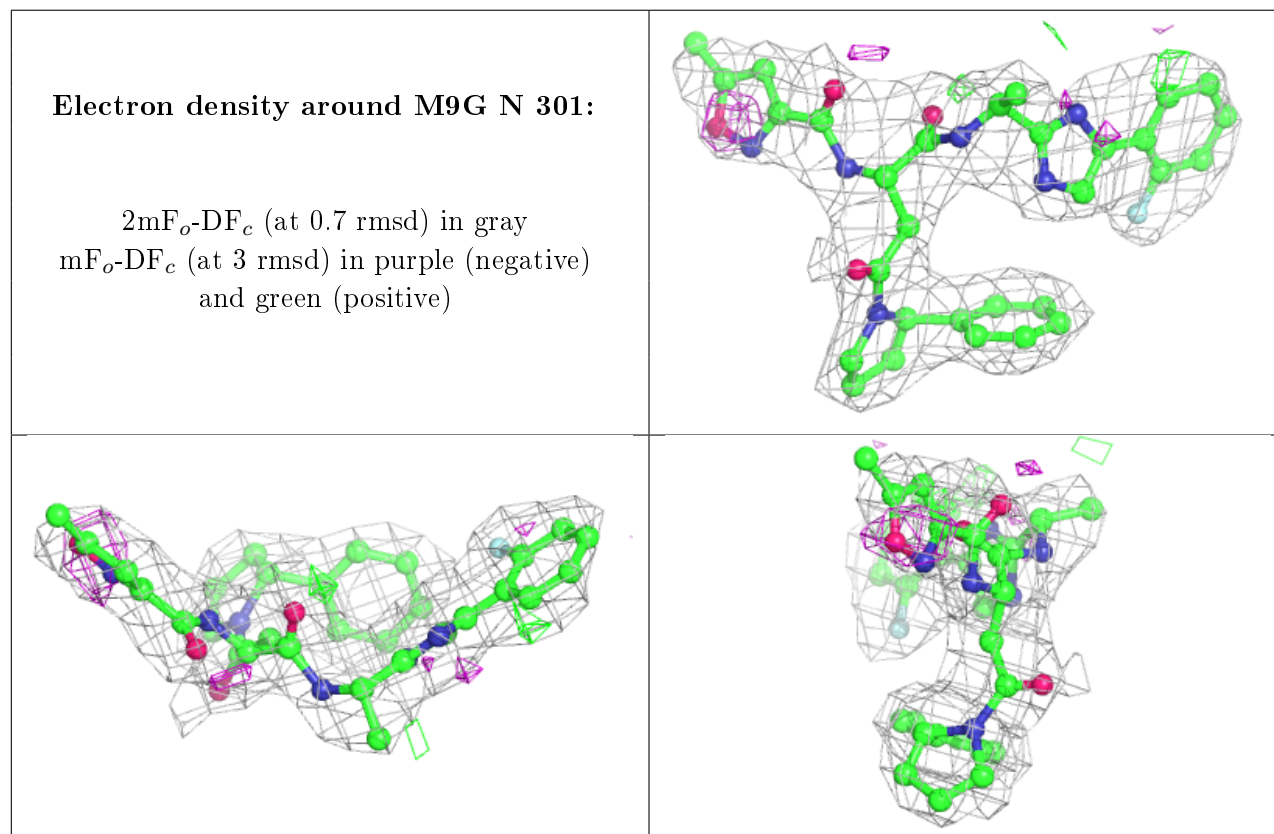
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	M9G	N	301	41/41	0.94	0.19	13,24,36,49	0
3	M9G	M	301	41/41	0.95	0.21	18,26,40,51	0
3	M9G	H	301	41/41	0.95	0.20	17,24,36,50	0
3	M9G	V	301	41/41	0.95	0.20	19,24,41,53	0
3	M9G	W	301	41/41	0.95	0.20	19,28,38,48	0
3	M9G	J	301	41/41	0.95	0.21	18,27,38,42	0
3	M9G	X	301	41/41	0.96	0.16	18,26,39,45	0

