



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:43 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 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	:	4-5-2 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

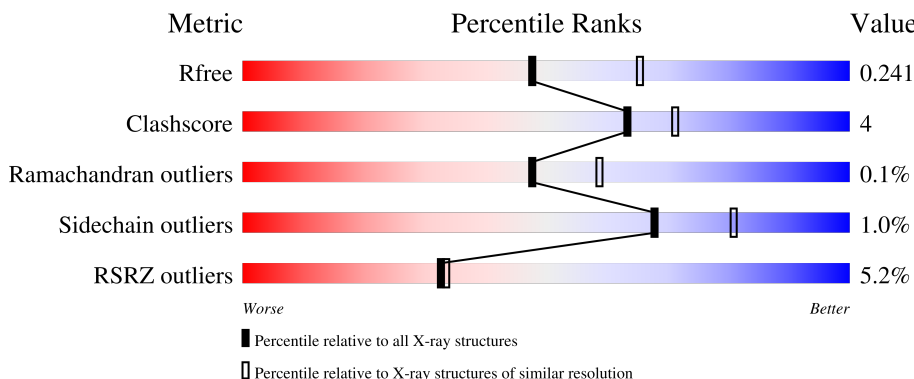
1 Overall quality at a glance

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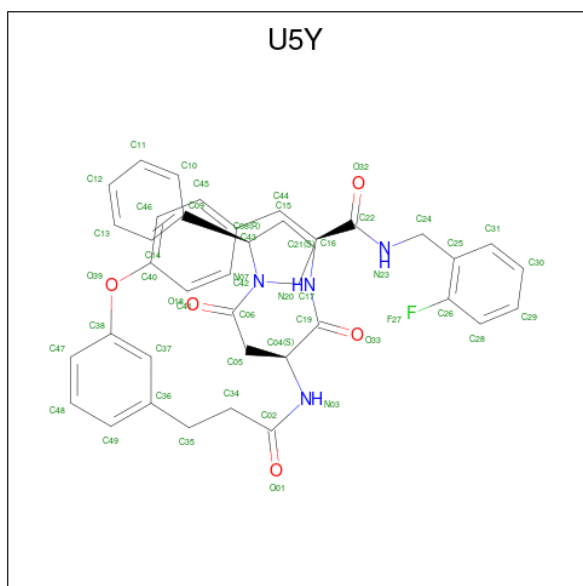
Chain	Residue	Modelled	Actual	Comment	Reference
N	235	HIS	-	expression tag	UNP A5U4D6
N	236	HIS	-	expression tag	UNP A5U4D6
N	237	HIS	-	expression tag	UNP A5U4D6
N	238	HIS	-	expression tag	UNP A5U4D6
N	239	HIS	-	expression tag	UNP A5U4D6
N	240	HIS	-	expression tag	UNP A5U4D6
V	235	HIS	-	expression tag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



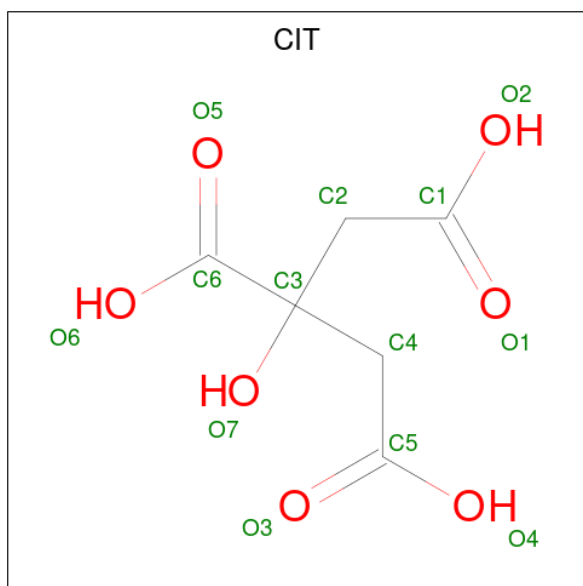
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	I	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	J	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	K	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	L	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	M	1	Total	C	F	N	O	0	0
			49	39	1	4	5		
3	N	1	Total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



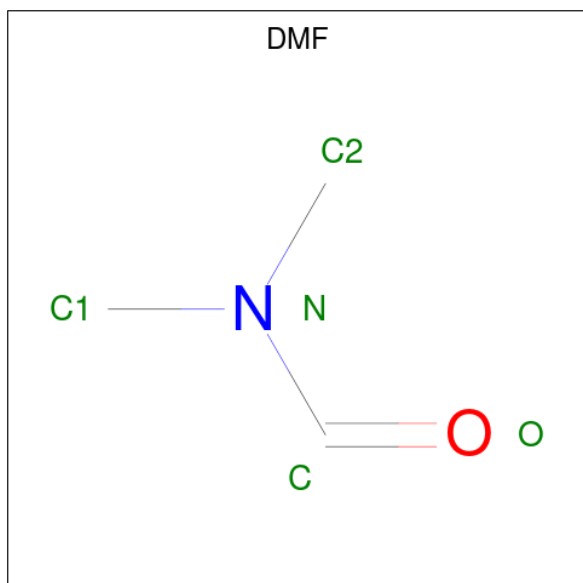
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			13	6	7		
4	I	1	Total	C	O	0	0
			13	6	7		
4	J	1	Total	C	O	0	0
			13	6	7		
4	K	1	Total	C	O	0	0
			13	6	7		

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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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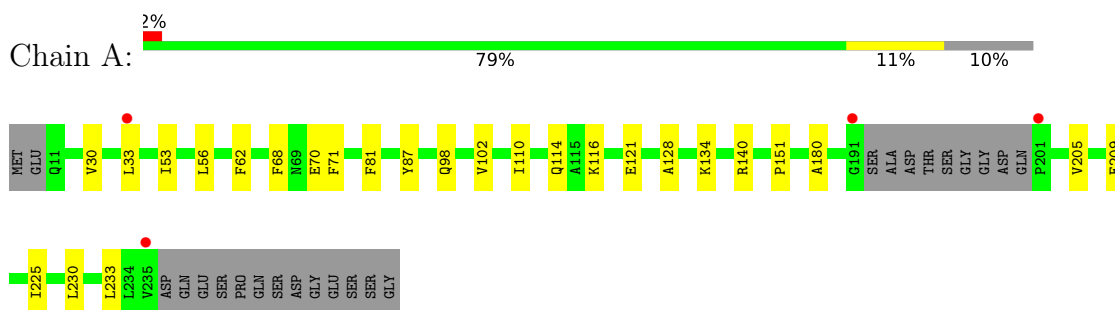
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	43	Total 43	O 43	0	0
6	N	64	Total 64	O 64	0	0
6	O	23	Total 23	O 23	0	0
6	P	30	Total 30	O 30	0	0
6	Q	32	Total 32	O 32	0	0
6	R	48	Total 48	O 48	0	0
6	S	12	Total 12	O 12	0	0
6	T	10	Total 10	O 10	0	0
6	U	13	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

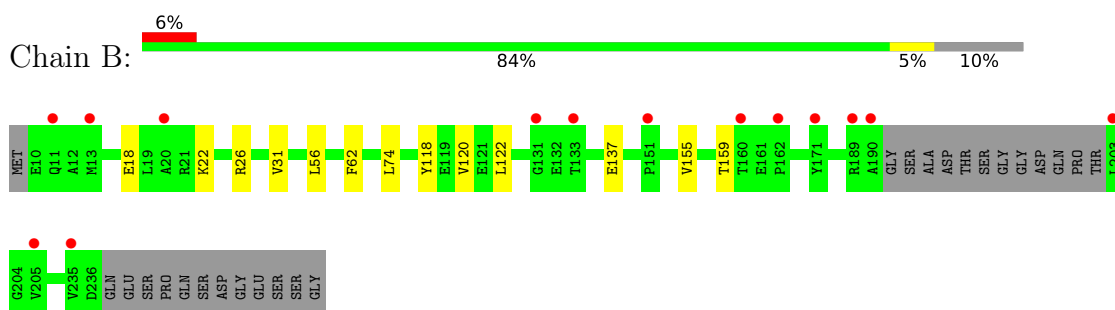
3 Residue-property plots [i](#)

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.

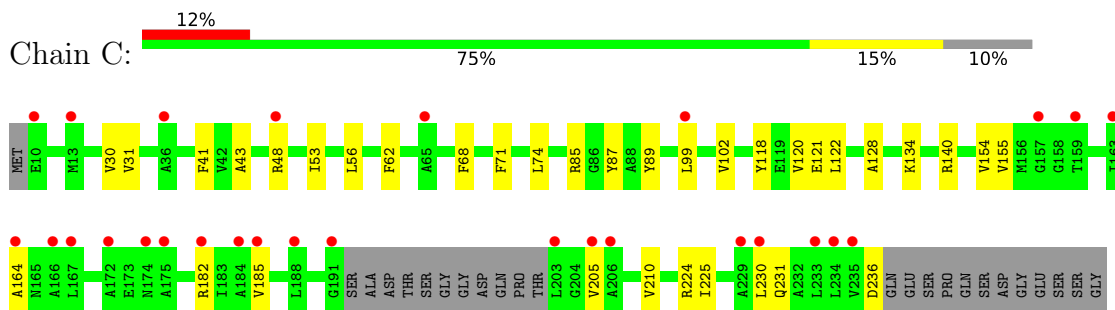
- Molecule 1: Proteasome subunit alpha



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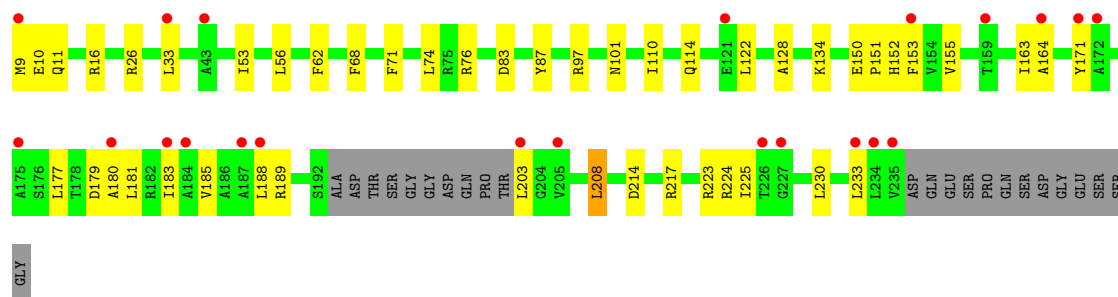


- Molecule 1: Proteasome subunit alpha

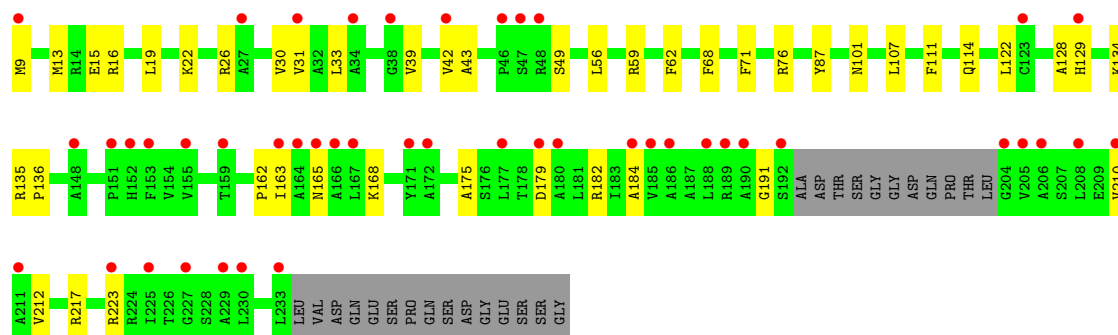


- Molecule 1: Proteasome subunit alpha

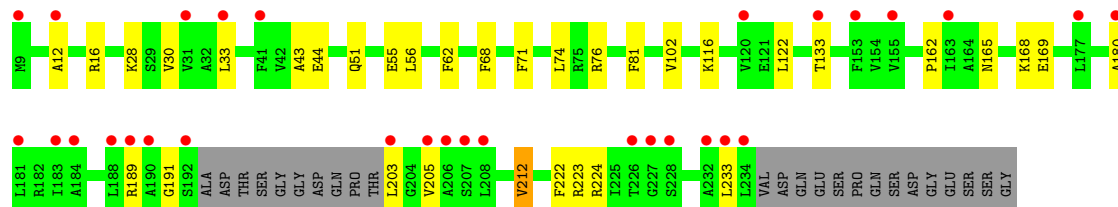
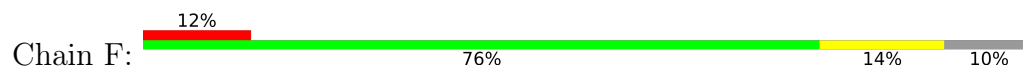




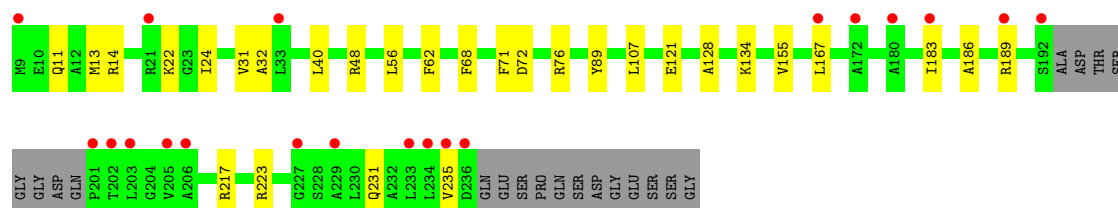
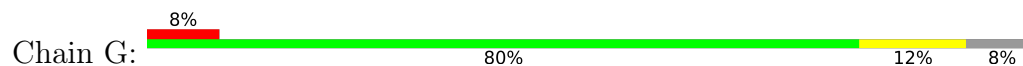
• Molecule 1: Proteasome subunit alpha



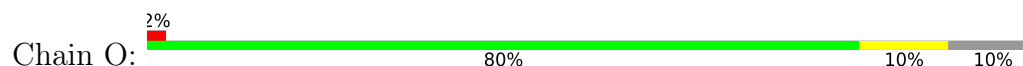
• Molecule 1: Proteasome subunit alpha

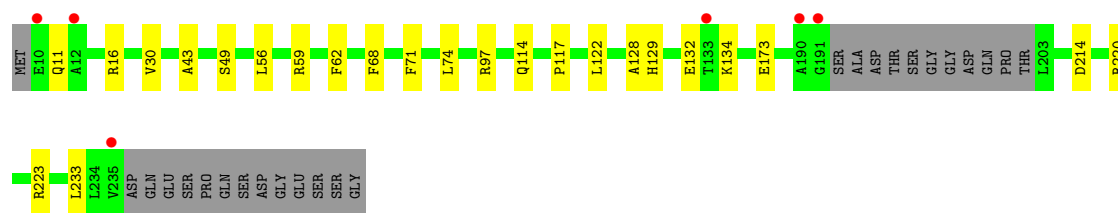


• Molecule 1: Proteasome subunit alpha

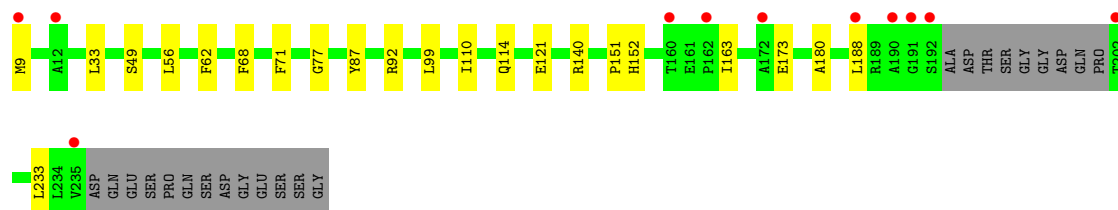
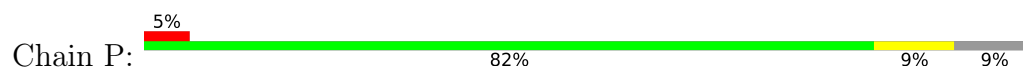


• Molecule 1: Proteasome subunit alpha

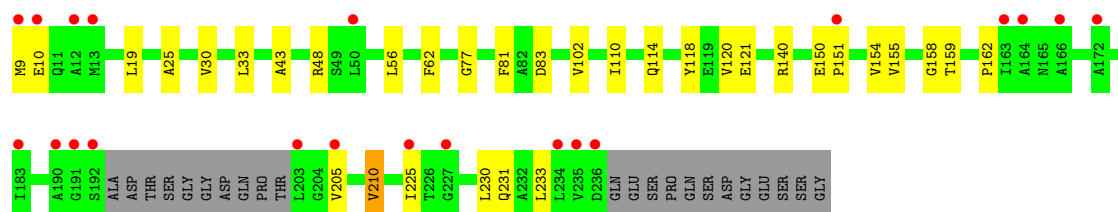
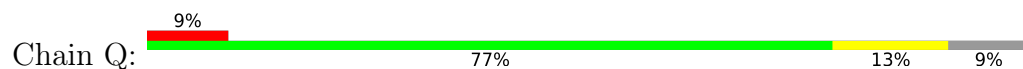




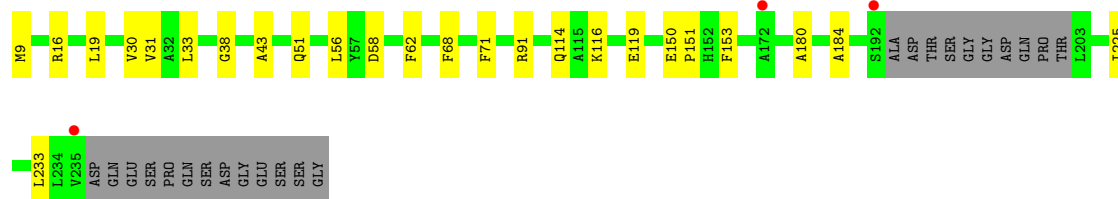
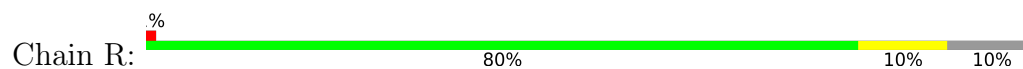
• Molecule 1: Proteasome subunit alpha



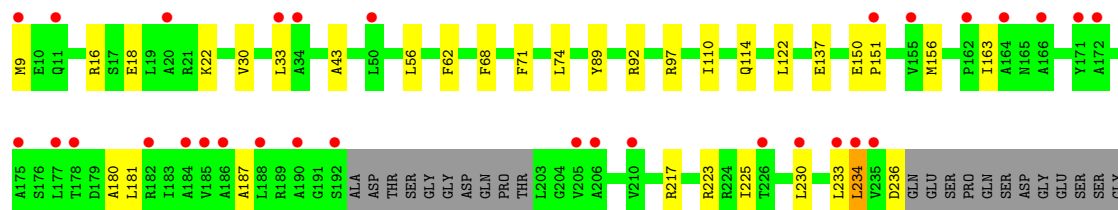
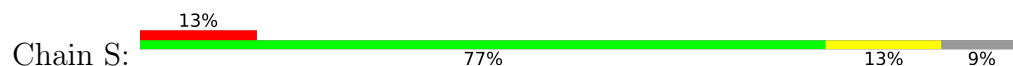
• Molecule 1: Proteasome subunit alpha



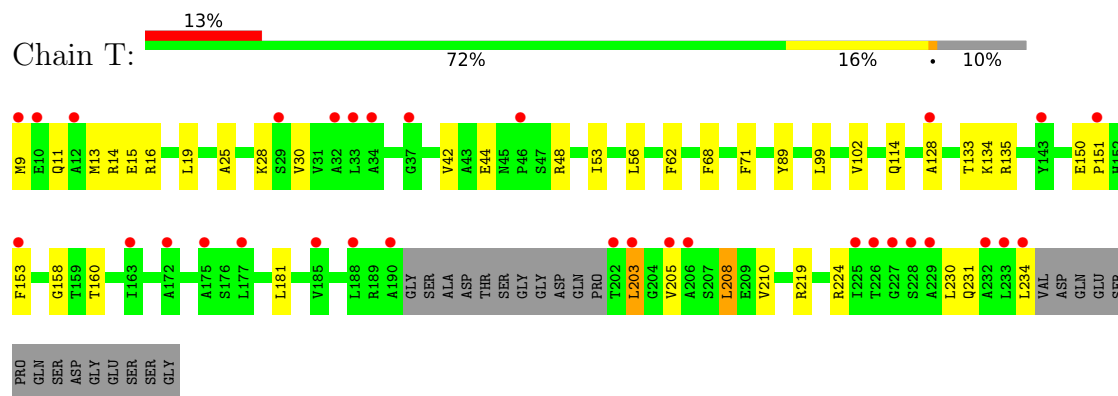
• Molecule 1: Proteasome subunit alpha



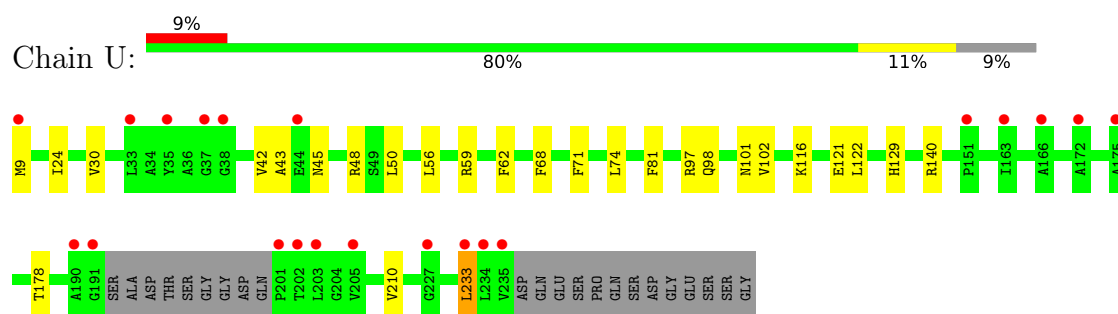
• Molecule 1: Proteasome subunit alpha



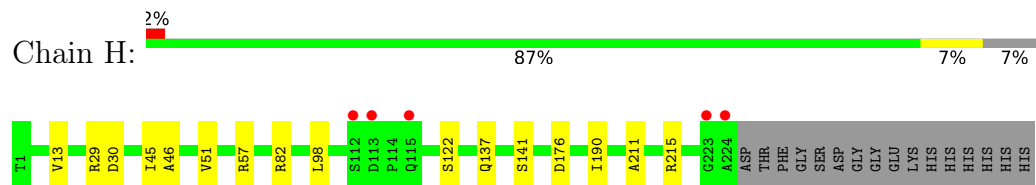
- Molecule 1: Proteasome subunit alpha



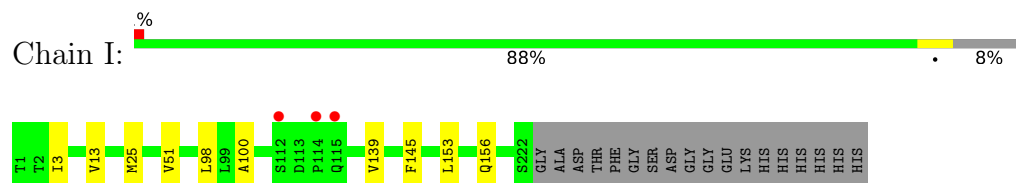
- Molecule 1: Proteasome subunit alpha



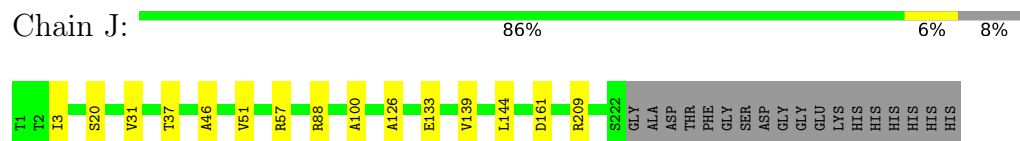
- Molecule 2: Proteasome subunit beta



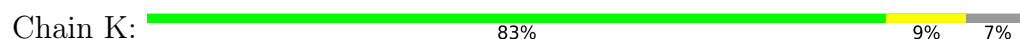
- Molecule 2: Proteasome subunit beta

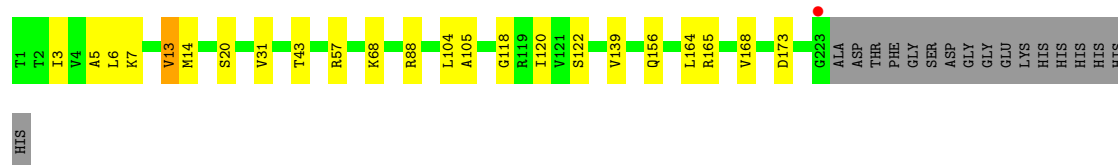


- Molecule 2: Proteasome subunit beta

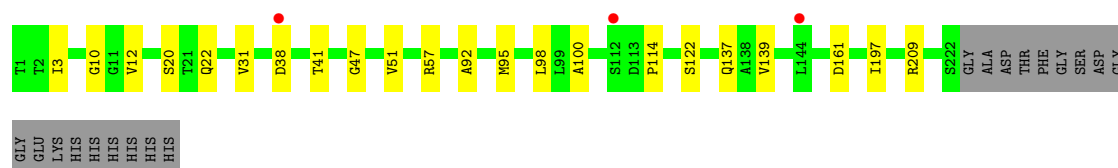
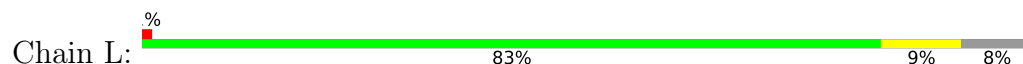


