



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 2, 2026 – 02:20 AM UTC

PDB ID : 6OCZ / pdb_00006ocz
Title : Crystal Structure of Mycobacterium tuberculosis Proteasome in Complex with Phenylimidazole-based Inhibitor A86
Authors : Hsu, H.C.; Li, H.
Deposited on : 2019-03-25
Resolution : 2.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

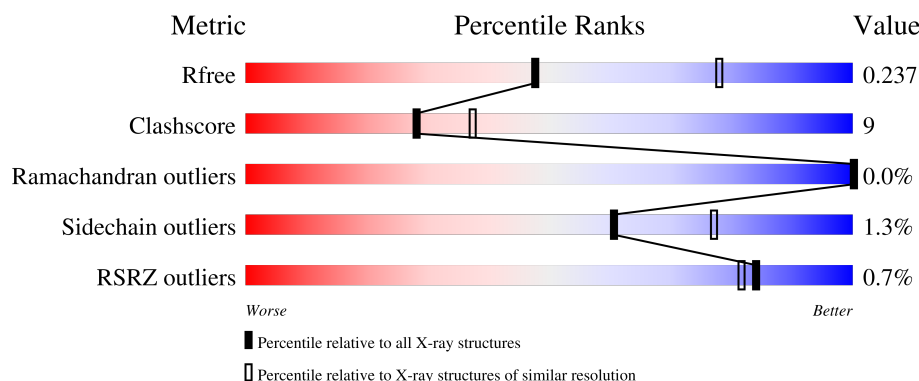
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



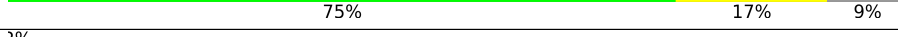
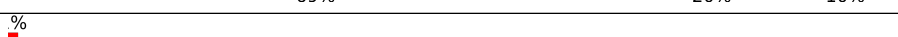
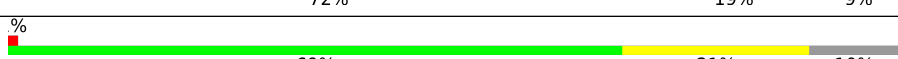
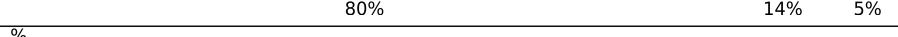
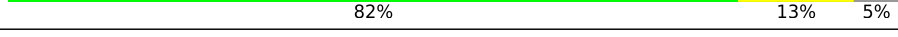
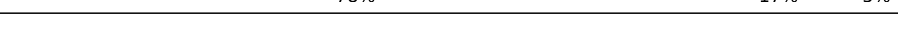
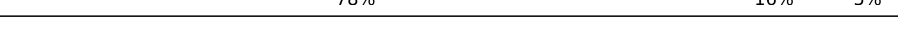
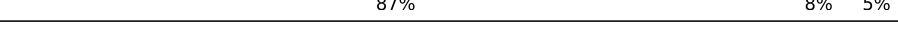
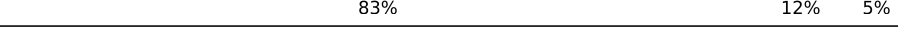
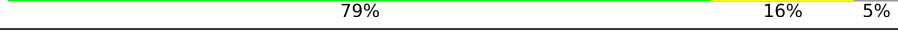
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	
1	B	240	
1	C	240	
1	D	240	
1	E	240	

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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	234	
2	I	234	
2	J	234	
2	K	234	
2	L	234	
2	M	234	
2	N	234	
2	V	234	
2	W	234	
2	X	234	
2	Y	234	
2	Z	234	
2	a	234	
2	b	234	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 48235 atoms, of which 210 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	B	215	Total	C	N	O	S	0	0	0
			1660	1041	303	312	4			
1	C	217	Total	C	N	O	S	0	0	0
			1672	1047	305	316	4			
1	D	215	Total	C	N	O	S	0	0	0
			1655	1035	303	313	4			
1	E	217	Total	C	N	O	S	0	0	0
			1670	1046	305	315	4			
1	F	216	Total	C	N	O	S	0	0	0
			1663	1041	304	314	4			
1	G	216	Total	C	N	O	S	0	0	0
			1661	1039	304	314	4			
1	O	217	Total	C	N	O	S	0	0	0
			1670	1045	305	316	4			
1	P	219	Total	C	N	O	S	0	0	0
			1685	1054	307	320	4			
1	Q	216	Total	C	N	O	S	0	0	0
			1668	1045	304	315	4			
1	R	215	Total	C	N	O	S	0	0	0
			1657	1038	303	312	4			
1	S	218	Total	C	N	O	S	0	0	0
			1678	1050	306	318	4			
1	T	217	Total	C	N	O	S	0	0	0
			1671	1047	305	315	4			
1	U	216	Total	C	N	O	S	0	0	0
			1664	1043	304	313	4			

There are 14 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is a protein called Proteasome subunit beta.

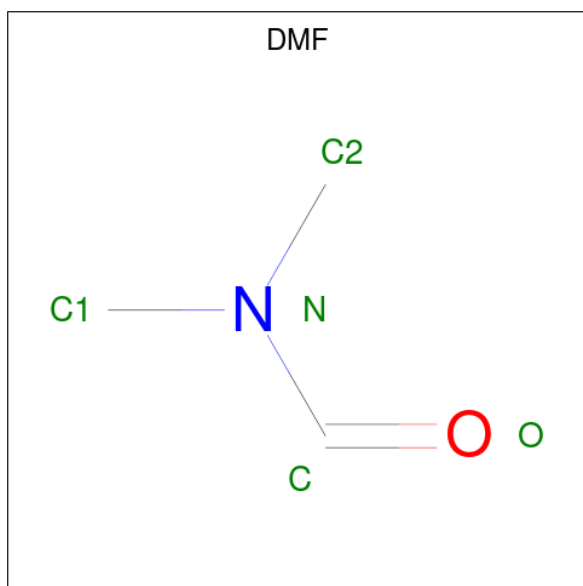
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	I	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	J	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	K	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	L	223	Total	C	N	O	S	0	0	0
			1642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

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

- Molecule 3 is DIMETHYLFORMAMIDE (CCD ID: DMF) (formula: C_3H_7NO).



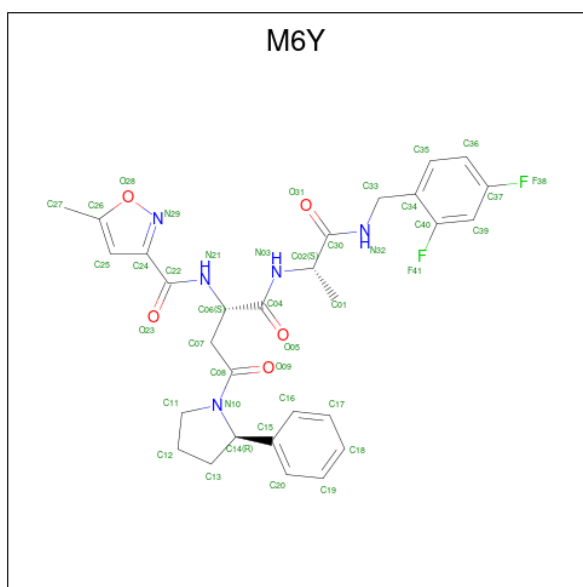
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	B	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	C	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	E	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	F	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	F	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	G	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	G	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	I	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	J	1	Total	C	H	N	O	0	0
			12	3	7	1	1		

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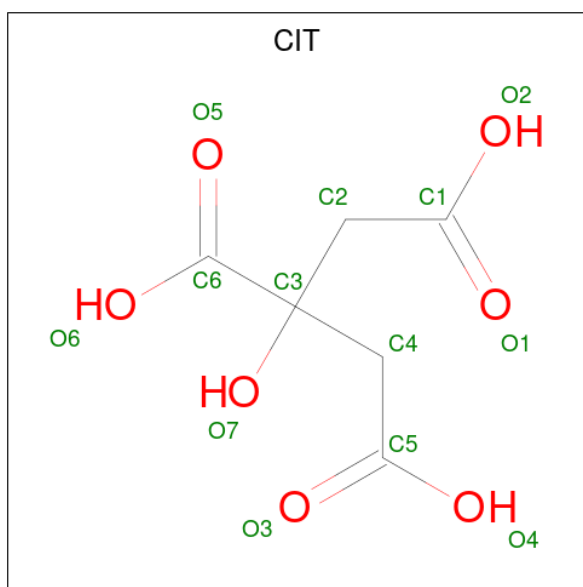
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	J	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	O	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	P	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	Q	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	R	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	R	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	S	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	S	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	T	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	U	1	Total	C	H	N	O	0	0
			12	3	7	1	1		

- Molecule 4 is N-{(2S)-1-((2S)-1-[(2,4-difluorobenzyl)amino]-1-oxopropan-2-yl)amino)-1,4-dioxo-4-[(2R)-2-phenylpyrrolidin-1-yl]butan-2-yl}-5-methyl-1,2-oxazole-3-carboxamide (non-preferred name) (CCD ID: M6Y) (formula: C₂₉H₃₁F₂N₅O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	I	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	J	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	K	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	L	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	M	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	N	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	V	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	W	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	X	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	Y	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	Z	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	a	1	Total 41	C 29	F 2	N 5	O 5	0	0
4	b	1	Total 41	C 29	F 2	N 5	O 5	0	0

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	H	O	0	0
			18	6	5	7		
5	I	1	Total	C	H	O	0	0
			18	6	5	7		
5	J	1	Total	C	H	O	0	0
			18	6	5	7		
5	K	1	Total	C	H	O	0	0
			18	6	5	7		
5	L	1	Total	C	H	O	0	0
			18	6	5	7		
5	M	1	Total	C	H	O	0	0
			18	6	5	7		
5	N	1	Total	C	H	O	0	0
			18	6	5	7		
5	V	1	Total	C	H	O	0	0
			18	6	5	7		
5	W	1	Total	C	H	O	0	0
			18	6	5	7		
5	X	1	Total	C	H	O	0	0
			18	6	5	7		
5	Y	1	Total	C	H	O	0	0
			18	6	5	7		
5	Z	1	Total	C	H	O	0	0
			18	6	5	7		
5	a	1	Total	C	H	O	0	0
			18	6	5	7		
5	b	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	27	Total O 27 27	0	0
6	B	20	Total O 20 20	0	0
6	C	29	Total O 29 29	0	0
6	D	20	Total O 20 20	0	0
6	E	24	Total O 24 24	0	0
6	F	16	Total O 16 16	0	0
6	G	21	Total O 21 21	0	0
6	H	36	Total O 36 36	0	0
6	I	49	Total O 49 49	0	0
6	J	36	Total O 36 36	0	0
6	K	41	Total O 41 41	0	0
6	L	42	Total O 42 42	0	0
6	M	35	Total O 35 35	0	0
6	N	34	Total O 34 34	0	0
6	O	17	Total O 17 17	0	0
6	P	26	Total O 26 26	0	0
6	Q	31	Total O 31 31	0	0
6	R	28	Total O 28 28	0	0
6	S	28	Total O 28 28	0	0
6	T	13	Total O 13 13	0	0
6	U	27	Total O 27 27	0	0

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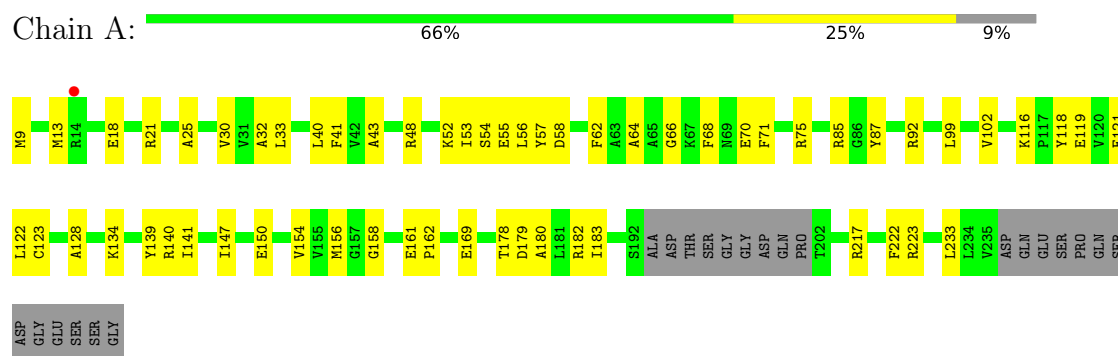
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	V	42	Total 42	O 42	0	0
6	W	39	Total 39	O 39	0	0
6	X	35	Total 35	O 35	0	0
6	Y	40	Total 40	O 40	0	0
6	Z	37	Total 37	O 37	0	0
6	a	29	Total 29	O 29	0	0
6	b	32	Total 32	O 32	0	0

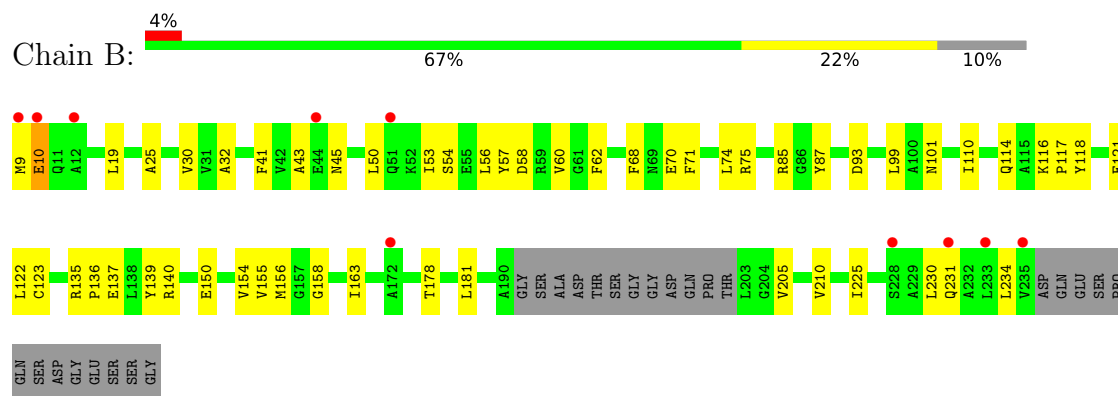
3 Residue-property plots

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.

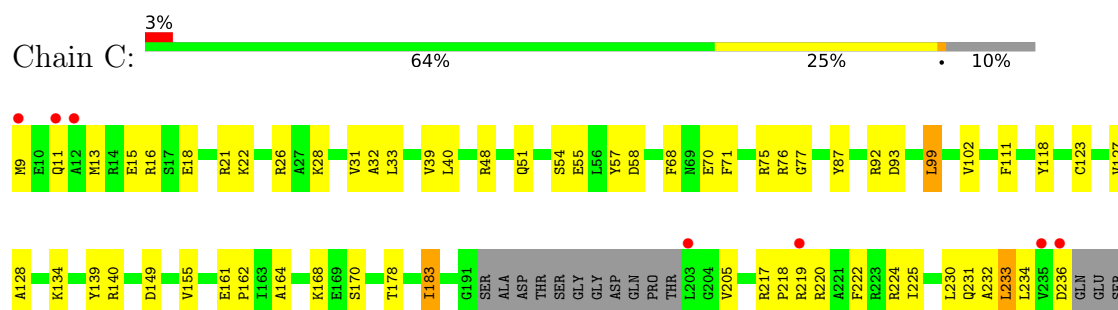
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha



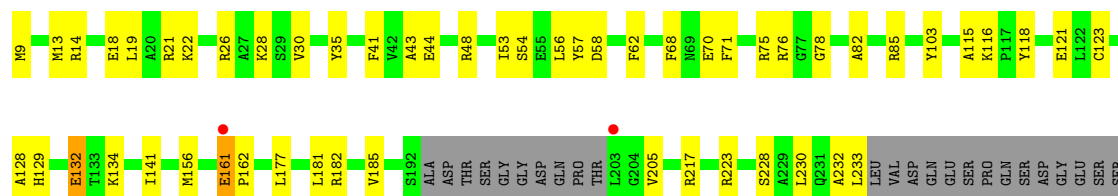
• Molecule 1: Proteasome subunit alpha



PRO
GLN
SER
ASP
GLY
GLU
SER
SER
GLY

• Molecule 1: Proteasome subunit alpha

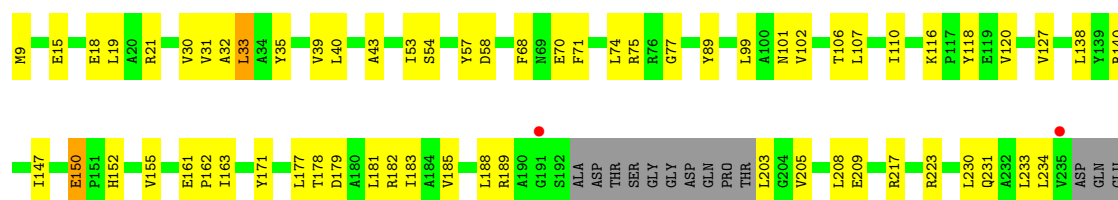
Chain D:  67% 22% 10%



GLY

• Molecule 1: Proteasome subunit alpha

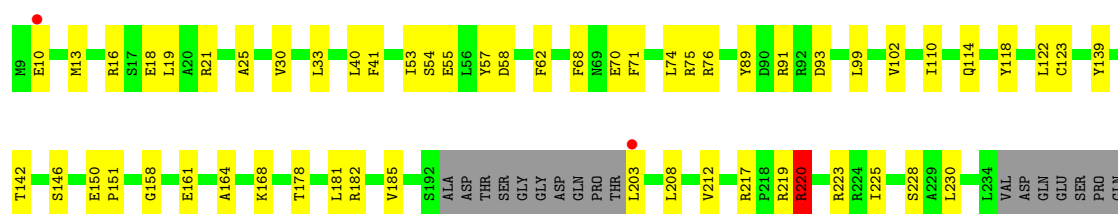
Chain E:  64% 25% 10%



SER
PRO
GLN
SER
SER
ASP
GLY
GLU
SER
SER
GLY

• Molecule 1: Proteasome subunit alpha

Chain F:  67% 23% 10%



SER
ASP
GLY
GLU
SER
SER
SER
GLY

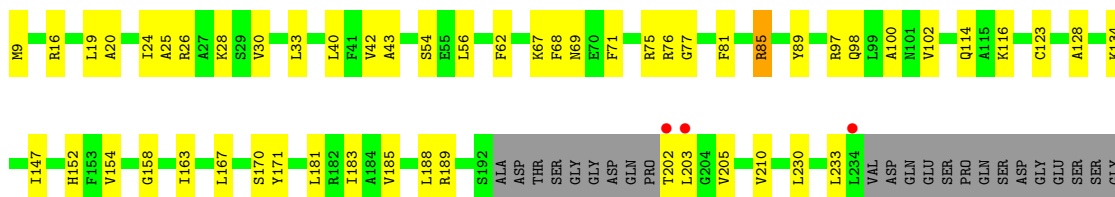
• Molecule 1: Proteasome subunit alpha

Chain G:  74% 16% 10%

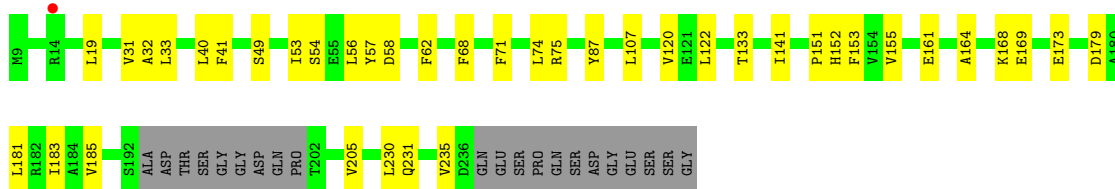




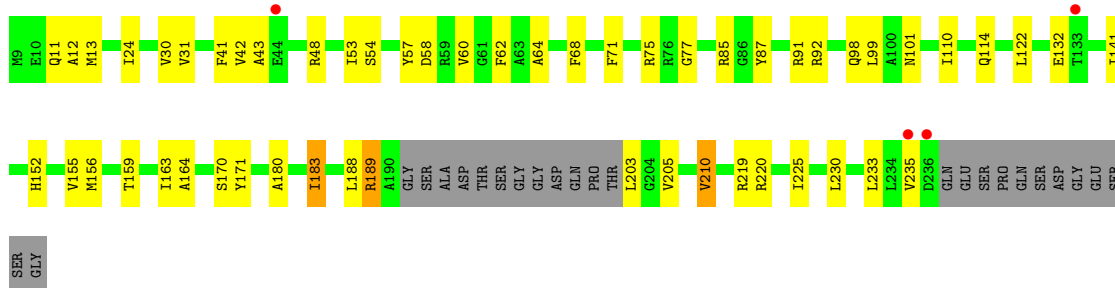
- Molecule 1: Proteasome subunit alpha



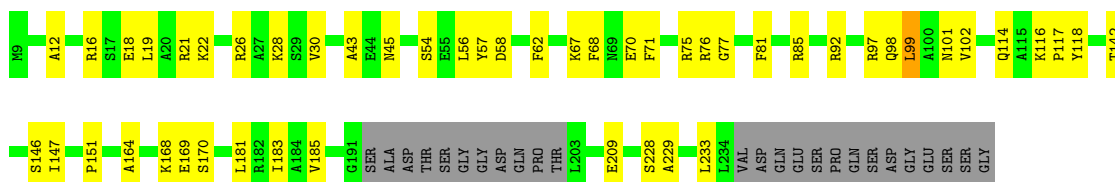
- Molecule 1: Proteasome subunit alpha



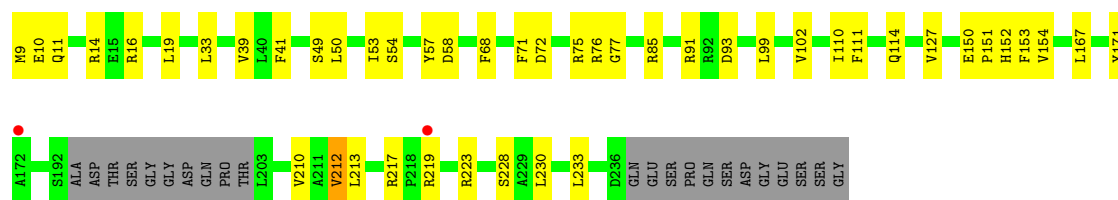
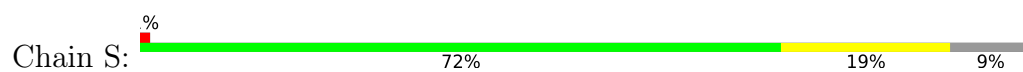
- Molecule 1: Proteasome subunit alpha



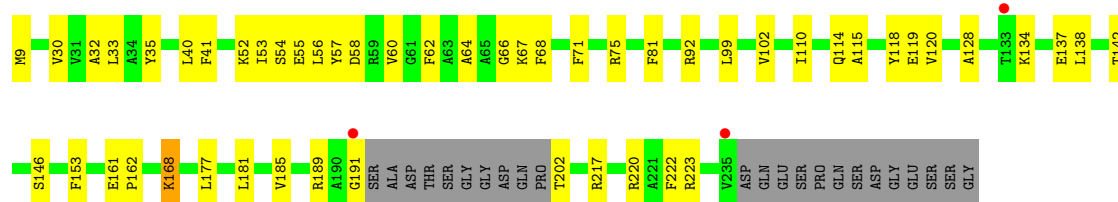
- Molecule 1: Proteasome subunit alpha



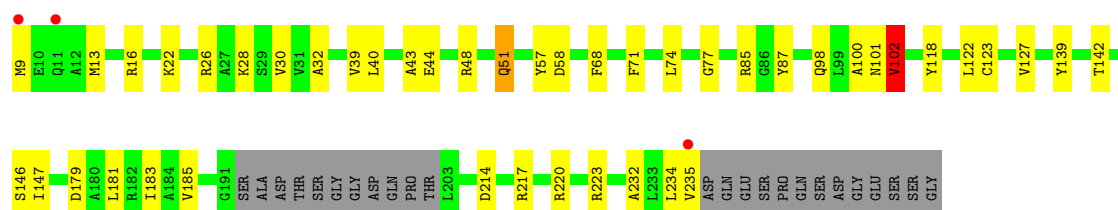
- Molecule 1: Proteasome subunit alpha



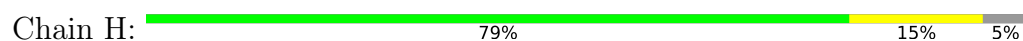
• Molecule 1: Proteasome subunit alpha



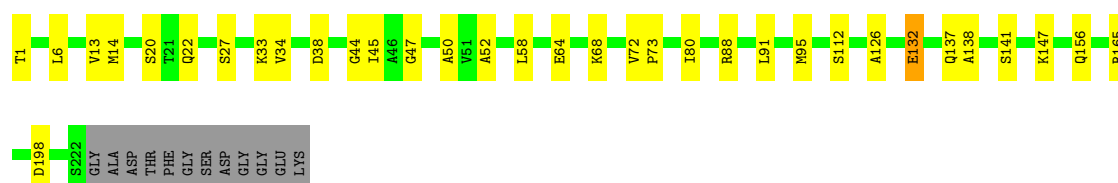
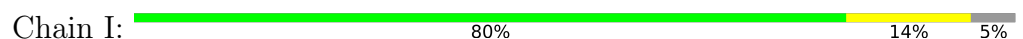
• Molecule 1: Proteasome subunit alpha



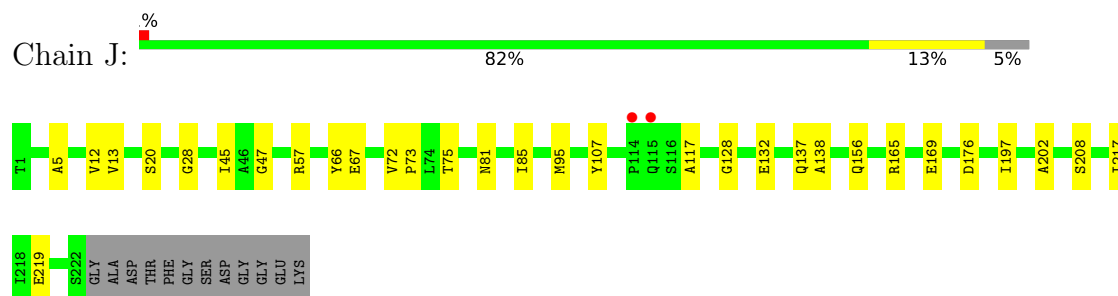
• Molecule 2: Proteasome subunit beta



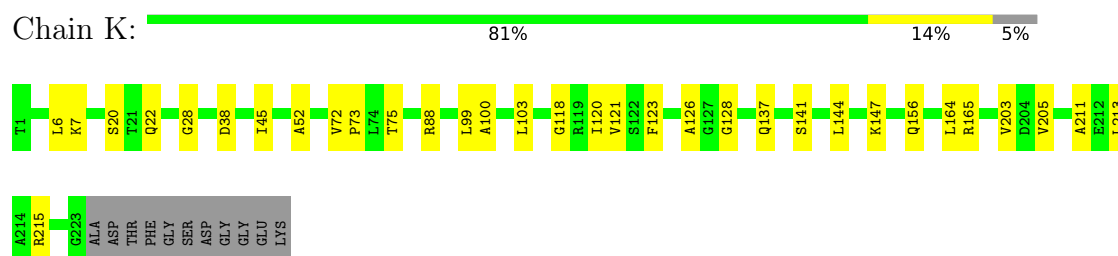
• Molecule 2: Proteasome subunit beta



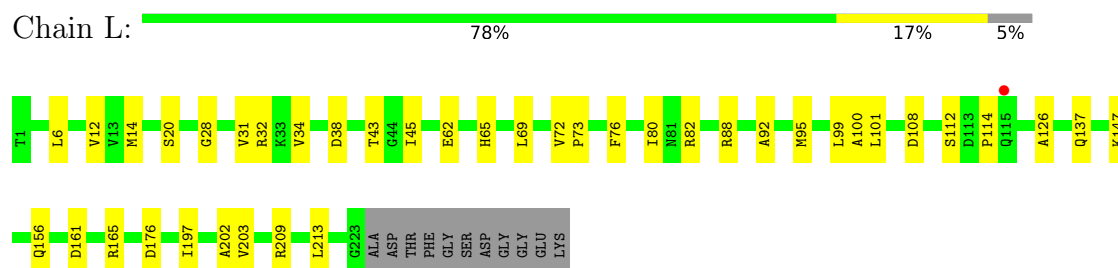
- Molecule 2: Proteasome subunit beta



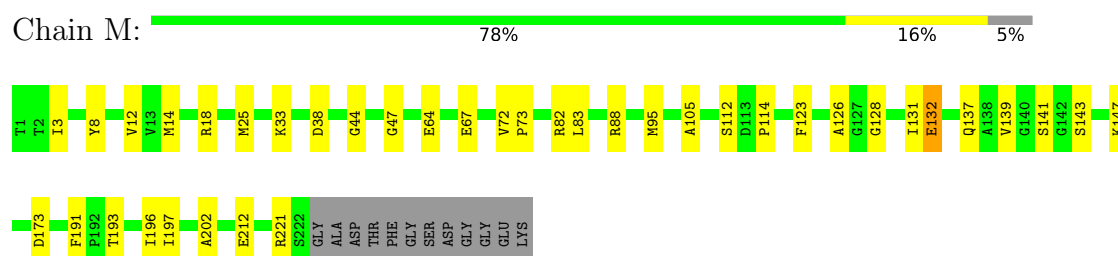
- Molecule 2: Proteasome subunit beta



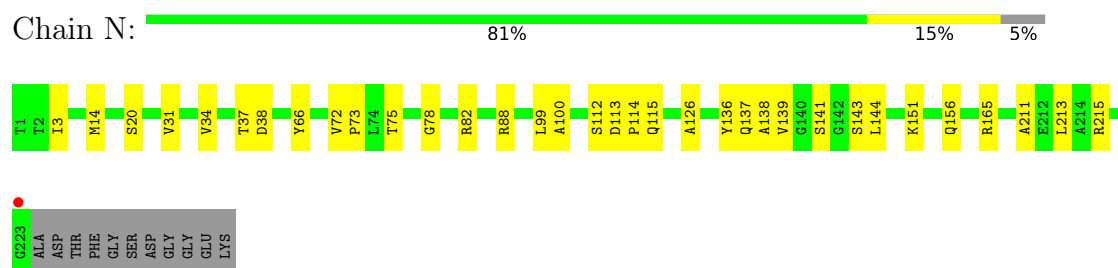
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



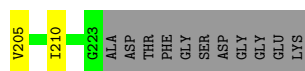
- Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

Chain V:  87% 8% 5%

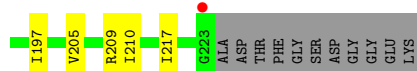
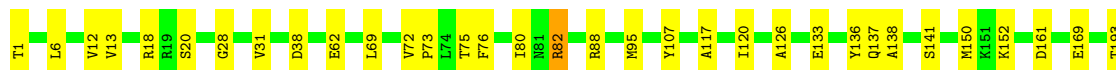
• Molecule 2: Proteasome subunit beta

Chain W:  81% 14% 5%

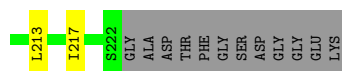
• Molecule 2: Proteasome subunit beta

Chain X:  83% 12% 5%

• Molecule 2: Proteasome subunit beta

Chain Y:  79% 16% 5%

• Molecule 2: Proteasome subunit beta

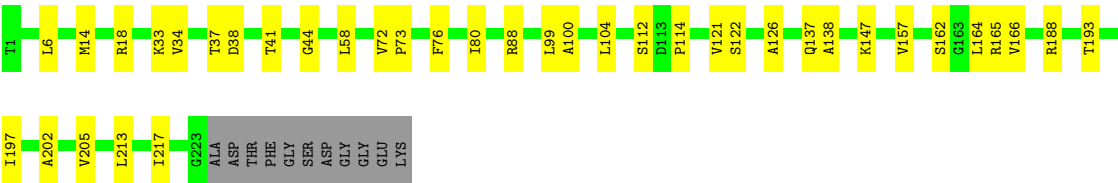
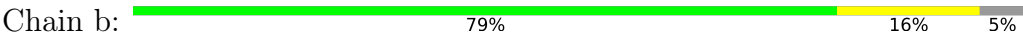
Chain Z:  80% 15% 5%

• Molecule 2: Proteasome subunit beta

Chain a:  82% 13% 5%



● Molecule 2: Proteasome subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.77Å 198.06Å 167.92Å 90.00° 103.72° 90.00°	Depositor
Resolution (Å)	42.92 – 2.65 42.92 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.5 (42.92-2.65) 93.5 (42.92-2.65)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.184 , 0.235 0.187 , 0.237	Depositor DCC
R_{free} test set	10233 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	48235	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, M6Y, DMF

