Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:10 AM EDT

PDB ID	:	6WNK
Title	:	Macrocyclic peptides TDI5575 that selectively inhibit the Mycobacterium tuberculosis proteasome
Authors	:	Hsu, H.C.; Li, H.
Deposited on	:	2020-04-22
Resolution	:	2.28 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

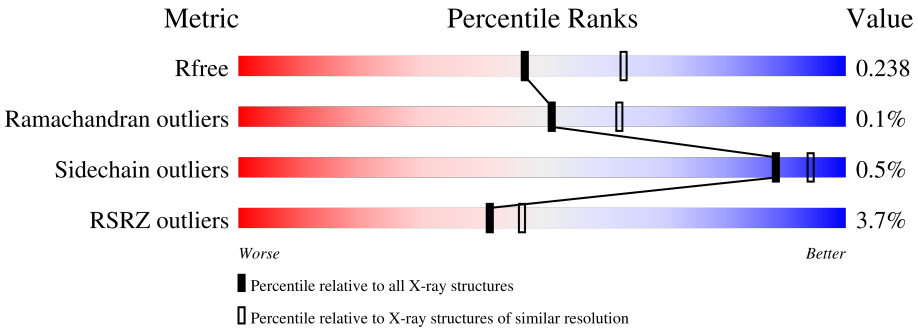
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.28 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	6980 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	240	89% · 10%
1	B	240	4% 89% 10%
1	C	240	9% 90% 10%
1	D	240	8% 90% 10%
1	E	240	12% 88% · 11%
1	F	240	15% 88% · 10%

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Mol	Chain	Length	Quality of chain
1	G	240	7% 92% 8%
1	O	240	2% 89% 10%
1	P	240	3% 91% 9%
1	Q	240	6% 90% 9%
1	R	240	1% 90% 10%
1	S	240	5% 90% 9%
1	T	240	12% 88% 10%
1	U	240	8% 90% 9%
2	H	240	93% 7%
2	I	240	92% 8%
2	J	240	91% 8%
2	K	240	92% 7%
2	L	240	92% 8%
2	M	240	92% 8%
2	N	240	92% 8%
2	V	240	92% 8%
2	W	240	92% 7%
2	X	240	92% 8%
2	Y	240	93% 7%
2	Z	240	92% 8%
2	a	240	92% 8%
2	b	240	1% 93% 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 48400 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	216	Total	C	N	O	S	0	0	0
			1661	1042	304	312	3			
1	B	215	Total	C	N	O	S	0	0	0
			1660	1040	303	314	3			
1	C	216	Total	C	N	O	S	0	0	0
			1664	1042	304	315	3			
1	D	217	Total	C	N	O	S	0	0	0
			1670	1046	305	315	4			
1	E	214	Total	C	N	O	S	0	0	0
			1647	1029	302	312	4			
1	F	216	Total	C	N	O	S	0	0	0
			1663	1041	304	314	4			
1	G	220	Total	C	N	O	S	0	0	0
			1692	1059	308	321	4			
1	O	215	Total	C	N	O	S	0	0	0
			1656	1038	303	312	3			
1	P	218	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	Q	218	Total	C	N	O	S	0	0	0
			1678	1050	306	318	4			
1	R	217	Total	C	N	O	S	0	0	0
			1670	1046	305	315	4			
1	S	218	Total	C	N	O	S	0	0	0
			1678	1050	306	318	4			
1	T	215	Total	C	N	O	S	0	0	0
			1660	1040	303	313	4			
1	U	218	Total	C	N	O	S	0	0	0
			1678	1052	306	316	4			

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	224	Total	C	N	O	S	0	0	0
			1647	1032	284	326	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	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	M	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	N	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	V	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	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	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	b	224	Total	C	N	O	S	0	0	0
			1647	1032	284	326	5			

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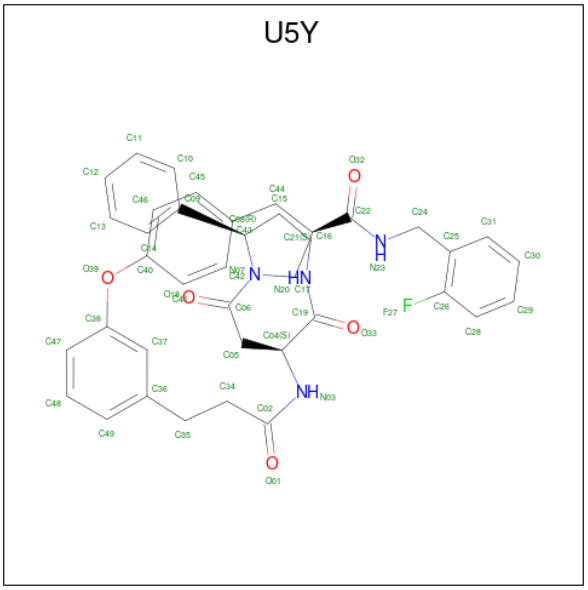
Chain	Residue	Modelled	Actual	Comment	Reference
b	235	HIS	-	expression tag	UNP A5U4D6
b	236	HIS	-	expression tag	UNP A5U4D6
b	237	HIS	-	expression tag	UNP A5U4D6
b	238	HIS	-	expression tag	UNP A5U4D6
b	239	HIS	-	expression tag	UNP A5U4D6
b	240	HIS	-	expression tag	UNP A5U4D6

- Molecule 3 is (12S,15S)-N-[(2-fluorophenyl)methyl]-10,13-dioxo-12-{2-oxo-2-[(2R)-2-phenylpyrrolidin-1-yl]ethyl}-2-oxa-11,14-diazatricyclo[15.2.2.1 3,7]docosa-1(19),3(22),4,6,17,20-hexaene-15-carboxamide (three-letter code: U5Y) (formula: $C_{39}H_{39}FN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	I	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	J	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	K	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	L	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	M	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	N	1	Total	C	F	N	O	0	0
			49	39	1	4	5		

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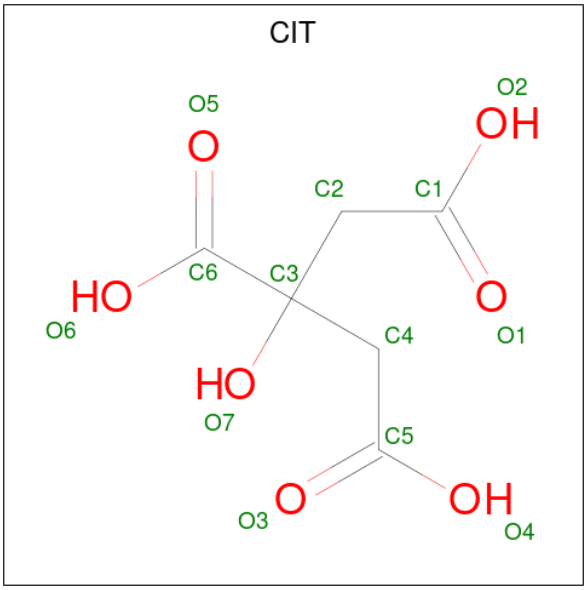
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	V	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	W	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	X	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	Y	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	Z	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	a	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	b	1	Total	C	F	N	O	0	0
			49	39	1	4	5		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			13	6	7		
4	I	1	Total	C	O	0	0
			13	6	7		
4	J	1	Total	C	O	0	0
			13	6	7		
4	K	1	Total	C	O	0	0
			13	6	7		

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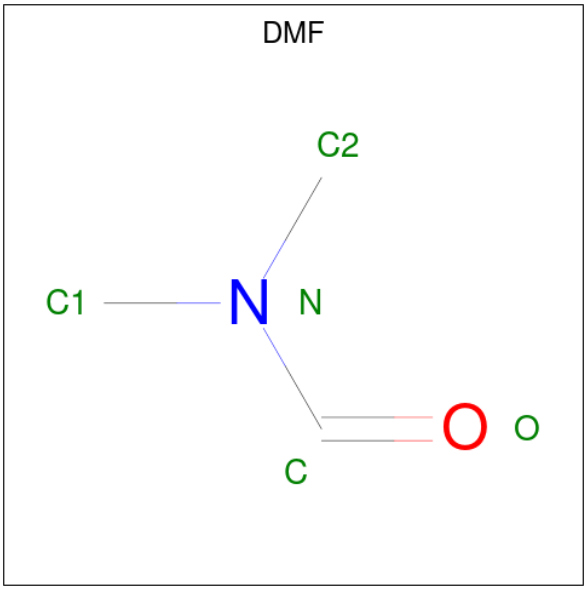
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 13 6 7	0	0
4	M	1	Total C O 13 6 7	0	0
4	N	1	Total C O 13 6 7	0	0
4	V	1	Total C O 13 6 7	0	0
4	W	1	Total C O 13 6 7	0	0
4	X	1	Total C O 13 6 7	0	0
4	Y	1	Total C O 13 6 7	0	0
4	Z	1	Total C O 13 6 7	0	0
4	a	1	Total C O 13 6 7	0	0
4	b	1	Total C O 13 6 7	0	0

- Molecule 5 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula: C_3H_7NO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	1	Total C N O 5 3 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	1	Total C N O 5 3 1 1	0	0
5	Q	1	Total C N O 5 3 1 1	0	0
5	R	1	Total C N O 5 3 1 1	0	0
5	R	1	Total C N O 5 3 1 1	0	0
5	S	1	Total C N O 5 3 1 1	0	0
5	W	1	Total C N O 5 3 1 1	0	0
5	X	1	Total C N O 5 3 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	34	Total O 34 34	0	0
6	B	14	Total O 14 14	0	0
6	C	12	Total O 12 12	0	0
6	D	13	Total O 13 13	0	0
6	E	9	Total O 9 9	0	0
6	F	9	Total O 9 9	0	0
6	G	22	Total O 22 22	0	0
6	H	74	Total O 74 74	0	0
6	I	98	Total O 98 98	0	0
6	J	69	Total O 69 69	0	0
6	K	46	Total O 46 46	0	0
6	L	37	Total O 37 37	0	0

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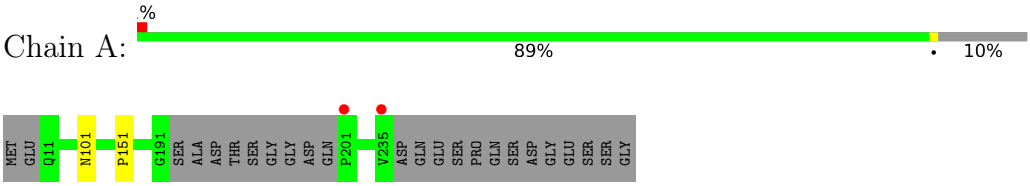
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	43	Total O 43 43	0	0
6	N	64	Total O 64 64	0	0
6	O	23	Total O 23 23	0	0
6	P	30	Total O 30 30	0	0
6	Q	32	Total O 32 32	0	0
6	R	48	Total O 48 48	0	0
6	S	12	Total O 12 12	0	0
6	T	10	Total O 10 10	0	0
6	U	13	Total O 13 13	0	0
6	V	45	Total O 45 45	0	0
6	W	73	Total O 73 73	0	0
6	X	103	Total O 103 103	0	0
6	Y	95	Total O 95 95	0	0
6	Z	63	Total O 63 63	0	0
6	a	41	Total O 41 41	0	0
6	b	44	Total O 44 44	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

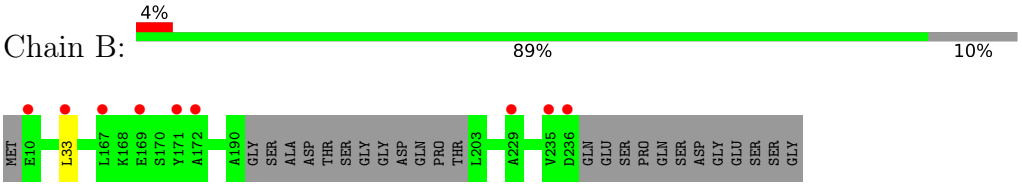
• Molecule 1: Proteasome subunit alpha

Chain A:



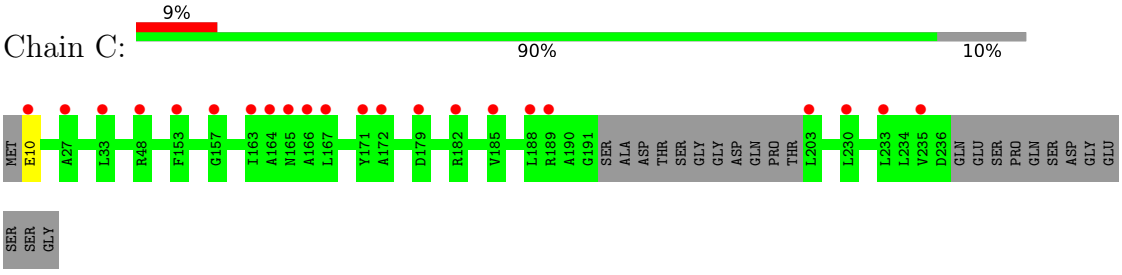
• Molecule 1: Proteasome subunit alpha

Chain B:



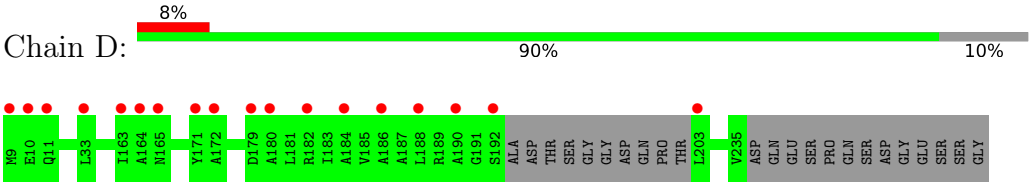
• Molecule 1: Proteasome subunit alpha

Chain C:



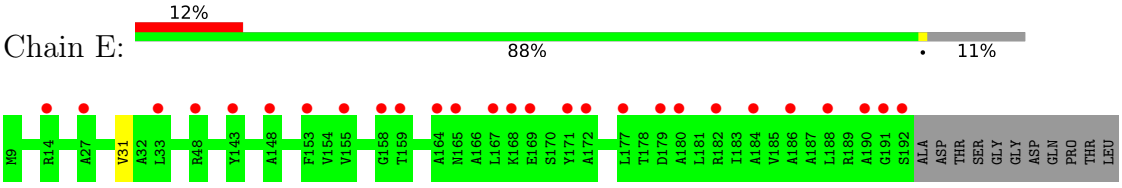
• Molecule 1: Proteasome subunit alpha

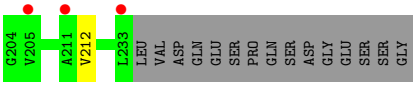
Chain D:



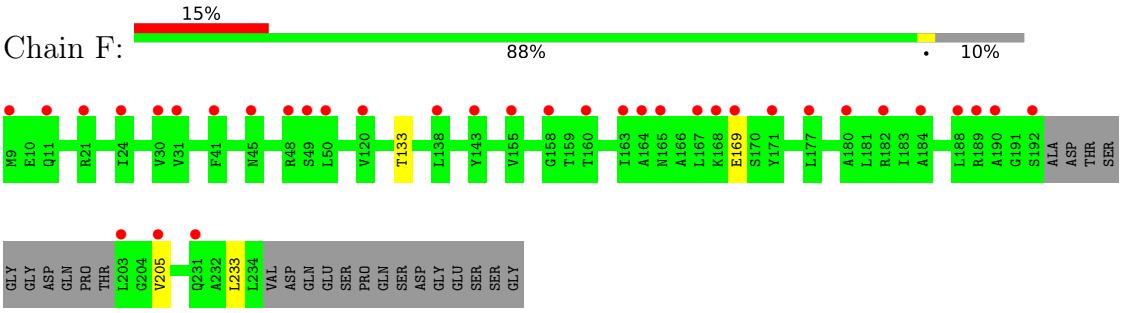
• Molecule 1: Proteasome subunit alpha

Chain E:

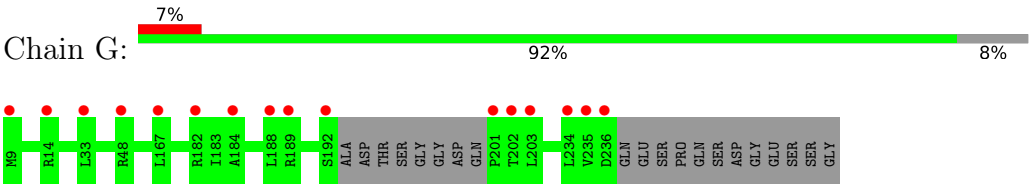




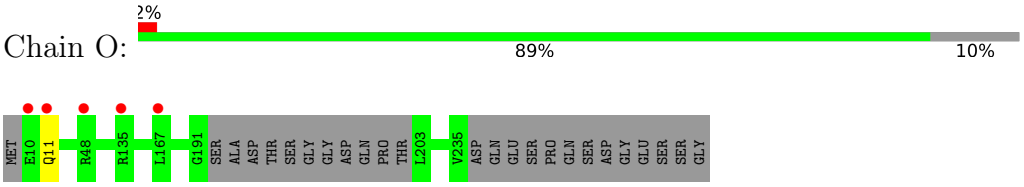
• Molecule 1: Proteasome subunit alpha



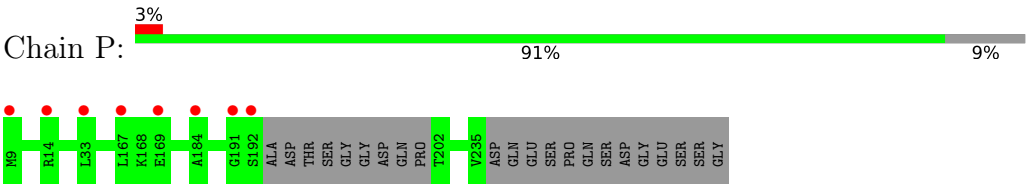
• Molecule 1: Proteasome subunit alpha



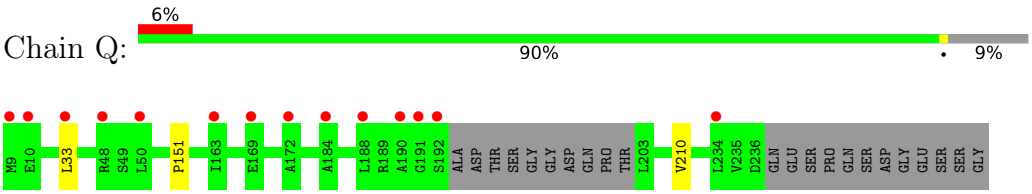
• Molecule 1: Proteasome subunit alpha



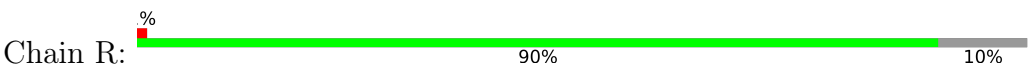
• Molecule 1: Proteasome subunit alpha

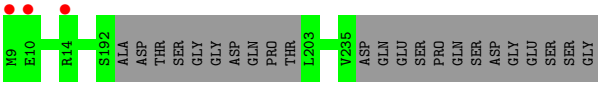


• Molecule 1: Proteasome subunit alpha

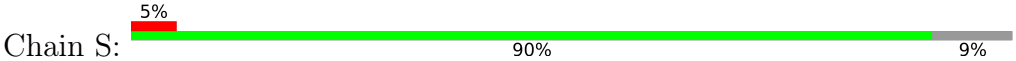


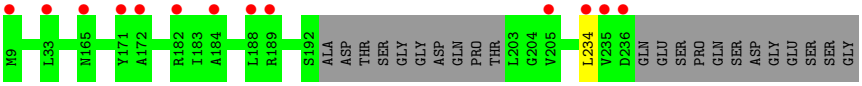
• Molecule 1: Proteasome subunit alpha



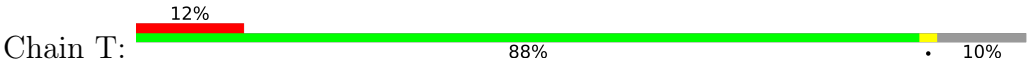


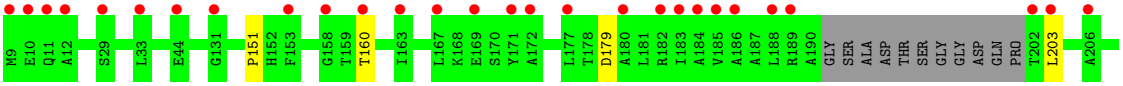
• Molecule 1: Proteasome subunit alpha

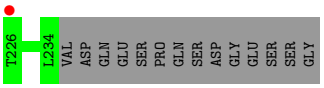




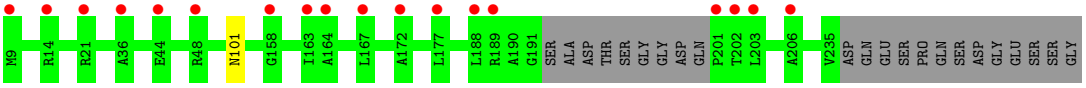
• Molecule 1: Proteasome subunit alpha



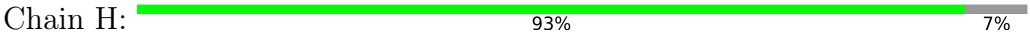


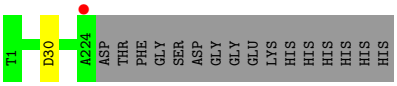


• Molecule 1: Proteasome subunit alpha

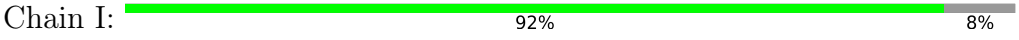


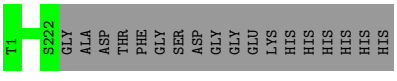
• Molecule 2: Proteasome subunit beta



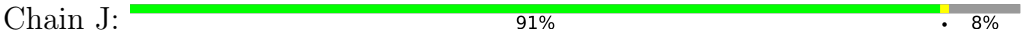


• Molecule 2: Proteasome subunit beta



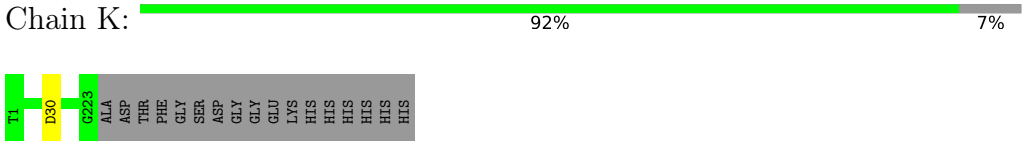


• Molecule 2: Proteasome subunit beta



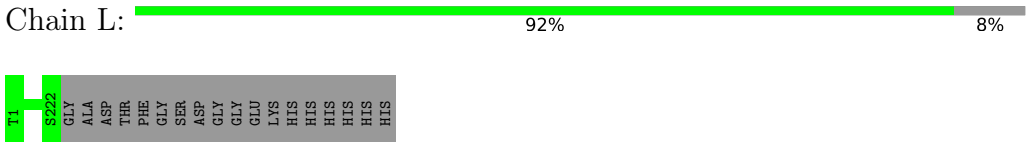
• Molecule 2: Proteasome subunit beta

Chain K:



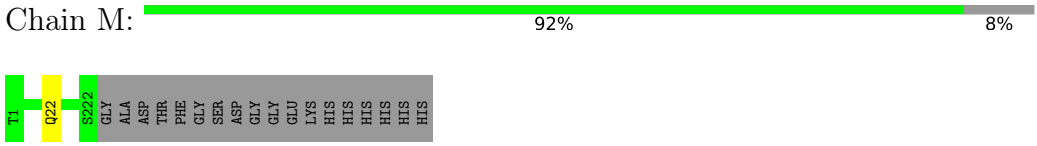
• Molecule 2: Proteasome subunit beta

Chain L:



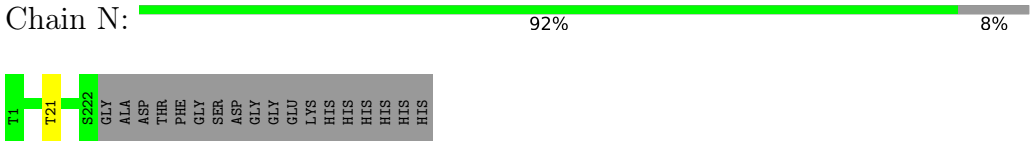
• Molecule 2: Proteasome subunit beta

Chain M:



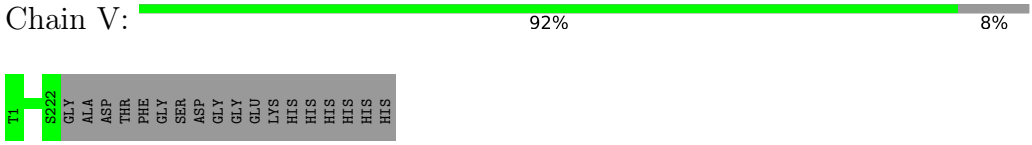
• Molecule 2: Proteasome subunit beta

Chain N:



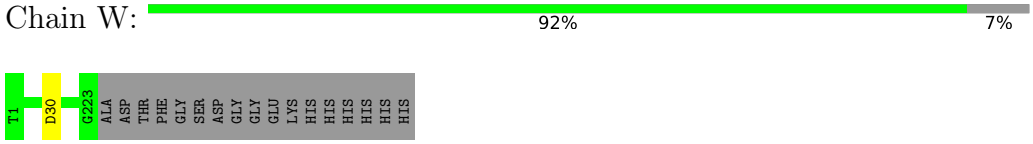
• Molecule 2: Proteasome subunit beta

Chain V:



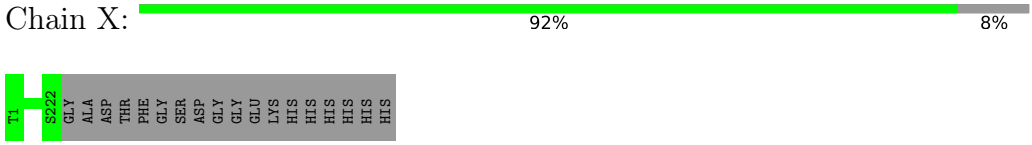
• Molecule 2: Proteasome subunit beta

Chain W:



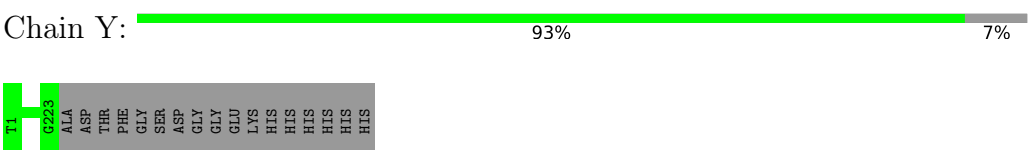
• Molecule 2: Proteasome subunit beta

Chain X:



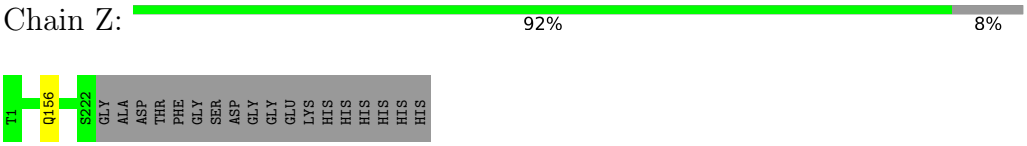
• Molecule 2: Proteasome subunit beta

Chain Y:



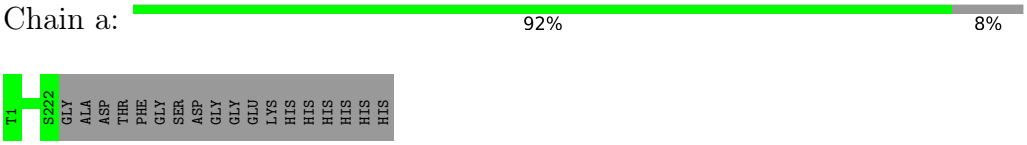
• Molecule 2: Proteasome subunit beta

Chain Z:



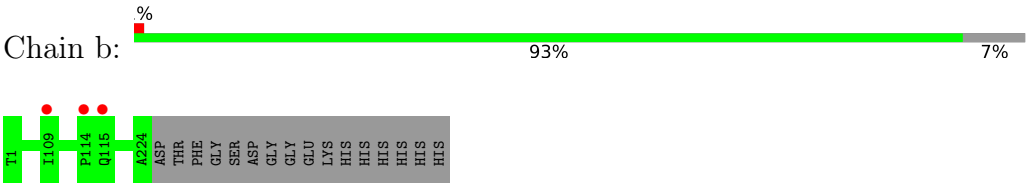
• Molecule 2: Proteasome subunit beta

Chain a:



• Molecule 2: Proteasome subunit beta

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	155.63Å 115.95Å 208.11Å 90.00° 91.58° 90.00°	Depositor
Resolution (Å)	87.59 – 2.28 87.59 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.1 (87.59-2.28) 98.1 (87.59-2.28)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.200 , 0.238 0.199 , 0.238	Depositor DCC
R_{free} test set	16401 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	48400	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, DMF, U5Y

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	0/1686	0.45	0/2278
1	B	0.26	0/1684	0.45	0/2275
1	C	0.25	0/1688	0.44	0/2280
1	D	0.25	0/1694	0.43	0/2287
1	E	0.25	0/1671	0.43	0/2255
1	F	0.26	0/1687	0.46	0/2277
1	G	0.26	0/1717	0.45	0/2319
1	O	0.25	0/1680	0.44	0/2269
1	P	0.26	0/1701	0.45	0/2297
1	Q	0.26	0/1702	0.45	0/2298
1	R	0.27	0/1694	0.46	0/2287
1	S	0.25	0/1702	0.45	0/2298
1	T	0.25	0/1684	0.46	0/2274
1	U	0.25	0/1703	0.45	0/2300
2	H	0.27	0/1671	0.48	0/2266
2	I	0.27	0/1662	0.49	0/2254
2	J	0.26	0/1662	0.48	0/2254
2	K	0.27	0/1666	0.47	0/2259
2	L	0.26	0/1662	0.46	0/2254
2	M	0.26	0/1662	0.48	0/2254
2	N	0.26	0/1662	0.47	0/2254
2	V	0.26	0/1662	0.47	0/2254
2	W	0.26	0/1666	0.47	0/2259
2	X	0.28	0/1662	0.49	0/2254
2	Y	0.27	0/1666	0.50	0/2259
2	Z	0.27	0/1662	0.48	0/2254
2	a	0.26	0/1662	0.47	0/2254
2	b	0.26	0/1671	0.48	0/2266
All	All	0.26	0/46991	0.46	0/63589

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	212/240 (88%)	208 (98%)	3 (1%)	1 (0%)	29	34
1	B	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
1	C	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
1	D	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
1	E	210/240 (88%)	205 (98%)	5 (2%)	0	100	100
1	F	212/240 (88%)	203 (96%)	9 (4%)	0	100	100
1	G	216/240 (90%)	211 (98%)	5 (2%)	0	100	100
1	O	211/240 (88%)	207 (98%)	4 (2%)	0	100	100
1	P	214/240 (89%)	210 (98%)	4 (2%)	0	100	100
1	Q	214/240 (89%)	208 (97%)	5 (2%)	1 (0%)	29	34
1	R	213/240 (89%)	206 (97%)	7 (3%)	0	100	100
1	S	214/240 (89%)	207 (97%)	6 (3%)	1 (0%)	29	34
1	T	211/240 (88%)	204 (97%)	6 (3%)	1 (0%)	29	34
1	U	214/240 (89%)	207 (97%)	7 (3%)	0	100	100
2	H	222/240 (92%)	217 (98%)	5 (2%)	0	100	100
2	I	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	J	220/240 (92%)	217 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	221/240 (92%)	220 (100%)	1 (0%)	0	100	100
2	L	220/240 (92%)	215 (98%)	5 (2%)	0	100	100
2	M	220/240 (92%)	213 (97%)	7 (3%)	0	100	100
2	N	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	V	220/240 (92%)	215 (98%)	5 (2%)	0	100	100
2	W	221/240 (92%)	216 (98%)	5 (2%)	0	100	100
2	X	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	Y	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	Z	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	a	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	b	222/240 (92%)	218 (98%)	4 (2%)	0	100	100
All	All	6064/6720 (90%)	5926 (98%)	134 (2%)	4 (0%)	51	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	234	LEU
1	A	151	PRO
1	Q	151	PRO
1	T	151	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	165/184 (90%)	164 (99%)	1 (1%)	86	93
1	B	165/184 (90%)	164 (99%)	1 (1%)	86	93
1	C	165/184 (90%)	164 (99%)	1 (1%)	86	93
1	D	166/184 (90%)	166 (100%)	0	100	100
1	E	163/184 (89%)	161 (99%)	2 (1%)	71	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	165/184 (90%)	161 (98%)	4 (2%)	49 63
1	G	169/184 (92%)	169 (100%)	0	100 100
1	O	164/184 (89%)	163 (99%)	1 (1%)	86 93
1	P	167/184 (91%)	167 (100%)	0	100 100
1	Q	167/184 (91%)	165 (99%)	2 (1%)	71 82
1	R	166/184 (90%)	166 (100%)	0	100 100
1	S	167/184 (91%)	167 (100%)	0	100 100
1	T	165/184 (90%)	162 (98%)	3 (2%)	59 72
1	U	167/184 (91%)	166 (99%)	1 (1%)	86 93
2	H	165/178 (93%)	164 (99%)	1 (1%)	86 93
2	I	165/178 (93%)	165 (100%)	0	100 100
2	J	165/178 (93%)	162 (98%)	3 (2%)	59 72
2	K	165/178 (93%)	164 (99%)	1 (1%)	86 93
2	L	165/178 (93%)	165 (100%)	0	100 100
2	M	165/178 (93%)	164 (99%)	1 (1%)	86 93
2	N	165/178 (93%)	164 (99%)	1 (1%)	86 93
2	V	165/178 (93%)	165 (100%)	0	100 100
2	W	165/178 (93%)	164 (99%)	1 (1%)	86 93
2	X	165/178 (93%)	165 (100%)	0	100 100
2	Y	165/178 (93%)	165 (100%)	0	100 100
2	Z	165/178 (93%)	164 (99%)	1 (1%)	86 93
2	a	165/178 (93%)	165 (100%)	0	100 100
2	b	165/178 (93%)	165 (100%)	0	100 100
All	All	4631/5068 (91%)	4606 (100%)	25 (0%)	88 94

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	B	33	LEU
1	C	10	GLU
1	E	31	VAL
1	E	212	VAL
1	F	133	THR

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Mol	Chain	Res	Type
1	F	169	GLU
1	F	205	VAL
1	F	233	LEU
2	H	30	ASP
2	J	37	THR
2	J	133	GLU
2	J	161	ASP
2	K	30	ASP
2	M	22	GLN
2	N	21	THR
1	O	11	GLN
1	Q	33	LEU
1	Q	210	VAL
1	T	160	THR
1	T	179	ASP
1	T	203	LEU
1	U	101	ASN
2	W	30	ASP
2	Z	156	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	101	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

36 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	U5Y	J	301	-	54,54,54	2.35	11 (20%)	73,74,74	1.27	11 (15%)
3	U5Y	Z	301	-	54,54,54	2.36	10 (18%)	73,74,74	1.28	10 (13%)
5	DMF	Q	301	-	4,4,4	0.35	0	4,4,4	0.48	0
5	DMF	R	302	-	4,4,4	0.33	0	4,4,4	0.44	0
5	DMF	S	301	-	4,4,4	0.33	0	4,4,4	0.44	0
3	U5Y	Y	301	-	54,54,54	2.33	11 (20%)	73,74,74	1.32	11 (15%)
4	CIT	a	302	-	12,12,12	1.00	0	17,17,17	2.10	5 (29%)
5	DMF	W	301	-	4,4,4	0.37	0	4,4,4	0.45	0
5	DMF	P	301	-	4,4,4	0.35	0	4,4,4	0.45	0
4	CIT	N	302	-	12,12,12	0.98	0	17,17,17	1.65	2 (11%)
3	U5Y	a	301	-	54,54,54	2.35	11 (20%)	73,74,74	1.28	10 (13%)
4	CIT	I	302	-	12,12,12	1.05	0	17,17,17	1.50	2 (11%)
4	CIT	Y	302	-	12,12,12	1.05	0	17,17,17	1.52	3 (17%)
3	U5Y	I	301	-	54,54,54	2.36	10 (18%)	73,74,74	1.25	9 (12%)
4	CIT	W	303	-	12,12,12	0.96	0	17,17,17	1.63	2 (11%)
3	U5Y	K	301	-	54,54,54	2.37	11 (20%)	73,74,74	1.37	13 (17%)
4	CIT	X	303	-	12,12,12	0.98	0	17,17,17	1.63	4 (23%)
3	U5Y	V	301	-	54,54,54	2.35	10 (18%)	73,74,74	1.34	12 (16%)
3	U5Y	b	301	-	54,54,54	2.35	10 (18%)	73,74,74	1.32	11 (15%)
3	U5Y	L	301	-	54,54,54	2.37	10 (18%)	73,74,74	1.37	11 (15%)
4	CIT	L	302	-	12,12,12	0.99	0	17,17,17	1.66	2 (11%)
3	U5Y	W	302	-	54,54,54	2.36	10 (18%)	73,74,74	1.28	9 (12%)
3	U5Y	H	301	-	54,54,54	2.35	10 (18%)	73,74,74	1.29	11 (15%)
5	DMF	X	301	-	4,4,4	0.37	0	4,4,4	0.40	0
4	CIT	K	302	-	12,12,12	0.98	0	17,17,17	1.59	3 (17%)
4	CIT	V	302	-	12,12,12	1.03	0	17,17,17	1.54	3 (17%)
5	DMF	O	301	-	4,4,4	0.32	0	4,4,4	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CIT	b	302	-	12,12,12	1.04	0	17,17,17	1.54	4 (23%)
5	DMF	R	301	-	4,4,4	0.36	0	4,4,4	0.36	0
3	U5Y	X	302	-	54,54,54	2.38	10 (18%)	73,74,74	1.28	10 (13%)
4	CIT	M	302	-	12,12,12	0.94	0	17,17,17	1.79	3 (17%)
4	CIT	Z	302	-	12,12,12	1.02	0	17,17,17	1.45	1 (5%)
3	U5Y	N	301	-	54,54,54	2.38	10 (18%)	73,74,74	1.31	12 (16%)
3	U5Y	M	301	-	54,54,54	2.35	11 (20%)	73,74,74	1.28	8 (10%)
4	CIT	J	302	-	12,12,12	0.97	0	17,17,17	1.79	5 (29%)
4	CIT	H	302	-	12,12,12	0.98	0	17,17,17	1.66	4 (23%)

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	U5Y	J	301	-	-	2/46/56/56	0/5/6/6
3	U5Y	Z	301	-	-	0/46/56/56	0/5/6/6
5	DMF	Q	301	-	-	0/2/2/2	-
5	DMF	R	302	-	-	2/2/2/2	-
5	DMF	S	301	-	-	0/2/2/2	-
3	U5Y	Y	301	-	-	2/46/56/56	0/5/6/6
4	CIT	a	302	-	-	6/16/16/16	-
5	DMF	W	301	-	-	2/2/2/2	-
5	DMF	P	301	-	-	0/2/2/2	-
4	CIT	N	302	-	-	6/16/16/16	-
3	U5Y	a	301	-	-	2/46/56/56	0/5/6/6
4	CIT	I	302	-	-	12/16/16/16	-
4	CIT	Y	302	-	-	11/16/16/16	-
3	U5Y	I	301	-	-	2/46/56/56	0/5/6/6
4	CIT	W	303	-	-	8/16/16/16	-
3	U5Y	K	301	-	-	0/46/56/56	0/5/6/6
4	CIT	X	303	-	-	9/16/16/16	-
3	U5Y	V	301	-	-	0/46/56/56	0/5/6/6
3	U5Y	b	301	-	-	3/46/56/56	0/5/6/6
3	U5Y	L	301	-	-	2/46/56/56	0/5/6/6
4	CIT	L	302	-	-	10/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	U5Y	W	302	-	-	2/46/56/56	0/5/6/6
3	U5Y	H	301	-	-	2/46/56/56	0/5/6/6
5	DMF	X	301	-	-	0/2/2/2	-
4	CIT	K	302	-	-	8/16/16/16	-
4	CIT	V	302	-	-	7/16/16/16	-
5	DMF	O	301	-	-	0/2/2/2	-
4	CIT	b	302	-	-	7/16/16/16	-
5	DMF	R	301	-	-	2/2/2/2	-
3	U5Y	X	302	-	-	4/46/56/56	0/5/6/6
4	CIT	M	302	-	-	7/16/16/16	-
4	CIT	Z	302	-	-	10/16/16/16	-
3	U5Y	N	301	-	-	0/46/56/56	0/5/6/6
3	U5Y	M	301	-	-	3/46/56/56	0/5/6/6
4	CIT	J	302	-	-	6/16/16/16	-
4	CIT	H	302	-	-	8/16/16/16	-

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	302	U5Y	C08-N07	-9.25	1.33	1.47
3	Z	301	U5Y	C08-N07	-9.10	1.33	1.47
3	N	301	U5Y	C08-N07	-9.07	1.33	1.47
3	b	301	U5Y	C08-N07	-9.05	1.33	1.47
3	I	301	U5Y	C08-N07	-9.00	1.33	1.47
3	V	301	U5Y	C08-N07	-8.97	1.33	1.47
3	a	301	U5Y	C08-N07	-8.93	1.33	1.47
3	H	301	U5Y	C08-N07	-8.92	1.33	1.47
3	L	301	U5Y	C08-N07	-8.86	1.33	1.47
3	Y	301	U5Y	C08-N07	-8.86	1.33	1.47
3	J	301	U5Y	C08-N07	-8.84	1.33	1.47
3	K	301	U5Y	C08-N07	-8.83	1.33	1.47
3	W	302	U5Y	C08-N07	-8.81	1.33	1.47
3	M	301	U5Y	C08-N07	-8.77	1.33	1.47
3	L	301	U5Y	C17-N07	8.64	1.64	1.47
3	X	302	U5Y	C17-N07	8.63	1.64	1.47
3	M	301	U5Y	C17-N07	8.60	1.64	1.47
3	W	302	U5Y	C17-N07	8.60	1.64	1.47
3	N	301	U5Y	C17-N07	8.58	1.64	1.47
3	H	301	U5Y	C17-N07	8.58	1.64	1.47
3	K	301	U5Y	C17-N07	8.56	1.64	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Z	301	U5Y	C17-N07	8.54	1.64	1.47
3	J	301	U5Y	C17-N07	8.52	1.64	1.47
3	b	301	U5Y	C17-N07	8.52	1.64	1.47
3	I	301	U5Y	C17-N07	8.49	1.64	1.47
3	a	301	U5Y	C17-N07	8.43	1.63	1.47
3	V	301	U5Y	C17-N07	8.41	1.63	1.47
3	Y	301	U5Y	C17-N07	8.31	1.63	1.47
3	V	301	U5Y	C19-N20	5.84	1.46	1.34
3	N	301	U5Y	C19-N20	5.82	1.46	1.34
3	W	302	U5Y	C19-N20	5.79	1.46	1.34
3	a	301	U5Y	C19-N20	5.75	1.46	1.34
3	K	301	U5Y	C19-N20	5.73	1.46	1.34
3	Z	301	U5Y	C19-N20	5.67	1.46	1.34
3	Y	301	U5Y	C19-N20	5.63	1.46	1.34
3	I	301	U5Y	C19-N20	5.63	1.46	1.34
3	J	301	U5Y	C19-N20	5.60	1.46	1.34
3	L	301	U5Y	C19-N20	5.59	1.46	1.34
3	M	301	U5Y	C19-N20	5.52	1.46	1.34
3	b	301	U5Y	C19-N20	5.50	1.46	1.34
3	H	301	U5Y	C19-N20	5.46	1.46	1.34
3	X	302	U5Y	C19-N20	5.44	1.46	1.34
3	N	301	U5Y	C22-N23	5.43	1.45	1.33
3	J	301	U5Y	C22-N23	5.42	1.45	1.33
3	M	301	U5Y	C22-N23	5.41	1.45	1.33
3	I	301	U5Y	C22-N23	5.41	1.45	1.33
3	Y	301	U5Y	C22-N23	5.38	1.45	1.33
3	H	301	U5Y	C02-N03	5.34	1.45	1.34
3	W	302	U5Y	C22-N23	5.30	1.45	1.33
3	N	301	U5Y	C02-N03	5.29	1.45	1.34
3	L	301	U5Y	C22-N23	5.29	1.45	1.33
3	H	301	U5Y	C22-N23	5.29	1.45	1.33
3	V	301	U5Y	C22-N23	5.27	1.45	1.33
3	X	302	U5Y	C02-N03	5.26	1.45	1.34
3	a	301	U5Y	C22-N23	5.25	1.45	1.33
3	Z	301	U5Y	C22-N23	5.25	1.45	1.33
3	K	301	U5Y	C02-N03	5.20	1.45	1.34
3	X	302	U5Y	C22-N23	5.19	1.44	1.33
3	W	302	U5Y	C02-N03	5.18	1.45	1.34
3	L	301	U5Y	C02-N03	5.17	1.45	1.34
3	b	301	U5Y	C02-N03	5.15	1.45	1.34
3	I	301	U5Y	C02-N03	5.11	1.44	1.34
3	K	301	U5Y	C22-N23	5.09	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	301	U5Y	C02-N03	5.06	1.44	1.34
3	b	301	U5Y	C22-N23	5.06	1.44	1.33
3	Z	301	U5Y	C02-N03	5.05	1.44	1.34
3	Y	301	U5Y	C02-N03	5.04	1.44	1.34
3	a	301	U5Y	C02-N03	5.03	1.44	1.34
3	V	301	U5Y	C02-N03	5.01	1.44	1.34
3	M	301	U5Y	C02-N03	4.90	1.44	1.34
3	a	301	U5Y	C16-C17	-4.06	1.37	1.51
3	Z	301	U5Y	C16-C17	-4.04	1.37	1.51
3	W	302	U5Y	C16-C17	-4.02	1.37	1.51
3	M	301	U5Y	C16-C17	-4.01	1.37	1.51
3	K	301	U5Y	C16-C17	-4.01	1.37	1.51
3	L	301	U5Y	C16-C17	-4.00	1.37	1.51
3	b	301	U5Y	C16-C17	-3.98	1.37	1.51
3	N	301	U5Y	C16-C17	-3.98	1.37	1.51
3	H	301	U5Y	C16-C17	-3.96	1.38	1.51
3	J	301	U5Y	C16-C17	-3.93	1.38	1.51
3	Y	301	U5Y	C16-C17	-3.93	1.38	1.51
3	V	301	U5Y	C16-C17	-3.90	1.38	1.51
3	X	302	U5Y	C16-C17	-3.90	1.38	1.51
3	I	301	U5Y	C16-C17	-3.88	1.38	1.51
3	K	301	U5Y	C06-N07	3.60	1.46	1.35
3	a	301	U5Y	C06-N07	3.55	1.46	1.35
3	L	301	U5Y	C06-N07	3.54	1.46	1.35
3	M	301	U5Y	C06-N07	3.52	1.46	1.35
3	H	301	U5Y	C06-N07	3.49	1.45	1.35
3	X	302	U5Y	C06-N07	3.48	1.45	1.35
3	b	301	U5Y	C06-N07	3.46	1.45	1.35
3	J	301	U5Y	C06-N07	3.45	1.45	1.35
3	V	301	U5Y	C06-N07	3.44	1.45	1.35
3	W	302	U5Y	C06-N07	3.44	1.45	1.35
3	N	301	U5Y	C06-N07	3.44	1.45	1.35
3	I	301	U5Y	C06-N07	3.40	1.45	1.35
3	Z	301	U5Y	C06-N07	3.38	1.45	1.35
3	Y	301	U5Y	C06-N07	3.35	1.45	1.35
3	K	301	U5Y	C15-C08	2.76	1.61	1.54
3	a	301	U5Y	C15-C08	2.70	1.61	1.54
3	L	301	U5Y	O32-C22	-2.65	1.18	1.23
3	I	301	U5Y	C15-C08	2.64	1.61	1.54
3	K	301	U5Y	O32-C22	-2.61	1.18	1.23
3	b	301	U5Y	C15-C08	2.60	1.61	1.54
3	L	301	U5Y	C15-C08	2.60	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	301	U5Y	C15-C08	2.59	1.61	1.54
3	Z	301	U5Y	C15-C08	2.59	1.61	1.54
3	W	302	U5Y	C15-C08	2.56	1.60	1.54
3	J	301	U5Y	C15-C08	2.56	1.60	1.54
3	V	301	U5Y	C15-C08	2.54	1.60	1.54
3	Y	301	U5Y	C15-C08	2.54	1.60	1.54
3	X	302	U5Y	C15-C08	2.50	1.60	1.54
3	H	301	U5Y	C15-C08	2.48	1.60	1.54
3	N	301	U5Y	C15-C08	2.45	1.60	1.54
3	N	301	U5Y	O32-C22	-2.43	1.18	1.23
3	J	301	U5Y	O32-C22	-2.37	1.18	1.23
3	I	301	U5Y	O32-C22	-2.36	1.18	1.23
3	a	301	U5Y	O32-C22	-2.34	1.18	1.23
3	Y	301	U5Y	O32-C22	-2.33	1.18	1.23
3	W	302	U5Y	O32-C22	-2.32	1.18	1.23
3	X	302	U5Y	O32-C22	-2.32	1.18	1.23
3	M	301	U5Y	O32-C22	-2.31	1.18	1.23
3	b	301	U5Y	O32-C22	-2.29	1.18	1.23
3	M	301	U5Y	O33-C19	-2.27	1.18	1.23
3	Z	301	U5Y	O32-C22	-2.24	1.18	1.23
3	V	301	U5Y	O32-C22	-2.23	1.19	1.23
3	Y	301	U5Y	O33-C19	-2.22	1.19	1.23
3	W	302	U5Y	O33-C19	-2.21	1.19	1.23
3	V	301	U5Y	O33-C19	-2.18	1.19	1.23
3	I	301	U5Y	O33-C19	-2.15	1.19	1.23
3	X	302	U5Y	O33-C19	-2.15	1.19	1.23
3	a	301	U5Y	O01-C02	-2.13	1.18	1.23
3	J	301	U5Y	O33-C19	-2.13	1.19	1.23
3	Y	301	U5Y	O01-C02	-2.12	1.19	1.23
3	L	301	U5Y	O33-C19	-2.12	1.19	1.23
3	K	301	U5Y	O33-C19	-2.11	1.19	1.23
3	H	301	U5Y	O32-C22	-2.11	1.19	1.23
3	a	301	U5Y	O33-C19	-2.08	1.19	1.23
3	Z	301	U5Y	O18-C06	-2.07	1.18	1.23
3	N	301	U5Y	O33-C19	-2.05	1.19	1.23
3	J	301	U5Y	O01-C02	-2.04	1.19	1.23
3	M	301	U5Y	O01-C02	-2.03	1.19	1.23
3	H	301	U5Y	O33-C19	-2.03	1.19	1.23
3	b	301	U5Y	O01-C02	-2.02	1.19	1.23
3	K	301	U5Y	O01-C02	-2.01	1.19	1.23

