



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:52 AM UTC

PDB ID : 6ODE / pdb_00006ode
Title : Crystal Structure of Mycobacterium tuberculosis Proteasome in Complex with Phenylimidazole-based Inhibitor B6
Authors : Hsu, H.C.; Li, H.
Deposited on : 2019-03-26
Resolution : 2.90 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

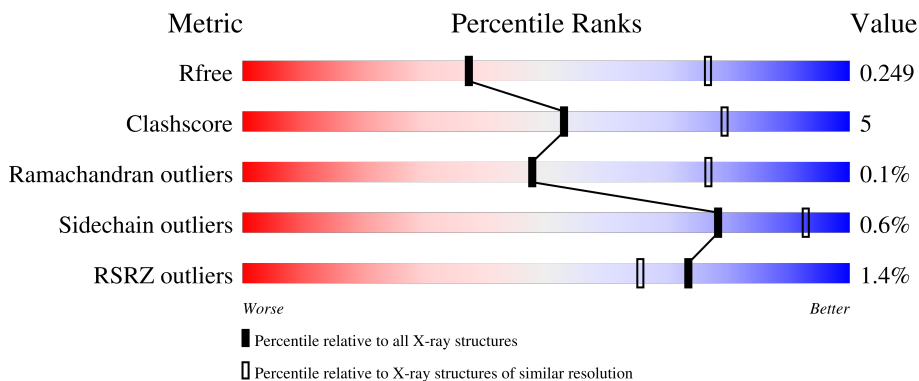
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.







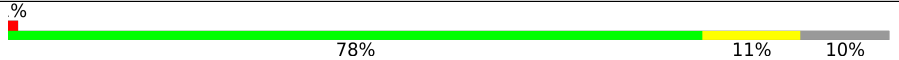
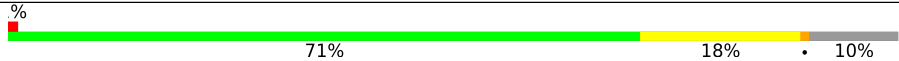
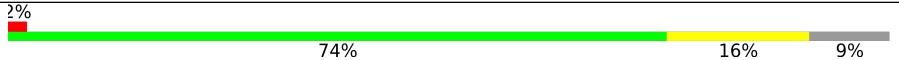
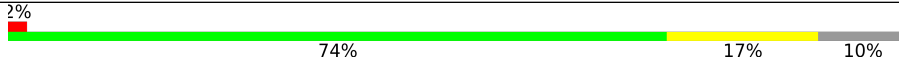
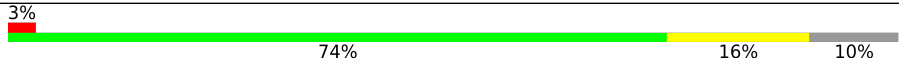
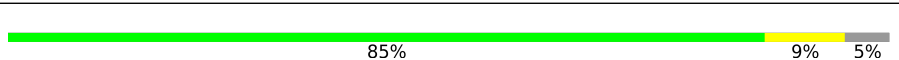
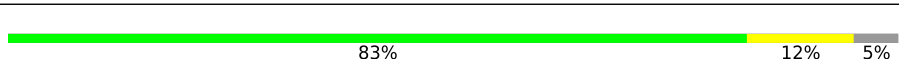


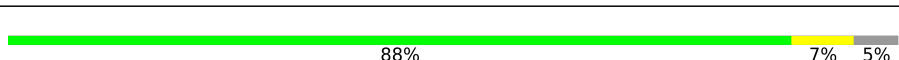

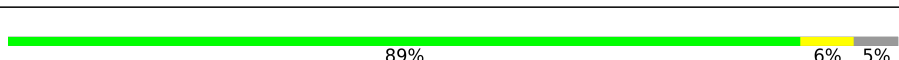
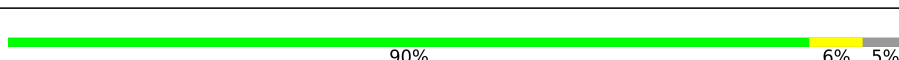
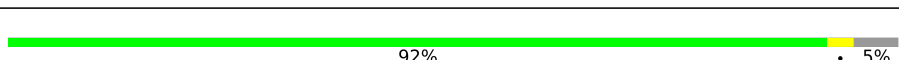
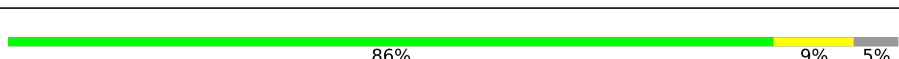
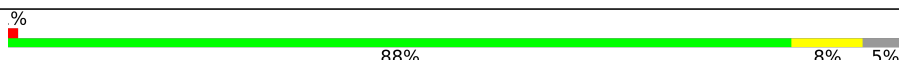
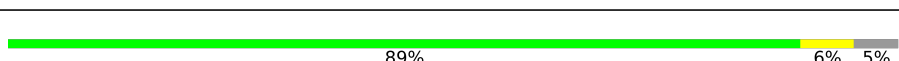
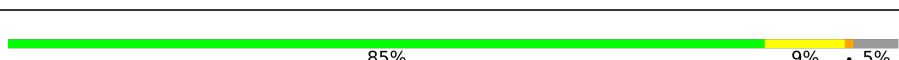
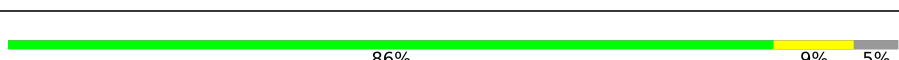
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">71% 20% 9%</p>
1	B	240	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">75% 15% 10%</p>
1	C	240	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">66% 24% 10%</p>
1	D	240	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">71% 17% 11%</p>
1	E	240	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">73% 18% 10%</p>

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Mol	Chain	Length	Quality of chain
1	F	240	 % 72% 17% 11%
1	G	240	 % 81% 9% 10%
1	O	240	 3% 71% 18% 10%
1	P	240	 % 73% 17% 9%
1	Q	240	 % 78% 11% 10%
1	R	240	 % 71% 18% 10%
1	S	240	 2% 74% 16% 9%
1	T	240	 2% 74% 17% 10%
1	U	240	 3% 74% 16% 10%
2	H	234	 85% 9% 5%
2	I	234	 83% 12% 5%
2	J	234	 85% 9% 5%
2	K	234	 88% 6% 5%
2	L	234	 88% 7% 5%
2	M	234	 88% 6% 5%
2	N	234	 89% 6% 5%
2	V	234	 90% 6% 5%
2	W	234	 92% 5%
2	X	234	 86% 9% 5%
2	Y	234	 % 88% 8% 5%
2	Z	234	 89% 6% 5%
2	a	234	 85% 9% 5%
2	b	234	 86% 9% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 47311 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	Total 1677	C 1050	N 306	O 317	S 4	0	0	0
1	B	215	Total 1660	C 1041	N 303	O 312	S 4	0	0	0
1	C	216	Total 1664	C 1043	N 304	O 313	S 4	0	0	0
1	D	214	Total 1649	C 1032	N 302	O 311	S 4	0	0	0
1	E	217	Total 1671	C 1047	N 305	O 315	S 4	0	0	0
1	F	214	Total 1653	C 1036	N 302	O 311	S 4	0	0	0
1	G	216	Total 1662	C 1040	N 304	O 314	S 4	0	0	0
1	O	216	Total 1664	C 1042	N 304	O 314	S 4	0	0	0
1	P	219	Total 1685	C 1054	N 307	O 320	S 4	0	0	0
1	Q	215	Total 1660	C 1041	N 303	O 312	S 4	0	0	0
1	R	215	Total 1657	C 1038	N 303	O 312	S 4	0	0	0
1	S	218	Total 1678	C 1050	N 306	O 318	S 4	0	0	0
1	T	217	Total 1671	C 1047	N 305	O 315	S 4	0	0	0
1	U	216	Total 1664	C 1043	N 304	O 313	S 4	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

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

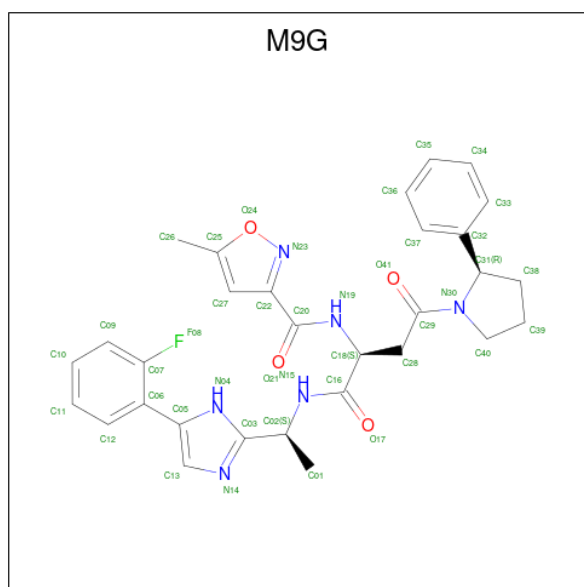
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	I	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	J	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	K	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	L	223	Total	C	N	O	S	0	0	0
			1642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

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

- Molecule 3 is N-((2S)-1-((1S)-1-[5-(2-fluorophenyl)-1H-imidazol-2-yl]ethyl)amino)-1,4-dioxo-4-[(2R)-2-phenylpyrrolidin-1-yl]butan-2-yl)-5-methyl-1,2-oxazole-3-carboxamide (CCD ID: M9G) (formula: C₃₀H₃₁FN₆O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	H	1	41	30	1	6	4	0	0
3	I	1	41	30	1	6	4	0	0
3	J	1	41	30	1	6	4	0	0
3	L	1	41	30	1	6	4	0	0
3	L	1	41	30	1	6	4	0	0
3	M	1	41	30	1	6	4	0	0
3	N	1	41	30	1	6	4	0	0
3	V	1	41	30	1	6	4	0	0
3	W	1	41	30	1	6	4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	X	1	Total 41	C 30	F 1	N 6	O 4	0	0
3	Y	1	Total 41	C 30	F 1	N 6	O 4	0	0
3	Z	1	Total 41	C 30	F 1	N 6	O 4	0	0
3	a	1	Total 41	C 30	F 1	N 6	O 4	0	0
3	b	1	Total 41	C 30	F 1	N 6	O 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total 15	O 15	0	0
4	B	11	Total 11	O 11	0	0
4	C	10	Total 10	O 10	0	0
4	D	6	Total 6	O 6	0	0
4	E	6	Total 6	O 6	0	0
4	F	9	Total 9	O 9	0	0
4	G	11	Total 11	O 11	0	0
4	H	14	Total 14	O 14	0	0
4	I	21	Total 21	O 21	0	0
4	J	28	Total 28	O 28	0	0
4	K	20	Total 20	O 20	0	0
4	L	24	Total 24	O 24	0	0
4	M	20	Total 20	O 20	0	0
4	N	22	Total 22	O 22	0	0

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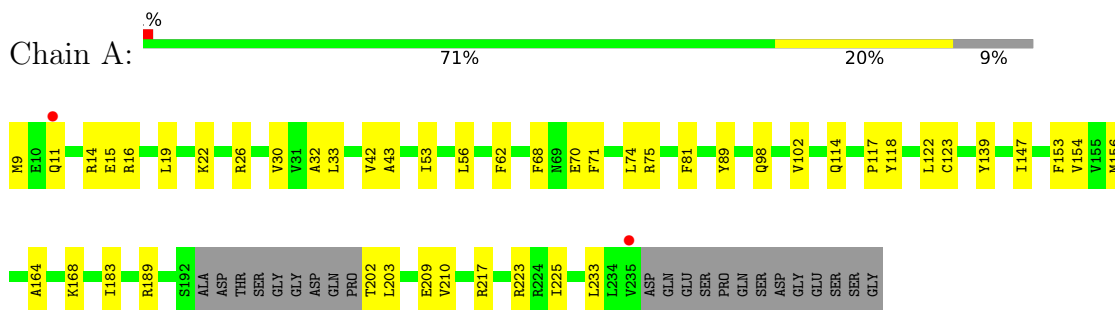
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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4	P	11	Total O 11 11	0	0
4	Q	15	Total O 15 15	0	0
4	R	15	Total O 15 15	0	0
4	S	10	Total O 10 10	0	0
4	T	12	Total O 12 12	0	0
4	U	11	Total O 11 11	0	0
4	V	27	Total O 27 27	0	0
4	W	21	Total O 21 21	0	0
4	X	27	Total O 27 27	0	0
4	Y	23	Total O 23 23	0	0
4	Z	23	Total O 23 23	0	0
4	a	16	Total O 16 16	0	0
4	b	19	Total O 19 19	0	0

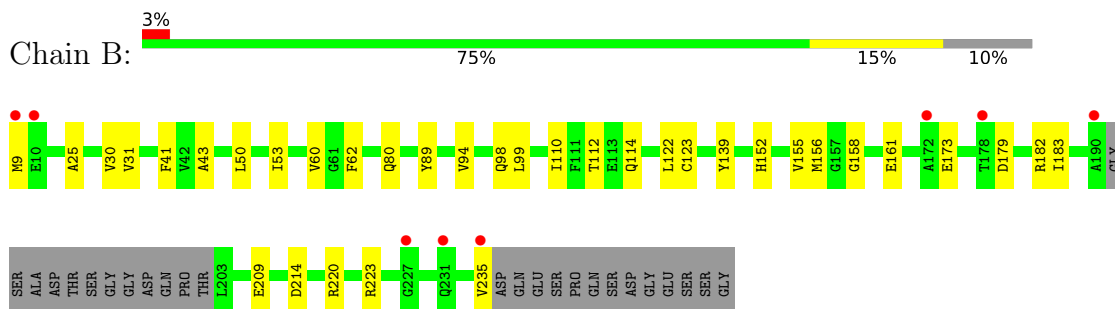
3 Residue-property plots [i](#)

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.

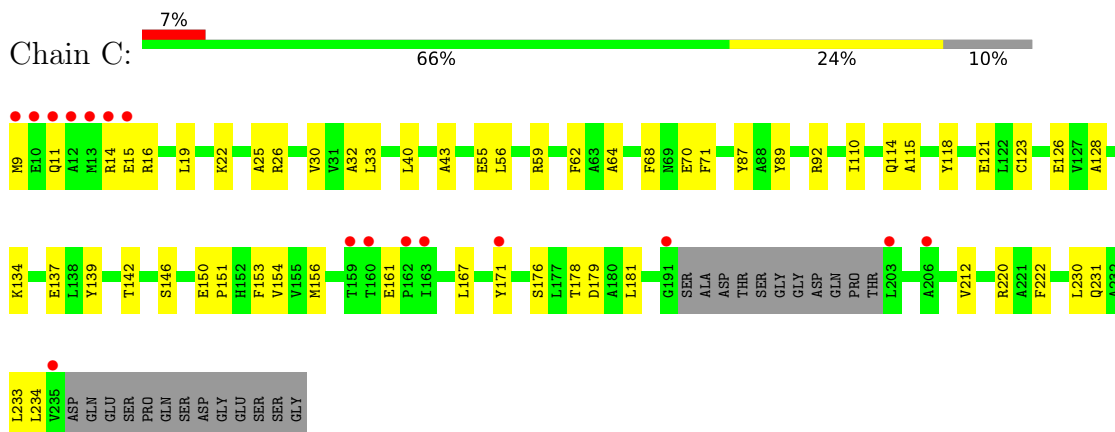
- Molecule 1: Proteasome subunit alpha



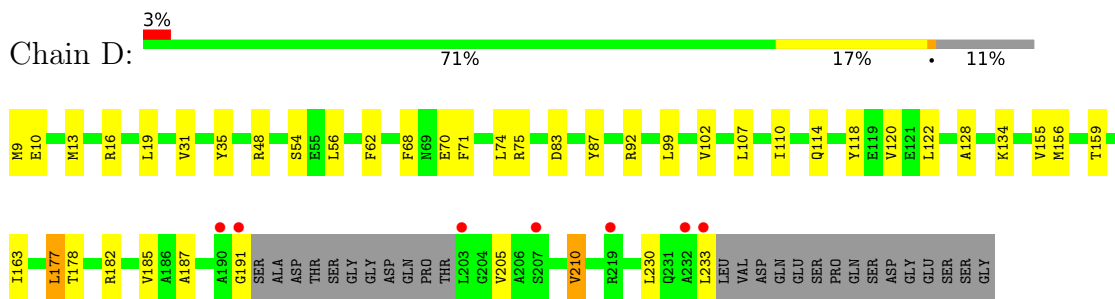
- Molecule 1: Proteasome subunit alpha



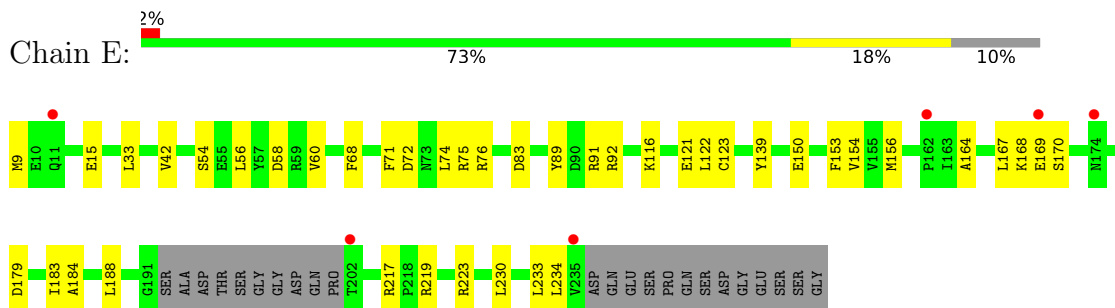
- Molecule 1: Proteasome subunit alpha



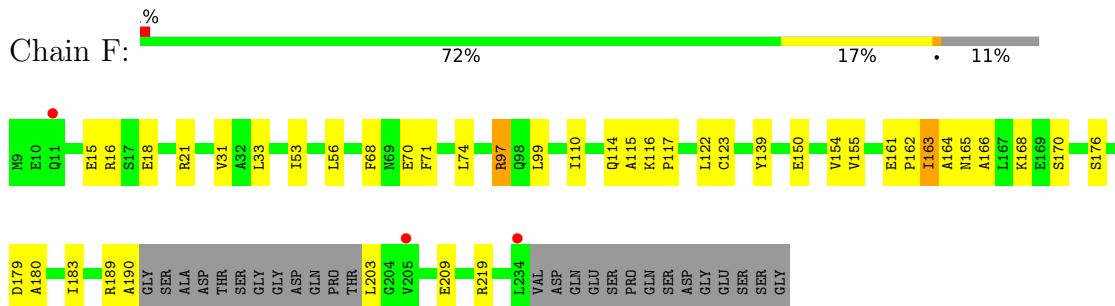
- Molecule 1: Proteasome subunit alpha



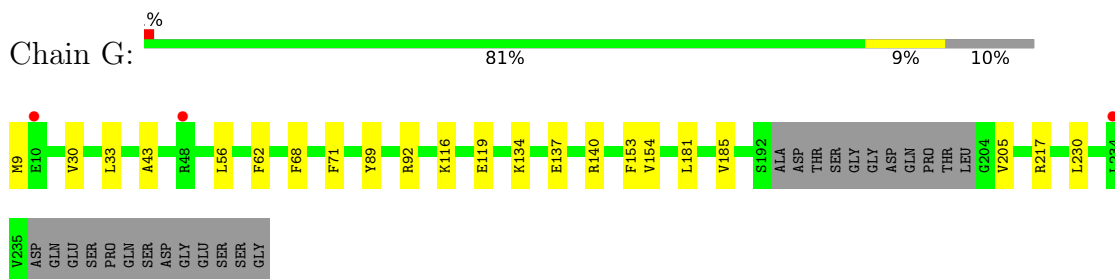
- Molecule 1: Proteasome subunit alpha



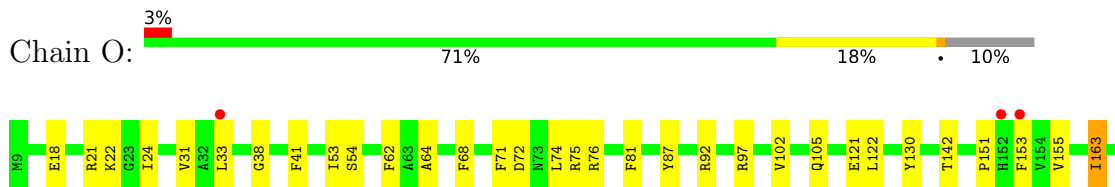
- Molecule 1: Proteasome subunit alpha



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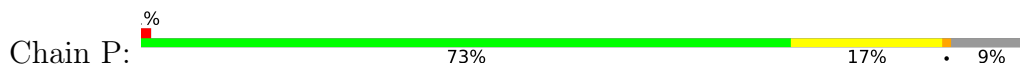


