



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 03:37 AM UTC

PDB ID : 6WNK / pdb_00006wnk
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

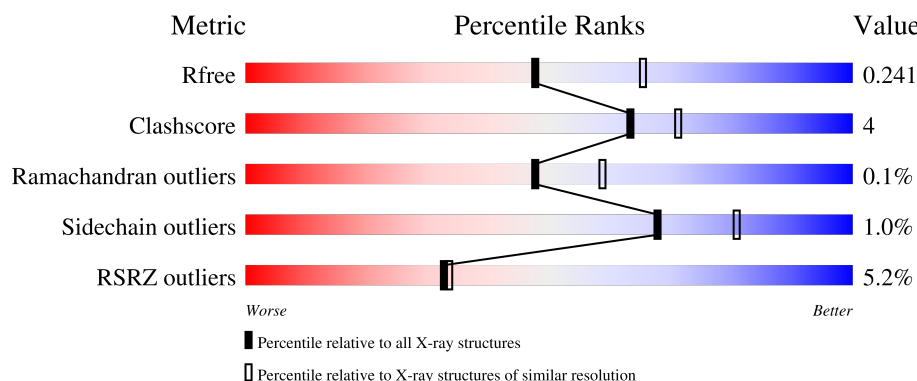
1 Overall quality at a glance

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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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 $\leq 5\%$. 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	2% 79% 11% 10%
1	B	240	6% 84% 5% 10%
1	C	240	12% 75% 15% 10%
1	D	240	9% 71% 19% 10%
1	E	240	19% 71% 18% 11%

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

2 Entry composition

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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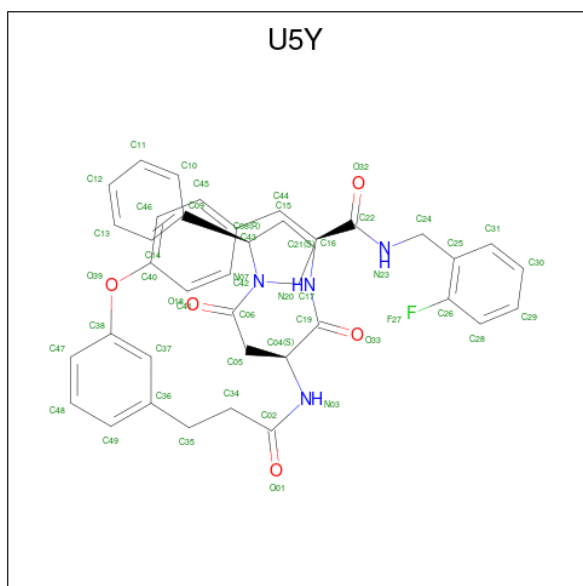
Chain	Residue	Modelled	Actual	Comment	Reference
N	235	HIS	-	expression tag	UNP A5U4D6
N	236	HIS	-	expression tag	UNP A5U4D6
N	237	HIS	-	expression tag	UNP A5U4D6
N	238	HIS	-	expression tag	UNP A5U4D6
N	239	HIS	-	expression tag	UNP A5U4D6
N	240	HIS	-	expression tag	UNP A5U4D6
V	235	HIS	-	expression tag	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 (1S,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 (CCD ID: U5Y) (formula: C₃₉H₃₉FN₄O₅) (labeled as "Ligand of Interest" by depositor).



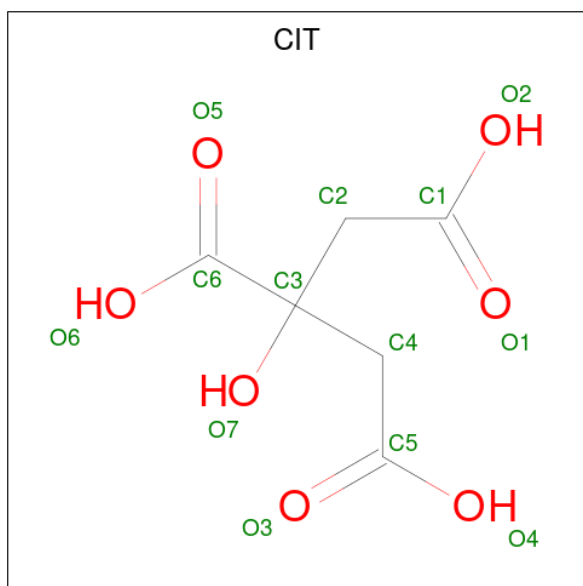
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	I	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	J	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	K	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	L	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	M	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	N	1	Total	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 (CCD ID: CIT) (formula: $C_6H_8O_7$).



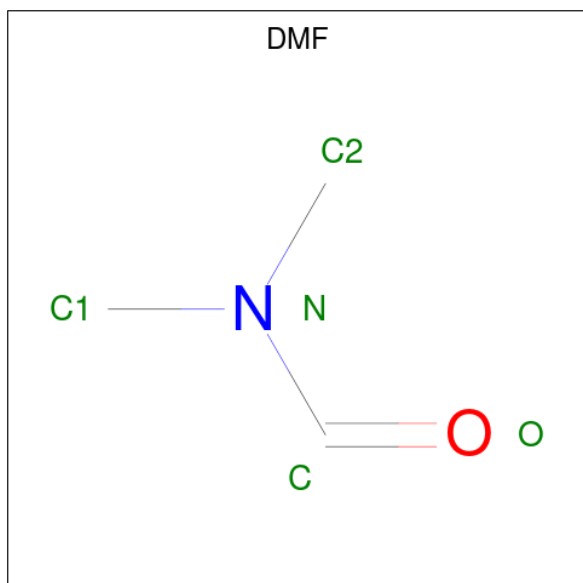
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			13	6	7		
4	I	1	Total	C	O	0	0
			13	6	7		
4	J	1	Total	C	O	0	0
			13	6	7		
4	K	1	Total	C	O	0	0
			13	6	7		

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

- Molecule 5 is DIMETHYLFORMAMIDE (CCD ID: DMF) (formula: C_3H_7NO).



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

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

- Molecule 6 is water.

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

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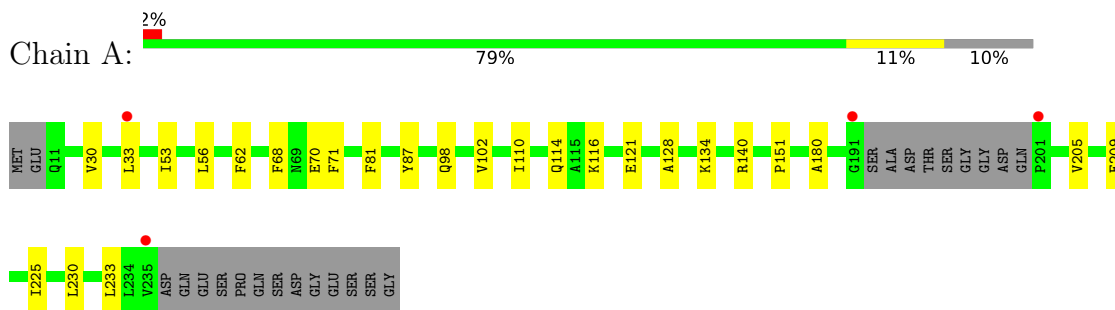
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	43	Total 43	O 43	0	0
6	N	64	Total 64	O 64	0	0
6	O	23	Total 23	O 23	0	0
6	P	30	Total 30	O 30	0	0
6	Q	32	Total 32	O 32	0	0
6	R	48	Total 48	O 48	0	0
6	S	12	Total 12	O 12	0	0
6	T	10	Total 10	O 10	0	0
6	U	13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

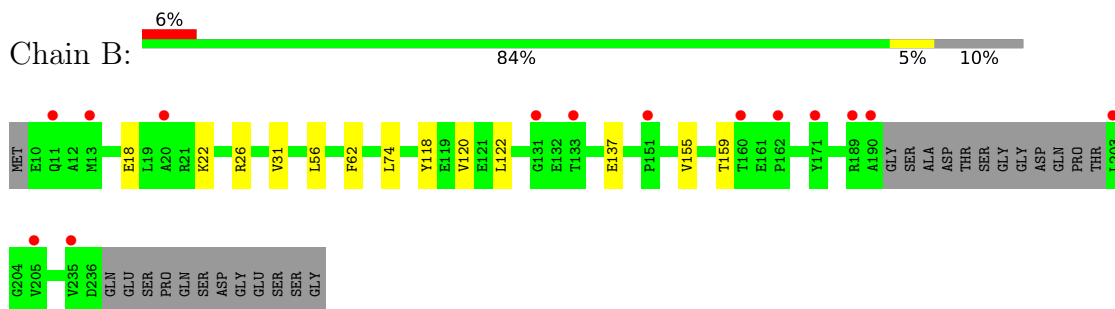
3 Residue-property plots [i](#)

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.

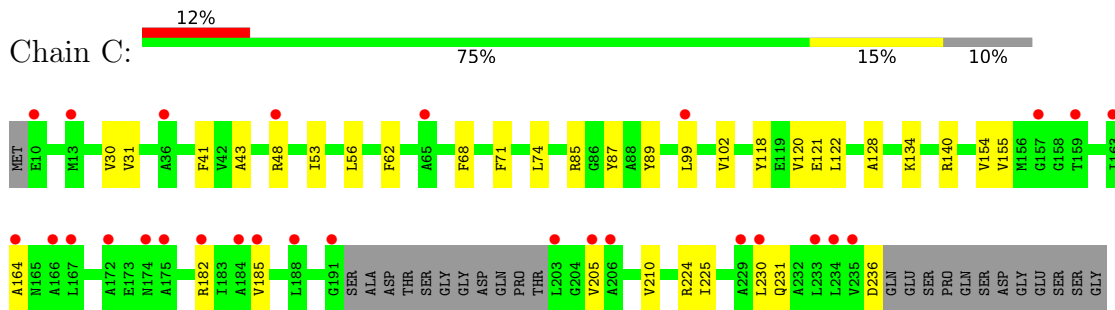
- Molecule 1: Proteasome subunit alpha



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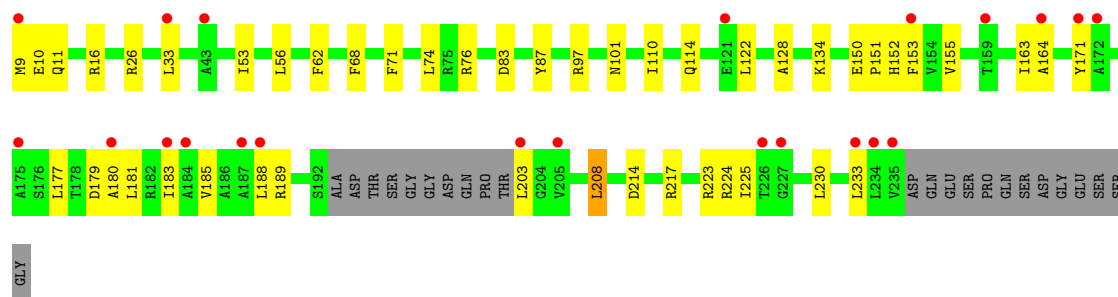


- Molecule 1: Proteasome subunit alpha

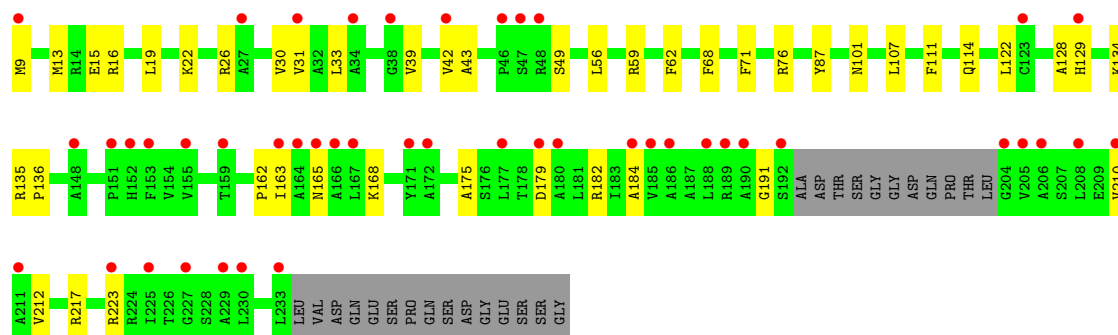


- Molecule 1: Proteasome subunit alpha

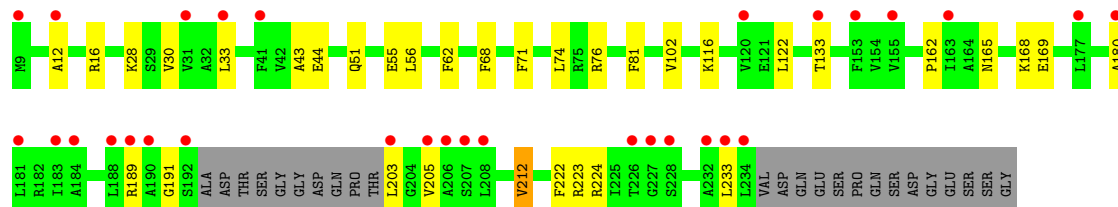
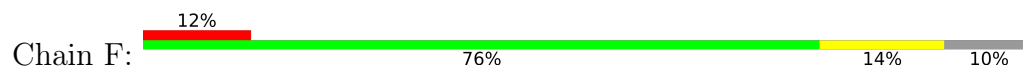




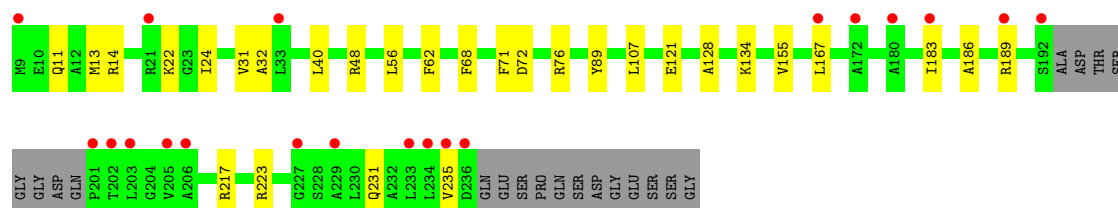
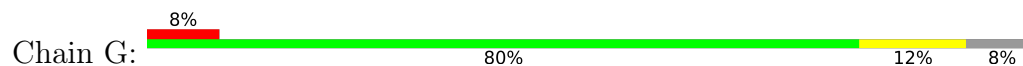
• Molecule 1: Proteasome subunit alpha



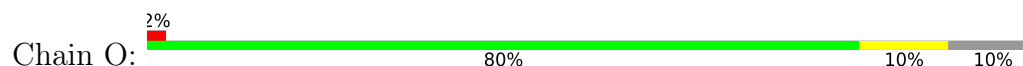
• Molecule 1: Proteasome subunit alpha

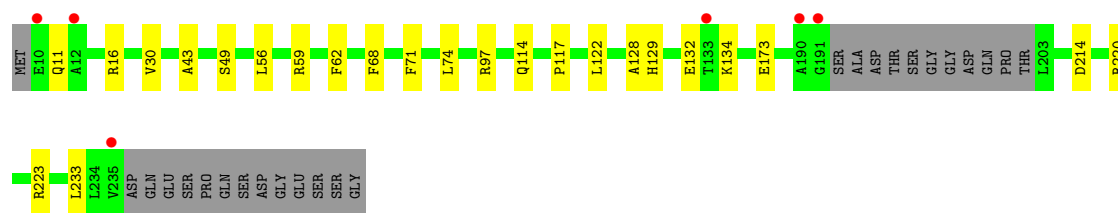


• Molecule 1: Proteasome subunit alpha

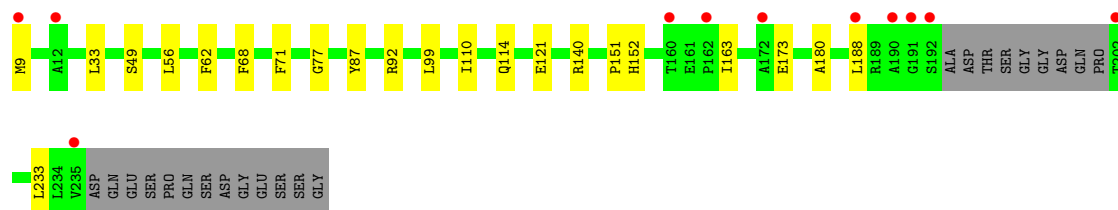
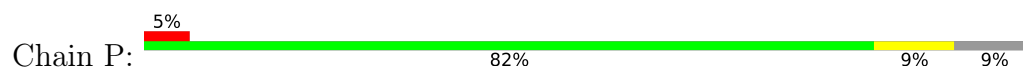


• Molecule 1: Proteasome subunit alpha

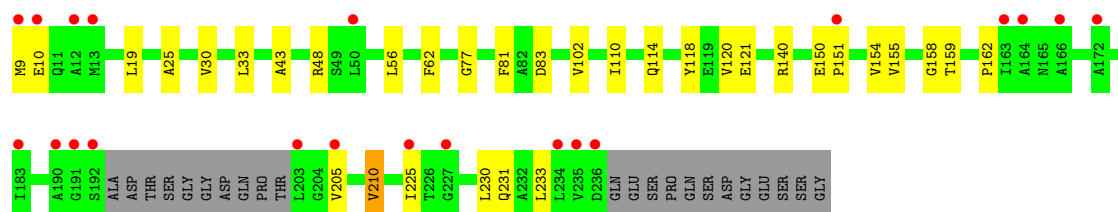
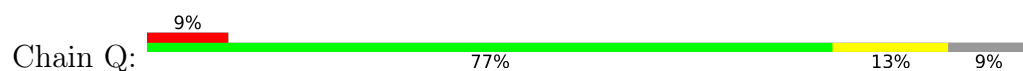