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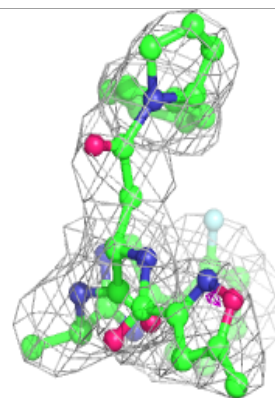
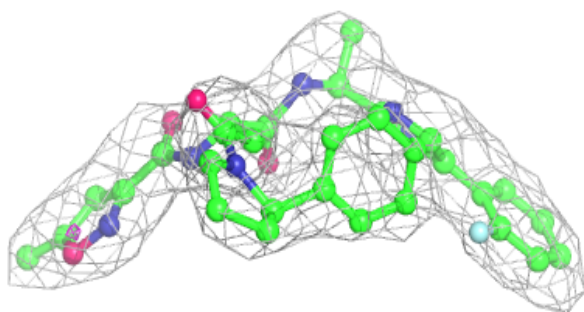
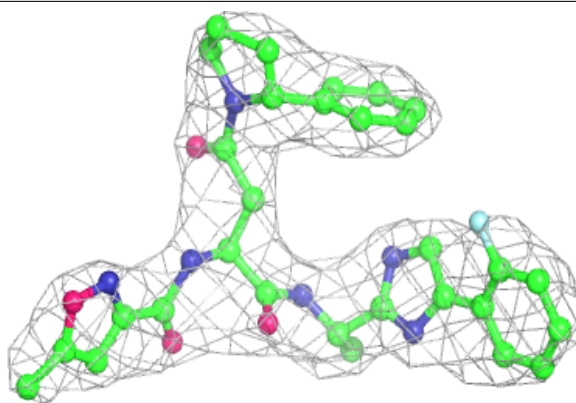
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	M9G	Y	301	41/41	0.96	0.20	13,24,35,45	0
3	M9G	L	302	41/41	0.96	0.20	17,26,36,48	0
3	M9G	b	301	41/41	0.96	0.18	15,24,35,40	0
3	M9G	Z	301	41/41	0.96	0.20	17,26,37,49	0
3	M9G	L	301	41/41	0.96	0.20	15,25,43,51	0
3	M9G	a	301	41/41	0.97	0.18	19,27,36,45	0
3	M9G	I	301	41/41	0.97	0.16	15,24,40,45	0

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

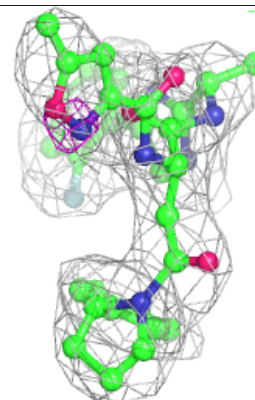
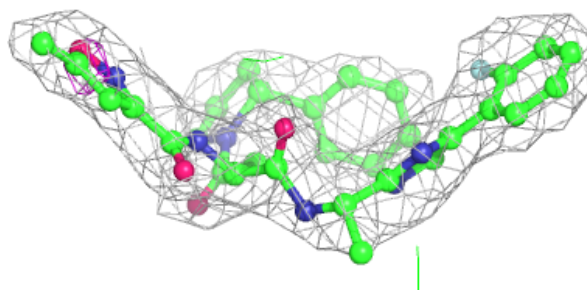
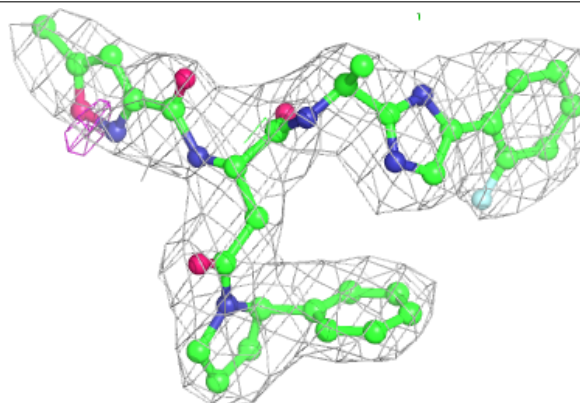