- Molecule 1: Proteasome subunit alpha

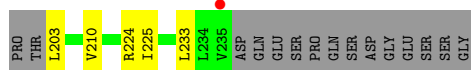
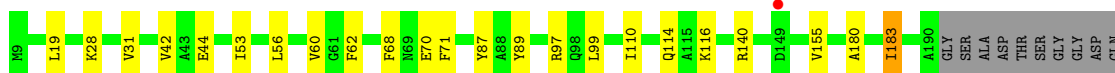
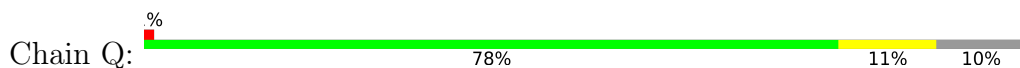




- Molecule 1: Proteasome subunit alpha



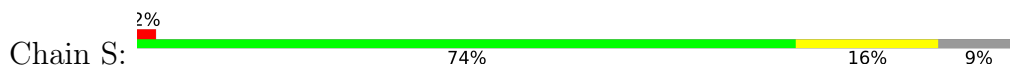
- Molecule 1: Proteasome subunit alpha



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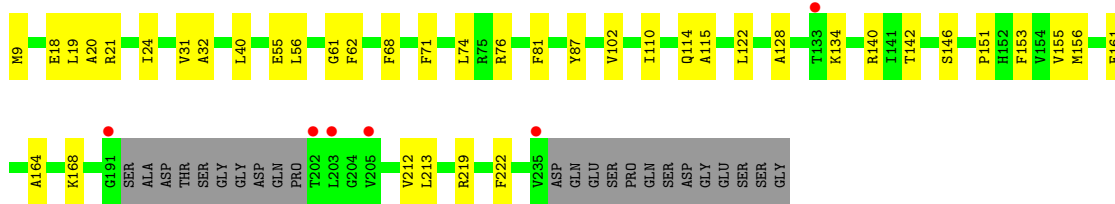


- Molecule 1: Proteasome subunit alpha

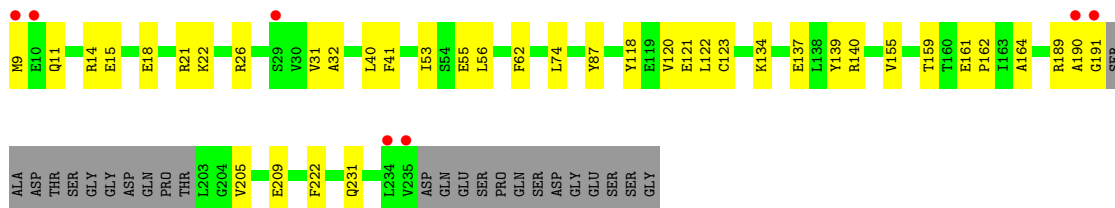
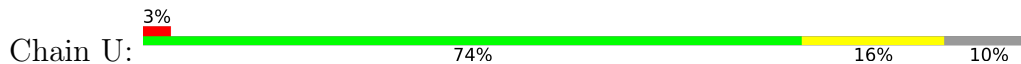


- Molecule 1: Proteasome subunit alpha

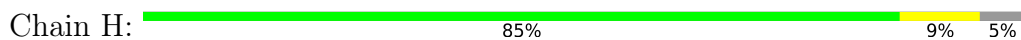




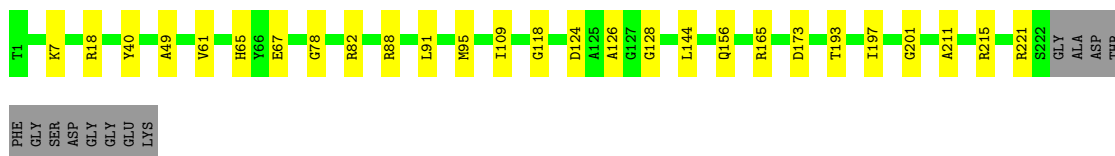
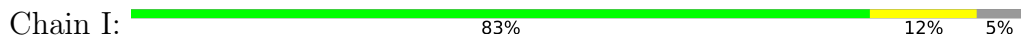
• Molecule 1: Proteasome subunit alpha



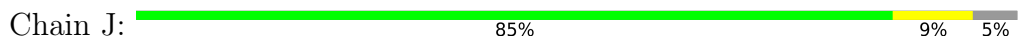
• Molecule 2: Proteasome subunit beta



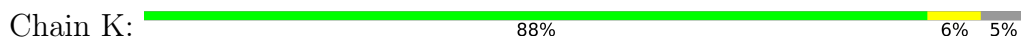
• Molecule 2: Proteasome subunit beta




• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta




• Molecule 2: Proteasome subunit beta

Chain L:  88% 7% 5%




• Molecule 2: Proteasome subunit beta

Chain M:  88% 6% 5%




• Molecule 2: Proteasome subunit beta

Chain N:  89% 6% 5%



• Molecule 2: Proteasome subunit beta

Chain V:  90% 6% 5%




• Molecule 2: Proteasome subunit beta

Chain W:  92% 5% 5%




• Molecule 2: Proteasome subunit beta

Chain X:  86% 9% 5%




• Molecule 2: Proteasome subunit beta

Chain Y:  88% 8% 5%



• Molecule 2: Proteasome subunit beta

Chain Z:  89% 6% 5%



- Molecule 2: Proteasome subunit beta

Chain a: 85% 9% 5%



- Molecule 2: Proteasome subunit beta

Chain b: 86% 9% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.60Å 198.38Å 166.51Å 90.00° 103.10° 90.00°	Depositor
Resolution (Å)	53.97 – 2.90 53.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (53.97-2.90) 99.8 (53.97-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.91Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.197 , 0.247 0.200 , 0.249	Depositor DCC
R_{free} test set	8411 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtrriage
Anisotropy	0.376	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	47311	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: M9G

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	0.23	1/1701 (0.1%)	0.38	0/2297
1	B	0.13	0/1684	0.36	0/2274
1	C	0.15	0/1688	0.39	0/2279
1	D	0.13	0/1673	0.38	0/2258
1	E	0.15	0/1695	0.39	0/2289
1	F	0.34	1/1677 (0.1%)	0.43	0/2264
1	G	0.12	0/1686	0.35	0/2276
1	O	0.16	0/1688	0.39	0/2279
1	P	0.20	0/1709	0.40	0/2308
1	Q	0.15	0/1684	0.36	0/2274
1	R	0.40	3/1681 (0.2%)	0.42	0/2269
1	S	0.13	0/1702	0.36	0/2298
1	T	0.13	0/1695	0.37	0/2289
1	U	0.12	0/1688	0.37	0/2279
2	H	0.13	0/1662	0.33	0/2254
2	I	0.14	0/1662	0.35	0/2254
2	J	0.14	0/1662	0.32	0/2254
2	K	0.13	0/1666	0.33	0/2259
2	L	0.13	0/1666	0.32	0/2259
2	M	0.12	0/1662	0.34	0/2254
2	N	0.14	0/1666	0.34	0/2259
2	V	0.14	0/1666	0.33	0/2259
2	W	0.13	0/1666	0.34	0/2259
2	X	0.14	0/1662	0.35	0/2254
2	Y	0.15	0/1666	0.34	0/2259
2	Z	0.12	0/1666	0.33	0/2259
2	a	0.14	0/1666	0.35	0/2259
2	b	0.13	0/1666	0.32	0/2259
All	All	0.17	5/46955 (0.0%)	0.36	0/63534

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	TYR	CA-C	-7.48	1.48	1.52
1	R	220	ARG	C-O	-6.56	1.16	1.24
1	R	219	ARG	C-O	-5.52	1.17	1.24
1	F	97	ARG	C-O	-5.19	1.18	1.24
1	R	221	ALA	C-O	-5.17	1.17	1.24

There are no bond angle outliers.

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	28	0
1	B	1660	0	1665	25	0
1	C	1664	0	1668	41	0
1	D	1649	0	1648	33	0
1	E	1671	0	1675	30	0
1	F	1653	0	1656	25	0
1	G	1662	0	1662	13	0
1	O	1664	0	1666	31	0
1	P	1685	0	1684	29	0
1	Q	1660	0	1665	18	0
1	R	1657	0	1659	26	0
1	S	1678	0	1677	26	0
1	T	1671	0	1675	23	0
1	U	1664	0	1668	20	0
2	H	1638	0	1633	13	0
2	I	1638	0	1633	15	0
2	J	1638	0	1633	16	0
2	K	1642	0	1636	11	0
2	L	1642	0	1636	12	0
2	M	1638	0	1633	12	0
2	N	1642	0	1636	8	0
2	V	1642	0	1636	8	0
2	W	1642	0	1636	4	0
2	X	1638	0	1633	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	1642	0	1636	11	0
2	Z	1642	0	1636	6	0
2	a	1642	0	1636	15	0
2	b	1642	0	1636	13	0
3	H	41	0	0	0	0
3	I	41	0	0	1	0
3	J	41	0	0	0	0
3	L	82	0	0	0	0
3	M	41	0	0	1	0
3	N	41	0	0	1	0
3	V	41	0	0	0	0
3	W	41	0	0	0	0
3	X	41	0	0	0	0
3	Y	41	0	0	0	0
3	Z	41	0	0	0	0
3	a	41	0	0	0	0
3	b	41	0	0	1	0
4	A	15	0	0	0	0
4	B	11	0	0	1	0
4	C	10	0	0	0	0
4	D	6	0	0	0	0
4	E	6	0	0	0	0
4	F	9	0	0	0	0
4	G	11	0	0	0	0
4	H	14	0	0	0	0
4	I	21	0	0	0	0
4	J	28	0	0	1	0
4	K	20	0	0	0	0
4	L	24	0	0	0	0
4	M	20	0	0	0	0
4	N	22	0	0	0	0
4	O	7	0	0	0	0
4	P	11	0	0	1	0
4	Q	15	0	0	0	0
4	R	15	0	0	1	0
4	S	10	0	0	1	0
4	T	12	0	0	0	0
4	U	11	0	0	0	0
4	V	27	0	0	0	0
4	W	21	0	0	0	0
4	X	27	0	0	0	0
4	Y	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Z	23	0	0	0	0
4	a	16	0	0	1	0
4	b	19	0	0	0	0
All	All	47311	0	46237	468	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 5.