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	0.15	0/1701	0.40	0/2297
1	B	0.14	0/1684	0.38	0/2274
1	C	0.14	0/1696	0.37	0/2290
1	D	0.14	0/1679	0.39	0/2266
1	E	0.14	0/1694	0.38	0/2287
1	F	0.32	1/1687 (0.1%)	0.41	0/2277
1	G	0.14	0/1684	0.38	0/2272
1	O	0.29	0/1694	0.43	1/2287 (0.0%)
1	P	0.14	0/1709	0.39	0/2308
1	Q	0.15	0/1692	0.41	0/2285
1	R	0.15	0/1681	0.41	0/2269
1	S	0.15	0/1702	0.39	0/2298
1	T	0.14	0/1695	0.38	0/2289
1	U	0.27	1/1688 (0.1%)	0.42	0/2279
2	H	0.16	0/1662	0.37	0/2254
2	I	0.16	0/1662	0.36	0/2254
2	J	0.16	0/1662	0.37	0/2254
2	K	0.17	0/1666	0.39	0/2259
2	L	0.15	0/1666	0.37	0/2259
2	M	0.15	0/1662	0.35	0/2254
2	N	0.14	0/1666	0.36	0/2259
2	V	0.25	1/1666 (0.1%)	0.37	0/2259
2	W	0.15	0/1666	0.36	0/2259
2	X	0.15	0/1662	0.36	0/2254
2	Y	0.30	2/1666 (0.1%)	0.38	0/2259
2	Z	0.15	0/1662	0.37	0/2254
2	a	0.24	1/1666 (0.1%)	0.35	0/2259
2	b	0.15	0/1666	0.35	0/2259
All	All	0.18	6/46986 (0.0%)	0.38	1/63574 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	220	ARG	C-O	-6.71	1.16	1.24
2	a	147	LYS	C-O	-6.44	1.16	1.24
2	Y	82	ARG	C-O	-5.36	1.17	1.24
1	U	102	VAL	C-O	-5.28	1.18	1.24
2	V	212	GLU	C-O	-5.15	1.18	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	85	ARG	CG-CD-NE	-5.72	99.41	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1677	0	1680	44	0
1	B	1660	0	1665	44	0
1	C	1672	0	1672	50	0
1	D	1655	0	1653	43	0
1	E	1670	0	1673	49	0
1	F	1663	0	1664	43	0
1	G	1661	0	1659	27	0
1	O	1670	0	1671	48	0
1	P	1685	0	1684	30	0
1	Q	1668	0	1669	42	0
1	R	1657	0	1659	41	0
1	S	1678	0	1677	39	0
1	T	1671	0	1675	38	0
1	U	1664	0	1668	34	0
2	H	1638	0	1633	27	0
2	I	1638	0	1633	24	0
2	J	1638	0	1633	24	0
2	K	1642	0	1636	22	0
2	L	1642	0	1636	29	0
2	M	1638	0	1633	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1642	0	1636	24	0
2	V	1642	0	1636	12	0
2	W	1642	0	1636	26	0
2	X	1638	0	1633	20	0
2	Y	1642	0	1636	26	0
2	Z	1638	0	1633	21	0
2	a	1642	0	1636	23	0
2	b	1642	0	1636	28	0
3	A	5	7	7	0	0
3	B	5	7	7	0	0
3	C	5	7	7	1	0
3	E	5	7	7	2	0
3	F	10	14	14	1	0
3	G	10	14	14	0	0
3	I	5	7	7	1	0
3	J	10	14	14	2	0
3	O	5	7	7	1	0
3	P	5	7	7	0	0
3	Q	5	7	7	1	0
3	R	10	14	14	2	0
3	S	10	14	14	2	0
3	T	5	7	7	0	0
3	U	5	7	7	1	0
4	H	41	0	0	1	0
4	I	41	0	0	1	0
4	J	41	0	0	0	0
4	K	41	0	0	0	0
4	L	41	0	0	0	0
4	M	41	0	0	0	0
4	N	41	0	0	0	0
4	V	41	0	0	0	0
4	W	41	0	0	0	0
4	X	41	0	0	0	0
4	Y	41	0	0	0	0
4	Z	41	0	0	0	0
4	a	41	0	0	0	0
4	b	41	0	0	0	0
5	H	13	5	5	0	0
5	I	13	5	5	3	0
5	J	13	5	5	1	0
5	K	13	5	5	2	0
5	L	13	5	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	13	5	5	2	0
5	N	13	5	5	1	0
5	V	13	5	5	0	0
5	W	13	5	5	1	0
5	X	13	5	5	3	0
5	Y	13	5	5	2	0
5	Z	13	5	5	1	0
5	a	13	5	5	2	0
5	b	13	5	5	0	0
6	A	27	0	0	4	0
6	B	20	0	0	2	0
6	C	29	0	0	2	0
6	D	20	0	0	3	0
6	E	24	0	0	1	0
6	F	16	0	0	0	0
6	G	21	0	0	1	0
6	H	36	0	0	0	0
6	I	49	0	0	2	0
6	J	36	0	0	0	0
6	K	41	0	0	0	0
6	L	42	0	0	1	0
6	M	35	0	0	3	0
6	N	34	0	0	0	0
6	O	17	0	0	3	0
6	P	26	0	0	2	0
6	Q	31	0	0	4	0
6	R	28	0	0	2	0
6	S	28	0	0	3	0
6	T	13	0	0	0	0
6	U	27	0	0	3	0
6	V	42	0	0	0	0
6	W	39	0	0	1	0
6	X	35	0	0	1	0
6	Y	40	0	0	1	0
6	Z	37	0	0	1	0
6	a	29	0	0	0	0
6	b	32	0	0	0	0
All	All	48025	210	46465	833	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 9.

The worst 5 of 833 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:U:217:ARG:HD2	1:U:223:ARG:HH21	0.99	1.08
1:D:9:MET:HE3	1:E:19:LEU:HD13	1.37	1.05
2:X:14:MET:HE3	2:X:34:VAL:HG13	1.37	1.04
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	1.42	1.00
1:U:217:ARG:HD2	1:U:223:ARG:NH2	1.78	0.97

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/240 (89%)	210 (98%)	4 (2%)	0	100	100
1	B	211/240 (88%)	201 (95%)	10 (5%)	0	100	100
1	C	213/240 (89%)	203 (95%)	10 (5%)	0	100	100
1	D	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
1	E	213/240 (89%)	207 (97%)	6 (3%)	0	100	100
1	F	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
1	G	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
1	O	213/240 (89%)	207 (97%)	6 (3%)	0	100	100
1	P	215/240 (90%)	209 (97%)	6 (3%)	0	100	100
1	Q	212/240 (88%)	204 (96%)	8 (4%)	0	100	100
1	R	211/240 (88%)	205 (97%)	5 (2%)	1 (0%)	24	39
1	S	214/240 (89%)	206 (96%)	7 (3%)	1 (0%)	24	39
1	T	213/240 (89%)	205 (96%)	8 (4%)	0	100	100
1	U	212/240 (88%)	203 (96%)	9 (4%)	0	100	100
2	H	220/234 (94%)	215 (98%)	5 (2%)	0	100	100
2	I	220/234 (94%)	210 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	220/234 (94%)	213 (97%)	7 (3%)	0	100	100
2	K	221/234 (94%)	216 (98%)	5 (2%)	0	100	100
2	L	221/234 (94%)	215 (97%)	6 (3%)	0	100	100
2	M	220/234 (94%)	216 (98%)	4 (2%)	0	100	100
2	N	221/234 (94%)	212 (96%)	9 (4%)	0	100	100
2	V	221/234 (94%)	218 (99%)	3 (1%)	0	100	100
2	W	221/234 (94%)	217 (98%)	4 (2%)	0	100	100
2	X	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
2	Y	221/234 (94%)	217 (98%)	4 (2%)	0	100	100
2	Z	220/234 (94%)	215 (98%)	5 (2%)	0	100	100
2	a	221/234 (94%)	215 (97%)	6 (3%)	0	100	100
2	b	221/234 (94%)	218 (99%)	3 (1%)	0	100	100
All	All	6063/6636 (91%)	5888 (97%)	173 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	151	PRO
1	R	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	167/184 (91%)	165 (99%)	2 (1%)	63	79
1	B	165/184 (90%)	163 (99%)	2 (1%)	63	79
1	C	166/184 (90%)	162 (98%)	4 (2%)	43	65
1	D	164/184 (89%)	160 (98%)	4 (2%)	43	65
1	E	166/184 (90%)	163 (98%)	3 (2%)	51	72
1	F	165/184 (90%)	162 (98%)	3 (2%)	51	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	165/184 (90%)	165 (100%)	0	100	100
1	O	166/184 (90%)	166 (100%)	0	100	100
1	P	168/184 (91%)	166 (99%)	2 (1%)	63	79
1	Q	166/184 (90%)	159 (96%)	7 (4%)	26	45
1	R	164/184 (89%)	161 (98%)	3 (2%)	51	72
1	S	167/184 (91%)	164 (98%)	3 (2%)	51	72
1	T	166/184 (90%)	165 (99%)	1 (1%)	78	88
1	U	165/184 (90%)	163 (99%)	2 (1%)	63	79
2	H	165/172 (96%)	162 (98%)	3 (2%)	51	72
2	I	165/172 (96%)	163 (99%)	2 (1%)	63	79
2	J	165/172 (96%)	163 (99%)	2 (1%)	63	79
2	K	165/172 (96%)	163 (99%)	2 (1%)	63	79
2	L	165/172 (96%)	164 (99%)	1 (1%)	78	88
2	M	165/172 (96%)	164 (99%)	1 (1%)	78	88
2	N	165/172 (96%)	164 (99%)	1 (1%)	78	88
2	V	165/172 (96%)	164 (99%)	1 (1%)	78	88
2	W	165/172 (96%)	164 (99%)	1 (1%)	78	88
2	X	165/172 (96%)	163 (99%)	2 (1%)	63	79
2	Y	165/172 (96%)	163 (99%)	2 (1%)	63	79
2	Z	165/172 (96%)	163 (99%)	2 (1%)	63	79
2	a	165/172 (96%)	163 (99%)	2 (1%)	63	79
2	b	165/172 (96%)	164 (99%)	1 (1%)	78	88
All	All	4630/4984 (93%)	4571 (99%)	59 (1%)	61	77

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	132	GLU
2	Z	144	LEU
1	Q	183	ILE
2	Z	31	VAL
2	W	57	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	174	ASN
2	Z	130	ASN
1	T	105	GLN
2	V	130	ASN
2	b	22	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

48 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	DMF	J	304	-	4,4,4	0.46	0	4,4,4	0.47	0
5	CIT	H	302	-	12,12,12	1.05	0	17,17,17	1.47	2 (11%)
3	DMF	F	301	-	4,4,4	0.36	0	4,4,4	0.43	0
4	M6Y	H	301	-	44,44,44	2.86	13 (29%)	58,61,61	2.16	15 (25%)
4	M6Y	J	301	-	44,44,44	2.85	14 (31%)	58,61,61	2.20	17 (29%)
4	M6Y	a	301	-	44,44,44	2.85	13 (29%)	58,61,61	2.17	15 (25%)
5	CIT	J	302	-	12,12,12	1.09	0	17,17,17	1.50	2 (11%)
4	M6Y	M	301	-	44,44,44	2.85	13 (29%)	58,61,61	2.12	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	M6Y	X	301	-	44,44,44	2.83	14 (31%)	58,61,61	2.13	18 (31%)
5	CIT	I	302	-	12,12,12	1.11	0	17,17,17	1.45	2 (11%)
3	DMF	R	301	-	4,4,4	0.37	0	4,4,4	0.44	0
4	M6Y	W	301	-	44,44,44	2.82	13 (29%)	58,61,61	2.21	20 (34%)
5	CIT	Z	302	-	12,12,12	1.02	0	17,17,17	1.54	1 (5%)
3	DMF	A	301	-	4,4,4	0.38	0	4,4,4	0.40	0
3	DMF	B	301	-	4,4,4	0.40	0	4,4,4	0.41	0
3	DMF	F	302	-	4,4,4	0.39	0	4,4,4	0.40	0
4	M6Y	b	301	-	44,44,44	3.63	27 (61%)	58,61,61	2.32	23 (39%)
3	DMF	G	301	-	4,4,4	0.36	0	4,4,4	0.35	0
4	M6Y	Z	301	-	44,44,44	2.84	13 (29%)	58,61,61	2.10	18 (31%)
5	CIT	V	302	-	12,12,12	1.11	0	17,17,17	1.38	1 (5%)
4	M6Y	V	301	-	44,44,44	2.88	13 (29%)	58,61,61	2.14	16 (27%)
4	M6Y	I	301	-	44,44,44	2.85	13 (29%)	58,61,61	2.14	15 (25%)
5	CIT	b	302	-	12,12,12	1.07	0	17,17,17	1.57	3 (17%)
3	DMF	O	301	-	4,4,4	0.34	0	4,4,4	0.33	0
4	M6Y	N	301	-	44,44,44	2.84	13 (29%)	58,61,61	2.13	16 (27%)
3	DMF	U	301	-	4,4,4	0.36	0	4,4,4	0.43	0
3	DMF	R	302	-	4,4,4	0.37	0	4,4,4	0.46	0
5	CIT	a	302	-	12,12,12	1.07	0	17,17,17	1.43	1 (5%)
3	DMF	C	301	-	4,4,4	0.40	0	4,4,4	0.46	0
3	DMF	S	301	-	4,4,4	0.42	0	4,4,4	0.46	0
5	CIT	N	302	-	12,12,12	1.06	0	17,17,17	1.49	2 (11%)
3	DMF	J	303	-	4,4,4	0.39	0	4,4,4	0.47	0
3	DMF	Q	301	-	4,4,4	0.37	0	4,4,4	0.34	0
3	DMF	E	301	-	4,4,4	0.39	0	4,4,4	0.38	0
5	CIT	M	302	-	12,12,12	1.03	0	17,17,17	1.70	5 (29%)
5	CIT	W	302	-	12,12,12	1.08	0	17,17,17	1.46	2 (11%)
5	CIT	L	302	-	12,12,12	1.04	0	17,17,17	1.59	3 (17%)
5	CIT	Y	302	-	12,12,12	1.07	0	17,17,17	1.48	1 (5%)
3	DMF	I	303	-	4,4,4	0.43	0	4,4,4	0.38	0
4	M6Y	K	301	-	44,44,44	2.85	13 (29%)	58,61,61	2.15	16 (27%)
5	CIT	X	302	-	12,12,12	1.08	0	17,17,17	1.42	1 (5%)
3	DMF	G	302	-	4,4,4	0.40	0	4,4,4	0.45	0
3	DMF	S	302	-	4,4,4	0.43	0	4,4,4	0.39	0
4	M6Y	L	301	-	44,44,44	2.87	14 (31%)	58,61,61	2.12	15 (25%)
5	CIT	K	302	-	12,12,12	1.01	0	17,17,17	1.64	3 (17%)
3	DMF	T	301	-	4,4,4	0.39	0	4,4,4	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	M6Y	Y	301	-	44,44,44	2.85	13 (29%)	58,61,61	2.20	18 (31%)
3	DMF	P	301	-	4,4,4	0.37	0	4,4,4	0.33	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
3	DMF	J	304	-	-	0/2/2/2	-
5	CIT	H	302	-	-	4/16/16/16	-
3	DMF	F	301	-	-	0/2/2/2	-
4	M6Y	H	301	-	-	0/37/47/47	0/4/4/4
4	M6Y	J	301	-	-	4/37/47/47	0/4/4/4
4	M6Y	a	301	-	-	4/37/47/47	0/4/4/4
5	CIT	J	302	-	-	1/16/16/16	-
4	M6Y	M	301	-	-	1/37/47/47	0/4/4/4
4	M6Y	X	301	-	-	4/37/47/47	0/4/4/4
5	CIT	I	302	-	-	2/16/16/16	-
3	DMF	R	301	-	-	2/2/2/2	-
4	M6Y	W	301	-	-	6/37/47/47	0/4/4/4
5	CIT	Z	302	-	-	7/16/16/16	-
3	DMF	A	301	-	-	0/2/2/2	-
3	DMF	B	301	-	-	0/2/2/2	-
3	DMF	F	302	-	-	0/2/2/2	-
4	M6Y	b	301	-	-	6/37/47/47	0/4/4/4
3	DMF	G	301	-	-	0/2/2/2	-
4	M6Y	Z	301	-	-	7/37/47/47	0/4/4/4
5	CIT	V	302	-	-	1/16/16/16	-
4	M6Y	V	301	-	-	6/37/47/47	0/4/4/4
4	M6Y	I	301	-	-	4/37/47/47	0/4/4/4
5	CIT	b	302	-	-	3/16/16/16	-
3	DMF	O	301	-	-	2/2/2/2	-
4	M6Y	N	301	-	-	1/37/47/47	0/4/4/4
3	DMF	U	301	-	-	2/2/2/2	-
3	DMF	R	302	-	-	2/2/2/2	-
5	CIT	a	302	-	-	7/16/16/16	-
3	DMF	C	301	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	S	301	-	-	0/2/2/2	-
5	CIT	N	302	-	-	9/16/16/16	-
3	DMF	J	303	-	-	2/2/2/2	-
3	DMF	Q	301	-	-	0/2/2/2	-
3	DMF	E	301	-	-	0/2/2/2	-
5	CIT	M	302	-	-	8/16/16/16	-
5	CIT	W	302	-	-	3/16/16/16	-
5	CIT	L	302	-	-	9/16/16/16	-
5	CIT	Y	302	-	-	5/16/16/16	-
3	DMF	I	303	-	-	0/2/2/2	-
4	M6Y	K	301	-	-	4/37/47/47	0/4/4/4
5	CIT	X	302	-	-	1/16/16/16	-
3	DMF	G	302	-	-	2/2/2/2	-
3	DMF	S	302	-	-	0/2/2/2	-
4	M6Y	L	301	-	-	5/37/47/47	0/4/4/4
5	CIT	K	302	-	-	4/16/16/16	-
3	DMF	T	301	-	-	2/2/2/2	-
4	M6Y	Y	301	-	-	5/37/47/47	0/4/4/4
3	DMF	P	301	-	-	0/2/2/2	-

The worst 5 of 199 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	301	M6Y	C11-N10	-10.13	1.28	1.47
4	V	301	M6Y	C14-N10	9.89	1.63	1.47
4	Y	301	M6Y	C14-N10	9.79	1.63	1.47
4	H	301	M6Y	C14-N10	9.78	1.63	1.47
4	K	301	M6Y	C14-N10	9.77	1.63	1.47

The worst 5 of 266 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	301	M6Y	O28-C26-C27	8.25	127.24	115.89
4	N	301	M6Y	O28-C26-C27	8.05	126.96	115.89
4	M	301	M6Y	O28-C26-C27	8.00	126.90	115.89
4	V	301	M6Y	O28-C26-C27	8.00	126.89	115.89
4	I	301	M6Y	O28-C26-C27	7.90	126.76	115.89

There are no chirality outliers.

