



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 11:31 PM EDT

PDB ID : 5TS0
Title : Structure of Mycobacterium tuberculosis proteasome in complex with N,C-capped dipeptide PKS2208
Authors : Hsu, H.-C.; Fan, H.; Singh, P.K.; Wang, R.; Sukenick, G.; Nathan, C.; Lin, G.; Li, H.
Deposited on : 2016-10-27
Resolution : 2.85 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 types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

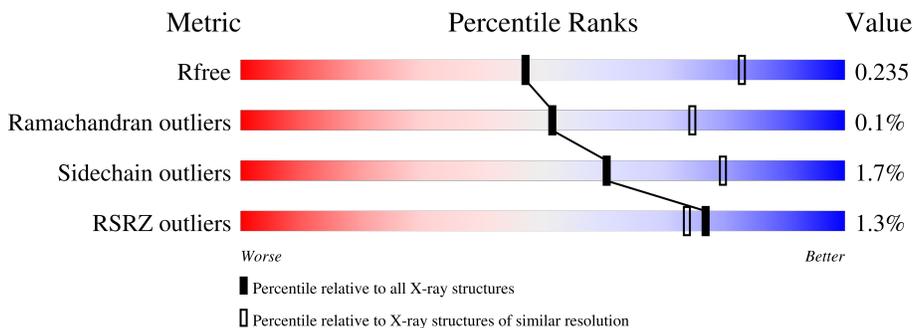
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1031 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	240	89% 9%
1	B	240	88% 10%
1	C	240	88% 10%
1	D	240	90% 10%
1	E	240	89% 9%
1	F	240	88% 10%

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Mol	Chain	Length	Quality of chain
1	G	240	2% 90% 8%
1	O	240	4% 89% 10%
1	P	240	2% 88% 9%
1	Q	240	2% 90% 9%
1	R	240	2% 90% 10%
1	S	240	2% 90% 9%
1	T	240	4% 88% 9%
1	U	240	2% 88% 10%
2	H	240	91% 8%
2	I	240	90% 8%
2	J	240	91% 8%
2	K	240	90% 7%
2	L	240	92% 7%
2	M	240	91% 8%
2	N	240	2% 90% 7%
2	V	240	92% 7%
2	W	240	91% 7%
2	X	240	92% 8%
2	Y	240	92% 7%
2	Z	240	91% 8%
2	a	240	91% 7%
2	b	240	92% 7%

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	218	1677	1050	306	317	4	0	0	0
1	B	216	1668	1045	304	315	4	0	0	0
1	C	217	1672	1047	305	316	4	0	0	0
1	D	217	1670	1046	305	315	4	0	0	0
1	E	218	1677	1050	306	317	4	0	0	0
1	F	215	1655	1035	303	313	4	0	0	0
1	G	220	1690	1057	308	321	4	0	0	0
1	O	216	1664	1043	304	313	4	0	0	0
1	P	218	1677	1050	306	317	4	0	0	0
1	Q	218	1678	1050	306	318	4	0	0	0
1	R	217	1670	1046	305	315	4	0	0	0
1	S	218	1678	1050	306	318	4	0	0	0
1	T	218	1679	1051	306	318	4	0	0	0
1	U	217	1670	1046	305	315	4	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP A5U4D5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	initiating methionine	UNP A5U4D5
C	9	MET	-	initiating methionine	UNP A5U4D5
D	9	MET	-	initiating methionine	UNP A5U4D5
E	9	MET	-	initiating methionine	UNP A5U4D5
F	9	MET	-	initiating methionine	UNP A5U4D5
G	9	MET	-	initiating methionine	UNP A5U4D5
O	9	MET	-	initiating methionine	UNP A5U4D5
P	9	MET	-	initiating methionine	UNP A5U4D5
Q	9	MET	-	initiating methionine	UNP A5U4D5
R	9	MET	-	initiating methionine	UNP A5U4D5
S	9	MET	-	initiating methionine	UNP A5U4D5
T	9	MET	-	initiating methionine	UNP A5U4D5
U	9	MET	-	initiating methionine	UNP A5U4D5

- 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	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	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
			Total	C	N	O	S			
2	b	223	1642	1029	283	325	5	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	235	HIS	-	expression tag	UNP A5U4D6
H	236	HIS	-	expression tag	UNP A5U4D6
H	237	HIS	-	expression tag	UNP A5U4D6
H	238	HIS	-	expression tag	UNP A5U4D6
H	239	HIS	-	expression tag	UNP A5U4D6
H	240	HIS	-	expression tag	UNP A5U4D6
I	235	HIS	-	expression tag	UNP A5U4D6
I	236	HIS	-	expression tag	UNP A5U4D6
I	237	HIS	-	expression tag	UNP A5U4D6
I	238	HIS	-	expression tag	UNP A5U4D6
I	239	HIS	-	expression tag	UNP A5U4D6
I	240	HIS	-	expression tag	UNP A5U4D6
J	235	HIS	-	expression tag	UNP A5U4D6
J	236	HIS	-	expression tag	UNP A5U4D6
J	237	HIS	-	expression tag	UNP A5U4D6
J	238	HIS	-	expression tag	UNP A5U4D6
J	239	HIS	-	expression tag	UNP A5U4D6
J	240	HIS	-	expression tag	UNP A5U4D6
K	235	HIS	-	expression tag	UNP A5U4D6
K	236	HIS	-	expression tag	UNP A5U4D6
K	237	HIS	-	expression tag	UNP A5U4D6
K	238	HIS	-	expression tag	UNP A5U4D6
K	239	HIS	-	expression tag	UNP A5U4D6
K	240	HIS	-	expression tag	UNP A5U4D6
L	235	HIS	-	expression tag	UNP A5U4D6
L	236	HIS	-	expression tag	UNP A5U4D6
L	237	HIS	-	expression tag	UNP A5U4D6
L	238	HIS	-	expression tag	UNP A5U4D6
L	239	HIS	-	expression tag	UNP A5U4D6
L	240	HIS	-	expression tag	UNP A5U4D6
M	235	HIS	-	expression tag	UNP A5U4D6
M	236	HIS	-	expression tag	UNP A5U4D6
M	237	HIS	-	expression tag	UNP A5U4D6
M	238	HIS	-	expression tag	UNP A5U4D6
M	239	HIS	-	expression tag	UNP A5U4D6
M	240	HIS	-	expression tag	UNP A5U4D6

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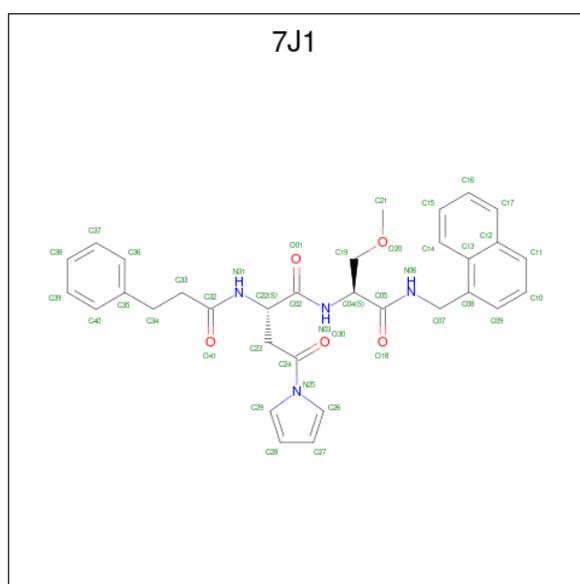
Chain	Residue	Modelled	Actual	Comment	Reference
N	235	HIS	-	expression tag	UNP A5U4D6
N	236	HIS	-	expression tag	UNP A5U4D6
N	237	HIS	-	expression tag	UNP A5U4D6
N	238	HIS	-	expression tag	UNP A5U4D6
N	239	HIS	-	expression tag	UNP A5U4D6
N	240	HIS	-	expression tag	UNP A5U4D6
V	235	HIS	-	expression tag	UNP A5U4D6
V	236	HIS	-	expression tag	UNP A5U4D6
V	237	HIS	-	expression tag	UNP A5U4D6
V	238	HIS	-	expression tag	UNP A5U4D6
V	239	HIS	-	expression tag	UNP A5U4D6
V	240	HIS	-	expression tag	UNP A5U4D6
W	235	HIS	-	expression tag	UNP A5U4D6
W	236	HIS	-	expression tag	UNP A5U4D6
W	237	HIS	-	expression tag	UNP A5U4D6
W	238	HIS	-	expression tag	UNP A5U4D6
W	239	HIS	-	expression tag	UNP A5U4D6
W	240	HIS	-	expression tag	UNP A5U4D6
X	235	HIS	-	expression tag	UNP A5U4D6
X	236	HIS	-	expression tag	UNP A5U4D6
X	237	HIS	-	expression tag	UNP A5U4D6
X	238	HIS	-	expression tag	UNP A5U4D6
X	239	HIS	-	expression tag	UNP A5U4D6
X	240	HIS	-	expression tag	UNP A5U4D6
Y	235	HIS	-	expression tag	UNP A5U4D6
Y	236	HIS	-	expression tag	UNP A5U4D6
Y	237	HIS	-	expression tag	UNP A5U4D6
Y	238	HIS	-	expression tag	UNP A5U4D6
Y	239	HIS	-	expression tag	UNP A5U4D6
Y	240	HIS	-	expression tag	UNP A5U4D6
Z	235	HIS	-	expression tag	UNP A5U4D6
Z	236	HIS	-	expression tag	UNP A5U4D6
Z	237	HIS	-	expression tag	UNP A5U4D6
Z	238	HIS	-	expression tag	UNP A5U4D6
Z	239	HIS	-	expression tag	UNP A5U4D6
Z	240	HIS	-	expression tag	UNP A5U4D6
a	235	HIS	-	expression tag	UNP A5U4D6
a	236	HIS	-	expression tag	UNP A5U4D6
a	237	HIS	-	expression tag	UNP A5U4D6
a	238	HIS	-	expression tag	UNP A5U4D6
a	239	HIS	-	expression tag	UNP A5U4D6
a	240	HIS	-	expression tag	UNP A5U4D6

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Chain	Residue	Modelled	Actual	Comment	Reference
b	235	HIS	-	expression tag	UNP A5U4D6
b	236	HIS	-	expression tag	UNP A5U4D6
b	237	HIS	-	expression tag	UNP A5U4D6
b	238	HIS	-	expression tag	UNP A5U4D6
b	239	HIS	-	expression tag	UNP A5U4D6
b	240	HIS	-	expression tag	UNP A5U4D6

- Molecule 3 is (2S)-N-{(2S)-3-methoxy-1-[(naphthalen-1-ylmethyl)amino]-1-oxopropan-2-yl}-4-oxo-2-[(3-phenylpropanoyl)amino]-4-(1H-pyrrol-1-yl)butanamide (non-preferred name) (three-letter code: 7J1) (formula: C₃₂H₃₄N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			41	32	4	5		
3	I	1	Total	C	N	O	0	0
			41	32	4	5		
3	J	1	Total	C	N	O	0	0
			41	32	4	5		
3	K	1	Total	C	N	O	0	0
			41	32	4	5		
3	L	1	Total	C	N	O	0	0
			41	32	4	5		
3	M	1	Total	C	N	O	0	0
			41	32	4	5		
3	N	1	Total	C	N	O	0	0
			41	32	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	V	1	Total	C	N	O	0	0
			41	32	4	5		
3	W	1	Total	C	N	O	0	0
			41	32	4	5		
3	X	1	Total	C	N	O	0	0
			41	32	4	5		
3	Y	1	Total	C	N	O	0	0
			41	32	4	5		
3	Z	1	Total	C	N	O	0	0
			41	32	4	5		
3	a	1	Total	C	N	O	0	0
			41	32	4	5		
3	b	1	Total	C	N	O	0	0
			41	32	4	5		

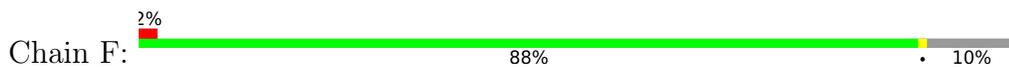
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	7	Total	O	0	0
			7	7		
4	C	9	Total	O	0	0
			9	9		
4	D	5	Total	O	0	0
			5	5		
4	E	7	Total	O	0	0
			7	7		
4	F	8	Total	O	0	0
			8	8		
4	G	4	Total	O	0	0
			4	4		
4	H	14	Total	O	0	0
			14	14		
4	I	25	Total	O	0	0
			25	25		
4	J	13	Total	O	0	0
			13	13		
4	K	19	Total	O	0	0
			19	19		
4	L	14	Total	O	0	0
			14	14		

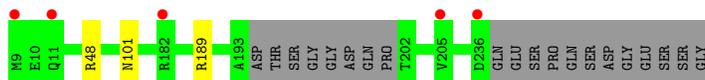
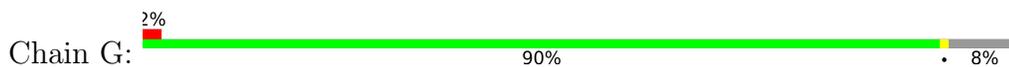
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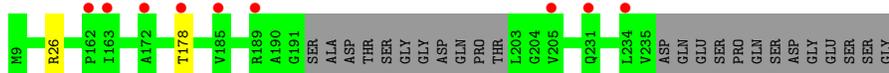
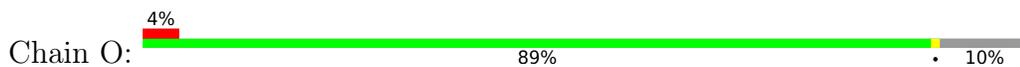
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	20	Total 20	O 20	0	0
4	N	11	Total 11	O 11	0	0
4	O	10	Total 10	O 10	0	0
4	P	4	Total 4	O 4	0	0
4	Q	5	Total 5	O 5	0	0
4	R	9	Total 9	O 9	0	0
4	S	15	Total 15	O 15	0	0
4	T	6	Total 6	O 6	0	0
4	U	10	Total 10	O 10	0	0
4	V	19	Total 19	O 19	0	0
4	W	12	Total 12	O 12	0	0
4	X	13	Total 13	O 13	0	0
4	Y	26	Total 26	O 26	0	0
4	Z	19	Total 19	O 19	0	0
4	a	16	Total 16	O 16	0	0
4	b	16	Total 16	O 16	0	0



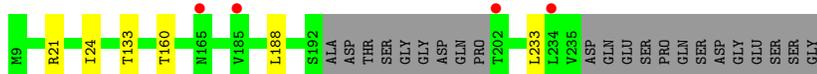
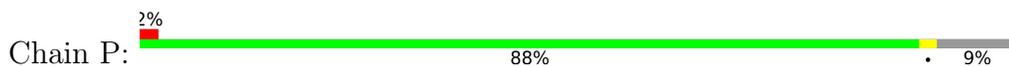
- Molecule 1: Proteasome subunit alpha