- Molecule 2: Proteasome subunit beta

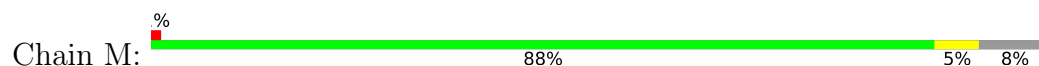




• Molecule 2: Proteasome subunit beta



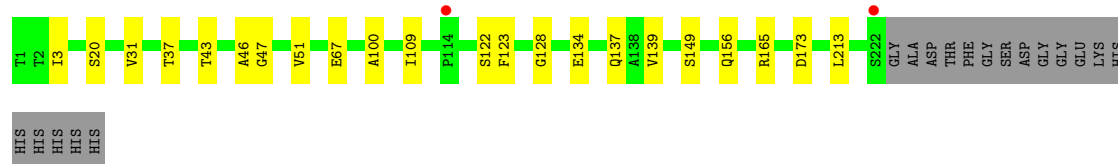
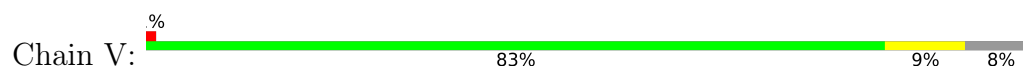
• Molecule 2: Proteasome subunit beta



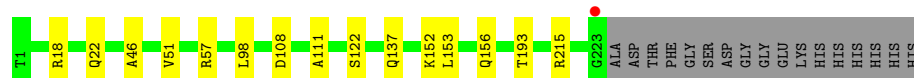
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

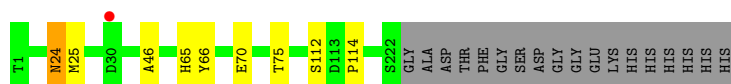


• Molecule 2: Proteasome subunit beta

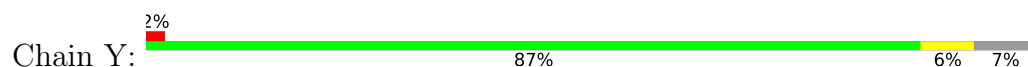


• Molecule 2: Proteasome subunit beta

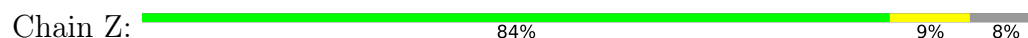




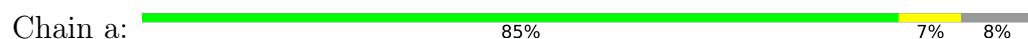
- Molecule 2: Proteasome subunit beta



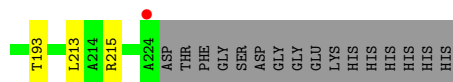
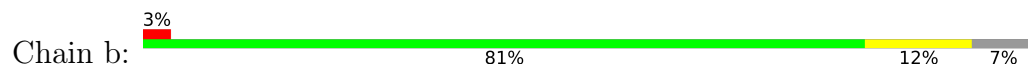
- Molecule 2: Proteasome subunit beta



- 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.

All (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
1:D:151:PRO:HG2	1:D:152:HIS:HD2	1.53	0.70
2:J:46:ALA:HB1	4:J:302:CIT:H42	1.73	0.70
1:D:87:TYR:O	2:K:57:ARG:NH2	2.25	0.70
2:W:46:ALA:HB1	4:W:303:CIT:H42	1.75	0.69
2:N:46:ALA:HB1	4:N:302:CIT:H21	1.73	0.69
1:T:219:ARG:NH1	2:a:64:GLU:OE2	2.26	0.69
2:Z:46:ALA:HB1	4:Z:302:CIT:H42	1.73	0.69
2:b:92:ALA:HA	2:b:95:MET:HE2	1.73	0.69
1:T:16:ARG:NH2	1:T:114:GLN:O	2.27	0.68
2:Z:209:ARG:NH1	2:Z:212:GLU:OE2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ARG:NH2	1:D:114:GLN:O	2.26	0.67
1:D:203:LEU:HG	1:D:208:LEU:HD21	1.77	0.67
1:C:210:VAL:HG11	1:C:230:LEU:HD13	1.76	0.66
1:E:30:VAL:HG13	1:E:43:ALA:HB2	1.77	0.66
1:C:30:VAL:HG13	1:C:43:ALA:HB2	1.76	0.66
1:R:33:LEU:HD11	1:R:180:ALA:HB1	1.77	0.66
1:S:9:MET:HE3	1:T:19:LEU:HD13	1.77	0.66
1:T:9:MET:HE1	1:U:116:LYS:HA	1.78	0.66
2:L:92:ALA:HA	2:L:95:MET:HE2	1.78	0.65
1:F:189:ARG:HG3	1:F:203:LEU:HD22	1.79	0.65
1:O:97:ARG:HD3	1:P:49:SER:HB2	1.78	0.65
1:C:87:TYR:O	2:J:57:ARG:NH2	2.29	0.65
2:Z:141:SER:HB3	4:Z:302:CIT:H21	1.78	0.65
1:E:13:MET:HE3	1:F:116:LYS:HB2	1.79	0.64
1:A:110:ILE:HG23	1:A:114:GLN:HG3	1.77	0.64
1:E:162:PRO:HG2	1:E:191:GLY:HA2	1.80	0.64
1:P:33:LEU:HD11	1:P:180:ALA:HB1	1.79	0.64
1:F:74:LEU:HD13	1:F:122:LEU:HD11	1.78	0.64
4:Y:302:CIT:O4	4:Y:302:CIT:O7	2.17	0.63
2:Y:141:SER:HB3	4:Y:302:CIT:H22	1.80	0.63
1:O:117:PRO:HD2	1:U:9:MET:HE2	1.80	0.63
1:T:210:VAL:HG21	1:T:230:LEU:HD13	1.81	0.62
1:D:189:ARG:HG3	1:D:203:LEU:HD22	1.81	0.62
1:U:56:LEU:HG	1:U:62:PHE:HB2	1.81	0.62
4:I:302:CIT:O2	4:I:302:CIT:O7	2.15	0.62
2:V:134:GLU:OE2	2:b:29:ARG:NH1	2.31	0.62
1:P:77:GLY:HA3	5:P:301:DMF:H13	1.81	0.61
1:S:33:LEU:HD11	1:S:180:ALA:HB1	1.81	0.61
2:X:46:ALA:HB1	4:X:303:CIT:H42	1.82	0.61
1:R:51:GLN:H	5:R:302:DMF:H12	1.65	0.61
2:V:165:ARG:HG3	2:V:213:LEU:HD22	1.83	0.61
1:C:31:VAL:HG12	1:C:155:VAL:HG12	1.83	0.61
1:E:165:ASN:HA	1:E:168:LYS:HD2	1.82	0.61
1:G:24:ILE:HD13	1:G:121:GLU:HG3	1.82	0.60
1:R:16:ARG:NH2	1:R:114:GLN:O	2.24	0.60
1:S:9:MET:N	1:T:15:GLU:OE2	2.34	0.60
2:L:12:VAL:HG12	2:L:197:ILE:HB	1.84	0.60
1:Q:110:ILE:HA	1:Q:114:GLN:HG3	1.83	0.60
1:D:97:ARG:HD3	1:E:49:SER:HB3	1.83	0.60
1:G:128:ALA:HB2	1:G:134:LYS:HB3	1.84	0.60
2:Y:25:MET:HE1	2:Z:144:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:42:VAL:HG23	1:T:210:VAL:HG12	1.85	0.59
2:K:5:ALA:HB1	2:K:120:ILE:HD12	1.84	0.59
1:A:87:TYR:O	2:H:57:ARG:NH2	2.30	0.59
2:a:20:SER:HB3	2:a:31:VAL:HG21	1.83	0.59
1:D:53:ILE:O	1:D:224:ARG:NH2	2.36	0.58
1:C:182:ARG:NH2	1:C:236:ASP:O	2.36	0.58
2:b:7:LYS:HE3	2:b:135:GLY:HA2	1.85	0.58
1:C:128:ALA:HB2	1:C:134:LYS:HB3	1.84	0.58
1:S:97:ARG:NH2	2:a:70:GLU:O	2.36	0.58
2:K:7:LYS:NZ	2:K:118:GLY:O	2.33	0.58
1:O:129:HIS:HB2	1:O:132:GLU:OE2	2.04	0.58
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	1.84	0.58
1:F:28:LYS:HD3	1:F:44:GLU:HG2	1.85	0.58
2:K:156:GLN:OE1	2:K:165:ARG:NH1	2.37	0.58
1:T:135:ARG:HD3	1:U:48:ARG:HH12	1.69	0.57
1:P:87:TYR:O	2:W:57:ARG:NH2	2.33	0.57
1:D:217:ARG:HH21	1:D:223:ARG:HH21	1.51	0.57
1:Q:140:ARG:HD3	1:Q:154:VAL:HG13	1.86	0.57
2:L:47:GLY:N	4:L:302:CIT:O6	2.36	0.56
1:E:163:ILE:HG13	1:E:191:GLY:HA3	1.88	0.55
1:A:53:ILE:HD12	1:A:209:GLU:HG2	1.87	0.55
1:G:76:ARG:NH2	2:N:70:GLU:OE2	2.38	0.55
1:O:214:ASP:OD2	1:O:223:ARG:NH2	2.39	0.55
1:Q:9:MET:HE3	1:R:16:ARG:HG2	1.88	0.55
1:Q:121:GLU:OE1	1:Q:140:ARG:NH2	2.39	0.55
2:b:38:ASP:OD2	2:b:79:LYS:NZ	2.37	0.55
1:S:137:GLU:HG2	1:T:48:ARG:HH21	1.72	0.55
1:D:128:ALA:HB2	1:D:134:LYS:HB3	1.87	0.55
1:B:31:VAL:HG12	1:B:155:VAL:HG22	1.89	0.55
1:F:212:VAL:HG13	1:F:223:ARG:HG3	1.89	0.55
2:N:47:GLY:HA2	4:N:302:CIT:H22	1.89	0.55
1:T:53:ILE:O	1:T:224:ARG:NH2	2.32	0.54
1:U:74:LEU:HD13	1:U:122:LEU:HD11	1.89	0.54
1:R:58:ASP:OD1	1:R:91:ARG:NH1	2.41	0.54
1:F:68:PHE:HA	1:F:71:PHE:CE2	2.43	0.54
1:U:59:ARG:HE	1:U:129:HIS:HA	1.72	0.54
1:A:33:LEU:HD11	1:A:180:ALA:HB1	1.89	0.54
1:T:205:VAL:HG11	1:T:231:GLN:HB2	1.90	0.54
1:E:56:LEU:HG	1:E:62:PHE:HB2	1.90	0.53
2:M:47:GLY:N	4:M:302:CIT:H41	2.24	0.53
1:S:92:ARG:HB2	2:a:75:THR:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:28:LYS:HB3	1:T:44:GLU:HB3	1.89	0.53
2:N:20:SER:HB3	2:N:28:GLY:HA3	1.90	0.53
1:U:68:PHE:HA	1:U:71:PHE:CE2	2.42	0.53
2:Y:13:VAL:HG22	2:Y:196:ILE:HG12	1.90	0.53
1:G:56:LEU:HG	1:G:62:PHE:HB2	1.90	0.52
1:G:68:PHE:HA	1:G:71:PHE:CE2	2.44	0.52
2:H:141:SER:HB3	4:H:302:CIT:H22	1.91	0.52
1:Q:205:VAL:HG22	1:Q:230:LEU:HG	1.90	0.52
1:A:128:ALA:HB2	1:A:134:LYS:HB3	1.91	0.52
1:S:217:ARG:HD2	1:S:223:ARG:HD3	1.92	0.52
1:F:30:VAL:HG13	1:F:43:ALA:HB2	1.90	0.52
1:Q:77:GLY:HA3	5:Q:301:DMF:H13	1.92	0.52
1:C:56:LEU:HG	1:C:62:PHE:HB2	1.91	0.52
2:M:165:ARG:HG3	2:M:213:LEU:HD22	1.91	0.52
1:C:155:VAL:HG21	1:C:164:ALA:HB2	1.92	0.52
1:D:33:LEU:HD11	1:D:180:ALA:HB1	1.90	0.52
1:U:178:THR:HB	1:U:233:LEU:HD12	1.91	0.52
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.91	0.52
1:E:33:LEU:HD21	1:E:184:ALA:HB2	1.92	0.52
2:b:3:ILE:HB	2:b:139:VAL:HG12	1.92	0.52
1:D:152:HIS:HD1	1:D:171:TYR:HE2	1.57	0.52
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.91	0.51
2:N:51:VAL:HG21	2:N:98:LEU:HB3	1.91	0.51
1:U:101:ASN:C	1:U:101:ASN:HD22	2.17	0.51
2:W:122:SER:HB3	2:W:137:GLN:HG2	1.92	0.51
1:P:151:PRO:HA	1:Q:48:ARG:HH22	1.74	0.51
2:X:24:ASN:OD1	2:X:24:ASN:N	2.38	0.51
1:F:162:PRO:HB2	1:F:191:GLY:HA2	1.93	0.51
2:I:153:LEU:O	2:I:156:GLN:HG2	2.11	0.51
1:A:116:LYS:HD2	1:G:13:MET:HE2	1.93	0.51
1:Q:205:VAL:HG21	1:Q:231:GLN:HG2	1.93	0.51
1:D:9:MET:N	1:E:15:GLU:OE1	2.44	0.51
1:D:163:ILE:HD13	1:D:188:LEU:HD23	1.93	0.50
1:T:11:GLN:HA	1:T:14:ARG:HB2	1.93	0.50
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.93	0.50
1:O:49:SER:HB2	1:U:97:ARG:HD3	1.93	0.50
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	1.94	0.50
1:S:68:PHE:HA	1:S:71:PHE:CE2	2.46	0.50
1:S:74:LEU:HD13	1:S:122:LEU:HD11	1.93	0.50
1:F:81:PHE:CZ	1:F:102:VAL:HG21	2.47	0.50
2:J:3:ILE:HB	2:J:139:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:230:LEU:O	1:T:234:LEU:HG	2.12	0.50
2:b:132:GLU:HG2	2:b:137:GLN:HG2	1.93	0.50
1:E:87:TYR:O	2:L:57:ARG:NH2	2.45	0.50
1:E:128:ALA:HB2	1:E:134:LYS:HB3	1.94	0.50
1:G:31:VAL:HG22	1:G:155:VAL:HG22	1.93	0.50
1:P:163:ILE:HD13	1:P:188:LEU:HD23	1.94	0.49
1:F:12:ALA:O	1:F:16:ARG:HG3	2.12	0.49
1:P:68:PHE:HA	1:P:71:PHE:CE2	2.48	0.49
1:C:85:ARG:HD3	1:C:89:TYR:CD2	2.47	0.49
1:D:225:ILE:HG22	1:D:230:LEU:HB2	1.93	0.49
2:Z:161:ASP:CG	2:Z:209:ARG:HH21	2.19	0.49
1:D:110:ILE:HA	1:D:114:GLN:HG3	1.93	0.49
1:O:220:ARG:HH22	2:V:67:GLU:CD	2.20	0.49
1:C:74:LEU:HD13	1:C:122:LEU:HD11	1.93	0.49
2:V:47:GLY:HA2	4:V:302:CIT:H22	1.94	0.49
1:G:186:ALA:O	1:G:189:ARG:HG2	2.13	0.49
2:b:88:ARG:NH2	6:b:401:HOH:O	2.44	0.49
1:F:56:LEU:HG	1:F:62:PHE:HB2	1.95	0.49
1:T:56:LEU:HG	1:T:62:PHE:HB2	1.95	0.49
1:A:98:GLN:O	1:A:102:VAL:HG23	2.12	0.49
1:B:118:TYR:HB3	1:B:120:VAL:HG22	1.93	0.49
2:H:176:ASP:O	2:Y:29:ARG:NH2	2.45	0.49
1:A:121:GLU:OE2	1:A:140:ARG:NH2	2.46	0.49
2:K:6:LEU:HB3	2:K:13:VAL:HG13	1.94	0.49
2:K:43:THR:HG22	2:K:104:LEU:HD12	1.95	0.49
2:W:153:LEU:O	2:W:156:GLN:HG2	2.14	0.48
2:L:22:GLN:HG2	3:L:301:U5Y:O01	2.12	0.48
1:P:9:MET:HE2	1:Q:19:LEU:HD13	1.95	0.48
1:P:56:LEU:HG	1:P:62:PHE:HB2	1.95	0.48
1:B:18:GLU:O	1:B:22:LYS:HB2	2.13	0.48
1:C:68:PHE:HA	1:C:71:PHE:CE2	2.48	0.48
1:D:10:GLU:HG2	1:E:19:LEU:HD13	1.94	0.48
1:S:110:ILE:HG23	1:S:114:GLN:HG3	1.95	0.48
1:T:68:PHE:HA	1:T:71:PHE:CE2	2.48	0.48
2:W:108:ASP:HB3	2:W:111:ALA:HB2	1.95	0.48
2:b:165:ARG:HG3	2:b:213:LEU:HD22	1.93	0.48
1:D:150:GLU:HG2	1:D:153:PHE:O	2.13	0.48
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.49	0.48
1:Q:25:ALA:O	1:Q:158:GLY:HA2	2.14	0.48
2:Z:141:SER:H	4:Z:302:CIT:HO7	1.60	0.48
1:E:16:ARG:NH2	1:E:114:GLN:O	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:150:GLU:HG2	1:R:153:PHE:O	2.14	0.48
2:M:51:VAL:HG12	2:M:100:ALA:HB2	1.96	0.48
1:O:16:ARG:NH1	1:O:114:GLN:O	2.24	0.48
1:Q:159:THR:HG22	1:Q:162:PRO:HD2	1.96	0.48
1:S:56:LEU:HG	1:S:62:PHE:HB2	1.94	0.48
2:b:32:ARG:HG2	2:b:193:THR:HG21	1.95	0.48
2:L:51:VAL:HG21	2:L:98:LEU:HB3	1.95	0.48
1:U:121:GLU:OE2	1:U:140:ARG:NH1	2.47	0.48
1:D:56:LEU:HG	1:D:62:PHE:HB2	1.96	0.47
2:V:46:ALA:HB1	4:V:302:CIT:H21	1.94	0.47
1:E:68:PHE:HA	1:E:71:PHE:CZ	2.49	0.47
2:M:20:SER:HB3	2:M:31:VAL:HG21	1.96	0.47
2:b:51:VAL:HG21	2:b:98:LEU:HB3	1.96	0.47
1:D:217:ARG:NH2	1:D:223:ARG:HD3	2.29	0.47
1:E:42:VAL:HG23	1:E:210:VAL:HG22	1.96	0.47
1:G:11:GLN:HA	1:G:14:ARG:HD2	1.95	0.47
2:H:46:ALA:HB1	4:H:302:CIT:H42	1.97	0.47
1:E:59:ARG:HE	1:E:129:HIS:HA	1.80	0.47
1:G:167:LEU:HD23	1:G:183:ILE:HG22	1.97	0.47
2:H:122:SER:HB3	2:H:137:GLN:HG2	1.96	0.47
2:L:10:GLY:HA2	2:L:114:PRO:O	2.14	0.47
1:S:163:ILE:HG23	1:S:187:ALA:HB1	1.97	0.47
1:U:81:PHE:CZ	1:U:102:VAL:HG21	2.50	0.47
1:E:101:ASN:OD1	1:F:76:ARG:NH2	2.40	0.47
1:Q:83:ASP:OD2	2:X:65:HIS:ND1	2.29	0.47
2:W:215:ARG:NH1	6:W:403:HOH:O	2.48	0.47
2:Z:101:LEU:HD23	2:Z:101:LEU:HA	1.81	0.47
2:a:141:SER:CB	4:a:302:CIT:H41	2.40	0.47
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.97	0.46
1:P:92:ARG:HB3	2:X:75:THR:HG21	1.96	0.46
1:R:9:MET:HE3	1:S:16:ARG:HG2	1.96	0.46
1:E:39:VAL:HG23	1:E:136:PRO:HB3	1.98	0.46
1:O:74:LEU:HD13	1:O:122:LEU:HD11	1.97	0.46
1:Q:210:VAL:HG11	1:Q:230:LEU:HD13	1.97	0.46
2:V:149:SER:OG	2:V:173:ASP:OD2	2.31	0.46
1:T:25:ALA:O	1:T:158:GLY:HA2	2.15	0.46
2:K:88:ARG:NH1	6:K:401:HOH:O	2.35	0.46
1:U:42:VAL:HG13	1:U:210:VAL:HG22	1.97	0.46
1:C:205:VAL:HG21	1:C:231:GLN:HG2	1.97	0.46
1:G:217:ARG:NH1	1:G:223:ARG:HB2	2.31	0.46
2:b:22:GLN:HG2	3:b:301:U5Y:O01	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:122:SER:HB3	2:M:137:GLN:HG2	1.97	0.46
1:D:11:GLN:H	1:D:11:GLN:CD	2.24	0.46
1:T:99:LEU:HA	1:T:102:VAL:HG12	1.98	0.46
2:W:22:GLN:HG2	3:W:302:U5Y:O01	2.16	0.46
2:b:101:LEU:HD23	2:b:101:LEU:HA	1.81	0.46
1:Q:150:GLU:HG3	1:Q:154:VAL:HG22	1.98	0.46
2:V:37:THR:OG1	2:V:43:THR:HG23	2.16	0.46
2:Z:161:ASP:OD2	2:Z:209:ARG:NH2	2.42	0.46
1:B:74:LEU:HD13	1:B:122:LEU:HD11	1.97	0.45
2:H:51:VAL:HG21	2:H:98:LEU:HB3	1.98	0.45
1:C:41:PHE:HB3	1:C:53:ILE:HG12	1.97	0.45
1:A:68:PHE:HA	1:A:71:PHE:CE2	2.52	0.45
2:I:51:VAL:HG21	2:I:98:LEU:HB3	1.98	0.45
1:O:59:ARG:NE	1:O:129:HIS:HA	2.32	0.45
1:P:110:ILE:HA	1:P:114:GLN:HG3	1.99	0.45
2:V:51:VAL:HG12	2:V:100:ALA:HB2	1.98	0.45
1:D:76:ARG:HD3	6:D:301:HOH:O	2.16	0.45
1:B:22:LYS:O	1:B:26:ARG:HG3	2.15	0.45
1:O:56:LEU:HG	1:O:62:PHE:HB2	1.99	0.45
2:Y:88:ARG:NH1	6:Y:406:HOH:O	2.49	0.45
2:Z:132:GLU:CD	2:Z:137:GLN:HE21	2.24	0.45
1:F:51:GLN:HG2	1:F:224:ARG:NH2	2.32	0.45
2:X:66:TYR:CZ	2:X:70:GLU:HG3	2.52	0.45
1:C:99:LEU:HA	1:C:102:VAL:HG12	1.99	0.44
1:R:31:VAL:HG21	1:R:184:ALA:HB1	1.99	0.44
1:E:107:LEU:HD11	1:E:122:LEU:HD13	1.99	0.44
1:E:175:ALA:HB1	1:E:179:ASP:HB3	1.99	0.44
2:b:165:ARG:HA	2:b:213:LEU:HD13	1.99	0.44
1:A:70:GLU:OE2	1:A:116:LYS:NZ	2.50	0.44
1:P:152:HIS:NE2	1:P:173:GLU:OE2	2.49	0.44
2:V:123:PHE:HA	2:V:128:GLY:O	2.17	0.44
1:E:16:ARG:NH1	1:E:111:PHE:O	2.51	0.44
2:K:20:SER:HB3	2:K:31:VAL:HG21	2.00	0.44
1:R:68:PHE:HA	1:R:71:PHE:CZ	2.53	0.44
1:S:89:TYR:CD1	2:a:82:ARG:HD3	2.53	0.44
2:Z:20:SER:HB3	2:Z:31:VAL:HG21	1.99	0.44
2:V:122:SER:HB3	2:V:137:GLN:HG2	2.00	0.44
2:Y:51:VAL:HG12	2:Y:100:ALA:HB2	2.00	0.44
1:C:118:TYR:HB3	1:C:120:VAL:HG22	2.00	0.43
1:D:214:ASP:HB3	1:D:217:ARG:HG2	2.00	0.43
2:L:51:VAL:HG12	2:L:100:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:225:ILE:HG21	1:R:233:LEU:HD12	1.99	0.43
2:a:51:VAL:HG12	2:a:100:ALA:HB2	1.99	0.43
1:C:182:ARG:HA	1:C:185:VAL:HG22	2.01	0.43
2:V:156:GLN:OE1	2:V:165:ARG:NH2	2.44	0.43
1:E:217:ARG:HH22	1:E:223:ARG:HB2	1.82	0.43
2:J:20:SER:HB3	2:J:31:VAL:HG21	2.00	0.43
1:P:121:GLU:OE2	1:P:140:ARG:NH1	2.52	0.43
1:T:89:TYR:CD1	2:b:82:ARG:HD3	2.54	0.43
2:I:145:PHE:HZ	2:X:25:MET:HE3	1.83	0.43
2:L:122:SER:HB3	2:L:137:GLN:HG2	2.01	0.43
2:X:112:SER:O	2:X:114:PRO:HD3	2.19	0.43
2:Z:47:GLY:N	4:Z:302:CIT:H41	2.33	0.43
1:G:231:GLN:O	1:G:235:VAL:HG22	2.18	0.43
2:Z:88:ARG:HD3	2:Z:126:ALA:O	2.18	0.43
2:a:153:LEU:O	2:a:156:GLN:HG2	2.18	0.43
1:E:22:LYS:O	1:E:26:ARG:HG2	2.18	0.43
2:I:25:MET:HE1	2:J:144:LEU:HD21	2.01	0.43
2:K:3:ILE:HB	2:K:139:VAL:HG12	1.99	0.43
2:Y:113:ASP:OD1	2:Y:113:ASP:N	2.45	0.43
2:a:3:ILE:HG21	2:a:44:GLY:HA3	2.01	0.43
1:A:205:VAL:HG13	1:A:230:LEU:HD23	2.01	0.43
2:K:173:ASP:OD2	2:W:152:LYS:NZ	2.48	0.43
2:M:101:LEU:HD23	2:M:101:LEU:HA	1.85	0.43
1:T:13:MET:HE2	1:U:116:LYS:HD3	2.01	0.43
2:N:64:GLU:HG2	2:N:68:LYS:HE2	2.01	0.43
1:U:24:ILE:HD13	1:U:121:GLU:HG3	2.01	0.43
1:A:225:ILE:HG21	1:A:233:LEU:HD12	2.01	0.42
1:C:140:ARG:HD3	1:C:154:VAL:HG13	2.01	0.42
2:Y:113:ASP:HA	2:Y:114:PRO:HD3	1.94	0.42
2:a:19:ARG:O	2:a:33:LYS:NZ	2.52	0.42
2:I:51:VAL:HG12	2:I:100:ALA:HB2	2.01	0.42
2:K:164:LEU:O	2:K:168:VAL:HG23	2.18	0.42
2:N:51:VAL:HG12	2:N:100:ALA:HB2	2.01	0.42
1:R:116:LYS:NZ	1:R:119:GLU:OE2	2.45	0.42
2:M:47:GLY:HA2	4:M:302:CIT:H41	2.01	0.42
2:a:150:MET:HG3	2:a:170:ALA:HB2	2.01	0.42
1:D:68:PHE:HA	1:D:71:PHE:CZ	2.54	0.42
1:D:110:ILE:HG23	1:D:114:GLN:HG3	2.01	0.42
1:D:101:ASN:OD1	1:E:76:ARG:NH2	2.48	0.42
2:Z:215:ARG:O	2:Z:219:GLU:HG2	2.19	0.42
1:D:74:LEU:HD13	1:D:122:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:ALA:HA	1:G:40:LEU:O	2.20	0.42
2:L:3:ILE:HB	2:L:139:VAL:HG12	2.02	0.42
2:L:161:ASP:OD2	2:L:209:ARG:NH1	2.48	0.42
1:U:98:GLN:O	1:U:102:VAL:HG23	2.20	0.42
2:V:3:ILE:HB	2:V:139:VAL:HG12	2.02	0.42
2:b:149:SER:OG	2:b:173:ASP:OD2	2.35	0.42
1:D:155:VAL:HG21	1:D:164:ALA:HB2	2.02	0.42
1:R:150:GLU:HA	1:R:151:PRO:HD3	1.86	0.42
1:S:30:VAL:HG13	1:S:43:ALA:HB2	2.01	0.42
1:U:45:ASN:ND2	1:U:50:LEU:O	2.44	0.42
2:W:51:VAL:HG21	2:W:98:LEU:HB3	2.01	0.42
2:Y:88:ARG:HD3	2:Y:126:ALA:O	2.20	0.42
1:D:177:LEU:HG	1:D:233:LEU:HD21	2.02	0.42
1:E:135:ARG:HG3	1:E:136:PRO:HD2	2.02	0.42
1:E:162:PRO:HG2	1:E:191:GLY:CA	2.49	0.42
1:F:165:ASN:HA	1:F:168:LYS:HD2	2.01	0.42
2:J:51:VAL:HG12	2:J:100:ALA:HB2	2.00	0.42
1:S:225:ILE:HG21	1:S:233:LEU:HD12	2.02	0.42
1:B:137:GLU:HG2	1:C:48:ARG:HH21	1.84	0.41
1:F:55:GLU:HB2	1:F:222:PHE:CG	2.55	0.41
2:J:161:ASP:OD2	2:J:209:ARG:NH2	2.37	0.41
1:R:38:GLY:HA2	5:R:301:DMF:H22	2.02	0.41
2:Z:217:ILE:O	2:Z:221:ARG:HG3	2.20	0.41
1:A:81:PHE:CZ	1:A:102:VAL:HG21	2.55	0.41
1:D:83:ASP:OD1	2:K:68:LYS:NZ	2.38	0.41
1:Q:10:GLU:HG2	1:R:19:LEU:HB2	2.02	0.41
1:T:150:GLU:HG2	1:T:153:PHE:O	2.21	0.41
2:N:222:SER:HB3	2:Z:187:VAL:HG13	2.03	0.41
1:O:128:ALA:HB2	1:O:134:LYS:HB3	2.02	0.41
1:R:51:GLN:N	5:R:302:DMF:H12	2.31	0.41
1:S:150:GLU:HA	1:S:151:PRO:HD3	1.89	0.41
2:b:19:ARG:O	2:b:33:LYS:NZ	2.54	0.41
1:S:230:LEU:HG	1:S:234:LEU:HD13	2.03	0.41
1:F:51:GLN:HG2	1:F:224:ARG:CZ	2.51	0.41
1:Q:225:ILE:HG21	1:Q:233:LEU:HD12	2.01	0.41
1:R:56:LEU:HG	1:R:62:PHE:HB2	2.02	0.41
1:S:236:ASP:OD1	1:S:236:ASP:N	2.53	0.41
2:V:20:SER:HB3	2:V:31:VAL:HG21	2.01	0.41
1:C:210:VAL:HG13	1:C:225:ILE:HB	2.03	0.41
1:Q:118:TYR:HB3	1:Q:120:VAL:HG22	2.03	0.41
1:S:18:GLU:OE1	1:S:22:LYS:NZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:85:ILE:HG12	2:b:88:ARG:NH1	2.36	0.41
1:C:30:VAL:HG22	1:C:43:ALA:HB1	2.02	0.41
1:E:9:MET:HE3	1:F:16:ARG:HG2	2.02	0.41
2:H:29:ARG:O	2:H:190:ILE:HG21	2.21	0.41
2:H:211:ALA:O	2:H:215:ARG:HG3	2.21	0.41
2:J:88:ARG:HD3	2:J:126:ALA:O	2.21	0.41
2:K:14:MET:HE3	2:K:105:ALA:HB2	2.03	0.41
2:L:38:ASP:HB3	2:L:41:THR:OG1	2.20	0.41
1:R:30:VAL:HG13	1:R:43:ALA:HB2	2.02	0.41
1:S:156:MET:HE3	1:S:156:MET:HB2	1.88	0.41
1:T:128:ALA:HB2	1:T:134:LYS:HB3	2.03	0.41
2:Y:101:LEU:HD23	2:Y:101:LEU:HA	1.87	0.41
2:Z:122:SER:HB3	2:Z:137:GLN:HG2	2.02	0.41
1:D:185:VAL:HG13	1:D:203:LEU:HD23	2.03	0.41
1:G:89:TYR:CD1	2:H:82:ARG:HD3	2.56	0.41
1:S:137:GLU:HA	1:T:48:ARG:NH2	2.36	0.41
1:C:68:PHE:HA	1:C:71:PHE:CZ	2.56	0.40
1:D:151:PRO:HG2	1:D:152:HIS:CD2	2.44	0.40
1:D:179:ASP:O	1:D:183:ILE:HG13	2.21	0.40
1:E:163:ILE:CG1	1:E:191:GLY:HA3	2.51	0.40
1:G:72:ASP:O	1:G:76:ARG:HG3	2.21	0.40
1:Q:81:PHE:CZ	1:Q:102:VAL:HG21	2.56	0.40
1:T:181:LEU:HD21	1:T:234:LEU:HD23	2.02	0.40
1:D:181:LEU:HD22	1:D:233:LEU:HD23	2.03	0.40
2:Z:86:MET:HB2	2:Z:86:MET:HE3	1.86	0.40
2:I:3:ILE:HB	2:I:139:VAL:HG12	2.04	0.40
2:L:20:SER:HB3	2:L:31:VAL:HG21	2.02	0.40
1:S:181:LEU:HD21	1:S:234:LEU:HD12	2.03	0.40
2:W:18:ARG:HD3	2:W:193:THR:HG23	2.03	0.40
1:G:107:LEU:HD23	1:G:107:LEU:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	B	159	THR
1	C	121	GLU
1	C	224	ARG
1	D	26	ARG
1	D	208	LEU
1	E	31	VAL
1	E	212	VAL
1	F	133	THR
1	F	169	GLU
1	F	205	VAL
1	F	212	VAL
1	F	233	LEU
1	G	22	LYS
1	G	48	ARG
2	H	13	VAL
2	H	30	ASP
2	H	45	ILE
2	I	13	VAL
2	J	37	THR
2	J	133	GLU
2	K	13	VAL
2	K	122	SER
2	M	22	GLN
2	N	21	THR
2	N	115	GLN
1	O	11	GLN
1	O	173	GLU