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	a	302	CIT	O6-C6-C3	5.26	122.18	113.05
4	M	302	CIT	O6-C6-C3	5.15	122.00	113.05
4	J	302	CIT	O6-C6-C3	4.82	121.42	113.05
4	L	302	CIT	O6-C6-C3	4.59	121.02	113.05
4	K	302	CIT	O6-C6-C3	4.58	121.00	113.05
4	W	303	CIT	O6-C6-C3	4.38	120.65	113.05
3	K	301	U5Y	C15-C08-N07	4.35	106.94	101.94
3	L	301	U5Y	C15-C08-N07	4.26	106.83	101.94
3	Z	301	U5Y	C15-C08-N07	4.20	106.76	101.94
3	b	301	U5Y	C15-C08-N07	4.03	106.56	101.94
4	N	302	CIT	O6-C6-C3	3.95	119.90	113.05
4	Z	302	CIT	O6-C6-C3	3.90	119.83	113.05
3	Y	301	U5Y	C15-C08-N07	3.89	106.41	101.94
3	I	301	U5Y	C15-C08-N07	3.86	106.37	101.94
4	Y	302	CIT	O6-C6-C3	3.83	119.71	113.05
4	H	302	CIT	O6-C6-C3	3.81	119.67	113.05
3	N	301	U5Y	C15-C08-N07	3.80	106.30	101.94
3	a	301	U5Y	C15-C08-N07	3.78	106.28	101.94
3	V	301	U5Y	C15-C08-N07	3.73	106.22	101.94
3	H	301	U5Y	C15-C08-N07	3.64	106.12	101.94
3	M	301	U5Y	C15-C08-N07	3.64	106.11	101.94
3	W	302	U5Y	C15-C08-N07	3.60	106.08	101.94
3	J	301	U5Y	C15-C08-N07	3.59	106.06	101.94
4	I	302	CIT	O6-C6-C3	3.55	119.21	113.05
4	X	303	CIT	O6-C6-C3	3.46	119.06	113.05
3	a	301	U5Y	C17-N07-C08	-3.44	107.83	111.83
4	b	302	CIT	O6-C6-C3	3.43	119.00	113.05
3	X	302	U5Y	C25-C24-N23	-3.35	105.97	113.03
3	X	302	U5Y	C15-C08-N07	3.28	105.71	101.94
3	L	301	U5Y	C16-C17-N07	3.28	109.00	103.25
3	J	301	U5Y	C40-O39-C38	-3.27	111.15	118.80
4	V	302	CIT	O6-C6-C3	3.25	118.69	113.05
3	K	301	U5Y	C17-N07-C08	-3.25	108.06	111.83
3	W	302	U5Y	C43-C44-C21	-3.19	104.58	113.39
3	a	301	U5Y	C40-O39-C38	-3.18	111.36	118.80
3	V	301	U5Y	C25-C24-N23	-3.10	106.48	113.03
3	L	301	U5Y	C43-C44-C21	-2.99	105.13	113.39
3	X	302	U5Y	C22-C21-N20	-2.95	103.12	111.16
3	K	301	U5Y	C43-C44-C21	-2.95	105.25	113.39
3	V	301	U5Y	C40-O39-C38	-2.93	111.95	118.80
3	X	302	U5Y	C17-N07-C08	-2.93	108.43	111.83
3	b	301	U5Y	C16-C17-N07	2.92	108.37	103.25
3	I	301	U5Y	C40-O39-C38	-2.91	112.01	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	301	U5Y	C16-C17-N07	2.90	108.33	103.25
3	I	301	U5Y	C16-C17-N07	2.89	108.33	103.25
3	K	301	U5Y	C15-C08-C09	-2.89	108.02	113.61
3	M	301	U5Y	C16-C17-N07	2.88	108.31	103.25
3	X	302	U5Y	C16-C17-N07	2.87	108.28	103.25
3	N	301	U5Y	C40-O39-C38	-2.86	112.10	118.80
3	Y	301	U5Y	C16-C17-N07	2.86	108.27	103.25
3	Y	301	U5Y	C43-C44-C21	-2.86	105.50	113.39
3	Z	301	U5Y	C16-C17-N07	2.86	108.27	103.25
3	Z	301	U5Y	C17-N07-C08	-2.85	108.52	111.83
3	H	301	U5Y	C40-O39-C38	-2.84	112.16	118.80
3	W	302	U5Y	C15-C08-C09	-2.84	108.11	113.61
3	I	301	U5Y	C17-N07-C08	-2.84	108.53	111.83
3	K	301	U5Y	C40-O39-C38	-2.82	112.21	118.80
3	H	301	U5Y	C17-N07-C08	-2.81	108.57	111.83
3	W	302	U5Y	C22-C21-N20	-2.79	103.56	111.16
3	J	301	U5Y	C17-N07-C08	-2.79	108.59	111.83
4	a	302	CIT	C2-C3-C6	2.77	116.07	110.11
3	N	301	U5Y	C43-C44-C21	-2.77	105.73	113.39
3	V	301	U5Y	C16-C17-N07	2.77	108.11	103.25
3	L	301	U5Y	C15-C08-C09	-2.75	108.27	113.61
3	N	301	U5Y	C17-N07-C08	-2.75	108.64	111.83
3	Y	301	U5Y	C40-O39-C38	-2.73	112.42	118.80
3	V	301	U5Y	C15-C08-C09	-2.72	108.34	113.61
3	J	301	U5Y	O01-C02-N03	-2.72	118.37	122.95
3	M	301	U5Y	C17-N07-C08	-2.71	108.68	111.83
3	W	302	U5Y	C16-C17-N07	2.70	107.99	103.25
3	Z	301	U5Y	C40-O39-C38	-2.68	112.54	118.80
3	M	301	U5Y	C43-C44-C21	-2.66	106.06	113.39
3	b	301	U5Y	C24-N23-C22	-2.65	118.52	122.34
3	Y	301	U5Y	C15-C08-C09	-2.65	108.48	113.61
3	V	301	U5Y	C43-C44-C21	-2.65	106.08	113.39
3	H	301	U5Y	C25-C24-N23	-2.65	107.45	113.03
3	b	301	U5Y	C22-C21-N20	-2.63	103.99	111.16
3	N	301	U5Y	C15-C08-C09	-2.63	108.52	113.61
3	Y	301	U5Y	C17-N07-C08	-2.62	108.79	111.83
3	N	301	U5Y	C16-C17-N07	2.62	107.85	103.25
3	b	301	U5Y	C25-C24-N23	-2.62	107.51	113.03
3	X	302	U5Y	C15-C08-C09	-2.60	108.57	113.61
3	Y	301	U5Y	O01-C02-N03	-2.59	118.58	122.95
3	L	301	U5Y	C25-C24-N23	-2.58	107.58	113.03
3	J	301	U5Y	C16-C17-N07	2.58	107.78	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	301	U5Y	C15-C08-C09	-2.57	108.64	113.61
3	V	301	U5Y	C04-C05-C06	2.56	117.31	112.25
3	W	302	U5Y	C40-O39-C38	-2.56	112.81	118.80
3	L	301	U5Y	C17-N07-C08	-2.56	108.86	111.83
3	L	301	U5Y	C04-C05-C06	2.55	117.30	112.25
4	H	302	CIT	O4-C5-C4	2.55	122.53	114.35
3	M	301	U5Y	O01-C02-N03	-2.55	118.65	122.95
3	W	302	U5Y	C17-N07-C08	-2.52	108.91	111.83
3	V	301	U5Y	C17-N07-C08	-2.50	108.93	111.83
3	K	301	U5Y	C16-C17-N07	2.49	107.62	103.25
3	I	301	U5Y	C22-C21-N20	-2.49	104.38	111.16
4	X	303	CIT	O4-C5-C4	2.49	122.34	114.35
3	Z	301	U5Y	C04-C05-C06	2.48	117.15	112.25
4	a	302	CIT	C4-C3-C2	2.47	115.61	109.16
3	Z	301	U5Y	C25-C24-N23	-2.47	107.82	113.03
3	V	301	U5Y	C05-C04-N03	-2.46	105.79	110.60
3	I	301	U5Y	C43-C44-C21	-2.45	106.62	113.39
3	a	301	U5Y	O01-C02-N03	-2.45	118.82	122.95
3	Z	301	U5Y	C15-C08-C09	-2.45	108.87	113.61
3	b	301	U5Y	O01-C02-N03	-2.44	118.84	122.95
3	J	301	U5Y	C04-C05-C06	2.43	117.06	112.25
3	Z	301	U5Y	C05-C04-N03	-2.42	105.86	110.60
4	N	302	CIT	O2-C1-C2	2.41	122.10	114.35
3	N	301	U5Y	C22-C21-N20	-2.41	104.60	111.16
3	H	301	U5Y	C15-C08-C09	-2.40	108.96	113.61
3	K	301	U5Y	C04-C05-C06	2.38	116.96	112.25
3	a	301	U5Y	C05-C04-N03	-2.36	105.98	110.60
3	H	301	U5Y	C22-C21-N20	-2.36	104.73	111.16
4	b	302	CIT	O2-C1-C2	2.35	121.91	114.35
3	a	301	U5Y	C25-C24-N23	-2.35	108.08	113.03
3	b	301	U5Y	C34-C02-N03	2.33	119.87	115.83
3	I	301	U5Y	O01-C02-N03	-2.32	119.03	122.95
3	b	301	U5Y	C17-N07-C08	-2.32	109.14	111.83
4	H	302	CIT	O4-C5-O3	-2.31	117.54	123.30
3	K	301	U5Y	C05-C04-N03	-2.31	106.08	110.60
4	a	302	CIT	O7-C3-C2	-2.31	104.00	109.40
3	b	301	U5Y	C15-C08-C09	-2.30	109.16	113.61
3	Y	301	U5Y	C22-C21-N20	-2.30	104.91	111.16
3	Y	301	U5Y	C05-C04-N03	-2.29	106.11	110.60
4	J	302	CIT	C3-C2-C1	-2.29	108.26	113.81
3	L	301	U5Y	C40-O39-C38	-2.29	113.45	118.80
4	X	303	CIT	C3-C2-C1	-2.29	108.27	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	301	U5Y	C05-C04-N03	-2.29	106.12	110.60
3	L	301	U5Y	C22-C21-N20	-2.28	104.95	111.16
4	J	302	CIT	O4-C5-O3	-2.28	117.61	123.30
4	L	302	CIT	O2-C1-C2	2.28	121.67	114.35
4	H	302	CIT	C3-C2-C1	-2.28	108.30	113.81
3	V	301	U5Y	C22-C21-N20	-2.27	104.97	111.16
3	X	302	U5Y	C43-C44-C21	-2.27	107.13	113.39
3	N	301	U5Y	C25-C24-N23	-2.27	108.25	113.03
3	W	302	U5Y	C25-C24-N23	-2.26	108.26	113.03
3	Z	301	U5Y	O01-C02-N03	-2.26	119.14	122.95
4	Y	302	CIT	O2-C1-C2	2.25	121.59	114.35
3	X	302	U5Y	C34-C02-N03	2.24	119.71	115.83
3	I	301	U5Y	C05-C04-N03	-2.23	106.23	110.60
4	V	302	CIT	O2-C1-C2	2.23	121.52	114.35
3	b	301	U5Y	C31-C25-C26	2.22	120.50	116.61
3	J	301	U5Y	C43-C44-C21	-2.22	107.25	113.39
4	M	302	CIT	O4-C5-C4	2.22	121.48	114.35
3	a	301	U5Y	C15-C08-C09	-2.22	109.31	113.61
3	a	301	U5Y	C04-C05-C06	2.22	116.64	112.25
3	W	302	U5Y	O01-C02-N03	-2.22	119.21	122.95
4	W	303	CIT	O2-C1-C2	2.21	121.46	114.35
3	V	301	U5Y	O01-C02-N03	-2.21	119.22	122.95
3	M	301	U5Y	C22-C21-N20	-2.20	105.16	111.16
4	a	302	CIT	O5-C6-C3	-2.20	119.14	122.25
3	Y	301	U5Y	C25-C24-N23	-2.20	108.39	113.03
3	N	301	U5Y	O01-C02-N03	-2.19	119.26	122.95
3	N	301	U5Y	C04-C05-C06	2.17	116.55	112.25
4	I	302	CIT	O2-C1-C2	2.17	121.33	114.35
4	b	302	CIT	C4-C3-C6	-2.17	105.44	110.11
3	Z	301	U5Y	C43-C44-C21	-2.17	107.40	113.39
3	M	301	U5Y	C05-C04-N03	-2.17	106.36	110.60
3	L	301	U5Y	C05-C04-N03	-2.16	106.37	110.60
3	N	301	U5Y	C34-C02-N03	2.16	119.58	115.83
4	K	302	CIT	O4-C5-O3	-2.16	117.92	123.30
3	I	301	U5Y	C25-C24-N23	-2.16	108.47	113.03
3	Y	301	U5Y	C34-C02-N03	2.16	119.57	115.83
3	N	301	U5Y	C05-C04-N03	-2.15	106.39	110.60
3	H	301	U5Y	C05-C04-C19	-2.15	105.37	110.42
3	K	301	U5Y	C08-N07-C06	2.15	127.27	120.83
3	M	301	U5Y	C15-C08-C09	-2.13	109.48	113.61
4	X	303	CIT	O4-C5-O3	-2.13	117.99	123.30
3	J	301	U5Y	C34-C02-N03	2.12	119.51	115.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	301	U5Y	C43-C44-C21	-2.11	107.56	113.39
3	L	301	U5Y	O01-C02-N03	-2.11	119.39	122.95
4	V	302	CIT	C4-C3-C6	-2.11	105.58	110.11
3	b	301	U5Y	C28-C26-C25	-2.10	119.78	123.61
3	J	301	U5Y	C25-C24-N23	-2.10	108.59	113.03
3	V	301	U5Y	C31-C25-C26	2.10	120.29	116.61
4	Y	302	CIT	O4-C5-C4	2.10	121.09	114.35
3	K	301	U5Y	C31-C25-C26	2.10	120.28	116.61
3	X	302	U5Y	O01-C02-N03	-2.10	119.41	122.95
3	H	301	U5Y	C43-C44-C21	-2.09	107.62	113.39
3	K	301	U5Y	C25-C24-N23	-2.08	108.64	113.03
4	J	302	CIT	O5-C6-C3	-2.07	119.32	122.25
4	M	302	CIT	O6-C6-O5	-2.06	117.27	123.82
3	J	301	U5Y	C31-C25-C26	2.06	120.21	116.61
4	K	302	CIT	O4-C5-C4	2.06	120.95	114.35
4	b	302	CIT	O2-C1-O1	-2.05	118.19	123.30
3	X	302	U5Y	C31-C25-C26	2.04	120.18	116.61
3	K	301	U5Y	C28-C26-C25	-2.03	119.91	123.61
4	J	302	CIT	O2-C1-C2	2.03	120.87	114.35
3	a	301	U5Y	C34-C02-N03	2.02	119.33	115.83
3	H	301	U5Y	C31-C25-C26	2.01	120.13	116.61
3	K	301	U5Y	C24-N23-C22	-2.00	119.45	122.34

There are no chirality outliers.

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	302	CIT	O7-C3-C6-O5
4	H	302	CIT	O7-C3-C6-O6
4	H	302	CIT	C4-C3-C6-O5
4	H	302	CIT	C4-C3-C6-O6
4	I	302	CIT	C1-C2-C3-O7
4	I	302	CIT	C1-C2-C3-C4
4	I	302	CIT	C1-C2-C3-C6
4	I	302	CIT	C2-C3-C4-C5
4	I	302	CIT	O7-C3-C4-C5
4	I	302	CIT	C6-C3-C4-C5
4	I	302	CIT	O7-C3-C6-O5
4	I	302	CIT	O7-C3-C6-O6
4	I	302	CIT	C4-C3-C6-O5
4	I	302	CIT	C4-C3-C6-O6
4	J	302	CIT	O7-C3-C6-O5

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Mol	Chain	Res	Type	Atoms
4	J	302	CIT	O7-C3-C6-O6
4	J	302	CIT	C4-C3-C6-O5
4	J	302	CIT	C4-C3-C6-O6
4	K	302	CIT	O7-C3-C6-O5
4	K	302	CIT	O7-C3-C6-O6
4	K	302	CIT	C4-C3-C6-O6
4	L	302	CIT	C1-C2-C3-O7
4	L	302	CIT	C1-C2-C3-C4
4	L	302	CIT	C1-C2-C3-C6
4	L	302	CIT	C2-C3-C6-O5
4	L	302	CIT	C2-C3-C6-O6
4	L	302	CIT	O7-C3-C6-O5
4	L	302	CIT	O7-C3-C6-O6
4	M	302	CIT	C2-C3-C4-C5
4	M	302	CIT	O7-C3-C4-C5
4	M	302	CIT	C6-C3-C4-C5
4	M	302	CIT	O7-C3-C6-O5
4	M	302	CIT	O7-C3-C6-O6
4	M	302	CIT	C4-C3-C6-O5
4	M	302	CIT	C4-C3-C6-O6
4	N	302	CIT	C2-C3-C6-O5
4	N	302	CIT	C2-C3-C6-O6
4	N	302	CIT	O7-C3-C6-O5
4	N	302	CIT	O7-C3-C6-O6
4	V	302	CIT	C2-C3-C6-O5
4	V	302	CIT	C2-C3-C6-O6
4	V	302	CIT	O7-C3-C6-O5
4	V	302	CIT	O7-C3-C6-O6
4	W	303	CIT	O7-C3-C6-O5
4	W	303	CIT	O7-C3-C6-O6
4	W	303	CIT	C4-C3-C6-O5
4	W	303	CIT	C4-C3-C6-O6
4	X	303	CIT	C1-C2-C3-O7
4	X	303	CIT	O7-C3-C6-O5
4	X	303	CIT	O7-C3-C6-O6
4	X	303	CIT	C4-C3-C6-O5
4	X	303	CIT	C4-C3-C6-O6
4	Y	302	CIT	C2-C3-C4-C5
4	Y	302	CIT	O7-C3-C4-C5
4	Y	302	CIT	C6-C3-C4-C5
4	Y	302	CIT	C2-C3-C6-O5
4	Y	302	CIT	C2-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
4	Y	302	CIT	O7-C3-C6-O5
4	Y	302	CIT	O7-C3-C6-O6
4	Z	302	CIT	C1-C2-C3-O7
4	Z	302	CIT	C1-C2-C3-C4
4	Z	302	CIT	C1-C2-C3-C6
4	Z	302	CIT	C2-C3-C4-C5
4	Z	302	CIT	O7-C3-C4-C5
4	Z	302	CIT	C6-C3-C4-C5
4	Z	302	CIT	O7-C3-C6-O5
4	Z	302	CIT	O7-C3-C6-O6
4	Z	302	CIT	C4-C3-C6-O5
4	Z	302	CIT	C4-C3-C6-O6
4	a	302	CIT	O7-C3-C6-O5
4	a	302	CIT	O7-C3-C6-O6
4	a	302	CIT	C4-C3-C6-O5
4	a	302	CIT	C4-C3-C6-O6
4	b	302	CIT	C2-C3-C6-O5
4	b	302	CIT	C2-C3-C6-O6
4	b	302	CIT	O7-C3-C6-O5
4	b	302	CIT	O7-C3-C6-O6
4	X	303	CIT	C1-C2-C3-C4
4	Y	302	CIT	C1-C2-C3-C4
5	W	301	DMF	O-C-N-C1
4	K	302	CIT	C4-C3-C6-O5
5	R	302	DMF	O-C-N-C1
4	H	302	CIT	C1-C2-C3-O7
4	H	302	CIT	C1-C2-C3-C4
4	J	302	CIT	C1-C2-C3-O7
4	K	302	CIT	C1-C2-C3-O7
4	L	302	CIT	C6-C3-C4-C5
4	W	303	CIT	C2-C3-C4-C5
4	Y	302	CIT	C1-C2-C3-O7
5	R	301	DMF	O-C-N-C1
3	X	302	U5Y	O01-C02-C34-C35
5	W	301	DMF	O-C-N-C2
4	b	302	CIT	O1-C1-C2-C3
4	J	302	CIT	C1-C2-C3-C4
4	L	302	CIT	O7-C3-C4-C5
4	b	302	CIT	O2-C1-C2-C3
3	X	302	U5Y	N03-C02-C34-C35
5	R	301	DMF	O-C-N-C2
5	R	302	DMF	O-C-N-C2

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Mol	Chain	Res	Type	Atoms
4	K	302	CIT	C2-C3-C6-O5
4	K	302	CIT	C2-C3-C6-O6
4	N	302	CIT	O1-C1-C2-C3
4	Y	302	CIT	C3-C4-C5-O3
4	Y	302	CIT	C3-C4-C5-O4
3	b	301	U5Y	O01-C02-C34-C35
4	L	302	CIT	C2-C3-C4-C5
4	V	302	CIT	C6-C3-C4-C5
4	X	303	CIT	C1-C2-C3-C6
4	N	302	CIT	O2-C1-C2-C3
3	b	301	U5Y	N03-C02-C34-C35
4	V	302	CIT	O7-C3-C4-C5
3	b	301	U5Y	C02-C34-C35-C36
4	I	302	CIT	O2-C1-C2-C3
4	I	302	CIT	O1-C1-C2-C3
4	K	302	CIT	C1-C2-C3-C4
4	W	303	CIT	O7-C3-C4-C5
4	a	302	CIT	C1-C2-C3-O7
4	b	302	CIT	C1-C2-C3-O7
4	V	302	CIT	C2-C3-C4-C5
4	W	303	CIT	C1-C2-C3-O7
4	W	303	CIT	C6-C3-C4-C5
4	a	302	CIT	O7-C3-C4-C5
3	M	301	U5Y	C02-C34-C35-C36
3	X	302	U5Y	C02-C34-C35-C36
3	L	301	U5Y	O01-C02-C34-C35
3	M	301	U5Y	O01-C02-C34-C35
4	X	303	CIT	C3-C4-C5-O3
3	J	301	U5Y	C04-C05-C06-O18
3	W	302	U5Y	C04-C05-C06-O18
3	Y	301	U5Y	O01-C02-C34-C35
3	a	301	U5Y	O01-C02-C34-C35
3	J	301	U5Y	C04-C05-C06-N07
3	W	302	U5Y	C04-C05-C06-N07
4	X	303	CIT	C3-C4-C5-O4
3	L	301	U5Y	N03-C02-C34-C35
3	M	301	U5Y	N03-C02-C34-C35
4	H	302	CIT	C3-C4-C5-O3
4	H	302	CIT	C3-C4-C5-O4
3	H	301	U5Y	O01-C02-C34-C35
3	Y	301	U5Y	N03-C02-C34-C35
3	a	301	U5Y	N03-C02-C34-C35

Continued on next page...