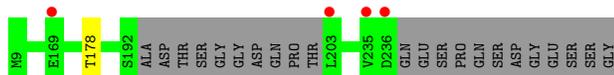
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



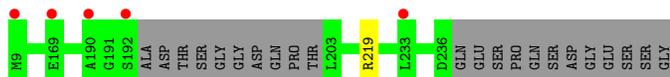
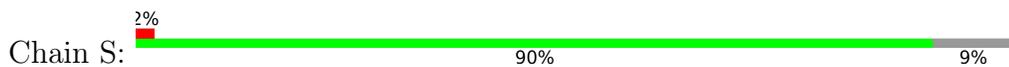
- Molecule 1: Proteasome subunit alpha



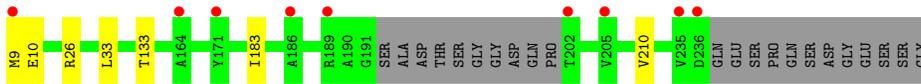
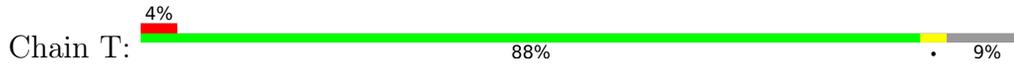
- Molecule 1: Proteasome subunit alpha



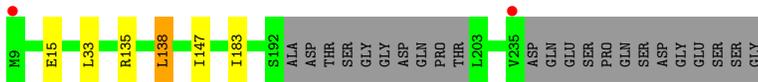
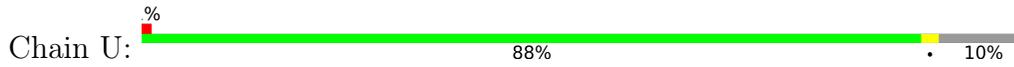
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



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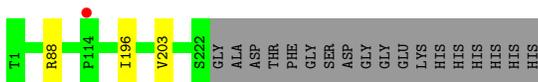
- Molecule 2: Proteasome subunit beta



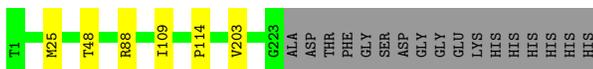
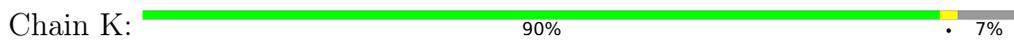
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta

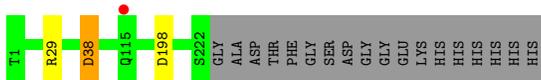


- Molecule 2: Proteasome subunit beta



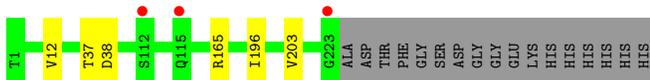
- Molecule 2: Proteasome subunit beta

Chain M:  91% 8%



- Molecule 2: Proteasome subunit beta

Chain N:  90% 7%



- Molecule 2: Proteasome subunit beta

Chain V:  92% 7%



- Molecule 2: Proteasome subunit beta

Chain W:  91% 7%



- Molecule 2: Proteasome subunit beta

Chain X:  92% 8%



- Molecule 2: Proteasome subunit beta

Chain Y:  92% 7%



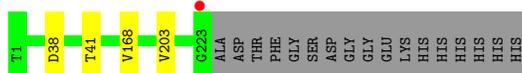
- Molecule 2: Proteasome subunit beta

Chain Z:  91% 8%



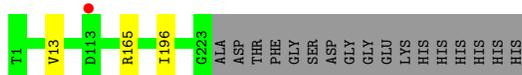
- Molecule 2: Proteasome subunit beta

Chain a:  91% 7%



• Molecule 2: Proteasome subunit beta

Chain b:  92% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.55Å 198.54Å 165.72Å 90.00° 103.24° 90.00°	Depositor
Resolution (Å)	49.61 – 2.85 49.83 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.61-2.85) 94.2 (49.83-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.86Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.177 , 0.235 0.178 , 0.235	Depositor DCC
R_{free} test set	8304 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtrriage
Anisotropy	0.092	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	47311	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 7J1

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	0.53	0/1701	0.72	0/2297
1	B	0.50	0/1692	0.73	2/2285 (0.1%)
1	C	0.48	0/1696	0.68	0/2290
1	D	0.53	1/1694 (0.1%)	0.72	0/2287
1	E	0.49	0/1701	0.71	0/2297
1	F	0.51	0/1679	0.71	0/2266
1	G	0.47	0/1714	0.71	0/2315
1	O	0.50	0/1688	0.70	0/2279
1	P	0.49	0/1701	0.72	3/2297 (0.1%)
1	Q	0.51	0/1702	0.72	0/2298
1	R	0.51	0/1694	0.73	0/2287
1	S	0.51	0/1702	0.72	1/2298 (0.0%)
1	T	0.56	2/1703 (0.1%)	0.77	3/2300 (0.1%)
1	U	0.57	2/1694 (0.1%)	0.81	3/2287 (0.1%)
2	H	0.49	0/1662	0.73	0/2254
2	I	0.52	1/1662 (0.1%)	0.75	0/2254
2	J	0.49	0/1662	0.75	0/2254
2	K	0.48	0/1666	0.76	0/2259
2	L	0.50	0/1666	0.72	0/2259
2	M	0.48	0/1662	0.72	2/2254 (0.1%)
2	N	0.49	0/1666	0.75	0/2259
2	V	0.48	0/1666	0.71	1/2259 (0.0%)
2	W	0.52	0/1666	0.76	1/2259 (0.0%)
2	X	0.52	0/1662	0.75	0/2254
2	Y	0.54	0/1666	0.73	1/2259 (0.0%)
2	Z	0.52	0/1662	0.75	1/2254 (0.0%)
2	a	0.49	0/1666	0.73	1/2259 (0.0%)
2	b	0.54	0/1666	0.74	0/2259
All	All	0.51	6/47061 (0.0%)	0.73	19/63679 (0.0%)

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
2	Y	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	15	GLU	CD-OE2	-7.91	1.17	1.25
1	T	10	GLU	CB-CG	6.17	1.63	1.52
1	D	216	ASN	C-N	-5.87	1.20	1.34
1	T	10	GLU	CG-CD	5.26	1.59	1.51
1	U	15	GLU	CD-OE1	-5.19	1.20	1.25

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	15	GLU	CA-CB-CG	-9.44	92.64	113.40
2	Y	82	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	T	9	MET	CB-CG-SD	6.70	132.49	112.40
1	T	9	MET	N-CA-C	6.67	129.00	111.00
1	S	219	ARG	NE-CZ-NH1	6.21	123.40	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Y	128	GLY	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	208 (97%)	6 (3%)	0	100	100
1	B	212/240 (88%)	208 (98%)	4 (2%)	0	100	100
1	C	213/240 (89%)	205 (96%)	5 (2%)	3 (1%)	11	24
1	D	213/240 (89%)	204 (96%)	9 (4%)	0	100	100
1	E	214/240 (89%)	207 (97%)	7 (3%)	0	100	100
1	F	211/240 (88%)	204 (97%)	7 (3%)	0	100	100
1	G	216/240 (90%)	211 (98%)	5 (2%)	0	100	100
1	O	212/240 (88%)	204 (96%)	8 (4%)	0	100	100
1	P	214/240 (89%)	208 (97%)	6 (3%)	0	100	100
1	Q	214/240 (89%)	207 (97%)	7 (3%)	0	100	100
1	R	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
1	S	214/240 (89%)	205 (96%)	9 (4%)	0	100	100
1	T	214/240 (89%)	207 (97%)	7 (3%)	0	100	100
1	U	213/240 (89%)	205 (96%)	8 (4%)	0	100	100
2	H	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	I	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	J	220/240 (92%)	215 (98%)	5 (2%)	0	100	100
2	K	221/240 (92%)	217 (98%)	3 (1%)	1 (0%)	29	51
2	L	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	M	220/240 (92%)	215 (98%)	5 (2%)	0	100	100
2	N	221/240 (92%)	215 (97%)	6 (3%)	0	100	100
2	V	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	W	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	X	220/240 (92%)	213 (97%)	6 (3%)	1 (0%)	29	51
2	Y	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	Z	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	a	221/240 (92%)	216 (98%)	5 (2%)	0	100	100
2	b	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
All	All	6075/6720 (90%)	5921 (98%)	149 (2%)	5 (0%)	51	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	190	ALA
1	C	234	LEU
1	C	151	PRO
2	X	114	PRO
2	K	114	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/184 (91%)	163 (98%)	4 (2%)	49	72
1	B	166/184 (90%)	164 (99%)	2 (1%)	71	85
1	C	166/184 (90%)	163 (98%)	3 (2%)	59	78
1	D	166/184 (90%)	165 (99%)	1 (1%)	86	93
1	E	167/184 (91%)	162 (97%)	5 (3%)	41	65
1	F	164/184 (89%)	161 (98%)	3 (2%)	59	78
1	G	168/184 (91%)	165 (98%)	3 (2%)	59	78
1	O	165/184 (90%)	163 (99%)	2 (1%)	71	85
1	P	167/184 (91%)	164 (98%)	3 (2%)	59	78
1	Q	167/184 (91%)	166 (99%)	1 (1%)	86	93
1	R	166/184 (90%)	164 (99%)	2 (1%)	71	85
1	S	167/184 (91%)	167 (100%)	0	100	100
1	T	167/184 (91%)	163 (98%)	4 (2%)	49	72
1	U	166/184 (90%)	162 (98%)	4 (2%)	49	72
2	H	165/178 (93%)	161 (98%)	4 (2%)	49	72
2	I	165/178 (93%)	160 (97%)	5 (3%)	41	65
2	J	165/178 (93%)	162 (98%)	3 (2%)	59	78
2	K	165/178 (93%)	160 (97%)	5 (3%)	41	65
2	L	165/178 (93%)	164 (99%)	1 (1%)	86	93
2	M	165/178 (93%)	163 (99%)	2 (1%)	71	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	165/178 (93%)	159 (96%)	6 (4%)	35	60
2	V	165/178 (93%)	164 (99%)	1 (1%)	86	93
2	W	165/178 (93%)	162 (98%)	3 (2%)	59	78
2	X	165/178 (93%)	164 (99%)	1 (1%)	86	93
2	Y	165/178 (93%)	164 (99%)	1 (1%)	86	93
2	Z	165/178 (93%)	162 (98%)	3 (2%)	59	78
2	a	165/178 (93%)	162 (98%)	3 (2%)	59	78
2	b	165/178 (93%)	162 (98%)	3 (2%)	59	78
All	All	4639/5068 (92%)	4561 (98%)	78 (2%)	60	80

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	183	ILE
2	Z	219	GLU
1	U	135	ARG
2	W	72	VAL
2	b	13	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	129	HIS
2	K	110	HIS
2	b	137	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	7J1	Y	301	-	42,44,44	2.06	9 (21%)	52,58,58	1.08	6 (11%)
3	7J1	X	301	-	42,44,44	2.17	8 (19%)	52,58,58	1.12	5 (9%)
3	7J1	H	301	-	42,44,44	2.55	8 (19%)	52,58,58	1.18	5 (9%)
3	7J1	L	301	-	42,44,44	2.44	8 (19%)	52,58,58	1.15	6 (11%)
3	7J1	a	301	-	42,44,44	2.46	9 (21%)	52,58,58	1.06	2 (3%)
3	7J1	Z	301	-	42,44,44	2.36	7 (16%)	52,58,58	1.14	5 (9%)
3	7J1	J	301	-	42,44,44	2.18	9 (21%)	52,58,58	1.27	7 (13%)
3	7J1	K	301	-	42,44,44	2.63	8 (19%)	52,58,58	1.10	3 (5%)
3	7J1	b	301	-	42,44,44	2.50	10 (23%)	52,58,58	1.06	3 (5%)
3	7J1	M	301	-	42,44,44	2.08	9 (21%)	52,58,58	1.28	9 (17%)
3	7J1	N	301	-	42,44,44	2.25	8 (19%)	52,58,58	1.04	3 (5%)
3	7J1	W	301	-	42,44,44	2.21	11 (26%)	52,58,58	1.22	4 (7%)
3	7J1	V	301	-	42,44,44	2.49	8 (19%)	52,58,58	1.07	5 (9%)
3	7J1	I	301	-	42,44,44	2.50	9 (21%)	52,58,58	1.08	2 (3%)

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	7J1	Y	301	-	-	2/33/37/37	0/4/4/4
3	7J1	X	301	-	-	3/33/37/37	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7J1	H	301	-	-	5/33/37/37	0/4/4/4
3	7J1	L	301	-	-	2/33/37/37	0/4/4/4
3	7J1	a	301	-	-	3/33/37/37	0/4/4/4
3	7J1	Z	301	-	-	3/33/37/37	0/4/4/4
3	7J1	J	301	-	-	3/33/37/37	0/4/4/4
3	7J1	K	301	-	-	6/33/37/37	0/4/4/4
3	7J1	b	301	-	-	1/33/37/37	0/4/4/4
3	7J1	M	301	-	-	2/33/37/37	0/4/4/4
3	7J1	N	301	-	-	3/33/37/37	0/4/4/4
3	7J1	W	301	-	-	5/33/37/37	0/4/4/4
3	7J1	V	301	-	-	3/33/37/37	0/4/4/4
3	7J1	I	301	-	-	3/33/37/37	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	301	7J1	C26-C27	8.98	1.57	1.38
3	K	301	7J1	C29-C28	8.77	1.57	1.38
3	K	301	7J1	C26-C27	8.55	1.56	1.38
3	a	301	7J1	C26-N25	8.53	1.51	1.39
3	Z	301	7J1	C29-C28	8.17	1.55	1.38

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	301	7J1	C33-C32-N31	4.06	122.88	115.83
3	I	301	7J1	C23-C22-C02	-3.86	101.33	110.42
3	H	301	7J1	C33-C32-N31	3.52	121.93	115.83
3	X	301	7J1	C19-C04-C05	-3.40	102.33	110.32
3	W	301	7J1	C23-C22-C02	-3.31	102.62	110.42

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	301	7J1	N03-C04-C19-O20
3	H	301	7J1	C05-C04-C19-O20
3	I	301	7J1	N03-C04-C19-O20
3	I	301	7J1	C05-C04-C19-O20