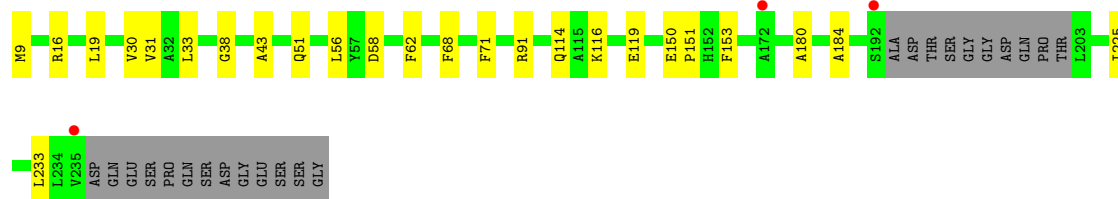
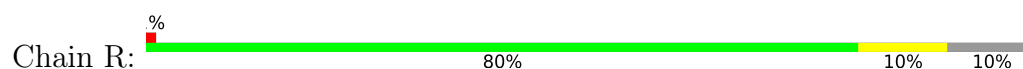
• Molecule 1: Proteasome subunit alpha



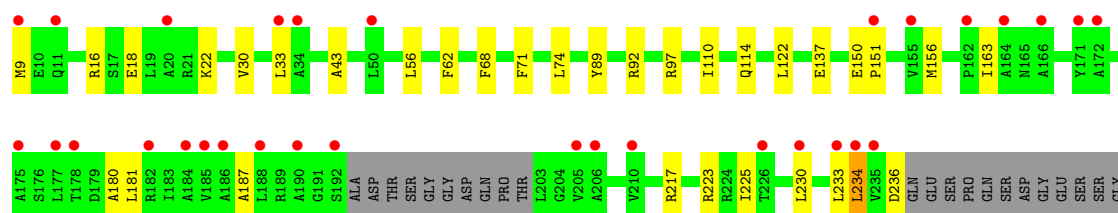
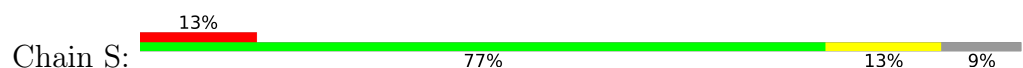
• Molecule 1: Proteasome subunit alpha



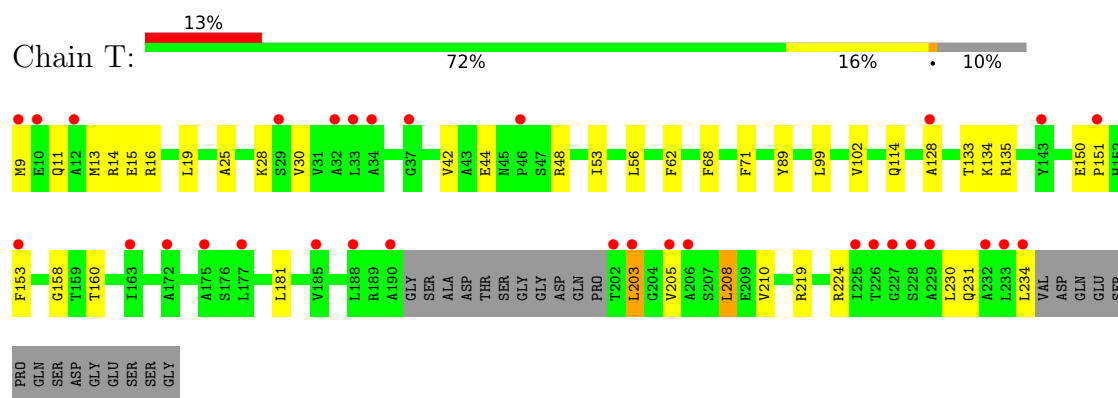
• Molecule 1: Proteasome subunit alpha



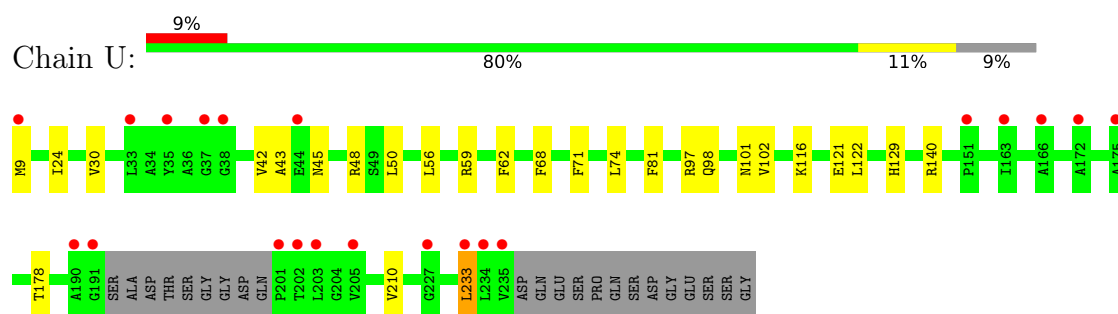
• Molecule 1: Proteasome subunit alpha



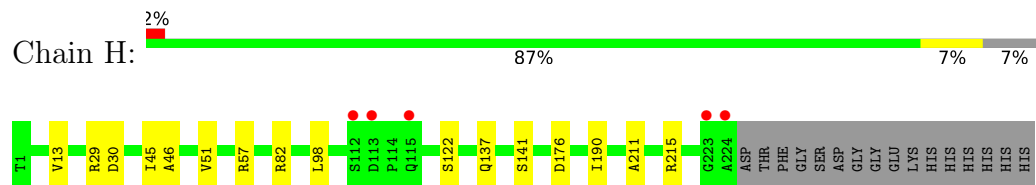
● Molecule 1: Proteasome subunit alpha



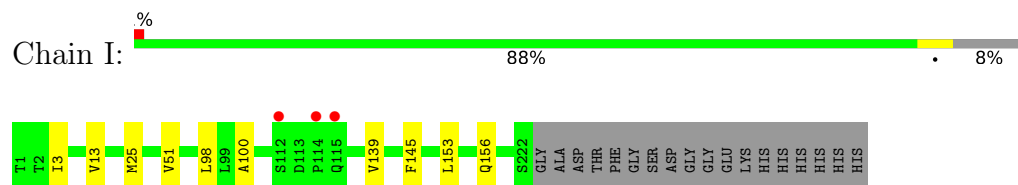
● Molecule 1: Proteasome subunit alpha



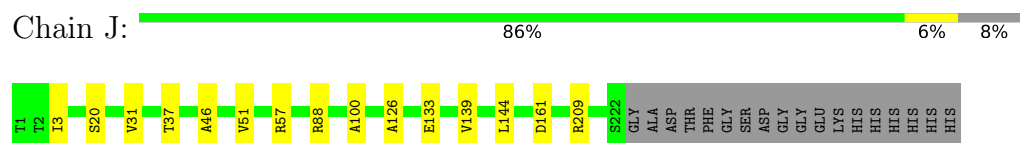
● Molecule 2: Proteasome subunit beta



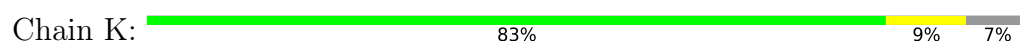
● Molecule 2: Proteasome subunit beta

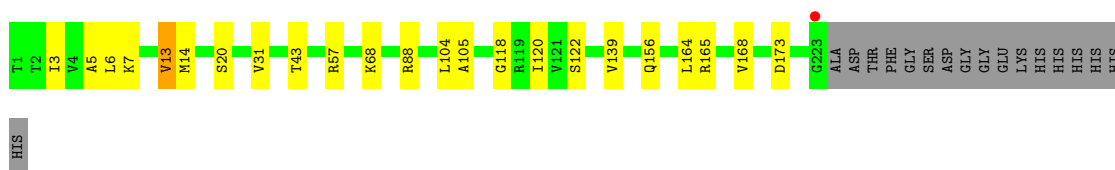


● Molecule 2: Proteasome subunit beta

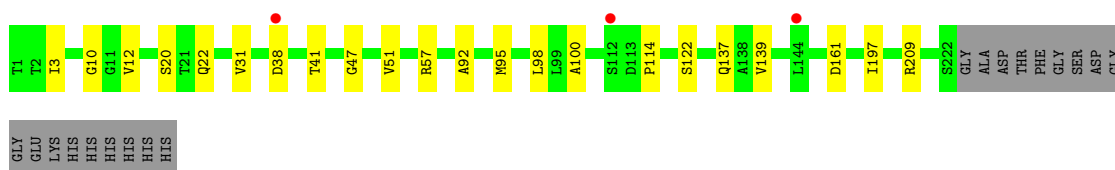
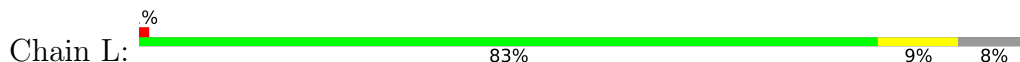


● Molecule 2: Proteasome subunit beta

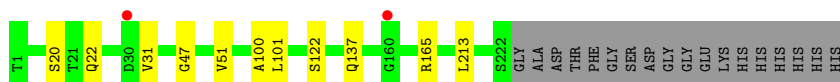
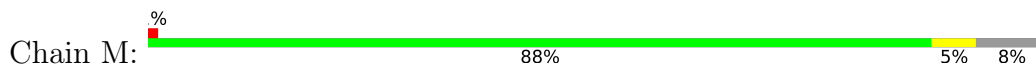




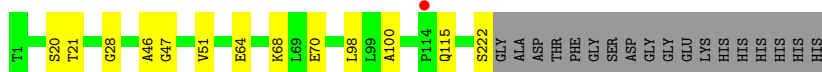
- Molecule 2: Proteasome subunit beta



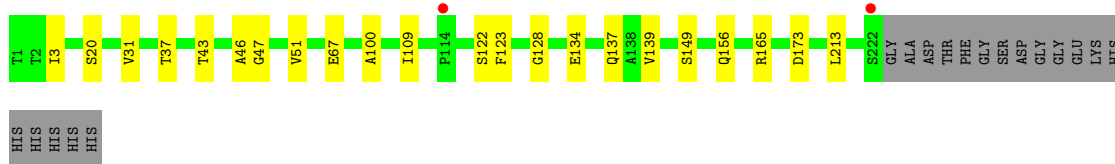
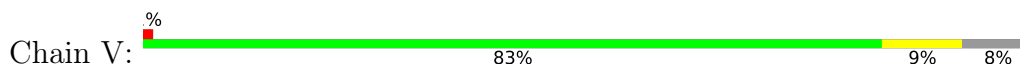
- Molecule 2: Proteasome subunit beta



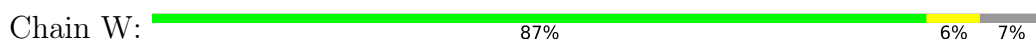
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta

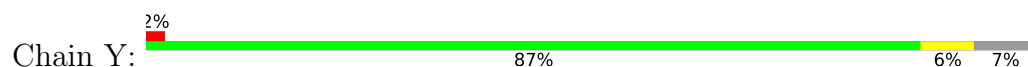


- Molecule 2: Proteasome subunit beta

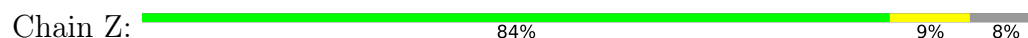




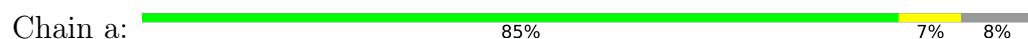
- Molecule 2: Proteasome subunit beta



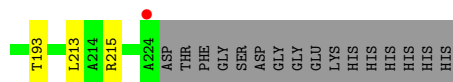
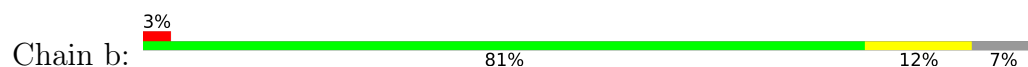
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.200 , 0.238 0.204 , 0.241	Depositor DCC
R_{free} test set	16408 reflections (4.85%)	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)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.14	0/1686	0.37	0/2278
1	B	0.14	0/1684	0.37	0/2275
1	C	0.13	0/1688	0.35	0/2280
1	D	0.13	0/1694	0.34	0/2287
1	E	0.13	0/1671	0.35	0/2255
1	F	0.15	0/1687	0.37	0/2277
1	G	0.13	0/1717	0.36	0/2319
1	O	0.14	0/1680	0.36	0/2269
1	P	0.14	0/1701	0.37	0/2297
1	Q	0.14	0/1702	0.37	0/2298
1	R	0.15	0/1694	0.38	0/2287
1	S	0.13	0/1702	0.37	0/2298
1	T	0.12	0/1684	0.36	0/2274
1	U	0.13	0/1703	0.36	0/2300
2	H	0.15	0/1671	0.34	0/2266
2	I	0.16	0/1662	0.35	0/2254
2	J	0.14	0/1662	0.34	0/2254
2	K	0.14	0/1666	0.32	0/2259
2	L	0.14	0/1662	0.33	0/2254
2	M	0.14	0/1662	0.33	0/2254
2	N	0.14	0/1662	0.33	0/2254
2	V	0.14	0/1662	0.33	0/2254
2	W	0.14	0/1666	0.33	0/2259
2	X	0.16	0/1662	0.35	0/2254
2	Y	0.16	0/1666	0.35	0/2259
2	Z	0.14	0/1662	0.34	0/2254
2	a	0.14	0/1662	0.32	0/2254
2	b	0.13	0/1671	0.34	0/2266
All	All	0.14	0/46991	0.35	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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1661	0	1668	14	0
1	B	1660	0	1660	7	0
1	C	1664	0	1663	21	0
1	D	1670	0	1673	33	0
1	E	1647	0	1642	29	0
1	F	1663	0	1664	18	0
1	G	1692	0	1692	16	0
1	O	1656	0	1659	13	0
1	P	1677	0	1680	13	0
1	Q	1678	0	1677	20	0
1	R	1670	0	1673	17	0
1	S	1678	0	1677	23	0
1	T	1660	0	1663	25	0
1	U	1678	0	1683	18	0
2	H	1647	0	1641	9	0
2	I	1638	0	1633	6	0
2	J	1638	0	1633	8	0
2	K	1642	0	1636	13	0
2	L	1638	0	1633	13	0
2	M	1638	0	1633	7	0
2	N	1638	0	1633	8	0
2	V	1638	0	1633	13	0
2	W	1642	0	1636	10	0
2	X	1638	0	1633	7	0
2	Y	1642	0	1636	11	0
2	Z	1638	0	1633	17	0
2	a	1638	0	1633	12	0
2	b	1647	0	1641	17	0
3	H	49	0	0	0	0
3	I	49	0	0	0	0
3	J	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	49	0	0	0	0
3	L	49	0	0	1	0
3	M	49	0	0	0	0
3	N	49	0	0	0	0
3	V	49	0	0	0	0
3	W	49	0	0	1	0
3	X	49	0	0	0	0
3	Y	49	0	0	0	0
3	Z	49	0	0	0	0
3	a	49	0	0	0	0
3	b	49	0	0	1	0
4	H	13	0	5	2	0
4	I	13	0	5	1	0
4	J	13	0	5	1	0
4	K	13	0	5	0	0
4	L	13	0	5	1	0
4	M	13	0	5	2	0
4	N	13	0	5	2	0
4	V	13	0	5	2	0
4	W	13	0	5	1	0
4	X	13	0	5	1	0
4	Y	13	0	5	2	0
4	Z	13	0	5	4	0
4	a	13	0	5	2	0
4	b	13	0	5	0	0
5	O	5	0	7	0	0
5	P	5	0	7	1	0
5	Q	5	0	7	1	0
5	R	10	0	14	3	0
5	S	5	0	7	0	0
5	W	5	0	7	0	0
5	X	5	0	7	0	0
6	A	34	0	0	0	0
6	B	14	0	0	0	0
6	C	12	0	0	0	0
6	D	13	0	0	1	0
6	E	9	0	0	0	0
6	F	9	0	0	0	0
6	G	22	0	0	0	0
6	H	74	0	0	0	0
6	I	98	0	0	0	0
6	J	69	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	46	0	0	1	0
6	L	37	0	0	0	0
6	M	43	0	0	0	0
6	N	64	0	0	0	0
6	O	23	0	0	0	0
6	P	30	0	0	0	0
6	Q	32	0	0	0	0
6	R	48	0	0	0	0
6	S	12	0	0	0	0
6	T	10	0	0	0	0
6	U	13	0	0	0	0
6	V	45	0	0	0	0
6	W	73	0	0	1	0
6	X	103	0	0	0	0
6	Y	95	0	0	1	0
6	Z	63	0	0	0	0
6	a	41	0	0	0	0
6	b	44	0	0	1	0
All	All	48400	0	46387	373	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 373 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:203:LEU:HB3	1:T:208:LEU:HD21	1.58	0.85
2:Y:132:GLU:HG3	2:Y:137:GLN:HG3	1.64	0.79
2:a:141:SER:HB3	4:a:302:CIT:H41	1.68	0.75
1:F:33:LEU:HD11	1:F:180:ALA:HB1	1.72	0.71
1:E:179:ASP:OD1	1:E:182:ARG:NH1	2.23	0.71