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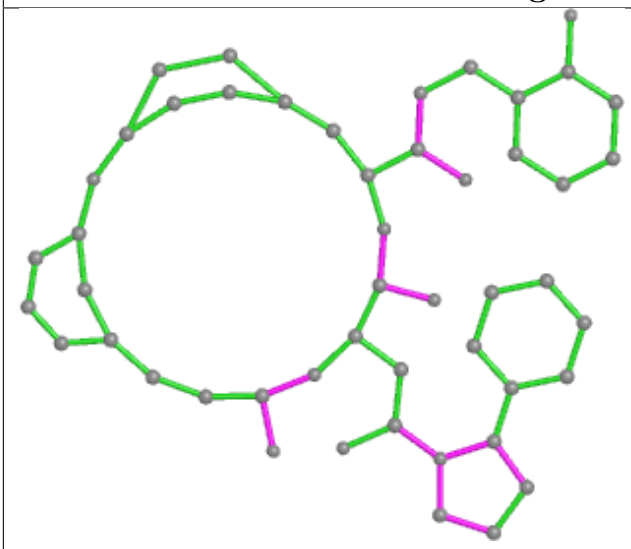
Mol	Chain	Res	Type	Atoms
3	H	301	U5Y	N03-C02-C34-C35
3	I	301	U5Y	O01-C02-C34-C35
3	I	301	U5Y	N03-C02-C34-C35
3	X	302	U5Y	C34-C35-C36-C49

There are no ring outliers.

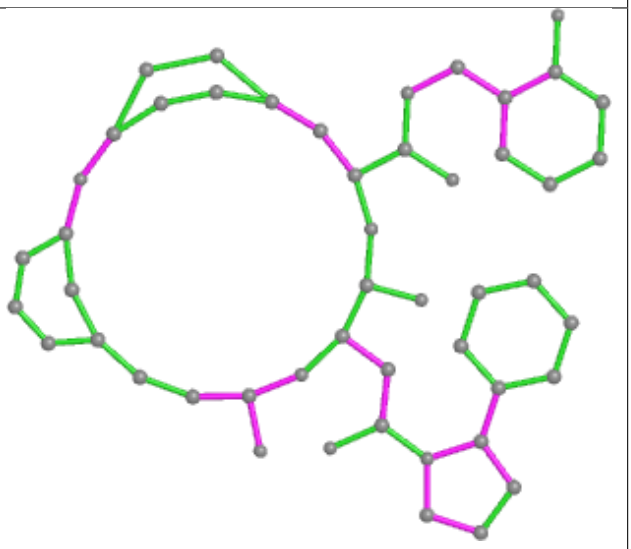
No monomer is involved in short contacts.

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 then 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 U5Y J 301



Bond lengths



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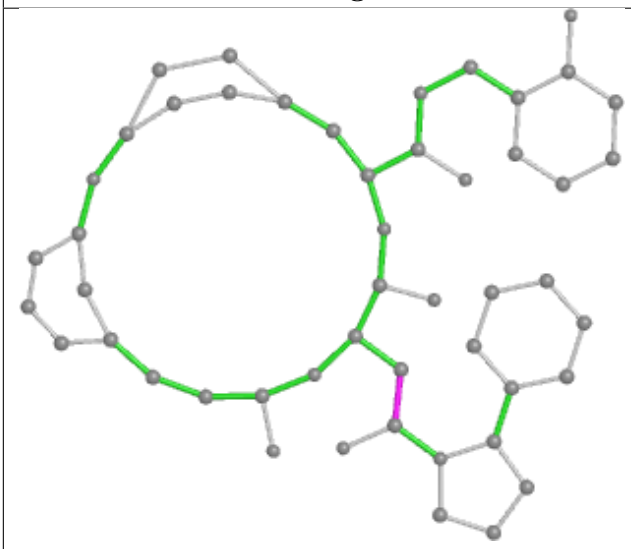

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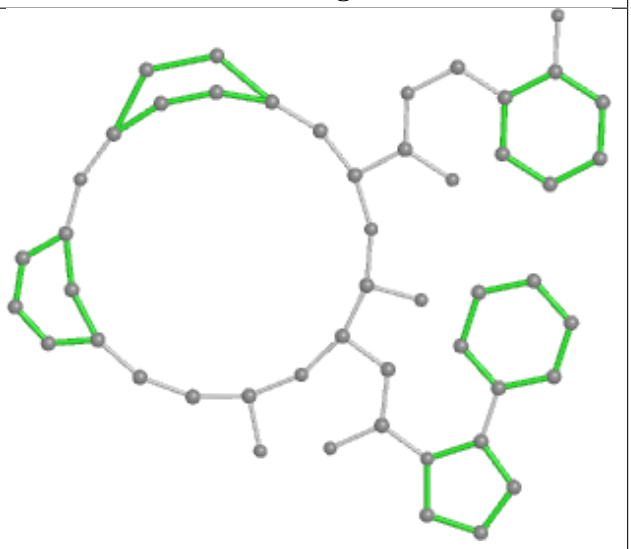
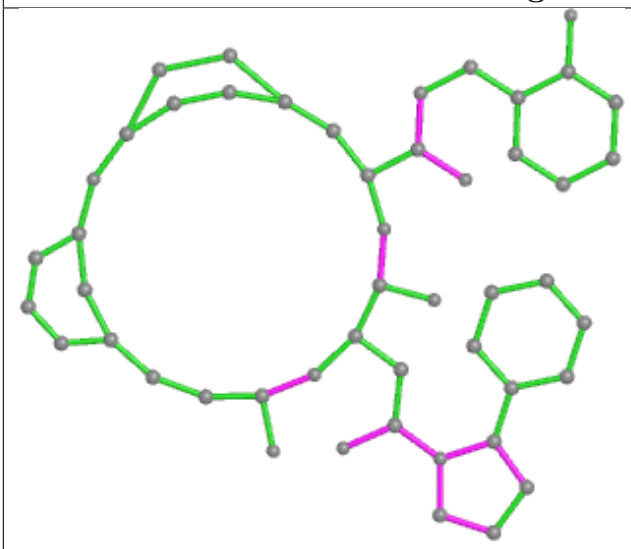


Rings

Ligand U5Y Z 301



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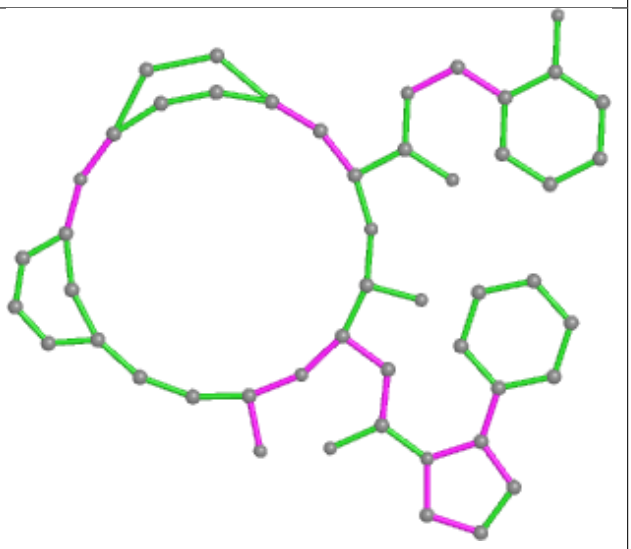

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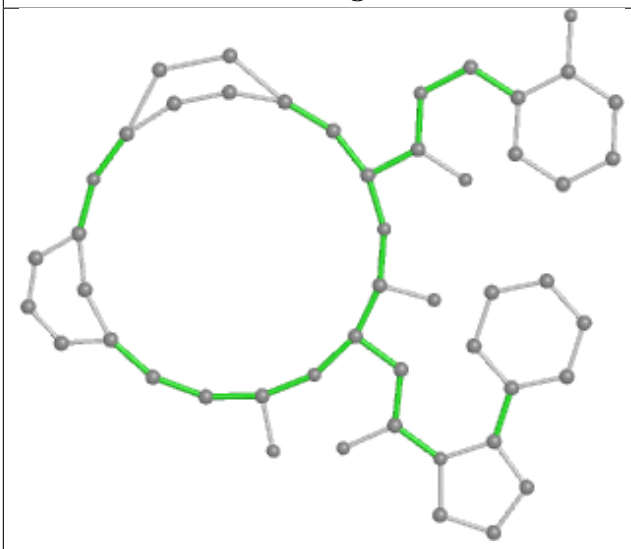

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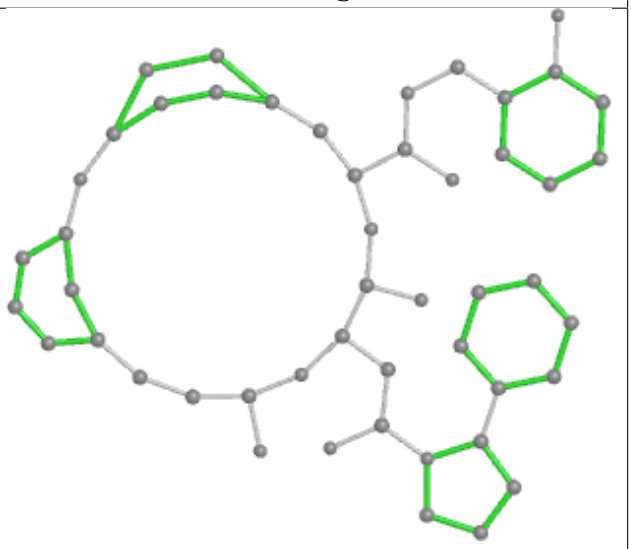
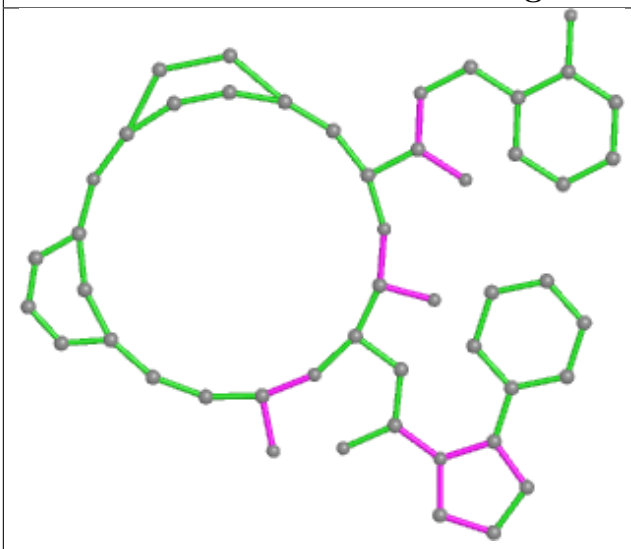


Rings

Ligand U5Y Y 301



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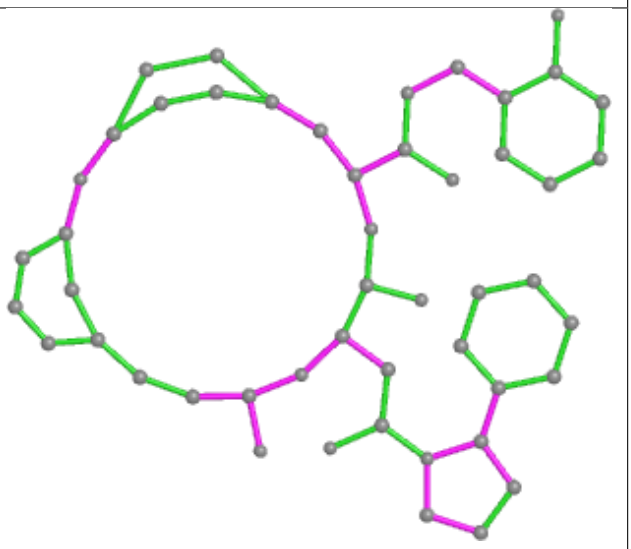

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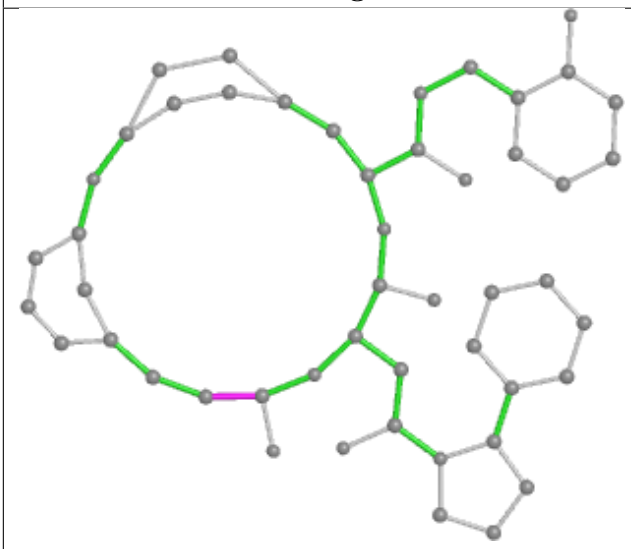

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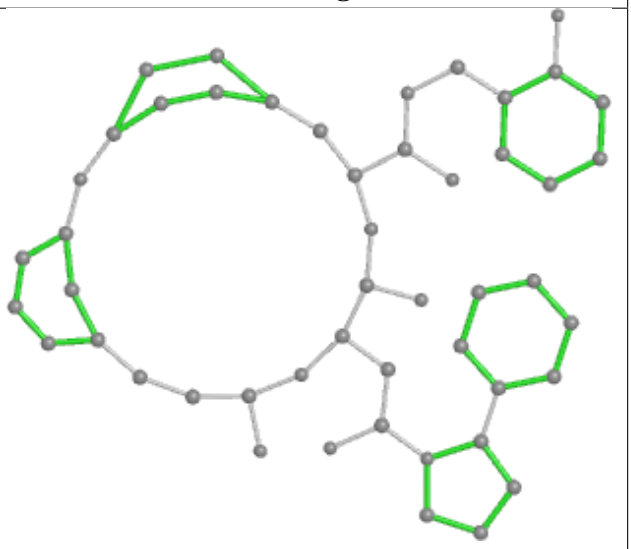
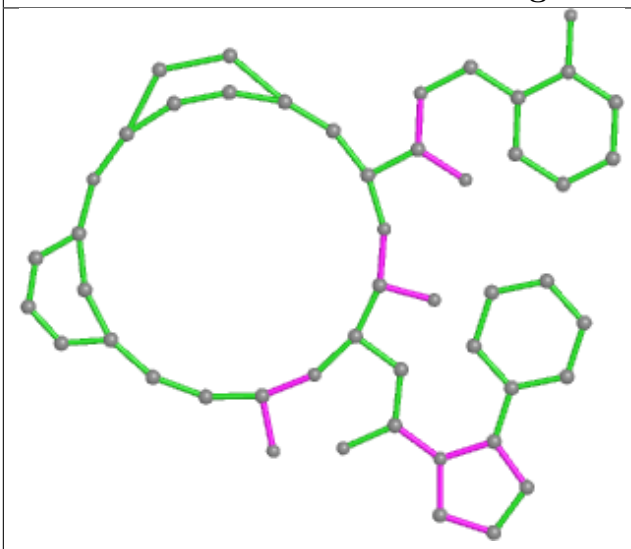


Rings

Ligand U5Y a 301



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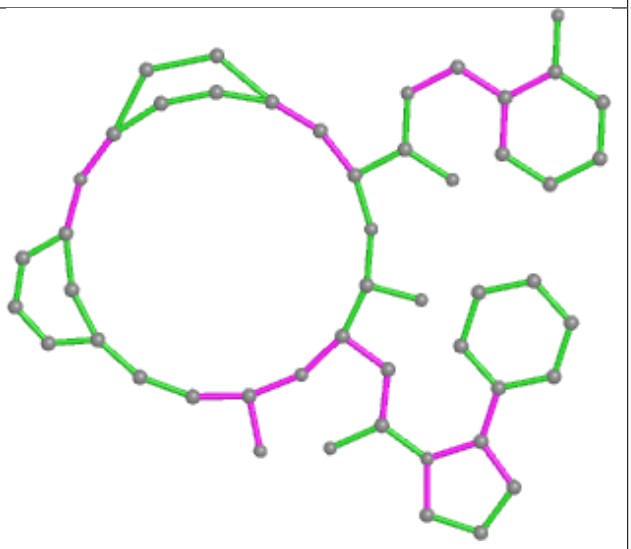

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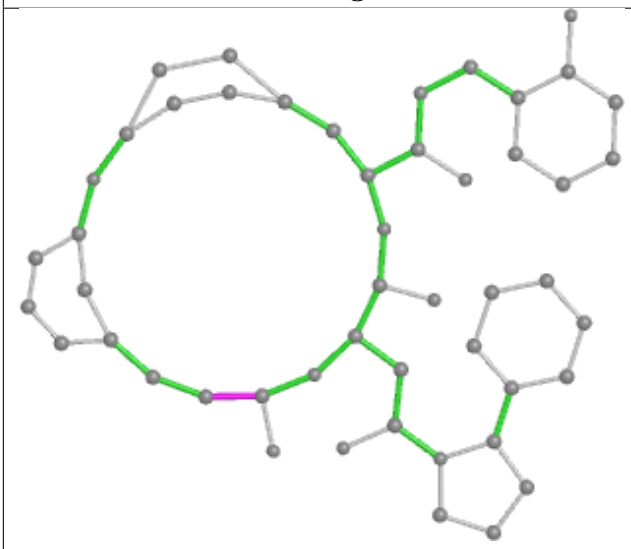

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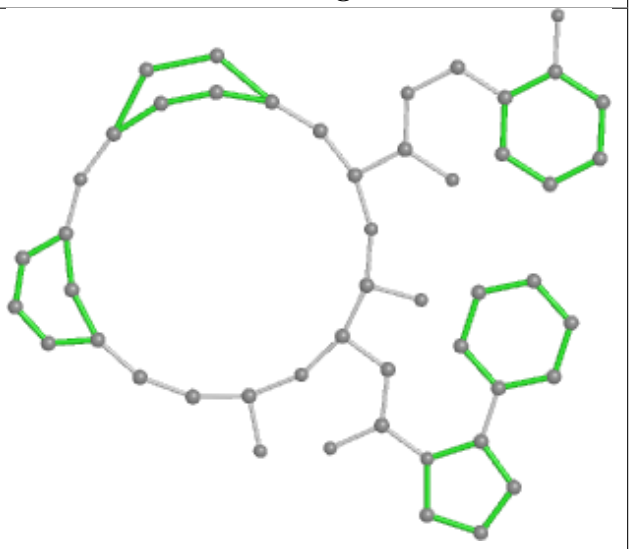
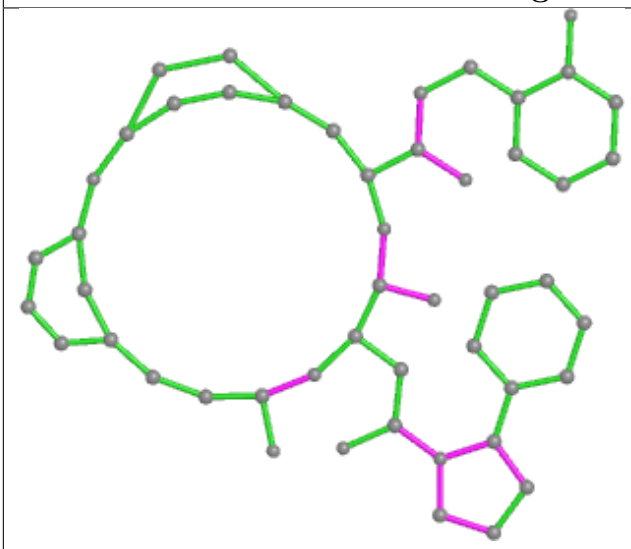


Rings

Ligand U5Y I 301



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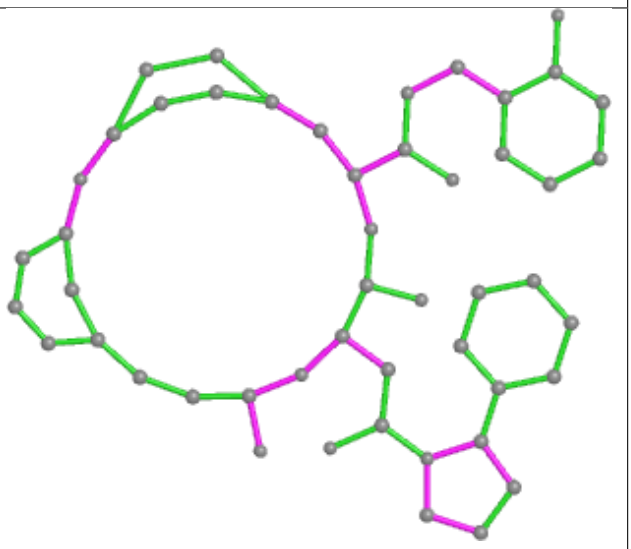

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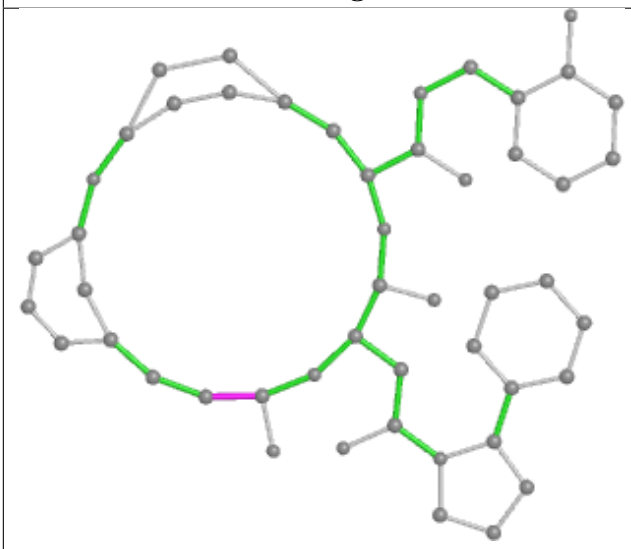

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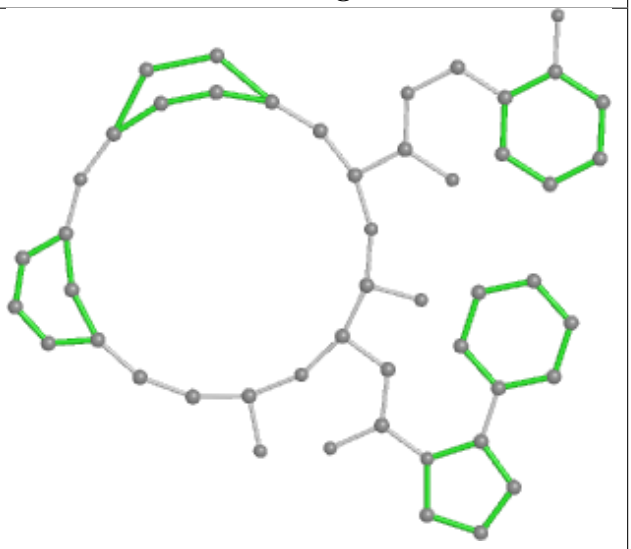