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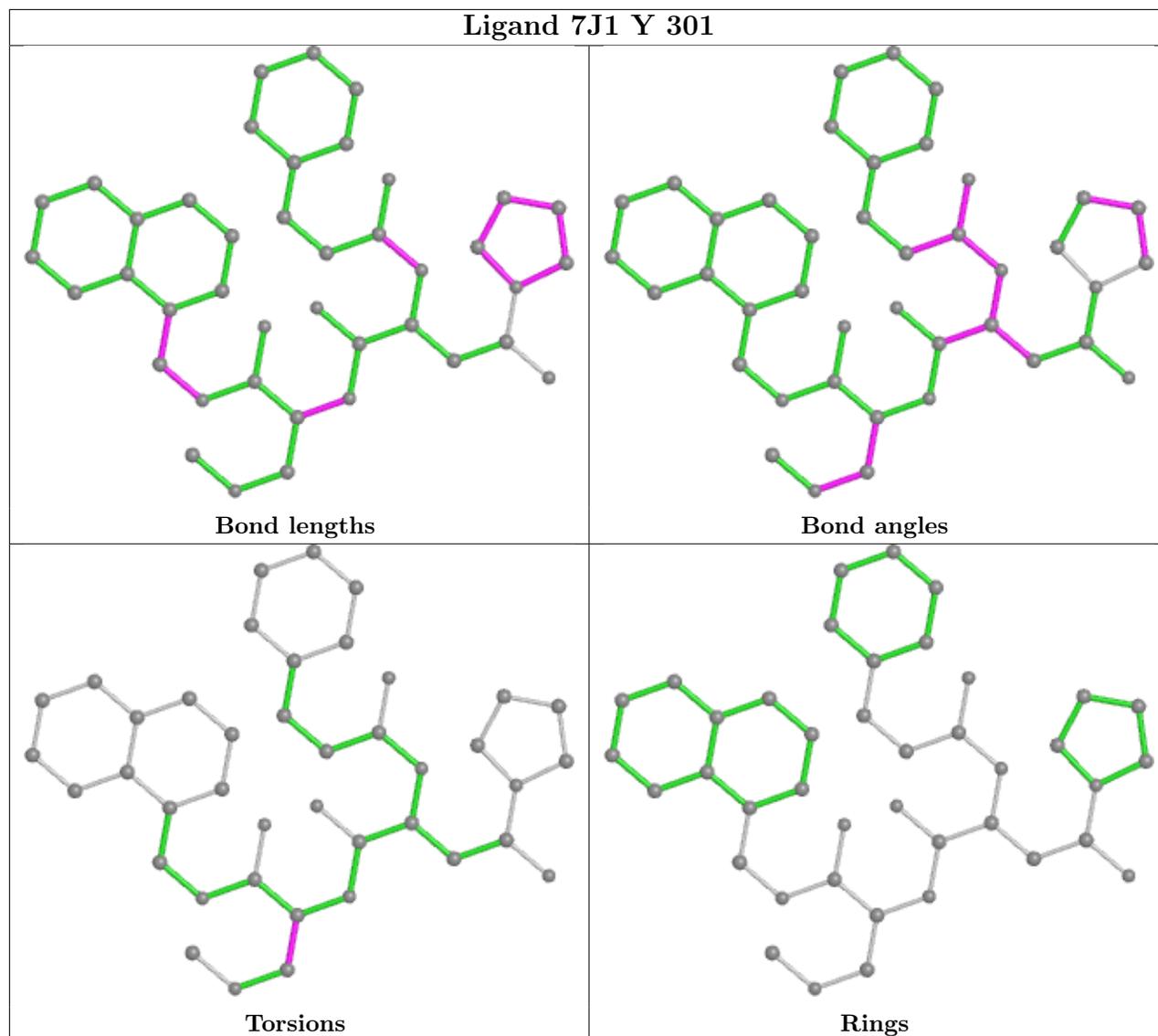
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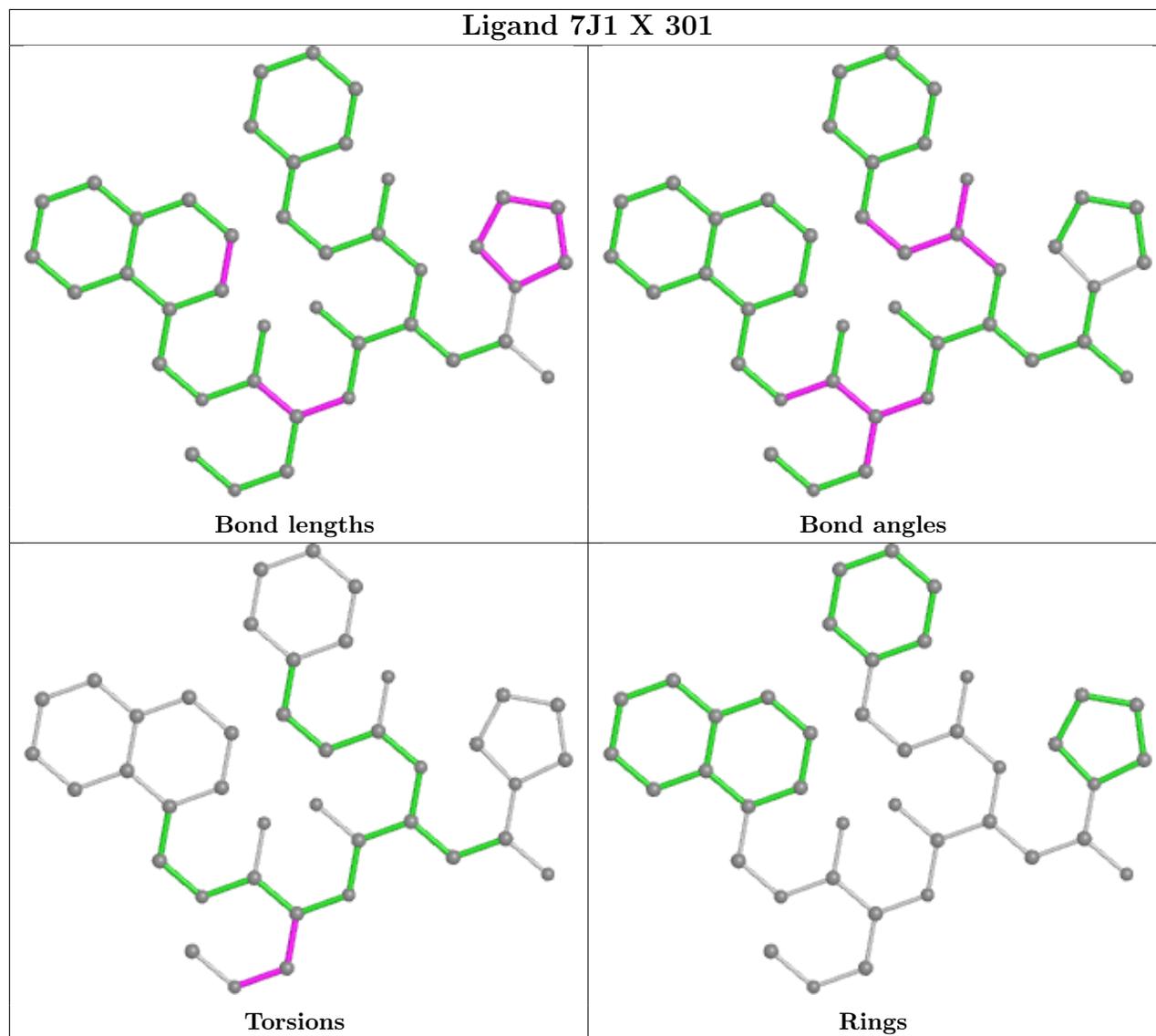
Mol	Chain	Res	Type	Atoms
3	J	301	7J1	C05-C04-C19-O20

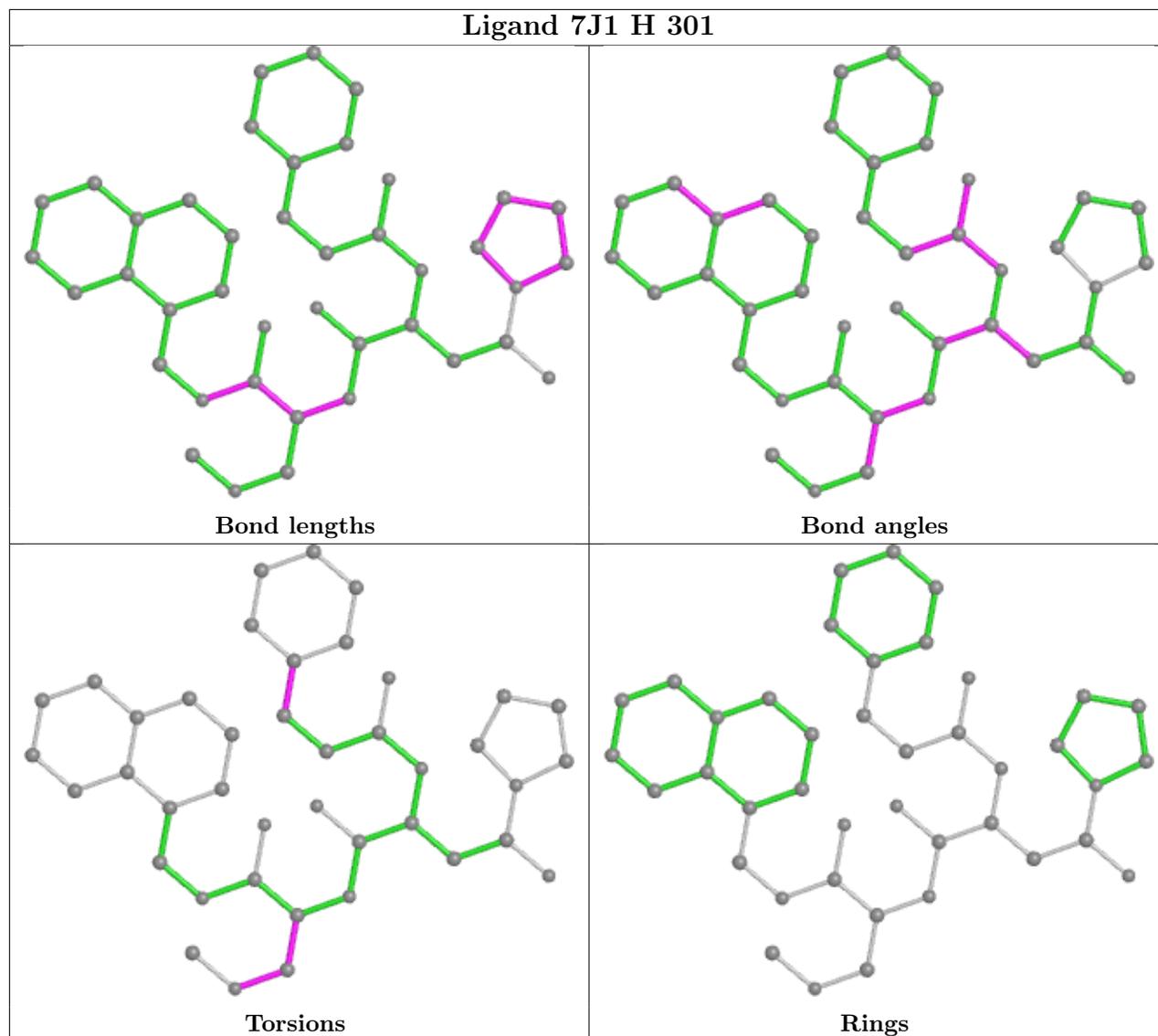
There are no ring outliers.

No monomer is involved in short contacts.

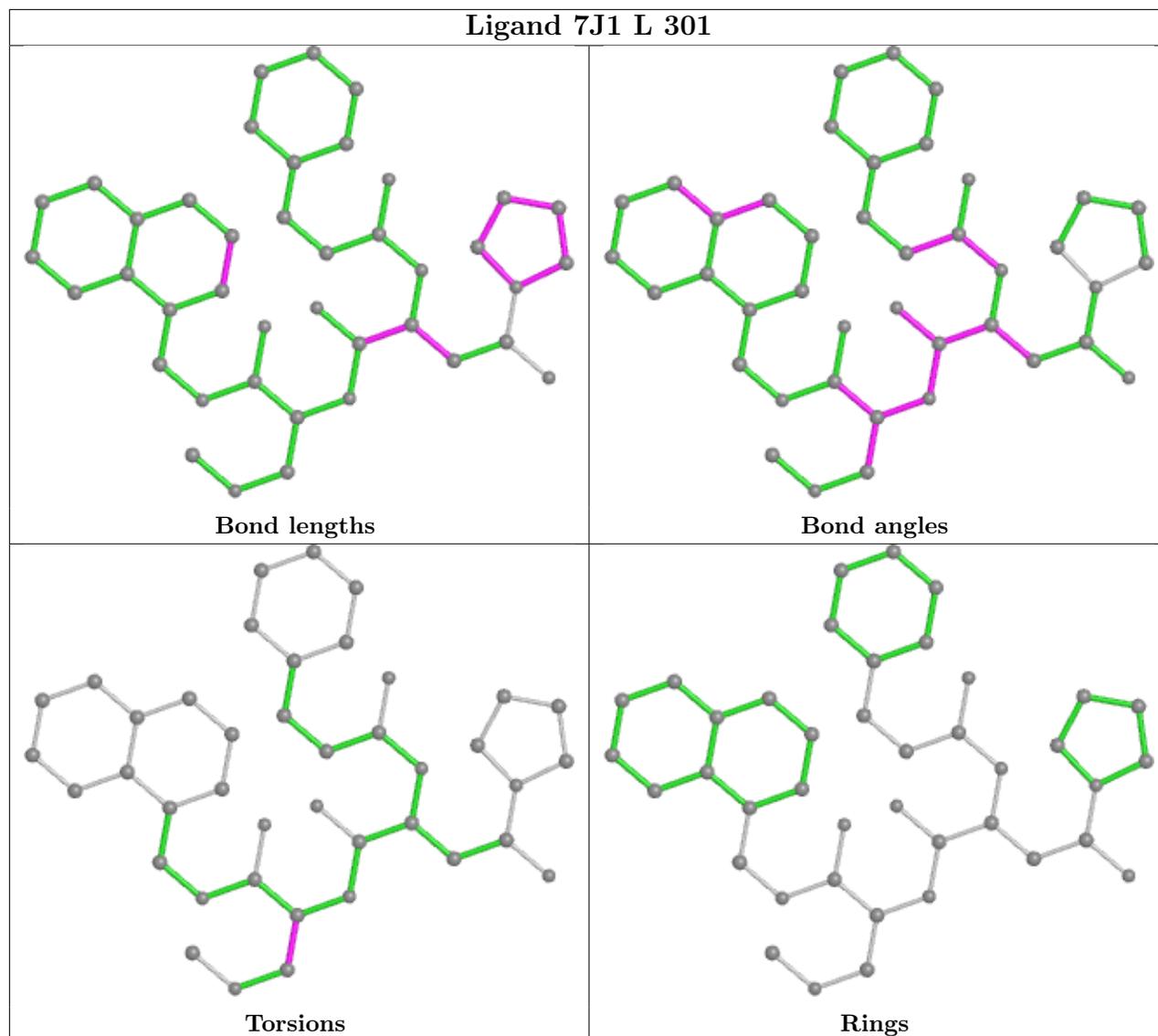
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