All (468) 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:O:31:VAL:HG12	1:O:155:VAL:HG22	1.64	0.78
1:P:161:GLU:HG2	1:P:162:PRO:HD3	1.65	0.78
1:F:161:GLU:O	1:F:165:ASN:ND2	2.19	0.76
1:C:231:GLN:HA	1:C:234:LEU:HD12	1.68	0.75
1:S:110:ILE:HG23	1:S:114:GLN:HG3	1.69	0.73
1:S:112:THR:HG22	1:S:113:GLU:HG3	1.69	0.73
1:A:16:ARG:NH1	1:A:114:GLN:O	2.23	0.72
1:P:189:ARG:NH1	1:P:203:LEU:HD11	2.05	0.72
2:b:22:GLN:NE2	3:b:301:M9G:O41	2.23	0.70
1:A:33:LEU:HD23	1:A:153:PHE:HB3	1.73	0.70
1:B:182:ARG:NH1	1:B:235:VAL:O	2.25	0.70
1:S:92:ARG:NH2	1:S:132:GLU:OE1	2.25	0.69
1:C:33:LEU:HD23	1:C:153:PHE:HB3	1.75	0.69
1:A:189:ARG:HE	1:A:202:THR:HG22	1.57	0.69
1:O:181:LEU:HD23	1:O:233:LEU:HD12	1.74	0.69
1:E:217:ARG:HH21	1:E:223:ARG:HD3	1.57	0.68
1:T:56:LEU:HG	1:T:62:PHE:HB2	1.75	0.66
1:U:74:LEU:HD13	1:U:122:LEU:HD11	1.77	0.66
1:C:30:VAL:HG13	1:C:43:ALA:HB2	1.78	0.66
1:P:135:ARG:HD2	1:P:136:PRO:HD2	1.77	0.66
1:S:92:ARG:HB3	2:a:75:THR:HG21	1.77	0.65
1:T:76:ARG:HD3	2:a:69:LEU:HD22	1.78	0.65
1:C:9:MET:HG3	1:D:19:LEU:HD13	1.79	0.65
1:D:210:VAL:HG11	1:D:230:LEU:HD13	1.78	0.65
1:A:189:ARG:HH21	1:A:203:LEU:H	1.45	0.65
1:P:16:ARG:NH1	1:P:114:GLN:O	2.28	0.64
1:E:42:VAL:HG11	1:E:184:ALA:HB1	1.78	0.64
2:I:173:ASP:OD1	2:I:221:ARG:NH2	2.31	0.64
1:F:219:ARG:NH2	2:M:64:GLU:OE2	2.26	0.64
2:L:165:ARG:NH2	2:L:169:GLU:OE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:31:VAL:HG12	1:U:155:VAL:HG12	1.77	0.64
1:U:41:PHE:HB3	1:U:53:ILE:HD13	1.79	0.64
1:A:74:LEU:HD13	1:A:122:LEU:HD11	1.80	0.63
1:P:116:LYS:NZ	1:P:119:GLU:OE1	2.30	0.63
1:F:56:LEU:HD13	1:F:99:LEU:HD23	1.80	0.63
1:B:110:ILE:HA	1:B:114:GLN:HG3	1.79	0.63
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.81	0.62
1:Q:225:ILE:HG21	1:Q:233:LEU:HD12	1.82	0.62
1:T:31:VAL:HG22	1:T:155:VAL:HG22	1.80	0.62
1:A:11:GLN:HA	1:A:14:ARG:HD2	1.81	0.62
1:R:42:VAL:HG11	1:R:184:ALA:HB1	1.82	0.61
2:L:165:ARG:HG2	2:L:213:LEU:HD22	1.80	0.61
1:F:53:ILE:HD12	1:F:209:GLU:HG2	1.82	0.61
2:J:18:ARG:NH2	4:J:401:HOH:O	2.33	0.61
1:D:9:MET:N	1:E:15:GLU:OE1	2.34	0.61
1:D:128:ALA:HB2	1:D:134:LYS:HB3	1.81	0.61
1:D:35:TYR:CZ	1:D:177:LEU:HD23	2.35	0.60
1:P:189:ARG:NH1	1:P:203:LEU:CD1	2.63	0.60
1:R:205:VAL:HG13	1:R:230:LEU:HD23	1.84	0.60
1:O:74:LEU:HD13	1:O:122:LEU:HD11	1.84	0.60
1:D:13:MET:HE3	1:E:116:LYS:HB2	1.84	0.60
2:Y:161:ASP:OD1	2:Y:209:ARG:NH2	2.34	0.60
2:J:20:SER:HB3	2:J:28:GLY:HA3	1.83	0.59
1:Q:31:VAL:HG12	1:Q:155:VAL:HG22	1.84	0.59
1:T:110:ILE:HA	1:T:114:GLN:HG3	1.84	0.59
1:E:74:LEU:HD13	1:E:122:LEU:HD11	1.85	0.59
1:P:9:MET:HE1	1:Q:19:LEU:HD13	1.83	0.59
1:P:33:LEU:HD23	1:P:153:PHE:HB3	1.84	0.59
1:E:164:ALA:O	1:E:168:LYS:HB2	2.03	0.59
1:C:92:ARG:HB3	2:K:75:THR:HG21	1.84	0.58
2:J:38:ASP:HB3	2:J:41:THR:OG1	2.03	0.58
1:D:163:ILE:HG13	1:D:187:ALA:O	2.02	0.58
1:O:205:VAL:HG21	1:O:231:GLN:HG3	1.84	0.58
1:U:11:GLN:HA	1:U:14:ARG:HB2	1.84	0.58
1:E:33:LEU:HD23	1:E:153:PHE:HB3	1.85	0.58
1:O:205:VAL:HG13	1:O:230:LEU:HD23	1.85	0.58
1:C:33:LEU:HD21	1:C:167:LEU:HD22	1.85	0.58
1:D:87:TYR:O	2:K:57:ARG:NH2	2.36	0.58
1:U:123:CYS:HA	1:U:139:TYR:O	2.05	0.57
1:B:152:HIS:NE2	1:B:173:GLU:OE2	2.37	0.57
1:B:53:ILE:HD12	1:B:209:GLU:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:97:ARG:NH2	1:R:49:SER:O	2.37	0.57
1:P:225:ILE:HG21	1:P:233:LEU:HD12	1.87	0.57
1:S:41:PHE:HB3	1:S:53:ILE:HD13	1.86	0.57
1:U:53:ILE:HD12	1:U:209:GLU:HG2	1.87	0.57
1:A:225:ILE:HG21	1:A:233:LEU:HD12	1.86	0.56
1:D:92:ARG:HB3	2:L:75:THR:HG21	1.86	0.56
1:R:89:TYR:CD1	2:Z:82:ARG:HD3	2.40	0.56
1:G:30:VAL:HG13	1:G:43:ALA:HB2	1.86	0.56
1:R:33:LEU:HD21	1:R:167:LEU:HD22	1.87	0.56
2:X:64:GLU:HG2	2:X:68:LYS:HE2	1.88	0.56
1:Q:60:VAL:HG11	1:Q:99:LEU:HD12	1.87	0.56
1:R:30:VAL:HG13	1:R:43:ALA:HB2	1.88	0.56
1:Q:28:LYS:HD2	1:Q:44:GLU:HG2	1.88	0.56
1:Q:110:ILE:HG23	1:Q:114:GLN:HG3	1.87	0.56
1:D:182:ARG:HA	1:D:185:VAL:HG22	1.87	0.55
1:F:31:VAL:HG12	1:F:155:VAL:HG12	1.86	0.55
1:F:166:ALA:O	1:F:170:SER:OG	2.11	0.55
2:H:156:GLN:OE1	2:H:165:ARG:NH2	2.39	0.55
1:O:41:PHE:HB3	1:O:53:ILE:HD13	1.88	0.55
2:L:176:ASP:OD2	2:b:188:ARG:NH1	2.40	0.55
2:a:13:VAL:HG22	2:a:196:ILE:HD12	1.88	0.55
1:G:56:LEU:HG	1:G:62:PHE:HB2	1.89	0.55
2:H:3:ILE:O	2:H:138:ALA:HA	2.07	0.55
1:F:74:LEU:HD13	1:F:122:LEU:HD11	1.88	0.55
2:H:38:ASP:OD2	2:H:39:ASP:N	2.39	0.55
1:E:150:GLU:HG3	1:E:154:VAL:HG22	1.89	0.55
1:P:30:VAL:HG13	1:P:43:ALA:HB2	1.89	0.55
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	1.89	0.55
2:Y:48:THR:HG21	2:Y:98:LEU:HD22	1.88	0.55
1:O:163:ILE:HD13	1:O:188:LEU:HA	1.89	0.55
1:E:68:PHE:HA	1:E:71:PHE:CE2	2.42	0.55
1:S:152:HIS:HB3	1:S:171:TYR:CZ	2.42	0.54
2:J:38:ASP:OD2	2:J:79:LYS:NZ	2.40	0.54
1:P:56:LEU:HG	1:P:62:PHE:HB2	1.89	0.54
1:D:74:LEU:HD13	1:D:122:LEU:HD11	1.90	0.54
1:F:162:PRO:HB2	1:F:190:ALA:O	2.07	0.54
2:J:64:GLU:HG2	2:J:68:LYS:HE2	1.87	0.54
1:O:153:PHE:CZ	1:O:167:LEU:HB3	2.42	0.54
1:U:134:LYS:NZ	1:U:137:GLU:OE2	2.40	0.54
1:O:205:VAL:HG22	1:O:230:LEU:HG	1.89	0.53
1:Q:140:ARG:NH1	1:Q:155:VAL:O	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:HA	1:D:102:VAL:HG12	1.90	0.53
1:F:18:GLU:OE1	1:F:21:ARG:NH1	2.41	0.53
2:K:95:MET:HE2	2:K:95:MET:HA	1.91	0.53
1:S:9:MET:HE2	1:T:19:LEU:HD13	1.90	0.53
1:T:18:GLU:OE1	1:T:21:ARG:NH2	2.41	0.53
2:a:216:ALA:O	2:a:220:SER:HB3	2.09	0.53
1:F:164:ALA:O	1:F:168:LYS:HG3	2.09	0.53
2:M:3:ILE:HB	2:M:139:VAL:HG12	1.91	0.53
2:Z:20:SER:HB3	2:Z:28:GLY:HA3	1.90	0.53
1:P:74:LEU:HD13	1:P:122:LEU:HD11	1.89	0.52
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.44	0.52
1:T:9:MET:N	1:U:15:GLU:OE1	2.42	0.52
1:U:32:ALA:HA	1:U:40:LEU:O	2.09	0.52
1:C:16:ARG:NH1	1:C:114:GLN:O	2.38	0.52
1:C:176:SER:OG	1:C:179:ASP:OD1	2.28	0.52
1:O:38:GLY:HA3	1:O:213:LEU:O	2.10	0.52
2:K:150:MET:O	2:K:154:TYR:HB2	2.10	0.52
1:R:203:LEU:N	4:R:301:HOH:O	2.43	0.52
1:C:161:GLU:N	1:C:161:GLU:OE1	2.43	0.52
1:E:230:LEU:O	1:E:234:LEU:HD12	2.09	0.52
1:G:33:LEU:HD23	1:G:153:PHE:HB3	1.91	0.52
1:P:92:ARG:NH1	1:P:132:GLU:OE1	2.37	0.52
1:A:16:ARG:HB3	1:A:117:PRO:HG3	1.91	0.52
1:B:9:MET:N	1:C:15:GLU:OE1	2.43	0.52
1:C:87:TYR:O	2:J:57:ARG:NH2	2.42	0.52
1:G:134:LYS:NZ	1:G:137:GLU:OE2	2.42	0.52
2:L:88:ARG:HD3	2:L:126:ALA:O	2.10	0.52
1:P:224:ARG:NH2	4:P:302:HOH:O	2.43	0.52
1:S:22:LYS:O	1:S:26:ARG:HG3	2.10	0.51
2:V:81:ASN:O	2:V:85:ILE:HG12	2.11	0.51
1:D:205:VAL:HG13	1:D:230:LEU:HD23	1.93	0.51
1:O:87:TYR:OH	2:V:54:GLU:OE1	2.24	0.51
1:R:51:GLN:OE1	1:R:224:ARG:NH2	2.43	0.51
1:C:150:GLU:HG3	1:C:154:VAL:HG22	1.92	0.51
1:G:116:LYS:NZ	1:G:119:GLU:OE1	2.39	0.51
1:R:128:ALA:HB2	1:R:134:LYS:HB3	1.92	0.51
2:H:5:ALA:HA	2:H:13:VAL:O	2.11	0.51
2:X:3:ILE:HG21	2:X:44:GLY:HA3	1.91	0.51
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.93	0.51
1:U:56:LEU:HG	1:U:62:PHE:HB2	1.93	0.51
1:P:28:LYS:HD3	1:P:44:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:36:ALA:HB2	1:S:174:ASN:HA	1.92	0.51
1:U:118:TYR:HB3	1:U:120:VAL:HG22	1.91	0.51
1:C:128:ALA:HB2	1:C:134:LYS:HB3	1.93	0.51
1:Q:87:TYR:O	2:X:57:ARG:NH1	2.44	0.51
1:O:41:PHE:O	1:O:210:VAL:HA	2.12	0.50
1:T:74:LEU:HD13	1:T:122:LEU:HD11	1.94	0.50
1:R:18:GLU:OE1	1:R:21:ARG:NH1	2.35	0.50
1:B:214:ASP:OD2	1:B:223:ARG:NH2	2.44	0.50
2:b:132:GLU:CD	2:b:137:GLN:HE21	2.19	0.50
2:I:91:LEU:HG	2:I:95:MET:HE2	1.93	0.50
2:M:1:THR:HG23	2:M:33:LYS:HD3	1.94	0.50
1:Q:70:GLU:OE2	1:Q:116:LYS:NZ	2.40	0.50
1:C:121:GLU:HG2	1:C:156:MET:HG2	1.93	0.49
1:P:118:TYR:HB3	1:P:120:VAL:HG22	1.94	0.49
1:P:51:GLN:OE1	1:P:224:ARG:NH2	2.45	0.49
1:S:68:PHE:HA	1:S:71:PHE:CE2	2.46	0.49
1:C:167:LEU:O	1:C:171:TYR:N	2.45	0.49
1:D:163:ILE:HG23	1:D:187:ALA:HB1	1.94	0.49
1:O:72:ASP:O	1:O:76:ARG:HG3	2.12	0.49
1:P:68:PHE:HA	1:P:71:PHE:CE2	2.48	0.49
1:S:56:LEU:HG	1:S:62:PHE:HB2	1.93	0.49
1:D:83:ASP:OD2	2:K:65:HIS:ND1	2.39	0.49
1:O:33:LEU:HA	1:O:153:PHE:HB3	1.95	0.49
1:B:9:MET:HB3	1:C:15:GLU:HB3	1.94	0.49
1:C:32:ALA:HA	1:C:40:LEU:O	2.13	0.49
1:E:56:LEU:HB2	1:E:60:VAL:HG12	1.95	0.49
2:M:20:SER:HB3	2:M:28:GLY:HA3	1.94	0.48
1:E:58:ASP:OD1	1:E:91:ARG:NH1	2.46	0.48
2:J:18:ARG:HD3	2:J:193:THR:HG23	1.96	0.48
2:a:17:ASP:OD2	2:a:18:ARG:N	2.46	0.48
2:K:64:GLU:HG2	2:K:68:LYS:HE2	1.95	0.48
1:O:97:ARG:NH1	1:P:49:SER:O	2.47	0.48
1:F:164:ALA:HB1	1:F:168:LYS:HE2	1.94	0.48
2:J:62:GLU:OE2	2:J:82:ARG:HD3	2.14	0.48
1:O:121:GLU:HG2	1:O:142:THR:HA	1.94	0.48
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.95	0.48
1:R:58:ASP:OD1	1:R:91:ARG:NH1	2.46	0.48
1:E:72:ASP:O	1:E:76:ARG:HG3	2.13	0.48
1:P:31:VAL:HG22	1:P:42:VAL:HG22	1.96	0.48
1:Q:42:VAL:HG22	1:Q:210:VAL:HG22	1.95	0.48
1:C:220:ARG:HH22	2:J:67:GLU:CD	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:GLY:O	2:H:82:ARG:HG2	2.14	0.48
2:I:78:GLY:O	2:I:82:ARG:HG2	2.13	0.48
2:J:132:GLU:HG3	2:J:137:GLN:HB2	1.96	0.48
2:X:1:THR:HG23	2:X:33:LYS:NZ	2.28	0.48
1:C:178:THR:HA	1:C:233:LEU:HD11	1.95	0.48
2:N:38:ASP:OD2	2:N:79:LYS:NZ	2.30	0.48
1:U:121:GLU:OE2	1:U:140:ARG:NH2	2.47	0.48
2:b:12:VAL:HG12	2:b:197:ILE:HB	1.96	0.48
1:A:42:VAL:HG13	1:A:210:VAL:HG22	1.95	0.48
1:B:94:VAL:HA	1:B:98:GLN:NE2	2.29	0.48
1:S:54:SER:OG	1:S:75:ARG:HD2	2.13	0.48
1:C:123:CYS:HA	1:C:139:TYR:O	2.14	0.47
1:D:110:ILE:HA	1:D:114:GLN:HG3	1.96	0.47
1:T:140:ARG:NH1	1:T:155:VAL:O	2.32	0.47
2:b:82:ARG:NH2	2:b:85:ILE:HD12	2.29	0.47
1:A:98:GLN:O	1:A:102:VAL:HG23	2.14	0.47
1:F:176:SER:HB3	1:F:179:ASP:OD1	2.14	0.47
2:J:109:ILE:HG13	2:J:110:HIS:ND1	2.29	0.47
2:a:194:ALA:HB3	2:a:205:VAL:HB	1.96	0.47
1:E:9:MET:HE1	1:F:115:ALA:O	2.14	0.47
2:M:6:LEU:HD21	2:M:163:GLY:O	2.14	0.47
2:Y:18:ARG:HB3	2:Y:30:ASP:HA	1.96	0.47
1:E:219:ARG:NH2	2:L:64:GLU:OE1	2.47	0.47
2:X:173:ASP:OD1	2:X:221:ARG:NH1	2.36	0.47
1:A:147:ILE:HG23	1:B:50:LEU:HD21	1.97	0.47
1:C:137:GLU:OE2	1:D:48:ARG:NH1	2.48	0.47
1:D:9:MET:HE3	1:D:9:MET:HB2	1.76	0.47
1:E:83:ASP:OD2	2:L:65:HIS:ND1	2.45	0.47
1:T:81:PHE:CZ	1:T:102:VAL:HG21	2.50	0.47
2:Y:88:ARG:HD3	2:Y:126:ALA:O	2.15	0.47
1:B:31:VAL:HG23	1:B:155:VAL:HG22	1.97	0.47
1:F:97:ARG:NH1	1:F:97:ARG:HG2	2.29	0.47
1:P:28:LYS:HZ1	1:P:46:PRO:HG3	1.80	0.47
1:D:56:LEU:HG	1:D:62:PHE:HB2	1.97	0.47
1:F:68:PHE:HA	1:F:71:PHE:CE2	2.50	0.47
1:O:130:TYR:HB2	1:O:218:PRO:HA	1.96	0.47
1:Q:53:ILE:O	1:Q:224:ARG:NH2	2.46	0.47
2:V:198:ASP:OD1	2:V:198:ASP:N	2.48	0.47
1:A:217:ARG:HD2	1:A:223:ARG:HD3	1.96	0.46
1:D:10:GLU:N	1:E:15:GLU:OE1	2.34	0.46
1:D:118:TYR:HB3	1:D:120:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:225:ILE:HG22	1:S:230:LEU:HB2	1.97	0.46
1:O:24:ILE:HD13	1:O:121:GLU:HG3	1.97	0.46
1:C:181:LEU:HD13	1:C:233:LEU:HD12	1.98	0.46
1:D:16:ARG:NH2	1:D:114:GLN:O	2.27	0.46
1:D:68:PHE:HA	1:D:71:PHE:CE2	2.50	0.46
1:O:210:VAL:HG21	1:O:230:LEU:HD13	1.98	0.46
1:T:68:PHE:HA	1:T:71:PHE:CE2	2.51	0.46
1:E:123:CYS:HA	1:E:139:TYR:O	2.16	0.46
1:A:156:MET:HE3	1:A:156:MET:HB2	1.83	0.46
1:D:178:THR:HG22	1:D:233:LEU:HG	1.97	0.46
1:F:70:GLU:OE2	1:F:116:LYS:NZ	2.49	0.46
1:P:33:LEU:HD12	1:P:184:ALA:HB2	1.98	0.46
1:S:21:ARG:HD3	4:S:307:HOH:O	2.16	0.46
2:Z:150:MET:O	2:Z:154:TYR:HB2	2.14	0.46
1:G:68:PHE:HA	1:G:71:PHE:CZ	2.51	0.46
1:A:9:MET:HE3	1:A:9:MET:HB2	1.81	0.46
1:B:41:PHE:HB3	1:B:53:ILE:HD13	1.96	0.46
1:T:164:ALA:O	1:T:168:LYS:HB2	2.15	0.46
1:F:123:CYS:HA	1:F:139:TYR:O	2.15	0.46
2:K:132:GLU:HG3	2:K:137:GLN:HB2	1.97	0.46
1:R:87:TYR:O	2:Y:57:ARG:NH2	2.48	0.46
1:S:11:GLN:HG3	1:S:14:ARG:NH1	2.31	0.46
1:S:219:ARG:NH2	2:Z:64:GLU:OE1	2.40	0.46
1:U:155:VAL:HG21	1:U:164:ALA:HB2	1.98	0.46
1:T:161:GLU:OE1	1:T:161:GLU:N	2.32	0.46
2:a:7:LYS:NZ	2:a:118:GLY:O	2.36	0.46
1:G:181:LEU:O	1:G:185:VAL:HG23	2.16	0.45
2:a:143:SER:O	2:a:147:LYS:HB2	2.16	0.45
1:C:40:LEU:HA	1:C:212:VAL:HG12	1.97	0.45