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Mol	Chain	Res	Type
1	O	233	LEU
1	P	99	LEU
1	P	233	LEU
1	Q	33	LEU
1	Q	155	VAL
1	Q	210	VAL
1	T	30	VAL
1	T	133	THR
1	T	160	THR
1	T	203	LEU
1	T	208	LEU
1	U	233	LEU
2	V	109	ILE
2	X	24	ASN
2	b	13	VAL
2	b	133	GLU
2	b	215	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	B	129	HIS
1	B	231	GLN
1	E	80	GLN
1	G	105	GLN
1	G	114	GLN
2	H	22	GLN
2	H	130	ASN
2	M	81	ASN
2	M	110	HIS
2	N	115	GLN
1	O	105	GLN
1	P	98	GLN
1	P	105	GLN
1	P	174	ASN
1	R	129	HIS
1	S	129	HIS
1	T	105	GLN
1	U	105	GLN
2	V	115	GLN
2	Y	22	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

All (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
3	V	301	U5Y	C08-N07	-9.31	1.33	1.47
3	a	301	U5Y	C08-N07	-9.26	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	U5Y	C08-N07	-9.24	1.33	1.47
3	L	301	U5Y	C08-N07	-9.19	1.33	1.47
3	Y	301	U5Y	C08-N07	-9.18	1.33	1.47
3	J	301	U5Y	C08-N07	-9.17	1.33	1.47
3	K	301	U5Y	C08-N07	-9.16	1.33	1.47
3	W	302	U5Y	C08-N07	-9.14	1.33	1.47
3	M	301	U5Y	C08-N07	-9.10	1.33	1.47
3	L	301	U5Y	C17-N07	8.61	1.64	1.47
3	X	302	U5Y	C17-N07	8.60	1.64	1.47
3	M	301	U5Y	C17-N07	8.57	1.64	1.47
3	W	302	U5Y	C17-N07	8.57	1.64	1.47
3	N	301	U5Y	C17-N07	8.56	1.64	1.47
3	H	301	U5Y	C17-N07	8.55	1.64	1.47
3	K	301	U5Y	C17-N07	8.53	1.64	1.47
3	Z	301	U5Y	C17-N07	8.51	1.64	1.47
3	J	301	U5Y	C17-N07	8.49	1.64	1.47
3	b	301	U5Y	C17-N07	8.49	1.64	1.47
3	I	301	U5Y	C17-N07	8.46	1.64	1.47
3	a	301	U5Y	C17-N07	8.40	1.63	1.47
3	V	301	U5Y	C17-N07	8.38	1.63	1.47
3	Y	301	U5Y	C17-N07	8.29	1.63	1.47
3	V	301	U5Y	C19-N20	5.99	1.46	1.34
3	N	301	U5Y	C19-N20	5.98	1.46	1.34
3	W	302	U5Y	C19-N20	5.95	1.46	1.34
3	a	301	U5Y	C19-N20	5.90	1.46	1.34
3	K	301	U5Y	C19-N20	5.88	1.46	1.34
3	Z	301	U5Y	C19-N20	5.82	1.46	1.34
3	Y	301	U5Y	C19-N20	5.78	1.46	1.34
3	I	301	U5Y	C19-N20	5.78	1.46	1.34
3	J	301	U5Y	C19-N20	5.75	1.46	1.34
3	L	301	U5Y	C19-N20	5.74	1.46	1.34
3	M	301	U5Y	C19-N20	5.67	1.46	1.34
3	b	301	U5Y	C19-N20	5.65	1.46	1.34
3	H	301	U5Y	C19-N20	5.60	1.46	1.34
3	X	302	U5Y	C19-N20	5.59	1.46	1.34
3	H	301	U5Y	C02-N03	5.38	1.45	1.34
3	N	301	U5Y	C02-N03	5.33	1.45	1.34
3	X	302	U5Y	C02-N03	5.30	1.45	1.34
3	K	301	U5Y	C02-N03	5.23	1.45	1.34
3	W	302	U5Y	C02-N03	5.21	1.45	1.34
3	L	301	U5Y	C02-N03	5.21	1.45	1.34
3	b	301	U5Y	C02-N03	5.19	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	301	U5Y	C02-N03	5.14	1.44	1.34
3	J	301	U5Y	C02-N03	5.10	1.44	1.34
3	Z	301	U5Y	C02-N03	5.08	1.44	1.34
3	Y	301	U5Y	C02-N03	5.07	1.44	1.34
3	a	301	U5Y	C02-N03	5.07	1.44	1.34
3	N	301	U5Y	C22-N23	5.05	1.45	1.33
3	V	301	U5Y	C02-N03	5.05	1.44	1.34
3	J	301	U5Y	C22-N23	5.05	1.45	1.33
3	M	301	U5Y	C22-N23	5.04	1.45	1.33
3	I	301	U5Y	C22-N23	5.03	1.45	1.33
3	Y	301	U5Y	C22-N23	5.01	1.45	1.33
3	M	301	U5Y	C02-N03	4.93	1.44	1.34
3	W	302	U5Y	C22-N23	4.93	1.45	1.33
3	L	301	U5Y	C22-N23	4.93	1.45	1.33
3	H	301	U5Y	C22-N23	4.92	1.45	1.33
3	V	301	U5Y	C22-N23	4.90	1.45	1.33
3	a	301	U5Y	C22-N23	4.88	1.45	1.33
3	Z	301	U5Y	C22-N23	4.88	1.45	1.33
3	X	302	U5Y	C22-N23	4.83	1.44	1.33
3	K	301	U5Y	C22-N23	4.73	1.44	1.33
3	b	301	U5Y	C22-N23	4.71	1.44	1.33
3	a	301	U5Y	C16-C17	-4.14	1.37	1.51
3	Z	301	U5Y	C16-C17	-4.12	1.37	1.51
3	W	302	U5Y	C16-C17	-4.10	1.37	1.51
3	M	301	U5Y	C16-C17	-4.09	1.37	1.51
3	K	301	U5Y	C16-C17	-4.09	1.37	1.51
3	L	301	U5Y	C16-C17	-4.08	1.37	1.51
3	b	301	U5Y	C16-C17	-4.06	1.37	1.51
3	N	301	U5Y	C16-C17	-4.06	1.37	1.51
3	H	301	U5Y	C16-C17	-4.04	1.38	1.51
3	J	301	U5Y	C16-C17	-4.01	1.38	1.51
3	Y	301	U5Y	C16-C17	-4.00	1.38	1.51
3	V	301	U5Y	C16-C17	-3.98	1.38	1.51
3	X	302	U5Y	C16-C17	-3.98	1.38	1.51
3	I	301	U5Y	C16-C17	-3.95	1.38	1.51
3	K	301	U5Y	C06-N07	3.78	1.46	1.35
3	a	301	U5Y	C06-N07	3.74	1.46	1.35
3	L	301	U5Y	C06-N07	3.72	1.46	1.35
3	M	301	U5Y	C06-N07	3.70	1.46	1.35
3	H	301	U5Y	C06-N07	3.67	1.45	1.35
3	X	302	U5Y	C06-N07	3.65	1.45	1.35
3	b	301	U5Y	C06-N07	3.64	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	301	U5Y	C06-N07	3.63	1.45	1.35
3	V	301	U5Y	C06-N07	3.62	1.45	1.35
3	W	302	U5Y	C06-N07	3.62	1.45	1.35
3	N	301	U5Y	C06-N07	3.61	1.45	1.35
3	I	301	U5Y	C06-N07	3.58	1.45	1.35
3	Z	301	U5Y	C06-N07	3.56	1.45	1.35
3	Y	301	U5Y	C06-N07	3.52	1.45	1.35
3	K	301	U5Y	C15-C08	2.81	1.61	1.54
3	a	301	U5Y	C15-C08	2.75	1.61	1.54
3	L	301	U5Y	O32-C22	-2.74	1.18	1.23
3	K	301	U5Y	O32-C22	-2.71	1.18	1.23
3	I	301	U5Y	C15-C08	2.69	1.61	1.54
3	b	301	U5Y	C15-C08	2.65	1.61	1.54
3	L	301	U5Y	C15-C08	2.65	1.61	1.54
3	M	301	U5Y	C15-C08	2.64	1.61	1.54
3	Z	301	U5Y	C15-C08	2.64	1.61	1.54
3	W	302	U5Y	C15-C08	2.61	1.60	1.54
3	J	301	U5Y	C15-C08	2.61	1.60	1.54
3	V	301	U5Y	C15-C08	2.59	1.60	1.54
3	Y	301	U5Y	C15-C08	2.59	1.60	1.54
3	X	302	U5Y	C15-C08	2.55	1.60	1.54
3	H	301	U5Y	C15-C08	2.53	1.60	1.54
3	N	301	U5Y	O32-C22	-2.51	1.18	1.23
3	N	301	U5Y	C15-C08	2.50	1.60	1.54
3	J	301	U5Y	O32-C22	-2.46	1.18	1.23
3	I	301	U5Y	O32-C22	-2.44	1.18	1.23
3	a	301	U5Y	O32-C22	-2.43	1.18	1.23
3	Y	301	U5Y	O32-C22	-2.41	1.18	1.23
3	W	302	U5Y	O32-C22	-2.41	1.18	1.23
3	X	302	U5Y	O32-C22	-2.40	1.18	1.23
3	M	301	U5Y	O32-C22	-2.40	1.18	1.23
3	b	301	U5Y	O32-C22	-2.38	1.18	1.23
3	M	301	U5Y	O33-C19	-2.35	1.18	1.23
3	Z	301	U5Y	O32-C22	-2.32	1.18	1.23
3	V	301	U5Y	O32-C22	-2.32	1.19	1.23
3	Y	301	U5Y	O33-C19	-2.30	1.19	1.23
3	W	302	U5Y	O33-C19	-2.29	1.19	1.23
3	V	301	U5Y	O33-C19	-2.26	1.19	1.23
3	I	301	U5Y	O33-C19	-2.23	1.19	1.23
3	X	302	U5Y	O33-C19	-2.23	1.19	1.23
3	J	301	U5Y	O33-C19	-2.21	1.19	1.23
3	L	301	U5Y	O33-C19	-2.20	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	301	U5Y	O33-C19	-2.19	1.19	1.23
3	H	301	U5Y	O32-C22	-2.18	1.19	1.23
3	a	301	U5Y	O01-C02	-2.18	1.18	1.23
3	Y	301	U5Y	O01-C02	-2.17	1.19	1.23
3	a	301	U5Y	O33-C19	-2.16	1.19	1.23
3	N	301	U5Y	O33-C19	-2.12	1.19	1.23
3	Z	301	U5Y	O18-C06	-2.11	1.18	1.23
3	H	301	U5Y	O33-C19	-2.10	1.19	1.23
3	J	301	U5Y	O01-C02	-2.08	1.19	1.23
3	M	301	U5Y	O01-C02	-2.08	1.19	1.23
3	b	301	U5Y	O01-C02	-2.06	1.19	1.23
3	K	301	U5Y	O01-C02	-2.06	1.19	1.23
3	b	301	U5Y	O33-C19	-2.06	1.19	1.23
3	Z	301	U5Y	O33-C19	-2.04	1.19	1.23
3	Y	301	U5Y	O18-C06	-2.03	1.18	1.23
3	L	301	U5Y	O01-C02	-2.03	1.19	1.23
3	H	301	U5Y	O01-C02	-2.03	1.19	1.23
3	X	302	U5Y	O01-C02	-2.01	1.19	1.23
3	I	301	U5Y	O01-C02	-2.00	1.19	1.23