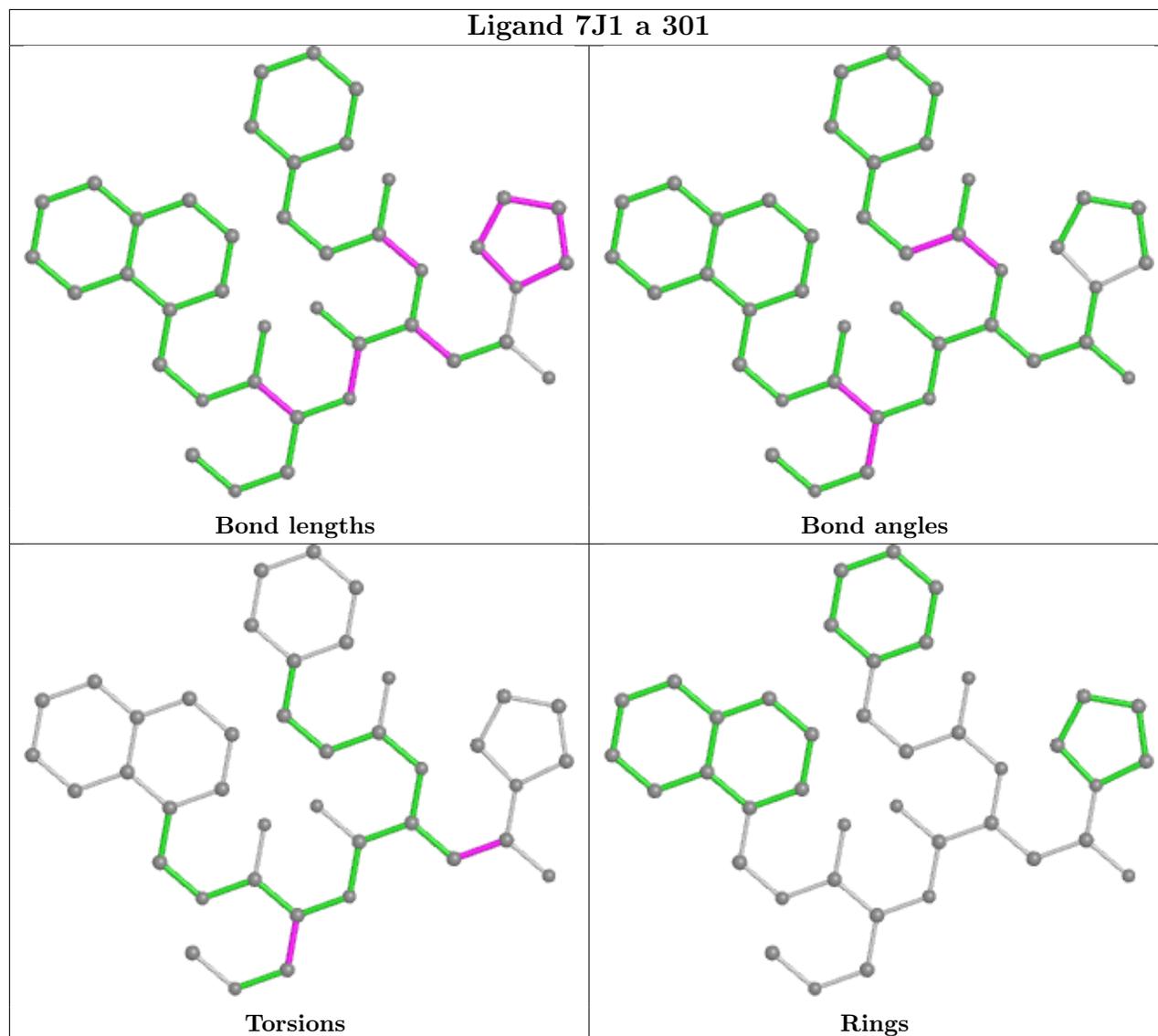




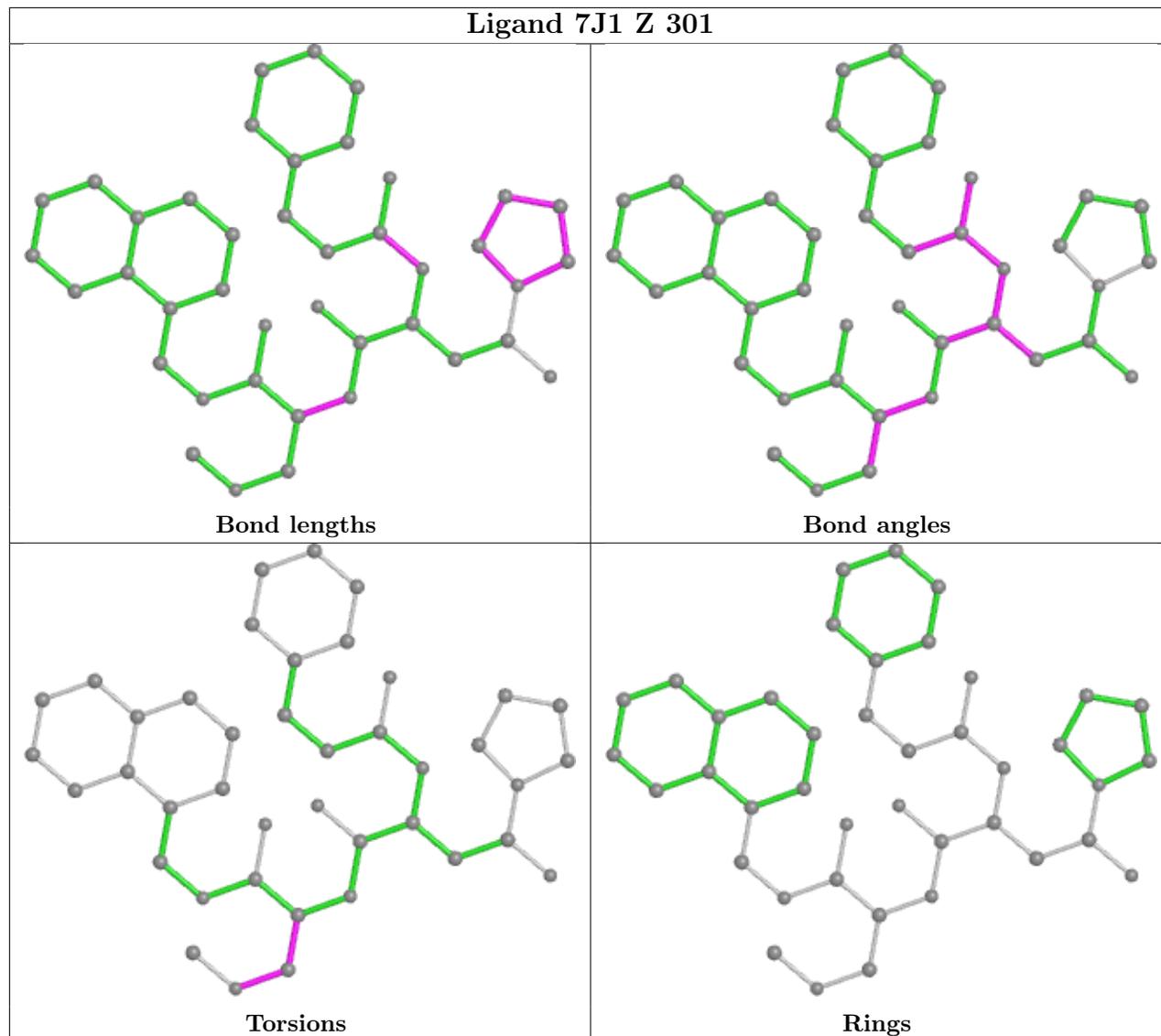


Ligand 7J1 L 301

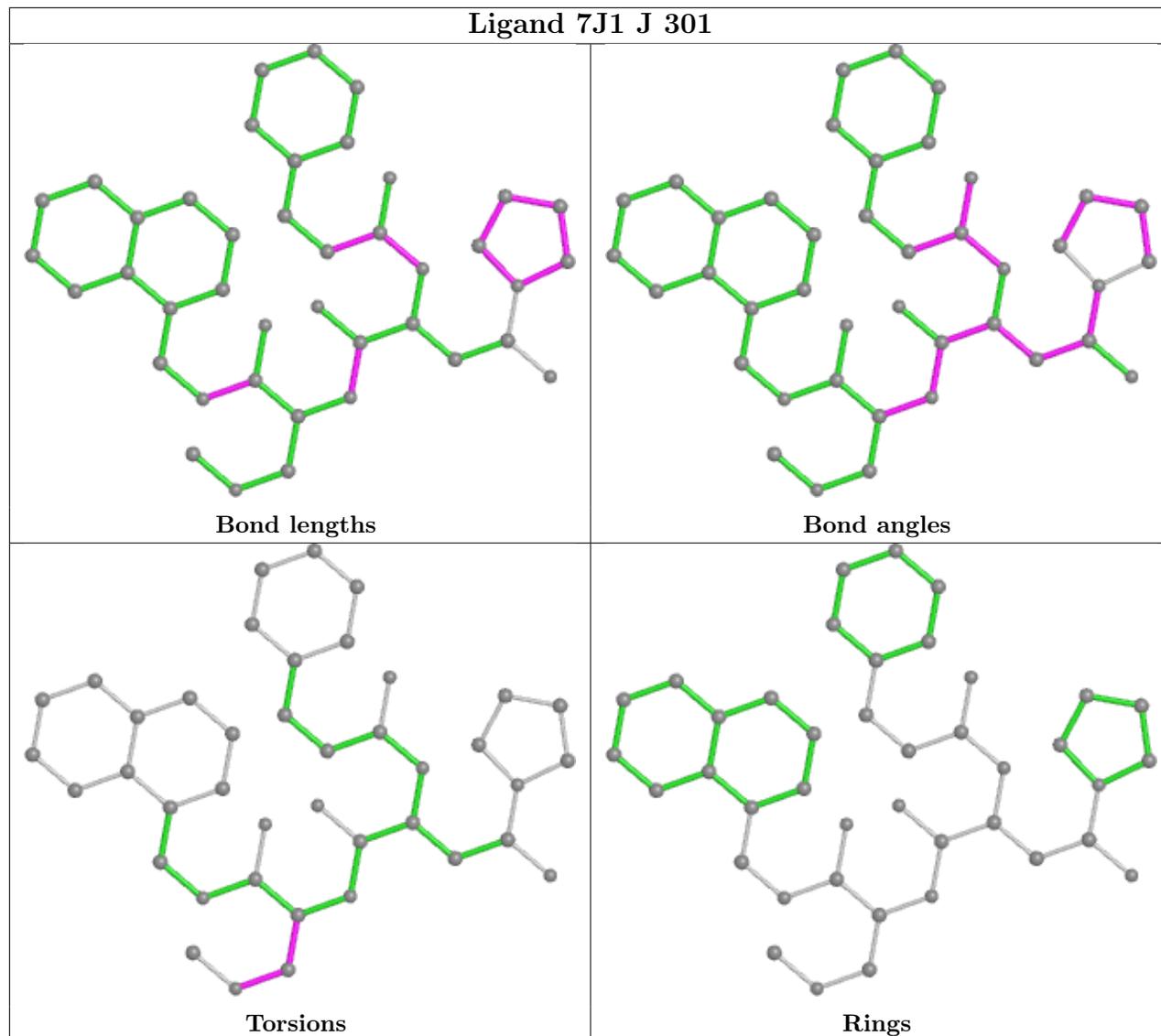


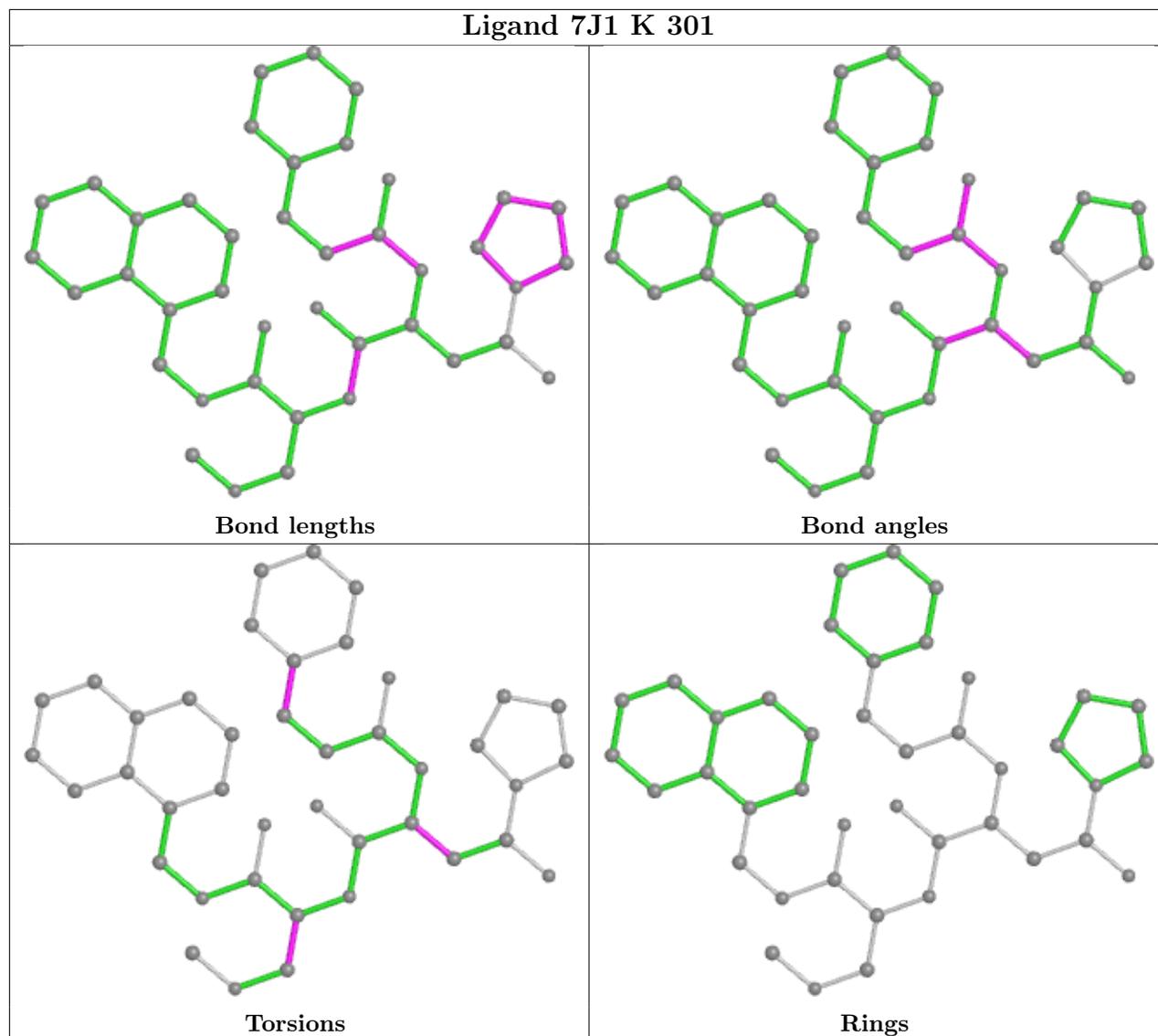


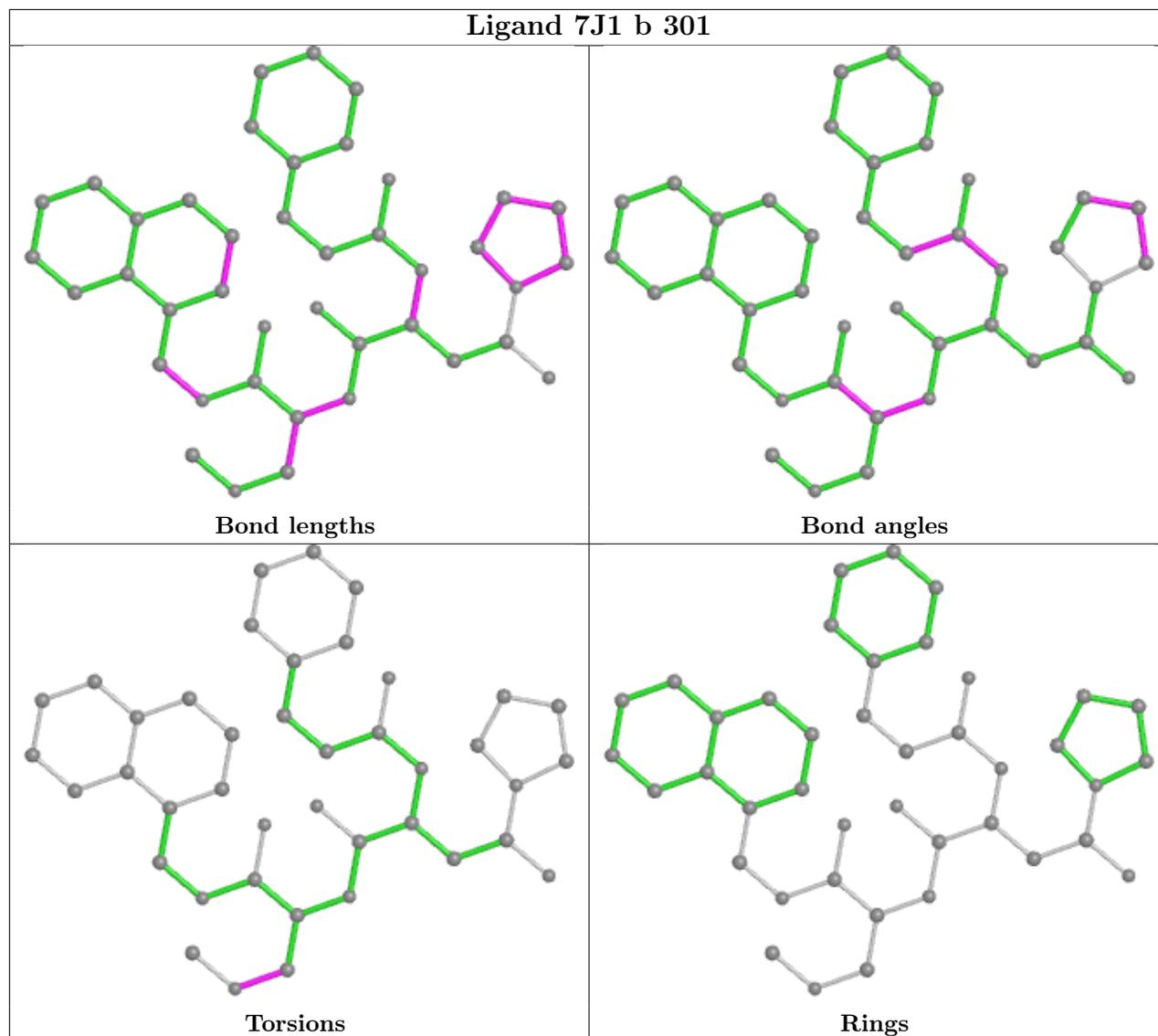
Ligand 7J1 Z 301

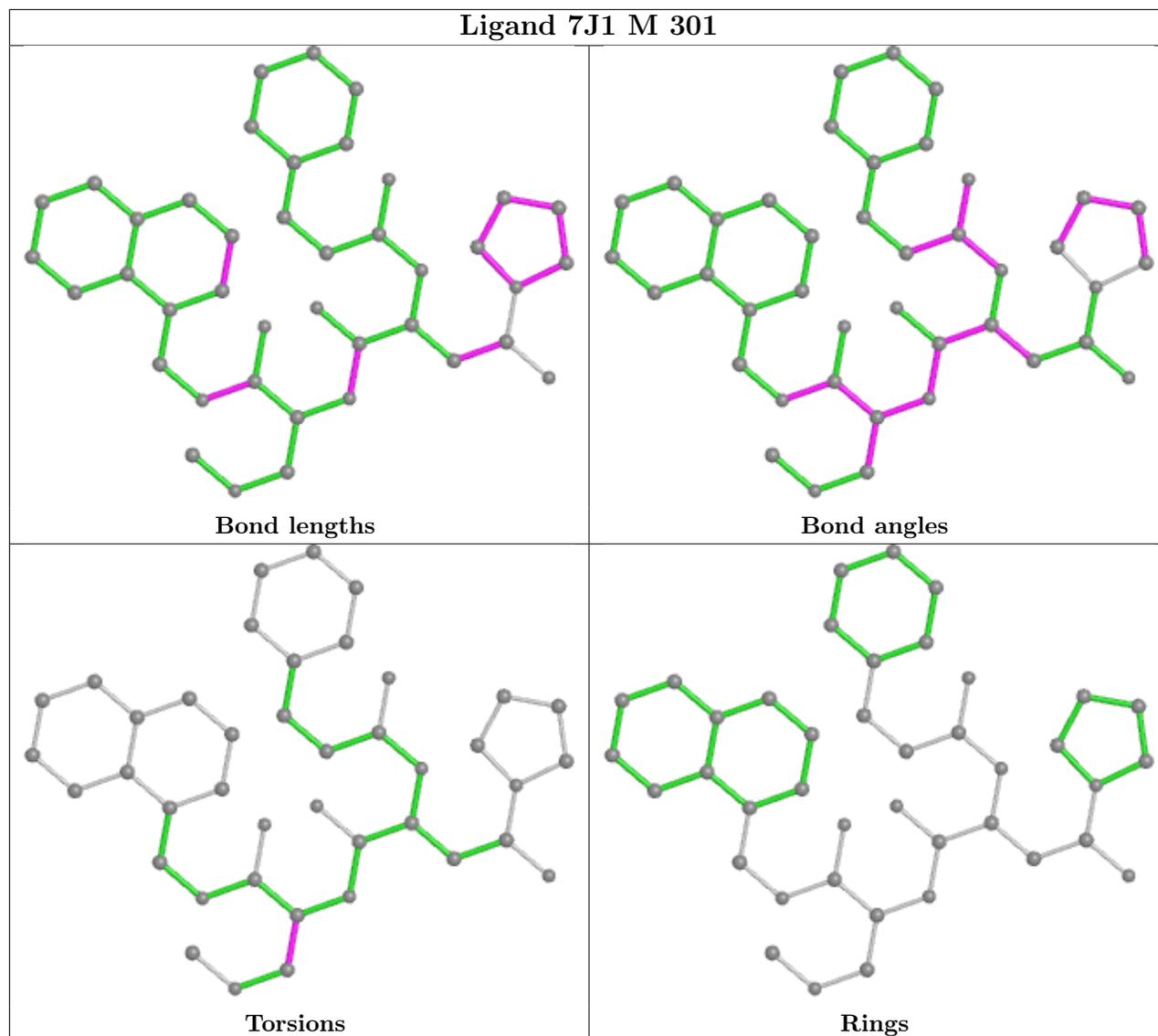


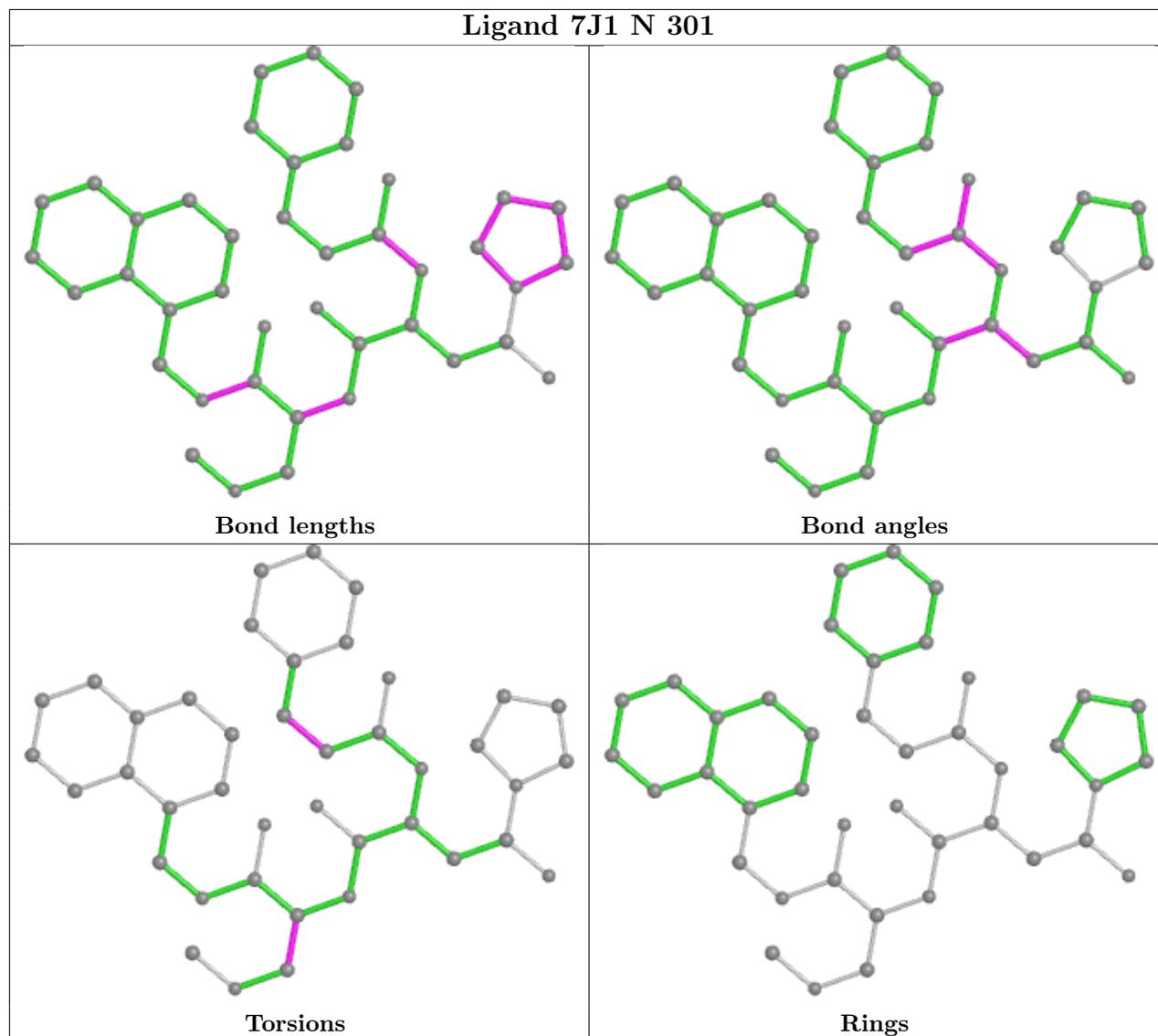
Ligand 7J1 J 301

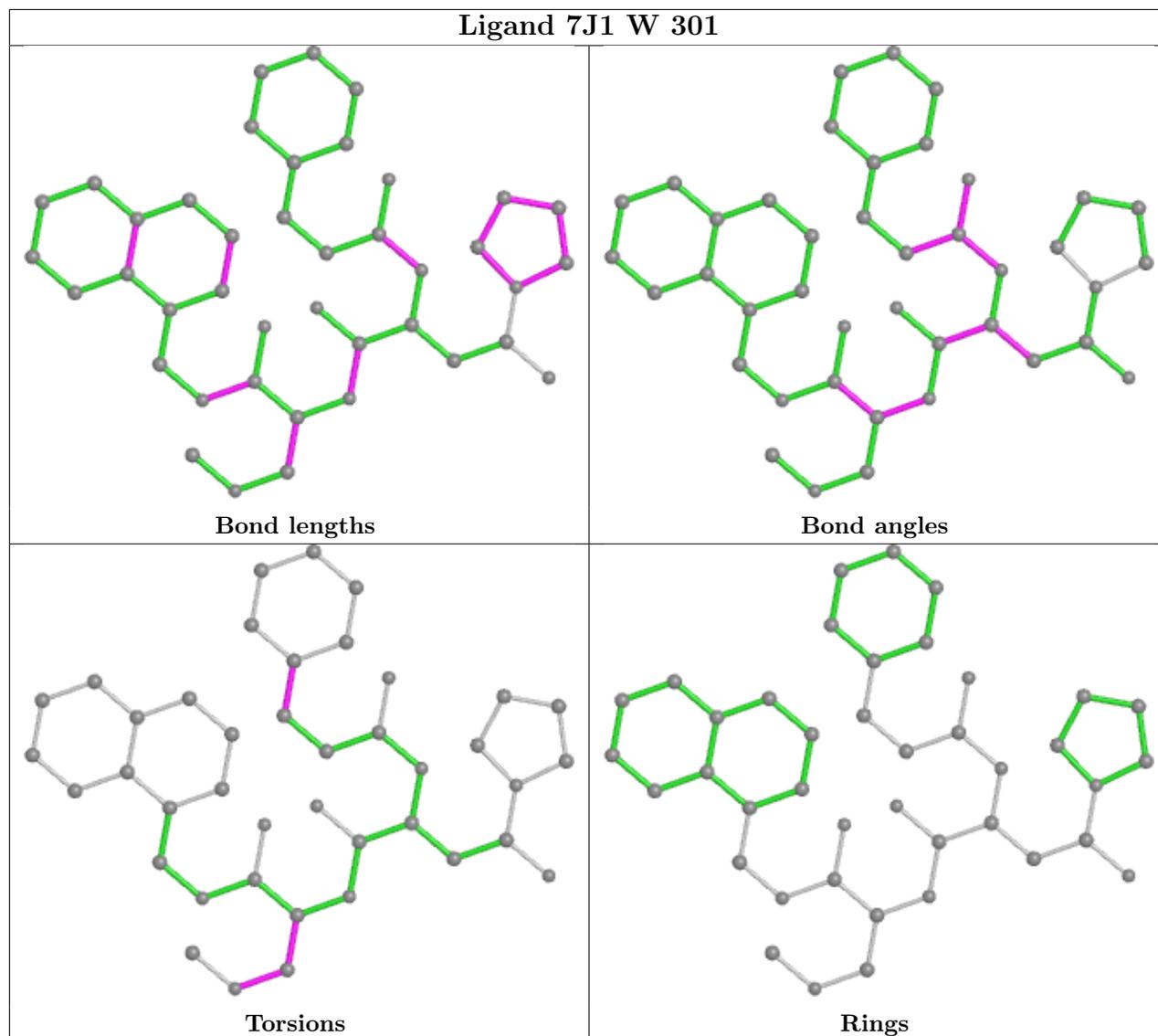


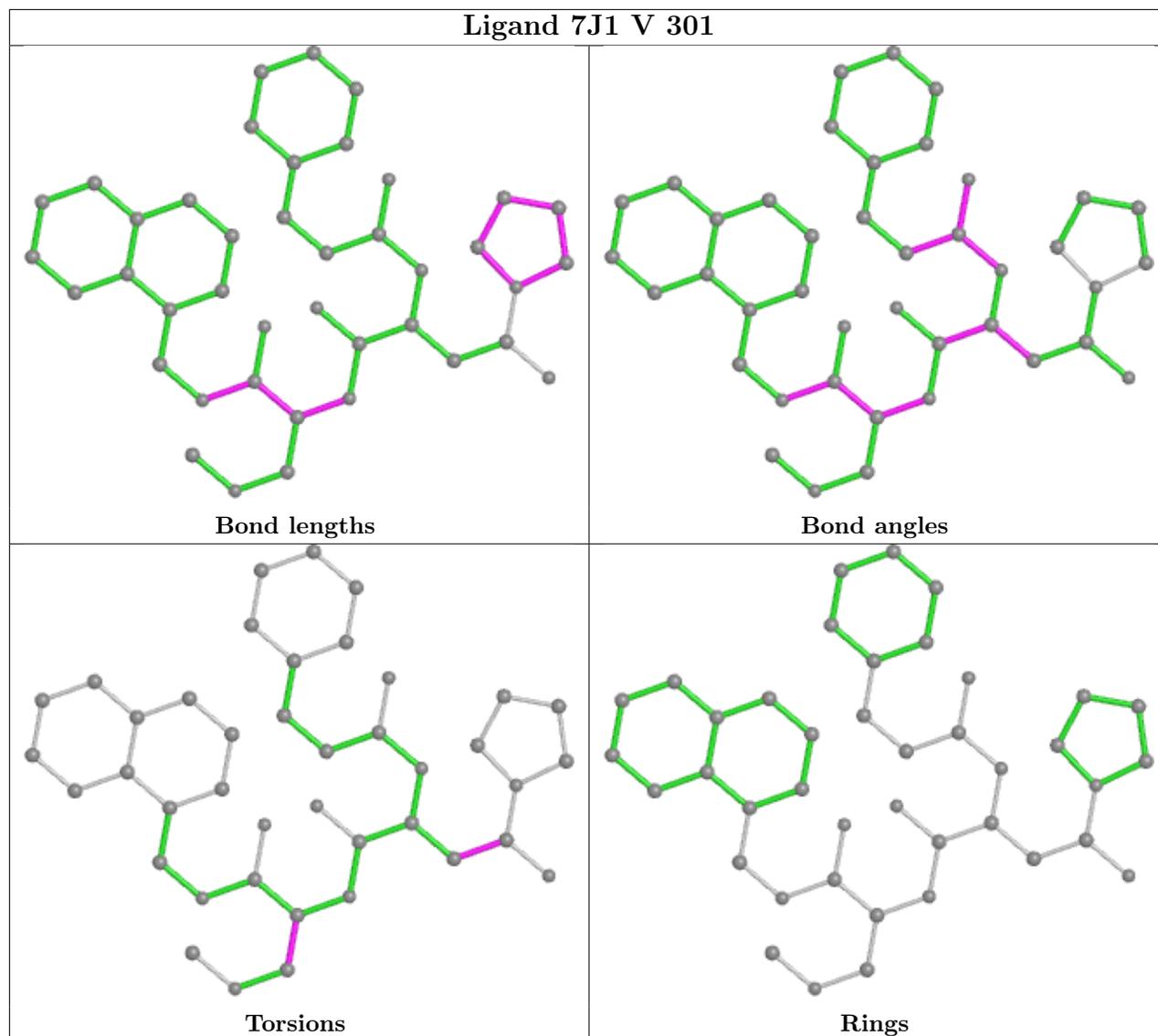


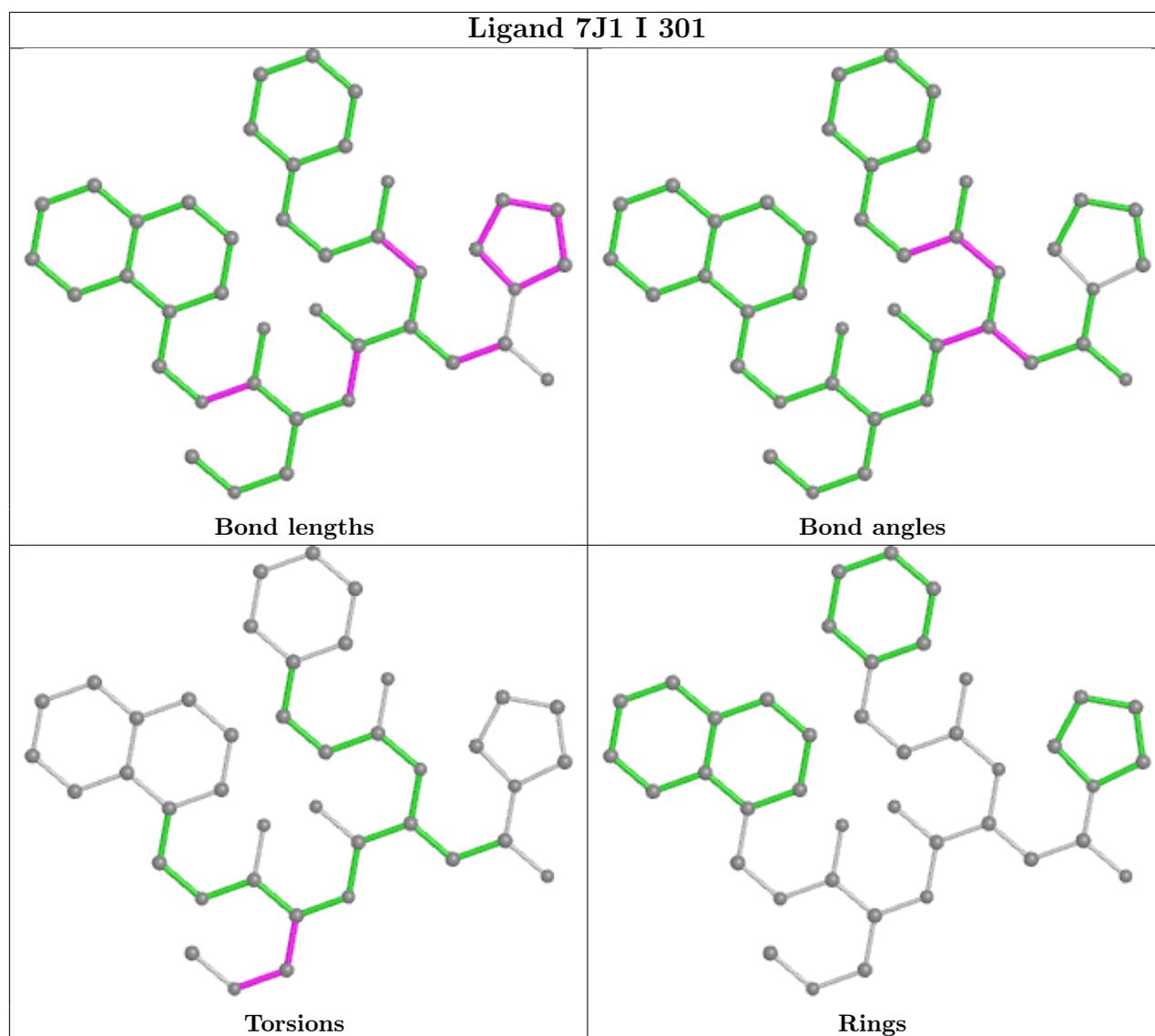












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/240 (90%)	-0.27	3 (1%) 75 71	30, 50, 78, 104	0
1	B	216/240 (90%)	-0.13	6 (2%) 53 47	34, 59, 93, 129	0
1	C	217/240 (90%)	-0.11	7 (3%) 47 41	34, 63, 97, 118	0
1	D	217/240 (90%)	-0.01	5 (2%) 60 55	34, 61, 91, 112	0
1	E	218/240 (90%)	-0.16	5 (2%) 60 55	28, 59, 87, 129	0
1	F	215/240 (89%)	-0.11	5 (2%) 60 55	34, 63, 93, 108	0
1	G	220/240 (91%)	-0.36	5 (2%) 60 55	33, 53, 83, 103	0