1:E:72:ASP:OD2	1:E:76:ARG:NH1	2.46	0.45
1:P:163:ILE:HG12	1:P:191:GLY:HA3	1.97	0.45
1:U:18:GLU:OE1	1:U:21:ARG:NH2	2.36	0.45
2:Y:18:ARG:HD3	2:Y:193:THR:HG23	1.98	0.45
1:G:205:VAL:HG13	1:G:230:LEU:HD23	1.97	0.45
1:B:112:THR:HG22	1:C:115:ALA:HB3	1.98	0.45
1:E:89:TYR:CD1	2:M:82:ARG:HD3	2.52	0.45
2:W:20:SER:HB3	2:W:28:GLY:HA3	1.99	0.45
2:b:5:ALA:HA	2:b:13:VAL:O	2.17	0.45
1:B:25:ALA:O	1:B:158:GLY:HA2	2.17	0.45
2:H:15:ALA:HA	2:H:193:THR:O	2.17	0.45
1:O:81:PHE:CZ	1:O:102:VAL:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:CYS:HA	1:A:139:TYR:O	2.16	0.45
1:G:92:ARG:HB3	2:H:75:THR:HG21	1.99	0.45
1:U:189:ARG:O	1:U:191:GLY:N	2.48	0.45
1:E:92:ARG:HB3	2:M:75:THR:HG21	1.97	0.45
2:I:40:TYR:CZ	2:I:109:ILE:HD11	2.52	0.45
2:N:109:ILE:HD12	2:N:110:HIS:CD2	2.52	0.45
1:O:151:PRO:HB3	1:P:48:ARG:HH12	1.82	0.45
1:Q:203:LEU:HD23	1:Q:203:LEU:HA	1.81	0.45
1:S:178:THR:O	1:S:182:ARG:HD3	2.17	0.45
2:Y:143:SER:O	2:Y:147:LYS:HB2	2.17	0.45
1:F:163:ILE:H	1:F:163:ILE:HG12	1.51	0.45
2:L:159:ASP:OD1	2:L:159:ASP:N	2.49	0.45
2:M:37:THR:OG1	2:M:41:THR:HG23	2.16	0.45
1:R:156:MET:HB2	1:R:156:MET:HE3	1.82	0.45
1:B:60:VAL:HG11	1:B:99:LEU:HD12	1.99	0.45
1:U:205:VAL:HG21	1:U:231:GLN:HB2	1.98	0.45
1:B:89:TYR:CE1	2:J:82:ARG:HD2	2.52	0.44
1:F:110:ILE:HA	1:F:114:GLN:HG3	1.98	0.44
1:R:68:PHE:HA	1:R:71:PHE:CZ	2.52	0.44
2:H:132:GLU:HG3	2:H:137:GLN:HB2	1.99	0.44
1:U:161:GLU:N	1:U:162:PRO:HD2	2.32	0.44
1:E:179:ASP:O	1:E:183:ILE:HG22	2.17	0.44
2:H:150:MET:O	2:H:154:TYR:HB2	2.18	0.44
1:T:128:ALA:HB2	1:T:134:LYS:HB3	1.99	0.44
1:C:70:GLU:HB3	1:C:118:TYR:CD2	2.52	0.44
1:U:22:LYS:O	1:U:26:ARG:HG3	2.18	0.44
2:V:61:VAL:O	2:V:65:HIS:HB2	2.17	0.44
1:C:11:GLN:HA	1:C:14:ARG:CD	2.47	0.44
2:K:13:VAL:HB	2:K:196:ILE:HD12	2.00	0.44
2:N:20:SER:HB3	2:N:28:GLY:HA3	1.99	0.44
1:O:97:ARG:HD3	1:P:49:SER:HB3	1.99	0.44
1:S:33:LEU:HD12	1:S:153:PHE:HB3	2.00	0.44
1:U:87:TYR:O	2:b:57:ARG:NH2	2.49	0.44
1:E:230:LEU:HG	1:E:234:LEU:HD11	2.00	0.44
2:V:20:SER:HB3	2:V:28:GLY:HA3	2.00	0.44
2:I:144:LEU:HD23	2:I:144:LEU:HA	1.83	0.44
1:P:140:ARG:NH2	1:P:155:VAL:O	2.49	0.44
1:S:172:ALA:HB3	1:S:175:ALA:HB2	2.00	0.44
2:Y:162:SER:O	2:Y:166:VAL:HG13	2.17	0.44
1:A:68:PHE:HA	1:A:71:PHE:CZ	2.53	0.43
2:I:124:ASP:OD1	2:I:128:GLY:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:116:SER:O	2:M:116:SER:OG	2.28	0.43
2:N:88:ARG:HD3	2:N:126:ALA:O	2.18	0.43
1:R:56:LEU:HB2	1:R:60:VAL:HG12	2.01	0.43
1:R:161:GLU:HB2	1:R:162:PRO:HD3	2.00	0.43
1:T:87:TYR:O	2:a:57:ARG:NH1	2.50	0.43
2:Y:164:LEU:O	2:Y:168:VAL:HG23	2.17	0.43
1:R:12:ALA:O	1:R:16:ARG:HG3	2.17	0.43
1:R:55:GLU:HB2	1:R:222:PHE:CG	2.53	0.43
2:X:1:THR:HG23	2:X:33:LYS:HZ3	1.83	0.43
2:Z:88:ARG:HD3	2:Z:126:ALA:O	2.18	0.43
1:R:56:LEU:HG	1:R:62:PHE:HB2	2.01	0.43
1:C:22:LYS:HD3	1:C:25:ALA:HB3	2.00	0.43
1:C:220:ARG:NH2	2:J:67:GLU:OE1	2.39	0.43
1:B:123:CYS:HA	1:B:139:TYR:O	2.18	0.43
1:B:179:ASP:O	1:B:183:ILE:HG13	2.18	0.43
1:E:33:LEU:HD21	1:E:167:LEU:HD22	1.99	0.43
1:E:169:GLU:OE1	1:E:170:SER:OG	2.36	0.43
1:A:62:PHE:CE1	1:A:75:ARG:HB2	2.53	0.43
1:B:156:MET:HE3	1:B:156:MET:HB2	1.89	0.43
2:I:49:ALA:HB2	3:I:301:M9G:C13	2.48	0.43
1:O:210:VAL:HG23	1:O:225:ILE:HB	2.00	0.43
1:C:22:LYS:HG3	1:C:26:ARG:NE	2.34	0.43
1:D:35:TYR:CE2	1:D:177:LEU:HD23	2.53	0.43
2:M:113:ASP:OD2	2:M:116:SER:N	2.50	0.43
1:O:105:GLN:NE2	1:P:73:ASN:OD1	2.52	0.43
1:A:32:ALA:HB3	1:A:154:VAL:HG22	2.00	0.43
2:N:49:ALA:HB2	3:N:301:M9G:C13	2.49	0.43
1:A:22:LYS:O	1:A:26:ARG:HG3	2.18	0.43
1:E:9:MET:HB3	1:F:15:GLU:OE1	2.19	0.43
2:J:176:ASP:OD1	2:W:188:ARG:NH1	2.52	0.43
2:b:3:ILE:O	2:b:138:ALA:HA	2.19	0.43
1:C:55:GLU:HB2	1:C:222:PHE:CG	2.54	0.42
2:L:18:ARG:HH11	2:L:193:THR:CG2	2.32	0.42
1:O:54:SER:CB	1:O:75:ARG:HD2	2.49	0.42
1:Q:68:PHE:HA	1:Q:71:PHE:CE2	2.54	0.42
2:V:37:THR:HG21	2:V:59:TYR:HD2	1.84	0.42
2:X:20:SER:HB3	2:X:28:GLY:HA3	2.01	0.42
2:b:88:ARG:HD3	2:b:126:ALA:O	2.18	0.42
2:J:211:ALA:O	2:J:215:ARG:HG3	2.19	0.42
2:W:104:LEU:HB3	2:W:121:VAL:HB	2.01	0.42
1:E:230:LEU:O	1:E:233:LEU:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:88:ARG:HD3	2:I:126:ALA:O	2.19	0.42
2:I:156:GLN:OE1	2:I:165:ARG:NH2	2.52	0.42
2:K:8:TYR:CE2	2:K:196:ILE:HD11	2.55	0.42
2:X:29:ARG:NH1	2:Y:134:GLU:OE2	2.52	0.42
1:A:70:GLU:HB3	1:A:118:TYR:CD2	2.54	0.42
2:H:88:ARG:HD3	2:H:126:ALA:O	2.19	0.42
1:B:80:GLN:HG3	4:B:311:HOH:O	2.20	0.42
1:E:54:SER:CB	1:E:75:ARG:HD2	2.50	0.42
2:M:47:GLY:O	3:M:301:M9G:N04	2.52	0.42
1:T:32:ALA:O	1:T:153:PHE:HA	2.20	0.42
2:X:83:LEU:O	2:X:87:VAL:HG23	2.20	0.42
1:B:94:VAL:HA	1:B:98:GLN:HE21	1.85	0.42
2:H:20:SER:HB2	2:H:31:VAL:HG21	2.01	0.42
2:I:61:VAL:O	2:I:65:HIS:HB2	2.19	0.42
2:a:20:SER:O	2:a:27:SER:N	2.45	0.42
1:C:64:ALA:HA	1:C:121:GLU:O	2.20	0.42
1:G:89:TYR:CD1	2:H:82:ARG:HD3	2.55	0.42
1:G:217:ARG:HD3	1:G:217:ARG:HA	1.95	0.42
1:A:189:ARG:HH21	1:A:202:THR:N	2.18	0.42
2:N:3:ILE:O	2:N:138:ALA:HA	2.19	0.42
1:S:11:GLN:NE2	1:S:15:GLU:OE2	2.51	0.42
1:U:55:GLU:HB2	1:U:222:PHE:CG	2.55	0.42
1:C:150:GLU:HA	1:C:151:PRO:HD3	1.90	0.42
1:F:150:GLU:HG3	1:F:154:VAL:HG22	2.02	0.42
2:I:7:LYS:NZ	2:I:118:GLY:O	2.52	0.42
1:O:92:ARG:HE	1:O:92:ARG:HB3	1.66	0.42
2:b:161:ASP:OD1	2:b:209:ARG:NH1	2.52	0.42
1:A:164:ALA:O	1:A:168:LYS:HB2	2.20	0.41
1:C:68:PHE:HA	1:C:71:PHE:CE2	2.54	0.41
1:D:68:PHE:HA	1:D:71:PHE:CZ	2.55	0.41
2:I:18:ARG:HD3	2:I:193:THR:HG23	2.02	0.41
1:Q:180:ALA:HA	1:Q:183:ILE:HG22	2.02	0.41
1:R:10:GLU:HG3	1:R:11:GLN:N	2.34	0.41
1:C:181:LEU:HD21	1:C:234:LEU:HD23	2.03	0.41
2:L:150:MET:O	2:L:154:TYR:HB2	2.19	0.41
1:T:55:GLU:HB2	1:T:222:PHE:CG	2.55	0.41
2:a:20:SER:HB2	2:a:31:VAL:HG21	2.02	0.41
2:a:96:GLN:HG2	4:a:413:HOH:O	2.19	0.41
1:A:11:GLN:O	1:A:15:GLU:HG3	2.20	0.41
1:A:19:LEU:HD13	1:G:9:MET:HG3	2.02	0.41
2:L:29:ARG:NH2	2:b:177:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:67:LYS:HG2	1:R:69:ASN:OD1	2.20	0.41
1:S:112:THR:HG23	1:T:115:ALA:HB3	2.02	0.41
1:B:9:MET:HG3	1:C:19:LEU:HD13	2.01	0.41
1:B:30:VAL:HG13	1:B:43:ALA:HB2	2.02	0.41
1:B:62:PHE:CE1	1:B:122:LEU:HD22	2.56	0.41
1:F:33:LEU:HD22	1:F:180:ALA:HB1	2.01	0.41
2:N:165:ARG:HA	2:N:213:LEU:HD13	2.02	0.41
1:G:140:ARG:HD2	1:G:154:VAL:HG13	2.01	0.41
1:Q:44:GLU:OE1	1:Q:203:LEU:HD21	2.20	0.41
2:X:197:ILE:HA	2:X:201:GLY:O	2.21	0.41
1:F:16:ARG:HB3	1:F:117:PRO:HG3	2.03	0.41
2:N:150:MET:O	2:N:154:TYR:HB2	2.20	0.41
1:O:18:GLU:O	1:O:22:LYS:HG3	2.20	0.41
1:S:68:PHE:HA	1:S:71:PHE:CZ	2.56	0.41
2:a:78:GLY:O	2:a:82:ARG:HG2	2.19	0.41
1:C:110:ILE:HG23	1:C:114:GLN:HG3	2.01	0.41
1:T:142:THR:OG1	1:T:146:SER:HB2	2.20	0.41
2:b:121:VAL:HG22	2:b:131:ILE:HG12	2.02	0.41
1:D:70:GLU:HB3	1:D:118:TYR:CD2	2.56	0.41
1:D:159:THR:O	1:D:163:ILE:HD13	2.21	0.41
2:I:211:ALA:O	2:I:215:ARG:HG3	2.20	0.41
2:b:116:SER:O	2:b:116:SER:OG	2.34	0.41
1:A:81:PHE:CZ	1:A:102:VAL:HG21	2.56	0.41
1:B:161:GLU:OE1	1:B:161:GLU:N	2.53	0.41
1:D:31:VAL:HG12	1:D:155:VAL:HG22	2.02	0.41
1:D:74:LEU:HD11	1:D:107:LEU:HD21	2.03	0.41
1:D:156:MET:HE3	1:D:156:MET:HB2	1.86	0.41
1:F:189:ARG:HG3	1:F:203:LEU:HD12	2.03	0.41
2:K:29:ARG:NH2	2:V:176:ASP:O	2.48	0.41
1:O:62:PHE:CZ	1:O:64:ALA:HB2	2.56	0.41
1:O:153:PHE:HE2	1:O:171:TYR:HB2	1.86	0.41
1:Q:89:TYR:CD1	2:Y:82:ARG:HD3	2.56	0.41
1:S:89:TYR:CD1	2:a:82:ARG:HD3	2.56	0.41
2:W:83:LEU:HD21	2:W:102:PRO:HG3	2.03	0.41
2:Z:211:ALA:O	2:Z:215:ARG:HG2	2.20	0.41
1:A:53:ILE:HD12	1:A:209:GLU:HG2	2.03	0.41
1:B:220:ARG:HH22	2:I:67:GLU:CD	2.29	0.41
1:C:56:LEU:HG	1:C:62:PHE:HB2	2.03	0.41
1:E:121:GLU:HG2	1:E:156:MET:HG2	2.02	0.41
2:I:197:ILE:HA	2:I:201:GLY:O	2.21	0.41
2:J:61:VAL:O	2:J:65:HIS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:68:PHE:HA	1:R:71:PHE:CE2	2.56	0.41
1:T:20:ALA:O	1:T:24:ILE:HG13	2.21	0.41
1:T:61:GLY:N	1:T:213:LEU:HD11	2.36	0.41
2:X:150:MET:O	2:X:154:TYR:HB2	2.21	0.41
1:C:68:PHE:HA	1:C:71:PHE:CZ	2.57	0.40
1:P:42:VAL:HG23	1:P:188:LEU:HD11	2.02	0.40
1:T:219:ARG:HH22	2:a:64:GLU:CD	2.28	0.40
1:D:163:ILE:HD11	1:D:191:GLY:HA3	2.03	0.40
1:F:180:ALA:HA	1:F:183:ILE:HG22	2.04	0.40
1:P:56:LEU:HD23	1:P:56:LEU:HA	1.88	0.40
1:T:32:ALA:HA	1:T:40:LEU:O	2.21	0.40
2:V:112:SER:O	2:V:114:PRO:HD3	2.22	0.40
1:C:59:ARG:O	1:C:126:GLU:HA	2.21	0.40
1:C:142:THR:OG1	1:C:146:SER:HB2	2.21	0.40
2:L:157:VAL:HG22	2:L:163:GLY:HA2	2.03	0.40
1:R:61:GLY:N	1:R:213:LEU:HD11	2.36	0.40
1:R:219:ARG:HB2	1:R:220:ARG:H	1.70	0.40
1:S:32:ALA:O	1:S:153:PHE:HA	2.21	0.40
1:S:39:VAL:HB	1:S:213:LEU:HB2	2.03	0.40
2:X:105:ALA:HA	2:X:119:ARG:O	2.20	0.40
1:C:89:TYR:CE1	2:K:82:ARG:HD3	2.57	0.40
2:H:7:LYS:HB3	2:H:7:LYS:HE3	1.88	0.40
2:M:1:THR:HG21	2:M:46:ALA:HA	2.02	0.40
1:O:18:GLU:OE1	1:O:21:ARG:NE	2.55	0.40
1:R:180:ALA:O	1:R:183:ILE:HG13	2.21	0.40
1:D:54:SER:CB	1:D:75:ARG:HD2	2.52	0.40
1:E:188:LEU:HD23	1:E:188:LEU:HA	1.95	0.40
1:R:44:GLU:HA	1:R:208:LEU:HD23	2.04	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	214/240 (89%)	207 (97%)	7 (3%)	0	100	100
1	B	211/240 (88%)	202 (96%)	9 (4%)	0	100	100
1	C	212/240 (88%)	202 (95%)	10 (5%)	0	100	100
1	D	210/240 (88%)	199 (95%)	11 (5%)	0	100	100
1	E	213/240 (89%)	207 (97%)	6 (3%)	0	100	100
1	F	210/240 (88%)	207 (99%)	3 (1%)	0	100	100
1	G	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
1	O	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
1	P	215/240 (90%)	207 (96%)	8 (4%)	0	100	100
1	Q	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
1	R	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
1	S	214/240 (89%)	206 (96%)	8 (4%)	0	100	100
1	T	213/240 (89%)	205 (96%)	7 (3%)	1 (0%)	24	54
1	U	212/240 (88%)	202 (95%)	9 (4%)	1 (0%)	24	54
2	H	220/234 (94%)	213 (97%)	7 (3%)	0	100	100
2	I	220/234 (94%)	215 (98%)	5 (2%)	0	100	100
2	J	220/234 (94%)	212 (96%)	8 (4%)	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%)	214 (97%)	6 (3%)	0	100	100
2	N	221/234 (94%)	215 (97%)	6 (3%)	0	100	100
2	V	221/234 (94%)	219 (99%)	2 (1%)	0	100	100
2	W	221/234 (94%)	217 (98%)	4 (2%)	0	100	100
2	X	220/234 (94%)	215 (98%)	4 (2%)	1 (0%)	24	54
2	Y	221/234 (94%)	214 (97%)	7 (3%)	0	100	100
2	Z	221/234 (94%)	215 (97%)	5 (2%)	1 (0%)	24	54
2	a	221/234 (94%)	217 (98%)	3 (1%)	1 (0%)	24	54
2	b	221/234 (94%)	215 (97%)	6 (3%)	0	100	100
All	All	6059/6636 (91%)	5876 (97%)	178 (3%)	5 (0%)	48	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	190	ALA
1	T	151	PRO
2	a	9	PRO
2	Z	9	PRO
2	X	9	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/184 (91%)	166 (99%)	1 (1%)	78	93
1	B	165/184 (90%)	165 (100%)	0	100	100
1	C	165/184 (90%)	164 (99%)	1 (1%)	78	93
1	D	163/184 (89%)	161 (99%)	2 (1%)	63	86
1	E	166/184 (90%)	166 (100%)	0	100	100
1	F	164/184 (89%)	163 (99%)	1 (1%)	78	93
1	G	165/184 (90%)	165 (100%)	0	100	100
1	O	165/184 (90%)	162 (98%)	3 (2%)	51	80
1	P	168/184 (91%)	166 (99%)	2 (1%)	63	86
1	Q	165/184 (90%)	164 (99%)	1 (1%)	78	93
1	R	164/184 (89%)	164 (100%)	0	100	100
1	S	167/184 (91%)	166 (99%)	1 (1%)	78	93
1	T	166/184 (90%)	164 (99%)	2 (1%)	63	86
1	U	165/184 (90%)	163 (99%)	2 (1%)	63	86
2	H	165/172 (96%)	165 (100%)	0	100	100
2	I	165/172 (96%)	165 (100%)	0	100	100
2	J	165/172 (96%)	165 (100%)	0	100	100
2	K	165/172 (96%)	163 (99%)	2 (1%)	63	86
2	L	165/172 (96%)	165 (100%)	0	100	100
2	M	165/172 (96%)	163 (99%)	2 (1%)	63	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	165/172 (96%)	164 (99%)	1 (1%)	78	93
2	V	165/172 (96%)	165 (100%)	0	100	100
2	W	165/172 (96%)	165 (100%)	0	100	100
2	X	165/172 (96%)	165 (100%)	0	100	100
2	Y	165/172 (96%)	165 (100%)	0	100	100
2	Z	165/172 (96%)	161 (98%)	4 (2%)	43	75
2	a	165/172 (96%)	163 (99%)	2 (1%)	63	86
2	b	165/172 (96%)	165 (100%)	0	100	100
All	All	4625/4984 (93%)	4598 (99%)	27 (1%)	78	93