Electron density around M9G M 301:

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

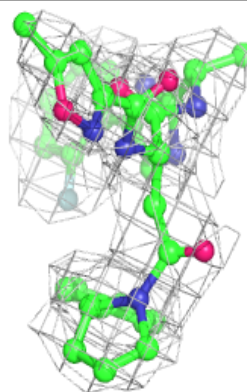
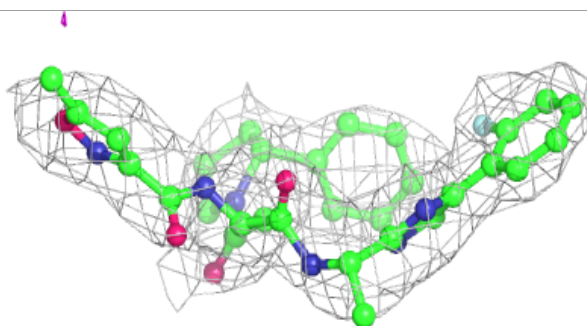
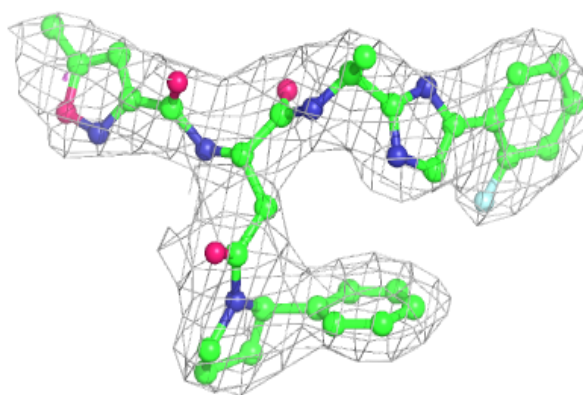
**Electron density around M9G H 301:**

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

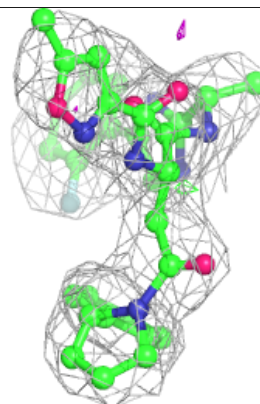
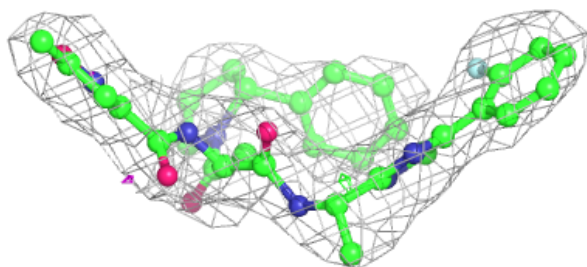
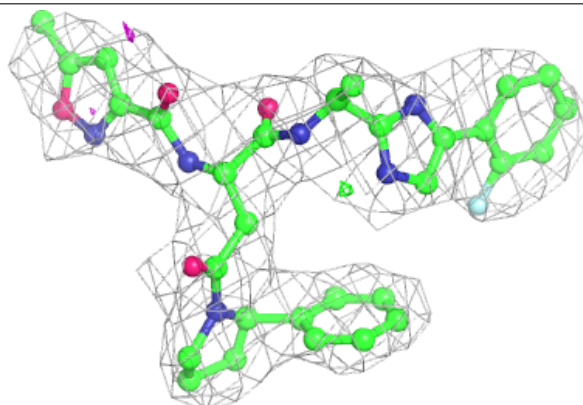