1	O	216/240 (90%)	-0.00	9 (4%) 36 28	30, 65, 99, 127	0
1	P	218/240 (90%)	-0.18	4 (1%) 68 63	34, 58, 90, 117	0
1	Q	218/240 (90%)	-0.18	4 (1%) 68 63	30, 53, 81, 124	0
1	R	217/240 (90%)	-0.15	4 (1%) 68 63	30, 53, 81, 99	0
1	S	218/240 (90%)	-0.21	5 (2%) 60 55	28, 50, 89, 104	0
1	T	218/240 (90%)	-0.08	9 (4%) 37 29	33, 59, 91, 118	0
1	U	217/240 (90%)	-0.29	2 (0%) 84 83	32, 52, 87, 105	0
2	H	222/240 (92%)	-0.32	1 (0%) 91 89	30, 44, 67, 111	0
2	I	222/240 (92%)	-0.45	0 100 100	29, 40, 60, 78	0
2	J	222/240 (92%)	-0.52	1 (0%) 91 89	30, 42, 65, 103	0
2	K	223/240 (92%)	-0.41	0 100 100	28, 45, 66, 84	0
2	L	223/240 (92%)	-0.43	1 (0%) 92 91	31, 43, 70, 95	0
2	M	222/240 (92%)	-0.42	1 (0%) 91 89	30, 44, 68, 111	0
2	N	223/240 (92%)	-0.31	3 (1%) 77 74	34, 49, 76, 115	0
2	V	223/240 (92%)	-0.39	0 100 100	31, 41, 63, 79	0
2	W	223/240 (92%)	-0.38	1 (0%) 92 91	30, 42, 66, 92	0