All (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
4	J	302	CIT	O6-C6-C3	4.32	121.42	113.14
3	b	301	U5Y	C15-C08-N07	4.16	106.56	101.93
4	L	302	CIT	O6-C6-C3	4.11	121.02	113.14
4	K	302	CIT	O6-C6-C3	4.10	121.00	113.14
3	Y	301	U5Y	C15-C08-N07	4.02	106.41	101.93
3	I	301	U5Y	C15-C08-N07	3.99	106.37	101.93
3	N	301	U5Y	C15-C08-N07	3.93	106.30	101.93
4	W	303	CIT	O6-C6-C3	3.92	120.65	113.14
3	a	301	U5Y	C15-C08-N07	3.91	106.28	101.93
3	V	301	U5Y	C15-C08-N07	3.86	106.22	101.93
3	H	301	U5Y	C15-C08-N07	3.76	106.12	101.93
3	M	301	U5Y	C15-C08-N07	3.76	106.11	101.93
3	W	302	U5Y	C15-C08-N07	3.72	106.08	101.93
3	J	301	U5Y	C15-C08-N07	3.71	106.06	101.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	301	U5Y	C17-N07-C08	-3.60	107.83	111.88
3	X	302	U5Y	C25-C24-N23	-3.56	105.97	113.15
4	N	302	CIT	O6-C6-C3	3.53	119.90	113.14
4	Z	302	CIT	O6-C6-C3	3.49	119.83	113.14
4	Y	302	CIT	O6-C6-C3	3.42	119.71	113.14
4	H	302	CIT	O6-C6-C3	3.40	119.67	113.14
3	K	301	U5Y	C17-N07-C08	-3.39	108.06	111.88
3	X	302	U5Y	C15-C08-N07	3.39	105.71	101.93
3	L	301	U5Y	C16-C17-N07	3.35	109.00	103.24
3	J	301	U5Y	C40-O39-C38	-3.34	111.15	118.78
3	V	301	U5Y	C25-C24-N23	-3.31	106.48	113.15
3	W	302	U5Y	C43-C44-C21	-3.30	104.58	113.36
3	a	301	U5Y	C40-O39-C38	-3.25	111.36	118.78
4	I	302	CIT	O6-C6-C3	3.16	119.21	113.14
3	L	301	U5Y	C43-C44-C21	-3.09	105.13	113.36
4	X	303	CIT	O6-C6-C3	3.09	119.06	113.14
3	X	302	U5Y	C17-N07-C08	-3.07	108.43	111.88
4	b	302	CIT	O6-C6-C3	3.05	119.00	113.14
3	K	301	U5Y	C43-C44-C21	-3.05	105.25	113.36
3	V	301	U5Y	C40-O39-C38	-2.99	111.95	118.78
3	Z	301	U5Y	C17-N07-C08	-2.99	108.52	111.88
3	b	301	U5Y	C16-C17-N07	2.98	108.37	103.24
3	I	301	U5Y	C17-N07-C08	-2.97	108.53	111.88
3	I	301	U5Y	C40-O39-C38	-2.97	112.01	118.78
3	H	301	U5Y	C16-C17-N07	2.96	108.33	103.24
3	I	301	U5Y	C16-C17-N07	2.96	108.33	103.24
3	Y	301	U5Y	C43-C44-C21	-2.96	105.50	113.36
3	X	302	U5Y	C22-C21-N20	-2.95	103.12	111.11
3	M	301	U5Y	C16-C17-N07	2.95	108.31	103.24
3	H	301	U5Y	C17-N07-C08	-2.94	108.57	111.88
3	X	302	U5Y	C16-C17-N07	2.93	108.28	103.24
3	Y	301	U5Y	C16-C17-N07	2.93	108.27	103.24
3	N	301	U5Y	C40-O39-C38	-2.92	112.10	118.78
3	Z	301	U5Y	C16-C17-N07	2.92	108.27	103.24
3	J	301	U5Y	C17-N07-C08	-2.92	108.59	111.88
3	H	301	U5Y	C40-O39-C38	-2.90	112.16	118.78
4	V	302	CIT	O6-C6-C3	2.90	118.69	113.14
3	N	301	U5Y	C17-N07-C08	-2.88	108.64	111.88
3	K	301	U5Y	C40-O39-C38	-2.87	112.21	118.78
3	N	301	U5Y	C43-C44-C21	-2.87	105.73	113.36
3	M	301	U5Y	C17-N07-C08	-2.84	108.68	111.88
3	K	301	U5Y	C15-C08-C09	-2.84	108.02	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	301	U5Y	C16-C17-N07	2.83	108.11	103.24
3	H	301	U5Y	C25-C24-N23	-2.83	107.45	113.15
3	b	301	U5Y	C25-C24-N23	-2.80	107.51	113.15
3	W	302	U5Y	C15-C08-C09	-2.79	108.11	113.69
3	W	302	U5Y	C22-C21-N20	-2.79	103.56	111.11
3	Y	301	U5Y	C40-O39-C38	-2.79	112.42	118.78
3	W	302	U5Y	C16-C17-N07	2.76	107.99	103.24
3	L	301	U5Y	C25-C24-N23	-2.76	107.58	113.15
3	Y	301	U5Y	C17-N07-C08	-2.75	108.79	111.88
3	M	301	U5Y	C43-C44-C21	-2.74	106.06	113.36
3	b	301	U5Y	C24-N23-C22	-2.74	118.52	122.29
3	V	301	U5Y	C43-C44-C21	-2.74	106.08	113.36
3	Z	301	U5Y	C40-O39-C38	-2.73	112.54	118.78
4	a	302	CIT	C2-C3-C6	2.73	116.07	110.03
3	L	301	U5Y	C15-C08-C09	-2.71	108.27	113.69
3	J	301	U5Y	O01-C02-N03	-2.71	118.37	122.95
3	L	301	U5Y	C17-N07-C08	-2.69	108.86	111.88
3	N	301	U5Y	C16-C17-N07	2.68	107.85	103.24
3	V	301	U5Y	C15-C08-C09	-2.68	108.34	113.69
3	W	302	U5Y	C17-N07-C08	-2.64	108.91	111.88
3	Z	301	U5Y	C25-C24-N23	-2.64	107.82	113.15
3	J	301	U5Y	C16-C17-N07	2.64	107.78	103.24
3	b	301	U5Y	C22-C21-N20	-2.63	103.99	111.11
3	V	301	U5Y	C17-N07-C08	-2.62	108.93	111.88
3	W	302	U5Y	C40-O39-C38	-2.61	112.81	118.78
3	Y	301	U5Y	C15-C08-C09	-2.61	108.48	113.69
3	N	301	U5Y	C15-C08-C09	-2.59	108.52	113.69
3	Y	301	U5Y	O01-C02-N03	-2.58	118.58	122.95
4	H	302	CIT	O4-C5-C4	2.58	122.53	114.35
3	X	302	U5Y	C15-C08-C09	-2.56	108.57	113.69
3	K	301	U5Y	C16-C17-N07	2.55	107.62	103.24
3	V	301	U5Y	C04-C05-C06	2.55	117.31	112.22
3	V	301	U5Y	C05-C04-N03	-2.54	105.79	110.64
3	L	301	U5Y	C04-C05-C06	2.54	117.30	112.22
3	M	301	U5Y	O01-C02-N03	-2.54	118.65	122.95
3	I	301	U5Y	C43-C44-C21	-2.53	106.62	113.36
3	J	301	U5Y	C15-C08-C09	-2.53	108.64	113.69
4	X	303	CIT	O4-C5-C4	2.52	122.34	114.35
3	a	301	U5Y	C25-C24-N23	-2.52	108.08	113.15
3	Z	301	U5Y	C05-C04-N03	-2.50	105.86	110.64
3	I	301	U5Y	C22-C21-N20	-2.49	104.38	111.11
3	Z	301	U5Y	C04-C05-C06	2.47	117.15	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	302	CIT	C4-C3-C2	2.45	115.61	109.31
4	N	302	CIT	O2-C1-C2	2.45	122.10	114.35
3	a	301	U5Y	C05-C04-N03	-2.44	105.98	110.64
3	a	301	U5Y	O01-C02-N03	-2.44	118.82	122.95
3	b	301	U5Y	C17-N07-C08	-2.43	109.14	111.88
3	N	301	U5Y	C25-C24-N23	-2.43	108.25	113.15
3	b	301	U5Y	O01-C02-N03	-2.43	118.84	122.95
3	W	302	U5Y	C25-C24-N23	-2.42	108.26	113.15
3	J	301	U5Y	C04-C05-C06	2.42	117.06	112.22
3	Z	301	U5Y	C15-C08-C09	-2.41	108.87	113.69
3	N	301	U5Y	C22-C21-N20	-2.41	104.60	111.11
3	K	301	U5Y	C05-C04-N03	-2.39	106.08	110.64
4	b	302	CIT	O2-C1-C2	2.39	121.91	114.35
3	K	301	U5Y	C04-C05-C06	2.37	116.96	112.22
3	Y	301	U5Y	C05-C04-N03	-2.37	106.11	110.64
3	H	301	U5Y	C15-C08-C09	-2.37	108.96	113.69
3	H	301	U5Y	C05-C04-N03	-2.36	106.12	110.64
3	Y	301	U5Y	C25-C24-N23	-2.36	108.39	113.15
4	a	302	CIT	O7-C3-C2	-2.36	104.00	109.38
3	H	301	U5Y	C22-C21-N20	-2.36	104.73	111.11
3	X	302	U5Y	C43-C44-C21	-2.34	107.13	113.36
3	L	301	U5Y	C40-O39-C38	-2.33	113.45	118.78
3	I	301	U5Y	C25-C24-N23	-2.32	108.47	113.15
3	I	301	U5Y	O01-C02-N03	-2.31	119.03	122.95
4	L	302	CIT	O2-C1-C2	2.31	121.67	114.35
3	I	301	U5Y	C05-C04-N03	-2.31	106.23	110.64
3	J	301	U5Y	C43-C44-C21	-2.30	107.25	113.36
3	Y	301	U5Y	C22-C21-N20	-2.29	104.91	111.11
4	Y	302	CIT	O2-C1-C2	2.29	121.59	114.35
3	L	301	U5Y	C22-C21-N20	-2.28	104.95	111.11
3	b	301	U5Y	C34-C02-N03	2.27	119.87	115.86
3	V	301	U5Y	C22-C21-N20	-2.27	104.97	111.11
3	b	301	U5Y	C15-C08-C09	-2.27	109.16	113.69
4	V	302	CIT	O2-C1-C2	2.26	121.52	114.35
3	J	301	U5Y	C25-C24-N23	-2.26	108.59	113.15
3	b	301	U5Y	C31-C25-C26	2.26	120.50	116.62
4	H	302	CIT	O4-C5-O3	-2.25	117.54	123.33
4	M	302	CIT	O4-C5-C4	2.25	121.48	114.35
3	Z	301	U5Y	O01-C02-N03	-2.25	119.14	122.95
4	W	303	CIT	O2-C1-C2	2.25	121.46	114.35
3	M	301	U5Y	C05-C04-N03	-2.24	106.36	110.64
3	L	301	U5Y	C05-C04-N03	-2.24	106.37	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	301	U5Y	C43-C44-C21	-2.24	107.40	113.36
3	K	301	U5Y	C25-C24-N23	-2.24	108.64	113.15
3	N	301	U5Y	C05-C04-N03	-2.23	106.39	110.64
4	J	302	CIT	O4-C5-O3	-2.22	117.61	123.33
3	W	302	U5Y	O01-C02-N03	-2.21	119.21	122.95
3	a	301	U5Y	C04-C05-C06	2.21	116.64	112.22
4	I	302	CIT	O2-C1-C2	2.21	121.33	114.35
3	H	301	U5Y	C05-C04-C19	-2.21	105.37	110.57
3	V	301	U5Y	O01-C02-N03	-2.20	119.22	122.95
3	M	301	U5Y	C22-C21-N20	-2.20	105.16	111.11
3	a	301	U5Y	C15-C08-C09	-2.19	109.31	113.69
3	X	302	U5Y	C34-C02-N03	2.18	119.71	115.86
3	N	301	U5Y	O01-C02-N03	-2.18	119.26	122.95
3	a	301	U5Y	C43-C44-C21	-2.18	107.56	113.36
3	K	301	U5Y	C08-N07-C06	2.17	127.27	120.83
3	N	301	U5Y	C04-C05-C06	2.17	116.55	112.22
3	H	301	U5Y	C43-C44-C21	-2.16	107.62	113.36
3	b	301	U5Y	C28-C26-C25	-2.15	119.78	123.60
3	V	301	U5Y	C31-C25-C26	2.13	120.29	116.62
3	K	301	U5Y	C31-C25-C26	2.13	120.28	116.62
4	Y	302	CIT	O4-C5-C4	2.13	121.09	114.35
3	N	301	U5Y	C34-C02-N03	2.11	119.58	115.86
4	K	302	CIT	O4-C5-O3	-2.11	117.92	123.33
3	M	301	U5Y	C15-C08-C09	-2.10	109.48	113.69
3	L	301	U5Y	O01-C02-N03	-2.10	119.39	122.95
3	Y	301	U5Y	C34-C02-N03	2.10	119.57	115.86
3	X	302	U5Y	O01-C02-N03	-2.09	119.41	122.95
3	J	301	U5Y	C31-C25-C26	2.09	120.21	116.62
4	K	302	CIT	O4-C5-C4	2.08	120.95	114.35
3	K	301	U5Y	C28-C26-C25	-2.08	119.91	123.60
4	b	302	CIT	C4-C3-C6	-2.08	105.44	110.03
4	X	303	CIT	O4-C5-O3	-2.08	117.99	123.33
3	X	302	U5Y	C31-C25-C26	2.07	120.18	116.62
3	J	301	U5Y	C34-C02-N03	2.07	119.51	115.86
4	J	302	CIT	C3-C2-C1	-2.07	108.26	113.92
4	X	303	CIT	C3-C2-C1	-2.07	108.27	113.92
3	K	301	U5Y	C24-N23-C22	-2.06	119.45	122.29
4	M	302	CIT	O6-C6-O5	-2.06	117.27	123.86
4	J	302	CIT	O2-C1-C2	2.06	120.87	114.35
4	H	302	CIT	C3-C2-C1	-2.06	108.30	113.92
3	H	301	U5Y	C31-C25-C26	2.04	120.13	116.62
3	a	301	U5Y	C31-C25-C26	2.03	120.11	116.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	302	CIT	O4-C5-C4	2.02	120.74	114.35
4	V	302	CIT	C4-C3-C6	-2.01	105.58	110.03
3	W	302	U5Y	C08-N07-C06	2.01	126.79	120.83
3	Y	301	U5Y	C31-C25-C26	2.01	120.07	116.62
3	b	301	U5Y	C40-O39-C38	-2.00	114.20	118.78
4	b	302	CIT	O2-C1-O1	-2.00	118.19	123.33

There are no chirality outliers.

All (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
4	I	302	CIT	C1-C2-C3-C6
4	I	302	CIT	C2-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
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-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	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

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Mol	Chain	Res	Type	Atoms
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
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	C2-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	I	302	CIT	C1-C2-C3-C4
4	I	302	CIT	O7-C3-C4-C5

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

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Mol	Chain	Res	Type	Atoms
3	M	301	U5Y	C02-C34-C35-C36
3	X	302	U5Y	C02-C34-C35-C36
4	J	302	CIT	C1-C2-C3-C4
4	K	302	CIT	C1-C2-C3-C4
4	W	303	CIT	O7-C3-C4-C5
4	W	303	CIT	C6-C3-C4-C5
3	L	301	U5Y	O01-C02-C34-C35
3	M	301	U5Y	O01-C02-C34-C35
4	V	302	CIT	C2-C3-C4-C5
4	a	302	CIT	C1-C2-C3-O7
4	b	302	CIT	C1-C2-C3-O7
3	Y	301	U5Y	O01-C02-C34-C35
3	a	301	U5Y	O01-C02-C34-C35
3	L	301	U5Y	N03-C02-C34-C35
3	M	301	U5Y	N03-C02-C34-C35
4	W	303	CIT	C1-C2-C3-O7
4	a	302	CIT	O7-C3-C4-C5
3	J	301	U5Y	C04-C05-C06-O18
3	W	302	U5Y	C04-C05-C06-O18
4	X	303	CIT	C3-C4-C5-O3
3	a	301	U5Y	N03-C02-C34-C35
3	H	301	U5Y	O01-C02-C34-C35
3	L	301	U5Y	C04-C05-C06-N07
3	N	301	U5Y	C04-C05-C06-N07
3	Z	301	U5Y	C04-C05-C06-N07
3	H	301	U5Y	N03-C02-C34-C35
3	Y	301	U5Y	N03-C02-C34-C35
4	X	303	CIT	C3-C4-C5-O4
3	I	301	U5Y	O01-C02-C34-C35
4	H	302	CIT	C3-C4-C5-O3
3	I	301	U5Y	N03-C02-C34-C35
4	H	302	CIT	C3-C4-C5-O4
3	X	302	U5Y	C34-C35-C36-C49
3	X	302	U5Y	C34-C35-C36-C37
3	K	301	U5Y	O01-C02-C34-C35
3	Z	301	U5Y	O01-C02-C34-C35

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

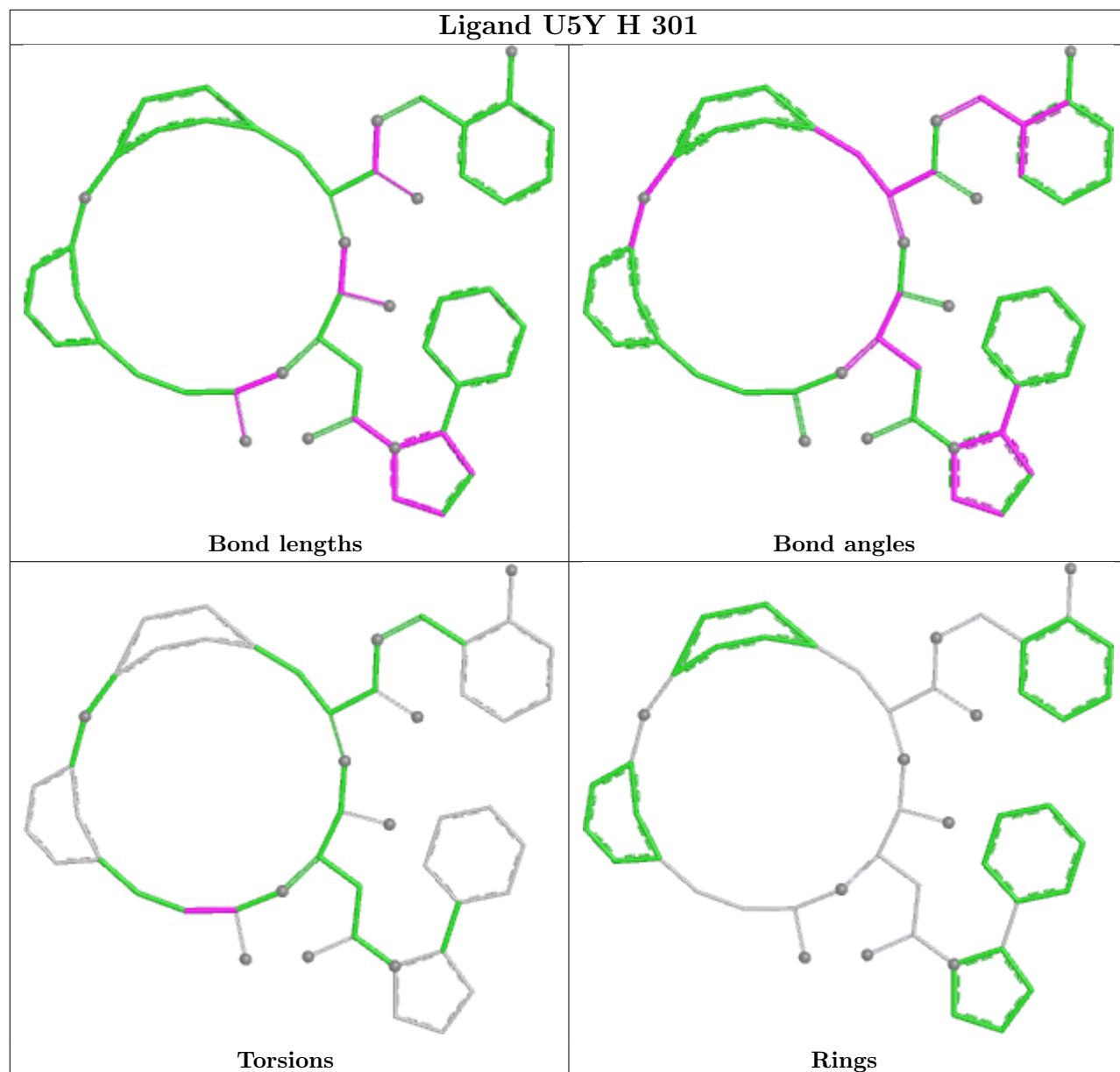
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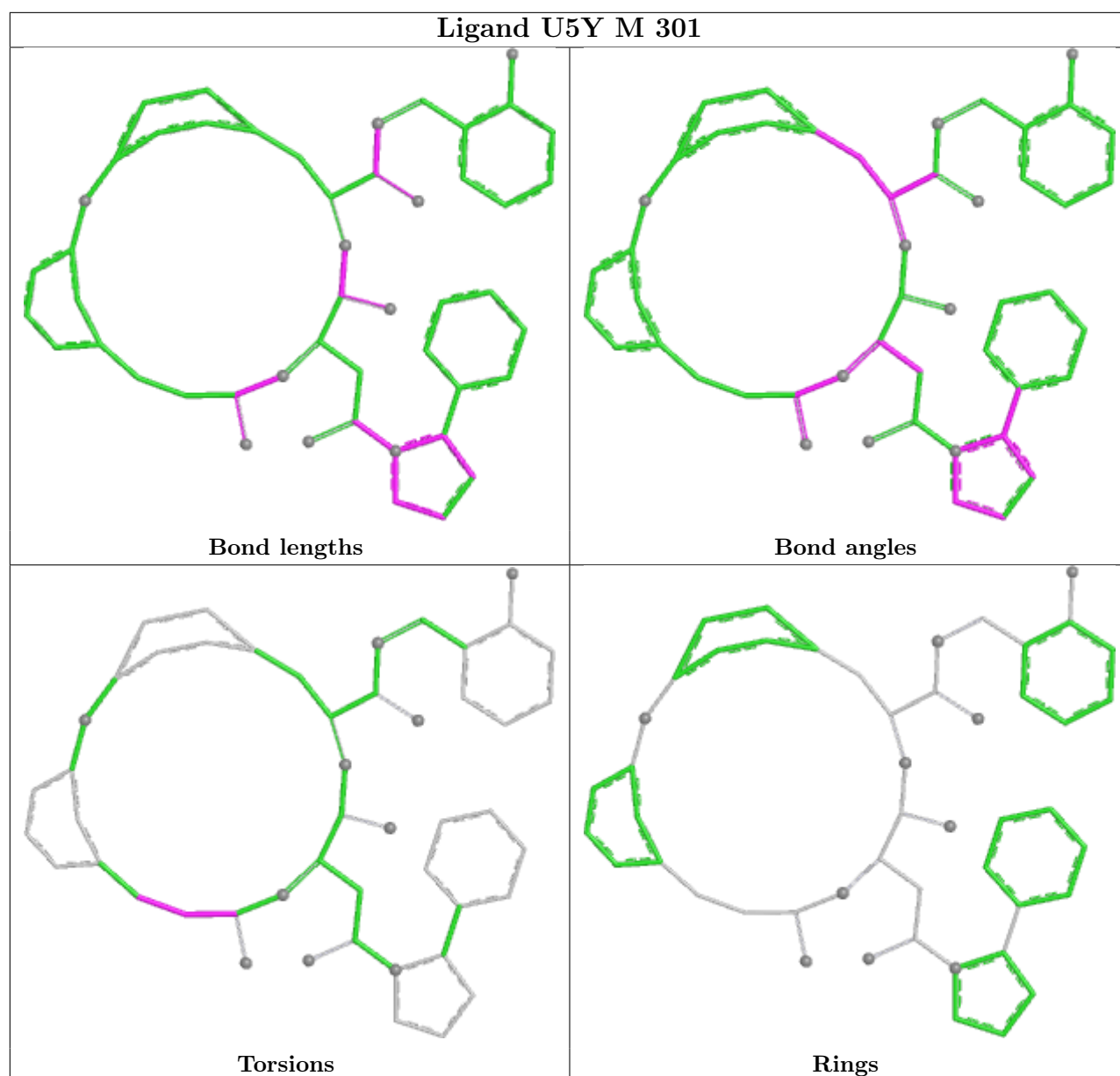
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	302	DMF	2	0
4	W	303	CIT	1	0
4	X	303	CIT	1	0
4	N	302	CIT	2	0
3	W	302	U5Y	1	0
5	P	301	DMF	1	0
4	J	302	CIT	1	0
4	a	302	CIT	2	0
4	L	302	CIT	1	0
4	Z	302	CIT	4	0
3	b	301	U5Y	1	0
4	V	302	CIT	2	0
4	Y	302	CIT	2	0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