5 of 137 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	301	M6Y	O23-C22-C24-C25
4	I	301	M6Y	N21-C22-C24-C25
4	I	301	M6Y	O23-C22-C24-N29
4	I	301	M6Y	N21-C22-C24-N29
4	J	301	M6Y	O23-C22-C24-C25

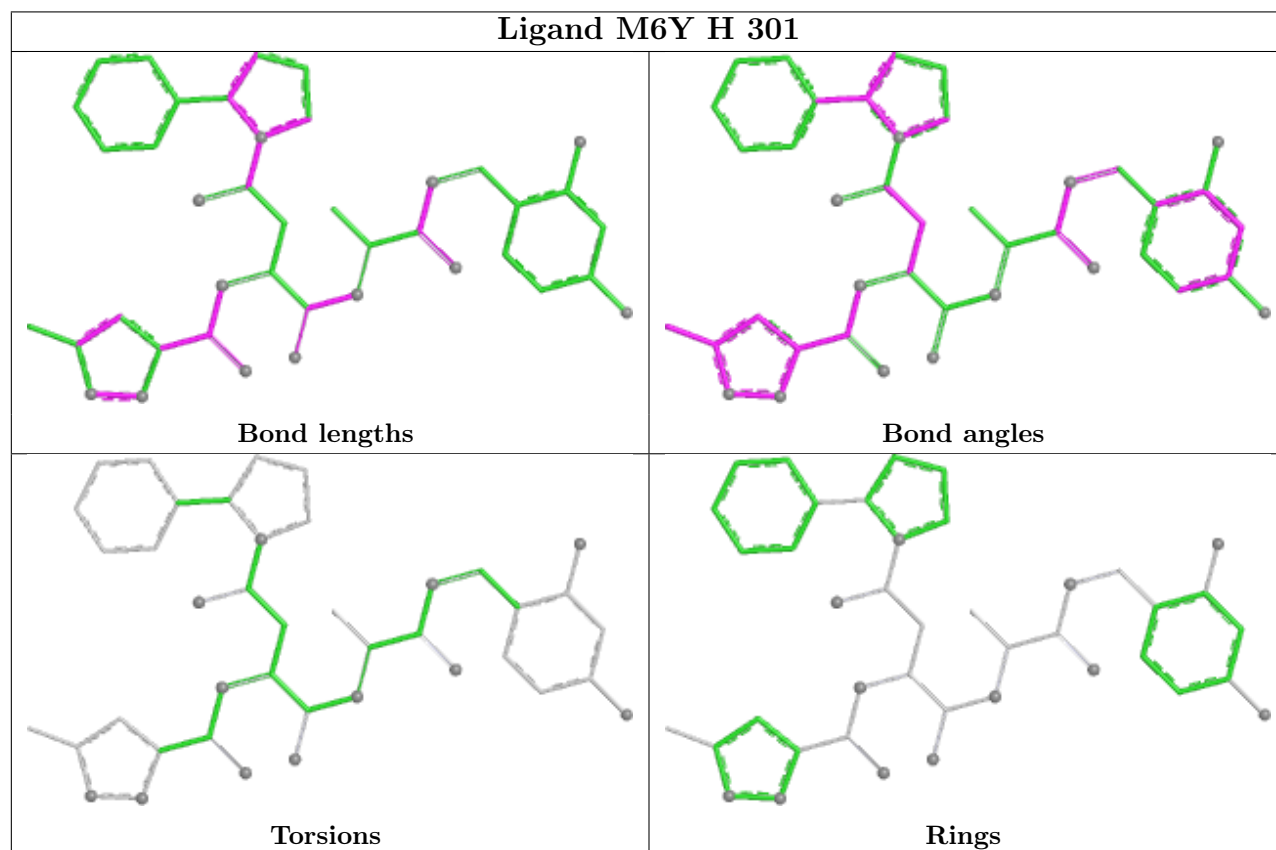
There are no ring outliers.

23 monomers are involved in 34 short contacts:

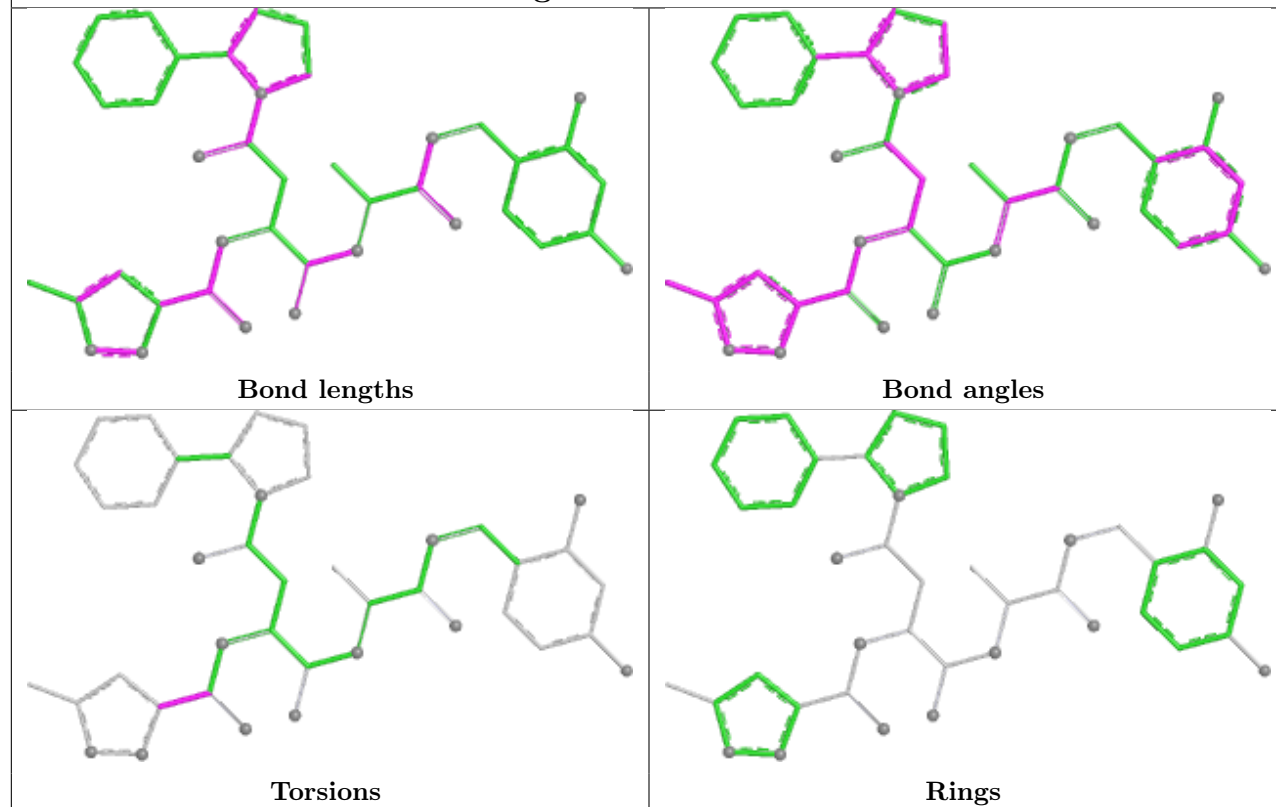
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	304	DMF	1	0
3	F	301	DMF	1	0
4	H	301	M6Y	1	0
5	J	302	CIT	1	0
5	I	302	CIT	3	0
3	R	301	DMF	2	0
5	Z	302	CIT	1	0
4	I	301	M6Y	1	0
3	O	301	DMF	1	0
3	U	301	DMF	1	0
5	a	302	CIT	2	0
3	C	301	DMF	1	0
3	S	301	DMF	2	0
5	N	302	CIT	1	0
3	J	303	DMF	1	0
3	Q	301	DMF	1	0
3	E	301	DMF	2	0
5	M	302	CIT	2	0
5	W	302	CIT	1	0
5	Y	302	CIT	2	0
3	I	303	DMF	1	0
5	X	302	CIT	3	0
5	K	302	CIT	2	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

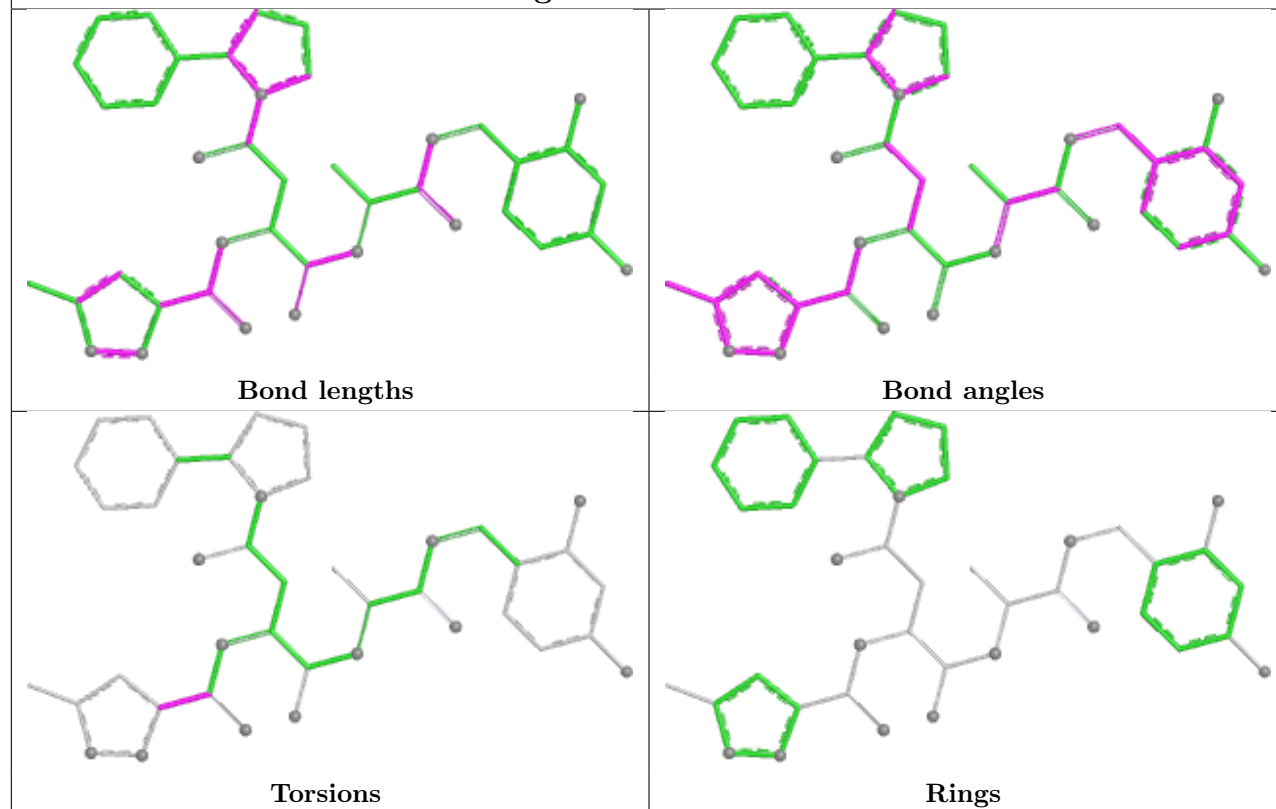
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

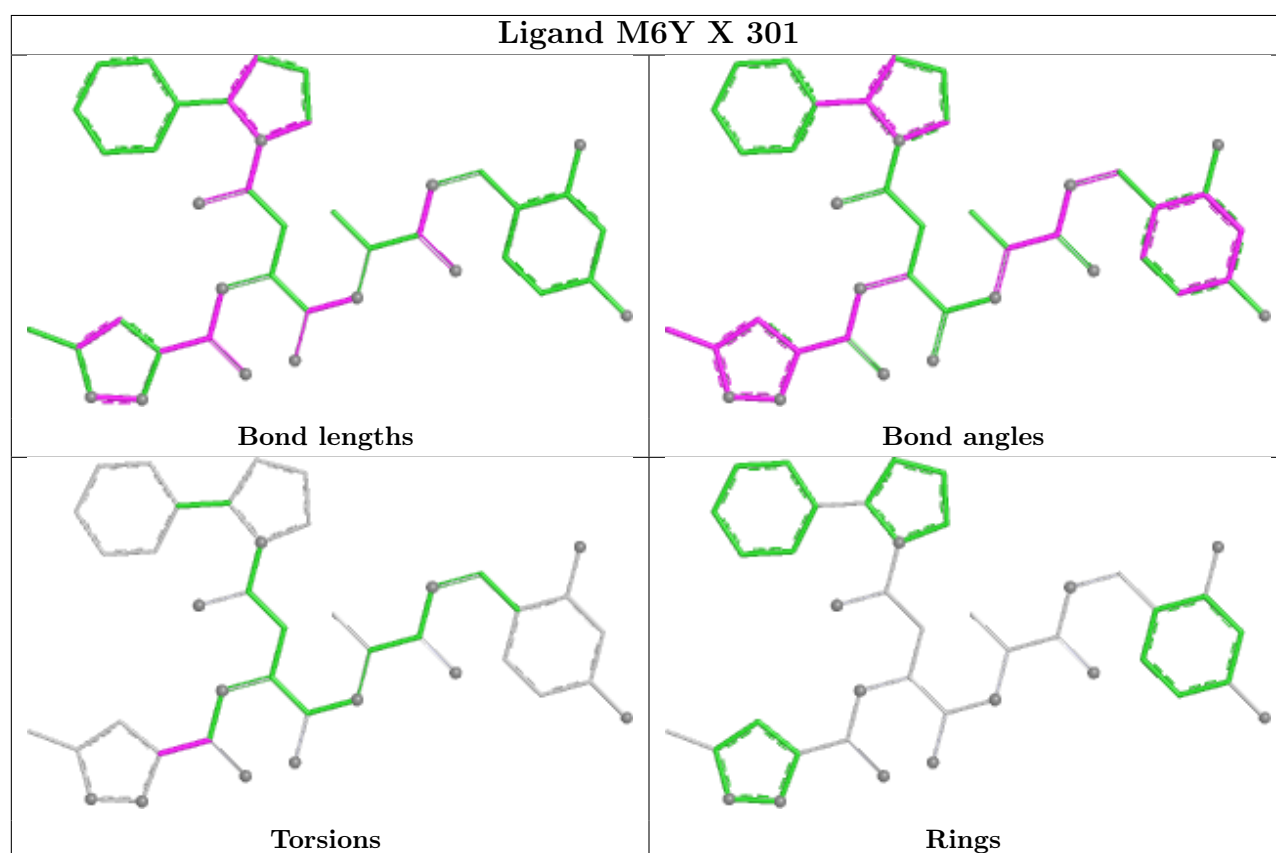
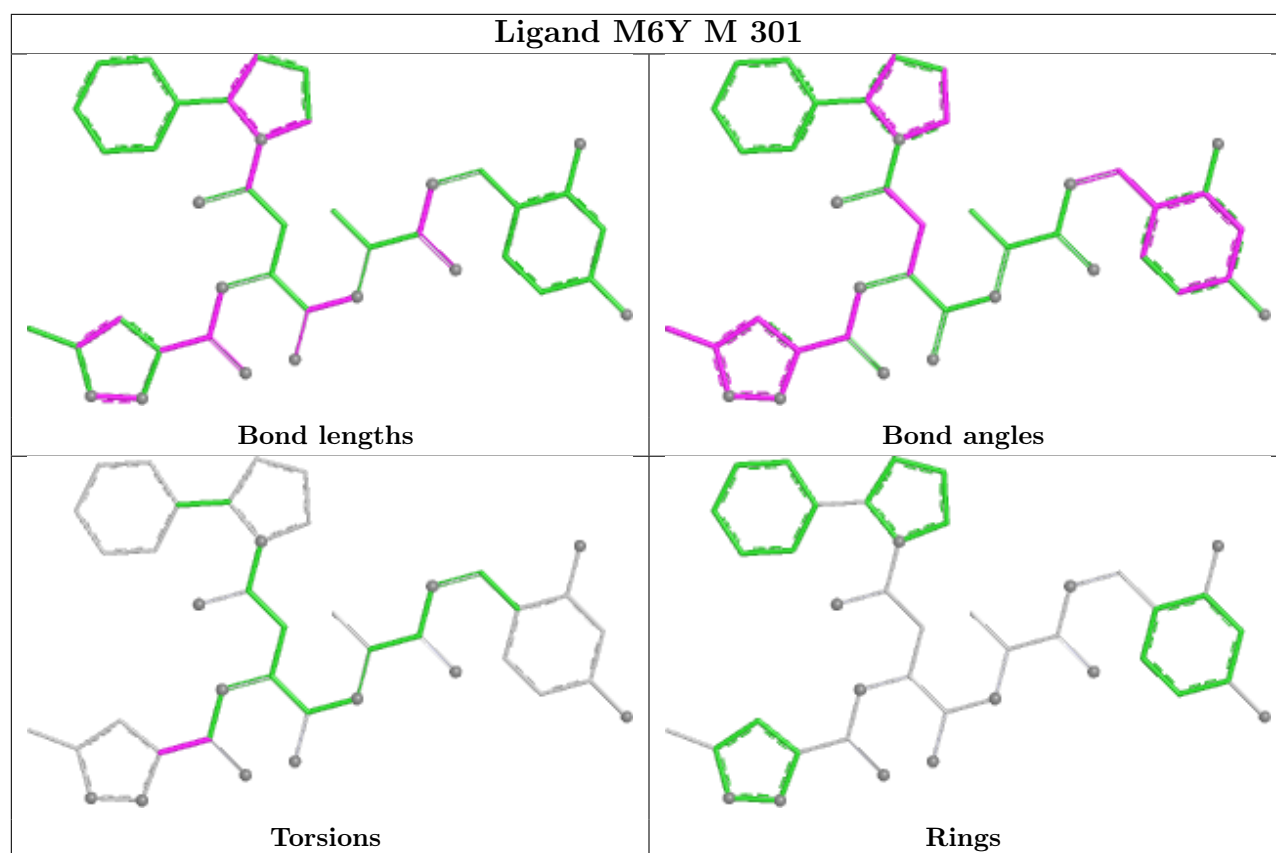