Electron density around M9G V 301:

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

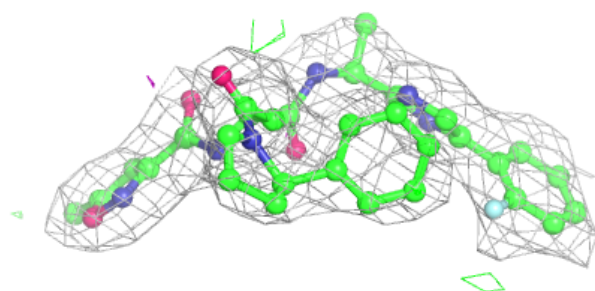
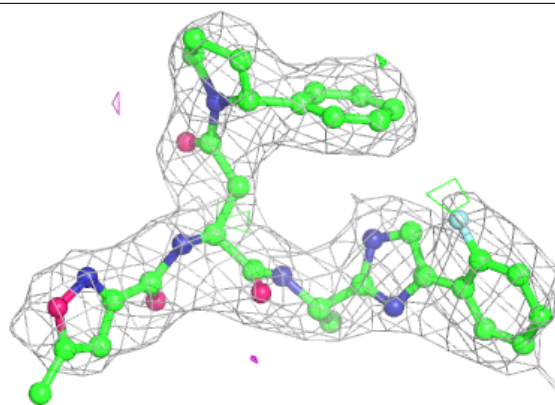
**Electron density around M9G W 301:**

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

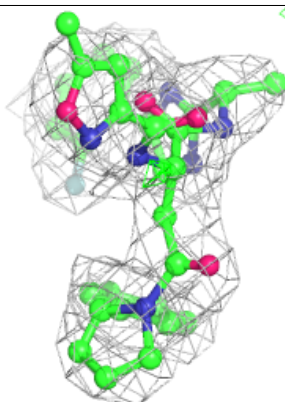
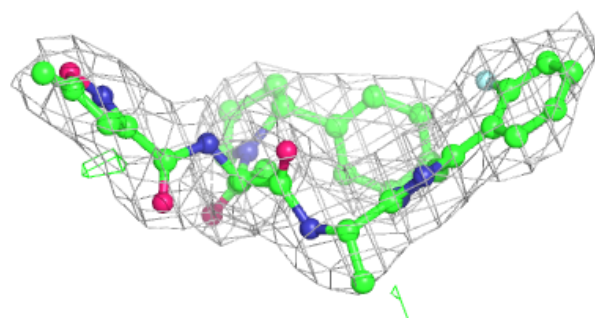
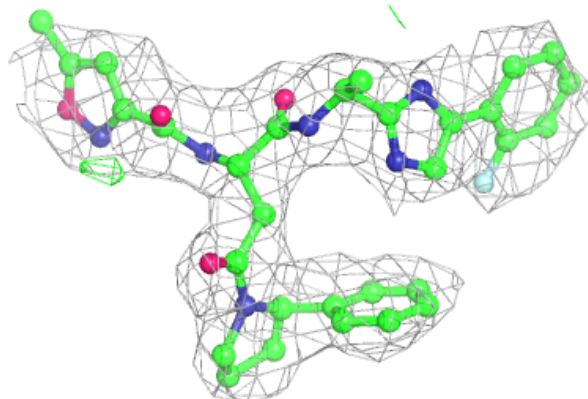


Electron density around M9G J 301:

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

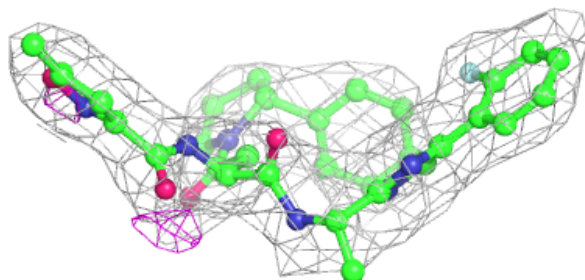
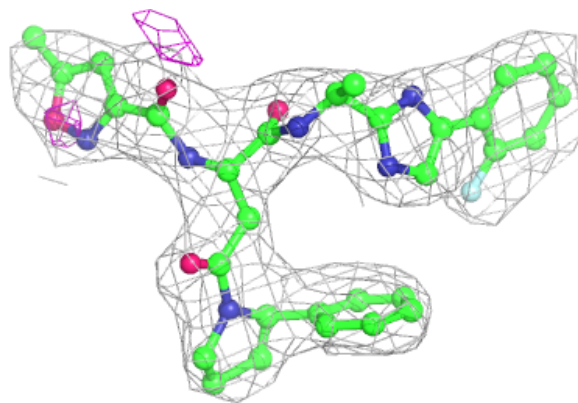
**Electron density around M9G X 301:**

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

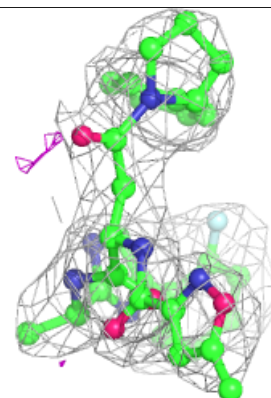
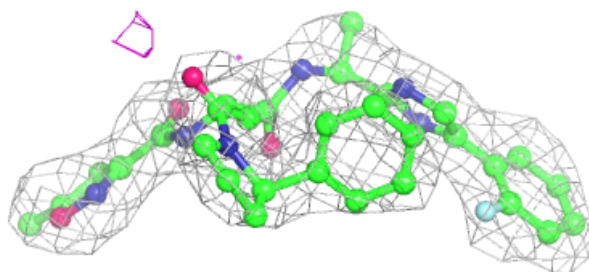
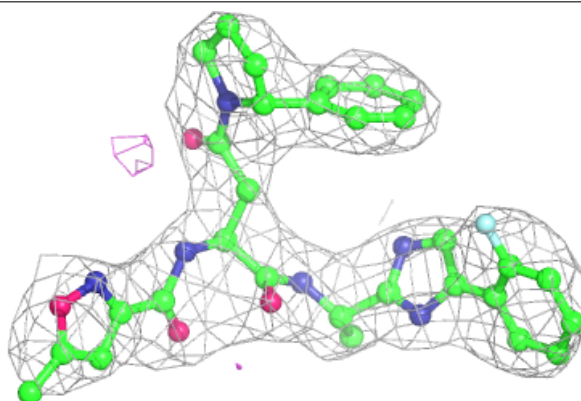


Electron density around M9G Y 301:

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

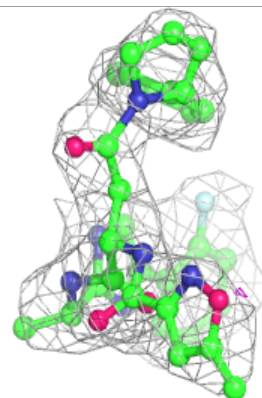
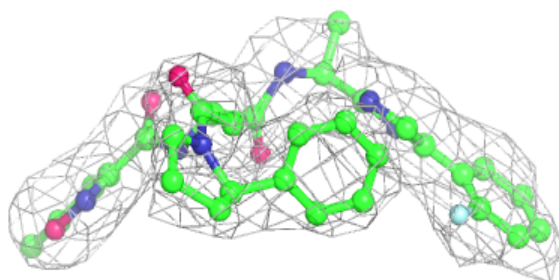
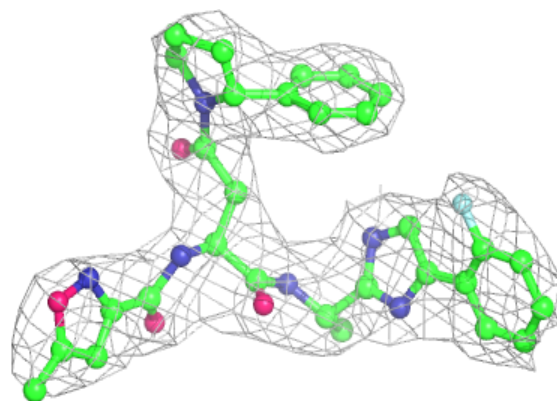
**Electron density around M9G L 302:**