2	X	222/240 (92%)	-0.49	0 100 100	29, 40, 64, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	Y	223/240 (92%)	-0.44	0 100 100	28, 41, 63, 99	0
2	Z	222/240 (92%)	-0.44	0 100 100	29, 42, 68, 95	0
2	a	223/240 (92%)	-0.42	1 (0%) 92 91	32, 46, 75, 99	0
2	b	223/240 (92%)	-0.40	1 (0%) 92 91	28, 42, 64, 97	0
All	All	6159/6720 (91%)	-0.29	83 (1%) 77 74	28, 48, 86, 129	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	223	GLY	7.3
1	A	183	ILE	4.9
1	U	9	MET	4.3
2	N	115	GLN	4.3
1	T	189	ARG	3.9

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

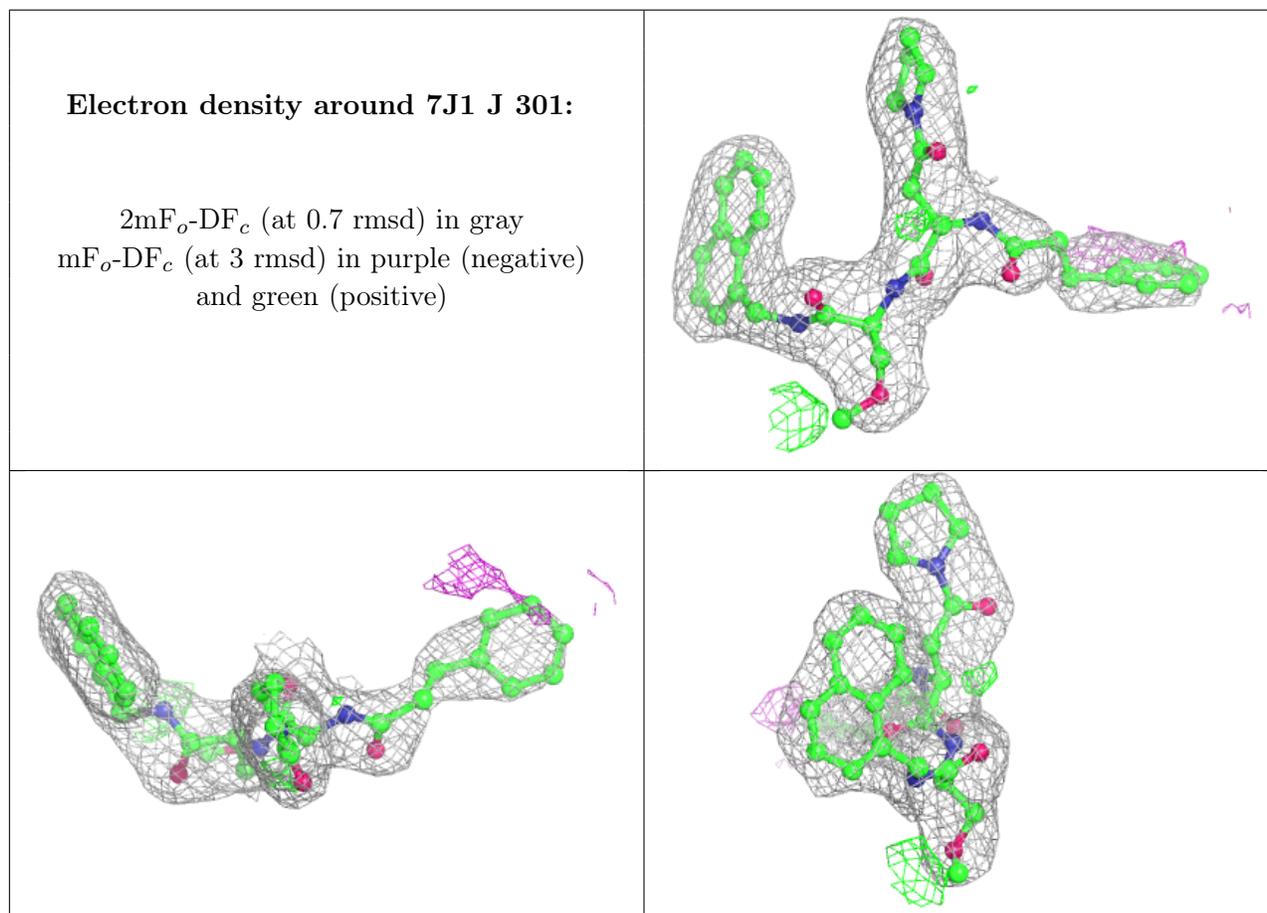
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	7J1	J	301	41/41	0.93	0.19	20,33,54,57	0
3	7J1	K	301	41/41	0.94	0.18	39,50,63,72	0
3	7J1	X	301	41/41	0.94	0.18	29,36,57,63	0
3	7J1	L	301	41/41	0.95	0.17	23,38,55,59	0
3	7J1	M	301	41/41	0.95	0.17	30,37,53,58	0
3	7J1	N	301	41/41	0.95	0.17	35,46,62,67	0
3	7J1	V	301	41/41	0.95	0.17	31,43,50,55	0