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	ILE
1	C	230	LEU
1	D	177	LEU
1	D	210	VAL
1	F	163	ILE
2	K	122	SER
2	K	196	ILE
2	M	37	THR
2	M	41	THR
2	N	109	ILE
1	O	163	ILE
1	O	168	LYS
1	O	233	LEU
1	P	161	GLU
1	P	203	LEU
1	Q	183	ILE
1	S	112	THR
1	T	156	MET
1	T	212	VAL
1	U	9	MET
1	U	159	THR
2	Z	72	VAL
2	Z	187	VAL
2	Z	207	GLU
2	Z	208	SER
2	a	196	ILE

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Mol	Chain	Res	Type
2	a	220	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	B	231	GLN
1	C	129	HIS
1	D	98	GLN
1	D	129	HIS
1	E	80	GLN
1	E	105	GLN
1	G	69	ASN
1	G	129	HIS
2	I	81	ASN
2	J	130	ASN
2	K	90	ASN
2	K	96	GLN
2	L	81	ASN
2	L	90	ASN
2	M	22	GLN
1	O	174	ASN
1	P	105	GLN
1	P	129	HIS
1	P	174	ASN
1	R	105	GLN
1	S	98	GLN
1	S	129	HIS
1	T	80	GLN
1	T	129	HIS
1	U	129	HIS
2	W	115	GLN
2	X	96	GLN
2	X	137	GLN
2	Y	115	GLN
2	Z	24	ASN
2	Z	90	ASN
2	Z	110	HIS
2	Z	130	ASN
2	a	96	GLN
2	b	22	GLN
2	b	96	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](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	M9G	X	301	-	44,45,45	3.28	16 (36%)	54,63,63	2.44	17 (31%)
3	M9G	W	301	-	44,45,45	3.29	17 (38%)	54,63,63	2.27	16 (29%)
3	M9G	H	301	-	44,45,45	3.32	17 (38%)	54,63,63	2.19	14 (25%)
3	M9G	N	301	-	44,45,45	3.28	17 (38%)	54,63,63	2.20	14 (25%)
3	M9G	b	301	-	44,45,45	3.34	17 (38%)	54,63,63	2.16	15 (27%)
3	M9G	M	301	-	44,45,45	3.31	16 (36%)	54,63,63	2.16	13 (24%)
3	M9G	a	301	-	44,45,45	3.31	17 (38%)	54,63,63	2.20	17 (31%)
3	M9G	V	301	-	44,45,45	3.31	17 (38%)	54,63,63	2.30	18 (33%)
3	M9G	Z	301	-	44,45,45	3.32	17 (38%)	54,63,63	2.10	14 (25%)
3	M9G	L	302	-	44,45,45	3.35	17 (38%)	54,63,63	2.21	13 (24%)
3	M9G	J	301	-	44,45,45	3.29	16 (36%)	54,63,63	2.49	16 (29%)
3	M9G	L	301	-	44,45,45	3.32	16 (36%)	54,63,63	2.16	15 (27%)
3	M9G	Y	301	-	44,45,45	3.31	17 (38%)	54,63,63	2.07	13 (24%)
3	M9G	I	301	-	44,45,45	3.31	18 (40%)	54,63,63	2.16	15 (27%)

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	M9G	X	301	-	-	4/36/46/46	0/5/5/5
3	M9G	W	301	-	-	1/36/46/46	0/5/5/5
3	M9G	H	301	-	-	0/36/46/46	0/5/5/5
3	M9G	N	301	-	-	0/36/46/46	0/5/5/5
3	M9G	b	301	-	-	1/36/46/46	0/5/5/5
3	M9G	M	301	-	-	0/36/46/46	0/5/5/5
3	M9G	a	301	-	-	0/36/46/46	0/5/5/5
3	M9G	V	301	-	-	6/36/46/46	0/5/5/5
3	M9G	Z	301	-	-	1/36/46/46	0/5/5/5
3	M9G	L	302	-	-	0/36/46/46	0/5/5/5
3	M9G	J	301	-	-	1/36/46/46	0/5/5/5
3	M9G	L	301	-	-	0/36/46/46	0/5/5/5
3	M9G	Y	301	-	-	4/36/46/46	0/5/5/5
3	M9G	I	301	-	-	2/36/46/46	0/5/5/5

All (235) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	302	M9G	C38-C31	-9.30	1.30	1.54
3	I	301	M9G	C38-C31	-9.21	1.30	1.54
3	a	301	M9G	C38-C31	-9.21	1.30	1.54
3	N	301	M9G	C38-C31	-9.19	1.30	1.54
3	L	301	M9G	C38-C31	-9.15	1.30	1.54
3	b	301	M9G	C38-C31	-9.14	1.30	1.54
3	Y	301	M9G	C38-C31	-9.11	1.30	1.54
3	V	301	M9G	C38-C31	-9.11	1.30	1.54
3	X	301	M9G	C38-C31	-9.10	1.30	1.54
3	M	301	M9G	C38-C31	-9.09	1.30	1.54
3	J	301	M9G	C38-C31	-9.08	1.30	1.54
3	W	301	M9G	C38-C31	-9.08	1.30	1.54
3	H	301	M9G	C38-C31	-9.08	1.30	1.54
3	Z	301	M9G	C38-C31	-9.03	1.30	1.54
3	L	301	M9G	C16-N15	8.47	1.52	1.34
3	Y	301	M9G	C16-N15	8.46	1.52	1.34
3	H	301	M9G	C16-N15	8.36	1.52	1.34
3	V	301	M9G	C16-N15	8.33	1.51	1.34
3	W	301	M9G	C16-N15	8.32	1.51	1.34
3	L	302	M9G	C16-N15	8.31	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	b	301	M9G	C16-N15	8.29	1.51	1.34
3	a	301	M9G	C16-N15	8.28	1.51	1.34
3	N	301	M9G	C16-N15	8.27	1.51	1.34
3	M	301	M9G	C16-N15	8.27	1.51	1.34
3	X	301	M9G	C16-N15	8.23	1.51	1.34
3	Z	301	M9G	C31-N30	8.22	1.60	1.47
3	L	302	M9G	C20-N19	8.20	1.51	1.34
3	Z	301	M9G	C16-N15	8.18	1.51	1.34
3	J	301	M9G	C16-N15	8.17	1.51	1.34
3	I	301	M9G	C16-N15	8.16	1.51	1.34
3	M	301	M9G	C31-N30	8.10	1.60	1.47
3	a	301	M9G	C20-N19	8.05	1.51	1.34
3	L	301	M9G	C20-N19	8.04	1.51	1.34
3	b	301	M9G	C31-N30	8.02	1.60	1.47
3	b	301	M9G	C20-N19	8.02	1.50	1.34
3	H	301	M9G	C20-N19	8.01	1.50	1.34
3	M	301	M9G	C20-N19	7.99	1.50	1.34
3	Z	301	M9G	C20-N19	7.94	1.50	1.34
3	L	302	M9G	C31-N30	7.93	1.60	1.47
3	V	301	M9G	C31-N30	7.93	1.60	1.47
3	J	301	M9G	C31-N30	7.93	1.60	1.47
3	Y	301	M9G	C20-N19	7.86	1.50	1.34
3	H	301	M9G	C31-N30	7.84	1.60	1.47
3	J	301	M9G	C20-N19	7.83	1.50	1.34
3	X	301	M9G	C31-N30	7.82	1.60	1.47
3	Y	301	M9G	C31-N30	7.81	1.59	1.47
3	W	301	M9G	C20-N19	7.80	1.50	1.34
3	I	301	M9G	C31-N30	7.80	1.59	1.47
3	I	301	M9G	C20-N19	7.79	1.50	1.34
3	N	301	M9G	C20-N19	7.78	1.50	1.34
3	L	301	M9G	C31-N30	7.78	1.59	1.47
3	W	301	M9G	C31-N30	7.76	1.59	1.47
3	a	301	M9G	C31-N30	7.75	1.59	1.47
3	V	301	M9G	C20-N19	7.74	1.50	1.34
3	X	301	M9G	C20-N19	7.73	1.50	1.34
3	N	301	M9G	C31-N30	7.58	1.59	1.47
3	L	302	M9G	C29-N30	6.03	1.52	1.35
3	Z	301	M9G	C29-N30	6.03	1.52	1.35
3	W	301	M9G	C29-N30	6.03	1.52	1.35
3	L	301	M9G	C29-N30	6.00	1.52	1.35
3	X	301	M9G	C29-N30	5.97	1.52	1.35
3	b	301	M9G	C29-N30	5.96	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	301	M9G	C29-N30	5.95	1.52	1.35
3	I	301	M9G	C29-N30	5.93	1.52	1.35
3	H	301	M9G	C29-N30	5.93	1.52	1.35
3	V	301	M9G	C29-N30	5.89	1.52	1.35
3	J	301	M9G	C29-N30	5.87	1.52	1.35
3	N	301	M9G	C29-N30	5.86	1.52	1.35
3	a	301	M9G	C29-N30	5.80	1.52	1.35
3	Y	301	M9G	C29-N30	5.76	1.51	1.35
3	L	302	M9G	C02-C03	5.67	1.61	1.50
3	H	301	M9G	C02-C03	5.51	1.60	1.50
3	J	301	M9G	C02-C03	5.50	1.60	1.50
3	L	301	M9G	C02-C03	5.41	1.60	1.50
3	I	301	M9G	C02-C03	5.38	1.60	1.50
3	a	301	M9G	C02-C03	5.38	1.60	1.50
3	b	301	M9G	C02-C03	5.34	1.60	1.50
3	M	301	M9G	C02-C03	5.31	1.60	1.50
3	Y	301	M9G	C02-C03	5.25	1.60	1.50
3	V	301	M9G	C02-C03	5.25	1.60	1.50
3	X	301	M9G	C02-C03	5.22	1.60	1.50
3	Z	301	M9G	C02-C03	5.12	1.60	1.50
3	W	301	M9G	C02-C03	5.09	1.60	1.50
3	N	301	M9G	C02-C03	5.05	1.60	1.50
3	Z	301	M9G	C32-C31	4.94	1.59	1.51
3	L	301	M9G	C39-C40	-4.93	1.34	1.51
3	J	301	M9G	C32-C31	4.91	1.59	1.51
3	M	301	M9G	C39-C40	-4.89	1.35	1.51
3	Z	301	M9G	C39-C40	-4.88	1.35	1.51
3	b	301	M9G	C39-C40	-4.88	1.35	1.51
3	Y	301	M9G	C39-C40	-4.88	1.35	1.51
3	V	301	M9G	C39-C40	-4.83	1.35	1.51
3	W	301	M9G	C39-C40	-4.82	1.35	1.51
3	V	301	M9G	C32-C31	4.81	1.59	1.51
3	J	301	M9G	C39-C40	-4.81	1.35	1.51
3	H	301	M9G	C39-C40	-4.81	1.35	1.51
3	N	301	M9G	C39-C40	-4.79	1.35	1.51
3	a	301	M9G	C32-C31	4.79	1.59	1.51
3	X	301	M9G	C39-C40	-4.79	1.35	1.51
3	L	302	M9G	C39-C40	-4.78	1.35	1.51
3	a	301	M9G	C39-C40	-4.76	1.35	1.51
3	I	301	M9G	C39-C40	-4.75	1.35	1.51
3	I	301	M9G	C32-C31	4.71	1.59	1.51
3	L	302	M9G	C32-C31	4.69	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	M9G	C32-C31	4.68	1.59	1.51
3	W	301	M9G	C32-C31	4.63	1.58	1.51
3	N	301	M9G	C32-C31	4.57	1.58	1.51
3	b	301	M9G	C32-C31	4.56	1.58	1.51
3	M	301	M9G	C32-C31	4.52	1.58	1.51
3	Y	301	M9G	C32-C31	4.52	1.58	1.51
3	X	301	M9G	C32-C31	4.50	1.58	1.51
3	L	301	M9G	C32-C31	4.41	1.58	1.51
3	N	301	M9G	C06-C05	-3.79	1.41	1.47
3	b	301	M9G	C06-C05	-3.77	1.41	1.47
3	V	301	M9G	C06-C05	-3.73	1.41	1.47
3	W	301	M9G	C06-C05	-3.64	1.41	1.47
3	Z	301	M9G	C06-C05	-3.61	1.41	1.47
3	a	301	M9G	C06-C05	-3.60	1.41	1.47
3	J	301	M9G	C06-C05	-3.56	1.41	1.47
3	X	301	M9G	C06-C05	-3.55	1.41	1.47
3	I	301	M9G	C06-C05	-3.55	1.41	1.47
3	Y	301	M9G	C06-C05	-3.54	1.41	1.47
3	L	302	M9G	C06-C05	-3.50	1.41	1.47
3	H	301	M9G	C06-C05	-3.50	1.41	1.47
3	M	301	M9G	C06-C05	-3.48	1.41	1.47
3	L	301	M9G	C06-C05	-3.34	1.41	1.47
3	Y	301	M9G	O24-N23	-3.31	1.36	1.42
3	N	301	M9G	O24-N23	-3.30	1.36	1.42
3	L	301	M9G	O24-N23	-3.29	1.36	1.42
3	V	301	M9G	O24-N23	-3.26	1.36	1.42
3	I	301	M9G	O24-N23	-3.26	1.36	1.42
3	L	302	M9G	O24-N23	-3.23	1.36	1.42
3	Y	301	M9G	O41-C29	-3.22	1.16	1.23
3	b	301	M9G	O24-N23	-3.21	1.36	1.42
3	Z	301	M9G	O24-N23	-3.19	1.36	1.42
3	a	301	M9G	O41-C29	-3.19	1.16	1.23
3	a	301	M9G	C39-C38	3.18	1.64	1.51
3	W	301	M9G	O24-N23	-3.18	1.36	1.42
3	M	301	M9G	O24-N23	-3.17	1.36	1.42
3	a	301	M9G	O24-N23	-3.14	1.36	1.42
3	I	301	M9G	C39-C38	3.14	1.64	1.51
3	N	301	M9G	C39-C38	3.13	1.64	1.51
3	J	301	M9G	C39-C38	3.13	1.64	1.51
3	X	301	M9G	O24-N23	-3.13	1.36	1.42
3	M	301	M9G	C39-C38	3.13	1.64	1.51
3	V	301	M9G	O41-C29	-3.12	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	301	M9G	C39-C38	3.12	1.64	1.51
3	V	301	M9G	C39-C38	3.12	1.64	1.51
3	W	301	M9G	C39-C38	3.11	1.64	1.51
3	X	301	M9G	C39-C38	3.11	1.64	1.51
3	H	301	M9G	C39-C38	3.11	1.64	1.51
3	H	301	M9G	O24-N23	-3.11	1.36	1.42
3	L	302	M9G	C39-C38	3.10	1.64	1.51
3	L	301	M9G	C39-C38	3.10	1.64	1.51
3	b	301	M9G	O41-C29	-3.10	1.16	1.23
3	b	301	M9G	C39-C38	3.10	1.64	1.51
3	I	301	M9G	O41-C29	-3.09	1.16	1.23
3	H	301	M9G	O41-C29	-3.08	1.16	1.23
3	M	301	M9G	O41-C29	-3.08	1.16	1.23
3	Z	301	M9G	C39-C38	3.08	1.64	1.51
3	N	301	M9G	O41-C29	-3.05	1.16	1.23
3	W	301	M9G	O41-C29	-3.03	1.16	1.23
3	L	301	M9G	O41-C29	-3.02	1.16	1.23
3	X	301	M9G	O41-C29	-3.02	1.16	1.23
3	H	301	M9G	C28-C29	2.99	1.56	1.51
3	J	301	M9G	O41-C29	-2.99	1.16	1.23
3	L	302	M9G	O41-C29	-2.97	1.16	1.23
3	Z	301	M9G	O41-C29	-2.94	1.16	1.23
3	L	302	M9G	C28-C29	2.94	1.56	1.51
3	X	301	M9G	C28-C29	2.89	1.56	1.51
3	J	301	M9G	O24-N23	-2.88	1.37	1.42
3	L	301	M9G	C28-C29	2.87	1.56	1.51
3	L	302	M9G	C40-N30	2.85	1.53	1.47
3	W	301	M9G	C28-C29	2.84	1.56	1.51
3	I	301	M9G	C28-C29	2.84	1.56	1.51
3	b	301	M9G	C28-C29	2.84	1.56	1.51
3	N	301	M9G	C40-N30	2.83	1.53	1.47
3	H	301	M9G	C40-N30	2.81	1.53	1.47
3	W	301	M9G	C40-N30	2.79	1.53	1.47
3	X	301	M9G	C40-N30	2.78	1.53	1.47
3	Z	301	M9G	C28-C29	2.77	1.56	1.51
3	Z	301	M9G	C40-N30	2.77	1.53	1.47
3	J	301	M9G	C40-N30	2.77	1.53	1.47
3	L	301	M9G	C40-N30	2.77	1.53	1.47
3	a	301	M9G	C40-N30	2.74	1.52	1.47
3	I	301	M9G	C40-N30	2.73	1.52	1.47
3	V	301	M9G	C40-N30	2.72	1.52	1.47
3	Y	301	M9G	C28-C29	2.70	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	301	M9G	C28-C29	2.69	1.56	1.51
3	b	301	M9G	C40-N30	2.67	1.52	1.47
3	Y	301	M9G	C40-N30	2.66	1.52	1.47
3	M	301	M9G	C40-N30	2.64	1.52	1.47
3	M	301	M9G	C28-C29	2.63	1.56	1.51
3	a	301	M9G	C28-C29	2.62	1.56	1.51
3	N	301	M9G	C28-C29	2.60	1.56	1.51
3	J	301	M9G	C28-C29	2.56	1.56	1.51
3	M	301	M9G	C13-N14	-2.51	1.32	1.37
3	L	301	M9G	C13-N14	-2.51	1.32	1.37
3	Y	301	M9G	C13-N14	-2.51	1.32	1.37
3	Z	301	M9G	C13-N14	-2.48	1.32	1.37
3	X	301	M9G	C13-N14	-2.46	1.32	1.37
3	W	301	M9G	C13-N14	-2.43	1.32	1.37
3	Y	301	M9G	C27-C25	2.41	1.39	1.34
3	H	301	M9G	C13-N14	-2.41	1.32	1.37
3	I	301	M9G	C13-N14	-2.40	1.32	1.37
3	V	301	M9G	C13-N14	-2.39	1.32	1.37
3	b	301	M9G	C13-N14	-2.36	1.33	1.37
3	a	301	M9G	C13-N14	-2.34	1.33	1.37
3	J	301	M9G	C13-N14	-2.34	1.33	1.37
3	N	301	M9G	C13-N14	-2.30	1.33	1.37
3	I	301	M9G	C27-C25	2.28	1.38	1.34
3	Z	301	M9G	C27-C25	2.28	1.38	1.34
3	N	301	M9G	C05-N04	-2.27	1.33	1.37
3	M	301	M9G	C27-C25	2.26	1.38	1.34
3	V	301	M9G	C27-C25	2.26	1.38	1.34
3	b	301	M9G	C27-C25	2.23	1.38	1.34
3	a	301	M9G	C27-C25	2.22	1.38	1.34
3	H	301	M9G	C27-C25	2.20	1.38	1.34
3	L	301	M9G	C27-C25	2.20	1.38	1.34
3	N	301	M9G	C27-C25	2.20	1.38	1.34
3	L	302	M9G	C27-C25	2.20	1.38	1.34
3	Z	301	M9G	C05-N04	-2.19	1.33	1.37
3	W	301	M9G	C27-C25	2.18	1.38	1.34
3	I	301	M9G	C05-N04	-2.17	1.33	1.37
3	L	302	M9G	C13-N14	-2.16	1.33	1.37
3	b	301	M9G	C05-N04	-2.15	1.33	1.37
3	X	301	M9G	C27-C25	2.13	1.38	1.34
3	a	301	M9G	C05-N04	-2.12	1.33	1.37
3	Y	301	M9G	C05-N04	-2.11	1.33	1.37
3	H	301	M9G	C05-N04	-2.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	301	M9G	C05-N04	-2.07	1.33	1.37
3	L	302	M9G	C05-N04	-2.07	1.33	1.37
3	I	301	M9G	C18-N19	-2.07	1.41	1.45
3	W	301	M9G	C05-N04	-2.06	1.33	1.37
3	V	301	M9G	C05-N04	-2.02	1.33	1.37