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/240 (88%)	208 (98%)	3 (1%)	1 (0%)	24	29
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%)	24	29
1	R	213/240 (89%)	206 (97%)	7 (3%)	0	100	100
1	S	214/240 (89%)	207 (97%)	6 (3%)	1 (0%)	24	29
1	T	211/240 (88%)	204 (97%)	6 (3%)	1 (0%)	24	29
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
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%)	48	59

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 ⓘ

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%)	78	87
1	B	165/184 (90%)	164 (99%)	1 (1%)	78	87
1	C	165/184 (90%)	163 (99%)	2 (1%)	63	77
1	D	166/184 (90%)	164 (99%)	2 (1%)	63	77
1	E	163/184 (89%)	161 (99%)	2 (1%)	63	77
1	F	165/184 (90%)	160 (97%)	5 (3%)	36	51
1	G	169/184 (92%)	167 (99%)	2 (1%)	63	77
1	O	164/184 (89%)	161 (98%)	3 (2%)	51	68
1	P	167/184 (91%)	165 (99%)	2 (1%)	63	77
1	Q	167/184 (91%)	164 (98%)	3 (2%)	51	68
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%)	160 (97%)	5 (3%)	36	51
1	U	167/184 (91%)	166 (99%)	1 (1%)	78	87
2	H	165/178 (93%)	162 (98%)	3 (2%)	51	68
2	I	165/178 (93%)	164 (99%)	1 (1%)	78	87
2	J	165/178 (93%)	163 (99%)	2 (1%)	63	77
2	K	165/178 (93%)	163 (99%)	2 (1%)	63	77
2	L	165/178 (93%)	165 (100%)	0	100	100
2	M	165/178 (93%)	164 (99%)	1 (1%)	78	87
2	N	165/178 (93%)	163 (99%)	2 (1%)	63	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	165/178 (93%)	164 (99%)	1 (1%)	78	87
2	W	165/178 (93%)	165 (100%)	0	100	100
2	X	165/178 (93%)	164 (99%)	1 (1%)	78	87
2	Y	165/178 (93%)	165 (100%)	0	100	100
2	Z	165/178 (93%)	165 (100%)	0	100	100
2	a	165/178 (93%)	165 (100%)	0	100	100
2	b	165/178 (93%)	162 (98%)	3 (2%)	51	68
All	All	4631/5068 (91%)	4586 (99%)	45 (1%)	68	81

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	233	LEU
1	T	133	THR
1	P	99	LEU
1	Q	155	VAL
1	T	203	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	174	ASN
1	T	105	GLN
2	Y	22	GLN
1	U	105	GLN
1	S	129	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
4	CIT	I	302	-	12,12,12	1.10	0	17,17,17	1.44	3 (17%)
3	U5Y	H	301	-	54,54,54	2.38	11 (20%)	72,74,74	1.32	11 (15%)
5	DMF	R	302	-	4,4,4	0.34	0	4,4,4	0.47	0
4	CIT	W	303	-	12,12,12	1.01	0	17,17,17	1.53	2 (11%)
3	U5Y	M	301	-	54,54,54	2.37	11 (20%)	72,74,74	1.31	8 (11%)
4	CIT	X	303	-	12,12,12	1.02	0	17,17,17	1.56	4 (23%)
4	CIT	b	302	-	12,12,12	1.09	0	17,17,17	1.46	4 (23%)
5	DMF	W	301	-	4,4,4	0.38	0	4,4,4	0.47	0
4	CIT	N	302	-	12,12,12	1.04	0	17,17,17	1.57	2 (11%)
3	U5Y	J	301	-	54,54,54	2.37	11 (20%)	72,74,74	1.30	11 (15%)
3	U5Y	W	302	-	54,54,54	2.39	10 (18%)	72,74,74	1.31	10 (13%)
5	DMF	P	301	-	4,4,4	0.36	0	4,4,4	0.48	0
3	U5Y	a	301	-	54,54,54	2.38	11 (20%)	72,74,74	1.30	10 (13%)
3	U5Y	V	301	-	54,54,54	2.38	10 (18%)	72,74,74	1.38	12 (16%)
4	CIT	J	302	-	12,12,12	1.02	0	17,17,17	1.65	4 (23%)
3	U5Y	K	301	-	54,54,54	2.40	11 (20%)	72,74,74	1.41	13 (18%)
3	U5Y	Y	301	-	54,54,54	2.36	12 (22%)	72,74,74	1.35	12 (16%)
4	CIT	a	302	-	12,12,12	1.05	0	17,17,17	1.98	4 (23%)
5	DMF	X	301	-	4,4,4	0.38	0	4,4,4	0.42	0
4	CIT	L	302	-	12,12,12	1.04	0	17,17,17	1.56	2 (11%)
4	CIT	Z	302	-	12,12,12	1.07	0	17,17,17	1.38	1 (5%)
3	U5Y	b	301	-	54,54,54	2.38	11 (20%)	72,74,74	1.35	12 (16%)
4	CIT	V	302	-	12,12,12	1.09	0	17,17,17	1.48	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	K	302	-	12,12,12	1.03	0	17,17,17	1.49	3 (17%)
4	CIT	Y	302	-	12,12,12	1.10	0	17,17,17	1.44	3 (17%)
5	DMF	S	301	-	4,4,4	0.34	0	4,4,4	0.46	0
5	DMF	O	301	-	4,4,4	0.33	0	4,4,4	0.41	0
5	DMF	R	301	-	4,4,4	0.37	0	4,4,4	0.38	0
3	U5Y	I	301	-	54,54,54	2.39	11 (20%)	72,74,74	1.29	9 (12%)
3	U5Y	N	301	-	54,54,54	2.41	10 (18%)	72,74,74	1.34	12 (16%)
3	U5Y	L	301	-	54,54,54	2.39	11 (20%)	72,74,74	1.40	11 (15%)
4	CIT	H	302	-	12,12,12	1.03	0	17,17,17	1.57	4 (23%)
4	CIT	M	302	-	12,12,12	0.98	0	17,17,17	1.70	3 (17%)
3	U5Y	Z	301	-	54,54,54	2.39	11 (20%)	72,74,74	1.31	10 (13%)
3	U5Y	X	302	-	54,54,54	2.41	11 (20%)	72,74,74	1.31	10 (13%)
5	DMF	Q	301	-	4,4,4	0.36	0	4,4,4	0.51	0

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
4	CIT	I	302	-	-	12/16/16/16	-
3	U5Y	H	301	-	-	2/46/56/56	0/5/6/6
5	DMF	R	302	-	-	2/2/2/2	-
4	CIT	W	303	-	-	8/16/16/16	-
3	U5Y	M	301	-	-	3/46/56/56	0/5/6/6
4	CIT	X	303	-	-	9/16/16/16	-
4	CIT	b	302	-	-	7/16/16/16	-
5	DMF	W	301	-	-	2/2/2/2	-
4	CIT	N	302	-	-	6/16/16/16	-
3	U5Y	J	301	-	-	2/46/56/56	0/5/6/6
3	U5Y	W	302	-	-	2/46/56/56	0/5/6/6
5	DMF	P	301	-	-	0/2/2/2	-
3	U5Y	a	301	-	-	2/46/56/56	0/5/6/6
3	U5Y	V	301	-	-	0/46/56/56	0/5/6/6
4	CIT	J	302	-	-	6/16/16/16	-
3	U5Y	K	301	-	-	1/46/56/56	0/5/6/6
3	U5Y	Y	301	-	-	2/46/56/56	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	a	302	-	-	6/16/16/16	-
5	DMF	X	301	-	-	0/2/2/2	-
4	CIT	L	302	-	-	10/16/16/16	-
4	CIT	Z	302	-	-	10/16/16/16	-
3	U5Y	b	301	-	-	3/46/56/56	0/5/6/6
4	CIT	V	302	-	-	7/16/16/16	-
4	CIT	K	302	-	-	8/16/16/16	-
4	CIT	Y	302	-	-	11/16/16/16	-
5	DMF	S	301	-	-	0/2/2/2	-
5	DMF	O	301	-	-	0/2/2/2	-
5	DMF	R	301	-	-	2/2/2/2	-
3	U5Y	I	301	-	-	2/46/56/56	0/5/6/6
3	U5Y	N	301	-	-	1/46/56/56	0/5/6/6
3	U5Y	L	301	-	-	3/46/56/56	0/5/6/6
4	CIT	H	302	-	-	8/16/16/16	-
4	CIT	M	302	-	-	7/16/16/16	-
3	U5Y	Z	301	-	-	2/46/56/56	0/5/6/6
3	U5Y	X	302	-	-	5/46/56/56	0/5/6/6
5	DMF	Q	301	-	-	0/2/2/2	-

The worst 5 of 152 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	302	U5Y	C08-N07	-9.60	1.33	1.47
3	Z	301	U5Y	C08-N07	-9.43	1.33	1.47
3	N	301	U5Y	C08-N07	-9.40	1.33	1.47
3	b	301	U5Y	C08-N07	-9.39	1.33	1.47
3	I	301	U5Y	C08-N07	-9.33	1.33	1.47

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	302	CIT	O6-C6-C3	4.71	122.18	113.14
4	M	302	CIT	O6-C6-C3	4.62	122.00	113.14
3	K	301	U5Y	C15-C08-N07	4.50	106.94	101.93
3	L	301	U5Y	C15-C08-N07	4.41	106.83	101.93
3	Z	301	U5Y	C15-C08-N07	4.34	106.76	101.93

There are no chirality outliers.

5 of 151 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

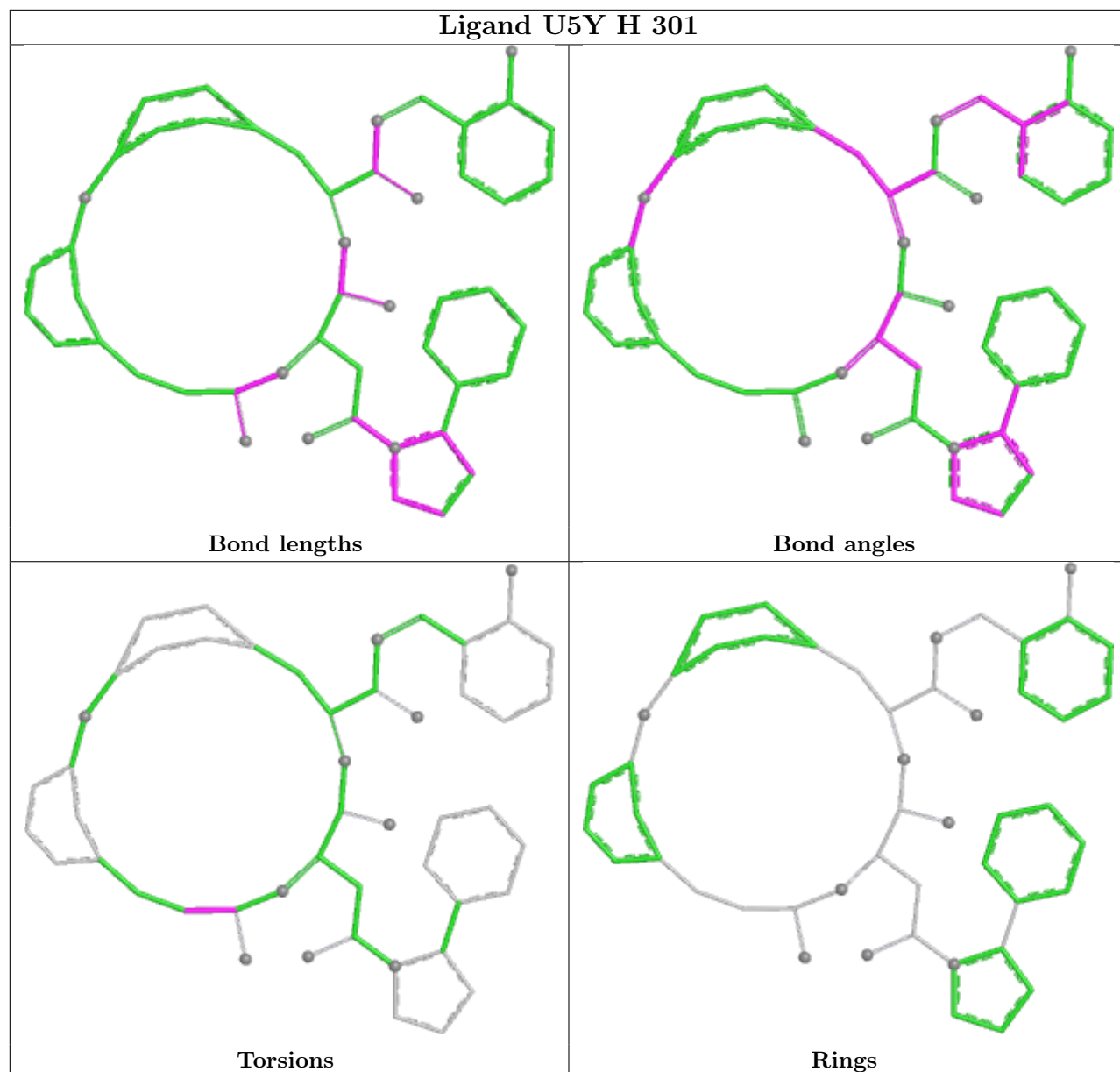
There are no ring outliers.

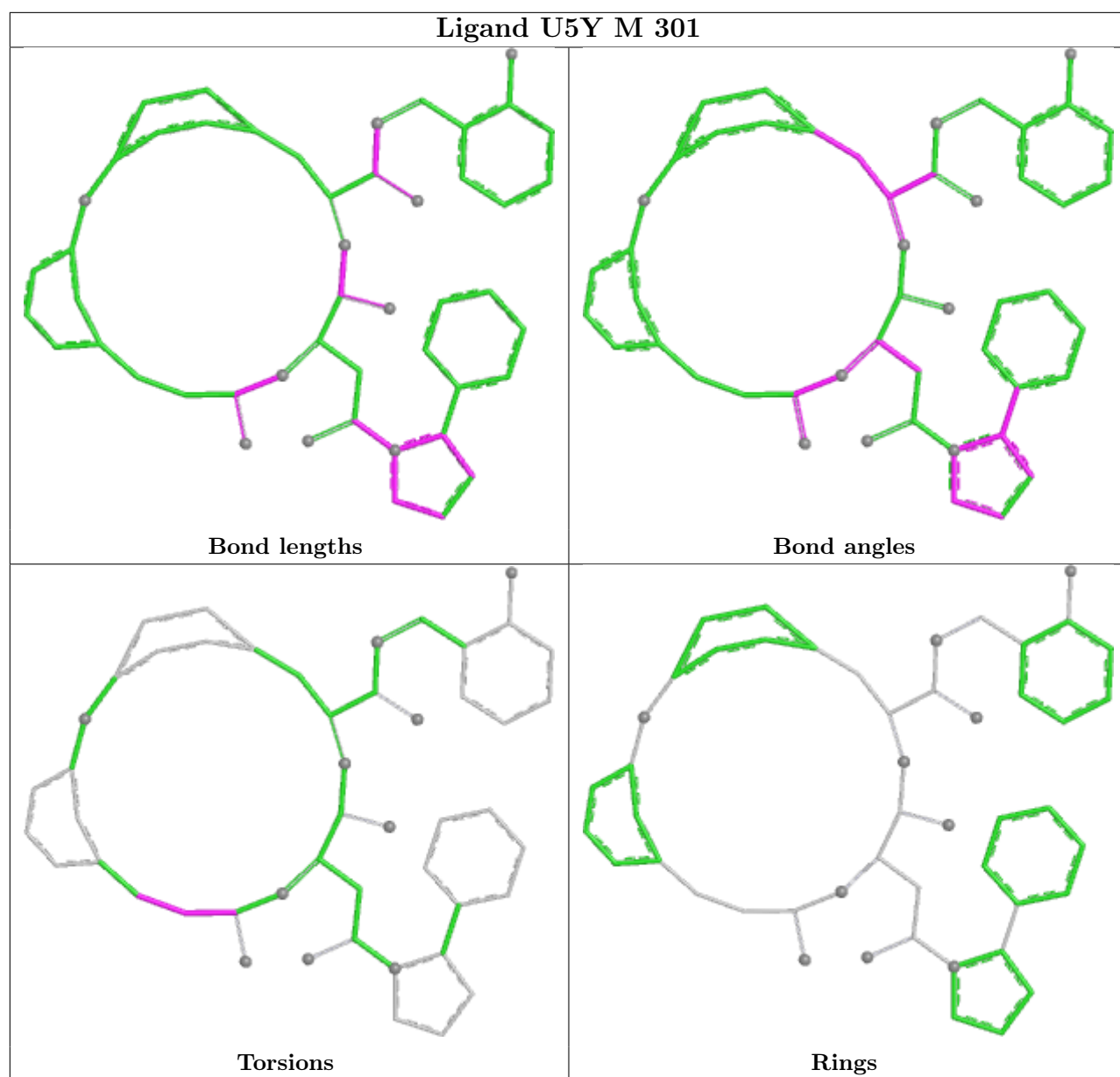
19 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	302	CIT	1	0
5	R	302	DMF	2	0
4	W	303	CIT	1	0
4	X	303	CIT	1	0
4	N	302	CIT	2	0
3	W	302	U5Y	1	0
5	P	301	DMF	1	0
4	J	302	CIT	1	0
4	a	302	CIT	2	0
4	L	302	CIT	1	0
4	Z	302	CIT	4	0
3	b	301	U5Y	1	0
4	V	302	CIT	2	0
4	Y	302	CIT	2	0
5	R	301	DMF	1	0
3	L	301	U5Y	1	0
4	H	302	CIT	2	0
4	M	302	CIT	2	0
5	Q	301	DMF	1	0