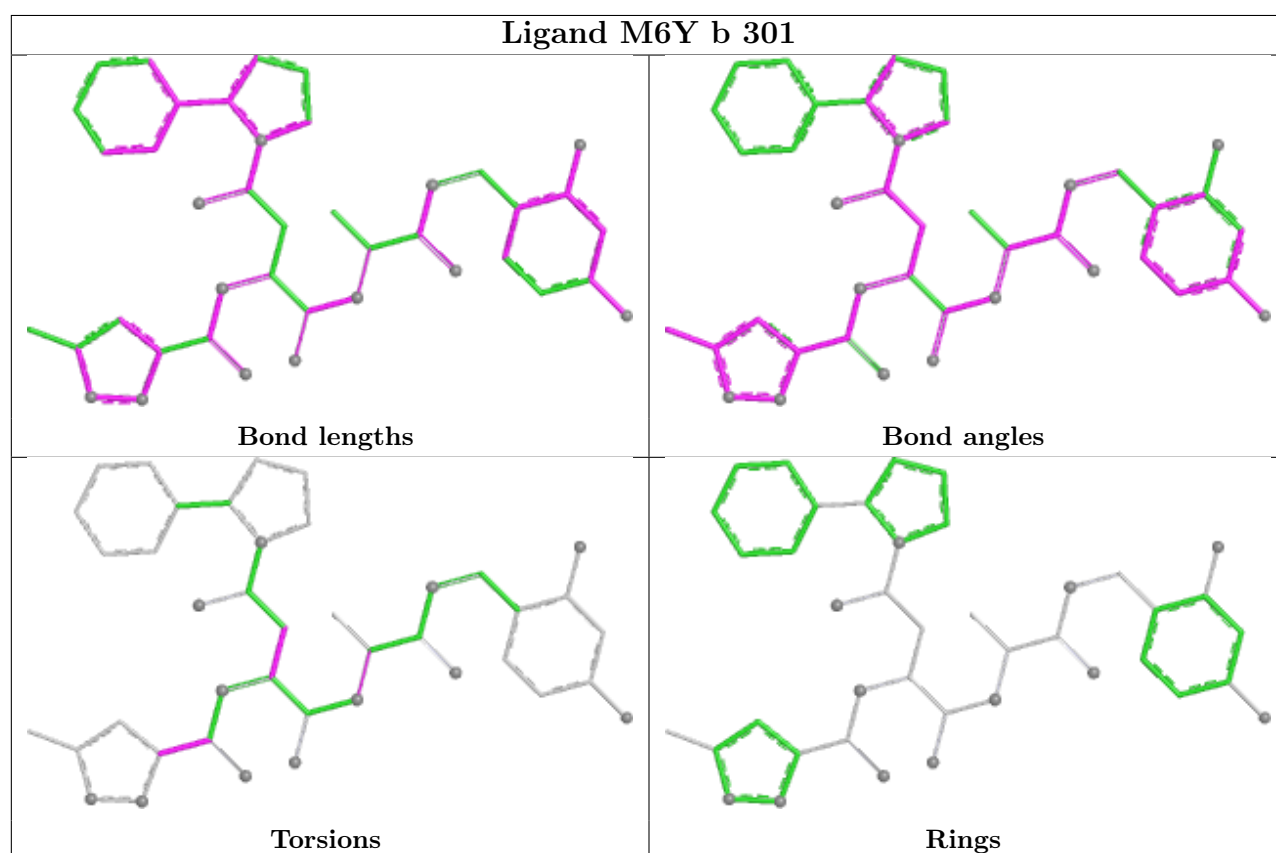
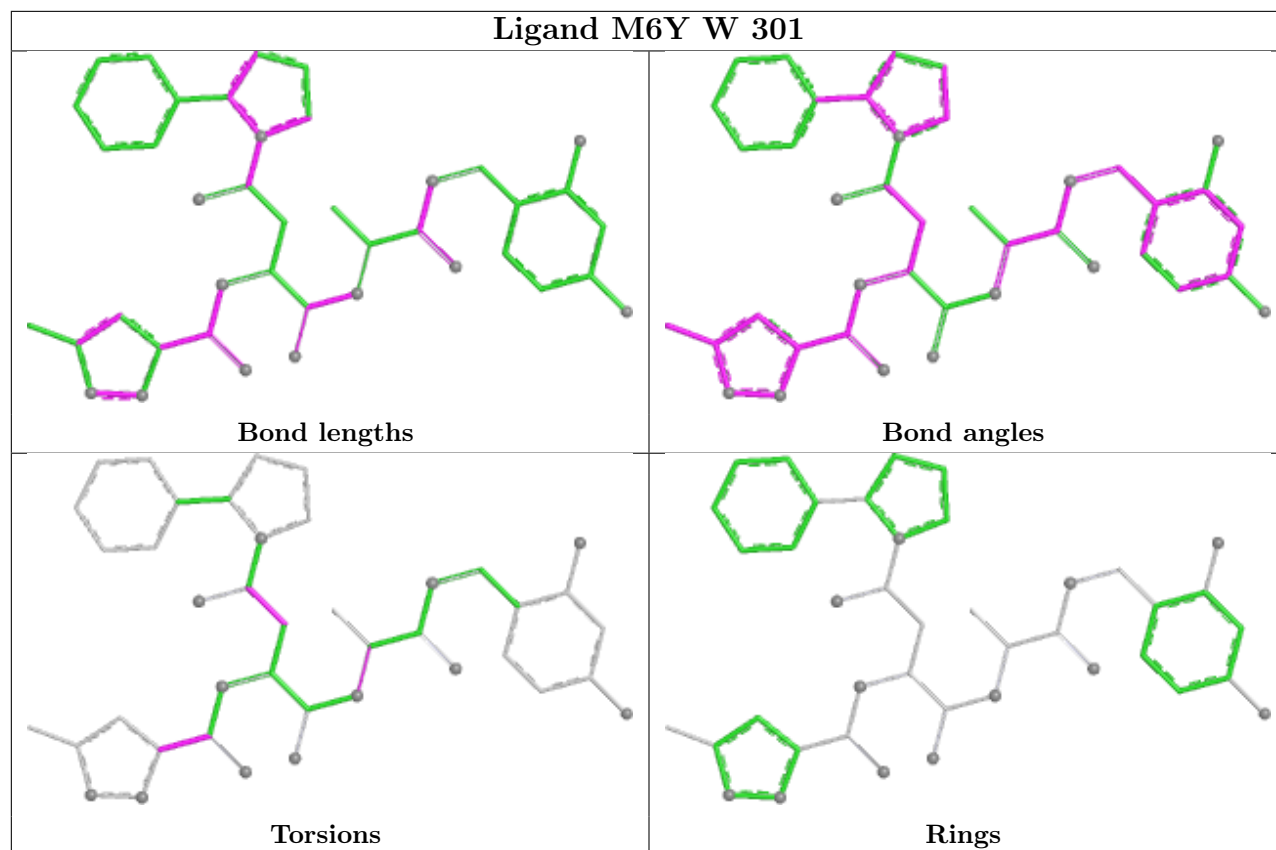
Ligand M6Y J 301