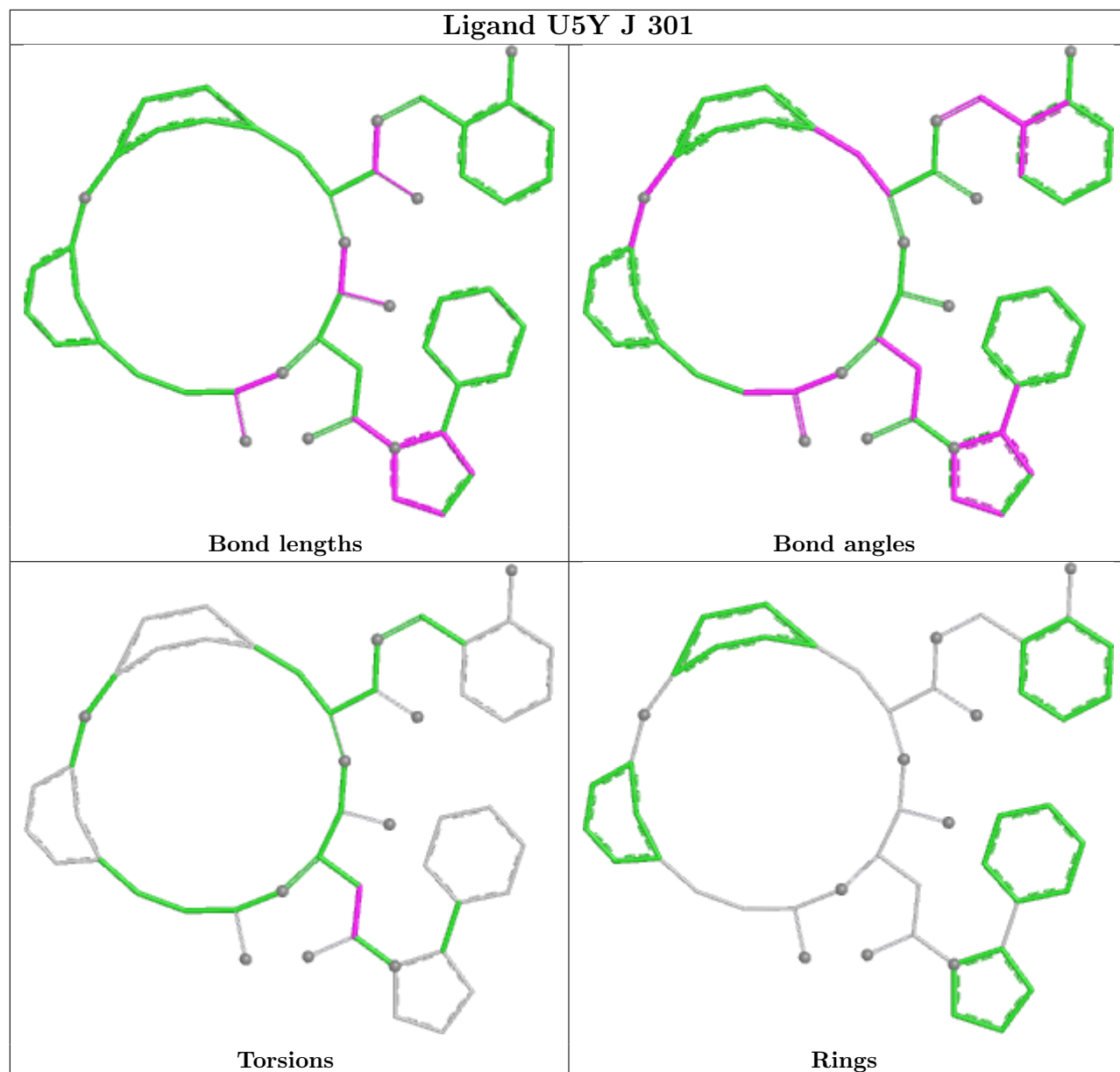
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