Rings

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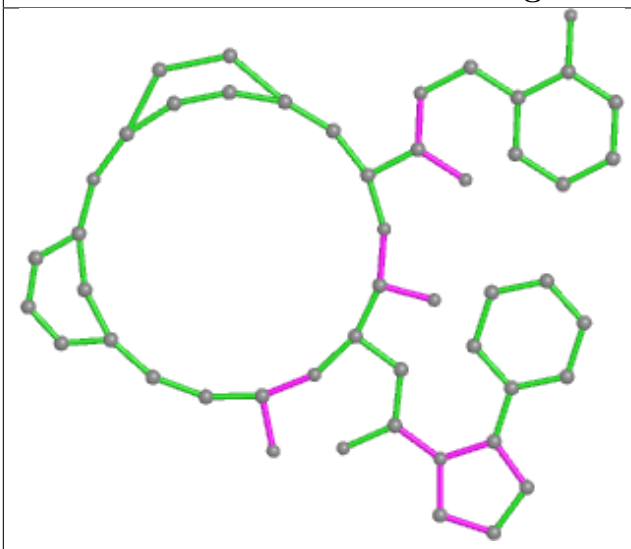

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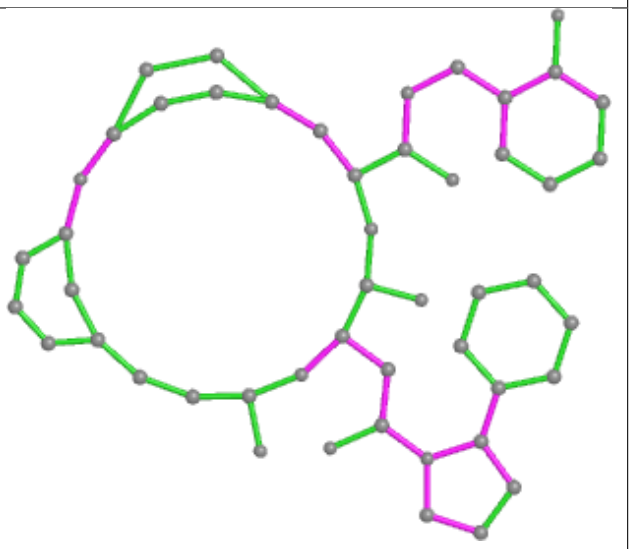

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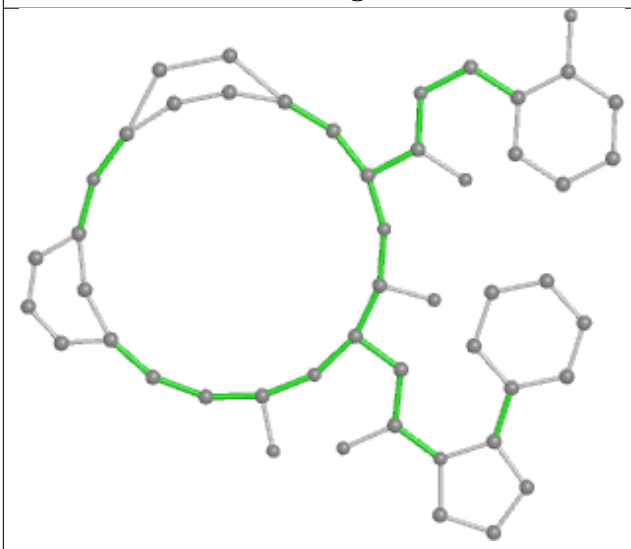

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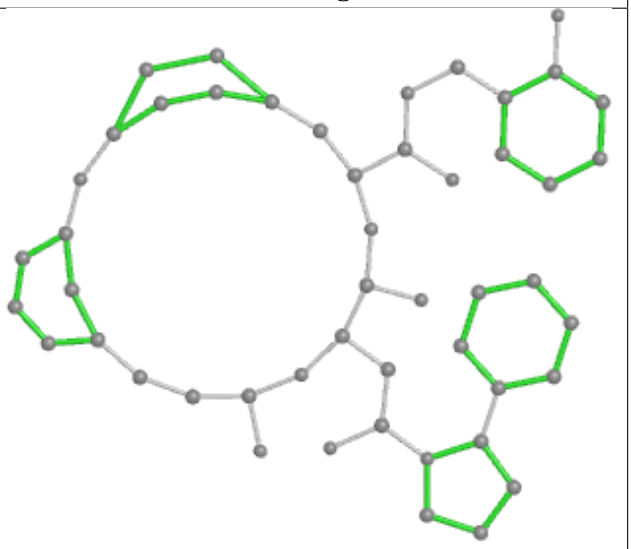
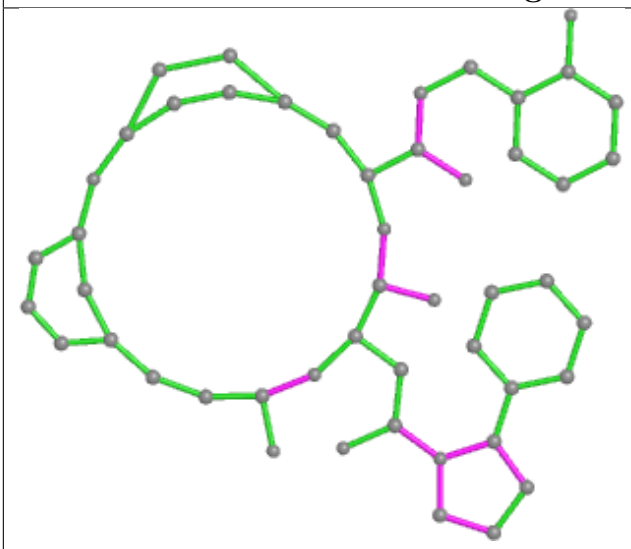


Rings

Ligand U5Y V 301



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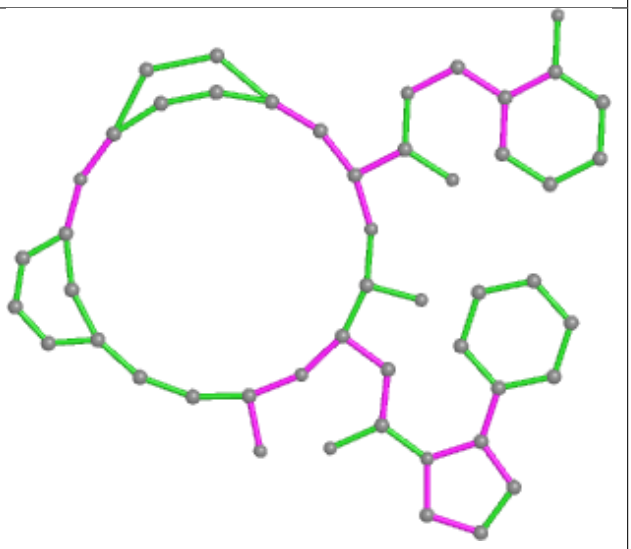

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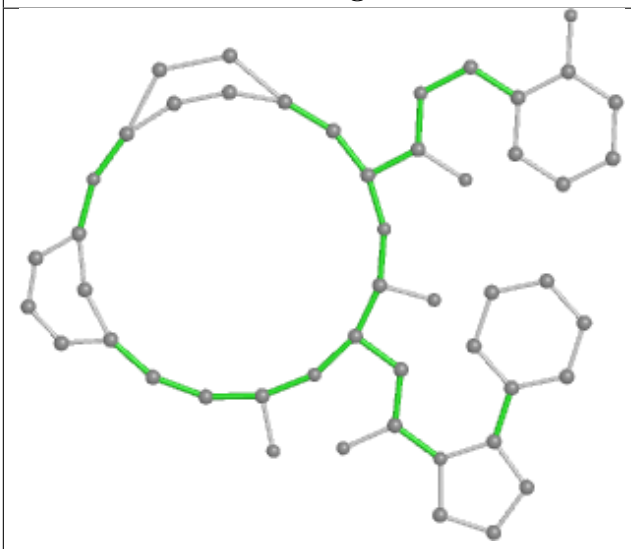

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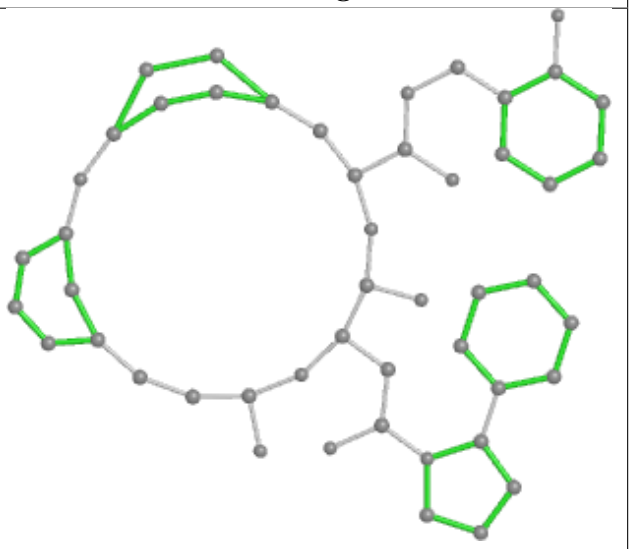
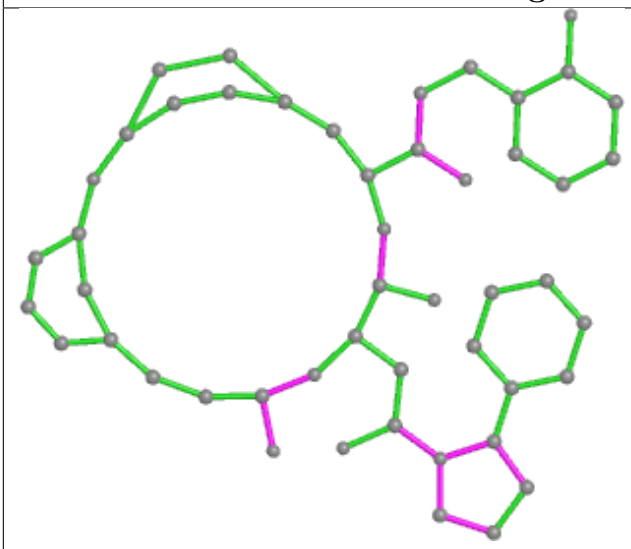


Rings

Ligand U5Y b 301



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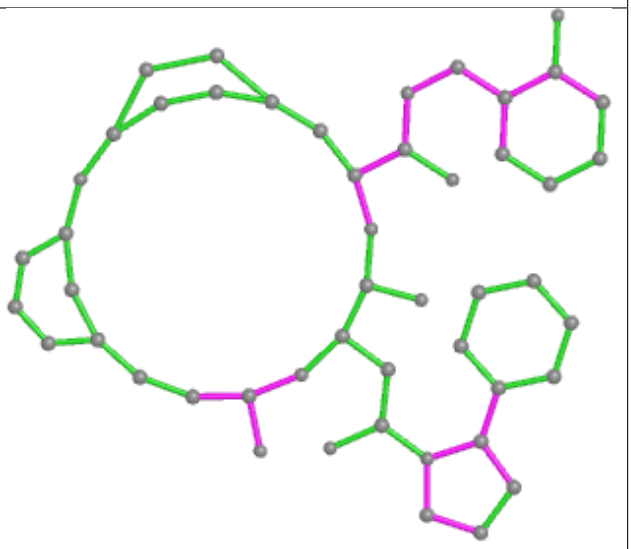

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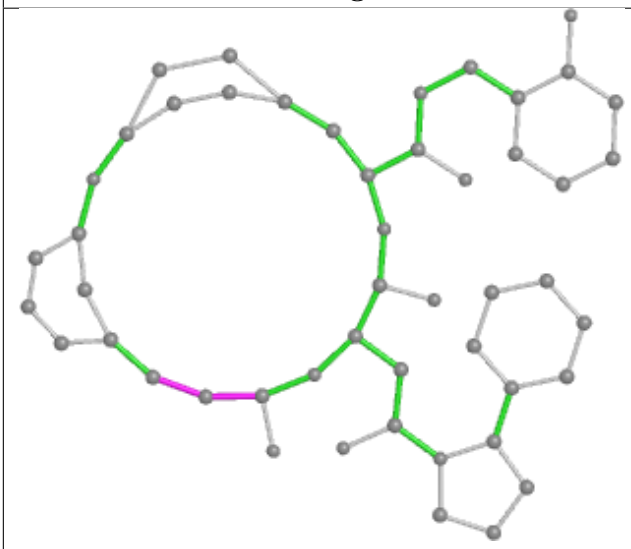

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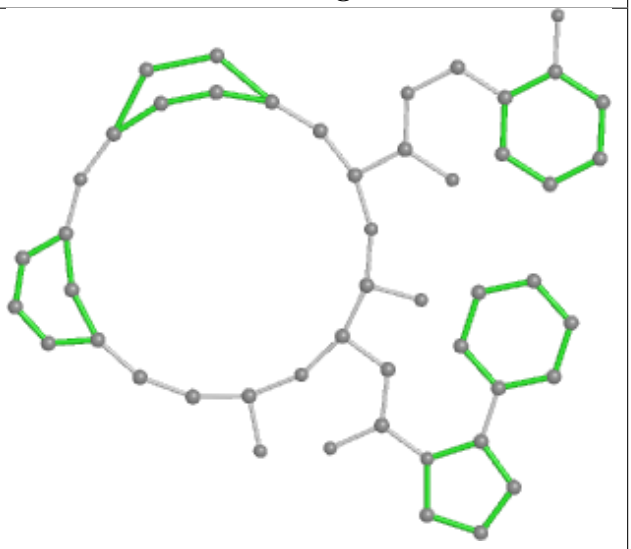
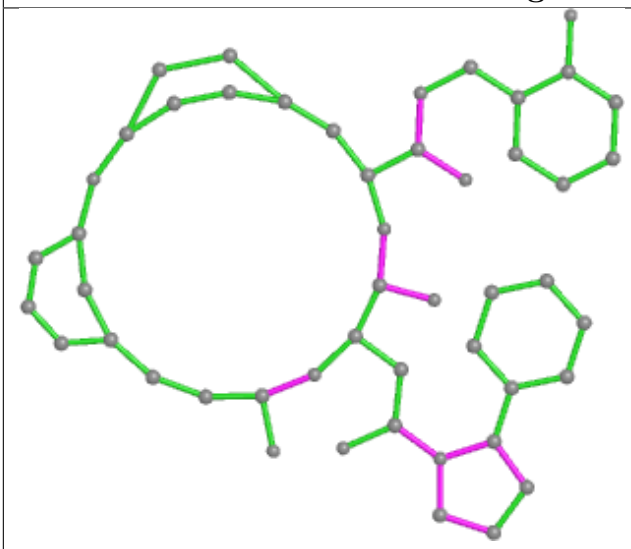


Rings

Ligand U5Y L 301



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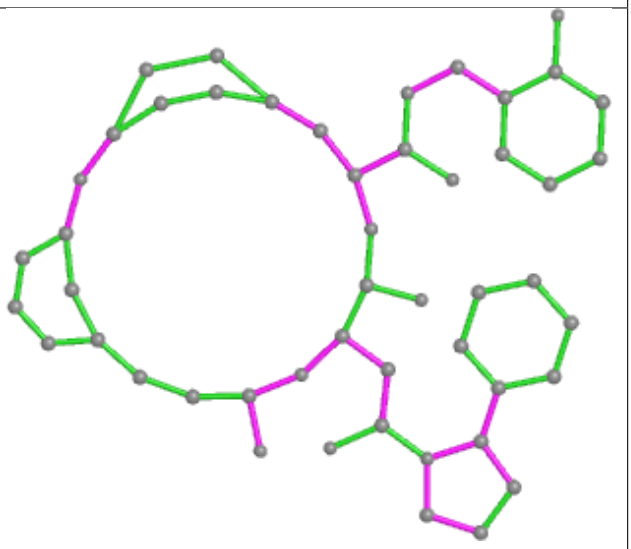

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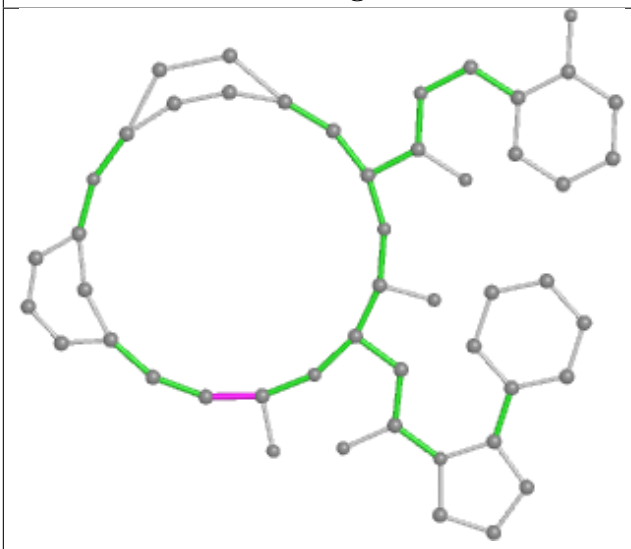

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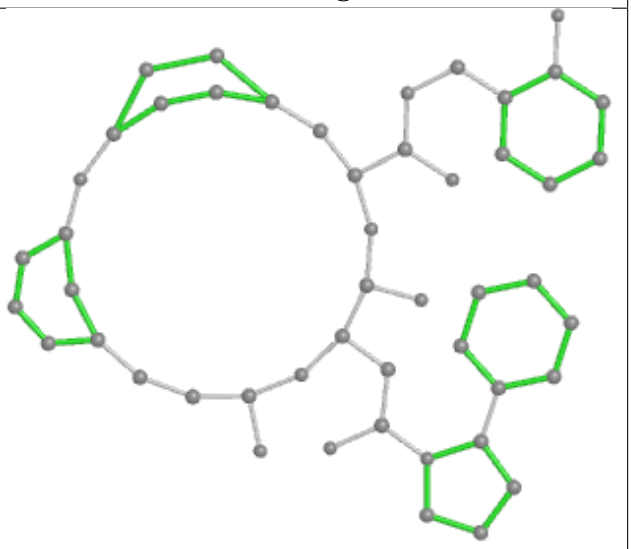
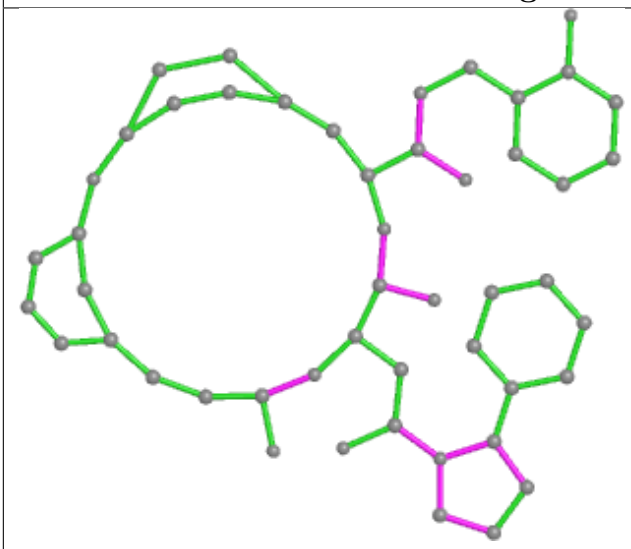


Rings

Ligand U5Y W 302



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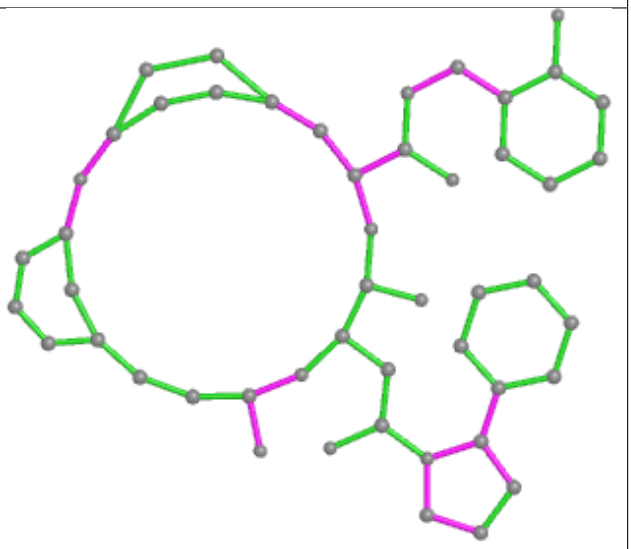

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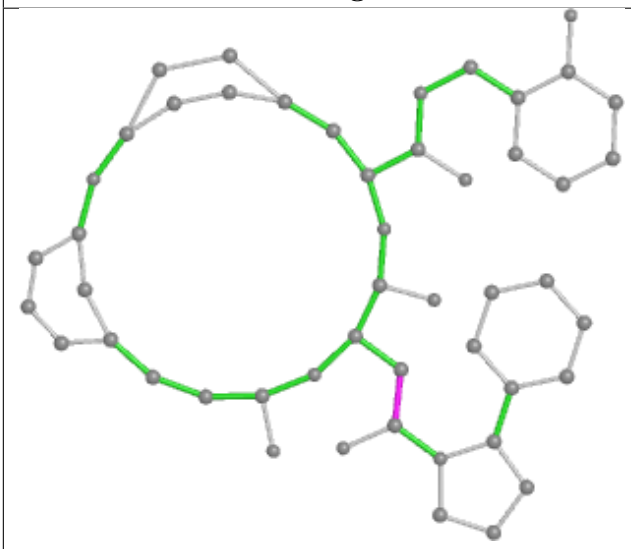

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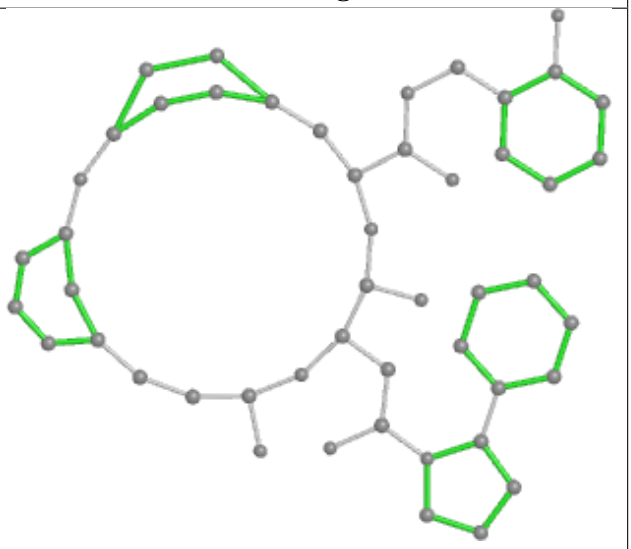
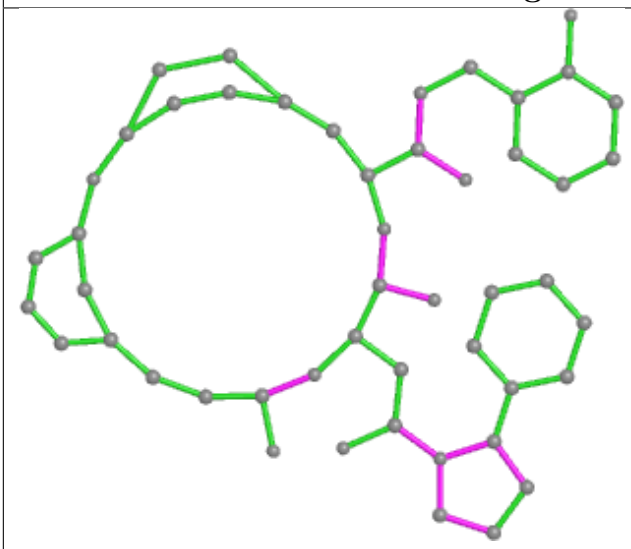


Rings

Ligand U5Y H 301



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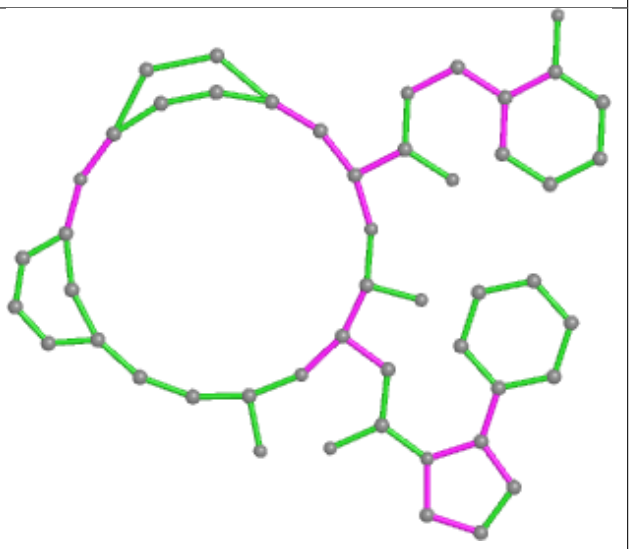