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

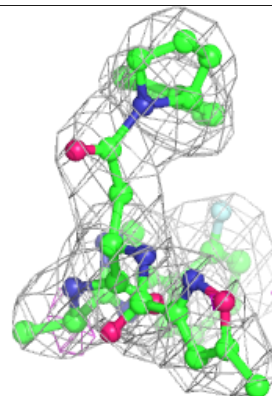
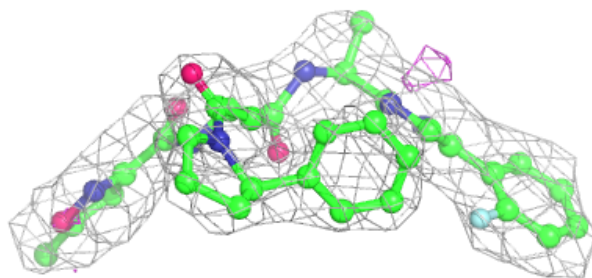
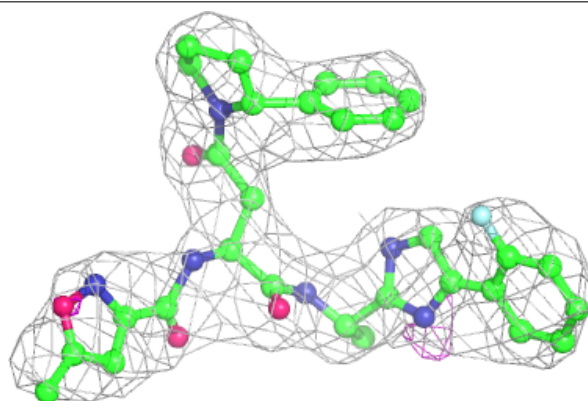


Electron density around M9G b 301:

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

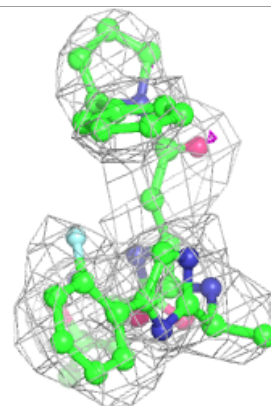
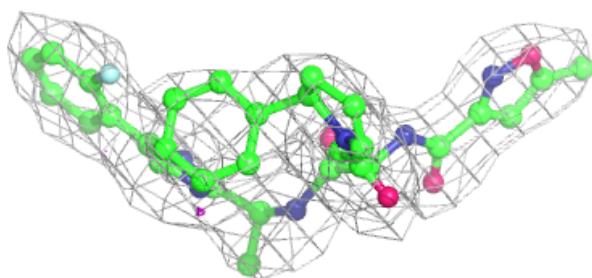
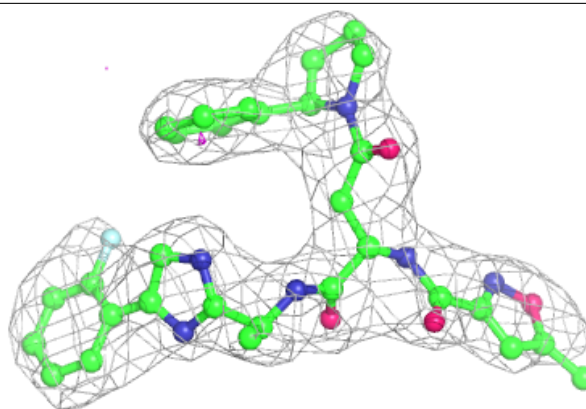
**Electron density around M9G Z 301:**