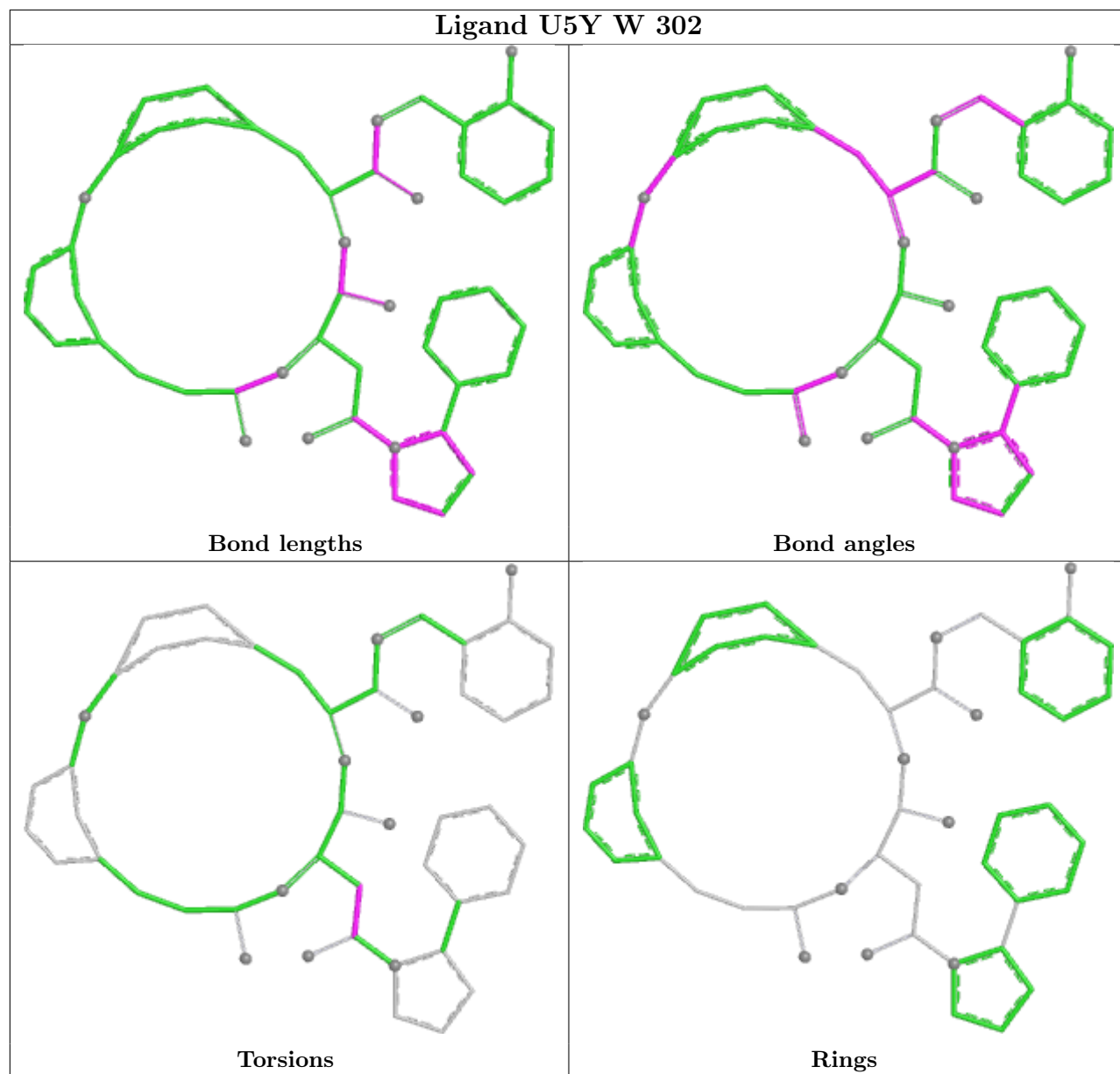
Ligand U5Y H 301



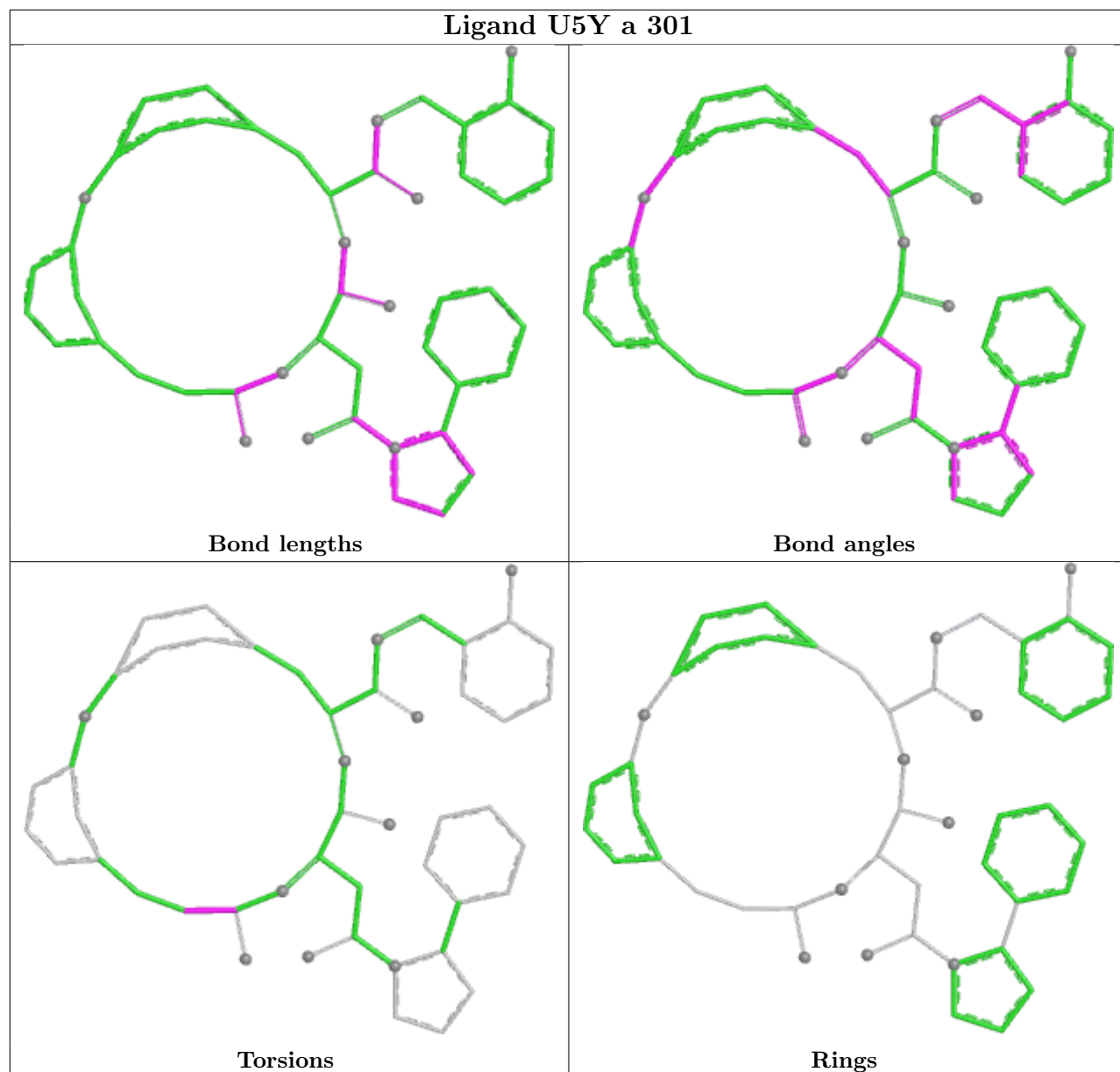


Ligand U5Y J 301

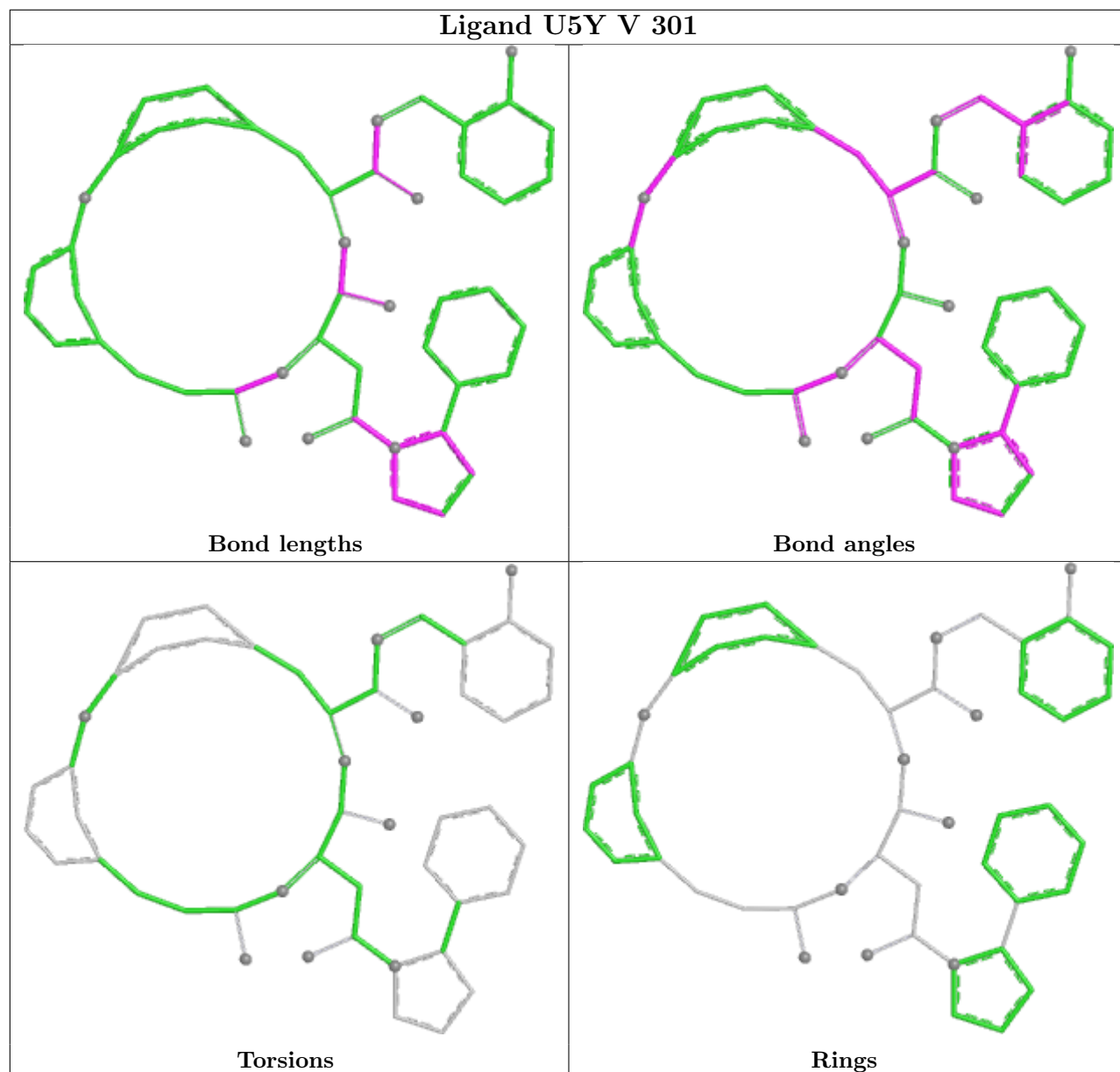




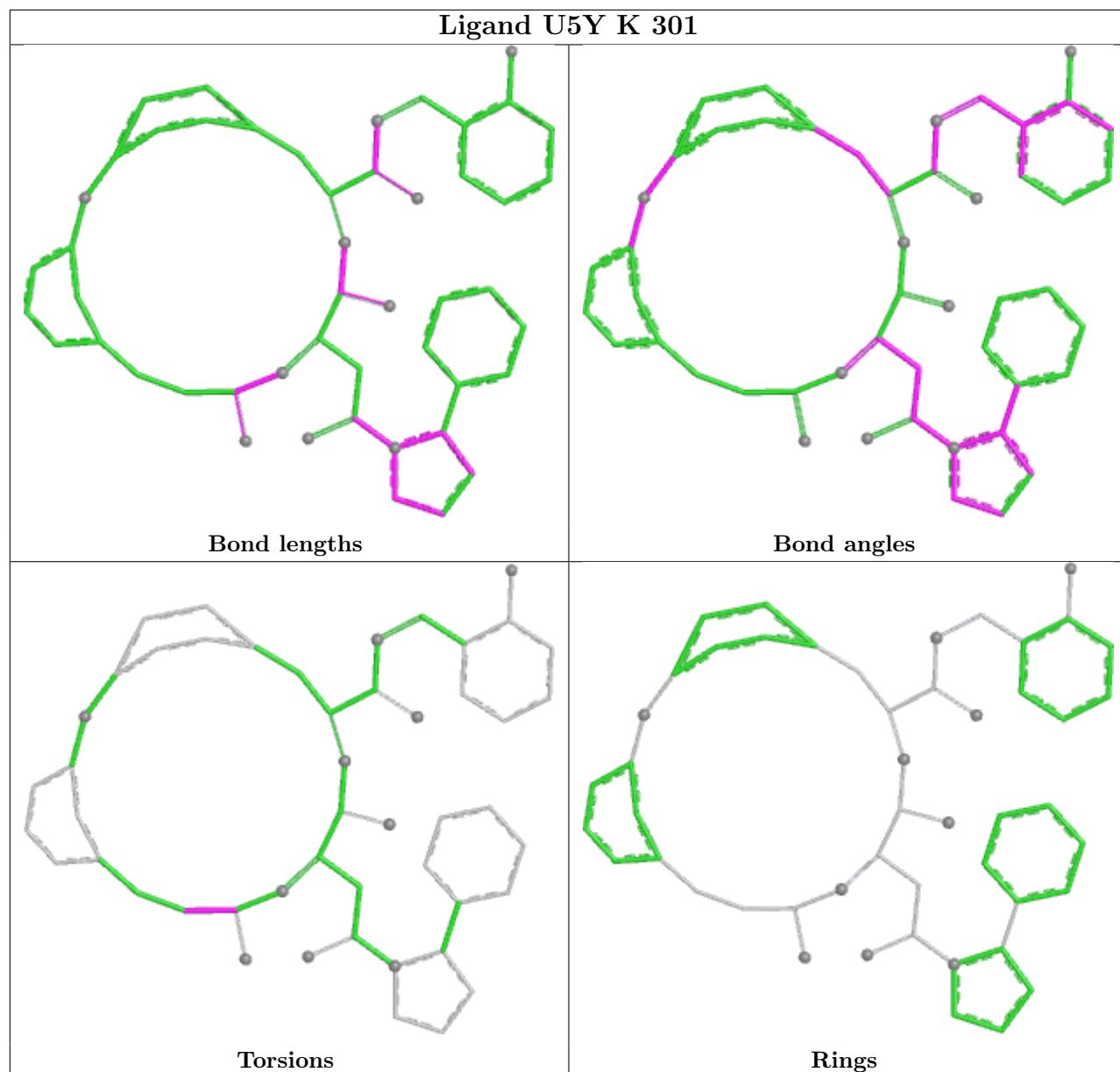
Ligand U5Y a 301



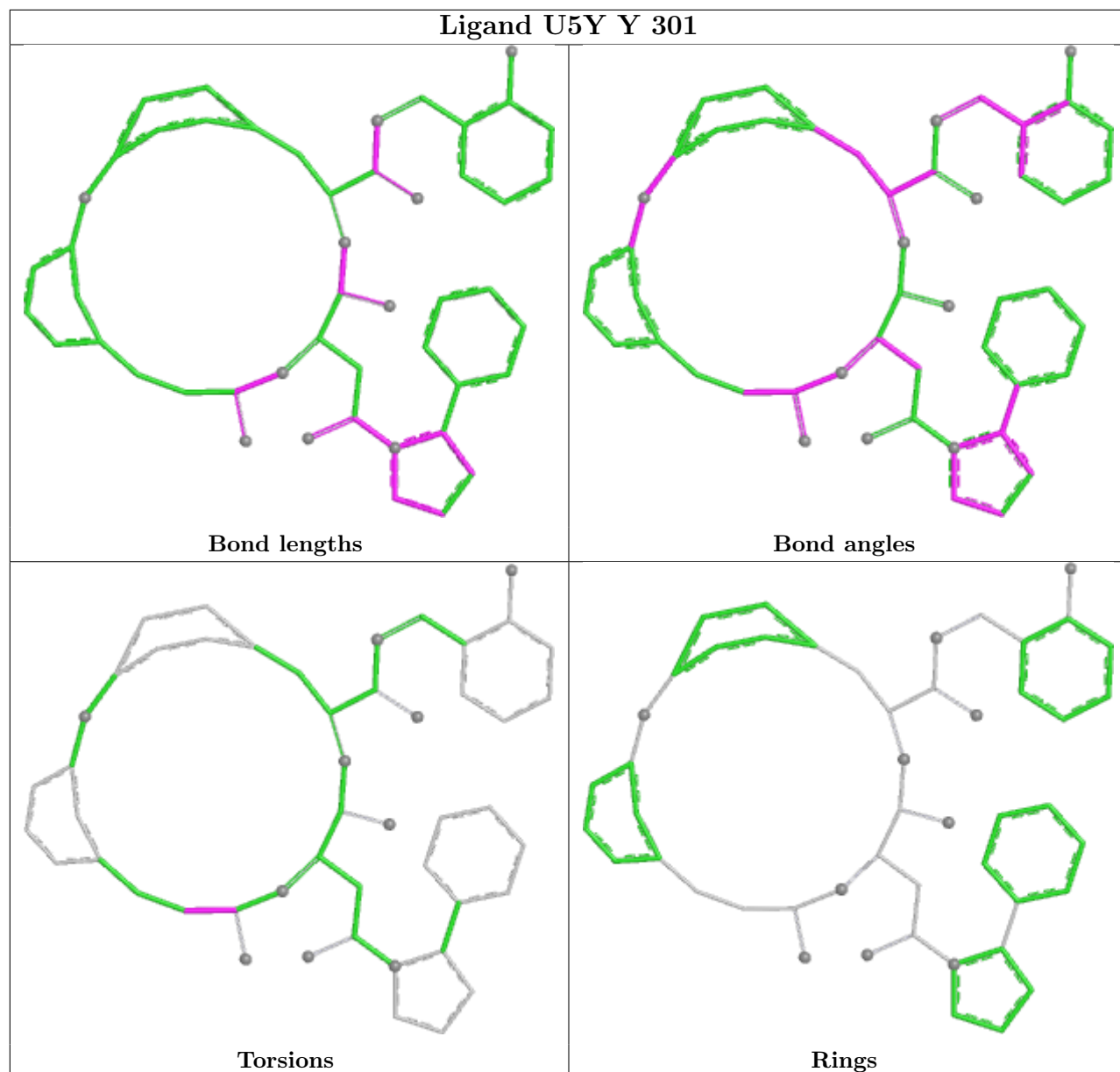
Ligand U5Y V 301



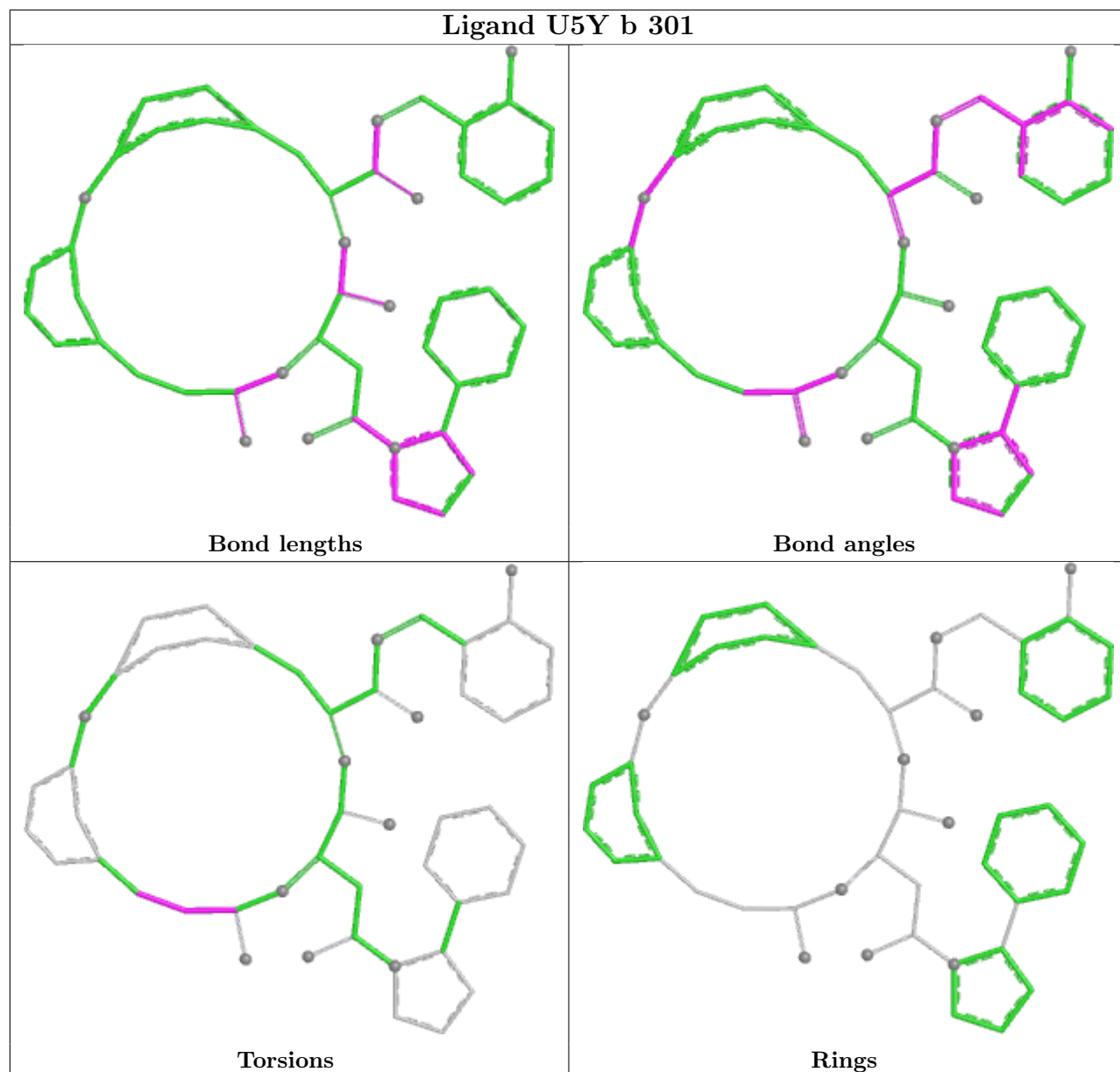
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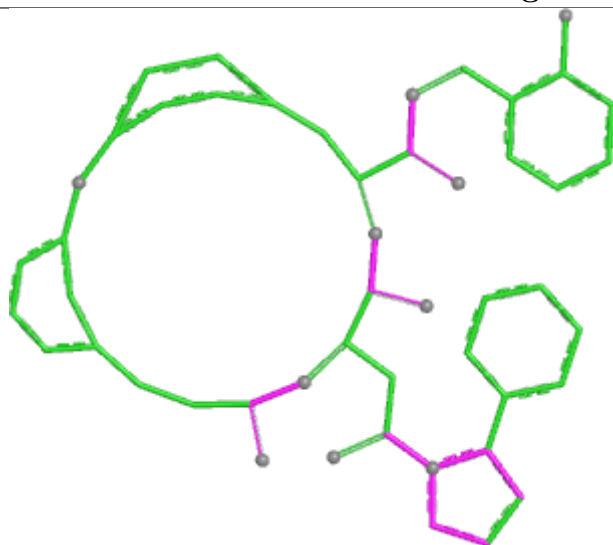
Ligand U5Y Y 301



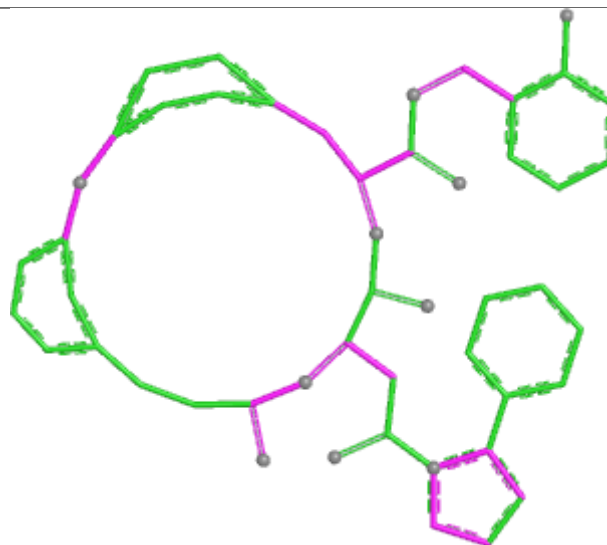
Ligand U5Y b 301



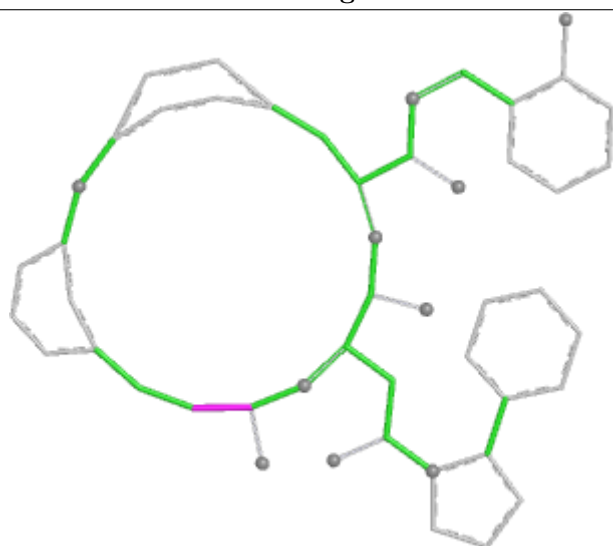
Ligand U5Y I 301



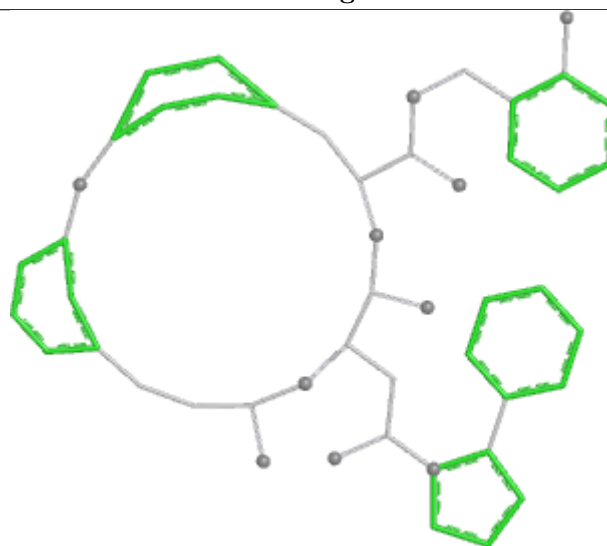
Bond lengths



Bond angles

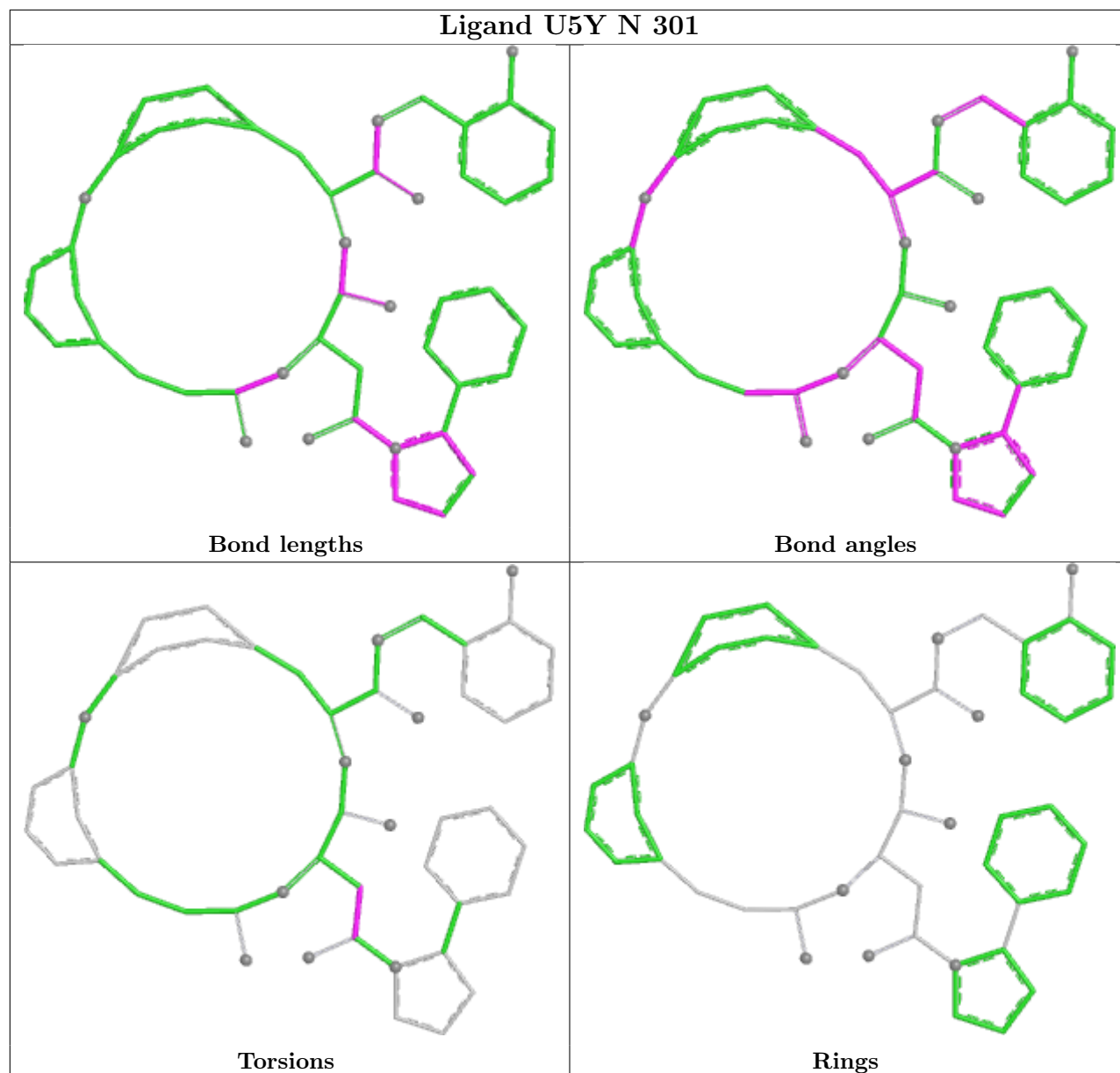


Torsions

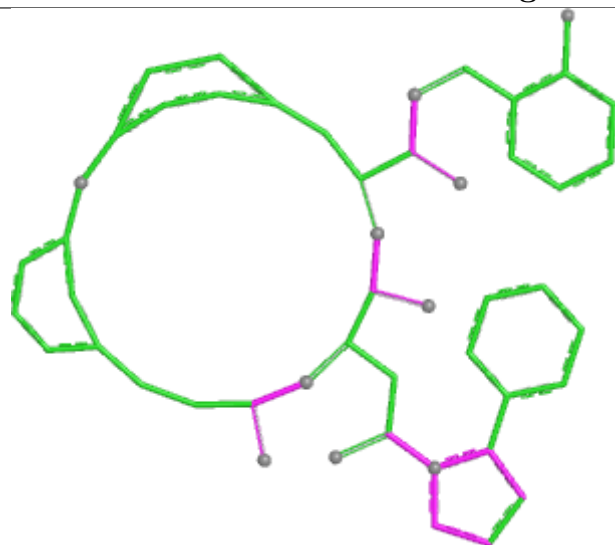


Rings

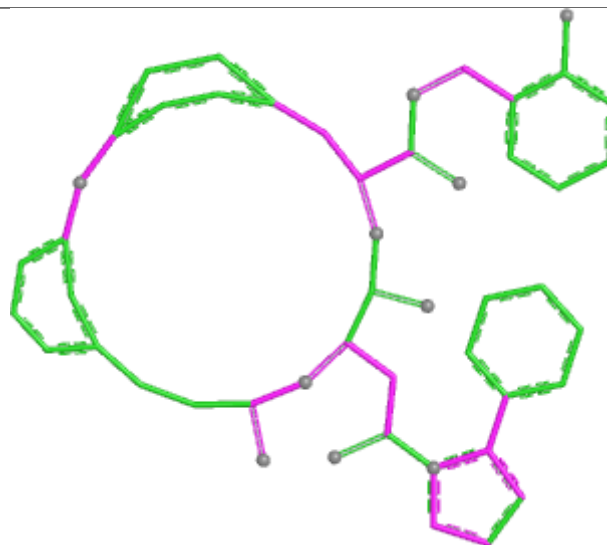
Ligand U5Y N 301



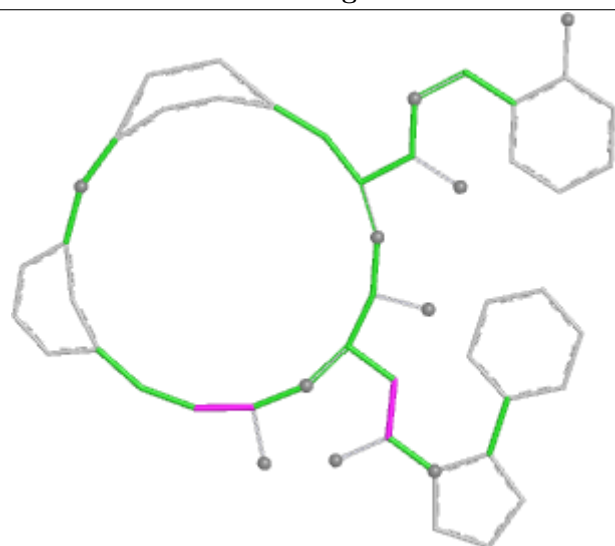
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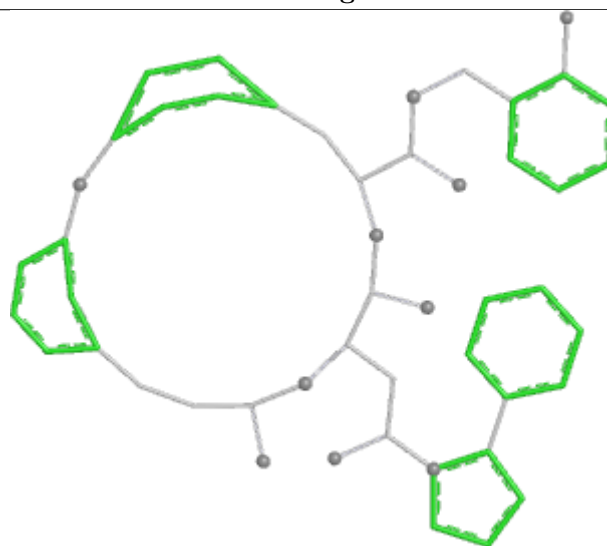
Bond lengths



Bond angles

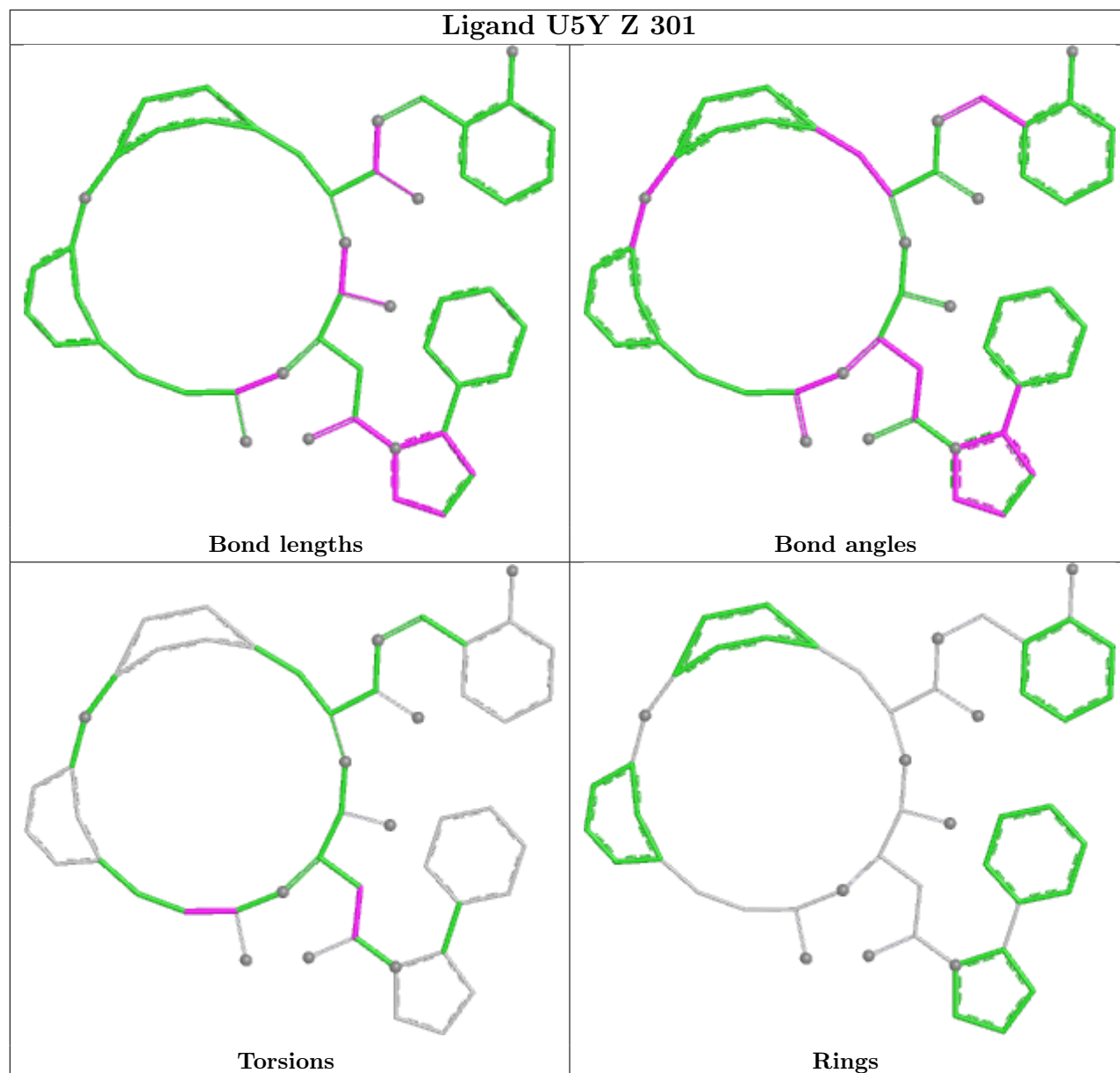


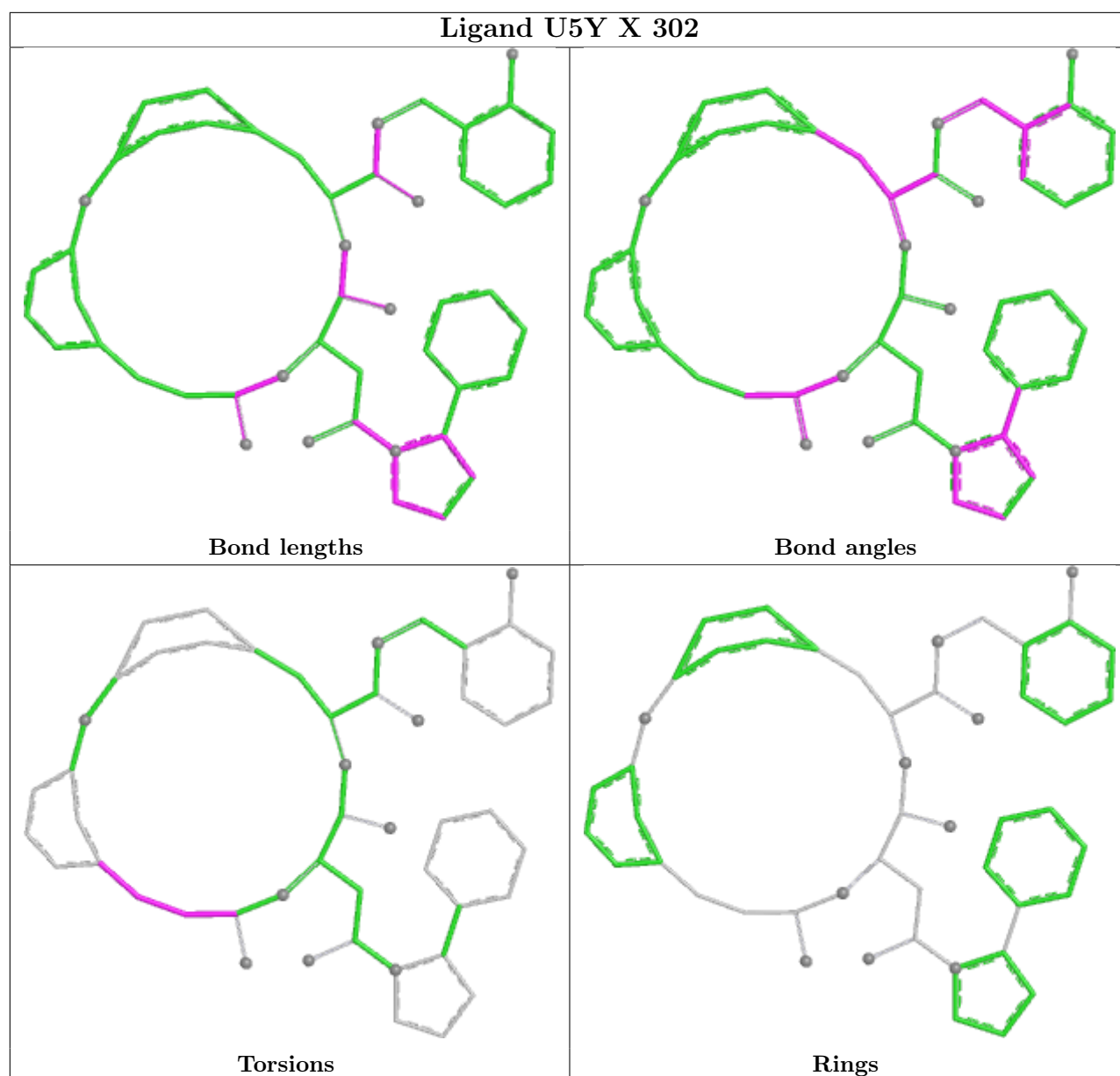
Torsions



Rings

Ligand U5Y Z 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, 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