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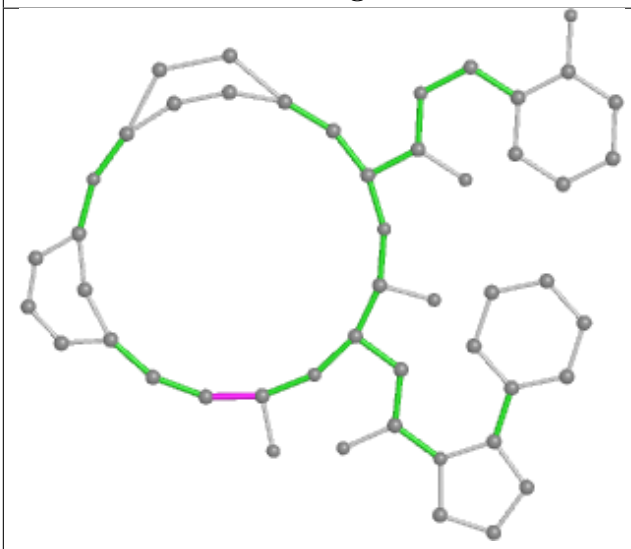

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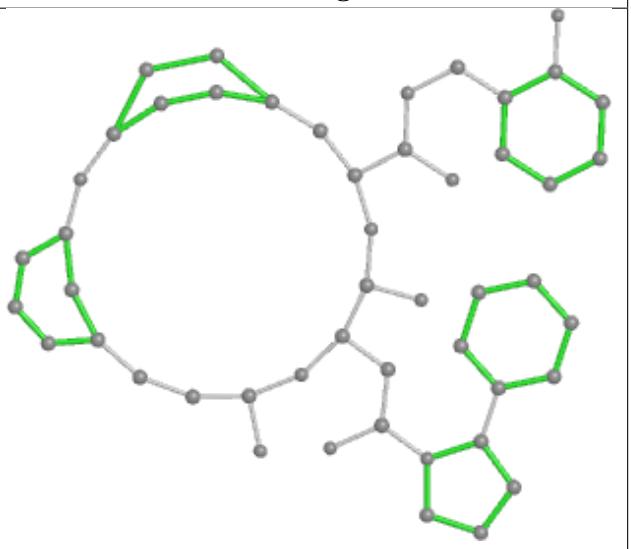

Rings

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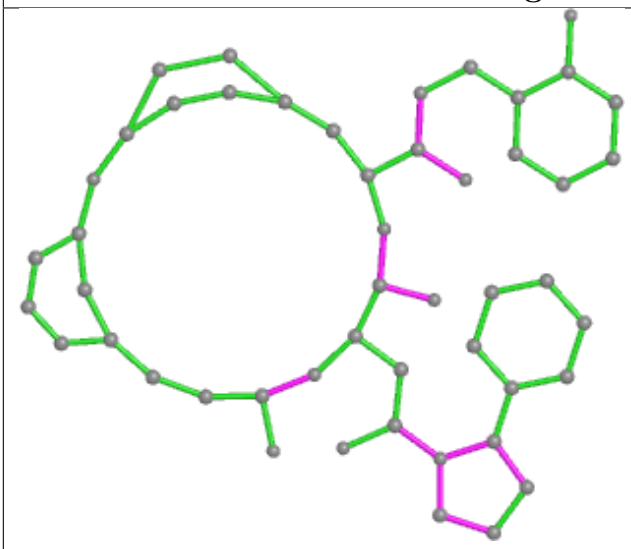

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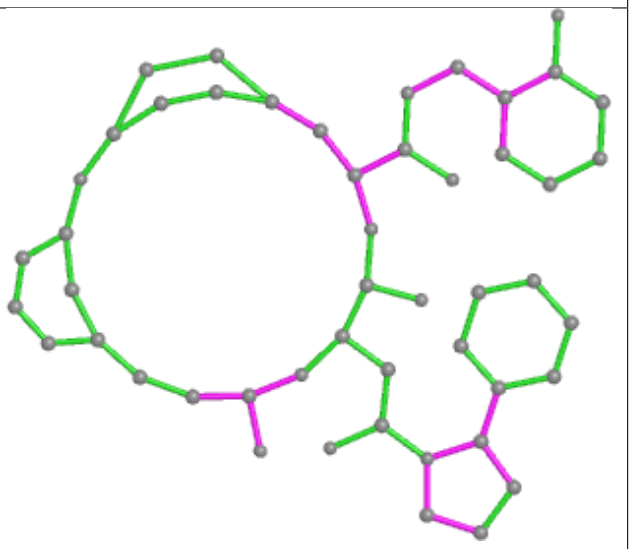

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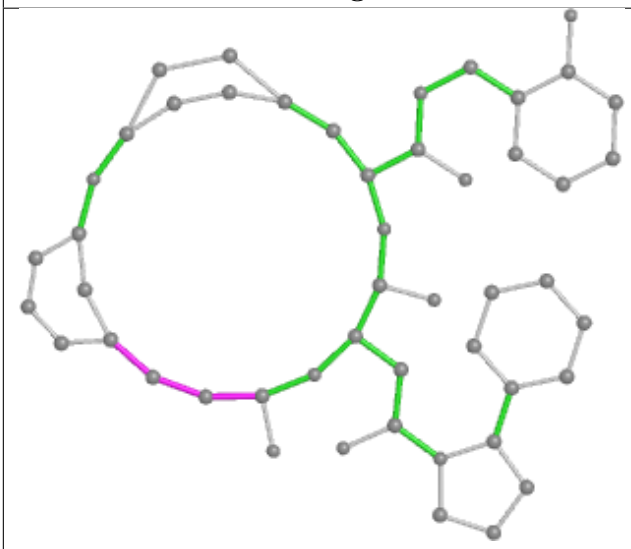
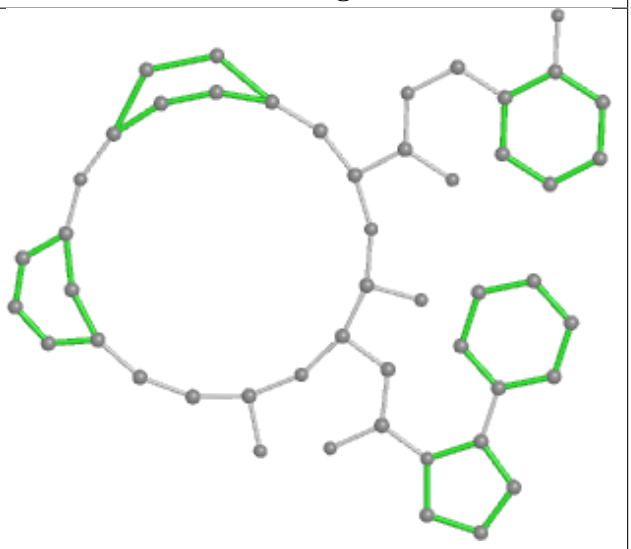
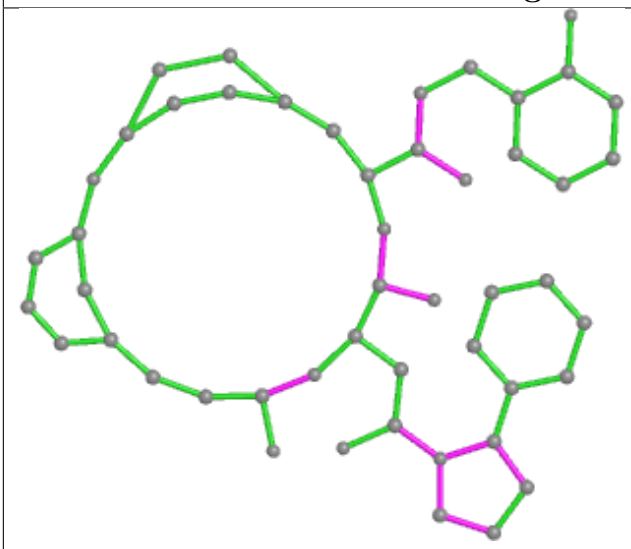


Torsions

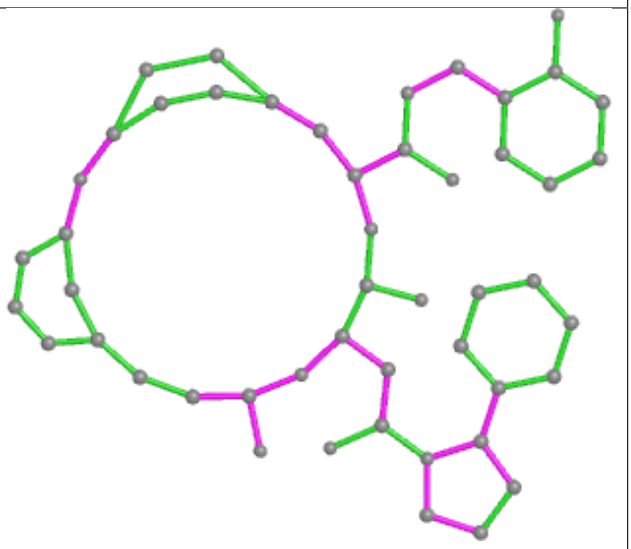


Rings

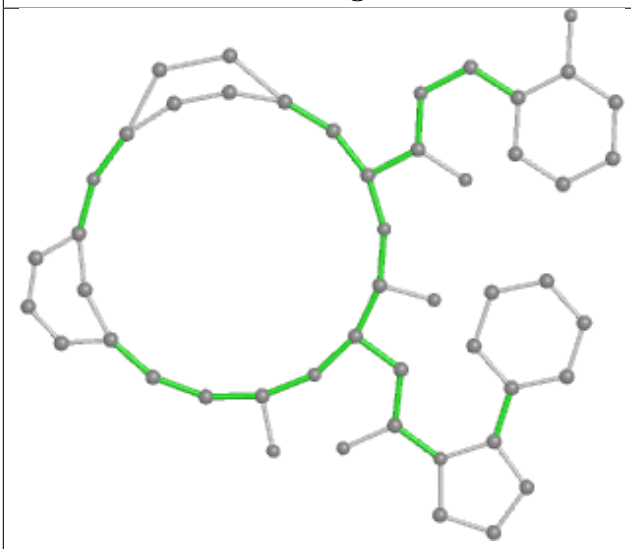
Ligand U5Y N 301



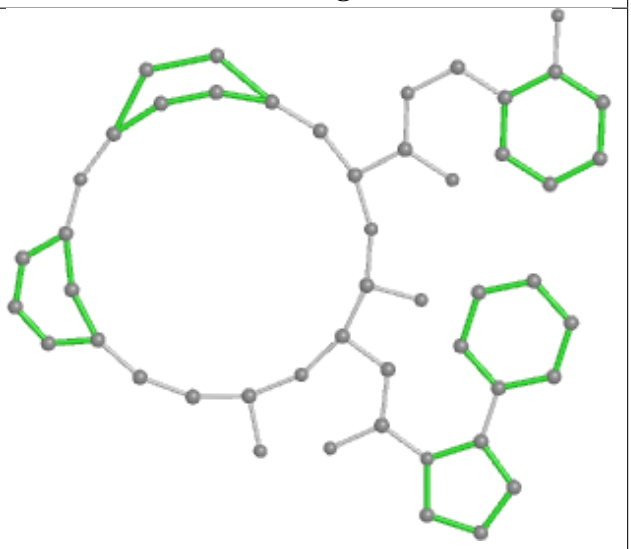
Bond lengths



Bond angles

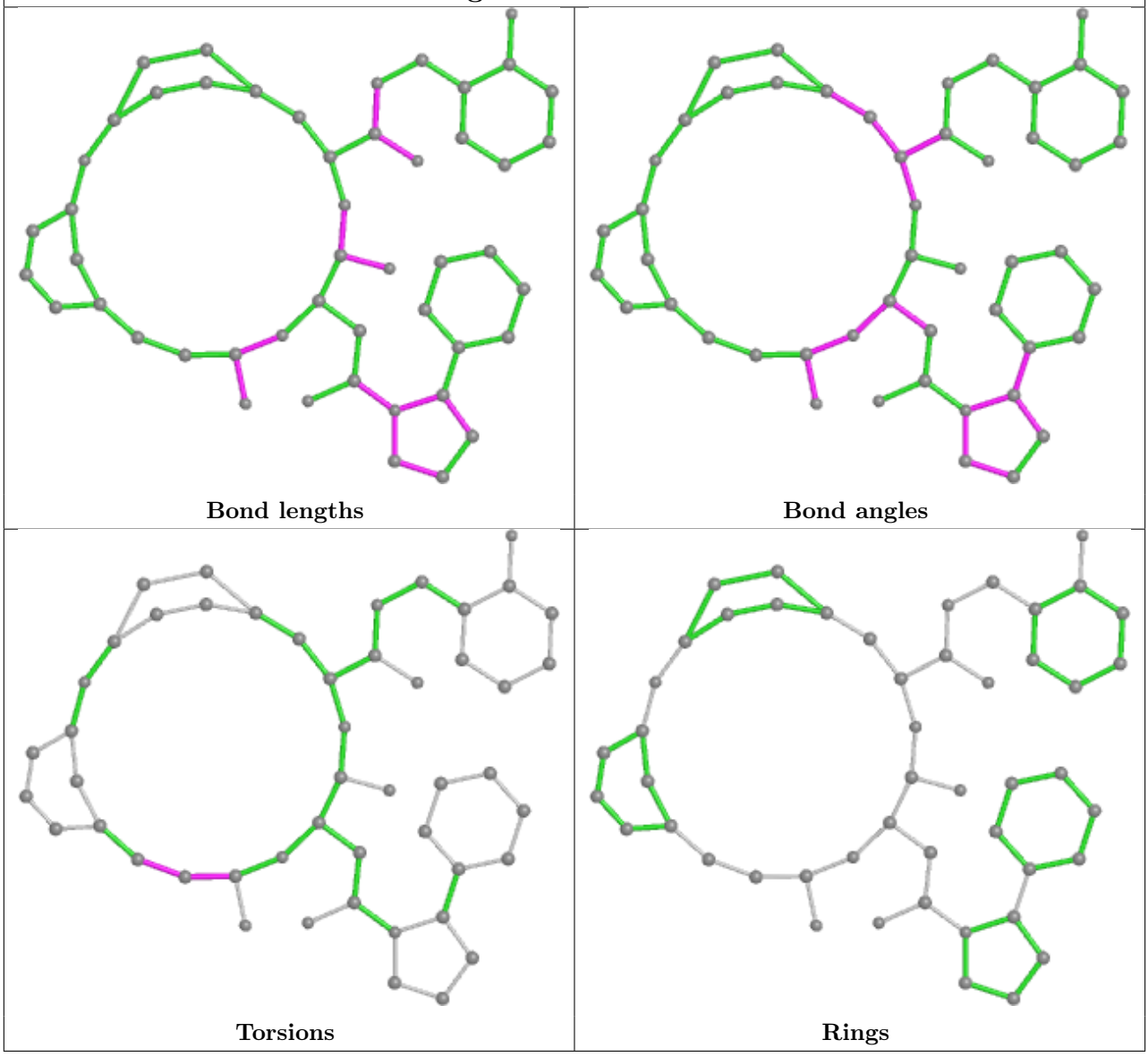


Torsions



Rings

Ligand U5Y M 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

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	216/240 (90%)	0.04	2 (0%) 84 87	34, 51, 75, 97	0
1	B	215/240 (89%)	0.32	9 (4%) 36 41	35, 58, 91, 105	0
1	C	216/240 (90%)	0.56	22 (10%) 6 8	39, 73, 100, 110	0
1	D	217/240 (90%)	0.59	18 (8%) 11 14	41, 70, 96, 101	0
1	E	214/240 (89%)	0.87	30 (14%) 2 3	39, 70, 98, 111	0
1	F	216/240 (90%)	0.81	35 (16%) 1 2	38, 71, 98, 106	0
1	G	220/240 (91%)	0.48	16 (7%) 15 18	36, 61, 92, 105	0
1	O	215/240 (89%)	0.10	5 (2%) 60 66	34, 53, 79, 91	0
1	P	218/240 (90%)	0.22	8 (3%) 41 47	32, 56, 85, 97	0
1	Q	218/240 (90%)	0.46	14 (6%) 19 23	30, 58, 87, 104	0
1	R	217/240 (90%)	0.01	3 (1%) 75 79	27, 47, 69, 88	0
1	S	218/240 (90%)	0.47	13 (5%) 21 26	39, 69, 96, 112	0
1	T	215/240 (89%)	0.70	29 (13%) 3 4	40, 71, 101, 112	0
1	U	218/240 (90%)	0.51	18 (8%) 11 14	38, 66, 93, 108	0
2	H	224/240 (93%)	0.02	1 (0%) 92 94	28, 38, 57, 87	0
2	I	222/240 (92%)	0.05	0 100 100	25, 34, 49, 83	0
2	J	222/240 (92%)	0.10	0 100 100	30, 39, 57, 65	0
2	K	223/240 (92%)	0.04	0 100 100	34, 44, 61, 71	0
2	L	222/240 (92%)	0.01	0 100 100	34, 45, 63, 77	0
2	M	222/240 (92%)	0.04	0 100 100	35, 46, 65, 93	0
2	N	222/240 (92%)	-0.01	0 100 100	33, 43, 62, 84	0
2	V	222/240 (92%)	-0.03	0 100 100	31, 42, 59, 86	0
2	W	223/240 (92%)	0.01	0 100 100	29, 40, 58, 81	0
2	X	222/240 (92%)	0.09	0 100 100	25, 34, 48, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	Y	223/240 (92%)	0.14	0 100 100	24, 33, 50, 84	0
2	Z	222/240 (92%)	0.19	0 100 100	28, 39, 59, 79	0
2	a	222/240 (92%)	0.07	0 100 100	33, 46, 63, 74	0
2	b	224/240 (93%)	0.06	3 (1%) 77 81	32, 46, 65, 91	0
All	All	6148/6720 (91%)	0.24	226 (3%) 41 47	24, 48, 90, 112	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	192	SER	8.8
1	T	188	LEU	6.7
1	G	202	THR	6.6
1	T	202	THR	5.8
1	C	167	LEU	5.4
1	T	9	MET	5.4
1	F	180	ALA	5.2
1	B	235	VAL	5.1
1	D	188	LEU	5.1
1	E	188	LEU	5.1
1	E	191	GLY	5.1
1	G	167	LEU	5.0
1	S	188	LEU	4.8
1	Q	9	MET	4.6
1	D	9	MET	4.5
1	S	172	ALA	4.5
1	B	171	TYR	4.5
1	C	10	GLU	4.4
1	E	167	LEU	4.4
2	b	109	ILE	4.4
1	E	177	LEU	4.2
1	E	48	ARG	4.2
1	G	9	MET	4.1
1	U	201	PRO	4.0
1	D	203	LEU	4.0
1	B	172	ALA	4.0
1	F	163	ILE	3.9
1	F	188	LEU	3.9
1	E	179	ASP	3.9
1	S	235	VAL	3.8
1	D	172	ALA	3.8
1	S	189	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	U	188	LEU	3.8
1	F	192	SER	3.8
1	E	180	ALA	3.7
1	E	205	VAL	3.7
1	F	203	LEU	3.7
1	R	9	MET	3.6
1	C	188	LEU	3.6
1	Q	48	ARG	3.6
1	O	10	GLU	3.5
1	C	157	GLY	3.5
1	T	186	ALA	3.4
1	F	189	ARG	3.4
1	S	184	ALA	3.4
1	U	9	MET	3.4
1	F	9	MET	3.4
1	Q	234	LEU	3.4
1	C	185	VAL	3.3
1	T	163	ILE	3.3
1	Q	188	LEU	3.3
1	P	9	MET	3.3
1	G	189	ARG	3.3
1	E	172	ALA	3.2
1	F	41	PHE	3.2
1	R	10	GLU	3.2
1	P	184	ALA	3.2
1	Q	191	GLY	3.2
1	E	27	ALA	3.2
1	F	120	VAL	3.2
1	T	180	ALA	3.2
1	U	14	ARG	3.1
1	T	33	LEU	3.1
1	U	202	THR	3.1
1	E	171	TYR	3.1
1	U	44	GLU	3.1
1	E	165	ASN	3.1
1	E	169	GLU	3.1
1	U	203	LEU	3.1
1	E	186	ALA	3.1
1	F	50	LEU	3.1
1	F	158	GLY	3.1
1	D	33	LEU	3.0
1	F	21	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	Q	184	ALA	3.0
1	T	131	GLY	3.0
1	F	138	LEU	3.0
1	T	189	ARG	3.0
1	F	167	LEU	2.9
1	D	192	SER	2.9
1	U	21	ARG	2.9
1	F	155	VAL	2.9
1	B	236	ASP	2.9
1	U	206	ALA	2.9
1	T	11	GLN	2.9
1	T	10	GLU	2.9
1	D	186	ALA	2.9
1	F	184	ALA	2.9
1	S	171	TYR	2.9
1	U	48	ARG	2.9
1	C	235	VAL	2.8
1	T	184	ALA	2.8
1	C	27	ALA	2.8
1	D	164	ALA	2.8
1	A	201	PRO	2.8
1	C	165	ASN	2.8
1	O	167	LEU	2.8
1	S	33	LEU	2.8
1	T	185	VAL	2.8
1	T	153	PHE	2.7
1	E	192	SER	2.7
1	F	168	LYS	2.7
1	C	172	ALA	2.7
1	D	10	GLU	2.7
1	U	177	LEU	2.7
1	C	48	ARG	2.7
1	S	182	ARG	2.7
1	D	11	GLN	2.7
1	E	153	PHE	2.7
1	C	230	LEU	2.7
1	T	169	GLU	2.7
1	U	164	ALA	2.7
1	C	171	TYR	2.7
1	G	235	VAL	2.7
1	P	167	LEU	2.7
1	R	14	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	T	206	ALA	2.7
1	E	182	ARG	2.6
1	T	182	ARG	2.6
1	E	148	ALA	2.6
1	D	163	ILE	2.6
1	E	184	ALA	2.6
1	E	190	ALA	2.6
1	G	192	SER	2.6
1	C	203	LEU	2.6
1	G	33	LEU	2.6
1	E	164	ALA	2.6
1	D	165	ASN	2.6
1	B	33	LEU	2.5
1	B	167	LEU	2.5
1	C	182	ARG	2.5
1	G	203	LEU	2.5
1	S	234	LEU	2.5
1	F	48	ARG	2.5
1	G	48	ARG	2.5
1	F	49	SER	2.5
1	T	172	ALA	2.5
1	S	9	MET	2.5
1	F	169	GLU	2.5
1	T	167	LEU	2.5
1	G	14	ARG	2.5
1	C	233	LEU	2.5
1	Q	172	ALA	2.4
1	D	179	ASP	2.4
1	G	182	ARG	2.4
1	U	189	ARG	2.4
1	P	192	SER	2.4
1	F	171	TYR	2.4
1	T	177	LEU	2.4
1	C	164	ALA	2.4
1	Q	10	GLU	2.4
1	E	233	LEU	2.4
1	E	168	LYS	2.4
1	T	158	GLY	2.4
1	F	24	ILE	2.4
1	E	33	LEU	2.4
1	G	234	LEU	2.4
1	Q	33	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	U	167	LEU	2.4
1	S	165	ASN	2.4
1	U	36	ALA	2.3
1	O	48	ARG	2.3
1	B	10	GLU	2.3
1	E	158	GLY	2.3
1	E	143	TYR	2.3
1	A	235	VAL	2.3
2	b	114	PRO	2.3
1	F	190	ALA	2.3
1	S	205	VAL	2.3
2	b	115	GLN	2.3
1	F	177	LEU	2.2
1	T	171	TYR	2.2
1	D	190	ALA	2.2
1	E	14	ARG	2.2
1	Q	190	ALA	2.2
1	T	226	THR	2.2
1	P	33	LEU	2.2
1	G	236	ASP	2.2
1	C	166	ALA	2.2
1	T	183	ILE	2.2
2	H	224	ALA	2.2
1	G	188	LEU	2.2
1	O	135	ARG	2.2
1	C	179	ASP	2.2
1	B	169	GLU	2.2
1	Q	169	GLU	2.2
1	E	159	THR	2.2
1	P	14	ARG	2.2
1	Q	50	LEU	2.2
1	F	31	VAL	2.2
1	U	172	ALA	2.2
1	C	33	LEU	2.2
1	F	231	GLN	2.1
1	G	201	PRO	2.1
1	D	182	ARG	2.1
1	C	153	PHE	2.1
1	T	12	ALA	2.1
1	C	163	ILE	2.1
1	F	165	ASN	2.1
1	F	182	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	44	GLU	2.1
1	D	171	TYR	2.1
1	E	155	VAL	2.1
1	F	45	ASN	2.1
1	P	191	GLY	2.1
1	F	205	VAL	2.1
1	T	29	SER	2.1
1	O	11	GLN	2.1
1	S	236	ASP	2.1
1	D	184	ALA	2.1
1	F	164	ALA	2.1
1	F	143	TYR	2.1
1	F	160	THR	2.0
1	Q	163	ILE	2.0
1	U	163	ILE	2.0
1	U	158	GLY	2.0
1	D	180	ALA	2.0
1	G	184	ALA	2.0
1	F	30	VAL	2.0
1	P	169	GLU	2.0
1	T	203	LEU	2.0
1	F	11	GLN	2.0
1	C	189	ARG	2.0
1	T	160	THR	2.0
1	B	229	ALA	2.0
1	E	211	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