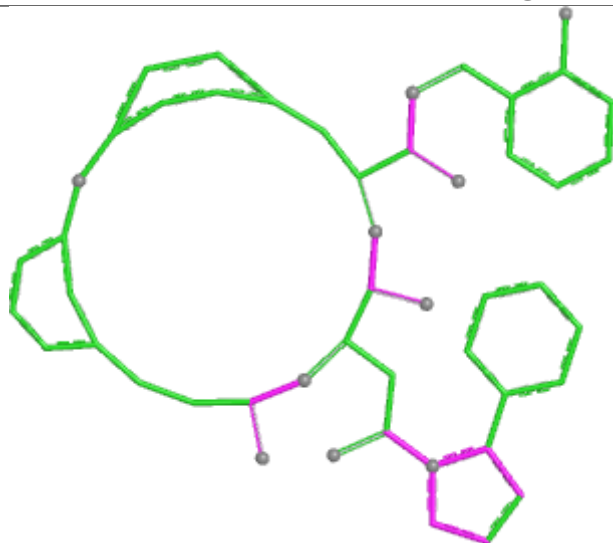
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand U5Y H 301

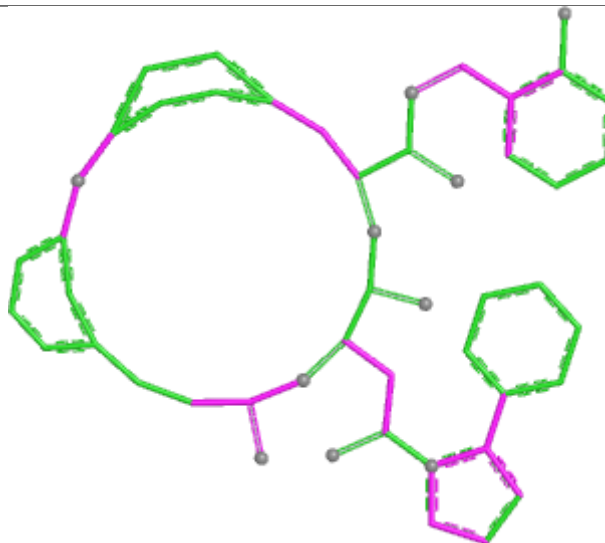




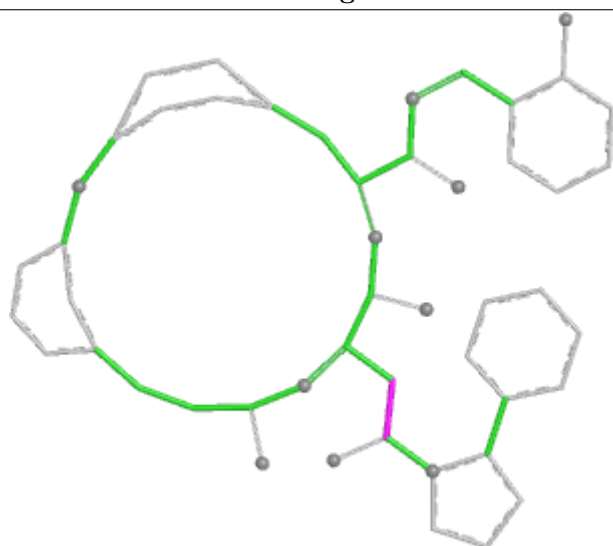
Ligand U5Y J 301



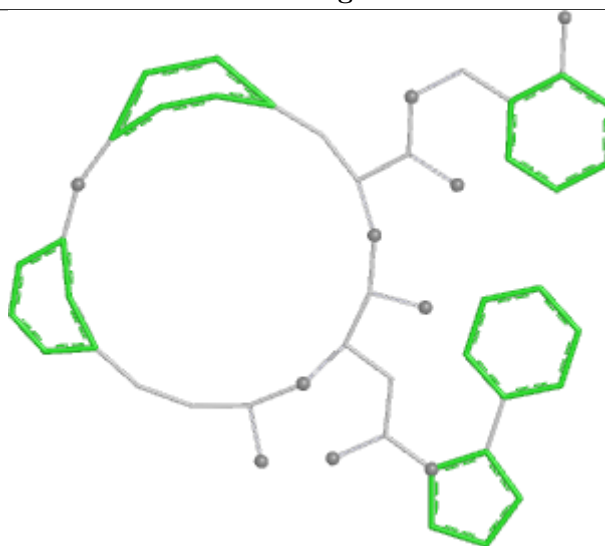
Bond lengths



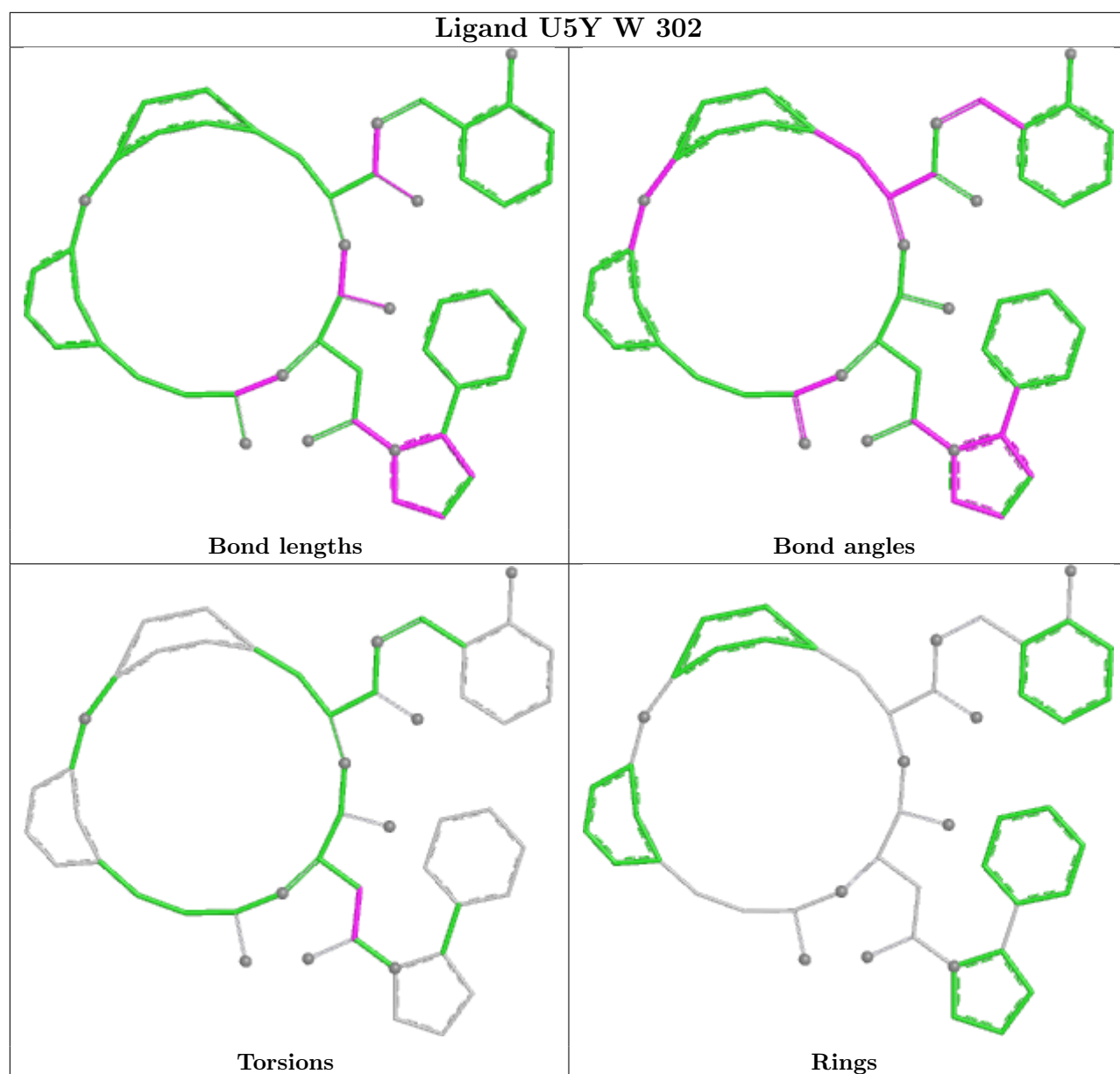
Bond angles



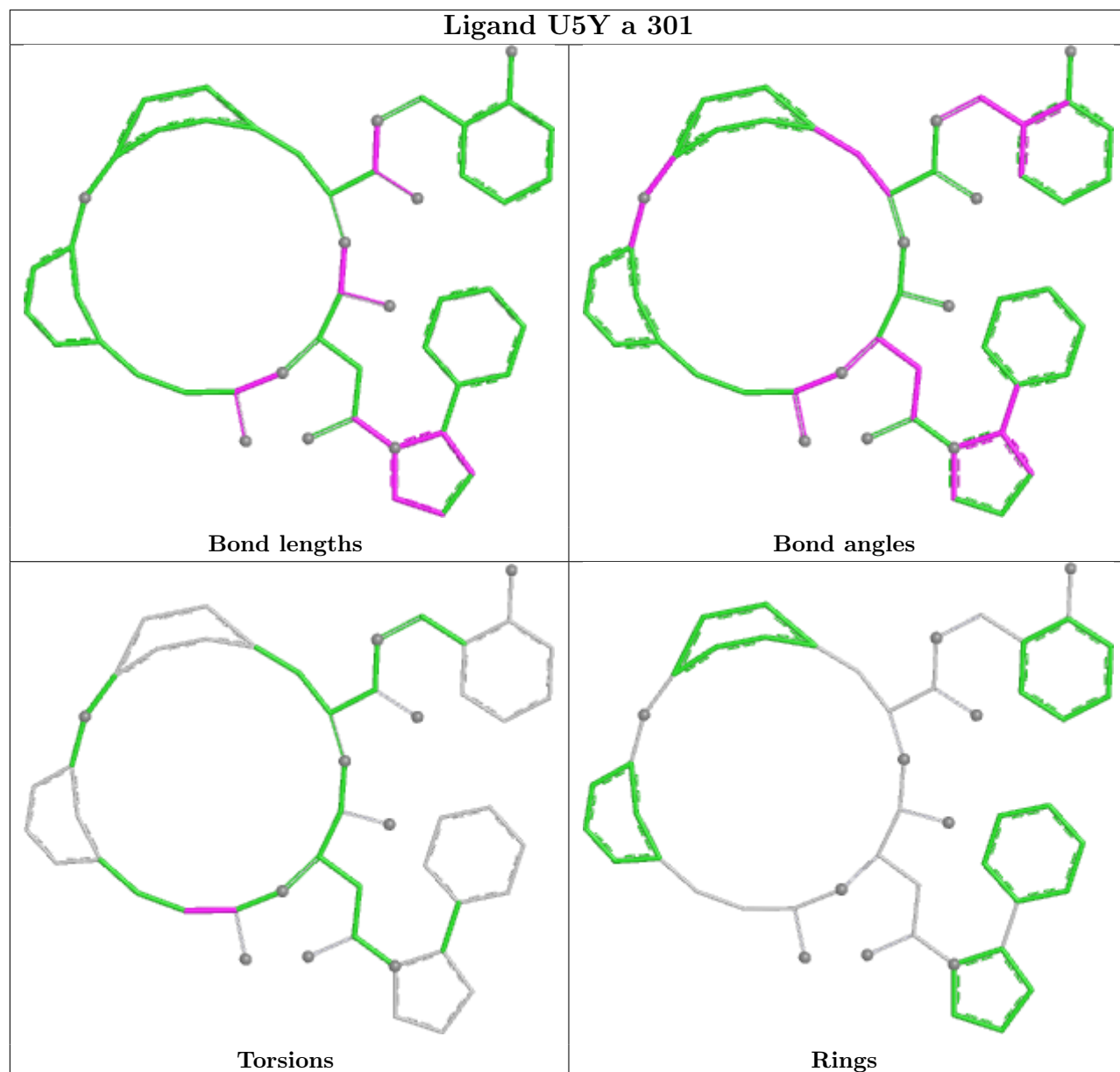
Torsions



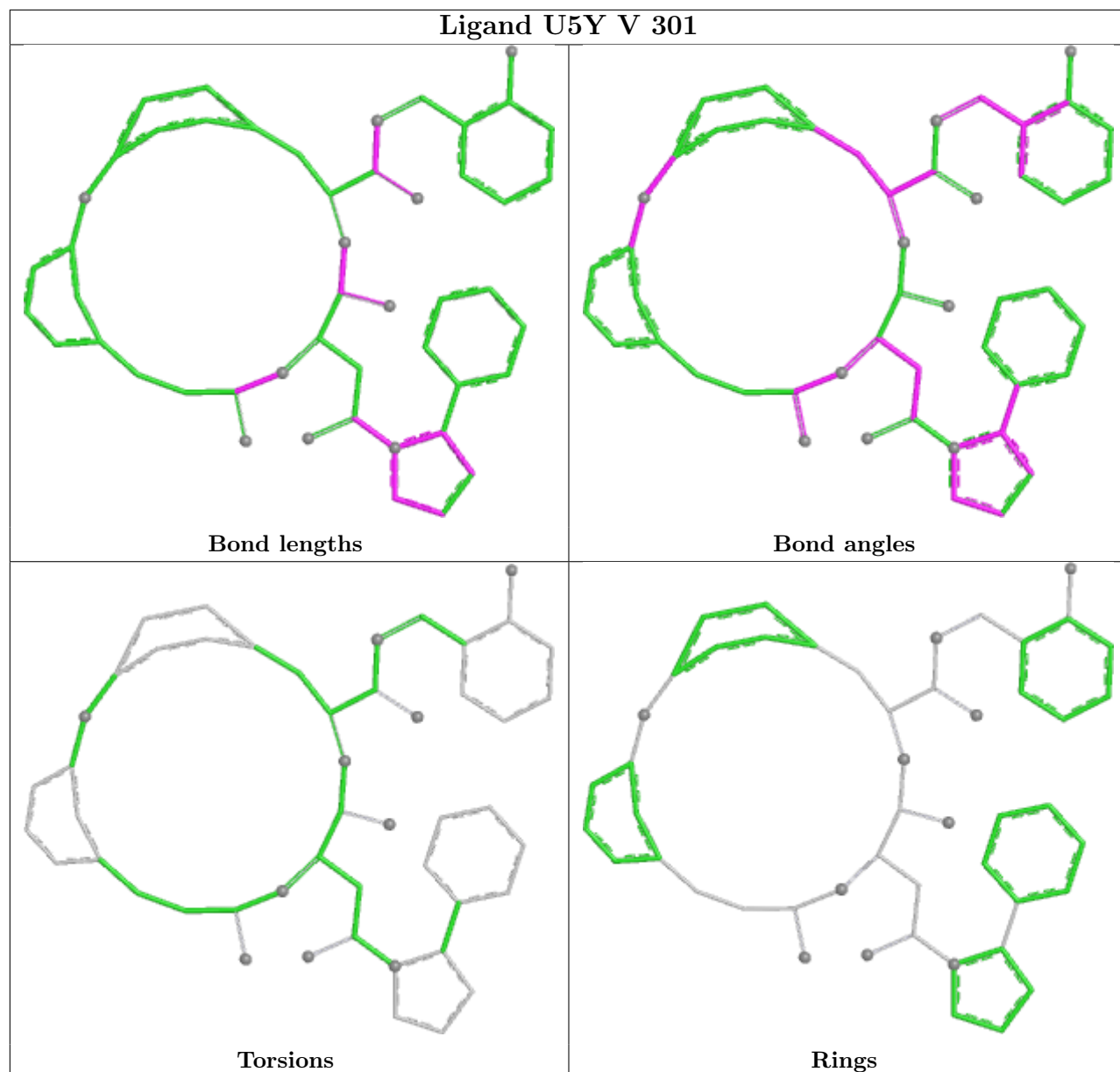
Rings



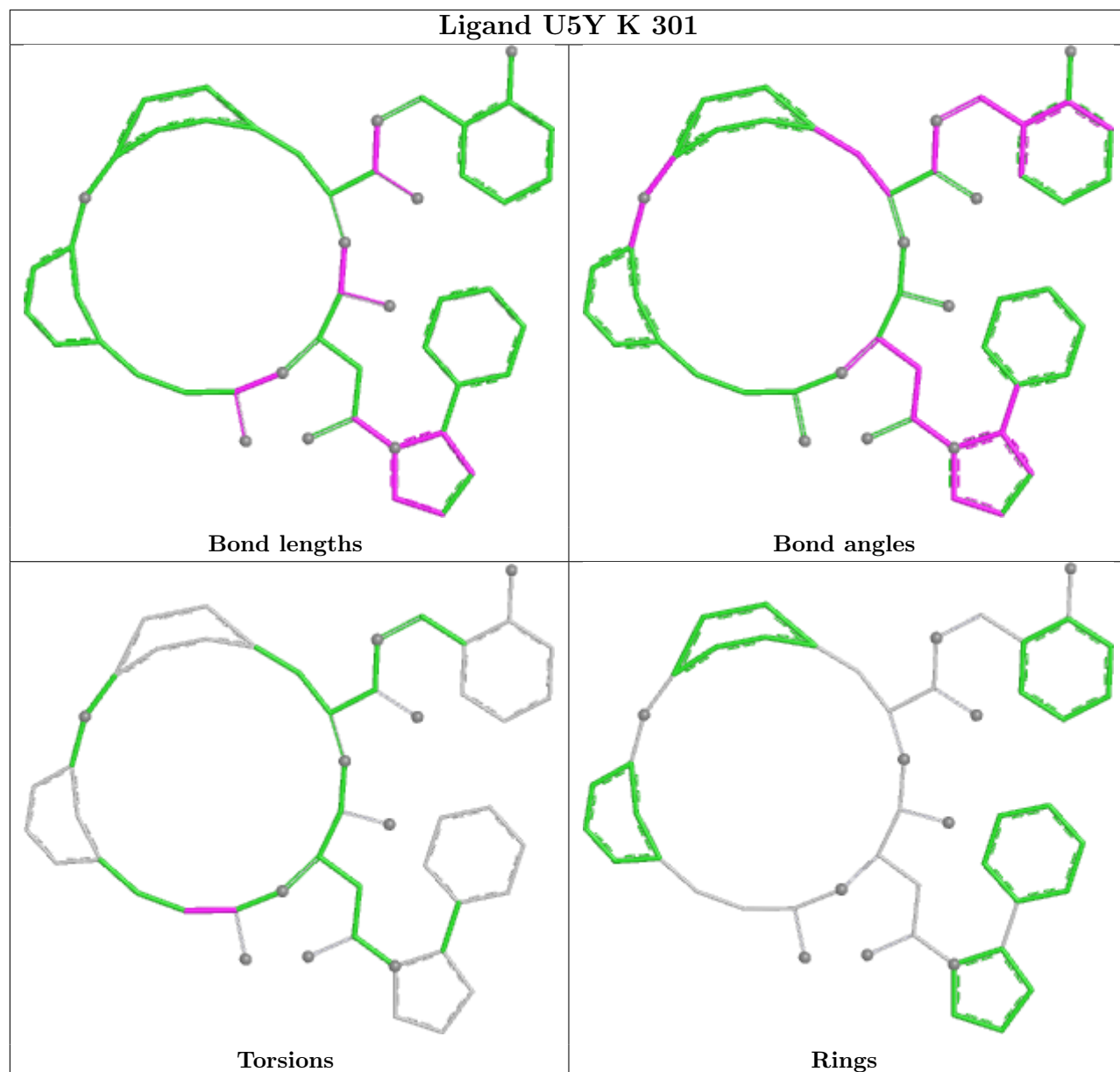
Ligand U5Y a 301



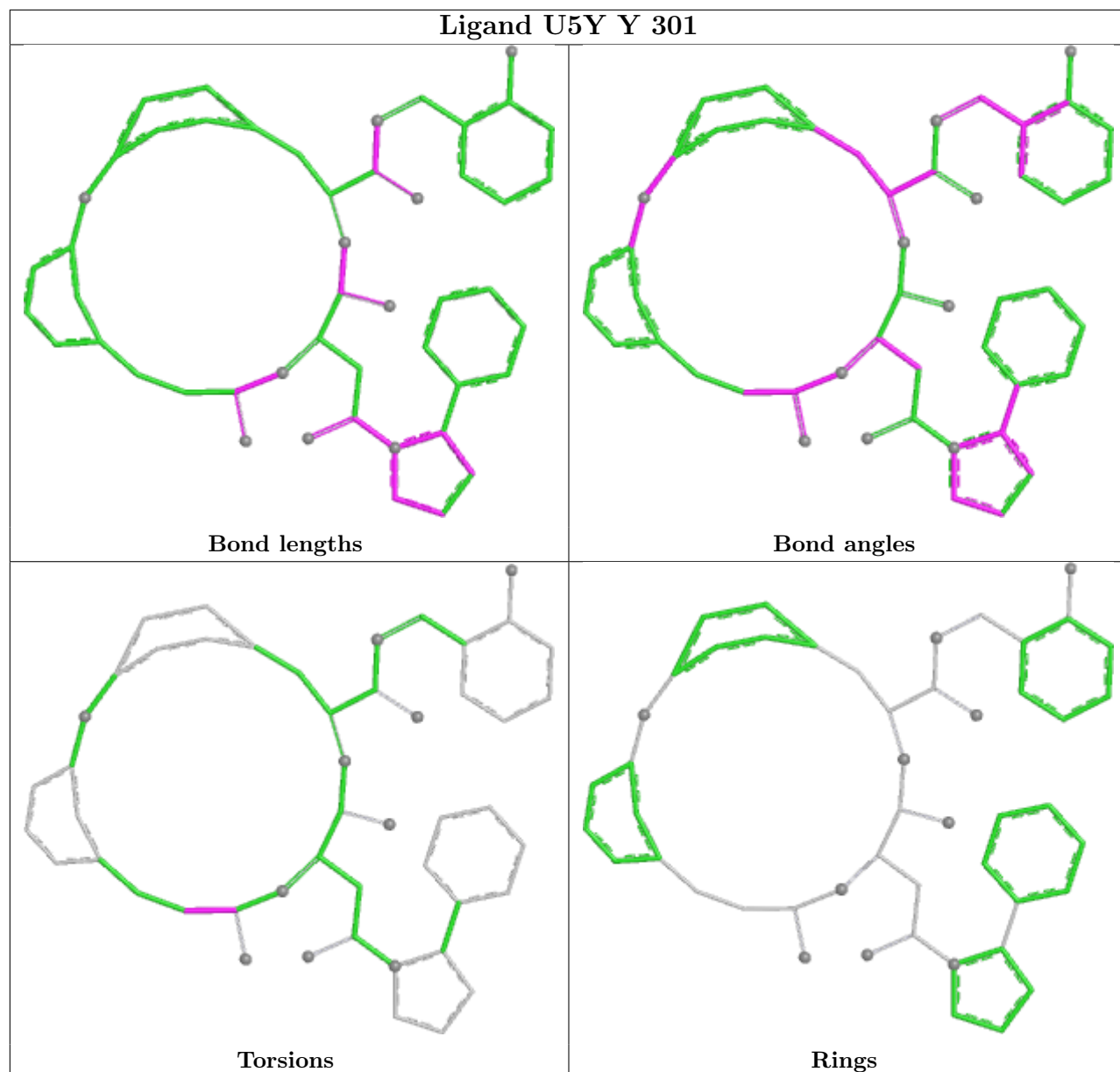
Ligand U5Y V 301



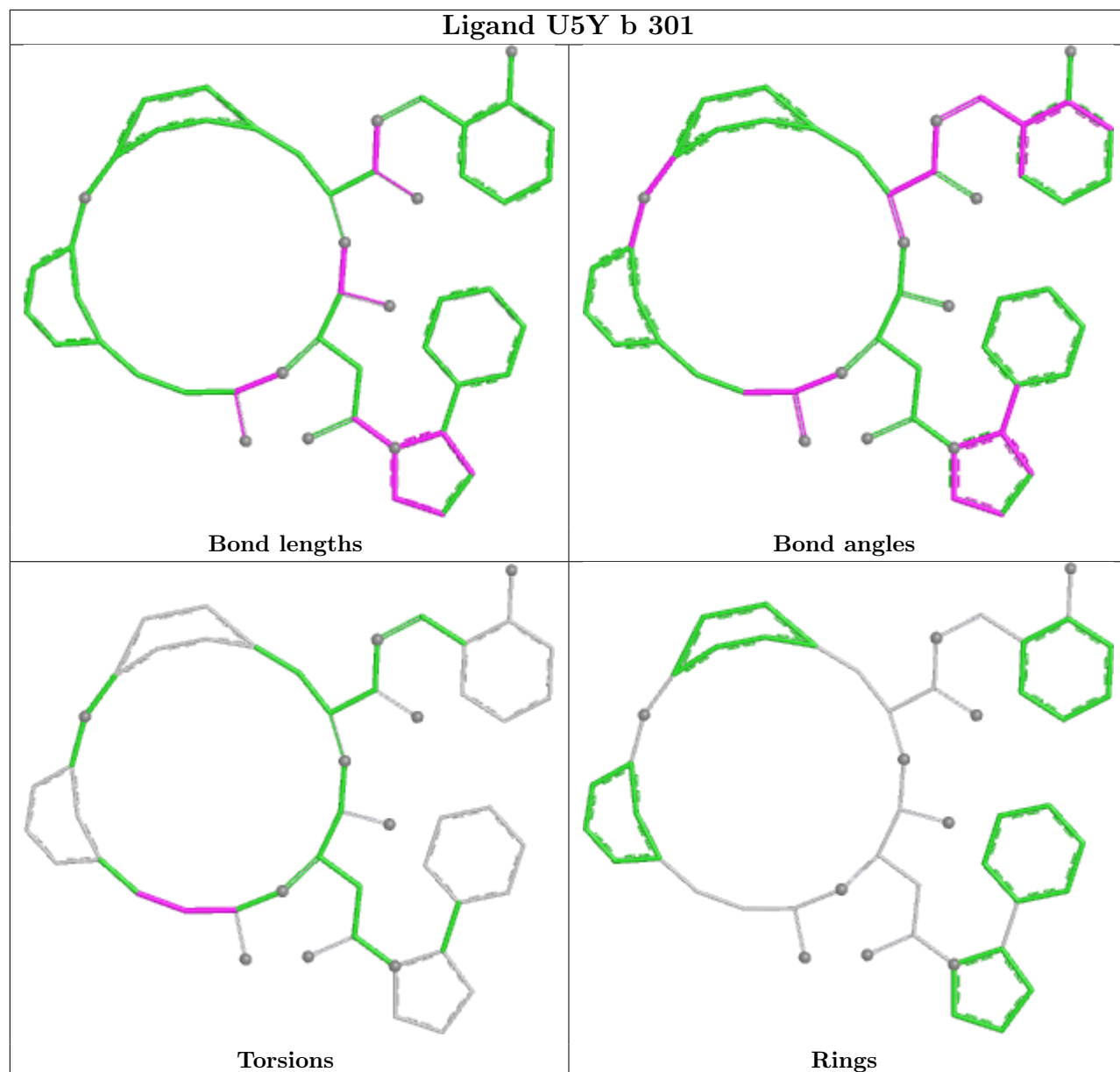
Ligand U5Y K 301



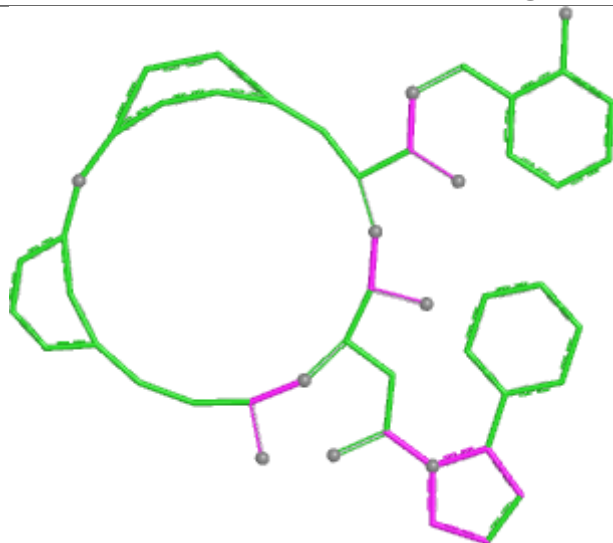
Ligand U5Y Y 301



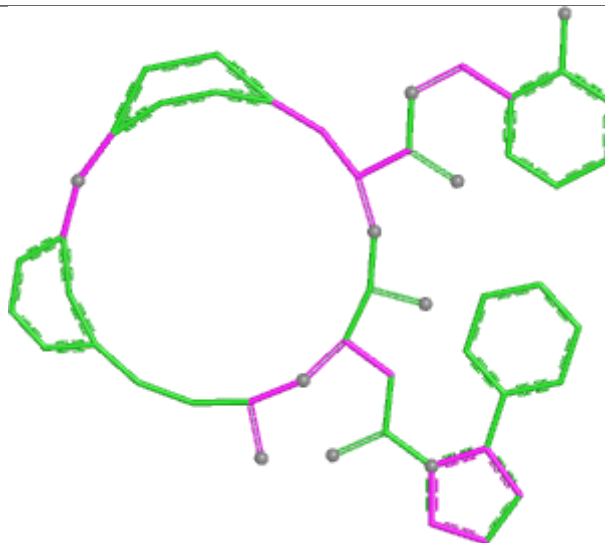
Ligand U5Y b 301



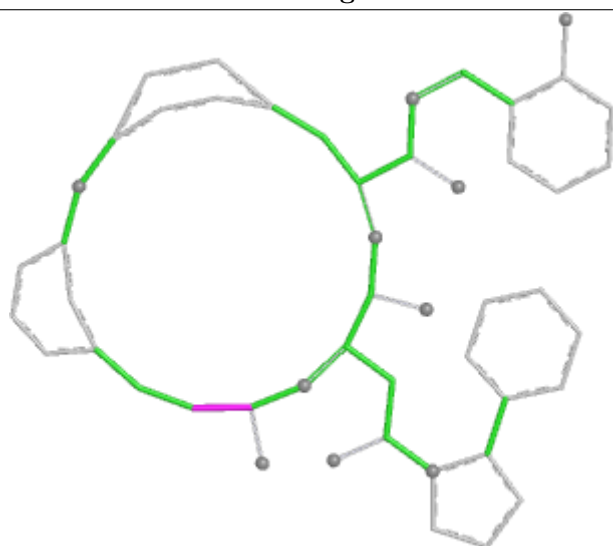
Ligand U5Y I 301



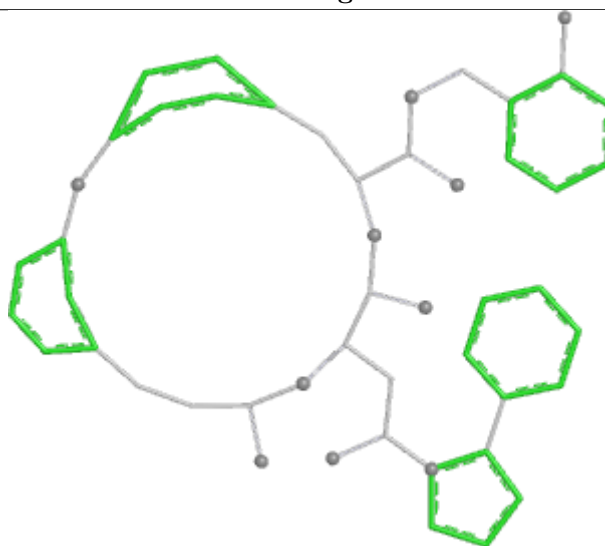
Bond lengths



Bond angles

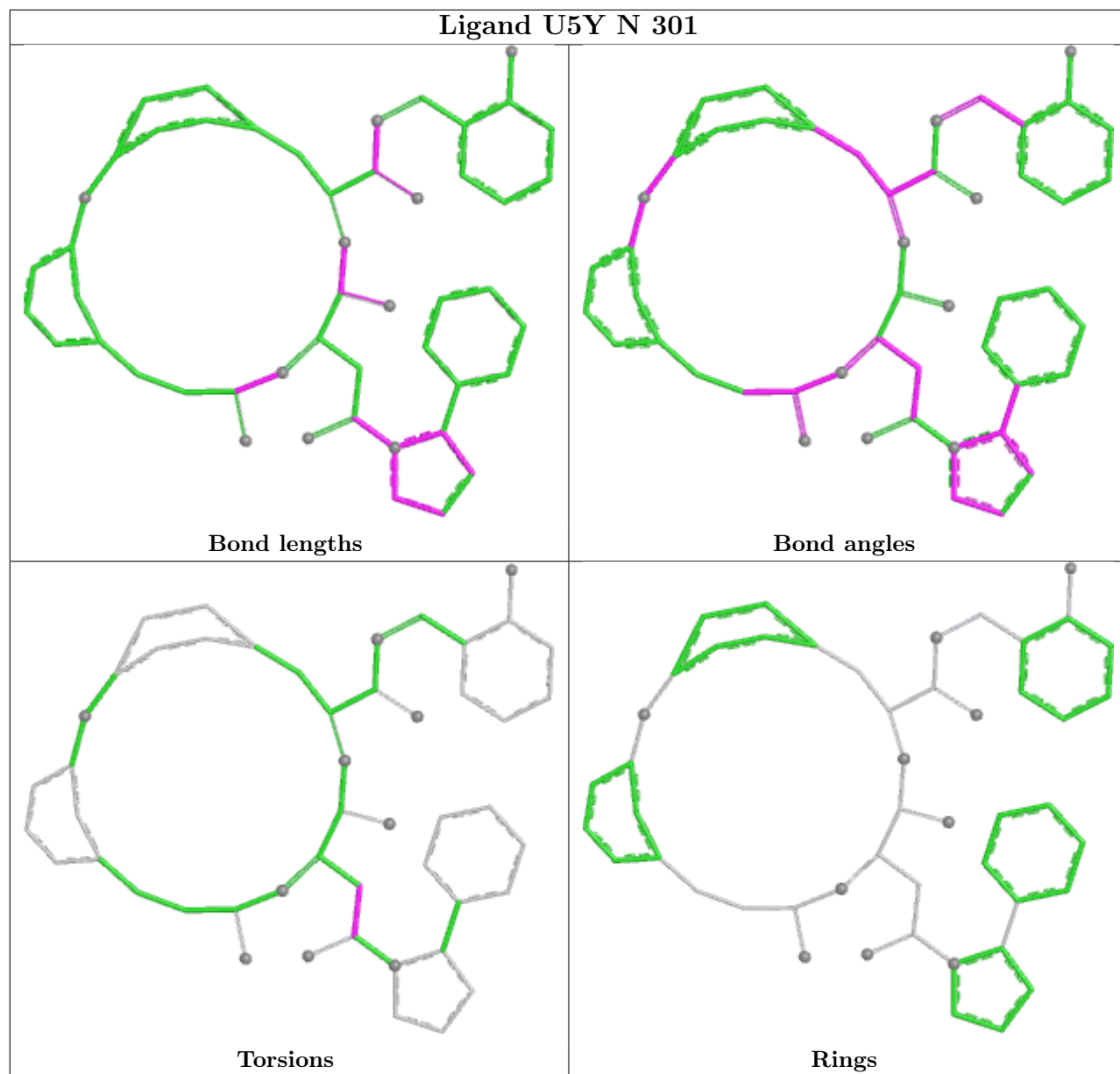


Torsions

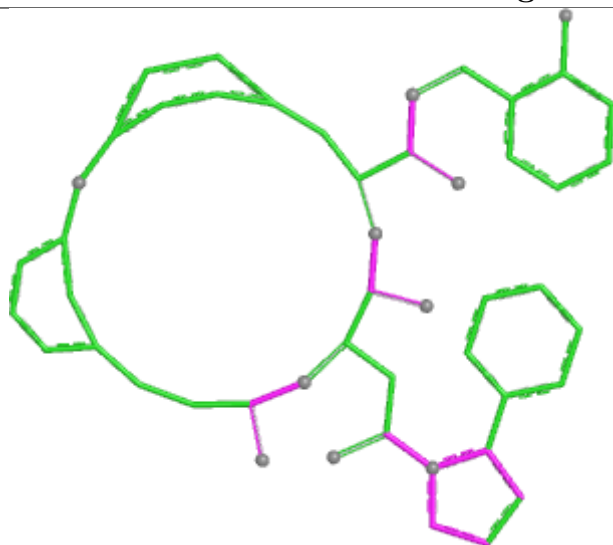


Rings

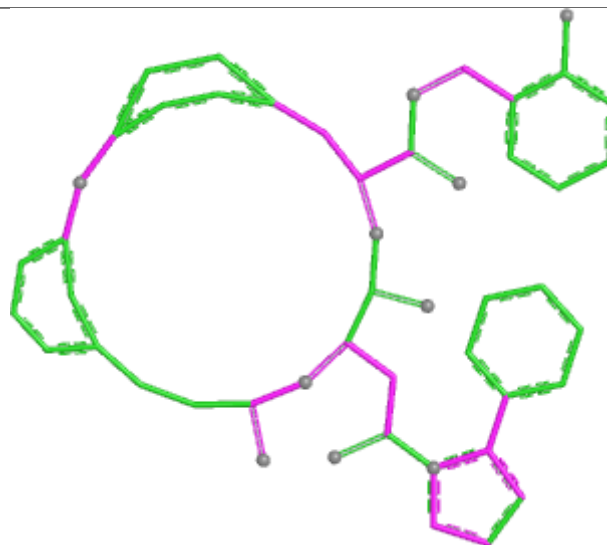
Ligand U5Y N 301



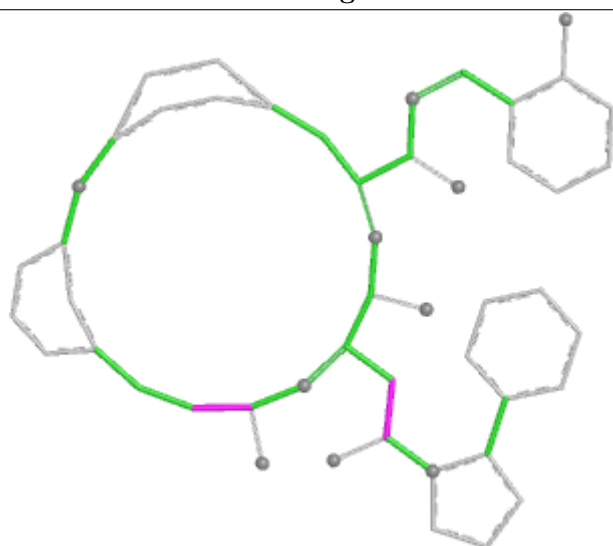
Ligand U5Y L 301



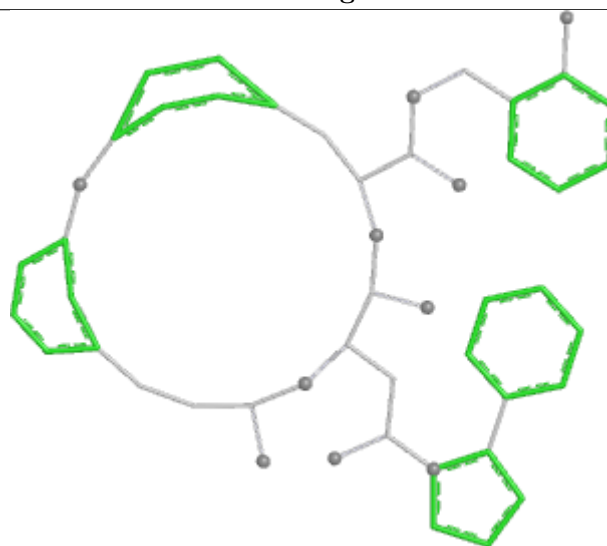
Bond lengths



Bond angles