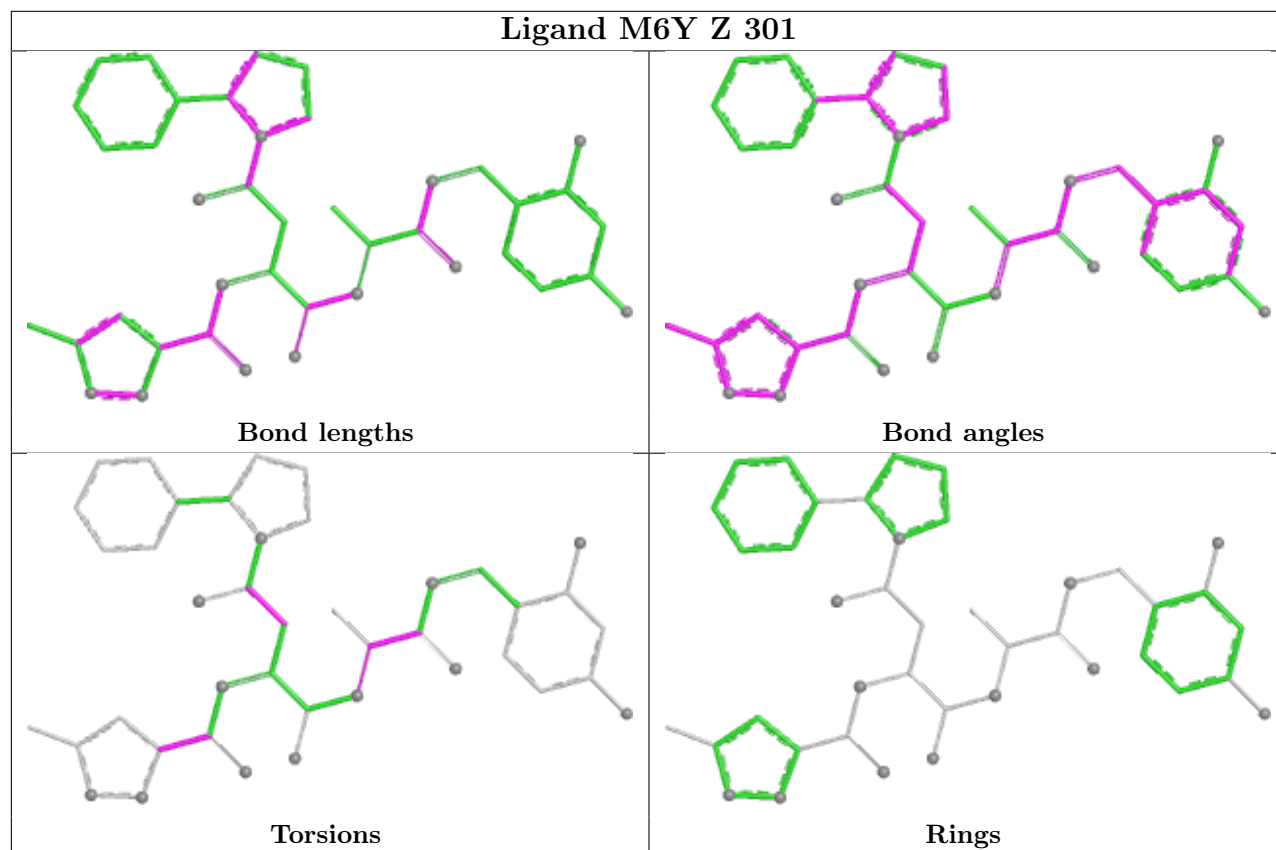
Ligand M6Y a 301



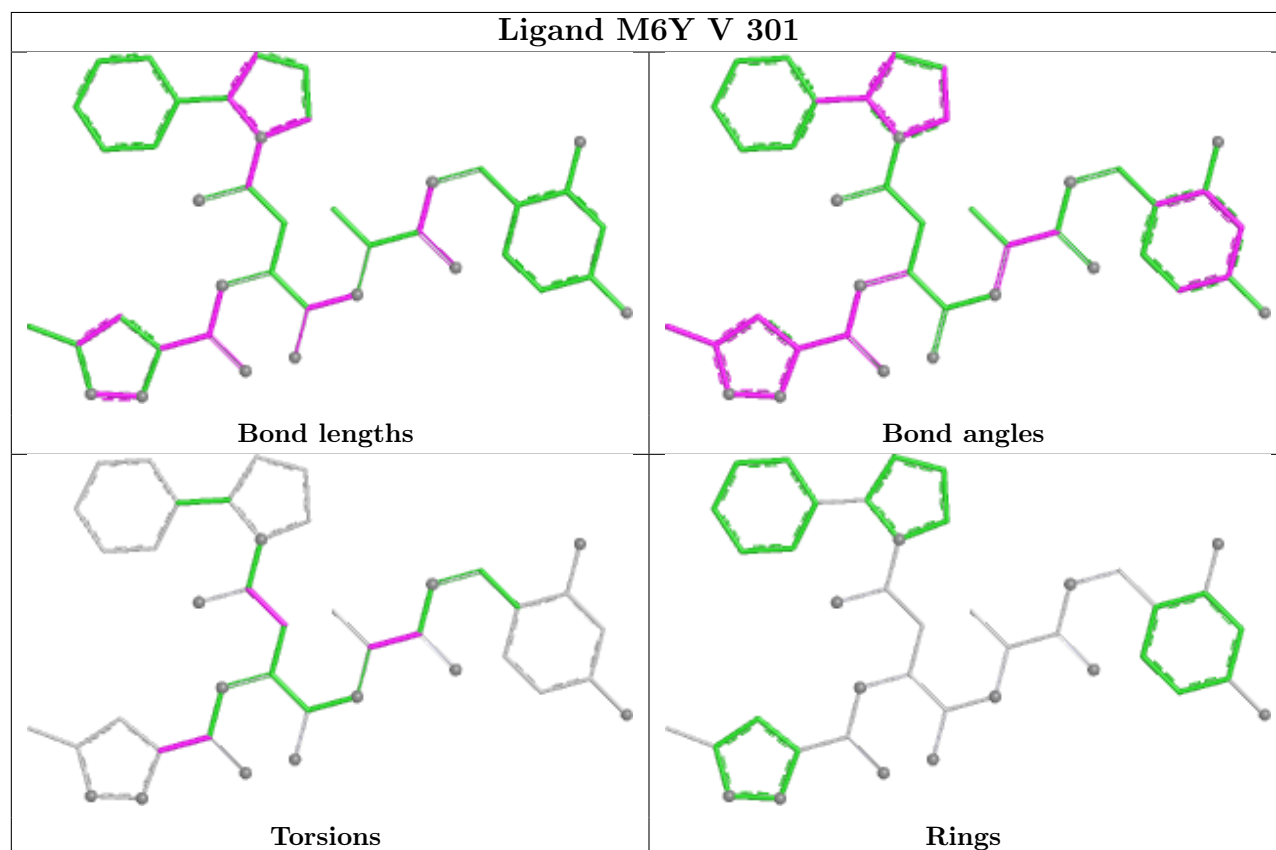




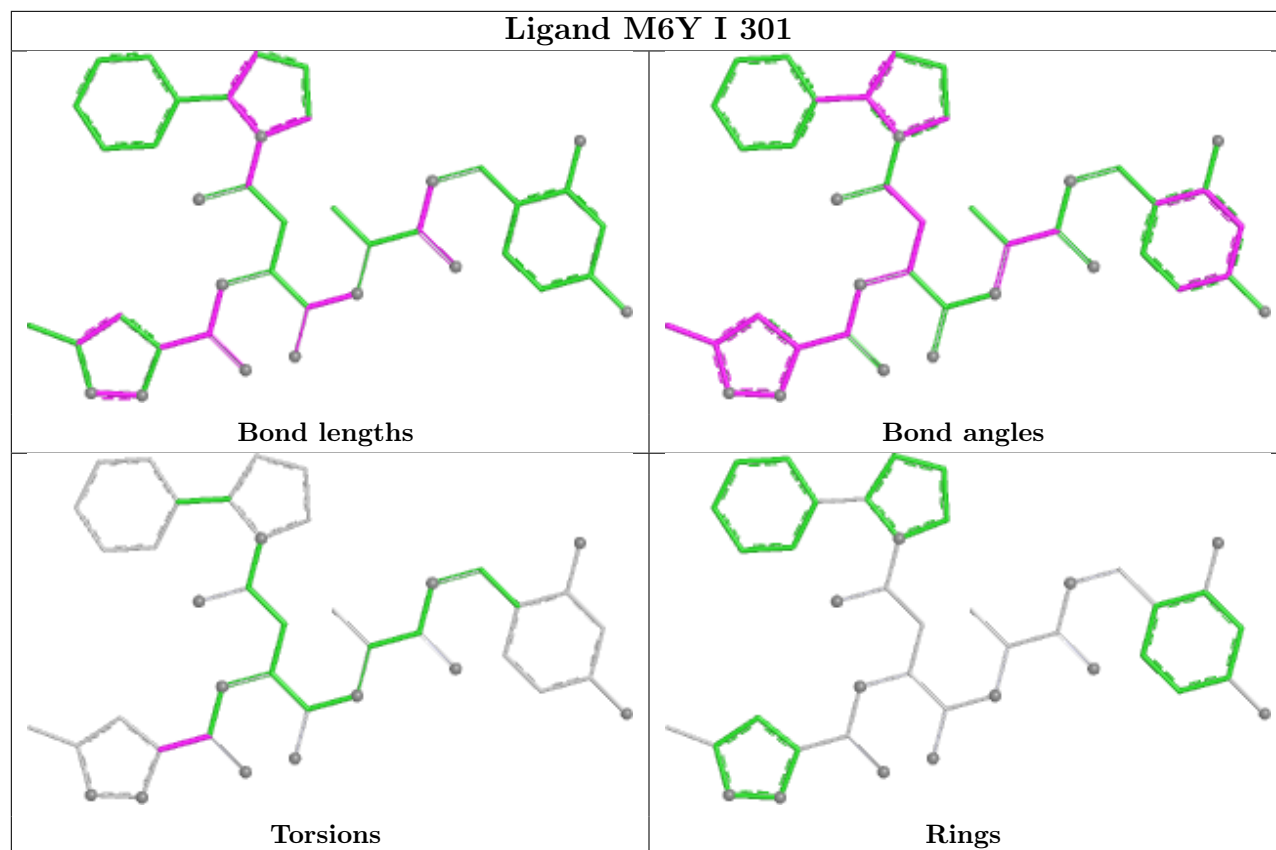
Ligand M6Y Z 301



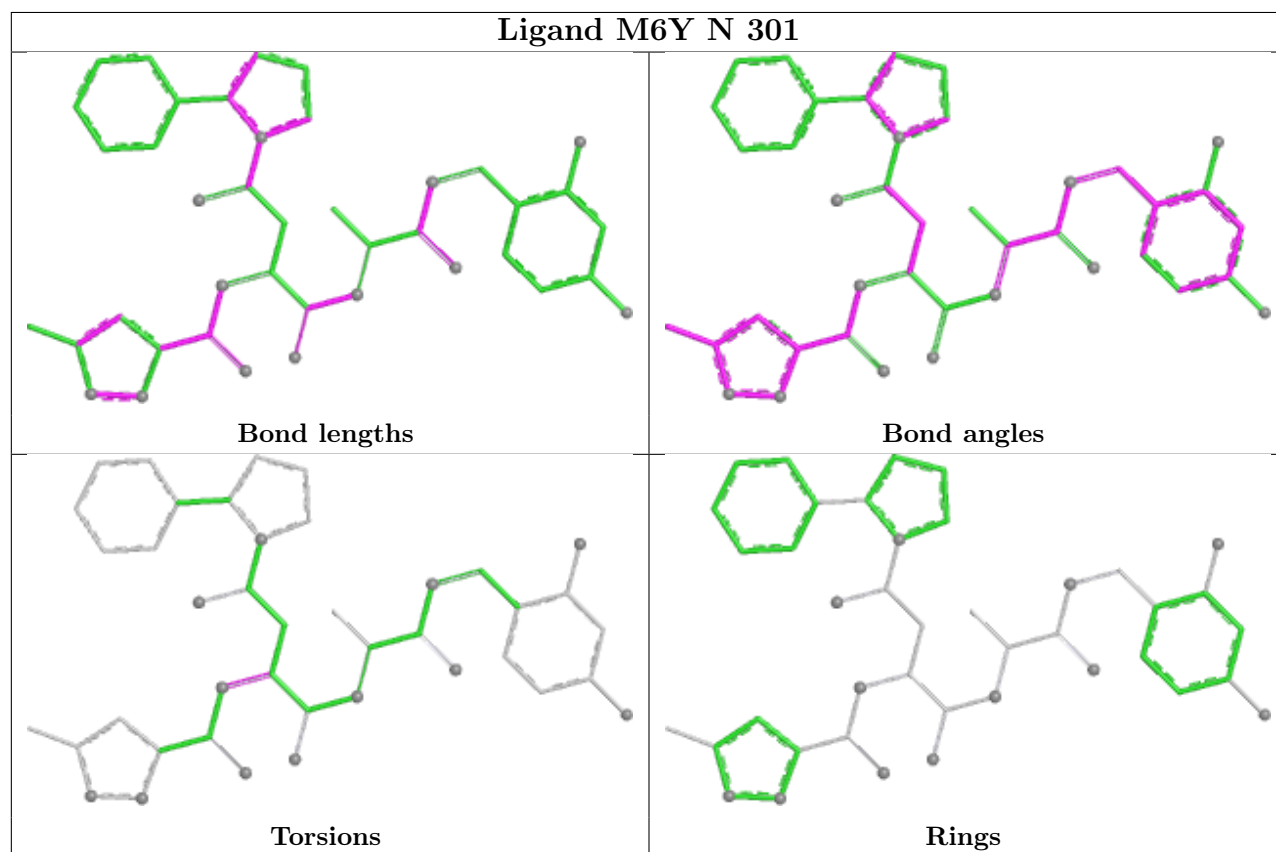
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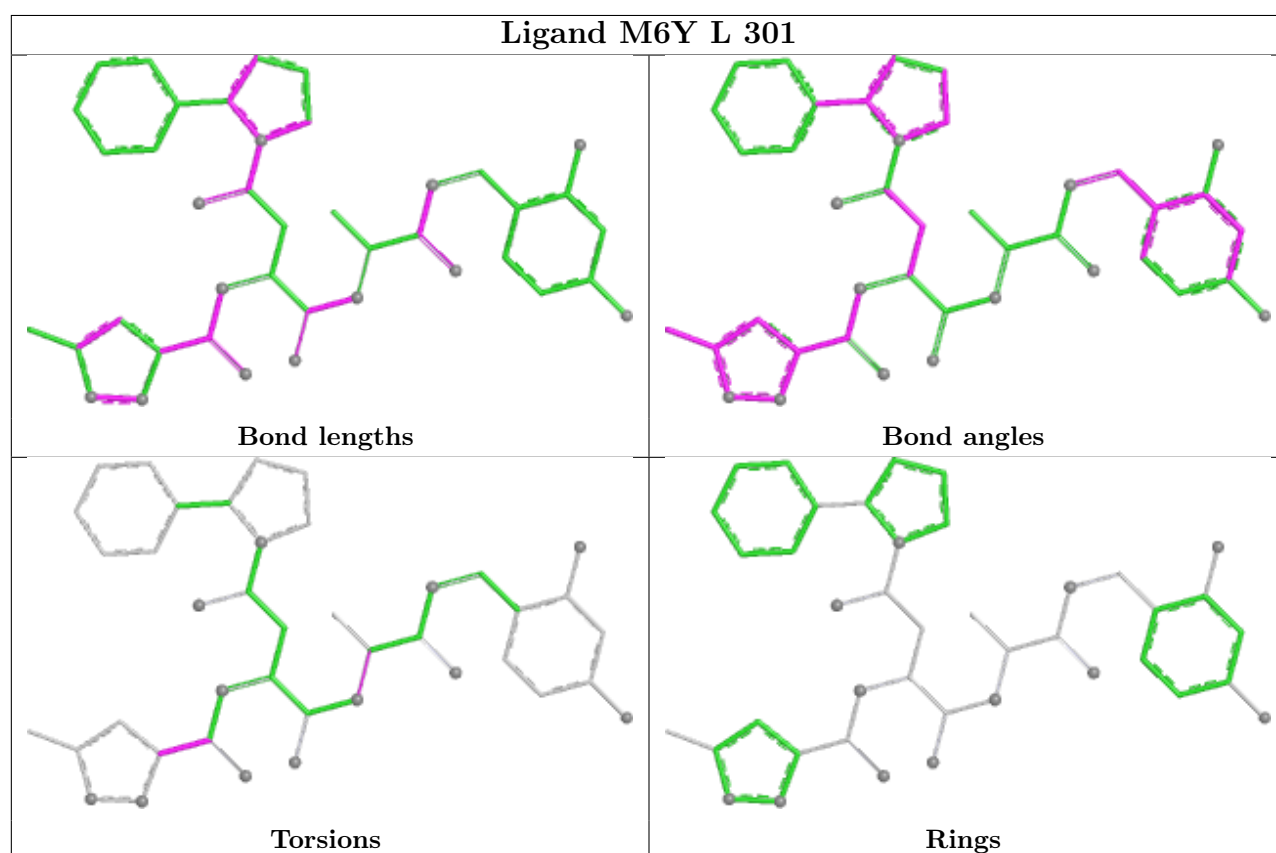
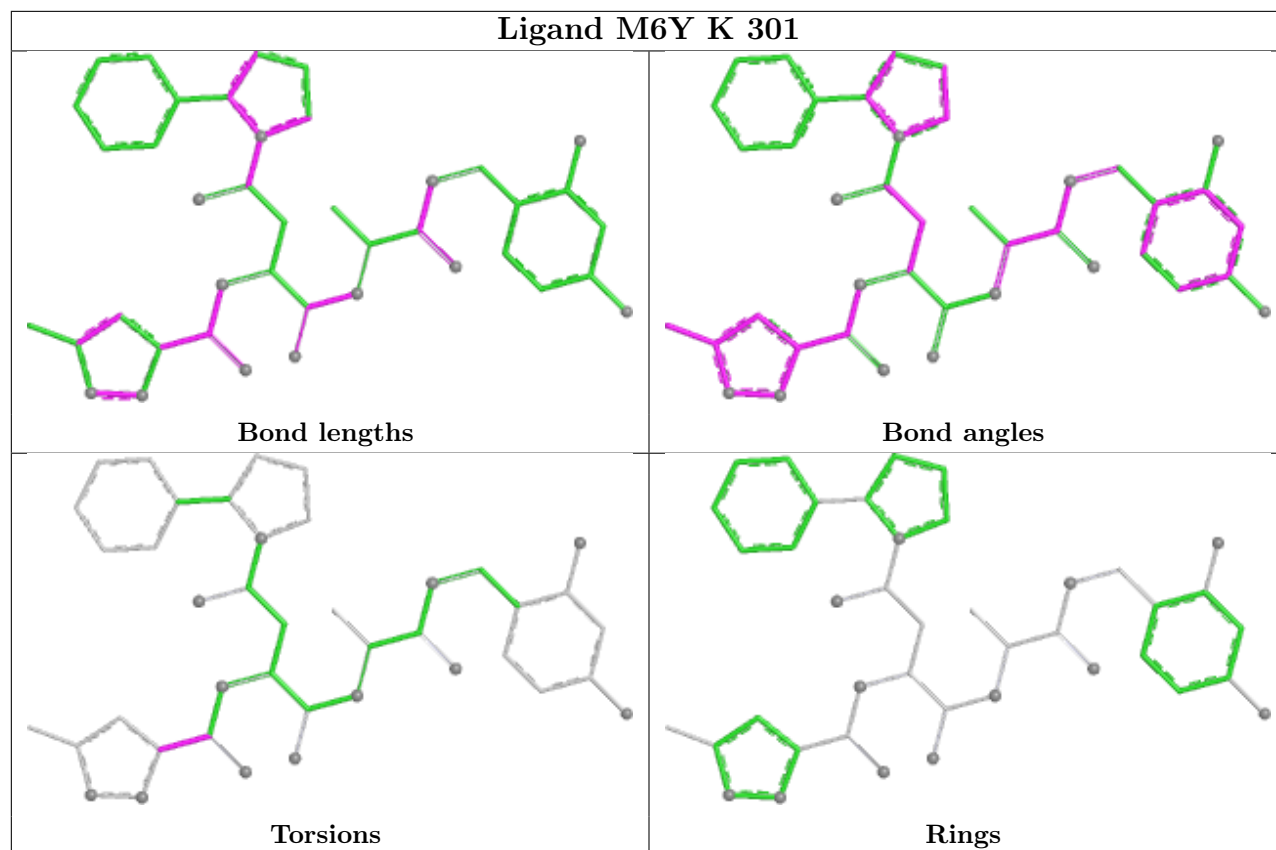


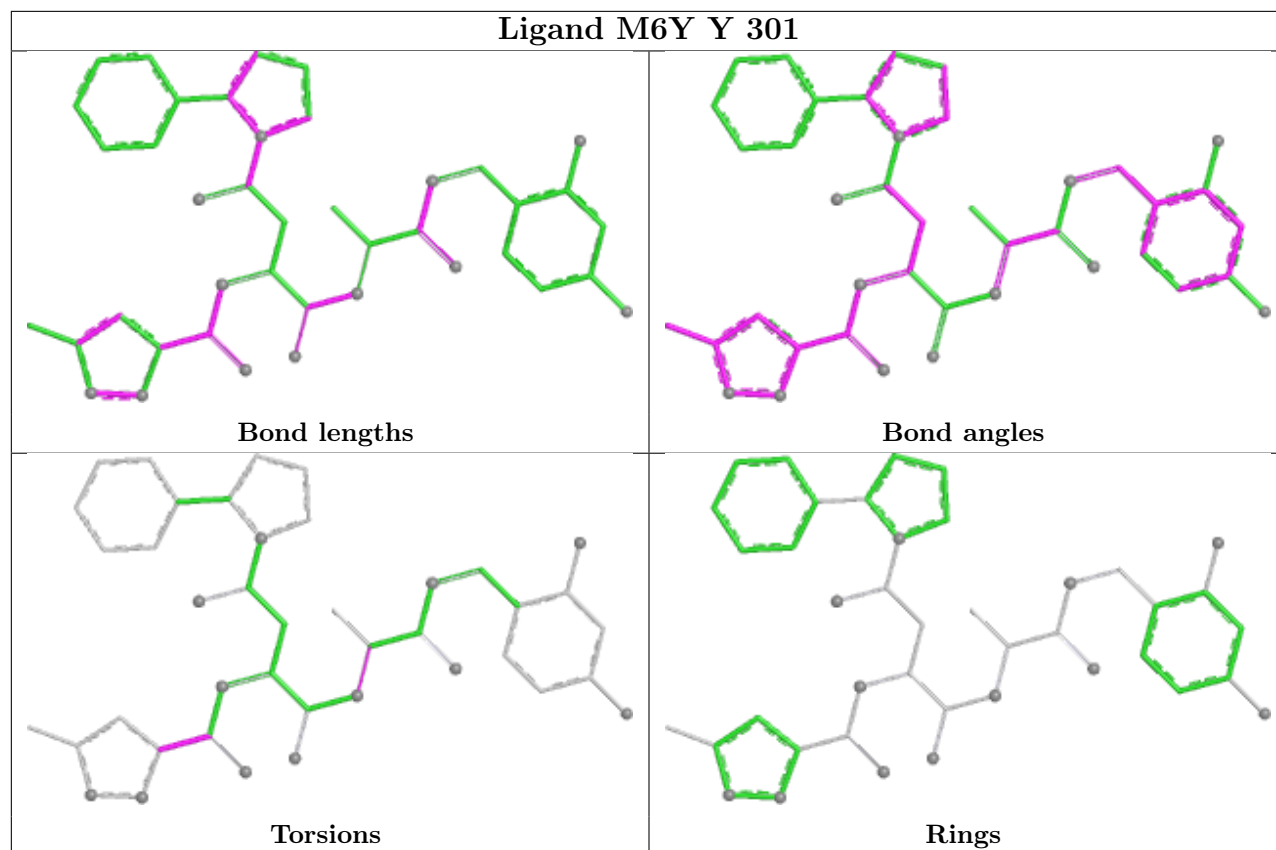
Ligand M6Y I 301



Ligand M6Y N 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	218/240 (90%)	-0.22	1 (0%) 87 85	19, 33, 55, 83	0
1	B	215/240 (89%)	0.18	10 (4%) 36 28	23, 44, 73, 89	0
1	C	217/240 (90%)	0.19	7 (3%) 50 42	21, 42, 73, 86	0
1	D	215/240 (89%)	-0.01	2 (0%) 81 78	20, 40, 66, 80	0
1	E	217/240 (90%)	0.09	2 (0%) 81 78	22, 41, 69, 83	0
1	F	216/240 (90%)	0.15	2 (0%) 81 78	21, 45, 70, 87	0
1	G	216/240 (90%)	-0.14	0 100 100	21, 35, 62, 71	0
1	O	217/240 (90%)	0.18	3 (1%) 73 69	23, 42, 74, 89	0
1	P	219/240 (91%)	-0.12	1 (0%) 87 85	20, 37, 64, 93	0
1	Q	216/240 (90%)	-0.09	4 (1%) 66 61	19, 35, 60, 99	0
1	R	215/240 (89%)	-0.19	0 100 100	19, 34, 59, 68	0
1	S	218/240 (90%)	-0.27	2 (0%) 81 78	19, 32, 60, 87	0
1	T	217/240 (90%)	0.00	3 (1%) 73 69	22, 43, 65, 93	0
1	U	216/240 (90%)	-0.12	3 (1%) 73 69	20, 36, 62, 79	0
2	H	222/234 (94%)	-0.45	0 100 100	18, 26, 44, 64	0
2	I	222/234 (94%)	-0.56	0 100 100	17, 25, 42, 58	0
2	J	222/234 (94%)	-0.53	2 (0%) 81 78	17, 25, 42, 80	0
2	K	223/234 (95%)	-0.51	0 100 100	14, 25, 42, 53	0
2	L	223/234 (95%)	-0.50	1 (0%) 88 87	17, 26, 42, 63	0
2	M	222/234 (94%)	-0.45	0 100 100	15, 27, 47, 69	0
2	N	223/234 (95%)	-0.42	1 (0%) 88 87	18, 29, 51, 68	0
2	V	223/234 (95%)	-0.53	0 100 100	15, 24, 41, 53	0
2	W	223/234 (95%)	-0.54	0 100 100	17, 25, 41, 58	0
2	X	222/234 (94%)	-0.48	0 100 100	18, 25, 40, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	Y	223/234 (95%)	-0.47	1 (0%) 88 87	16, 24, 41, 68	0
2	Z	222/234 (94%)	-0.51	0 100 100	17, 26, 44, 61	0
2	a	223/234 (95%)	-0.40	0 100 100	19, 28, 48, 66	0
2	b	223/234 (95%)	-0.44	0 100 100	17, 27, 44, 67	0
All	All	6148/6636 (92%)	-0.26	45 (0%) 84 82	14, 30, 63, 99	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	235	VAL	5.1
1	D	203	LEU	4.3
1	T	235	VAL	4.1
1	O	202	THR	3.8
1	O	234	LEU	3.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CIT	N	302	13/13	0.84	0.12	31,47,61,62	0
5	CIT	Z	302	13/13	0.84	0.12	32,42,51,67	0
3	DMF	J	304	5/5	0.85	0.21	26,41,50,54	0
3	DMF	B	301	5/5	0.87	0.18	27,39,47,47	0
5	CIT	b	302	13/13	0.87	0.11	31,40,56,58	0
3	DMF	J	303	5/5	0.88	0.18	30,37,47,50	0
3	DMF	F	301	5/5	0.88	0.15	25,34,44,46	0