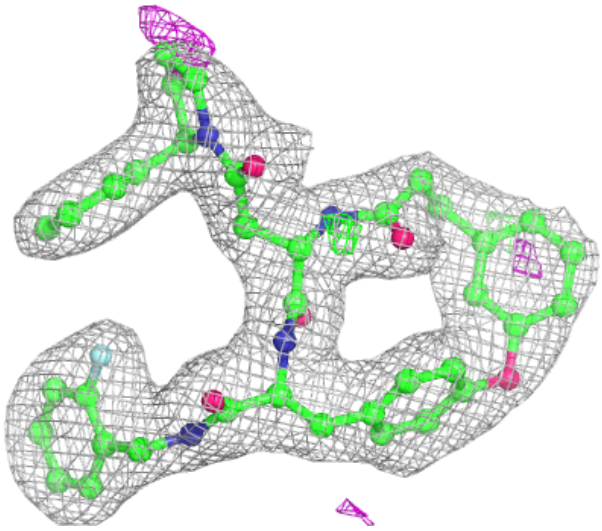
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

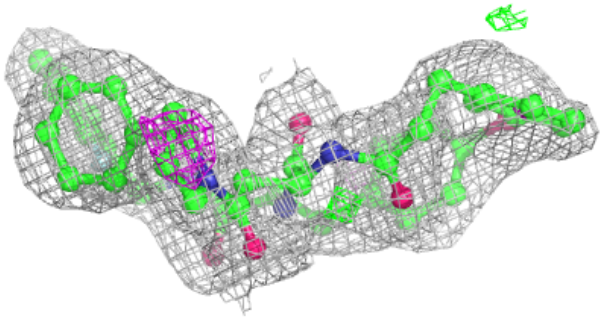
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CIT	a	302	13/13	0.80	0.22	47,56,70,80	0
5	DMF	R	301	5/5	0.80	0.20	50,51,56,59	0
5	DMF	X	301	5/5	0.80	0.18	40,46,55,57	0
4	CIT	M	302	13/13	0.82	0.26	41,58,70,71	0
4	CIT	L	302	13/13	0.82	0.26	48,57,69,73	0
4	CIT	X	303	13/13	0.83	0.17	35,47,64,66	0
4	CIT	V	302	13/13	0.83	0.24	41,55,67,74	0
4	CIT	K	302	13/13	0.84	0.18	49,58,67,77	0
4	CIT	I	302	13/13	0.84	0.15	37,50,62,66	0
4	CIT	Z	302	13/13	0.86	0.18	43,56,73,75	0
4	CIT	b	302	13/13	0.86	0.16	43,59,69,75	0
4	CIT	H	302	13/13	0.87	0.19	39,49,61,63	0
4	CIT	Y	302	13/13	0.88	0.14	34,50,64,71	0
4	CIT	J	302	13/13	0.88	0.14	41,53,59,66	0
5	DMF	R	302	5/5	0.89	0.27	48,57,59,60	0
4	CIT	W	303	13/13	0.89	0.26	39,51,66,69	0
5	DMF	Q	301	5/5	0.91	0.16	41,42,54,57	0
5	DMF	W	301	5/5	0.91	0.18	40,44,53,55	0
4	CIT	N	302	13/13	0.91	0.16	40,57,63,63	0
5	DMF	P	301	5/5	0.94	0.14	41,43,49,53	0
3	U5Y	J	301	49/49	0.95	0.16	27,37,51,57	0
3	U5Y	N	301	49/49	0.95	0.15	27,35,45,53	0
3	U5Y	V	301	49/49	0.95	0.15	28,34,46,51	0
3	U5Y	Y	301	49/49	0.95	0.16	23,31,42,51	0
3	U5Y	b	301	49/49	0.96	0.14	28,36,50,55	0
3	U5Y	K	301	49/49	0.96	0.14	30,37,46,53	0
3	U5Y	L	301	49/49	0.96	0.15	29,39,52,64	0
3	U5Y	X	302	49/49	0.96	0.17	22,29,44,51	0
3	U5Y	M	301	49/49	0.96	0.15	29,37,52,67	0
5	DMF	S	301	5/5	0.96	0.16	49,49,54,55	0
3	U5Y	Z	301	49/49	0.96	0.17	28,37,60,65	0
3	U5Y	a	301	49/49	0.96	0.16	29,38,51,54	0
5	DMF	O	301	5/5	0.97	0.15	35,43,47,52	0
3	U5Y	I	301	49/49	0.97	0.15	24,31,46,51	0
3	U5Y	W	302	49/49	0.97	0.16	25,31,46,52	0
3	U5Y	H	301	49/49	0.97	0.15	23,30,41,46	0

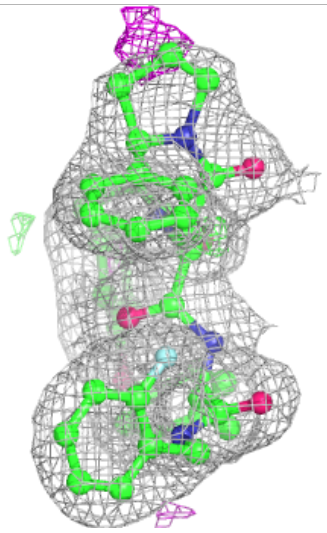
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U5Y J 301:

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

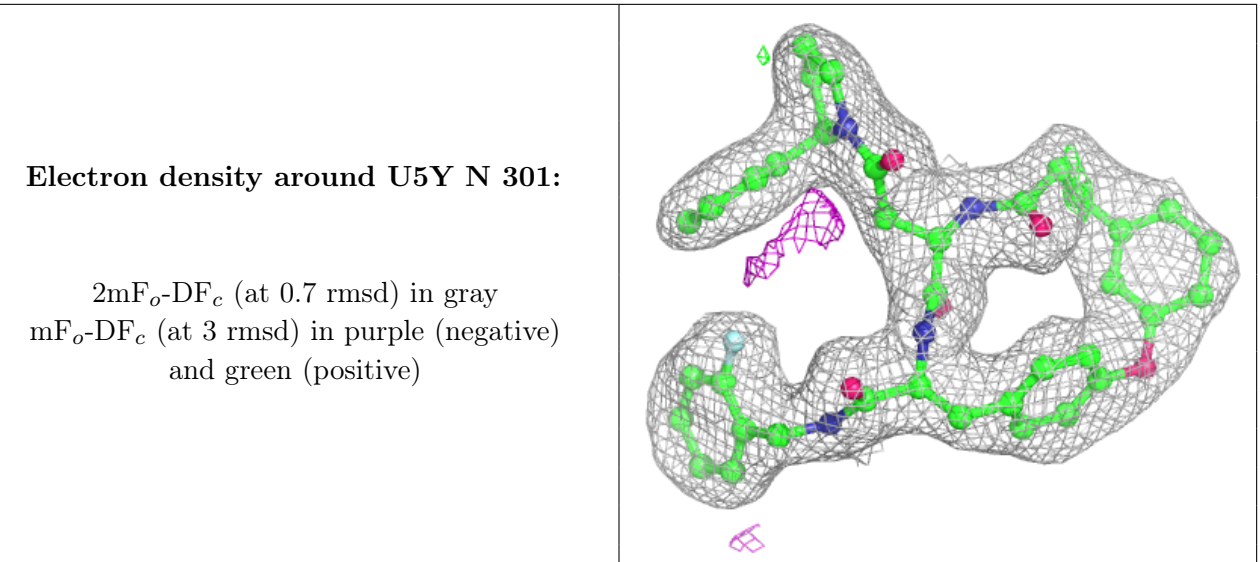


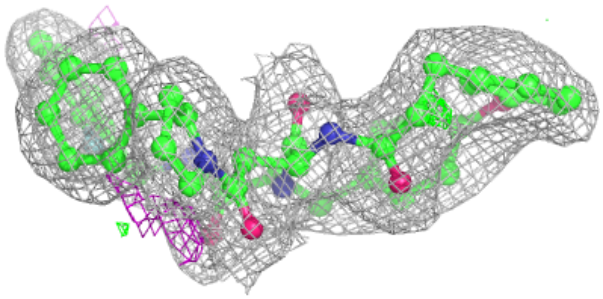


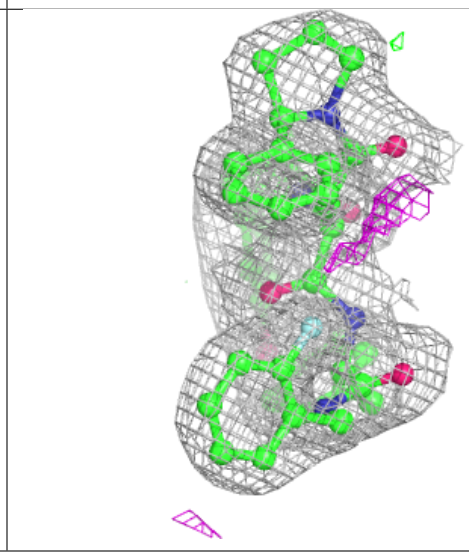


Electron density around U5Y N 301:

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

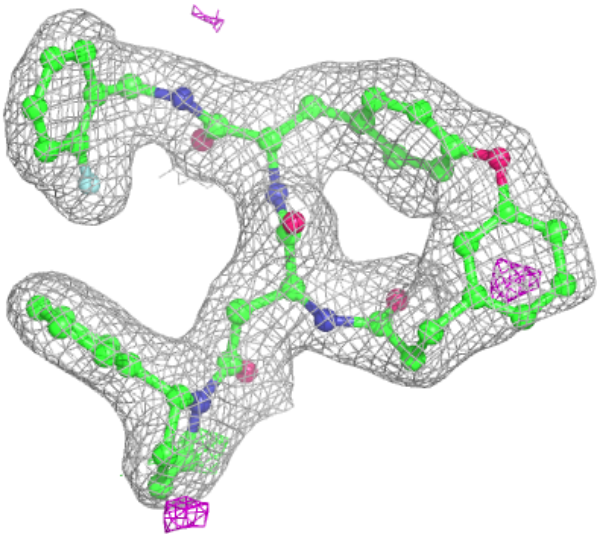


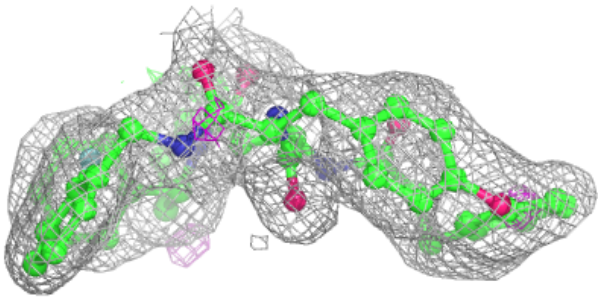


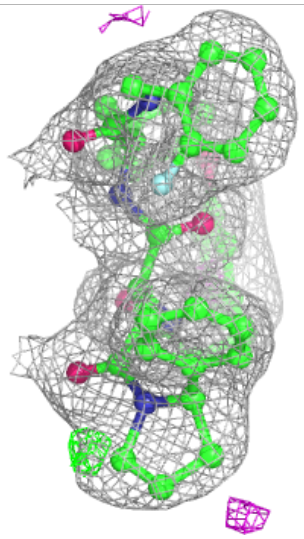


Electron density around U5Y V 301:

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

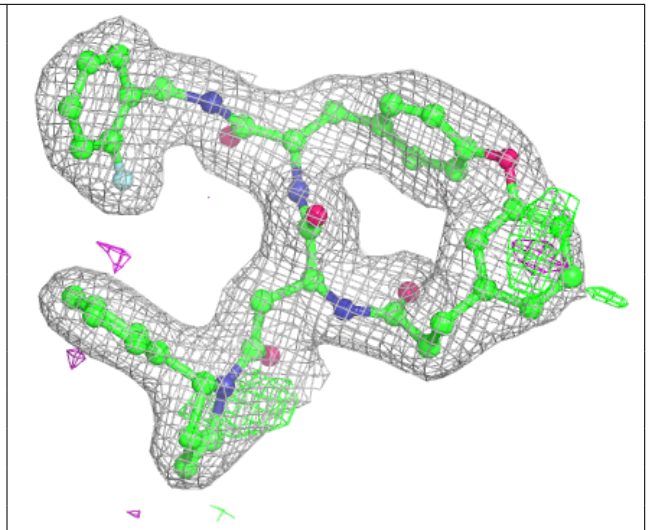


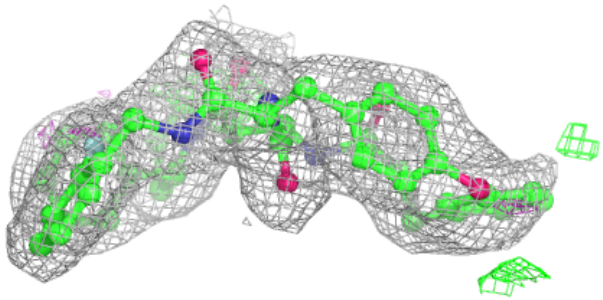


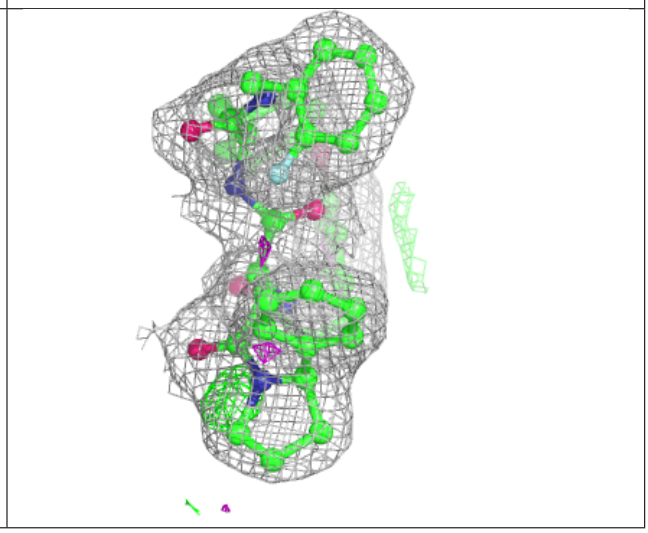


Electron density around U5Y Y 301:

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

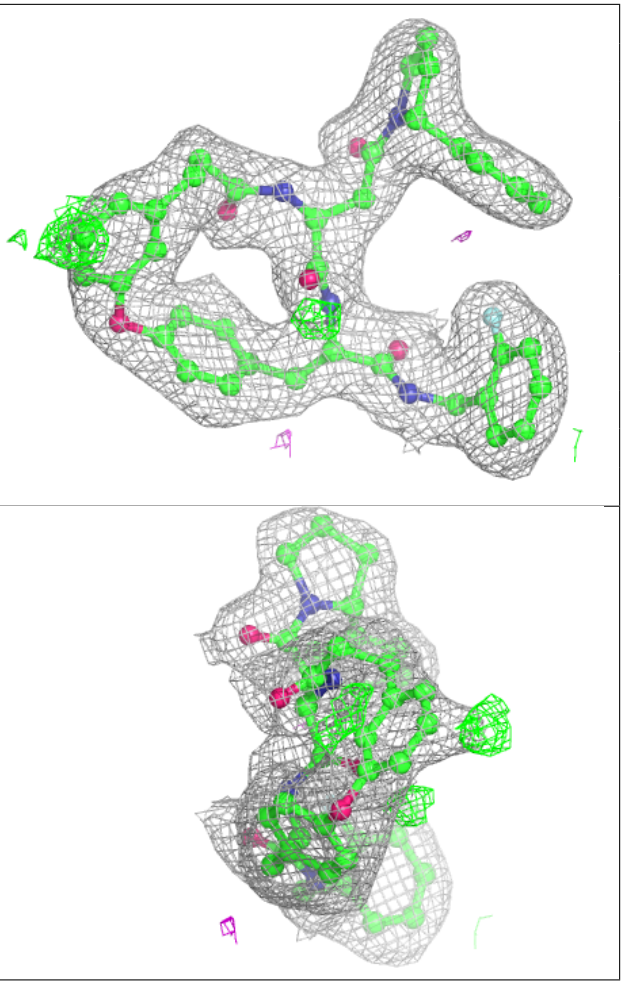






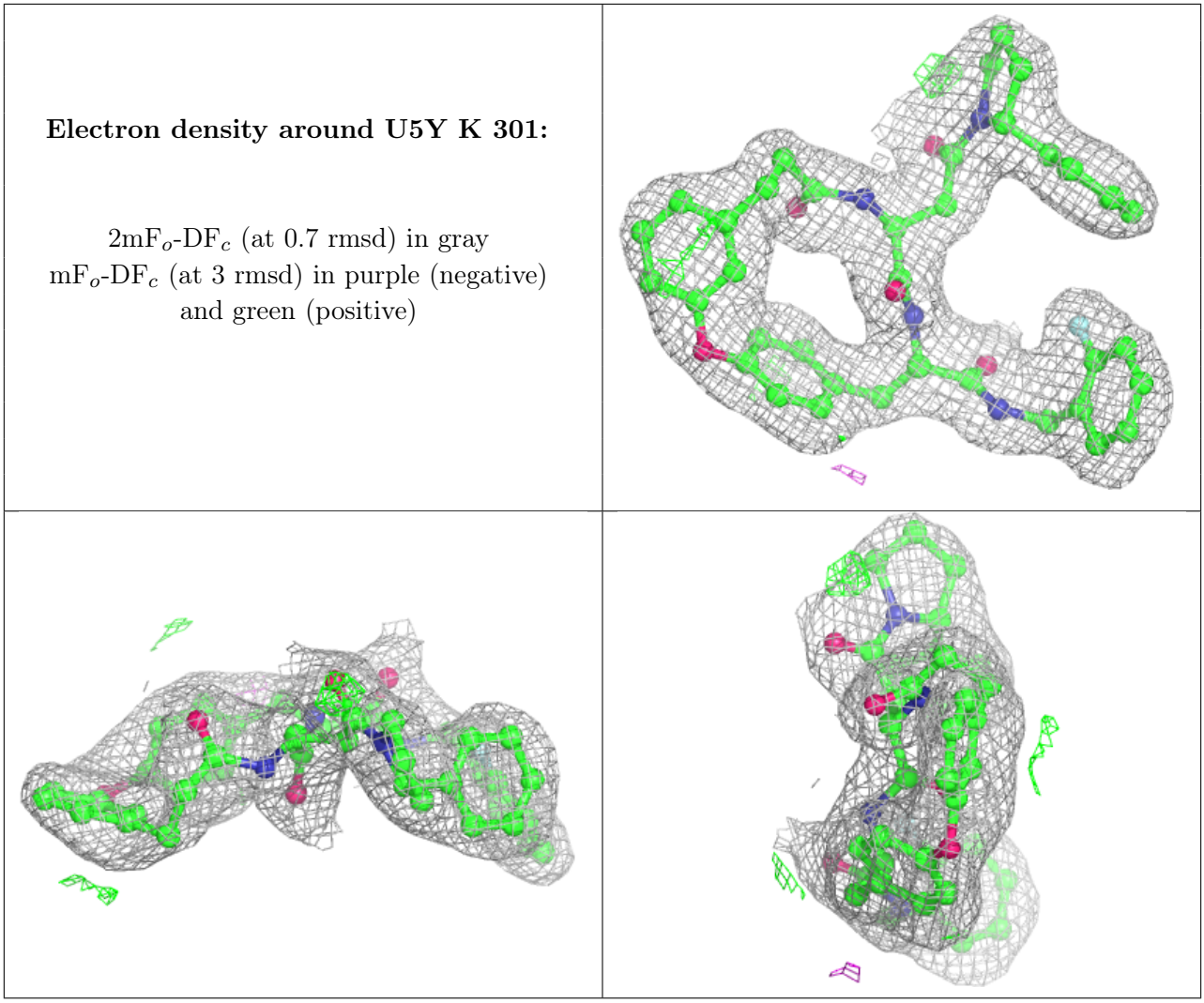
Electron density around U5Y b 301:

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



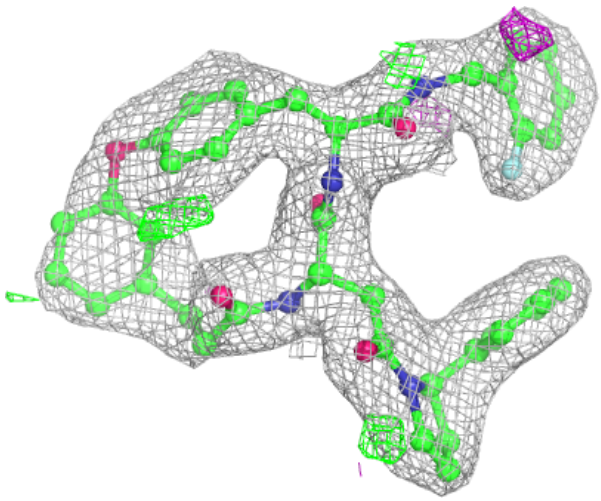
Electron density around U5Y K 301:

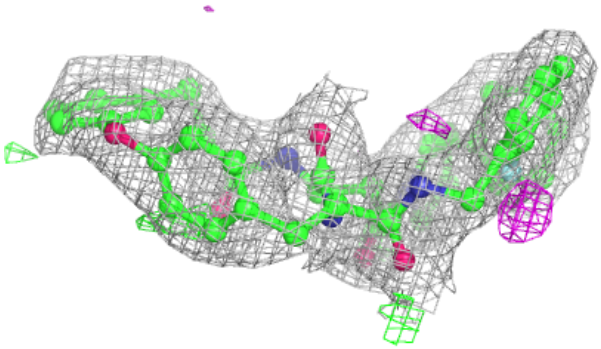
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

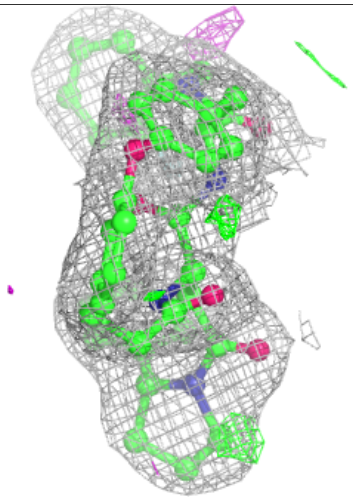


Electron density around U5Y L 301:

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

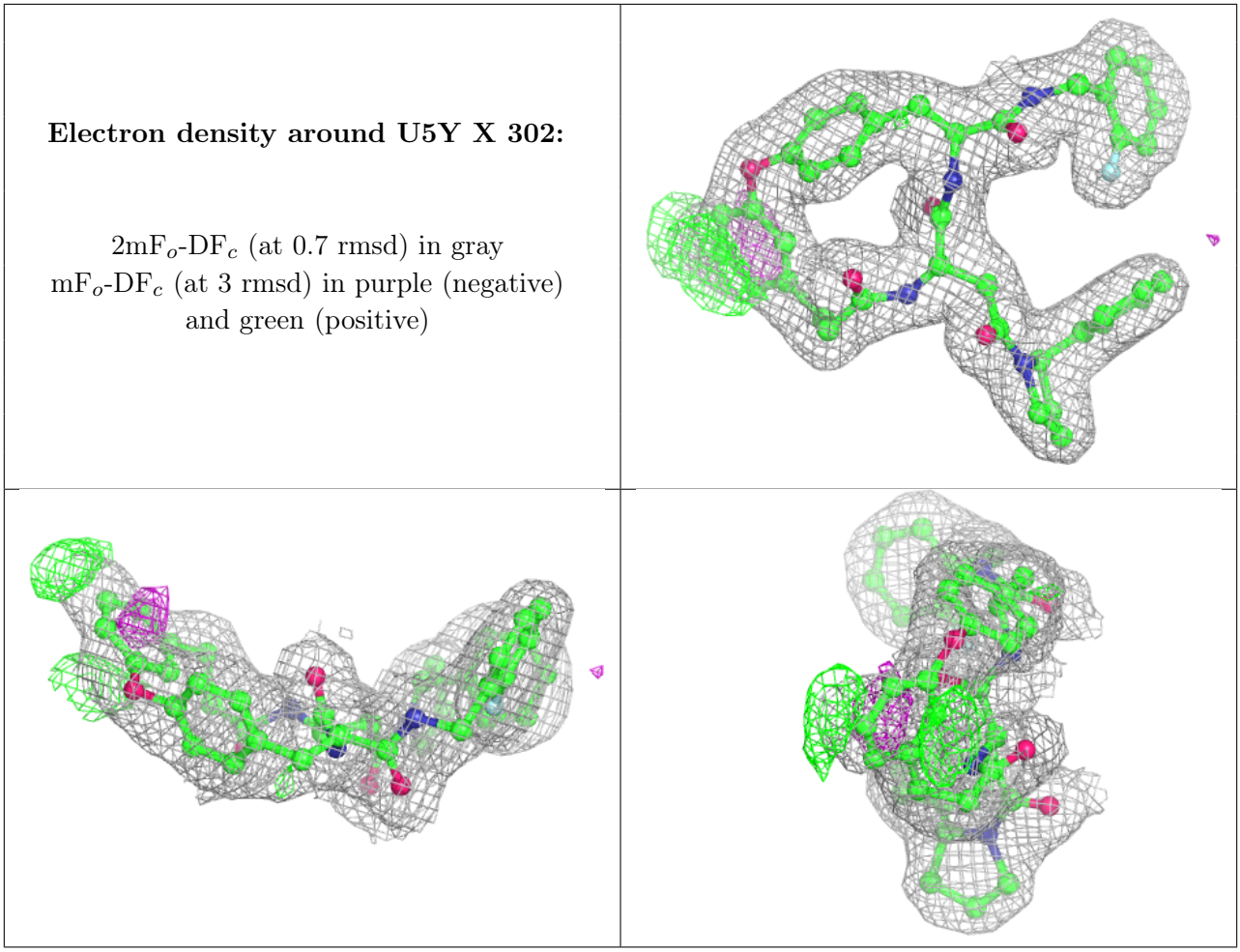






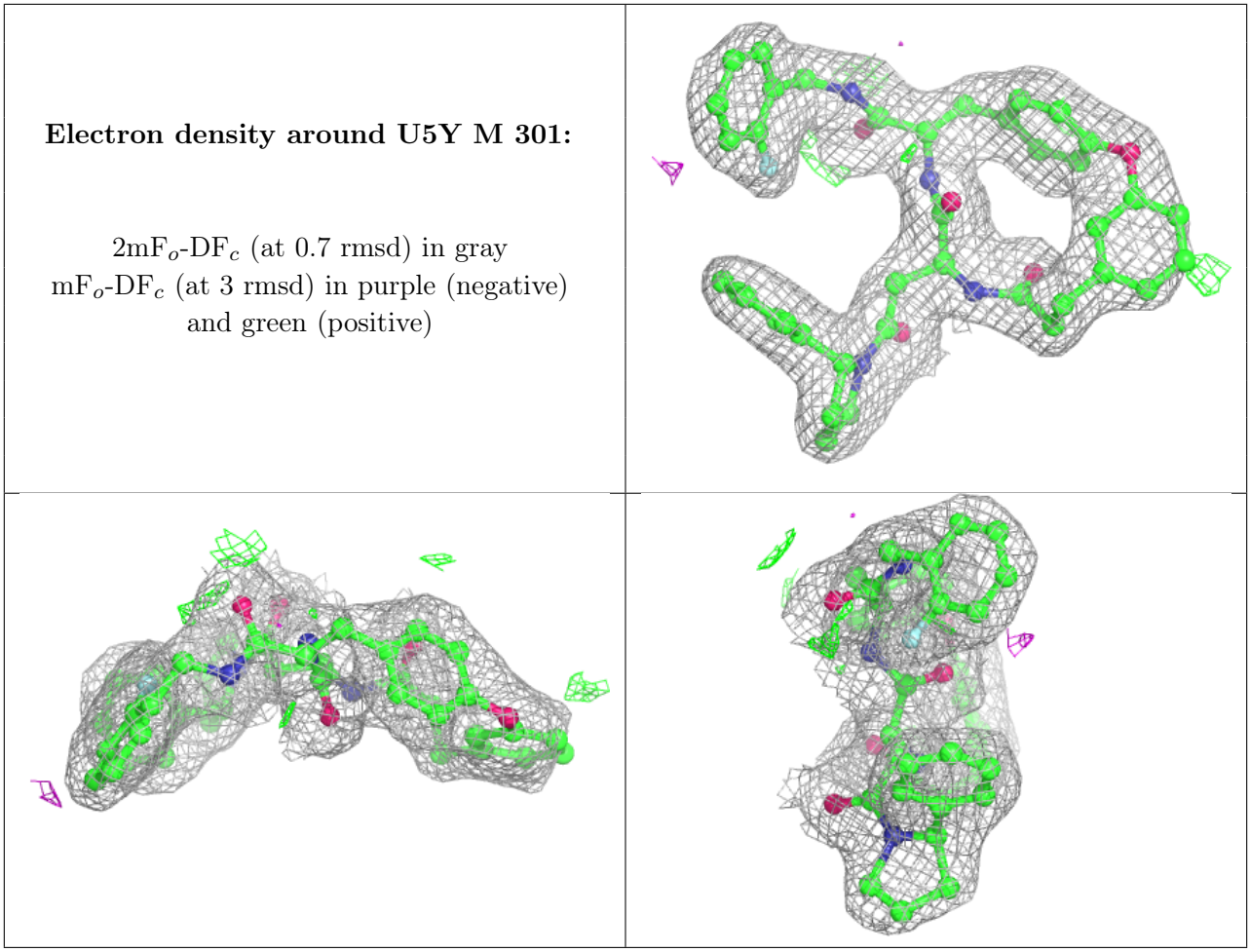
Electron density around U5Y X 302:

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



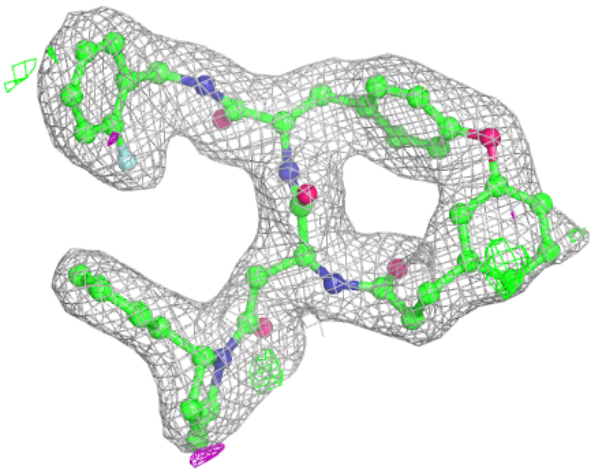
Electron density around U5Y M 301:

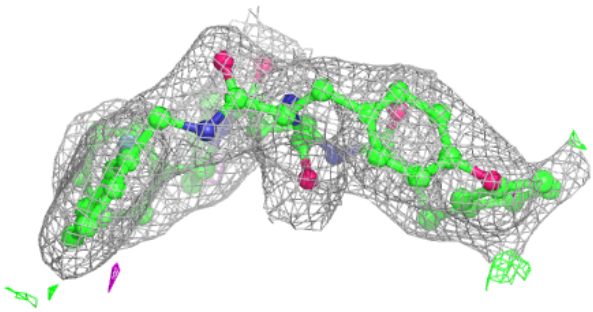
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

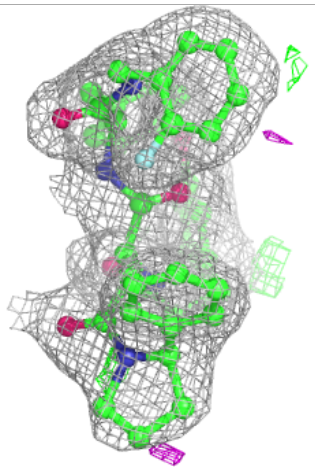


Electron density around U5Y Z 301:

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

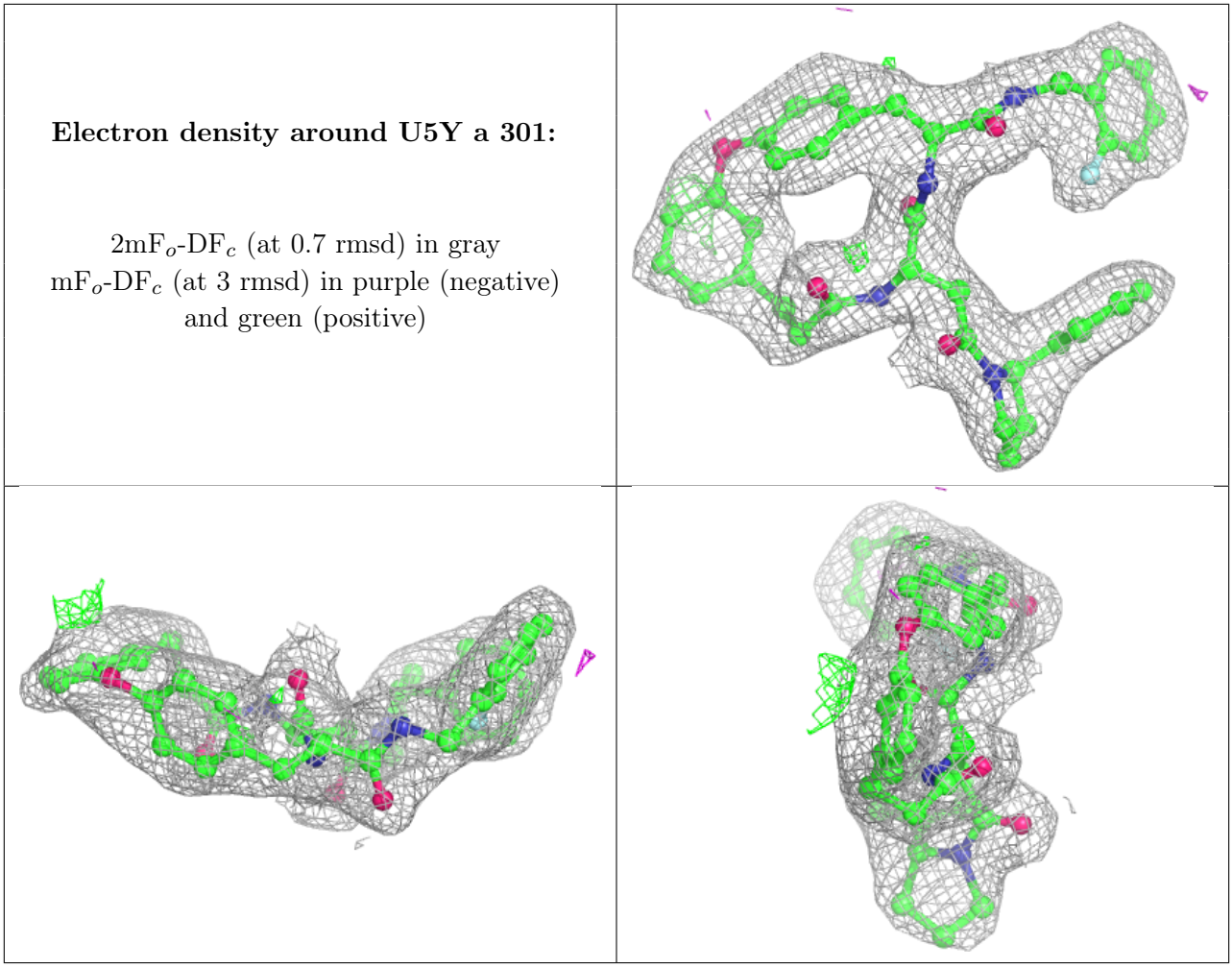






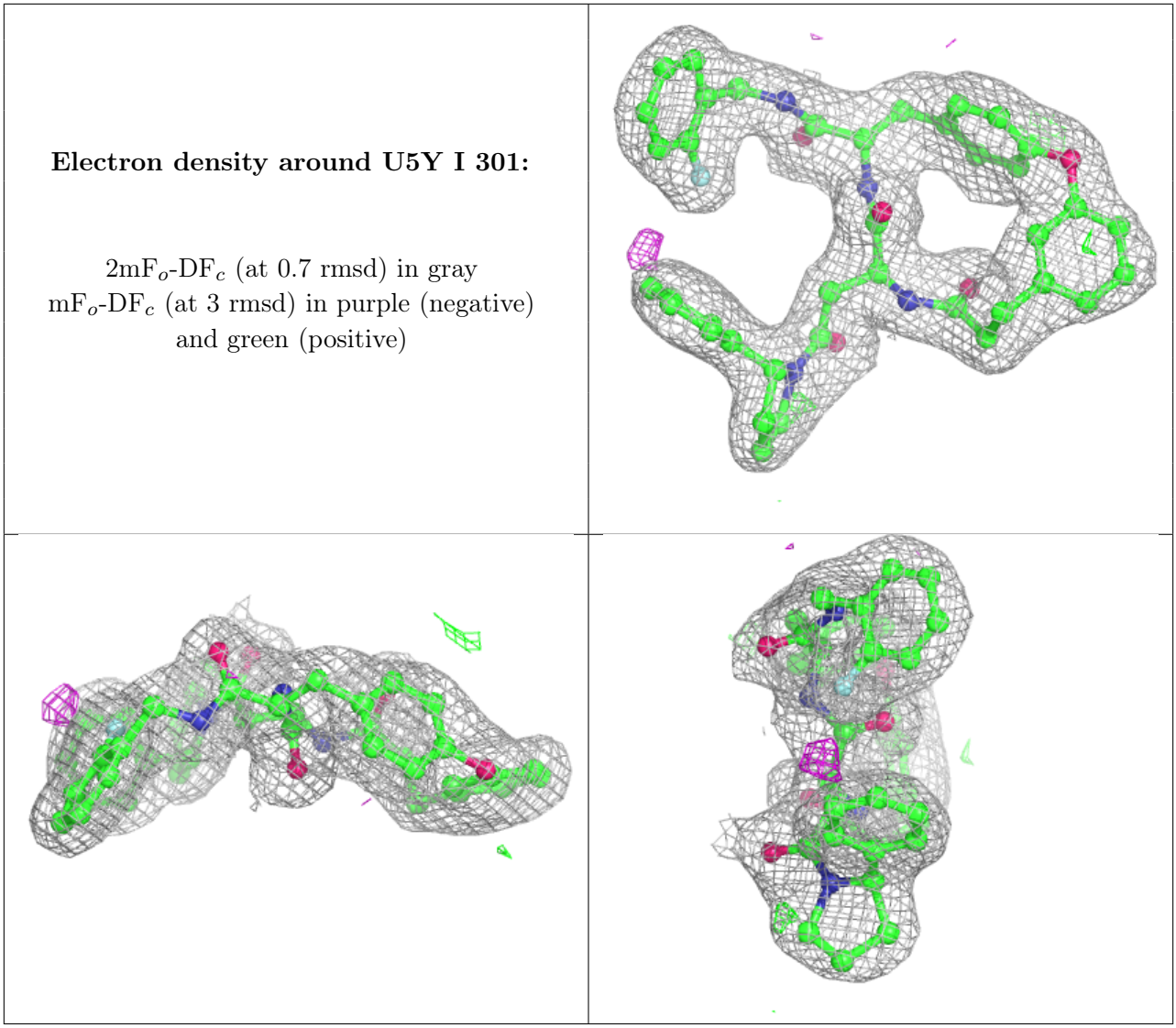
Electron density around U5Y a 301:

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



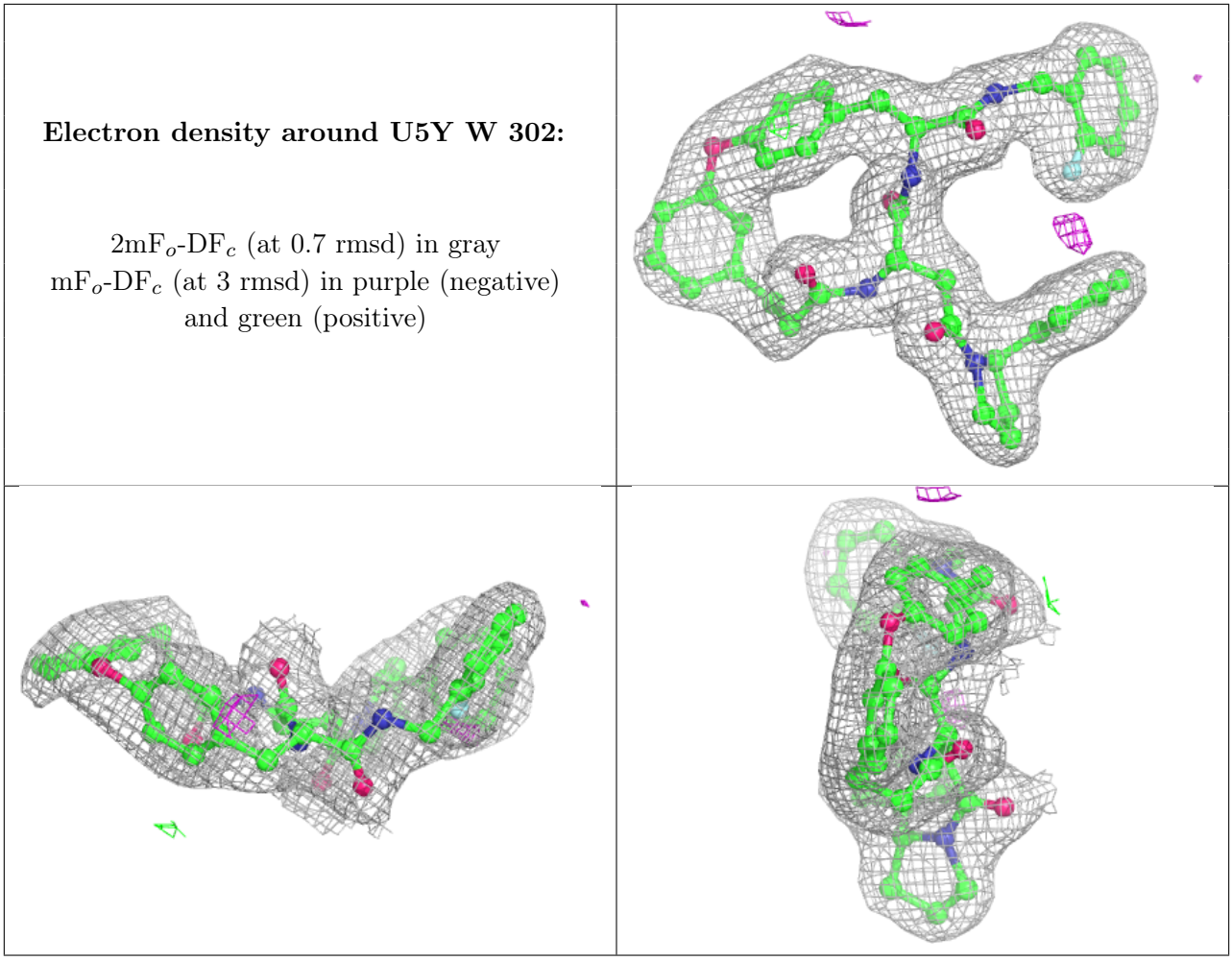
Electron density around U5Y I 301:

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



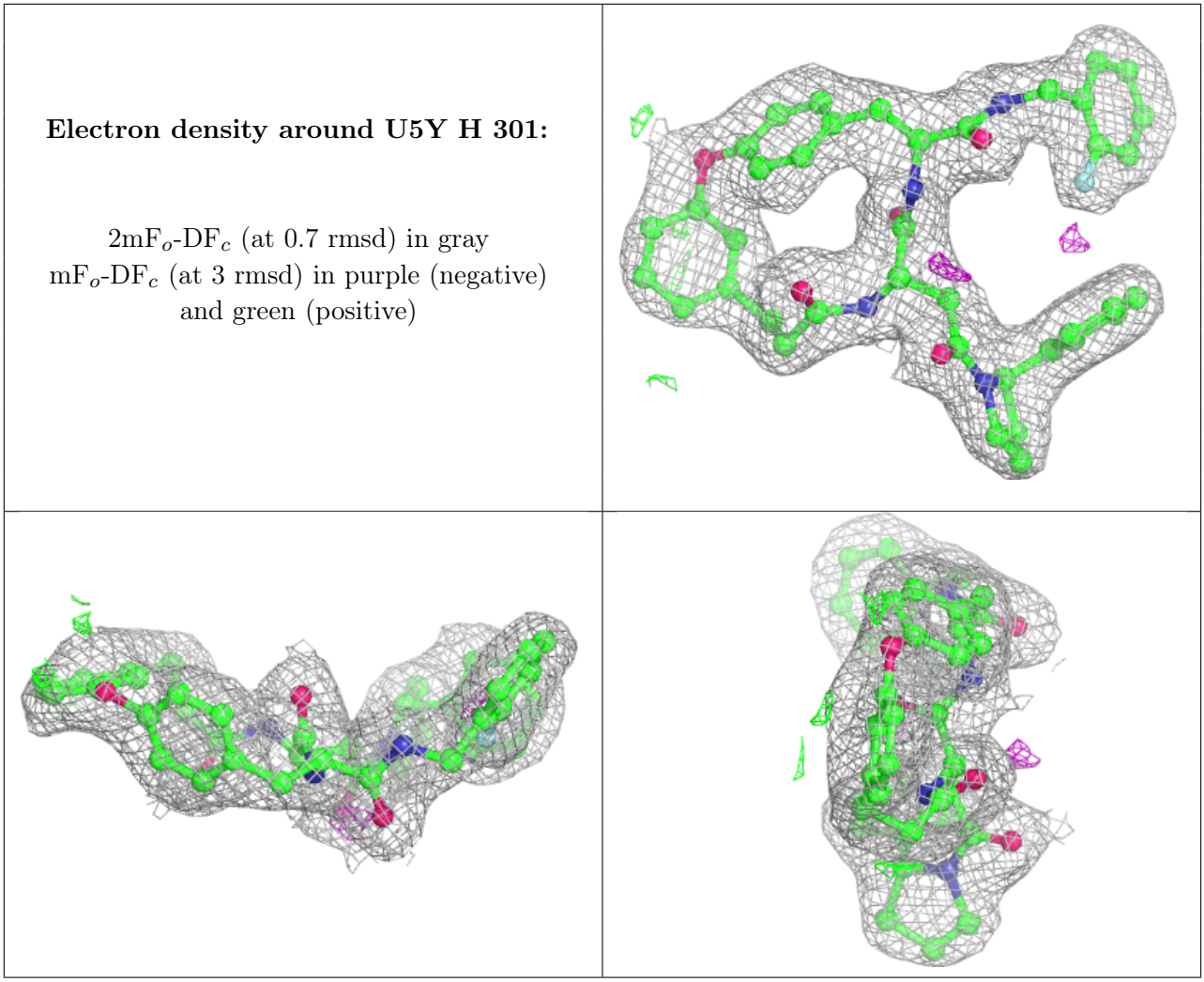
Electron density around U5Y W 302:

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



Electron density around U5Y 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)



6.5 Other polymers

There are no such residues in this entry.