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

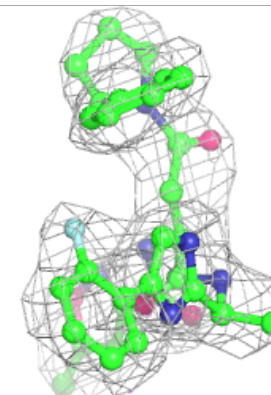
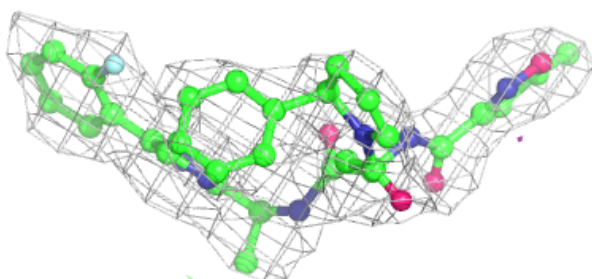
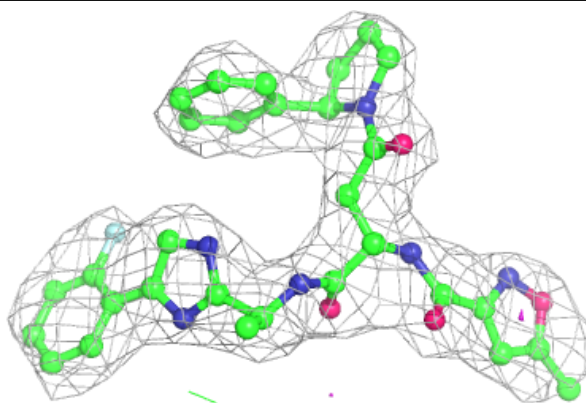


Electron density around M9G L 301:

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

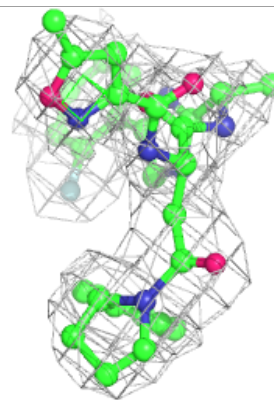
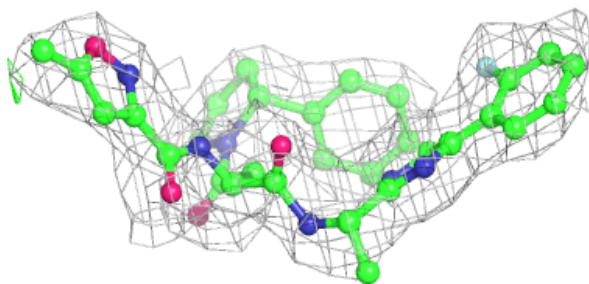
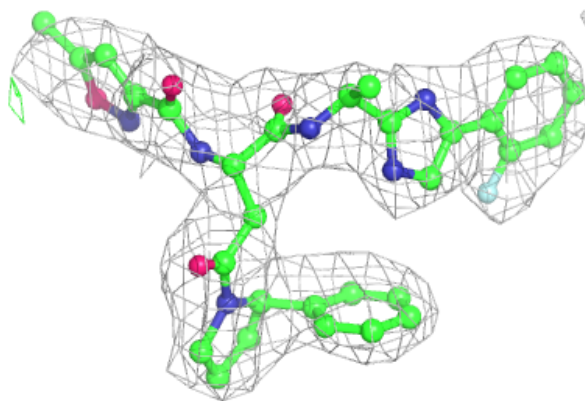
**Electron density around M9G a 301:**

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



Electron density around M9G I 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.