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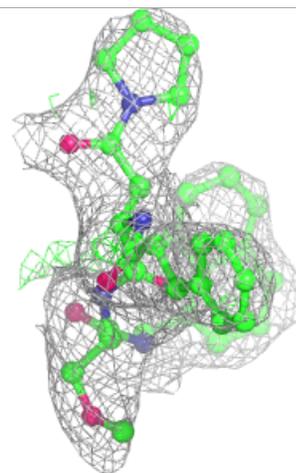
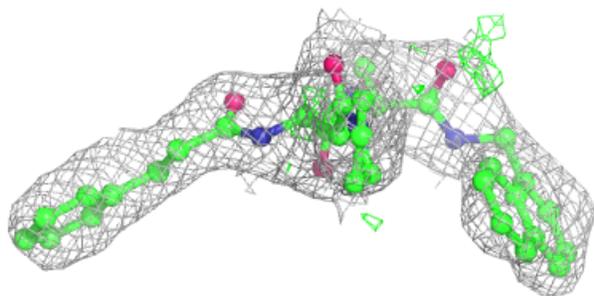
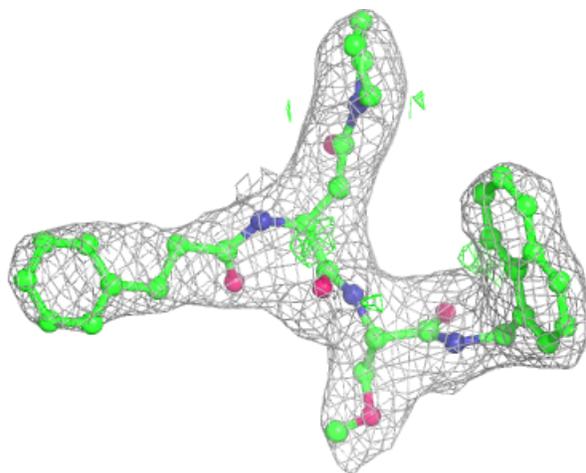
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	7J1	I	301	41/41	0.95	0.18	25,38,47,54	0
3	7J1	Y	301	41/41	0.95	0.16	21,38,57,63	0
3	7J1	Z	301	41/41	0.95	0.19	29,38,53,60	0
3	7J1	a	301	41/41	0.95	0.18	29,38,49,59	0
3	7J1	b	301	41/41	0.95	0.17	27,36,53,66	0
3	7J1	W	301	41/41	0.96	0.17	24,36,55,63	0
3	7J1	H	301	41/41	0.96	0.15	24,36,51,63	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.



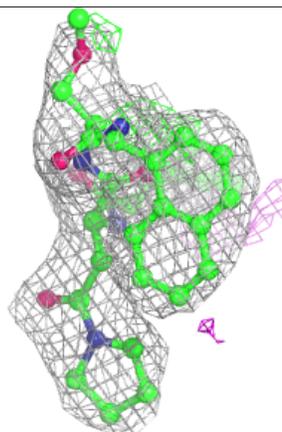
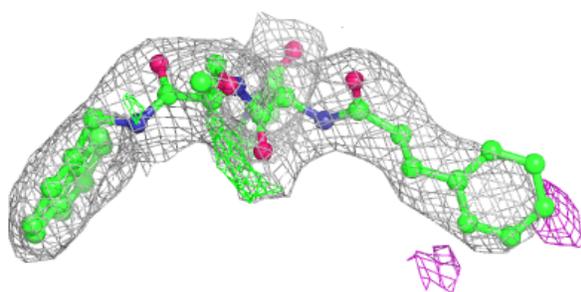
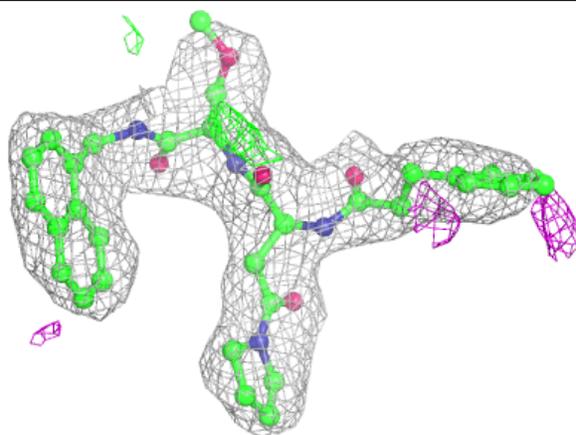
Electron density around 7J1 K 301:

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



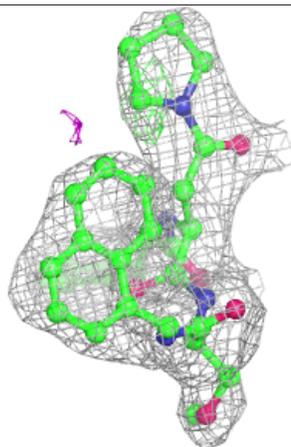
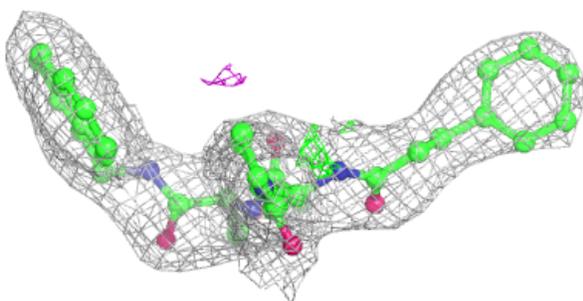
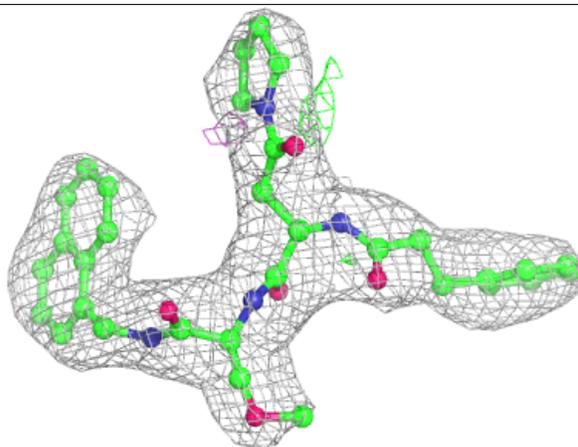
Electron density around 7J1 X 301:

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



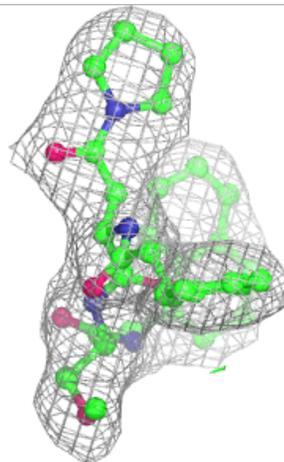
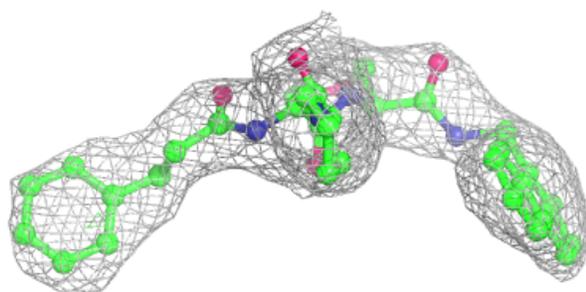
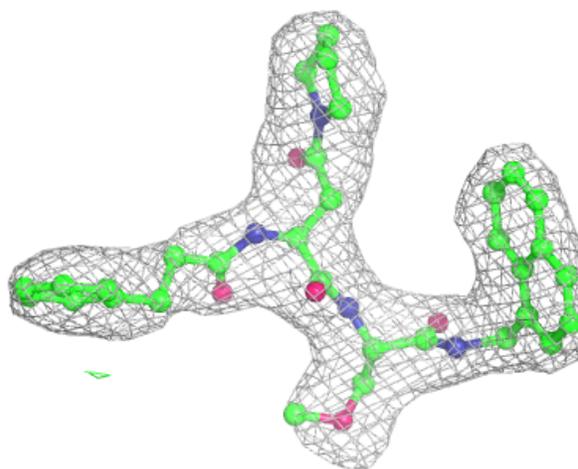
Electron density around 7J1 L 301:

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



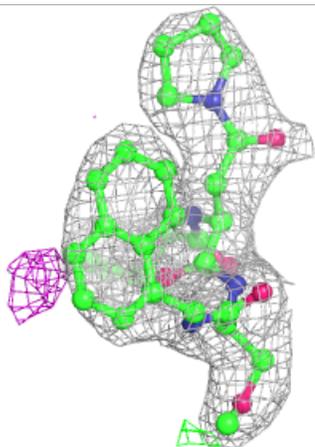
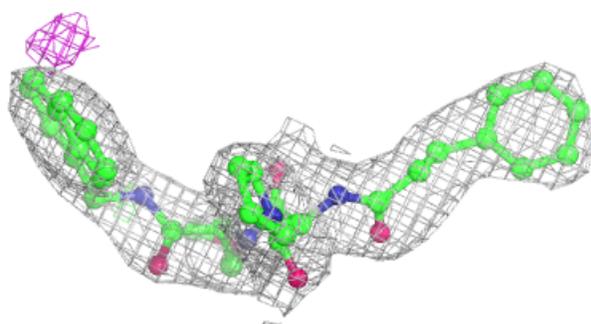
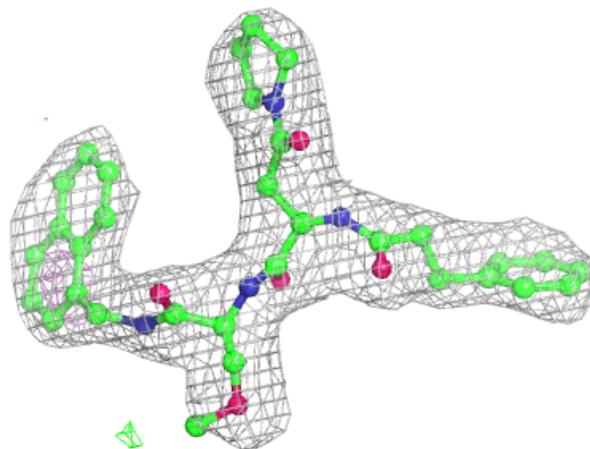
Electron density around 7J1 M 301:

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



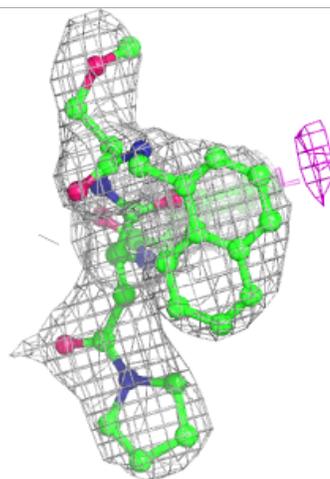
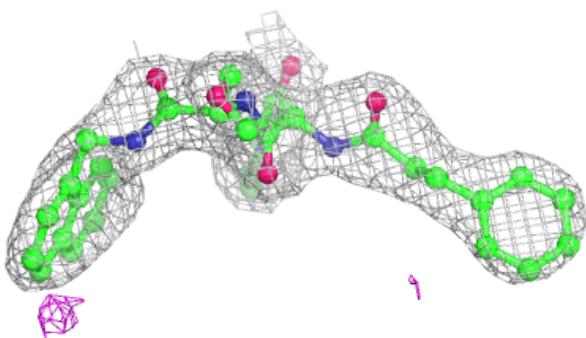
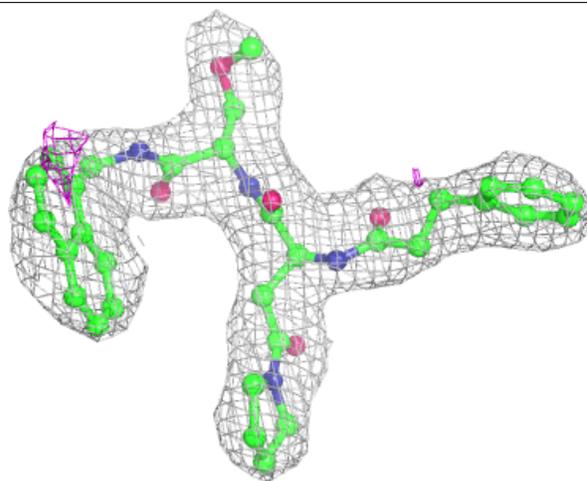
Electron density around 7J1 N 301:

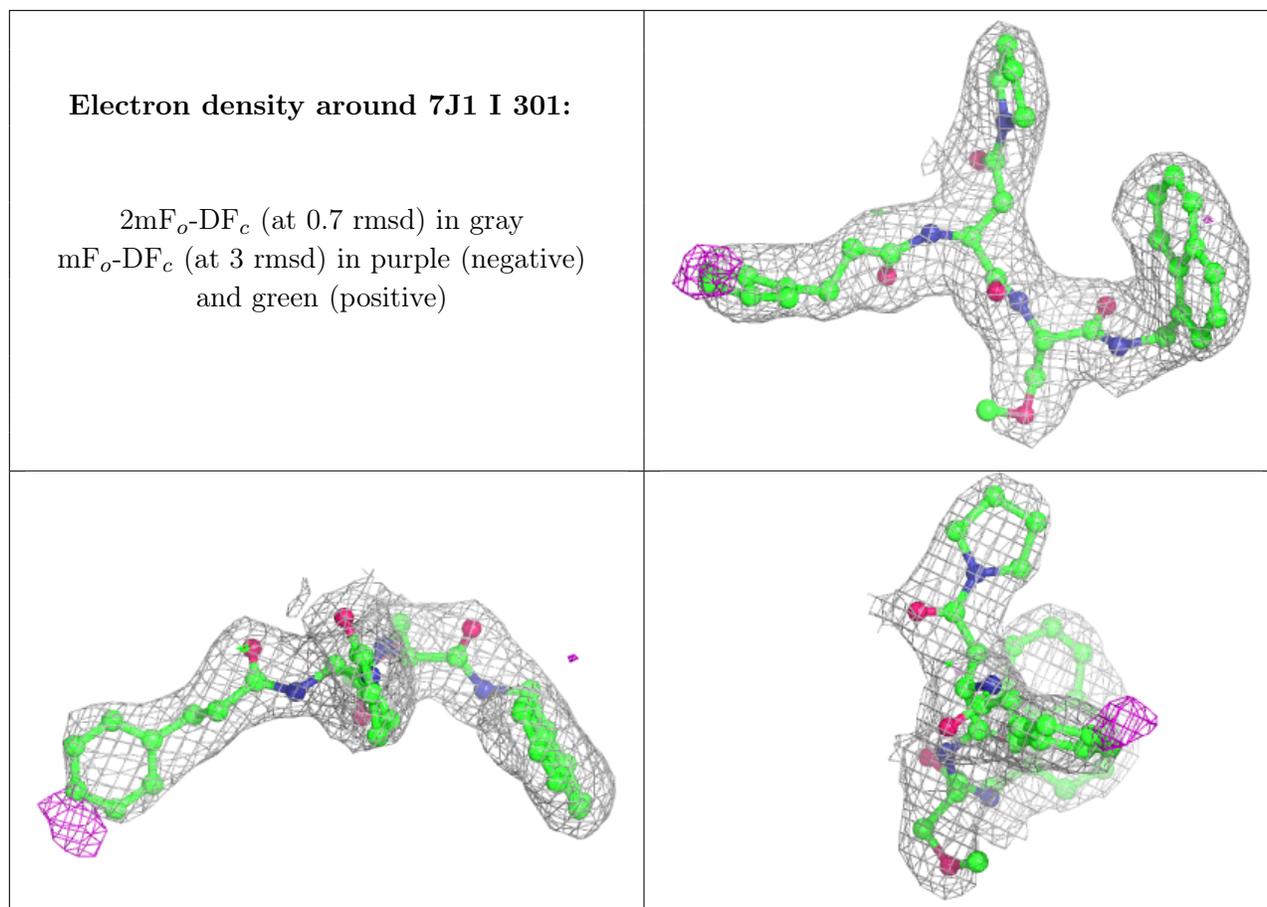
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 7J1 V 301:

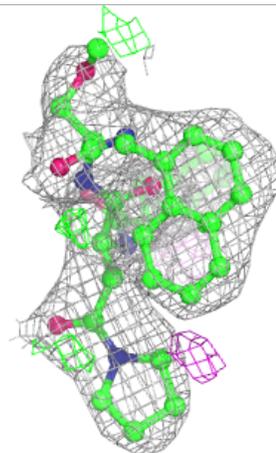
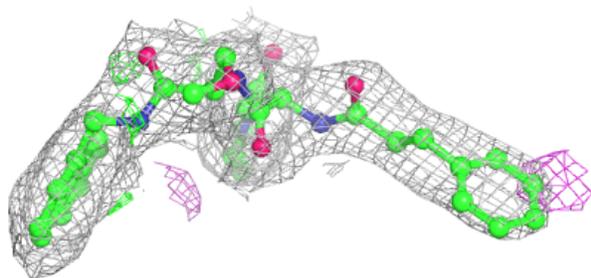
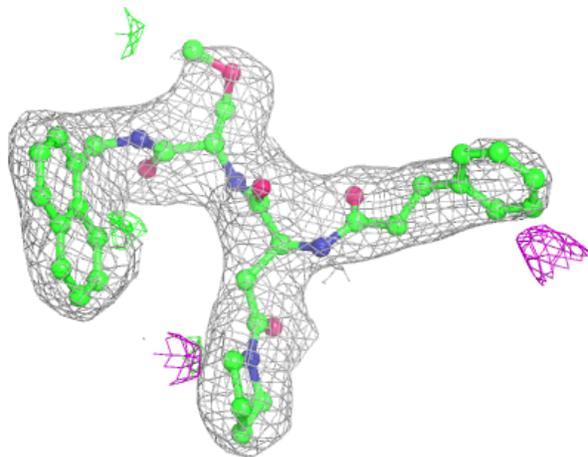
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





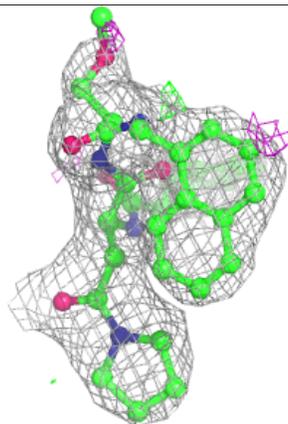
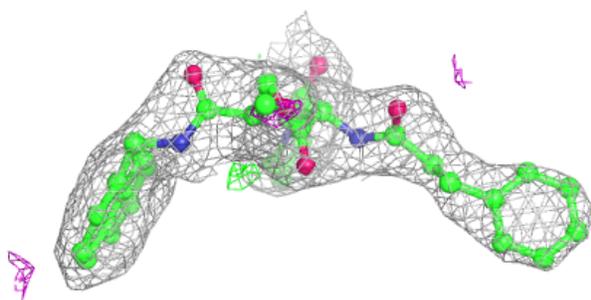
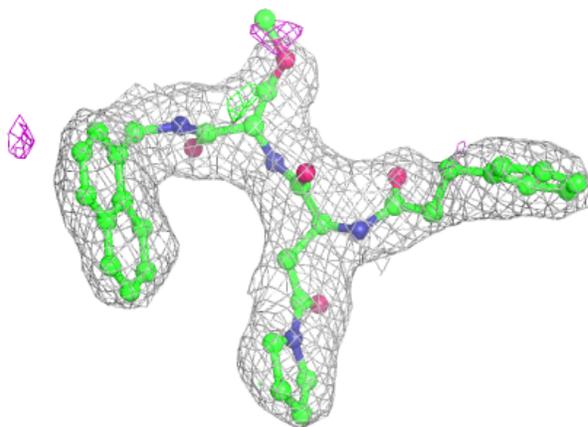
Electron density around 7J1 Y 301:

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



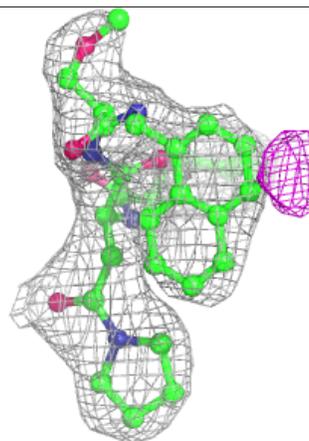
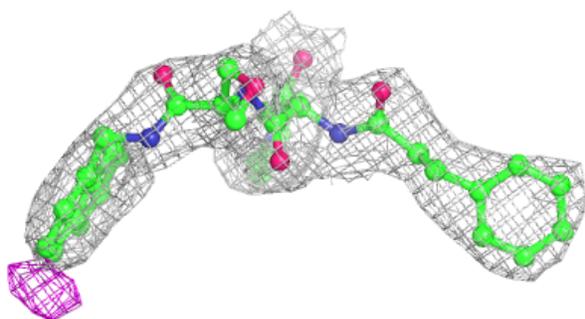
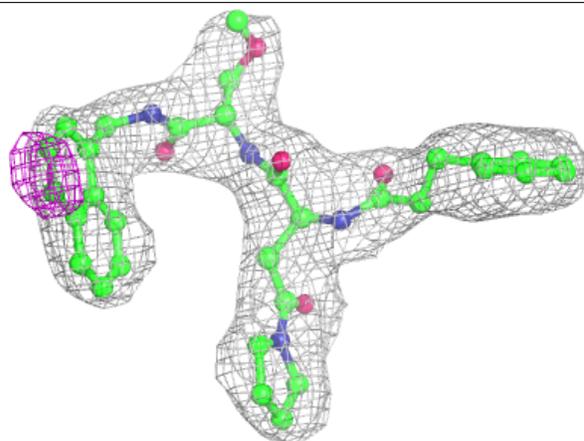
Electron density around 7J1 Z 301:

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



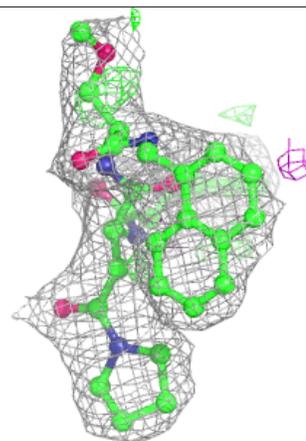
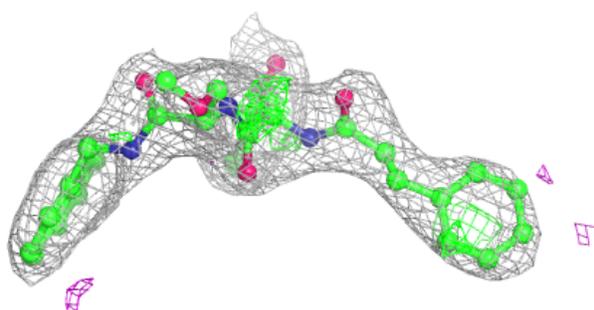
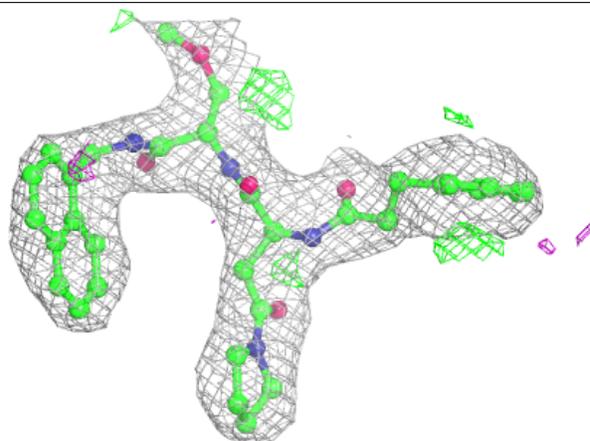
Electron density around 7J1 a 301:

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



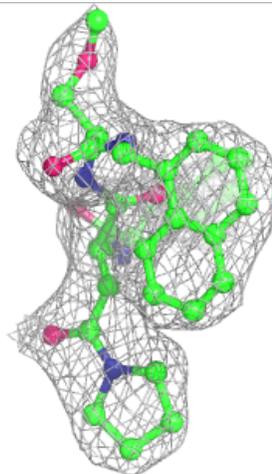
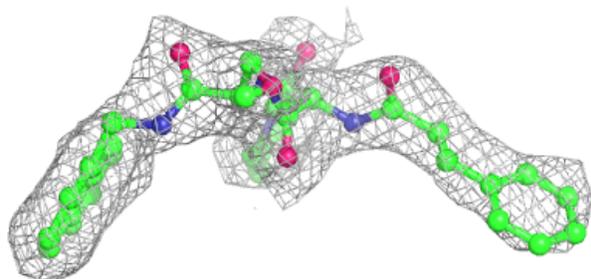
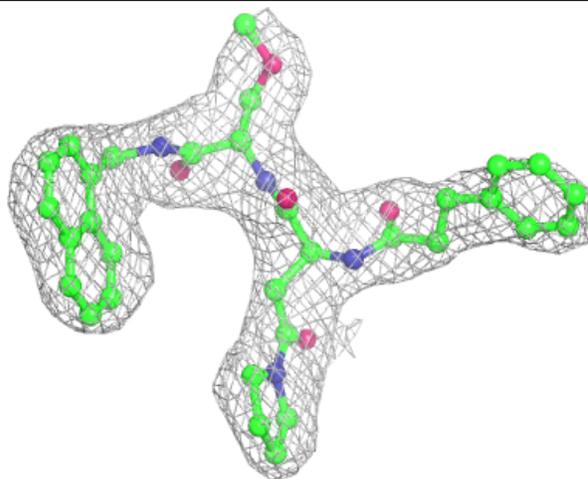
Electron density around 7J1 b 301:

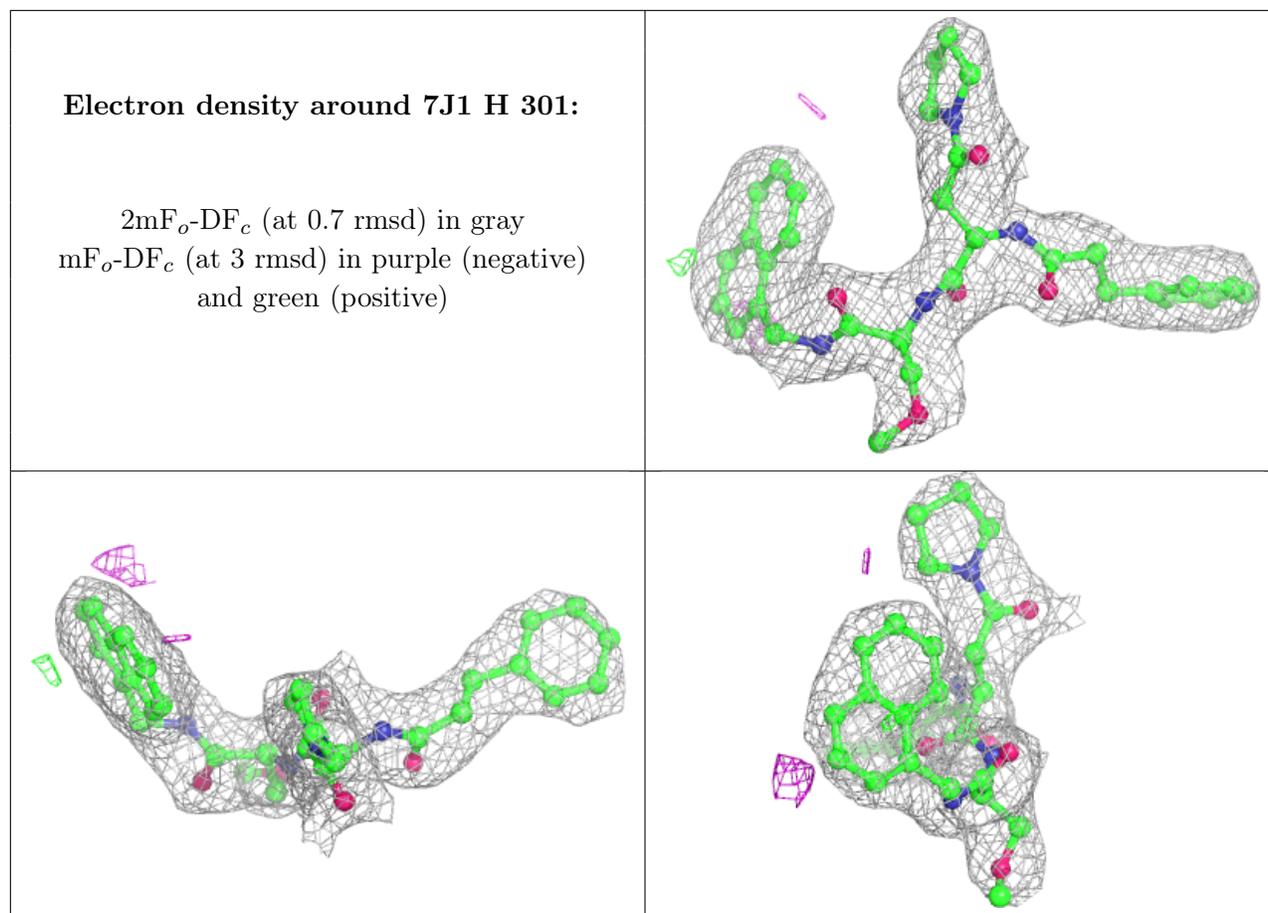
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 7J1 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.