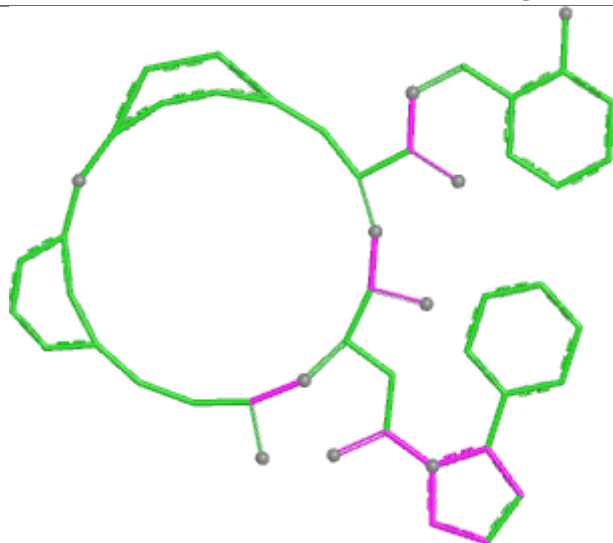


Torsions

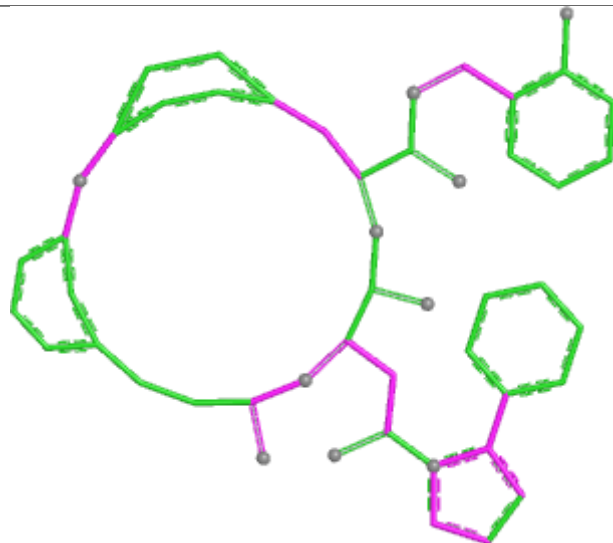


Rings

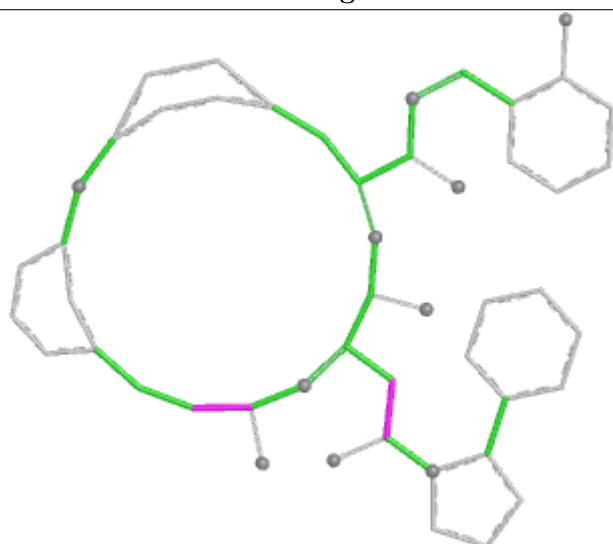
Ligand U5Y Z 301



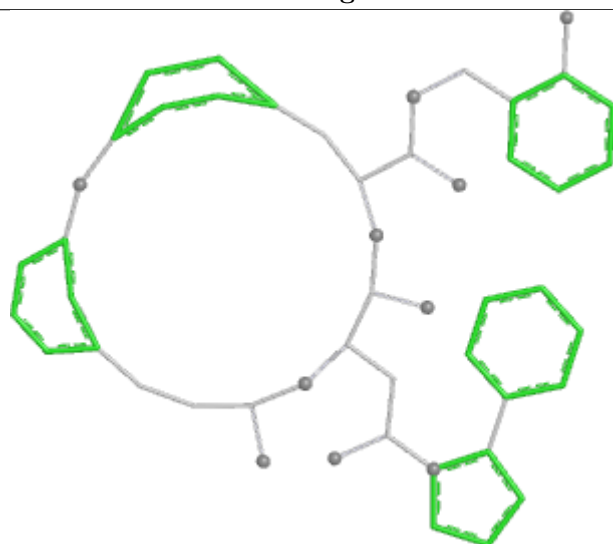
Bond lengths



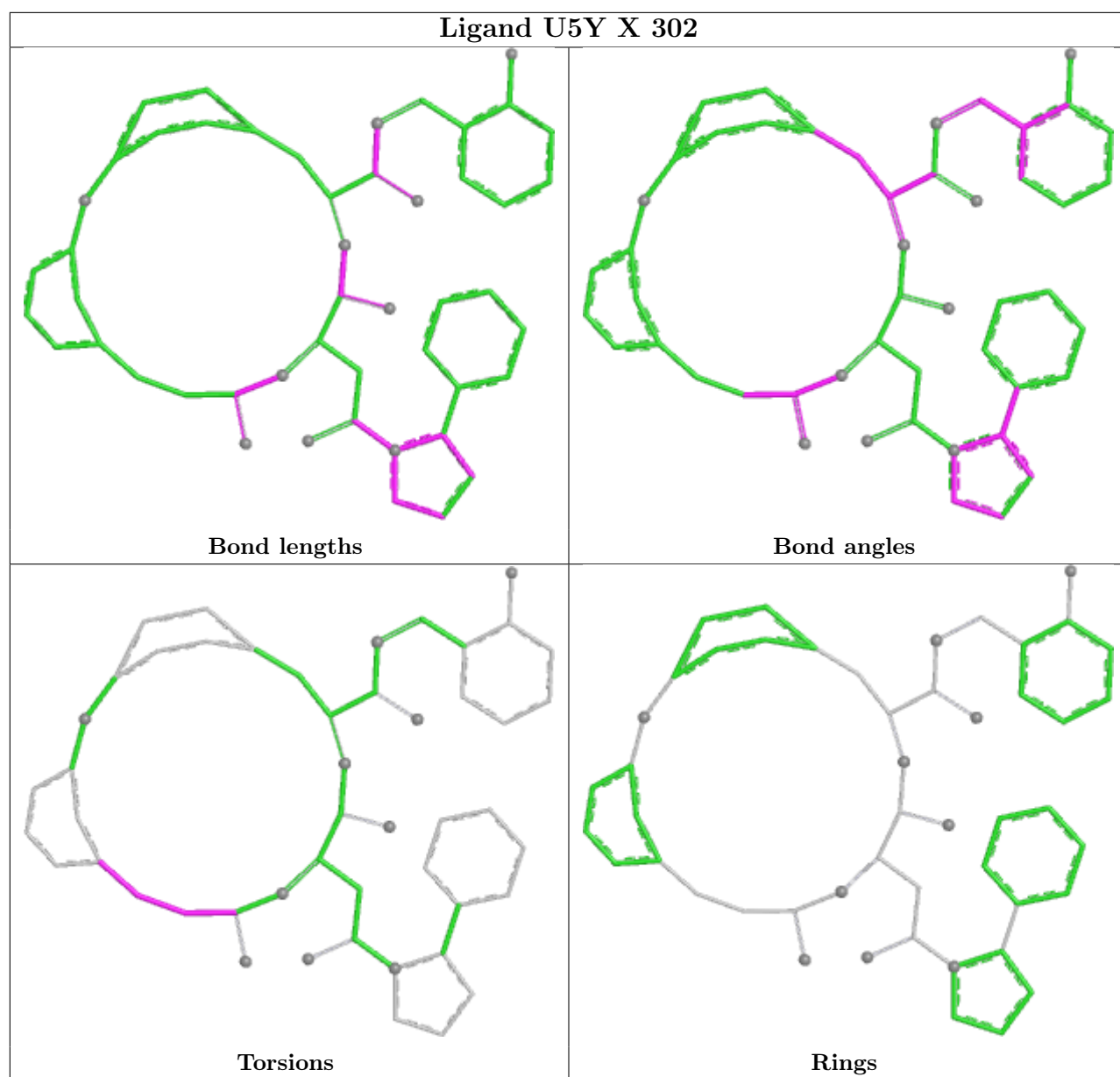
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	216/240 (90%)	0.39	4 (1%) 66 68	34, 51, 75, 97	0
1	B	215/240 (89%)	0.60	14 (6%) 25 26	35, 58, 91, 105	0
1	C	216/240 (90%)	1.16	28 (12%) 7 8	39, 73, 100, 110	0
1	D	217/240 (90%)	1.09	22 (10%) 12 13	41, 70, 96, 101	0
1	E	214/240 (89%)	1.32	46 (21%) 2 2	39, 70, 98, 111	0
1	F	216/240 (90%)	1.15	30 (13%) 6 7	38, 71, 98, 106	0
1	G	220/240 (91%)	0.87	20 (9%) 15 15	36, 61, 92, 105	0
1	O	215/240 (89%)	0.44	6 (2%) 55 56	34, 53, 79, 91	0
1	P	218/240 (90%)	0.56	11 (5%) 34 35	32, 56, 85, 97	0
1	Q	218/240 (90%)	0.66	21 (9%) 13 14	30, 58, 87, 104	0
1	R	217/240 (90%)	0.16	3 (1%) 73 75	27, 47, 69, 88	0
1	S	218/240 (90%)	0.95	31 (14%) 6 6	39, 69, 96, 112	0
1	T	215/240 (89%)	1.11	32 (14%) 5 6	40, 71, 101, 112	0
1	U	218/240 (90%)	0.94	21 (9%) 13 14	38, 66, 93, 108	0
2	H	224/240 (93%)	-0.13	5 (2%) 62 64	28, 38, 57, 87	0
2	I	222/240 (92%)	-0.33	3 (1%) 73 75	25, 34, 49, 83	0