All (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
1	T	226	THR	5.0
1	B	190	ALA	4.9
1	U	235	VAL	4.8
1	F	203	LEU	4.7
1	E	233	LEU	4.7
2	b	224	ALA	4.7
1	C	203	LEU	4.5
1	G	202	THR	4.4
1	G	201	PRO	4.3
1	T	234	LEU	4.2
1	B	235	VAL	4.1
1	O	191	GLY	4.0
1	R	235	VAL	3.9
1	A	191	GLY	3.9
1	Q	192	SER	3.9
1	E	205	VAL	3.9
1	P	235	VAL	3.9
1	T	188	LEU	3.9
2	H	224	ALA	3.9
1	C	172	ALA	3.8
1	U	191	GLY	3.7
1	O	235	VAL	3.7
1	C	233	LEU	3.7
1	S	235	VAL	3.6
1	T	205	VAL	3.6
1	F	163	ILE	3.5
1	C	235	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	b	114	PRO	3.5
1	D	172	ALA	3.5
1	E	164	ALA	3.5
1	T	12	ALA	3.5
1	G	234	LEU	3.4
1	Q	234	LEU	3.4
1	U	9	MET	3.4
1	D	164	ALA	3.4
1	E	172	ALA	3.4
1	F	233	LEU	3.4
1	F	9	MET	3.4
1	G	235	VAL	3.4
1	T	206	ALA	3.4
1	E	229	ALA	3.3
1	T	229	ALA	3.3
1	C	191	GLY	3.3
1	E	188	LEU	3.3
2	H	112	SER	3.3
1	U	190	ALA	3.3
1	E	171	TYR	3.3
1	C	206	ALA	3.3
1	F	120	VAL	3.3
1	O	133	THR	3.2
1	G	192	SER	3.2
1	E	227	GLY	3.1
1	Q	235	VAL	3.1
1	T	233	LEU	3.1
1	E	177	LEU	3.1
1	E	42	VAL	3.1
1	T	177	LEU	3.1
2	b	109	ILE	3.1
1	D	203	LEU	3.1
1	O	12	ALA	3.0
1	O	190	ALA	3.0
1	C	205	VAL	3.0
1	D	233	LEU	3.0
1	T	153	PHE	3.0
1	F	206	ALA	3.0
1	S	172	ALA	3.0
1	D	33	LEU	3.0
2	I	115	GLN	3.0
1	G	233	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	159	THR	2.9
1	F	208	LEU	2.9
2	W	223	GLY	2.9
2	I	114	PRO	2.9
1	C	175	ALA	2.9
1	E	166	ALA	2.8
1	G	229	ALA	2.8
1	T	202	THR	2.8
1	E	167	LEU	2.8
1	E	206	ALA	2.8
1	T	228	SER	2.8
1	C	167	LEU	2.8
1	D	234	LEU	2.8
1	E	190	ALA	2.8
1	S	166	ALA	2.8
1	S	175	ALA	2.8
1	D	9	MET	2.8
1	F	205	VAL	2.8
1	C	188	LEU	2.8
1	U	35	TYR	2.8
1	P	12	ALA	2.8
1	B	203	LEU	2.7
1	Q	13	MET	2.7
1	S	9	MET	2.7
1	S	233	LEU	2.7
1	T	190	ALA	2.7
1	D	188	LEU	2.7
1	F	190	ALA	2.7
1	F	192	SER	2.7
1	G	167	LEU	2.7
1	S	234	LEU	2.7
1	T	33	LEU	2.7
1	U	166	ALA	2.7
1	E	204	GLY	2.7
1	U	203	LEU	2.7
1	T	128	ALA	2.6
1	B	171	TYR	2.6
1	E	31	VAL	2.6
1	F	31	VAL	2.6
1	S	151	PRO	2.6
1	T	151	PRO	2.6
1	Q	236	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	166	ALA	2.6
1	E	27	ALA	2.6
1	G	33	LEU	2.6
1	C	157	GLY	2.6
1	F	41	PHE	2.6
1	B	205	VAL	2.6
1	S	192	SER	2.6
1	T	163	ILE	2.6
1	T	10	GLU	2.5
1	E	211	ALA	2.5
1	U	37	GLY	2.5
1	E	210	VAL	2.5
1	P	192	SER	2.5
1	B	189	ARG	2.5
1	C	13	MET	2.5
1	F	180	ALA	2.5
1	G	236	ASP	2.5
1	S	184	ALA	2.5
1	T	232	ALA	2.5
1	D	153	PHE	2.5
1	E	47	SER	2.5
1	G	205	VAL	2.5
1	T	185	VAL	2.5
1	E	223	ARG	2.5
1	S	188	LEU	2.5
1	E	179	ASP	2.5
2	b	113	ASP	2.5
1	B	162	PRO	2.5
1	E	46	PRO	2.5
1	E	225	ILE	2.5
1	C	230	LEU	2.5
1	E	230	LEU	2.5
1	S	50	LEU	2.5
1	T	9	MET	2.5
1	D	43	ALA	2.5
1	P	190	ALA	2.5
1	T	34	ALA	2.5
1	B	131	GLY	2.5
2	b	10	GLY	2.5
1	F	228	SER	2.4
1	E	185	VAL	2.4
1	F	12	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	180	ALA	2.4
1	Q	12	ALA	2.4
2	Y	223	GLY	2.4
1	P	160	THR	2.4
2	b	112	SER	2.4
2	X	30	ASP	2.4
2	b	115	GLN	2.4
1	C	164	ALA	2.4
1	D	175	ALA	2.4
1	Q	172	ALA	2.4
1	Q	191	GLY	2.4
1	E	159	THR	2.4
1	C	163	ILE	2.4
1	U	234	LEU	2.4
1	B	151	PRO	2.4
1	S	162	PRO	2.4
1	D	187	ALA	2.4
1	T	227	GLY	2.4
1	E	48	ARG	2.4
1	C	10	GLU	2.4
1	E	180	ALA	2.3
1	R	172	ALA	2.3
1	F	133	THR	2.3
1	F	207	SER	2.3
1	D	205	VAL	2.3
1	U	205	VAL	2.3
1	Q	227	GLY	2.3
1	S	186	ALA	2.3
1	P	202	THR	2.3
1	F	183	ILE	2.3
1	O	10	GLU	2.3
2	Y	113	ASP	2.3
1	E	186	ALA	2.3
1	F	226	THR	2.3
1	F	189	ARG	2.3
1	Q	50	LEU	2.3
1	S	33	LEU	2.3
1	E	165	ASN	2.3
1	Q	151	PRO	2.3
2	M	160	GLY	2.3
1	G	9	MET	2.3
1	S	171	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	184	ALA	2.3
1	B	133	THR	2.3
1	S	226	THR	2.3
1	E	163	ILE	2.3
1	S	210	VAL	2.3
1	E	151	PRO	2.2
1	T	46	PRO	2.2
1	U	151	PRO	2.2
1	B	20	ALA	2.2
1	S	34	ALA	2.2
1	S	164	ALA	2.2
1	S	190	ALA	2.2
1	B	160	THR	2.2
1	S	178	THR	2.2
1	Q	225	ILE	2.2
1	S	177	LEU	2.2
1	C	182	ARG	2.2
1	E	123	CYS	2.2
1	P	191	GLY	2.2
2	H	223	GLY	2.2
1	D	121	GLU	2.2
1	U	44	GLU	2.2
1	B	11	GLN	2.2
2	Y	115	GLN	2.2
1	E	34	ALA	2.2
1	E	184	ALA	2.2
1	P	172	ALA	2.2
1	T	175	ALA	2.2
1	D	171	TYR	2.2
1	D	183	ILE	2.2
1	T	225	ILE	2.2
1	E	208	LEU	2.2
1	U	233	LEU	2.2
2	L	38	ASP	2.2
1	G	227	GLY	2.2
1	U	38	GLY	2.2
2	K	223	GLY	2.2
1	E	148	ALA	2.2
1	G	206	ALA	2.2
1	T	172	ALA	2.2
2	Y	116	SER	2.2
1	F	177	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	T	203	LEU	2.2
1	U	33	LEU	2.2
1	C	185	VAL	2.2
1	E	153	PHE	2.2
1	C	65	ALA	2.2
1	D	159	THR	2.2
1	D	180	ALA	2.2
1	F	232	ALA	2.2
1	Q	190	ALA	2.2
1	T	29	SER	2.2
2	I	112	SER	2.2
1	C	99	LEU	2.1
1	F	188	LEU	2.1
1	G	183	ILE	2.1
2	L	144	LEU	2.1
1	Q	9	MET	2.1
1	S	205	VAL	2.1
2	H	113	ASP	2.1
2	N	114	PRO	2.1
2	V	114	PRO	2.1
1	U	202	THR	2.1
1	C	48	ARG	2.1
1	E	189	ARG	2.1
1	F	181	LEU	2.1
1	G	203	LEU	2.1
1	Q	183	ILE	2.1
1	Q	203	LEU	2.1
1	Q	205	VAL	2.1
2	H	115	GLN	2.1
2	Y	114	PRO	2.1
1	F	227	GLY	2.1
1	U	227	GLY	2.1
1	G	21	ARG	2.1
1	G	189	ARG	2.1
1	C	229	ALA	2.1
1	F	184	ALA	2.1
1	U	172	ALA	2.1
1	P	9	MET	2.1
1	P	188	LEU	2.1
1	T	143	TYR	2.1
2	M	30	ASP	2.1
1	S	11	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	155	VAL	2.1
1	F	153	PHE	2.1
1	D	227	GLY	2.1
1	E	38	GLY	2.1
1	D	226	THR	2.1
1	R	192	SER	2.1
2	V	222	SER	2.1
1	C	36	ALA	2.1
1	C	184	ALA	2.1
1	Q	164	ALA	2.1
1	Q	166	ALA	2.1
1	A	33	LEU	2.1
1	S	230	LEU	2.1
1	P	162	PRO	2.1
1	E	155	VAL	2.1
1	S	155	VAL	2.1
1	T	37	GLY	2.1
1	S	182	ARG	2.1
1	E	192	SER	2.0
2	L	112	SER	2.0
1	B	13	MET	2.0
1	E	9	MET	2.0
1	U	175	ALA	2.0
1	C	174	ASN	2.0
1	C	234	LEU	2.0
1	Q	163	ILE	2.0
1	U	163	ILE	2.0
2	Z	114	PRO	2.0
1	S	185	VAL	2.0
1	Q	10	GLU	2.0
1	G	172	ALA	2.0
1	S	20	ALA	2.0
1	S	206	ALA	2.0
1	T	32	ALA	2.0
1	E	129	HIS	2.0
1	E	152	HIS	2.0
1	F	33	LEU	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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
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

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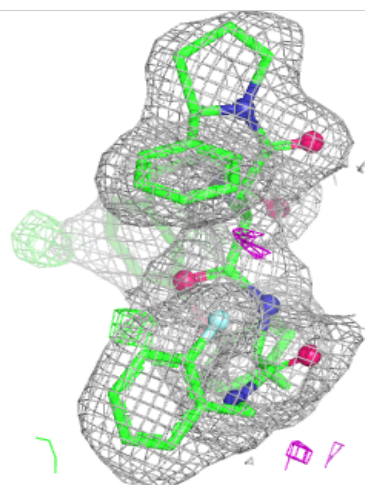
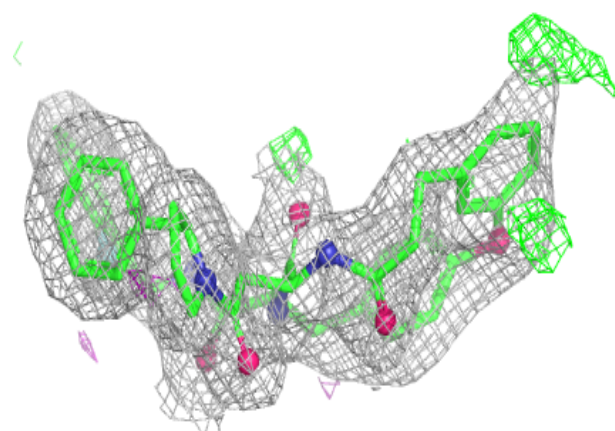
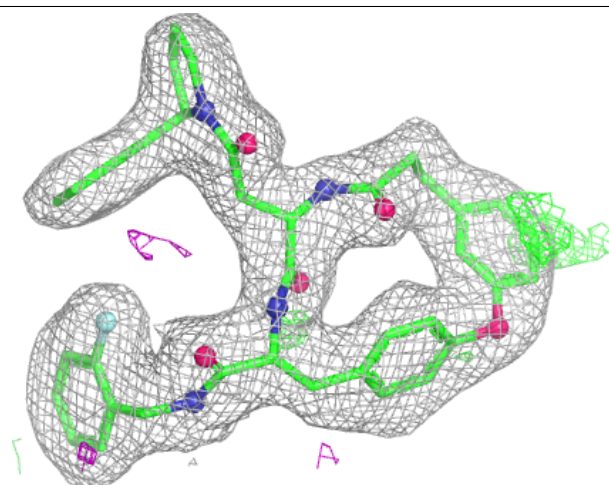
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	U5Y	Z	301	49/49	0.95	0.08	28,37,60,65	0
3	U5Y	H	301	49/49	0.96	0.07	23,30,41,46	0
3	U5Y	I	301	49/49	0.96	0.07	24,31,46,51	0
3	U5Y	W	302	49/49	0.96	0.07	25,31,46,52	0

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.

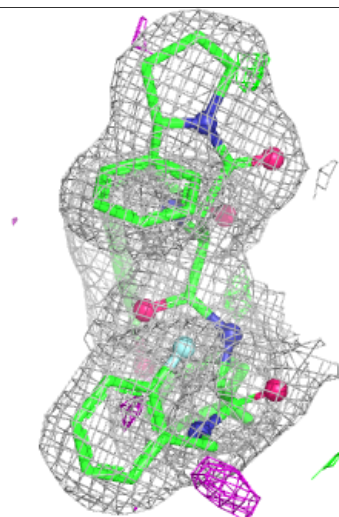
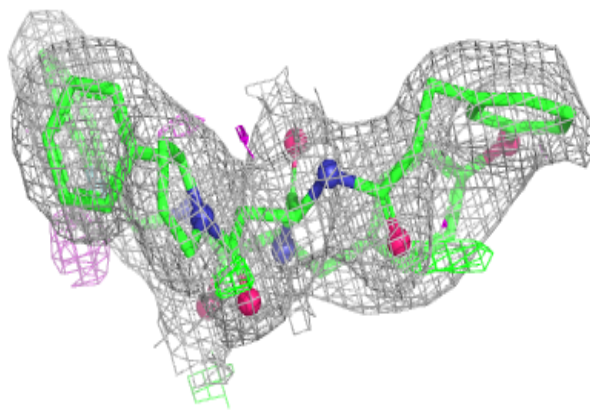
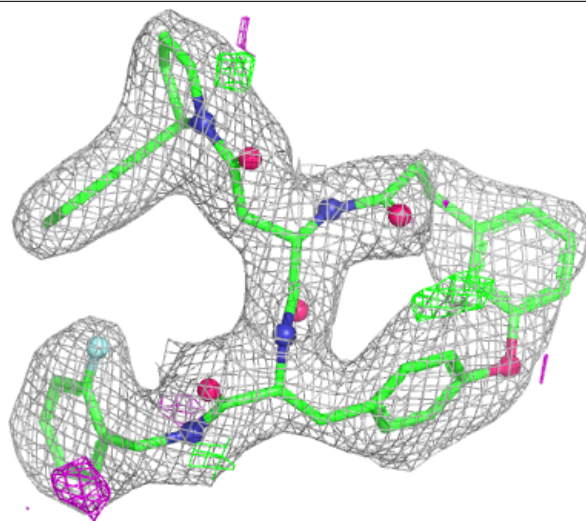
Electron density around U5Y b 301:

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



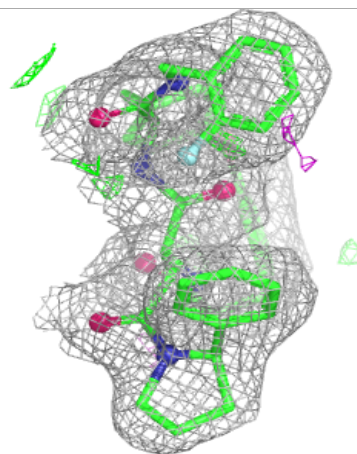
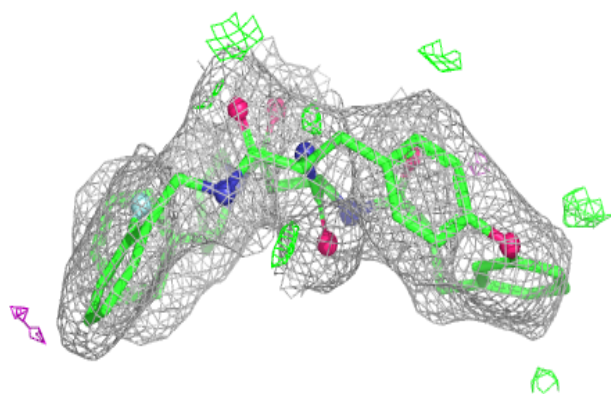
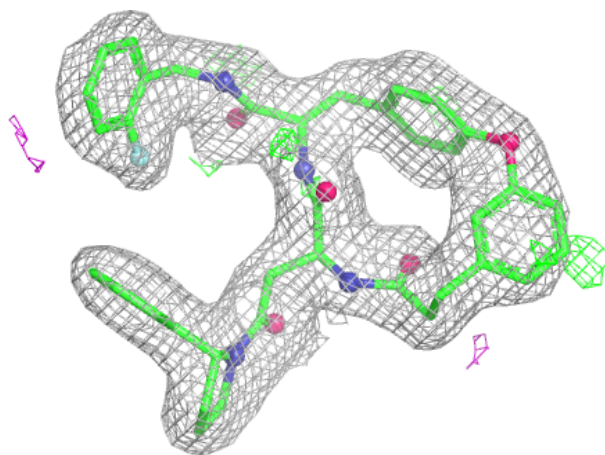
Electron density around U5Y L 301:

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



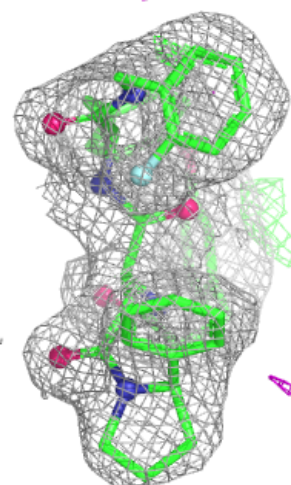
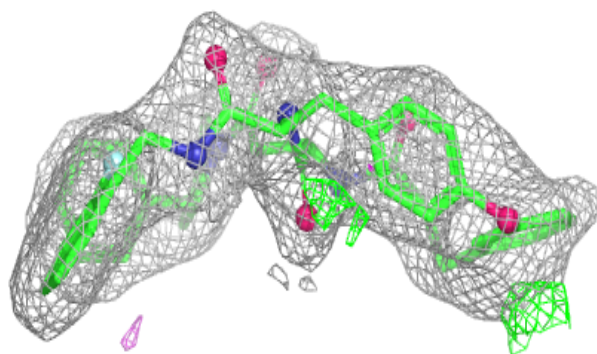
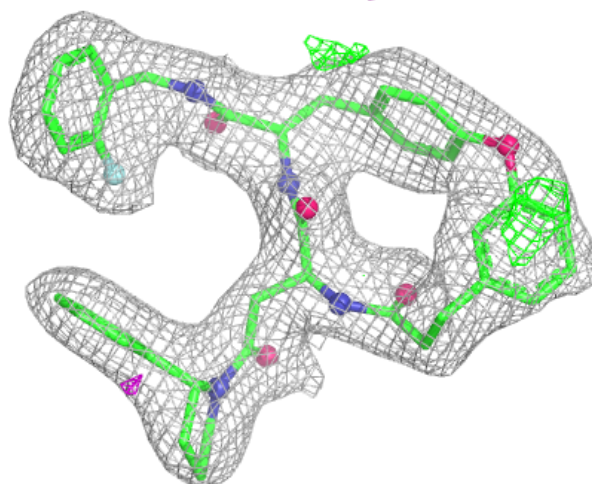
Electron density around U5Y M 301:

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



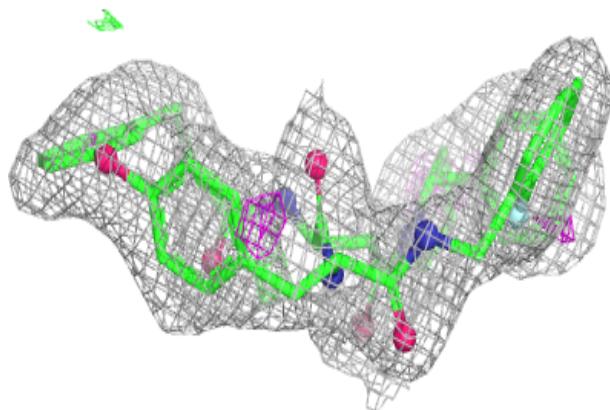
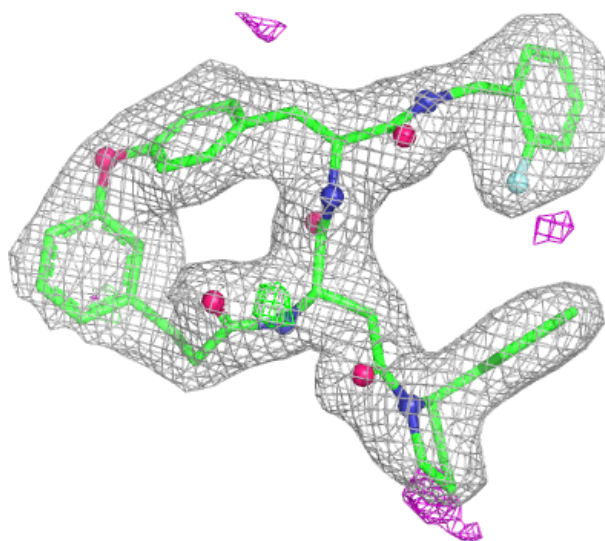
Electron density around U5Y a 301:

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



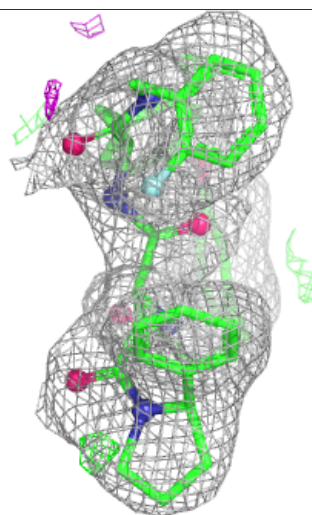
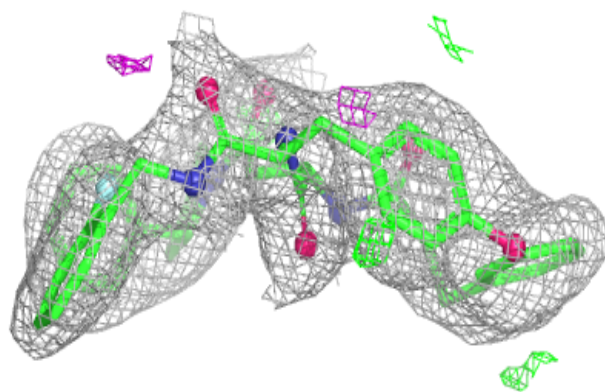
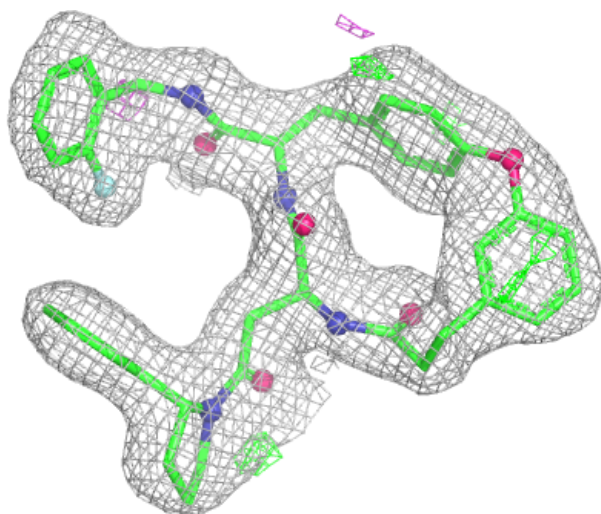
Electron density around U5Y J 301:

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



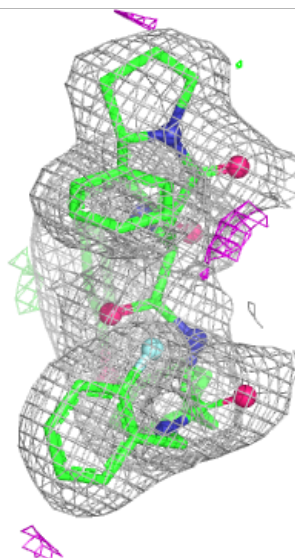
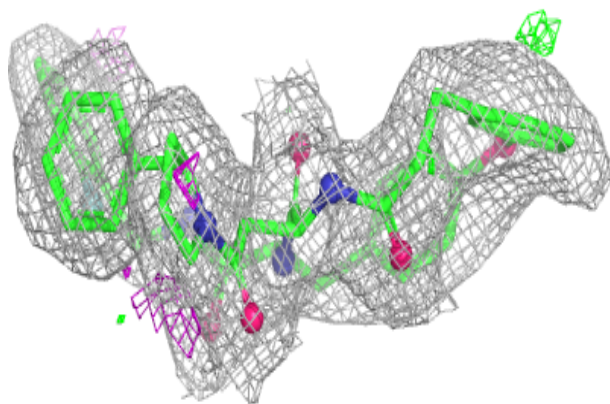
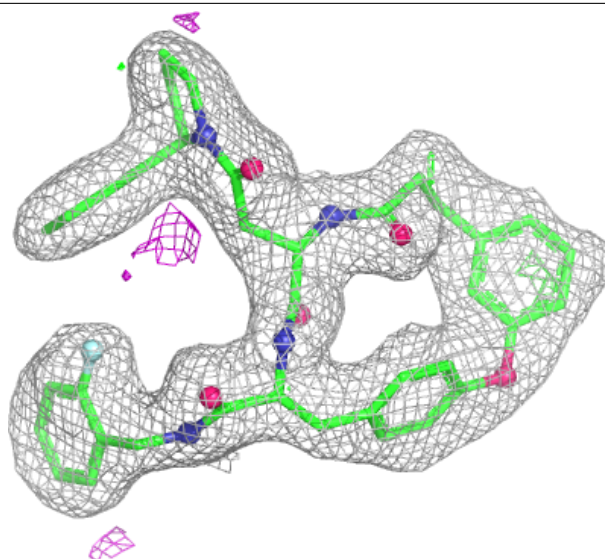
Electron density around U5Y K 301:

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



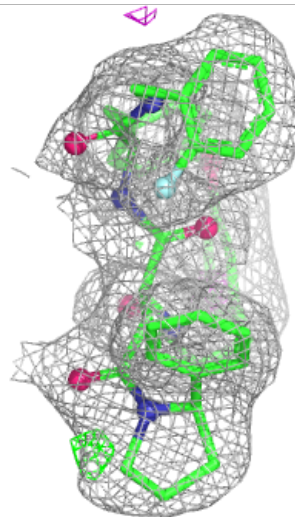
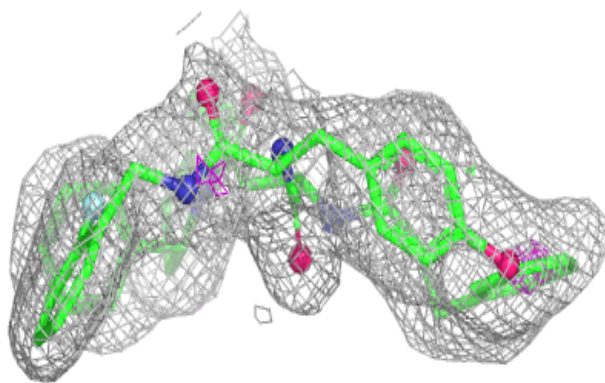
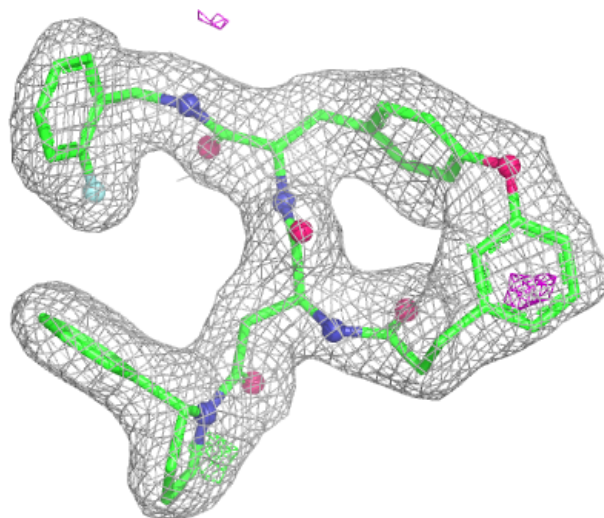
Electron density around U5Y N 301:

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



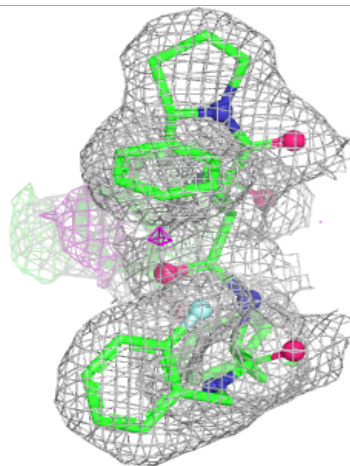
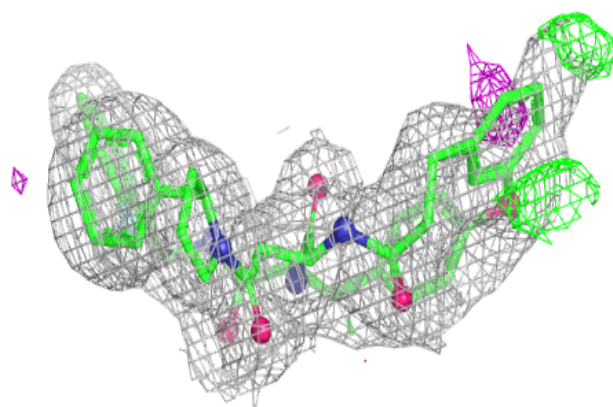
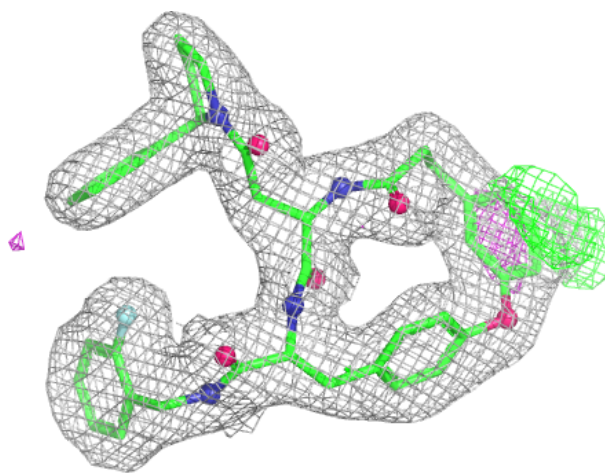
Electron density around U5Y V 301:

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



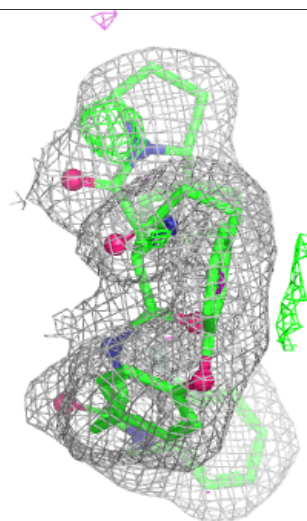
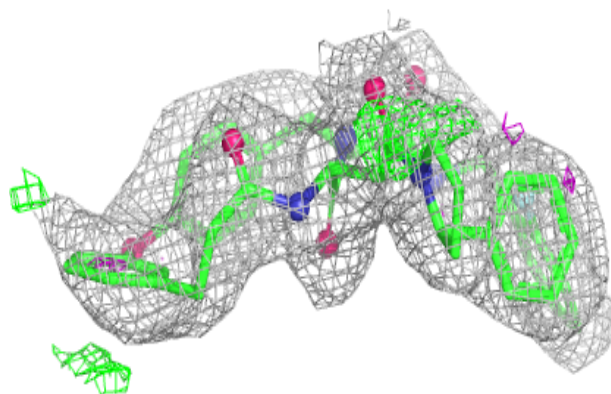
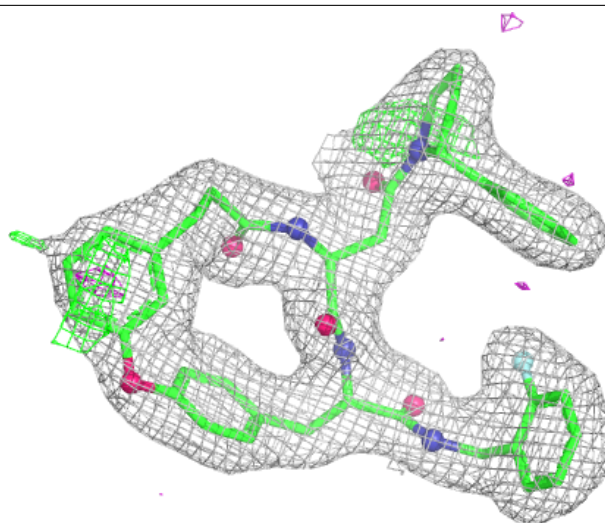
Electron density around U5Y X 302:

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



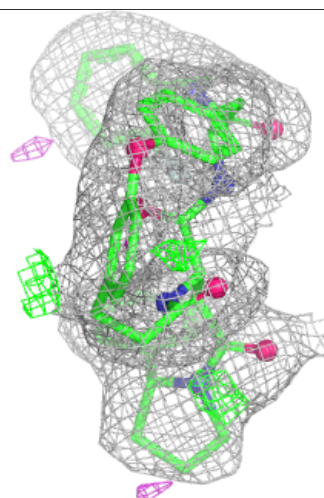
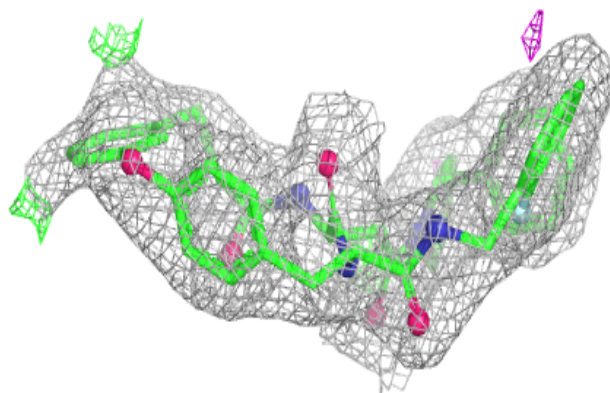
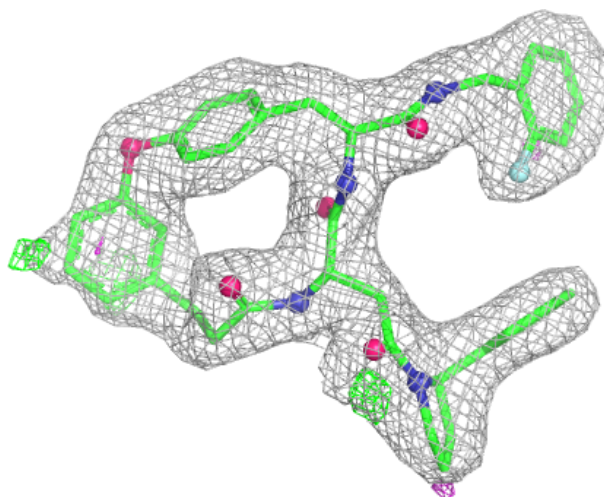
Electron density around U5Y Y 301:

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



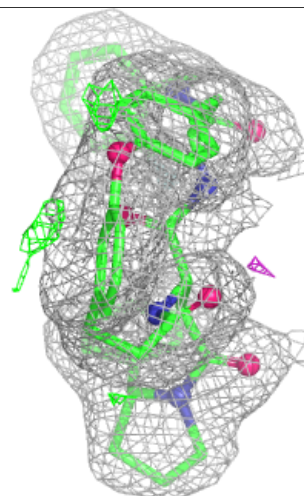
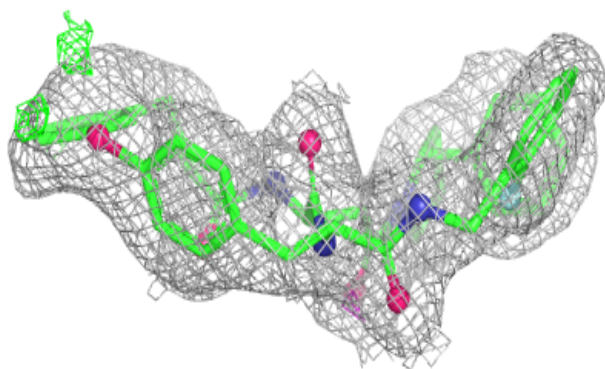
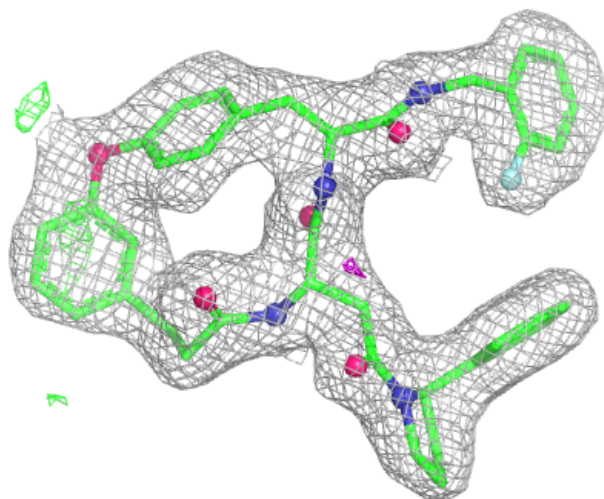
Electron density around U5Y Z 301:

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



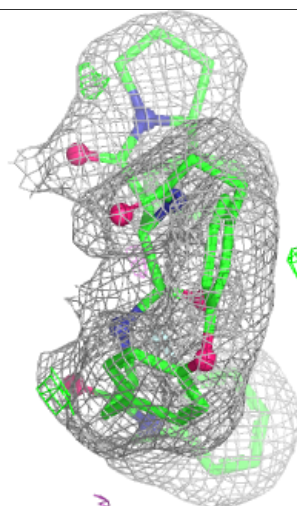
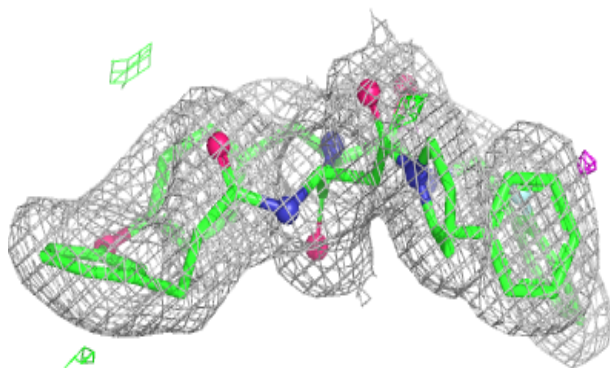
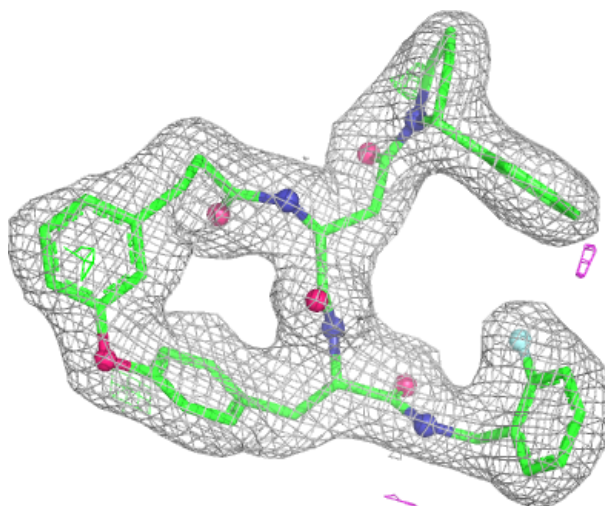
Electron density around U5Y H 301:

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



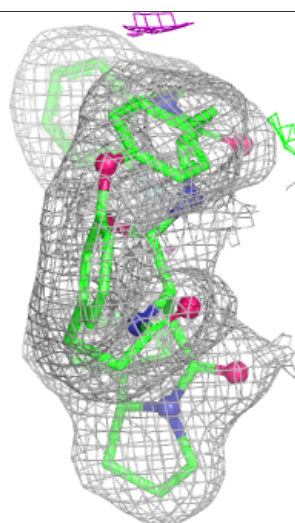
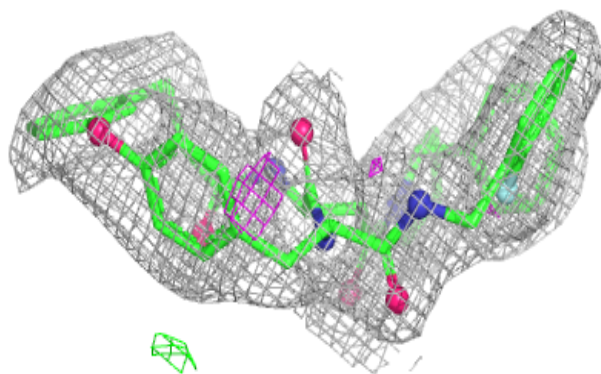
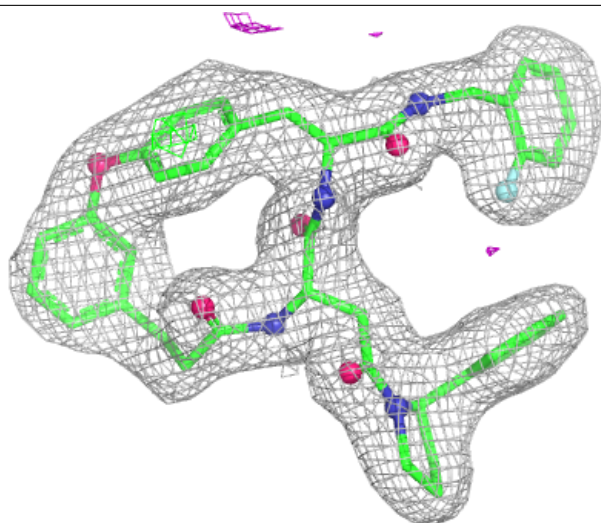
Electron density around U5Y I 301:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.