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	301	M9G	O24-C25-C26	8.41	127.45	115.89
3	W	301	M9G	O24-C25-C26	8.12	127.06	115.89
3	H	301	M9G	O24-C25-C26	8.02	126.92	115.89
3	M	301	M9G	O24-C25-C26	7.97	126.86	115.89
3	N	301	M9G	O24-C25-C26	7.97	126.86	115.89
3	X	301	M9G	O24-C25-C26	7.97	126.85	115.89
3	L	302	M9G	O24-C25-C26	7.87	126.71	115.89
3	a	301	M9G	O24-C25-C26	7.67	126.44	115.89
3	Z	301	M9G	O24-C25-C26	7.63	126.39	115.89
3	b	301	M9G	O24-C25-C26	7.61	126.35	115.89
3	V	301	M9G	O24-C25-C26	7.58	126.32	115.89
3	I	301	M9G	O24-C25-C26	7.58	126.31	115.89
3	L	301	M9G	O24-C25-C26	7.51	126.22	115.89
3	Y	301	M9G	O24-C25-C26	7.21	125.81	115.89
3	J	301	M9G	C22-C20-N19	6.18	124.00	115.22
3	J	301	M9G	C18-N19-C20	-5.64	112.50	122.00
3	Z	301	M9G	C40-N30-C31	-5.61	105.57	111.88
3	X	301	M9G	C40-N30-C31	-5.44	105.76	111.88
3	M	301	M9G	C40-N30-C31	-5.35	105.85	111.88
3	J	301	M9G	C40-N30-C31	-5.33	105.88	111.88
3	L	301	M9G	C40-N30-C31	-5.30	105.92	111.88
3	V	301	M9G	C40-N30-C31	-5.25	105.97	111.88
3	W	301	M9G	C40-N30-C31	-5.22	106.00	111.88
3	b	301	M9G	C40-N30-C31	-5.20	106.03	111.88
3	J	301	M9G	C26-C25-C27	-5.12	125.20	134.05
3	W	301	M9G	C26-C25-C27	-5.02	125.39	134.05
3	L	302	M9G	C40-N30-C31	-4.97	106.28	111.88
3	M	301	M9G	C27-C22-N23	-4.96	107.98	112.11
3	X	301	M9G	C22-C20-N19	4.94	122.24	115.22
3	N	301	M9G	C26-C25-C27	-4.93	125.54	134.05
3	X	301	M9G	C26-C25-C27	-4.85	125.68	134.05
3	M	301	M9G	C26-C25-C27	-4.83	125.70	134.05
3	H	301	M9G	C26-C25-C27	-4.80	125.76	134.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	301	M9G	C40-N30-C31	-4.78	106.50	111.88
3	W	301	M9G	C38-C31-N30	4.74	107.21	101.93
3	H	301	M9G	C40-N30-C31	-4.73	106.56	111.88
3	Y	301	M9G	C27-C22-N23	-4.72	108.18	112.11
3	X	301	M9G	C38-C31-N30	4.68	107.14	101.93
3	N	301	M9G	C38-C31-N30	4.65	107.11	101.93
3	H	301	M9G	C27-C22-N23	-4.64	108.25	112.11
3	L	302	M9G	C26-C25-C27	-4.64	126.04	134.05
3	X	301	M9G	C18-N19-C20	-4.61	114.23	122.00
3	b	301	M9G	C26-C25-C27	-4.61	126.08	134.05
3	Z	301	M9G	C26-C25-C27	-4.61	126.09	134.05
3	a	301	M9G	C26-C25-C27	-4.60	126.10	134.05
3	V	301	M9G	C26-C25-C27	-4.58	126.14	134.05
3	Y	301	M9G	C40-N30-C31	-4.54	106.77	111.88
3	L	302	M9G	C27-C22-N23	-4.54	108.33	112.11
3	I	301	M9G	C26-C25-C27	-4.53	126.23	134.05
3	L	301	M9G	C38-C31-N30	4.52	106.96	101.93
3	V	301	M9G	C27-C22-N23	-4.50	108.36	112.11
3	L	301	M9G	C26-C25-C27	-4.49	126.30	134.05
3	Z	301	M9G	C27-C22-N23	-4.49	108.37	112.11
3	I	301	M9G	C27-C22-N23	-4.48	108.38	112.11
3	a	301	M9G	C27-C22-N23	-4.47	108.39	112.11
3	I	301	M9G	C38-C31-N30	4.46	106.90	101.93
3	N	301	M9G	C40-N30-C31	-4.46	106.86	111.88
3	X	301	M9G	C27-C22-N23	-4.43	108.42	112.11
3	W	301	M9G	C27-C22-N23	-4.40	108.45	112.11
3	b	301	M9G	C27-C22-N23	-4.40	108.45	112.11
3	V	301	M9G	C38-C31-N30	4.39	106.81	101.93
3	L	302	M9G	C18-C28-C29	4.38	120.98	112.22
3	L	301	M9G	C27-C22-N23	-4.36	108.48	112.11
3	Y	301	M9G	C38-C31-N30	4.35	106.77	101.93
3	H	301	M9G	C38-C31-N30	4.33	106.75	101.93
3	a	301	M9G	C40-N30-C31	-4.31	107.02	111.88
3	M	301	M9G	C38-C31-N30	4.29	106.71	101.93
3	Y	301	M9G	C26-C25-C27	-4.29	126.65	134.05
3	L	302	M9G	C38-C31-N30	4.28	106.69	101.93
3	M	301	M9G	O24-N23-C22	4.21	109.48	104.91
3	J	301	M9G	C27-C22-N23	-4.21	108.60	112.11
3	Y	301	M9G	O24-N23-C22	4.19	109.45	104.91
3	b	301	M9G	C38-C31-N30	4.11	106.50	101.93
3	N	301	M9G	C27-C22-N23	-4.05	108.74	112.11
3	a	301	M9G	C22-C20-N19	4.02	120.93	115.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	301	M9G	C22-C20-N19	3.99	120.90	115.22
3	V	301	M9G	C18-N19-C20	-3.97	115.31	122.00
3	V	301	M9G	O24-N23-C22	3.94	109.19	104.91
3	J	301	M9G	C38-C31-N30	3.94	106.32	101.93
3	Z	301	M9G	O24-N23-C22	3.94	109.18	104.91
3	I	301	M9G	O24-N23-C22	3.92	109.16	104.91
3	H	301	M9G	O24-N23-C22	3.91	109.15	104.91
3	a	301	M9G	C38-C31-N30	3.87	106.24	101.93
3	N	301	M9G	C09-C07-C06	-3.85	118.92	123.07
3	W	301	M9G	O24-N23-C22	3.84	109.08	104.91
3	I	301	M9G	C18-C28-C29	3.84	119.89	112.22
3	b	301	M9G	O24-N23-C22	3.81	109.04	104.91
3	L	302	M9G	O24-N23-C22	3.79	109.02	104.91
3	b	301	M9G	C09-C07-C06	-3.78	119.00	123.07
3	V	301	M9G	C09-C07-C06	-3.77	119.01	123.07
3	Z	301	M9G	C38-C31-N30	3.75	106.11	101.93
3	X	301	M9G	O24-N23-C22	3.75	108.98	104.91
3	a	301	M9G	O24-N23-C22	3.73	108.96	104.91
3	N	301	M9G	O24-N23-C22	3.73	108.95	104.91
3	L	301	M9G	O24-N23-C22	3.73	108.95	104.91
3	J	301	M9G	C09-C07-C06	-3.65	119.14	123.07
3	V	301	M9G	C12-C06-C07	3.59	120.69	116.70
3	X	301	M9G	C09-C07-C06	-3.58	119.21	123.07
3	W	301	M9G	C09-C07-C06	-3.56	119.23	123.07
3	N	301	M9G	C12-C06-C07	3.48	120.56	116.70
3	L	301	M9G	C22-C20-N19	3.47	120.16	115.22
3	H	301	M9G	C09-C07-C06	-3.47	119.33	123.07
3	Z	301	M9G	C09-C07-C06	-3.44	119.36	123.07
3	a	301	M9G	C09-C07-C06	-3.44	119.37	123.07
3	L	302	M9G	C22-C20-N19	3.42	120.08	115.22
3	H	301	M9G	C18-C28-C29	3.39	119.00	112.22
3	b	301	M9G	C12-C06-C07	3.37	120.44	116.70
3	a	301	M9G	C18-C28-C29	3.34	118.89	112.22
3	X	301	M9G	C18-C28-C29	3.34	118.89	112.22
3	I	301	M9G	C09-C07-C06	-3.33	119.48	123.07
3	J	301	M9G	O24-N23-C22	3.31	108.49	104.91
3	X	301	M9G	C12-C06-C07	3.25	120.31	116.70
3	W	301	M9G	C12-C06-C07	3.20	120.25	116.70
3	Z	301	M9G	C12-C06-C07	3.19	120.24	116.70
3	J	301	M9G	C18-C28-C29	3.18	118.58	112.22
3	L	302	M9G	C09-C07-C06	-3.16	119.66	123.07
3	Y	301	M9G	C09-C07-C06	-3.16	119.66	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	301	M9G	C12-C06-C07	3.13	120.18	116.70
3	M	301	M9G	C09-C07-C06	-3.11	119.71	123.07
3	J	301	M9G	O21-C20-N19	-3.11	117.62	123.09
3	J	301	M9G	C12-C06-C07	3.10	120.14	116.70
3	H	301	M9G	C12-C06-C07	3.07	120.11	116.70
3	L	302	M9G	C12-C06-C07	3.07	120.10	116.70
3	N	301	M9G	C32-C31-N30	-3.04	107.66	113.03
3	a	301	M9G	C18-N19-C20	-3.03	116.89	122.00
3	W	301	M9G	C22-C20-N19	3.01	119.50	115.22
3	I	301	M9G	C12-C06-C07	2.99	120.02	116.70
3	X	301	M9G	O21-C20-N19	-2.95	117.90	123.09
3	Y	301	M9G	C12-C06-C07	2.92	119.94	116.70
3	J	301	M9G	C27-C22-C20	-2.92	122.80	127.35
3	L	301	M9G	C12-C06-C07	2.91	119.93	116.70
3	L	301	M9G	C18-C28-C29	2.89	117.99	112.22
3	V	301	M9G	O21-C20-N19	-2.82	118.13	123.09
3	W	301	M9G	C32-C31-N30	-2.81	108.06	113.03
3	L	301	M9G	C09-C07-C06	-2.78	120.07	123.07
3	b	301	M9G	C05-C13-N14	-2.73	106.47	110.81
3	M	301	M9G	C12-C06-C07	2.71	119.71	116.70
3	N	301	M9G	C05-C13-N14	-2.67	106.56	110.81
3	b	301	M9G	C22-C20-N19	2.67	119.02	115.22
3	V	301	M9G	C05-C13-N14	-2.67	106.57	110.81
3	X	301	M9G	C32-C31-N30	-2.60	108.42	113.03
3	X	301	M9G	C05-C13-N14	-2.58	106.72	110.81
3	a	301	M9G	C05-C13-N14	-2.57	106.72	110.81
3	Z	301	M9G	C05-C13-N14	-2.53	106.79	110.81
3	L	301	M9G	C05-C13-N14	-2.52	106.81	110.81
3	X	301	M9G	C38-C31-C32	-2.52	108.66	113.69
3	M	301	M9G	C38-C31-C32	-2.50	108.69	113.69
3	L	301	M9G	C38-C31-C32	-2.49	108.71	113.69
3	J	301	M9G	C05-C13-N14	-2.46	106.90	110.81
3	H	301	M9G	C05-C13-N14	-2.45	106.91	110.81
3	L	302	M9G	C05-C13-N14	-2.44	106.93	110.81
3	V	301	M9G	C03-C02-N15	-2.43	103.43	109.14
3	a	301	M9G	C28-C18-C16	-2.43	104.83	110.57
3	W	301	M9G	C18-N19-C20	-2.43	117.92	122.00
3	I	301	M9G	C05-C13-N14	-2.42	106.96	110.81
3	V	301	M9G	C18-C28-C29	2.42	117.06	112.22
3	H	301	M9G	C38-C31-C32	-2.41	108.87	113.69
3	b	301	M9G	C18-C28-C29	2.41	117.03	112.22
3	M	301	M9G	C31-N30-C29	2.40	127.93	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	301	M9G	C18-C28-C29	2.39	117.00	112.22
3	W	301	M9G	C05-C13-N14	-2.39	107.01	110.81
3	Y	301	M9G	C38-C31-C32	-2.36	108.98	113.69
3	H	301	M9G	C22-C20-N19	2.36	118.58	115.22
3	M	301	M9G	C05-C13-N14	-2.35	107.08	110.81
3	L	302	M9G	O24-C25-C27	-2.35	107.25	109.88
3	a	301	M9G	C38-C31-C32	-2.33	109.04	113.69
3	a	301	M9G	O21-C20-N19	-2.33	118.99	123.09
3	Z	301	M9G	C18-C28-C29	2.33	116.87	112.22
3	V	301	M9G	C32-C31-N30	-2.32	108.94	113.03
3	N	301	M9G	C38-C31-C32	-2.30	109.09	113.69
3	L	302	M9G	C32-C31-N30	-2.30	108.97	113.03
3	Y	301	M9G	C05-C13-N14	-2.29	107.17	110.81
3	H	301	M9G	O24-C25-C27	-2.28	107.32	109.88
3	Y	301	M9G	C18-C28-C29	2.27	116.75	112.22
3	J	301	M9G	C38-C31-C32	-2.26	109.17	113.69
3	J	301	M9G	O24-C25-C27	-2.26	107.35	109.88
3	W	301	M9G	C18-C28-C29	2.25	116.72	112.22
3	b	301	M9G	C31-N30-C29	2.25	127.50	120.83
3	Z	301	M9G	C31-N30-C29	2.25	127.50	120.83
3	b	301	M9G	C38-C31-C32	-2.25	109.20	113.69
3	Z	301	M9G	C38-C31-C32	-2.24	109.20	113.69
3	I	301	M9G	C39-C40-N30	2.20	107.03	103.24
3	X	301	M9G	C03-C02-N15	-2.20	103.98	109.14
3	N	301	M9G	C03-C02-N15	-2.18	104.03	109.14
3	M	301	M9G	O24-C25-C27	-2.17	107.44	109.88
3	I	301	M9G	C28-C18-C16	-2.17	105.46	110.57
3	a	301	M9G	O24-C25-C27	-2.16	107.46	109.88
3	I	301	M9G	O24-C25-C27	-2.16	107.46	109.88
3	L	301	M9G	C32-C31-N30	-2.15	109.23	113.03
3	X	301	M9G	O24-C25-C27	-2.15	107.47	109.88
3	I	301	M9G	C38-C31-C32	-2.15	109.40	113.69
3	L	301	M9G	O24-C25-C27	-2.13	107.48	109.88
3	V	301	M9G	C38-C31-C32	-2.13	109.44	113.69
3	L	301	M9G	C31-N30-C29	2.10	127.05	120.83
3	Z	301	M9G	O24-C25-C27	-2.10	107.53	109.88
3	Z	301	M9G	C22-C20-N19	2.10	118.20	115.22
3	V	301	M9G	O24-C25-C27	-2.09	107.53	109.88
3	b	301	M9G	C32-C31-N30	-2.09	109.34	113.03
3	Y	301	M9G	O24-C25-C27	-2.08	107.54	109.88
3	W	301	M9G	O24-C25-C27	-2.08	107.55	109.88
3	I	301	M9G	C32-C31-N30	-2.08	109.36	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	301	M9G	O21-C20-N19	-2.07	119.45	123.09
3	b	301	M9G	O24-C25-C27	-2.06	107.56	109.88
3	Y	301	M9G	C01-C02-C03	-2.06	108.61	111.44
3	a	301	M9G	C39-C40-N30	2.04	106.75	103.24
3	W	301	M9G	C38-C31-C32	-2.04	109.62	113.69
3	H	301	M9G	C39-C40-N30	2.04	106.74	103.24
3	V	301	M9G	C31-N30-C29	2.03	126.84	120.83
3	N	301	M9G	O24-C25-C27	-2.02	107.61	109.88
3	N	301	M9G	C39-C38-C31	2.01	109.24	104.24

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	V	301	M9G	O21-C20-C22-C27
3	V	301	M9G	N19-C20-C22-C27
3	V	301	M9G	O21-C20-C22-N23
3	V	301	M9G	N19-C20-C22-N23
3	X	301	M9G	O21-C20-C22-C27
3	X	301	M9G	N19-C20-C22-C27
3	X	301	M9G	O21-C20-C22-N23
3	X	301	M9G	N19-C20-C22-N23
3	Y	301	M9G	O21-C20-C22-C27
3	Y	301	M9G	N19-C20-C22-C27
3	Z	301	M9G	N19-C20-C22-C27
3	b	301	M9G	N19-C20-C22-C27
3	Y	301	M9G	N19-C20-C22-N23
3	Y	301	M9G	O21-C20-C22-N23
3	V	301	M9G	C18-C28-C29-N30
3	V	301	M9G	C18-C28-C29-O41
3	I	301	M9G	C18-C28-C29-N30
3	I	301	M9G	O17-C16-C18-N19
3	W	301	M9G	O17-C16-C18-N19
3	J	301	M9G	N19-C20-C22-C27

There are no ring outliers.