2	J	222/240 (92%)	-0.11	0 100 100	30, 39, 57, 65	0
2	K	223/240 (92%)	0.11	1 (0%) 88 89	34, 44, 61, 71	0
2	L	222/240 (92%)	0.30	3 (1%) 73 75	34, 45, 63, 77	0
2	M	222/240 (92%)	0.43	2 (0%) 81 82	35, 46, 65, 93	0
2	N	222/240 (92%)	0.16	1 (0%) 87 88	33, 43, 62, 84	0
2	V	222/240 (92%)	0.13	2 (0%) 81 82	31, 42, 59, 86	0
2	W	223/240 (92%)	-0.05	1 (0%) 88 89	29, 40, 58, 81	0
2	X	222/240 (92%)	-0.25	1 (0%) 87 88	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%)	-0.29	5 (2%) 62 64	24, 33, 50, 84	0
2	Z	222/240 (92%)	-0.09	1 (0%) 87 88	28, 39, 59, 79	0
2	a	222/240 (92%)	0.22	0 100 100	33, 46, 63, 74	0
2	b	224/240 (93%)	0.35	7 (3%) 51 53	32, 46, 65, 91	0
All	All	6148/6720 (91%)	0.42	321 (5%) 33 33	24, 48, 90, 112	0

The worst 5 of 321 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	PRO	5.6
1	A	235	VAL	5.3
1	F	234	LEU	5.3
1	D	235	VAL	5.2
1	U	201	PRO	5.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DMF	X	301	5/5	0.69	0.20	40,46,55,57	0
4	CIT	L	302	13/13	0.73	0.16	48,57,69,73	0
4	CIT	K	302	13/13	0.76	0.16	49,58,67,77	0
4	CIT	a	302	13/13	0.77	0.16	47,56,70,80	0
4	CIT	V	302	13/13	0.79	0.17	41,55,67,74	0
5	DMF	R	301	5/5	0.79	0.22	50,51,56,59	0
4	CIT	W	303	13/13	0.79	0.14	39,51,66,69	0