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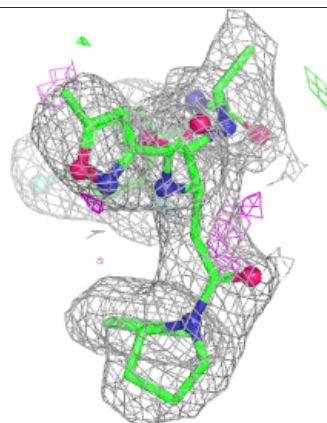
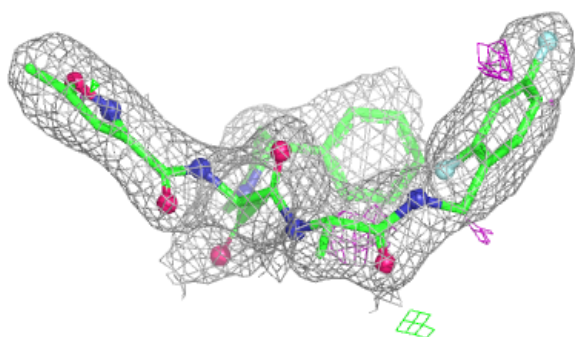
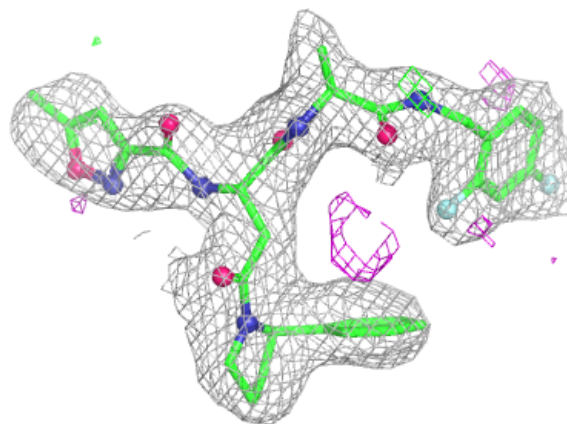
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CIT	L	302	13/13	0.88	0.11	31,40,52,55	0
3	DMF	I	303	5/5	0.89	0.17	24,35,42,44	0
5	CIT	M	302	13/13	0.90	0.10	30,47,57,63	0
3	DMF	S	301	5/5	0.90	0.15	22,28,35,36	0
3	DMF	S	302	5/5	0.90	0.14	34,47,56,57	0
3	DMF	F	302	5/5	0.90	0.16	27,34,56,56	0
5	CIT	J	302	13/13	0.91	0.16	31,39,47,47	0
3	DMF	R	302	5/5	0.91	0.16	36,43,52,52	0
5	CIT	a	302	13/13	0.91	0.09	29,35,48,52	0
5	CIT	I	302	13/13	0.91	0.09	33,38,49,52	0
5	CIT	Y	302	13/13	0.92	0.14	29,38,45,53	0
5	CIT	K	302	13/13	0.92	0.11	27,36,42,46	0
3	DMF	Q	301	5/5	0.92	0.14	21,33,40,46	0
5	CIT	V	302	13/13	0.92	0.09	28,35,54,57	0
5	CIT	X	302	13/13	0.93	0.17	27,36,44,55	0
3	DMF	T	301	5/5	0.93	0.14	27,37,44,45	0
5	CIT	H	302	13/13	0.93	0.11	26,39,50,56	0
3	DMF	E	301	5/5	0.93	0.10	26,34,45,45	0
5	CIT	W	302	13/13	0.93	0.15	26,38,47,52	0
3	DMF	G	301	5/5	0.94	0.10	22,30,37,37	0
3	DMF	G	302	5/5	0.94	0.11	34,41,51,51	0
3	DMF	C	301	5/5	0.94	0.09	21,37,41,48	0
3	DMF	R	301	5/5	0.94	0.10	26,31,38,38	0
4	M6Y	H	301	41/41	0.94	0.08	17,24,38,47	0
4	M6Y	N	301	41/41	0.94	0.08	19,26,37,44	0
4	M6Y	V	301	41/41	0.94	0.09	16,25,33,39	0
4	M6Y	Y	301	41/41	0.95	0.07	18,24,35,47	0
4	M6Y	Z	301	41/41	0.95	0.07	14,24,33,43	0
4	M6Y	a	301	41/41	0.95	0.08	17,24,35,39	0
4	M6Y	b	301	41/41	0.95	0.07	20,27,37,47	0
4	M6Y	L	301	41/41	0.95	0.08	15,25,34,42	0
4	M6Y	M	301	41/41	0.95	0.08	20,26,36,48	0
3	DMF	U	301	5/5	0.95	0.10	33,39,50,50	0
3	DMF	O	301	5/5	0.95	0.12	27,33,39,42	0
4	M6Y	X	301	41/41	0.95	0.08	20,26,35,47	0
4	M6Y	W	301	41/41	0.96	0.07	19,25,34,42	0
3	DMF	A	301	5/5	0.96	0.09	35,42,47,47	0
4	M6Y	I	301	41/41	0.96	0.08	17,27,38,46	0
4	M6Y	J	301	41/41	0.96	0.07	17,23,31,31	0
4	M6Y	K	301	41/41	0.96	0.07	17,24,36,41	0
3	DMF	P	301	5/5	0.97	0.10	30,36,41,41	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.

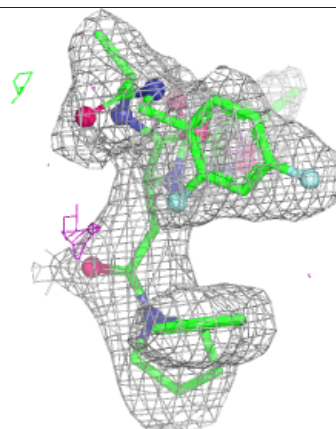
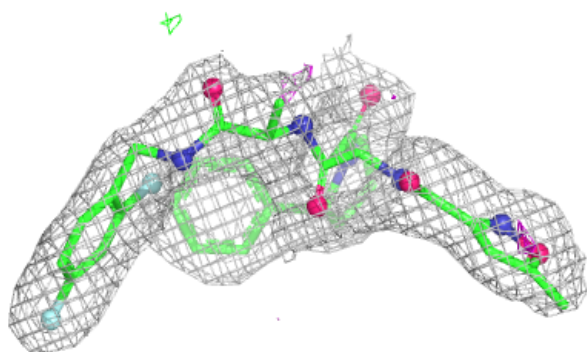
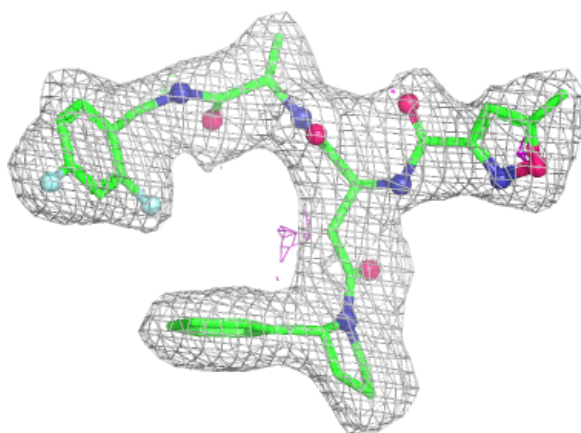
Electron density around M6Y H 301:

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



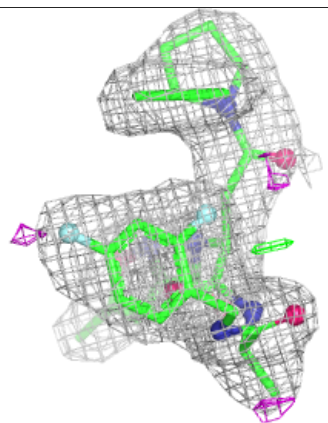
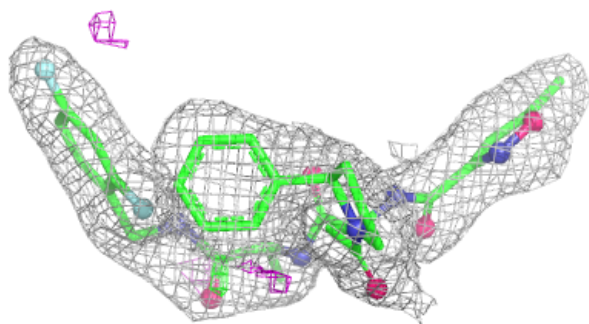
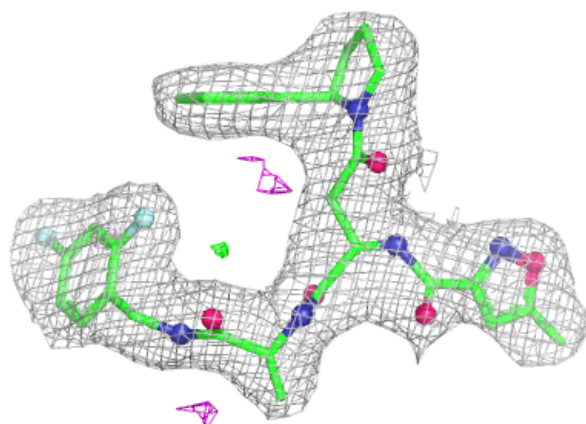
Electron density around M6Y N 301:

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

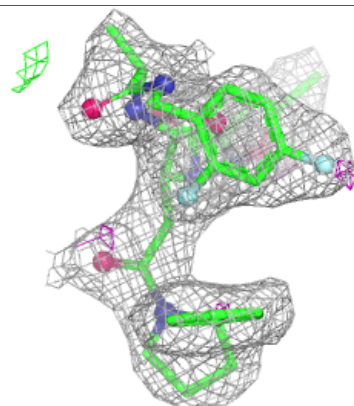
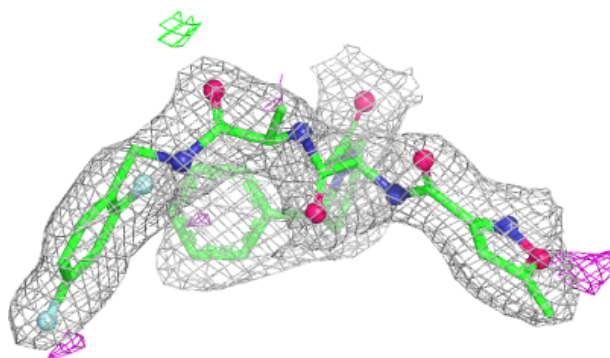
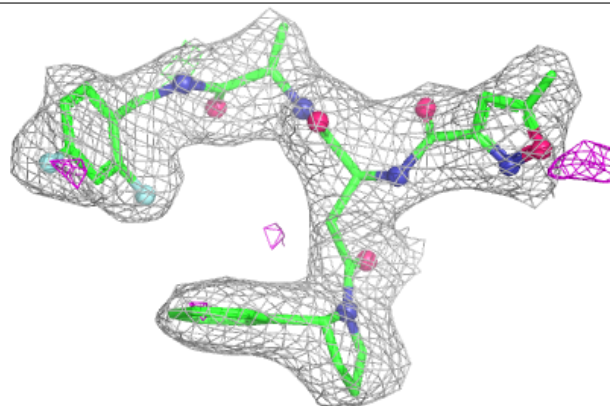


Electron density around M6Y V 301:

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

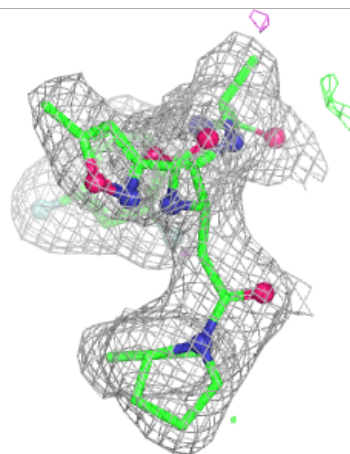
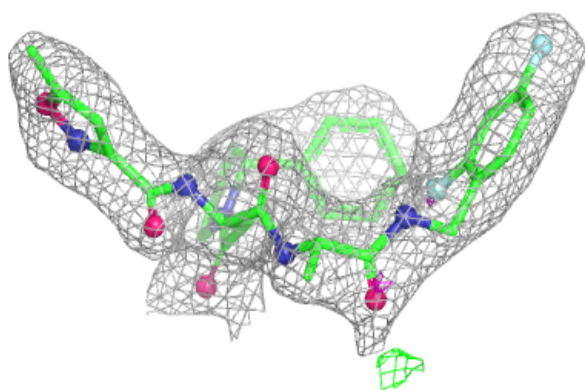
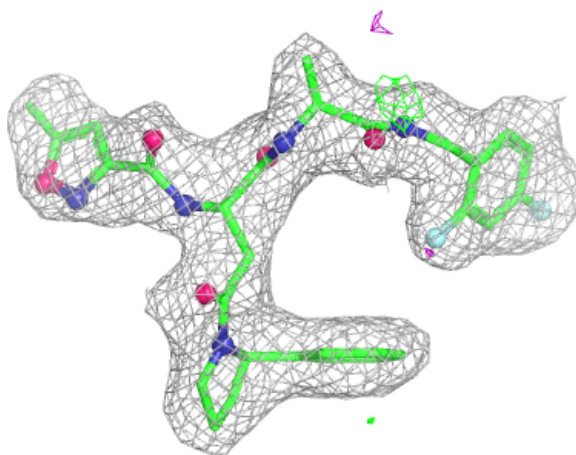
**Electron density around M6Y Y 301:**

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



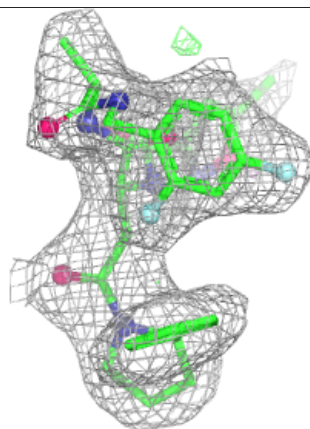
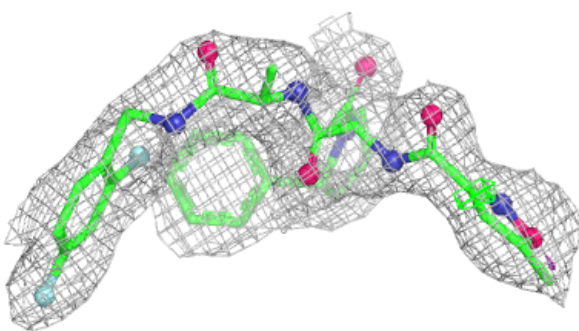
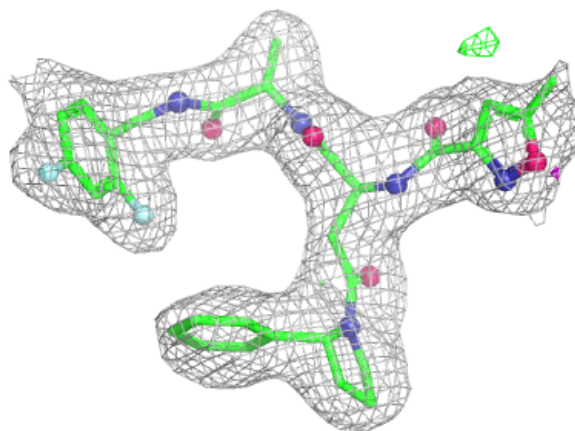
Electron density around M6Y Z 301:

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



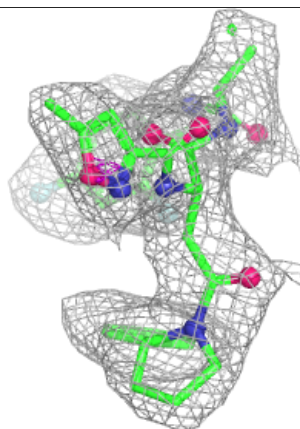
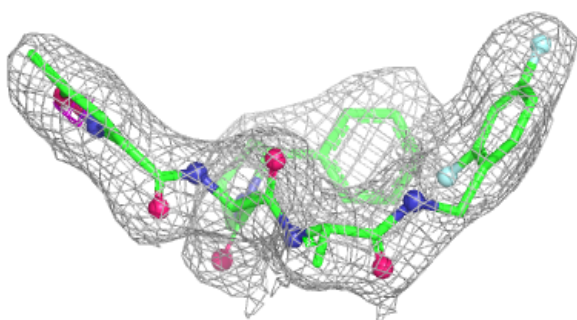
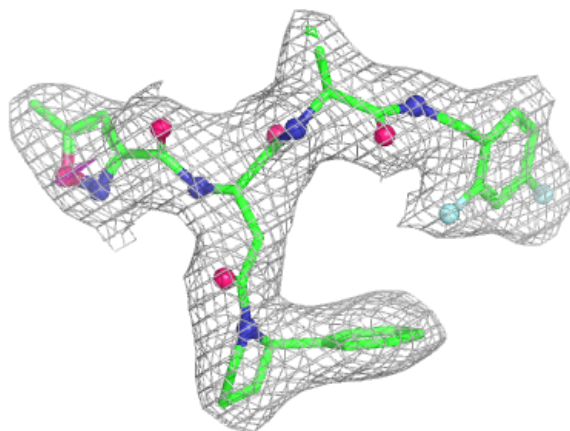
Electron density around M6Y a 301:

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



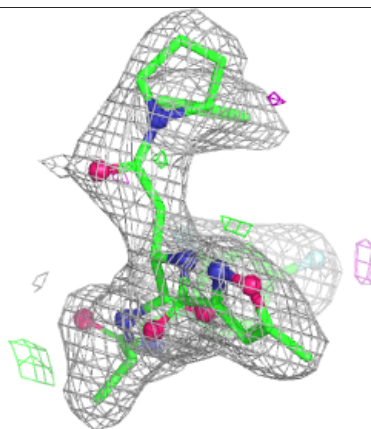
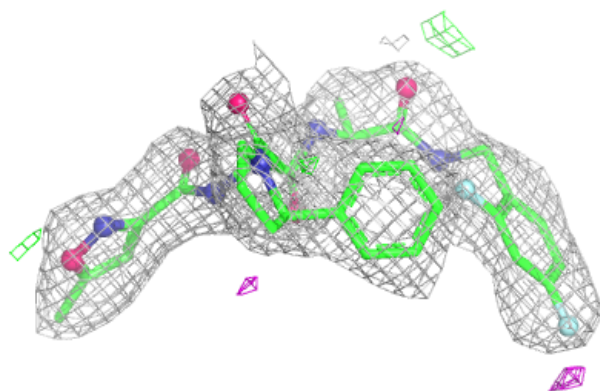
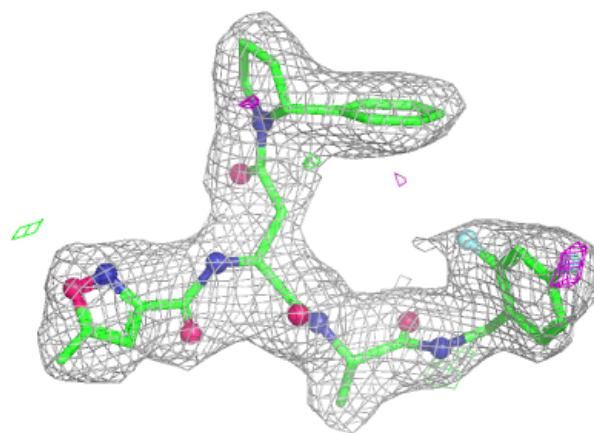
Electron density around M6Y b 301:

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

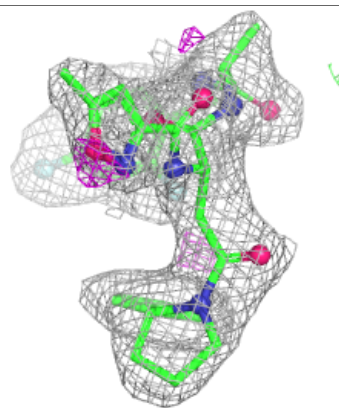
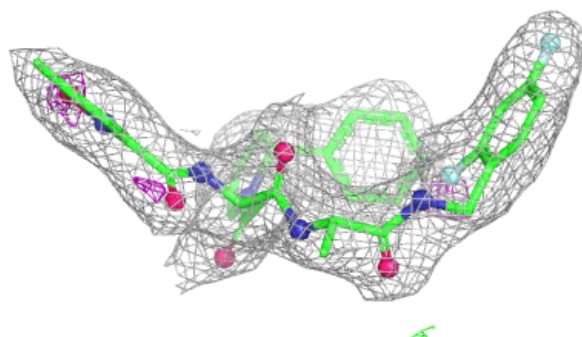
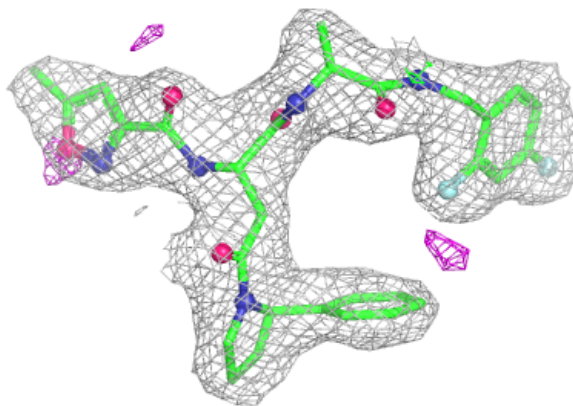


Electron density around M6Y L 301:

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

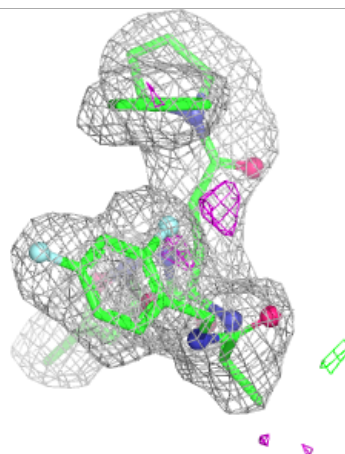
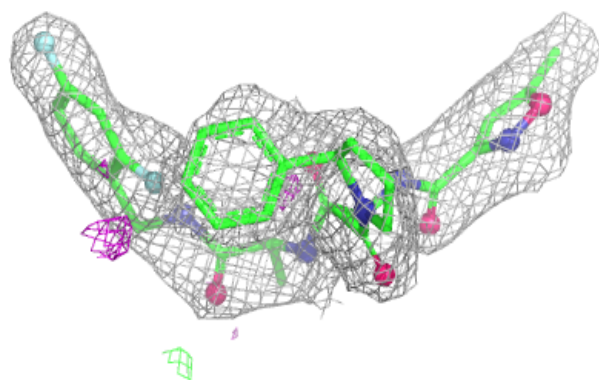
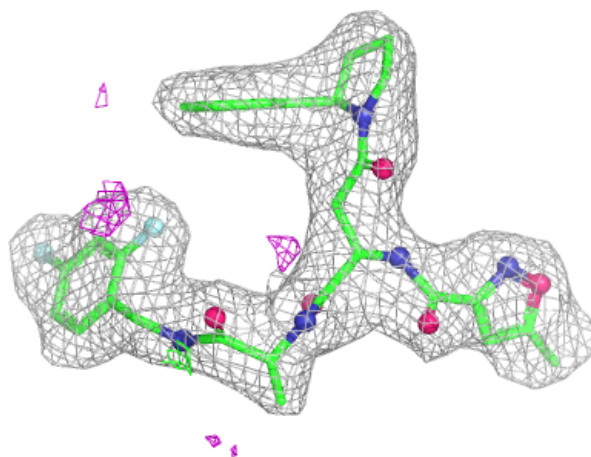
**Electron density around M6Y M 301:**

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



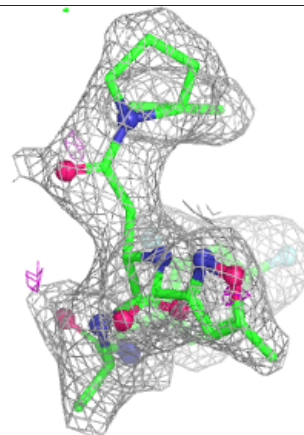
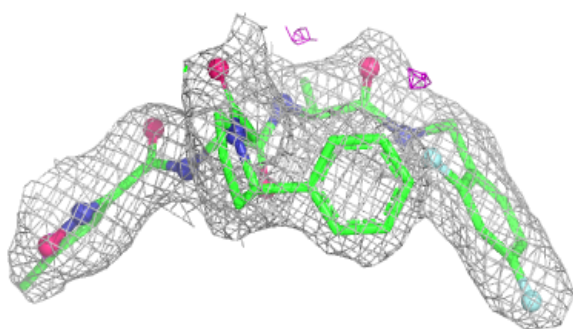
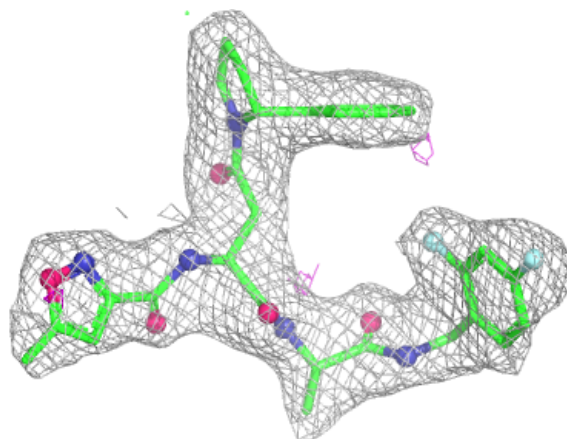
Electron density around M6Y X 301:

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



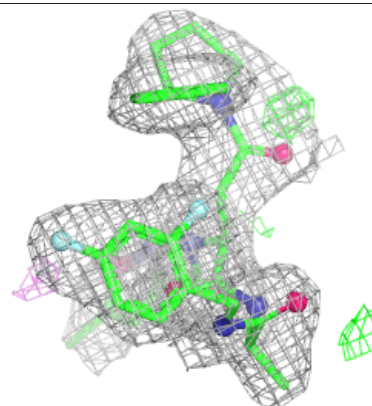
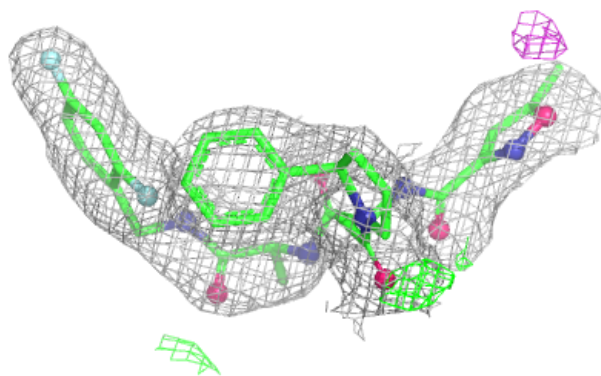
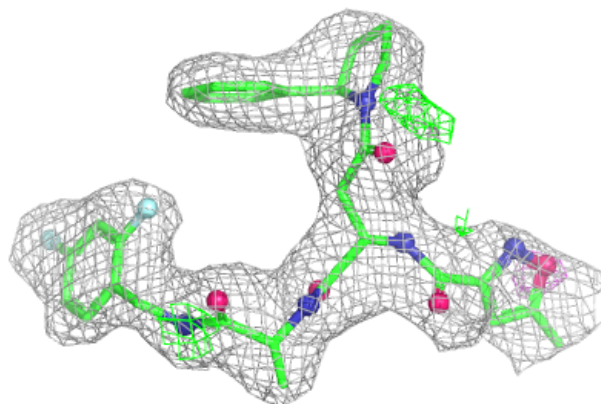
Electron density around M6Y W 301:

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

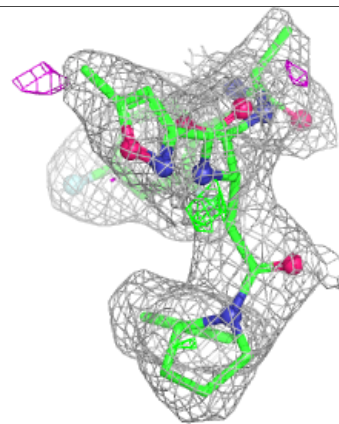
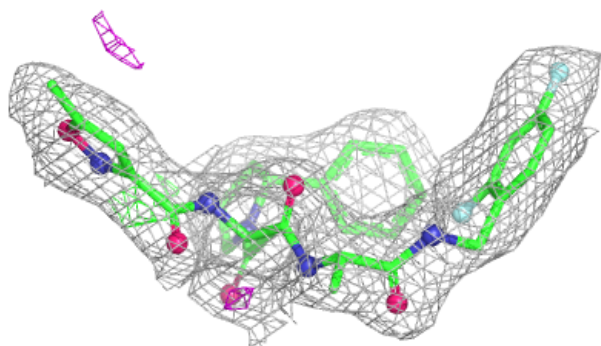
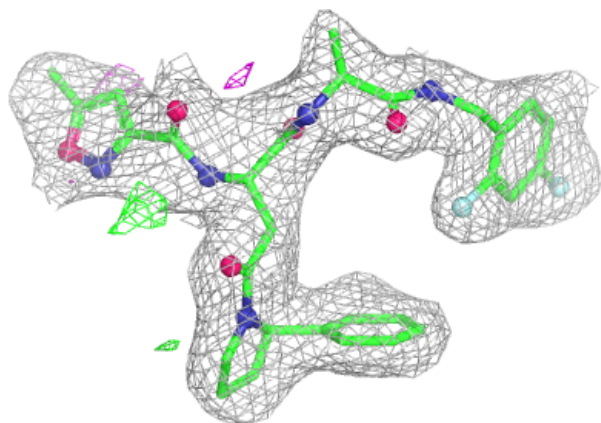


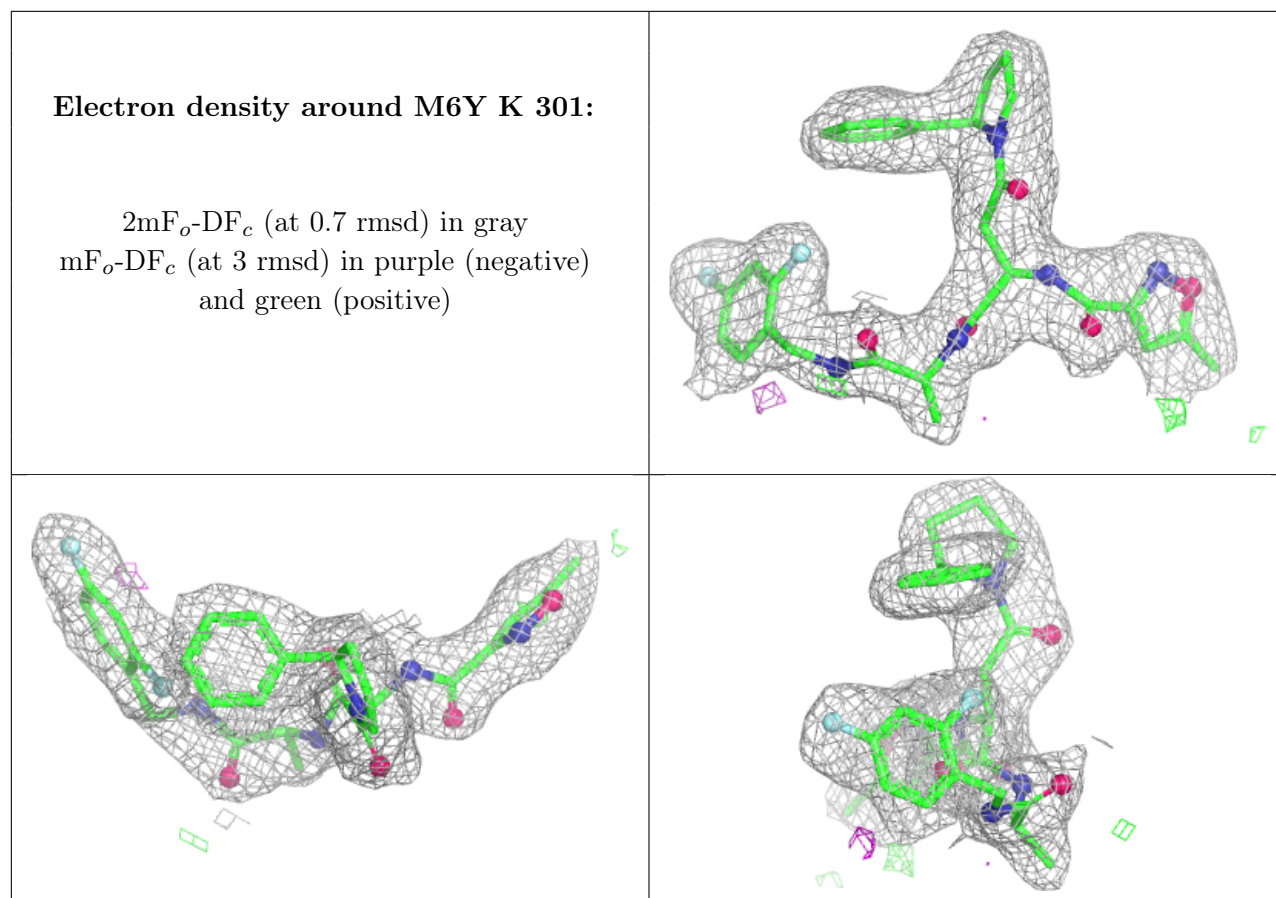
Electron density around M6Y I 301:

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

**Electron density around M6Y 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.