4 monomers are involved in 4 short contacts:

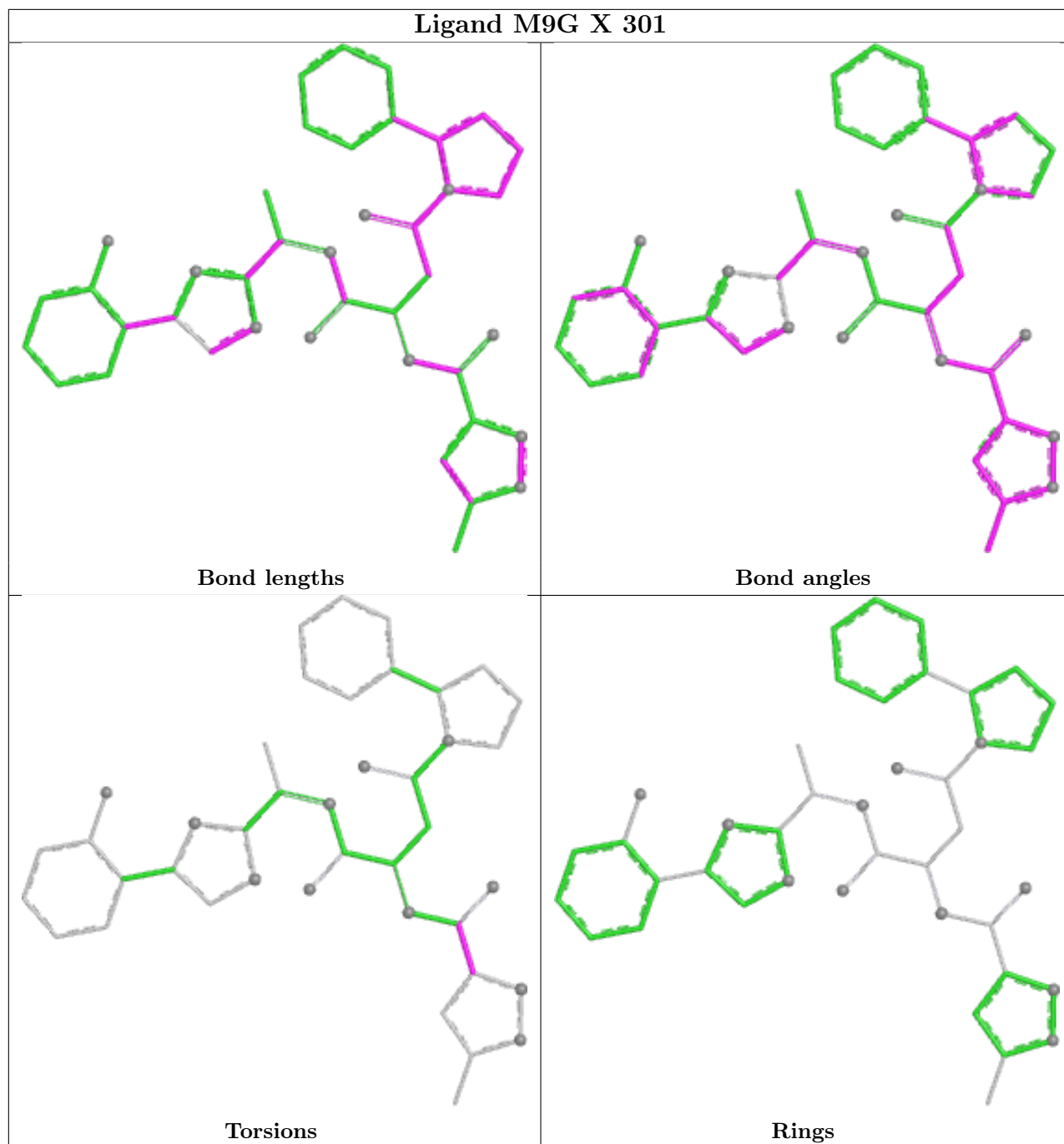
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	301	M9G	1	0
3	b	301	M9G	1	0

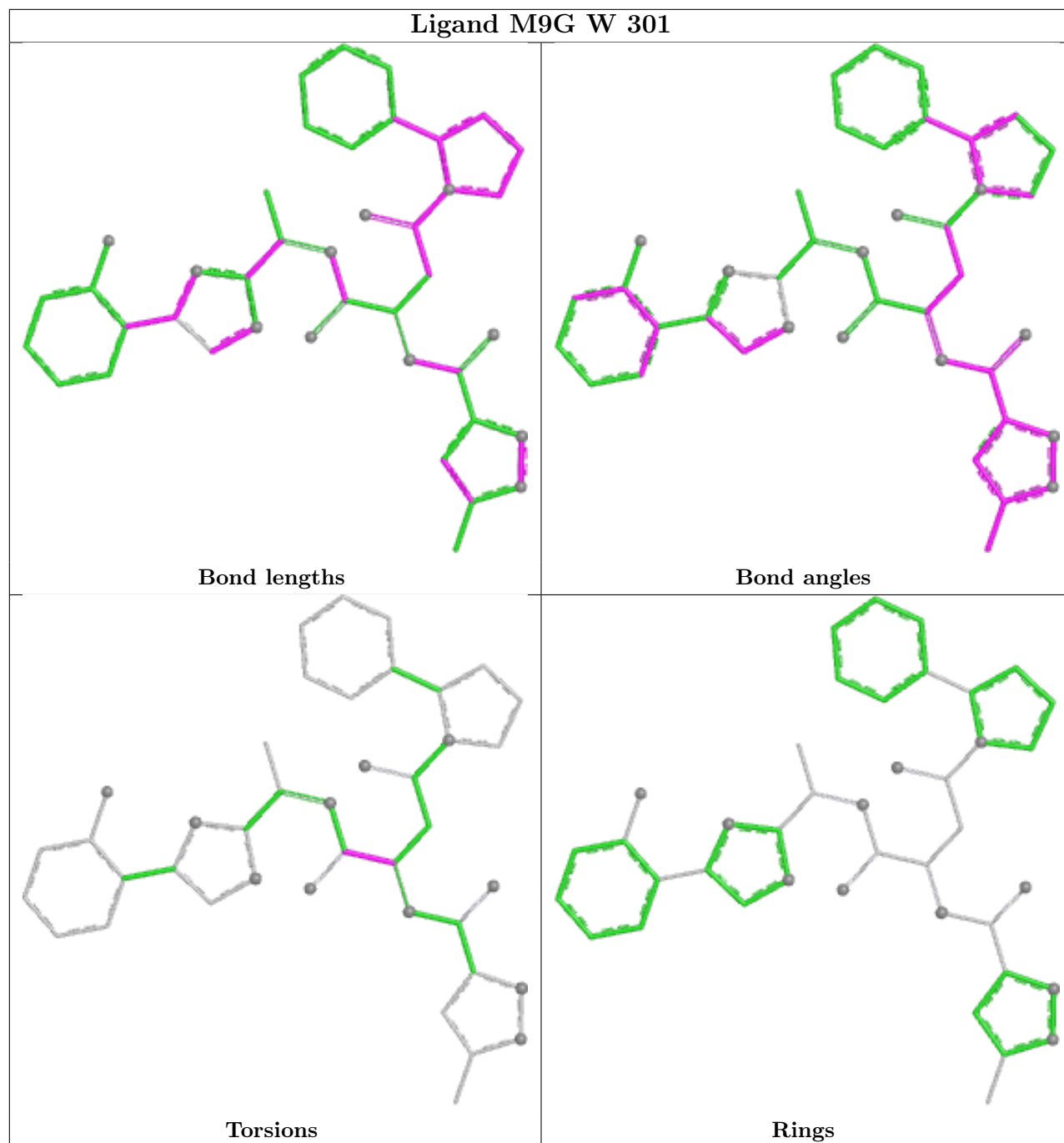
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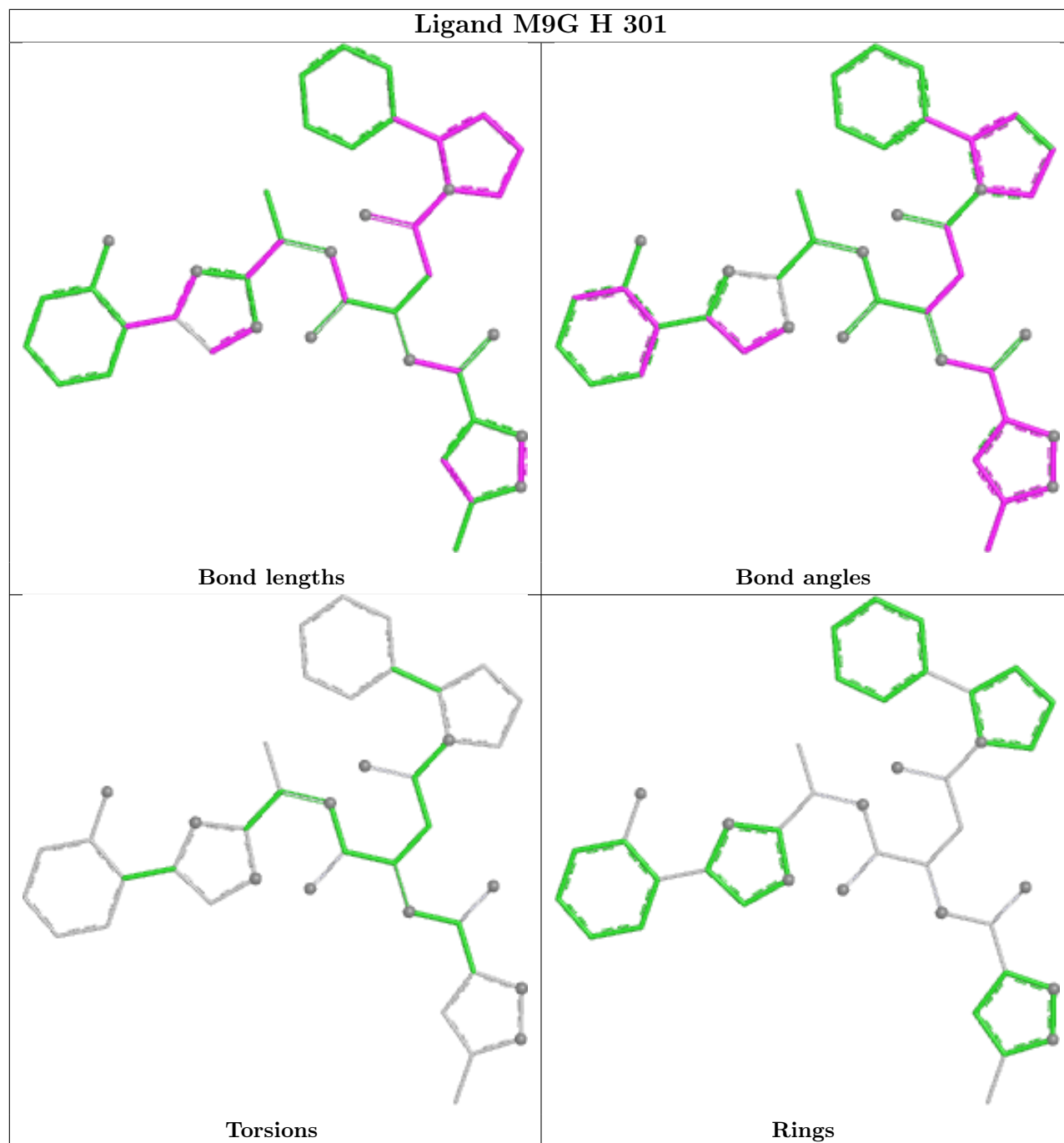
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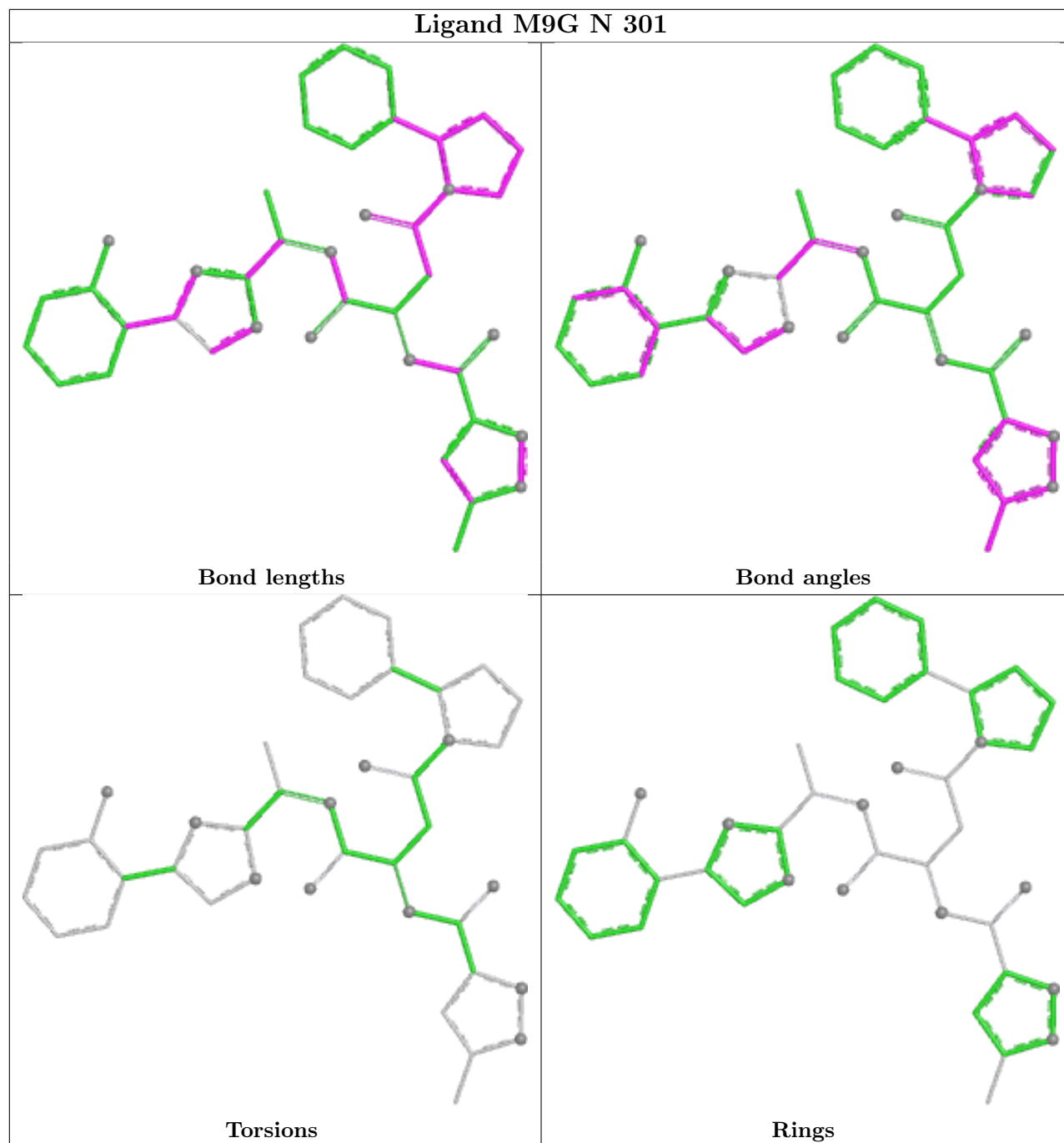
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	301	M9G	1	0
3	I	301	M9G	1	0

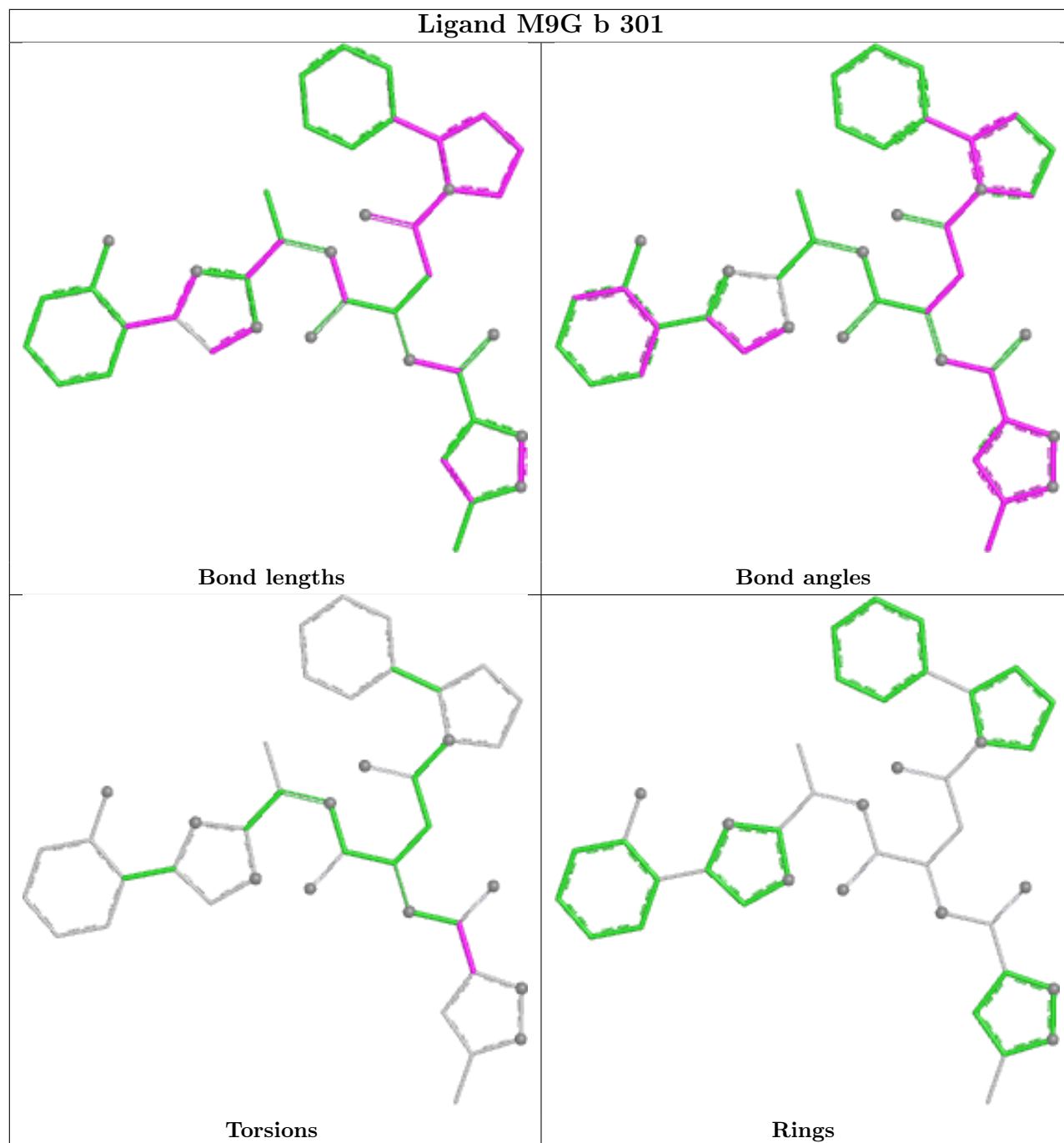
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