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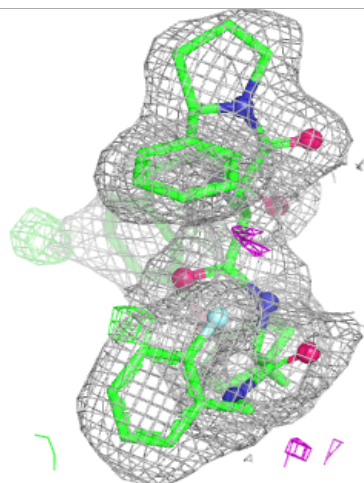
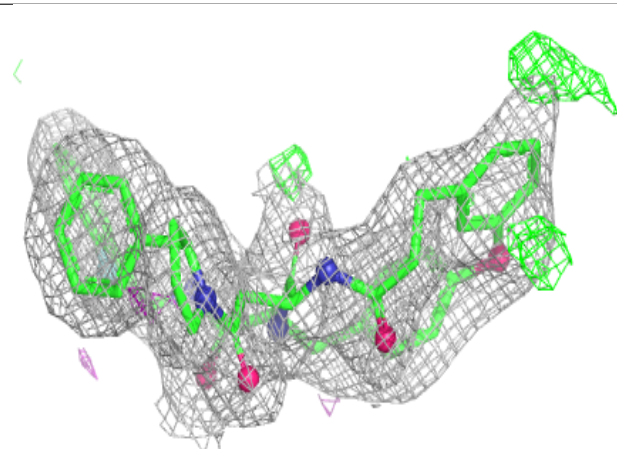
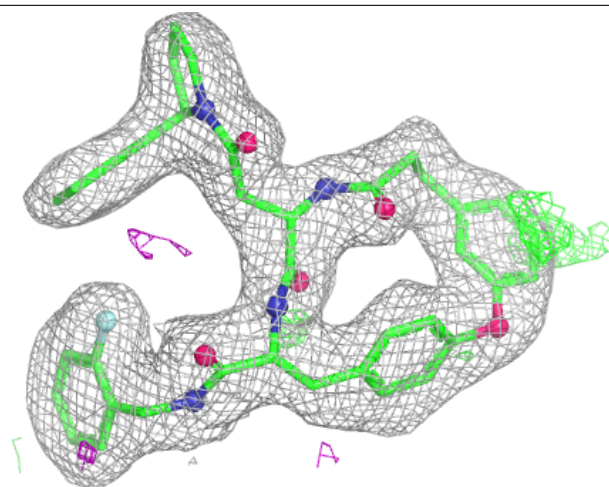
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CIT	H	302	13/13	0.80	0.14	39,49,61,63	0
4	CIT	M	302	13/13	0.81	0.15	41,58,70,71	0
4	CIT	b	302	13/13	0.82	0.15	43,59,69,75	0
4	CIT	Z	302	13/13	0.82	0.15	43,56,73,75	0
4	CIT	I	302	13/13	0.82	0.14	37,50,62,66	0
4	CIT	X	303	13/13	0.83	0.13	35,47,64,66	0
4	CIT	J	302	13/13	0.84	0.13	41,53,59,66	0
4	CIT	N	302	13/13	0.84	0.13	40,57,63,63	0
5	DMF	W	301	5/5	0.86	0.17	40,44,53,55	0
5	DMF	Q	301	5/5	0.86	0.16	41,42,54,57	0
5	DMF	R	302	5/5	0.87	0.18	48,57,59,60	0
4	CIT	Y	302	13/13	0.88	0.12	34,50,64,71	0
5	DMF	P	301	5/5	0.89	0.14	41,43,49,53	0
5	DMF	S	301	5/5	0.89	0.15	49,49,54,55	0
5	DMF	O	301	5/5	0.94	0.10	35,43,47,52	0
3	U5Y	b	301	49/49	0.94	0.08	28,36,50,55	0
3	U5Y	L	301	49/49	0.94	0.09	29,39,52,64	0
3	U5Y	M	301	49/49	0.94	0.09	29,37,52,67	0
3	U5Y	a	301	49/49	0.95	0.09	29,38,51,54	0
3	U5Y	J	301	49/49	0.95	0.09	27,37,51,57	0
3	U5Y	K	301	49/49	0.95	0.08	30,37,46,53	0
3	U5Y	N	301	49/49	0.95	0.08	27,35,45,53	0
3	U5Y	V	301	49/49	0.95	0.08	28,34,46,51	0
3	U5Y	X	302	49/49	0.95	0.08	22,29,44,51	0
3	U5Y	Y	301	49/49	0.95	0.08	23,31,42,51	0
3	U5Y	Z	301	49/49	0.95	0.08	28,37,60,65	0
3	U5Y	H	301	49/49	0.96	0.07	23,30,41,46	0
3	U5Y	I	301	49/49	0.96	0.07	24,31,46,51	0
3	U5Y	W	302	49/49	0.96	0.07	25,31,46,52	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.

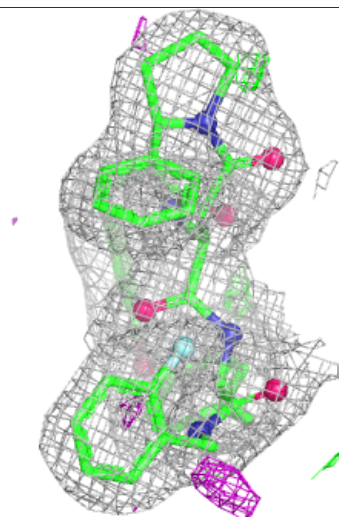
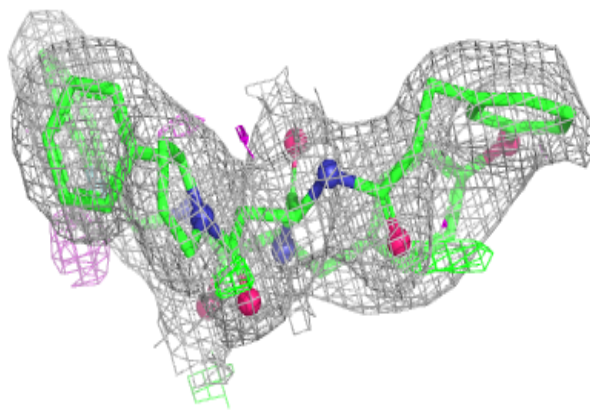
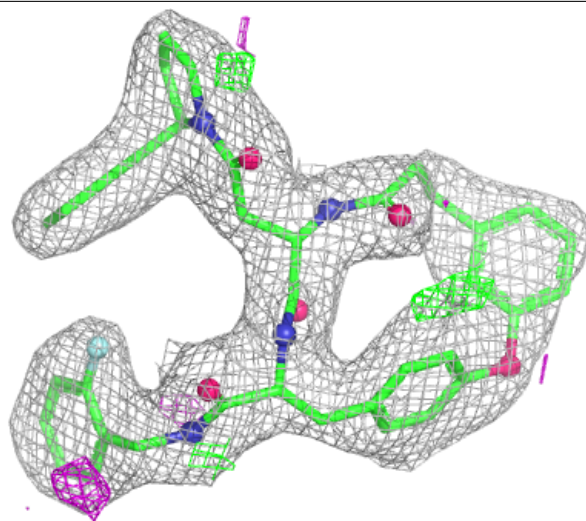
Electron density around U5Y b 301:

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



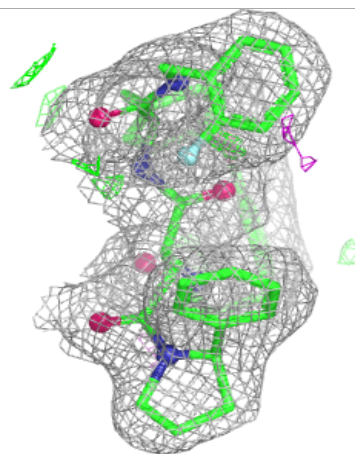
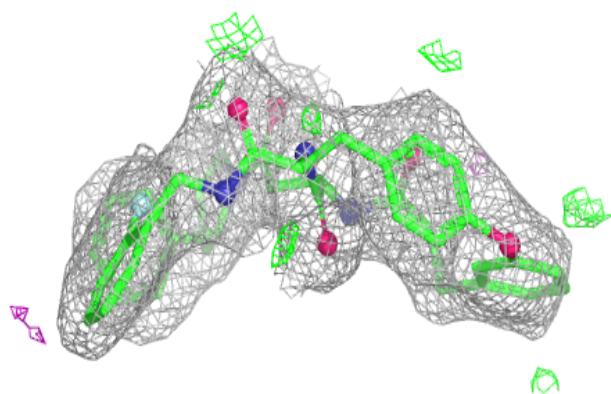
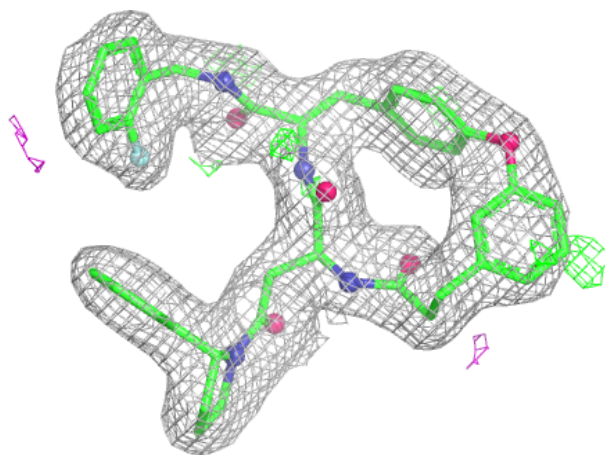
Electron density around U5Y L 301:

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



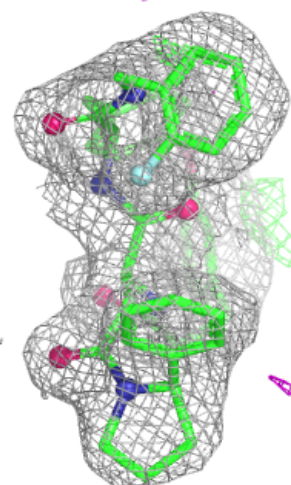
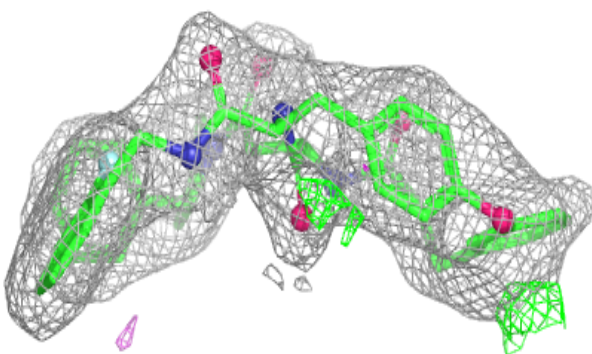
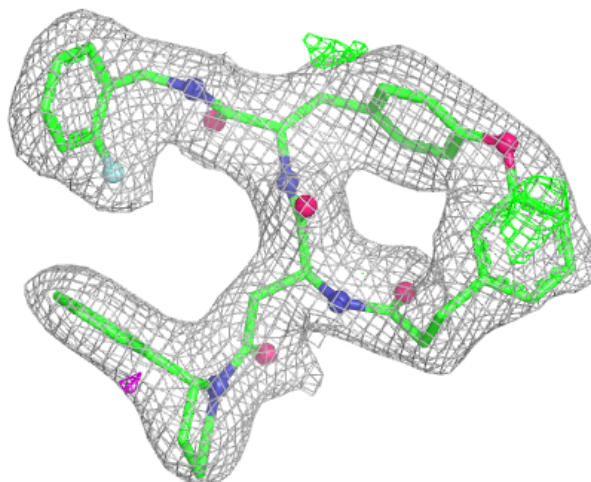
Electron density around U5Y M 301:

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and green (positive)



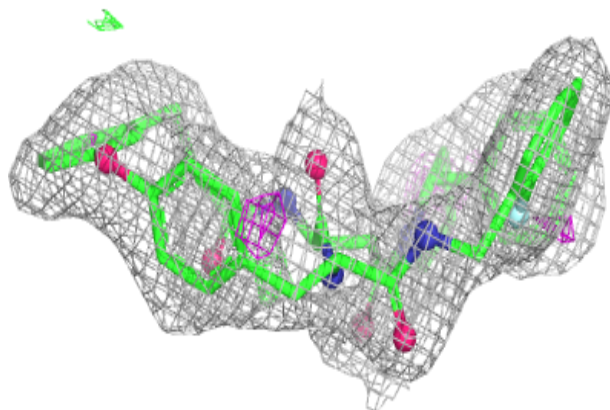
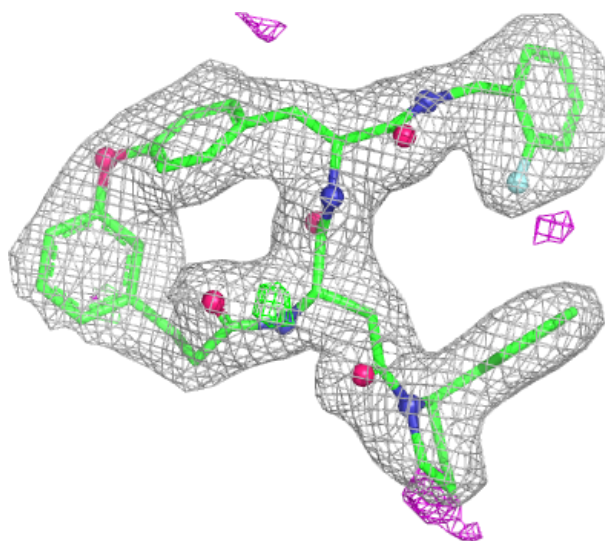
Electron density around U5Y a 301:

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and green (positive)



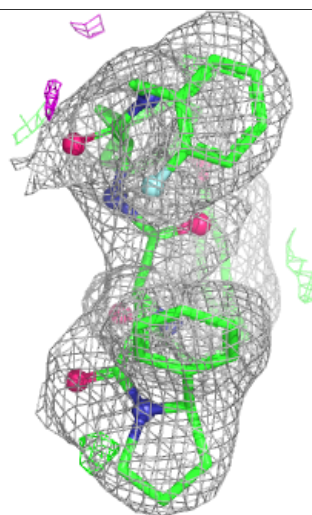
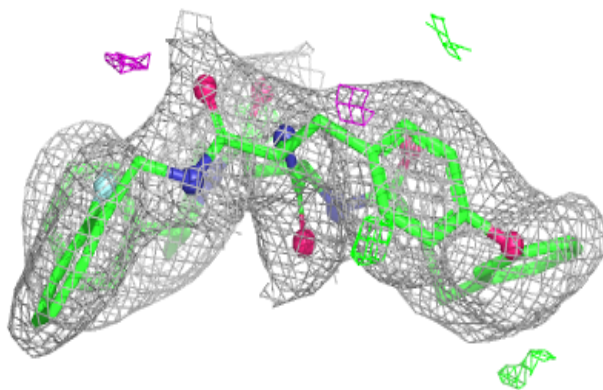
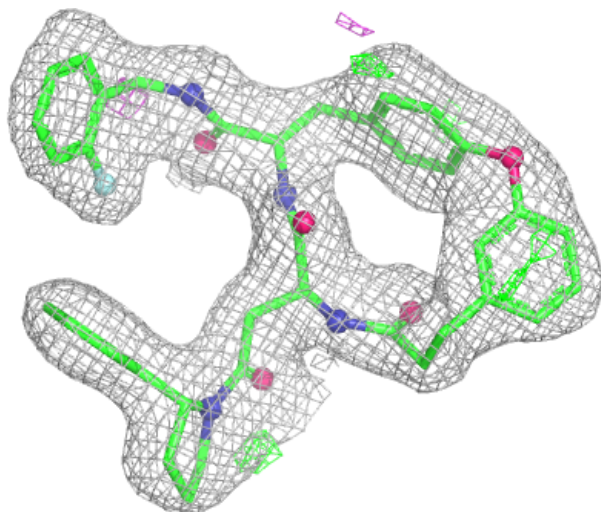
Electron density around U5Y J 301:

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and green (positive)



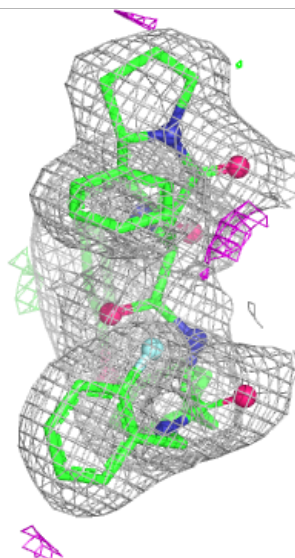
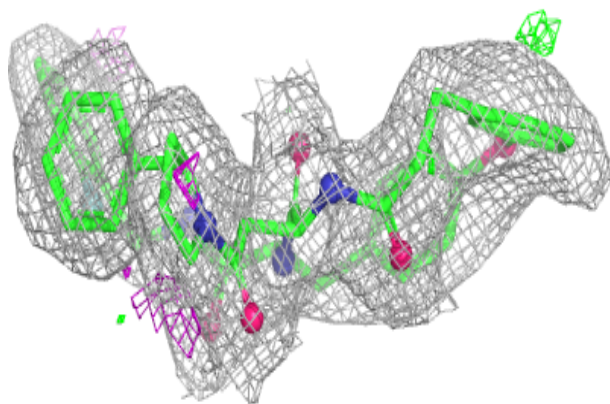
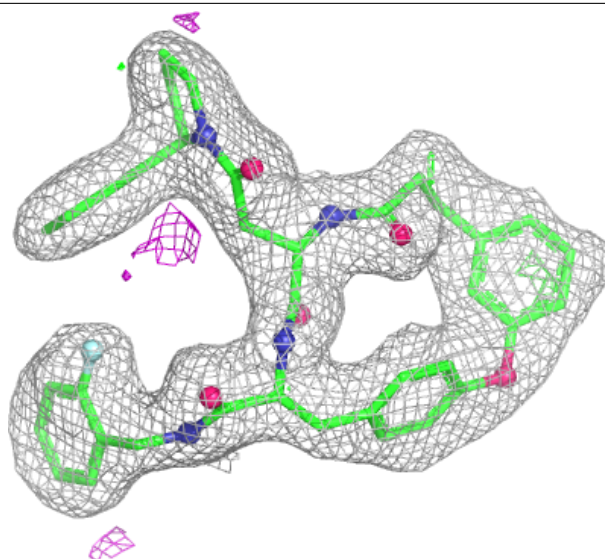
Electron density around U5Y K 301:

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and green (positive)



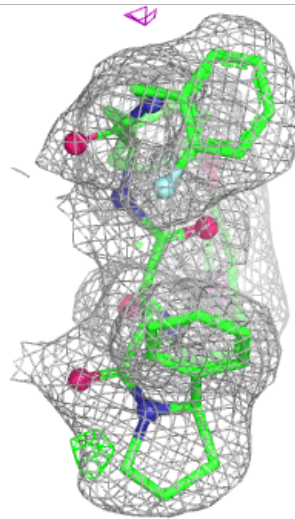
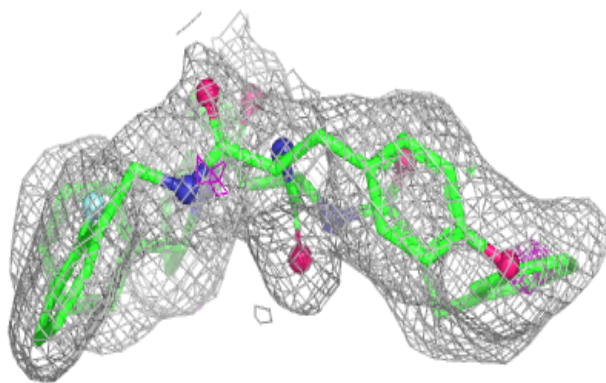
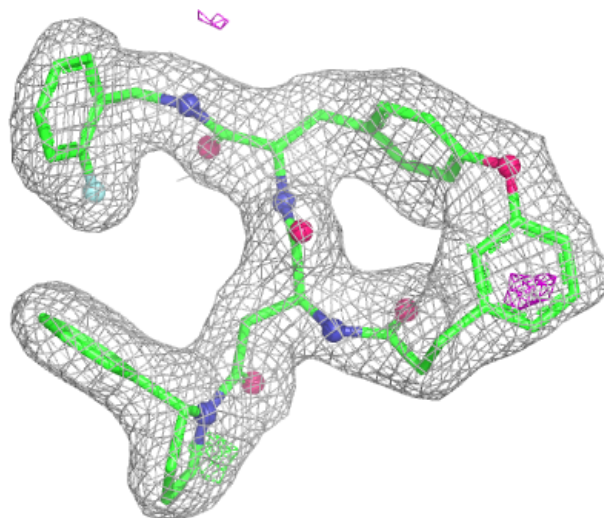
Electron density around U5Y N 301:

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and green (positive)



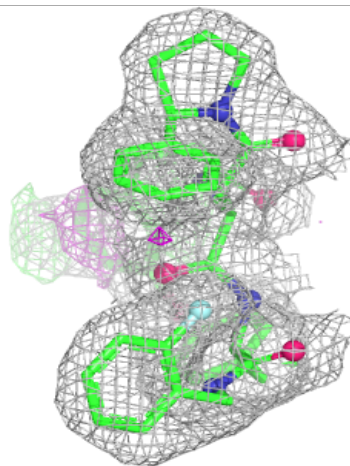
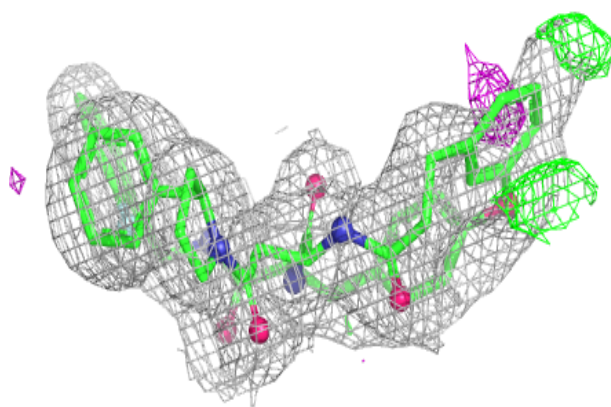
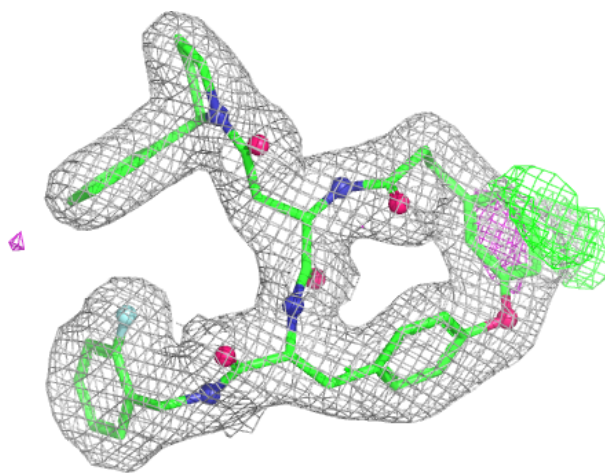
Electron density around U5Y V 301:

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and green (positive)



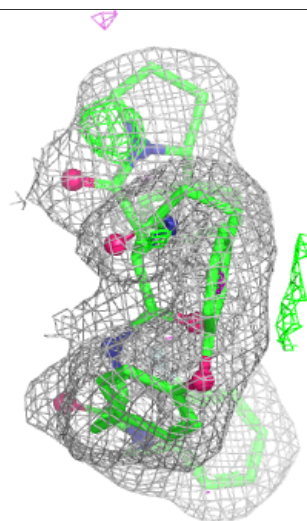
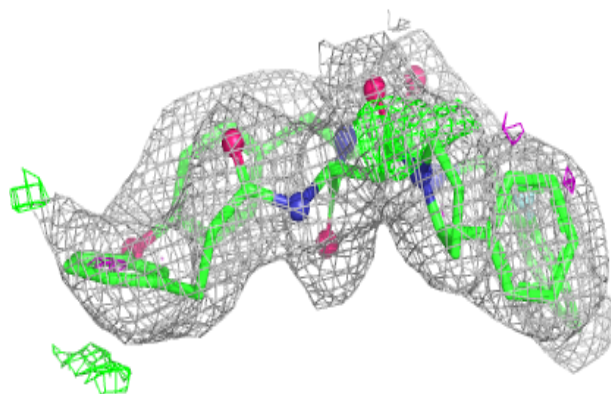
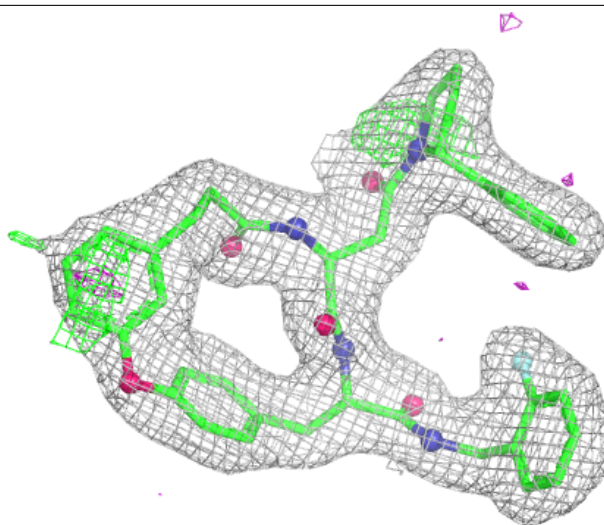
Electron density around U5Y X 302:

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and green (positive)



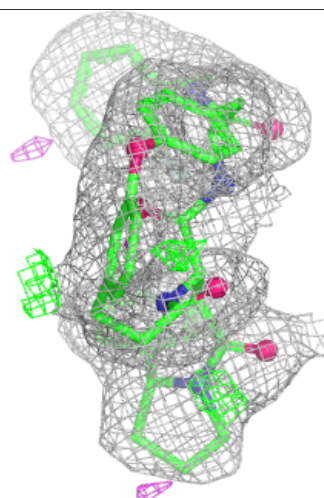
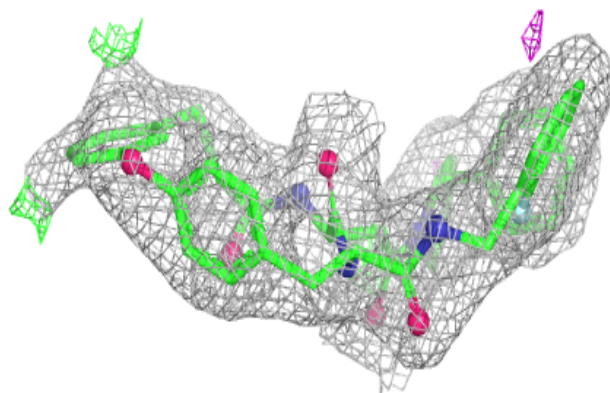
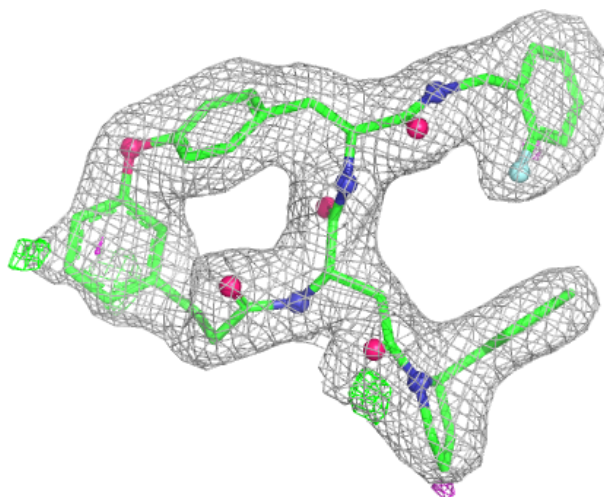
Electron density around U5Y Y 301:

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and green (positive)



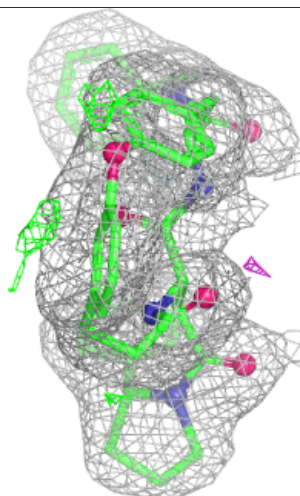
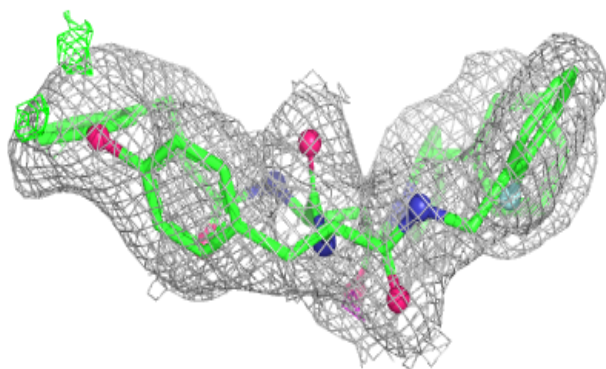
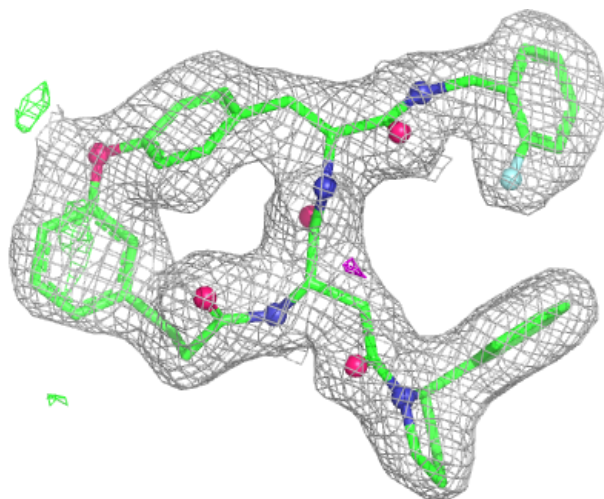
Electron density around U5Y Z 301:

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



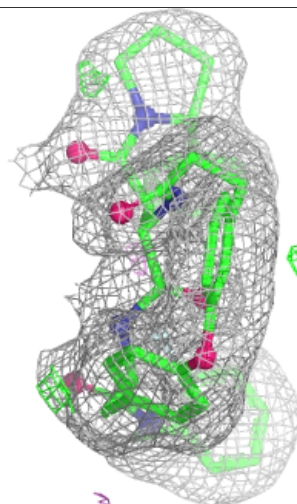
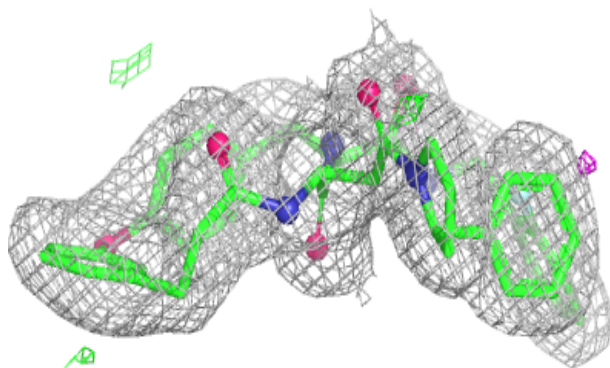
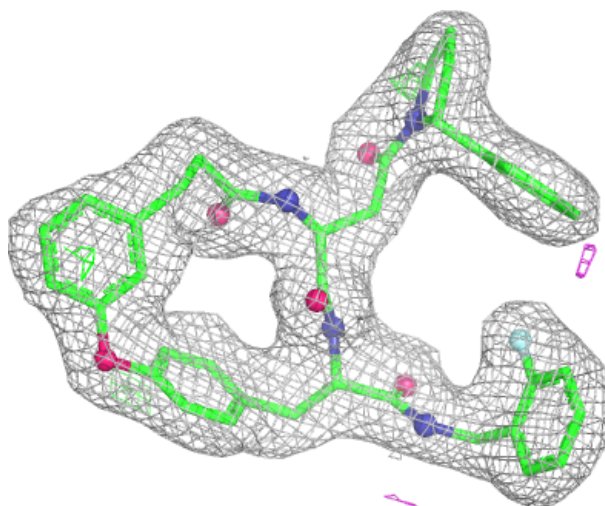
Electron density around U5Y H 301:

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and green (positive)



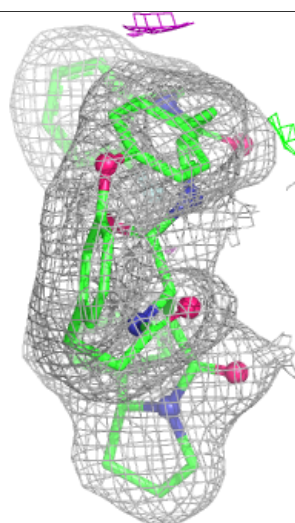
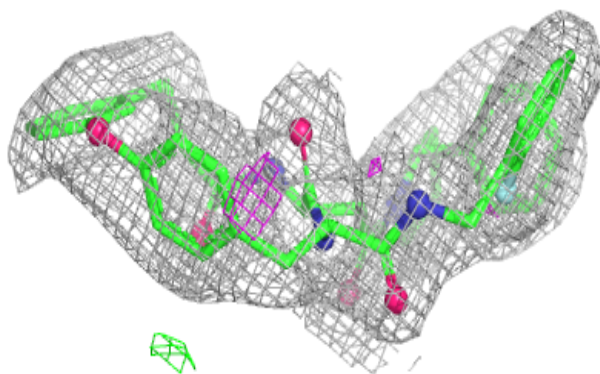
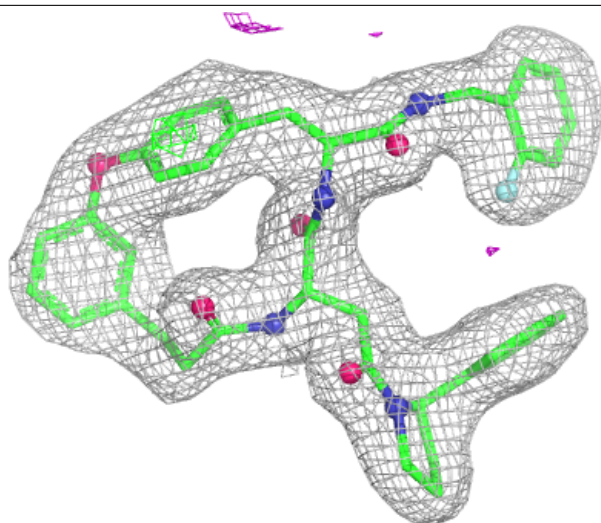
Electron density around U5Y I 301:

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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.