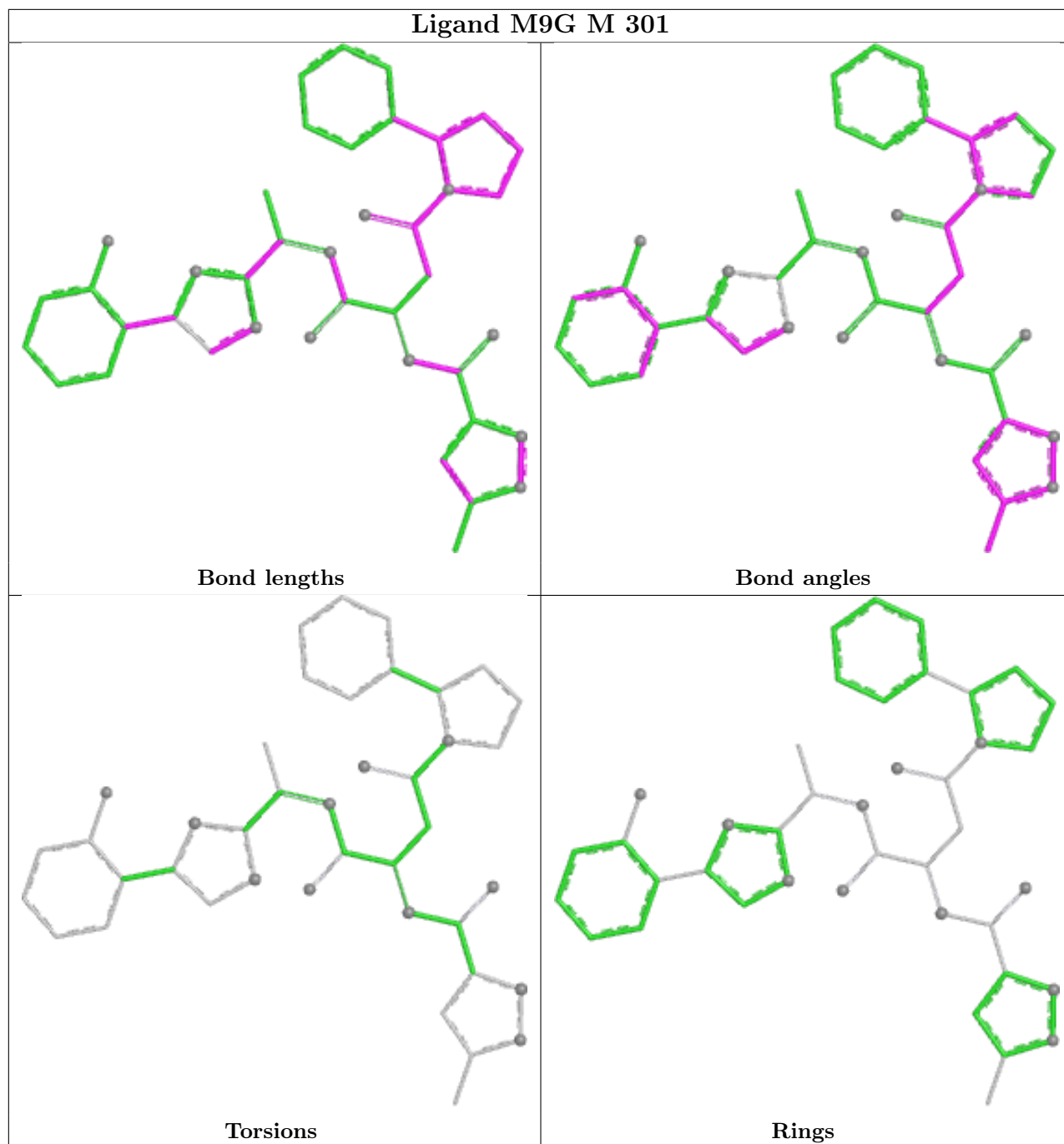


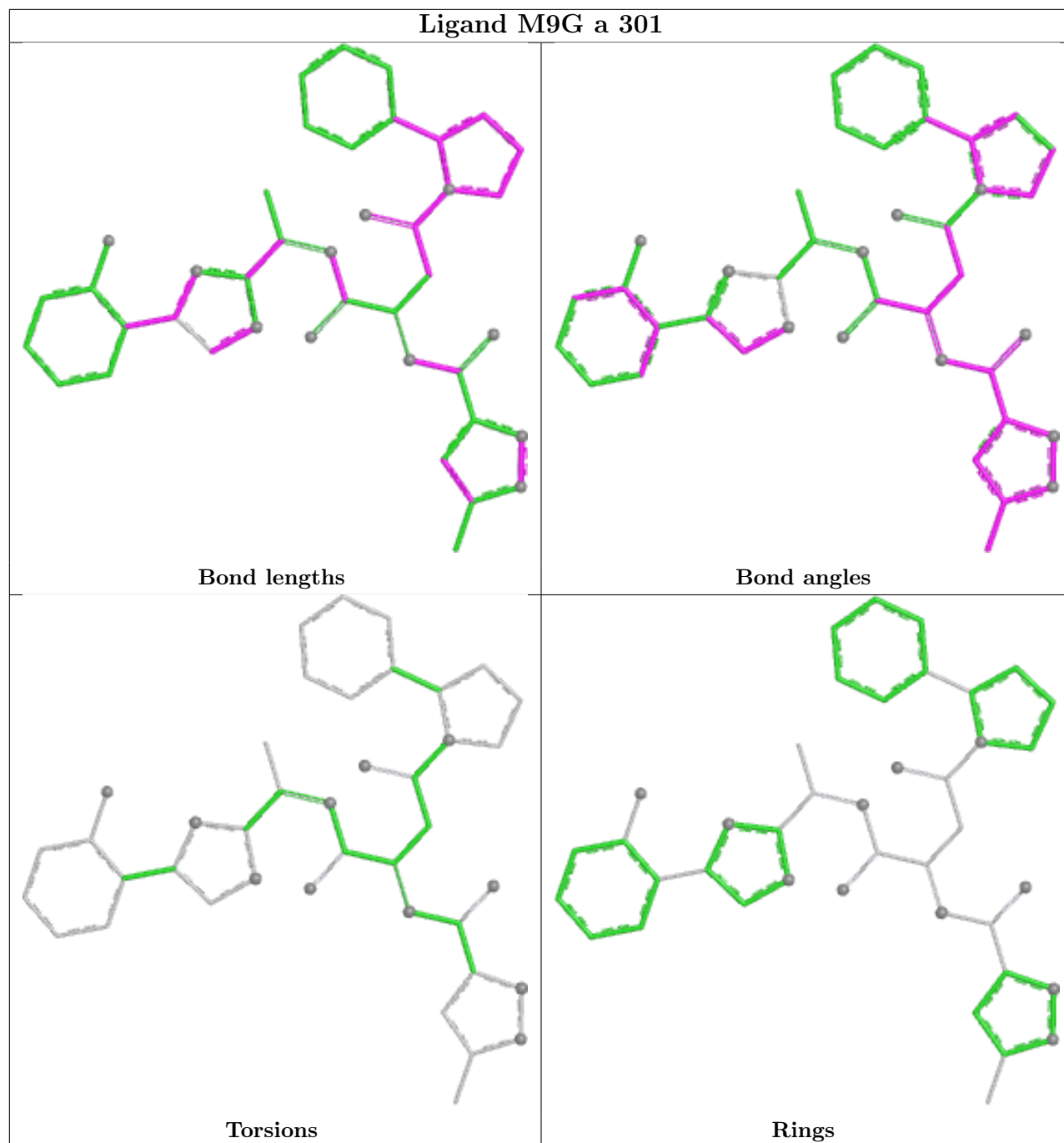


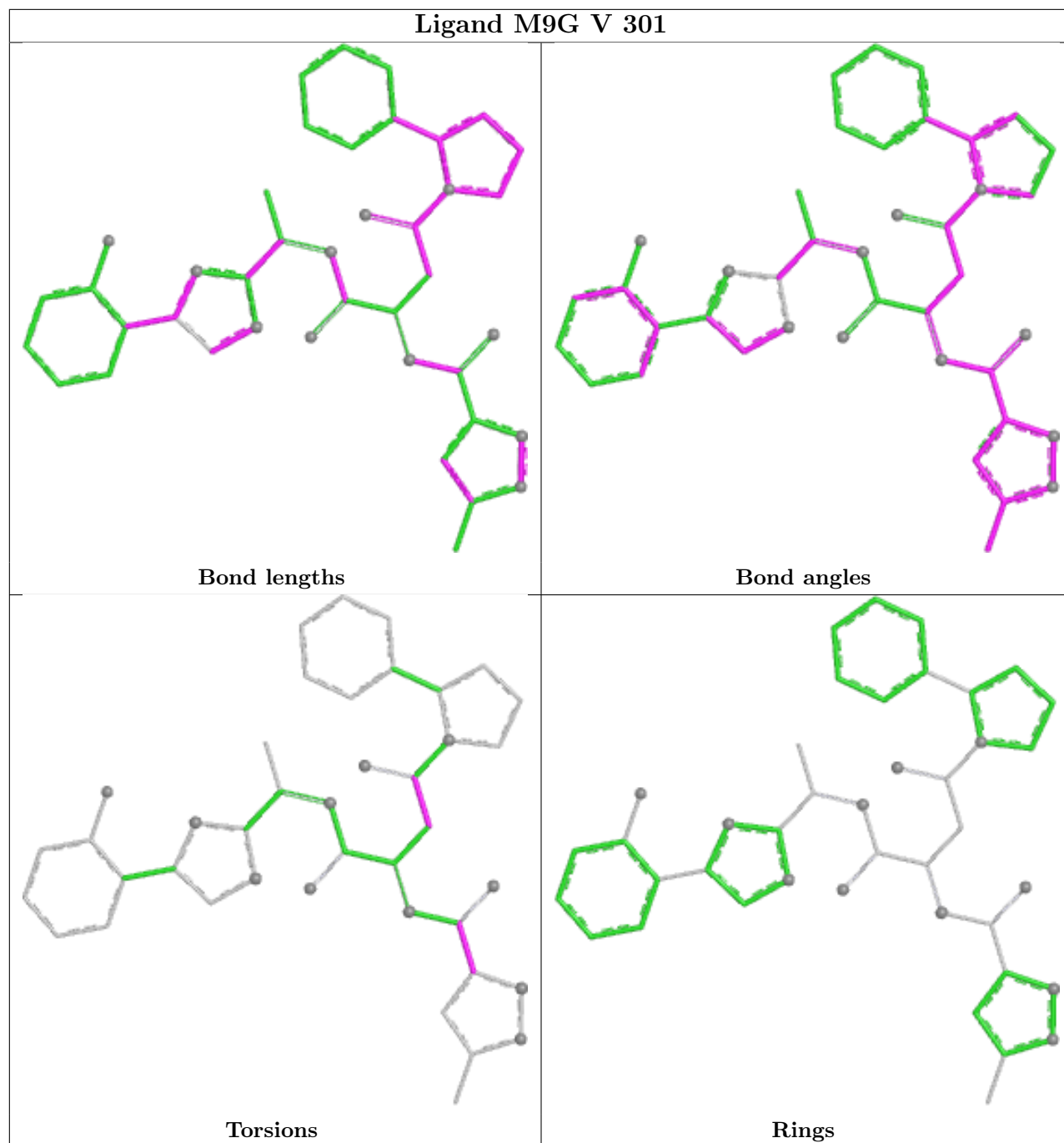


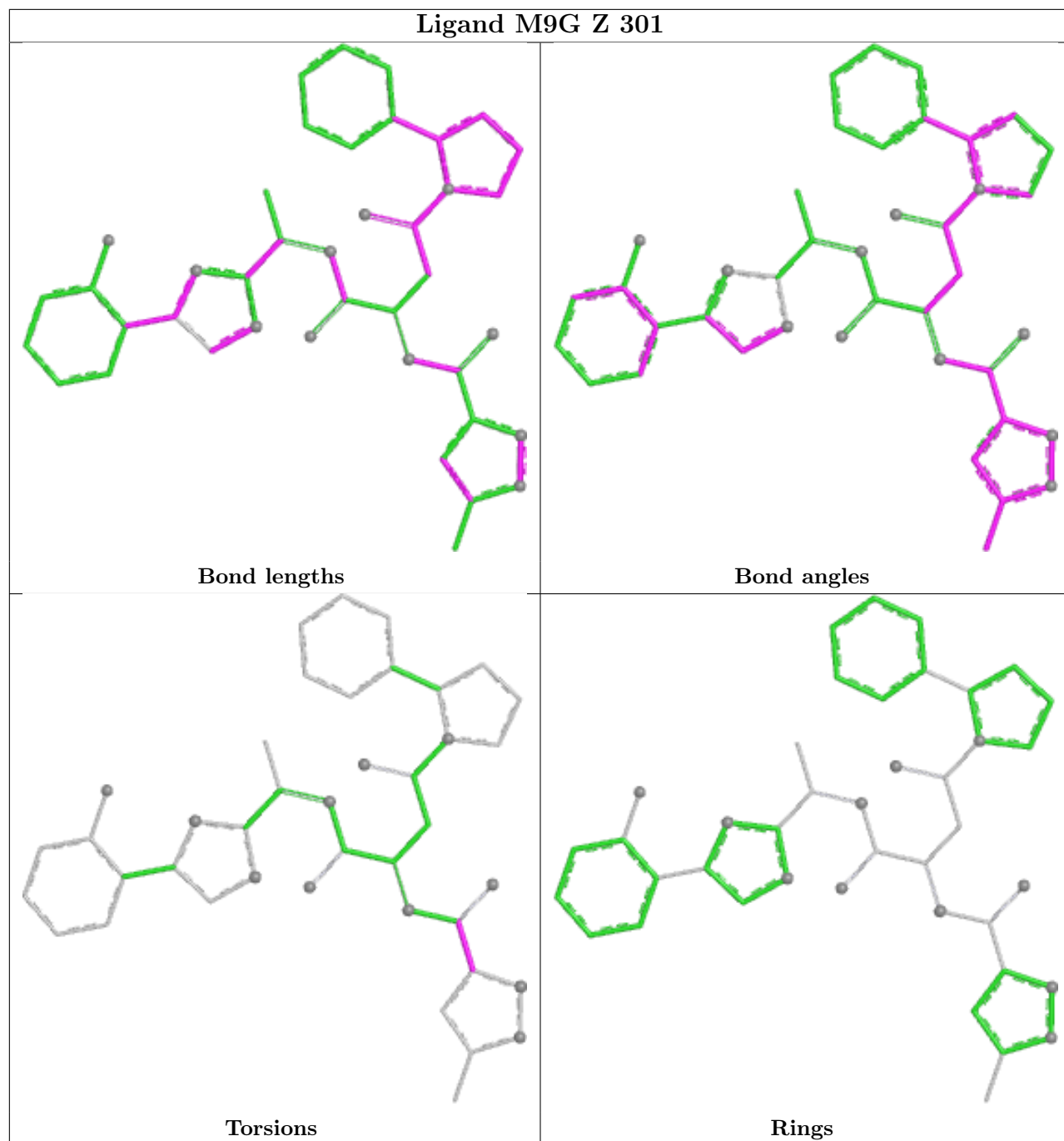


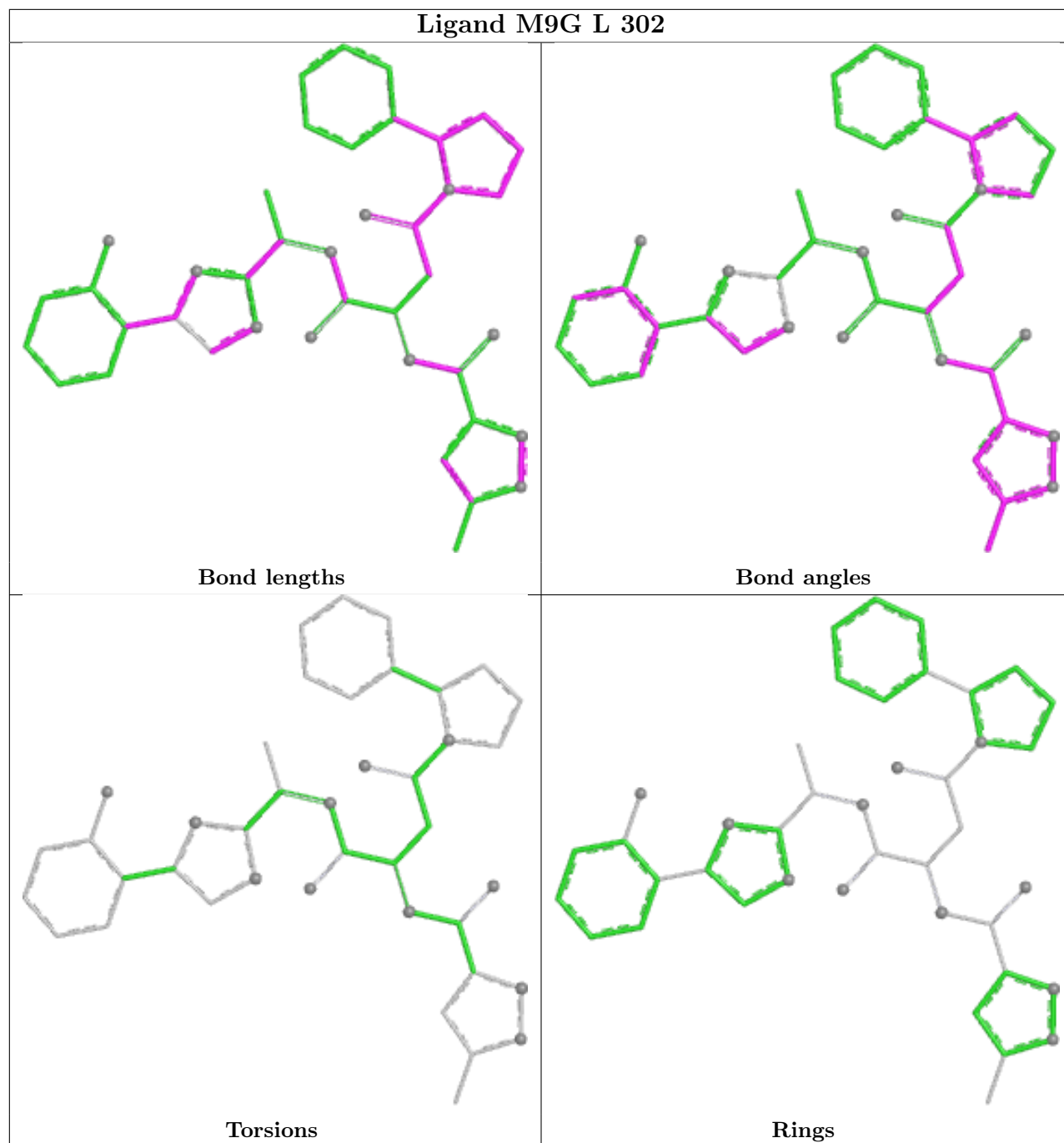


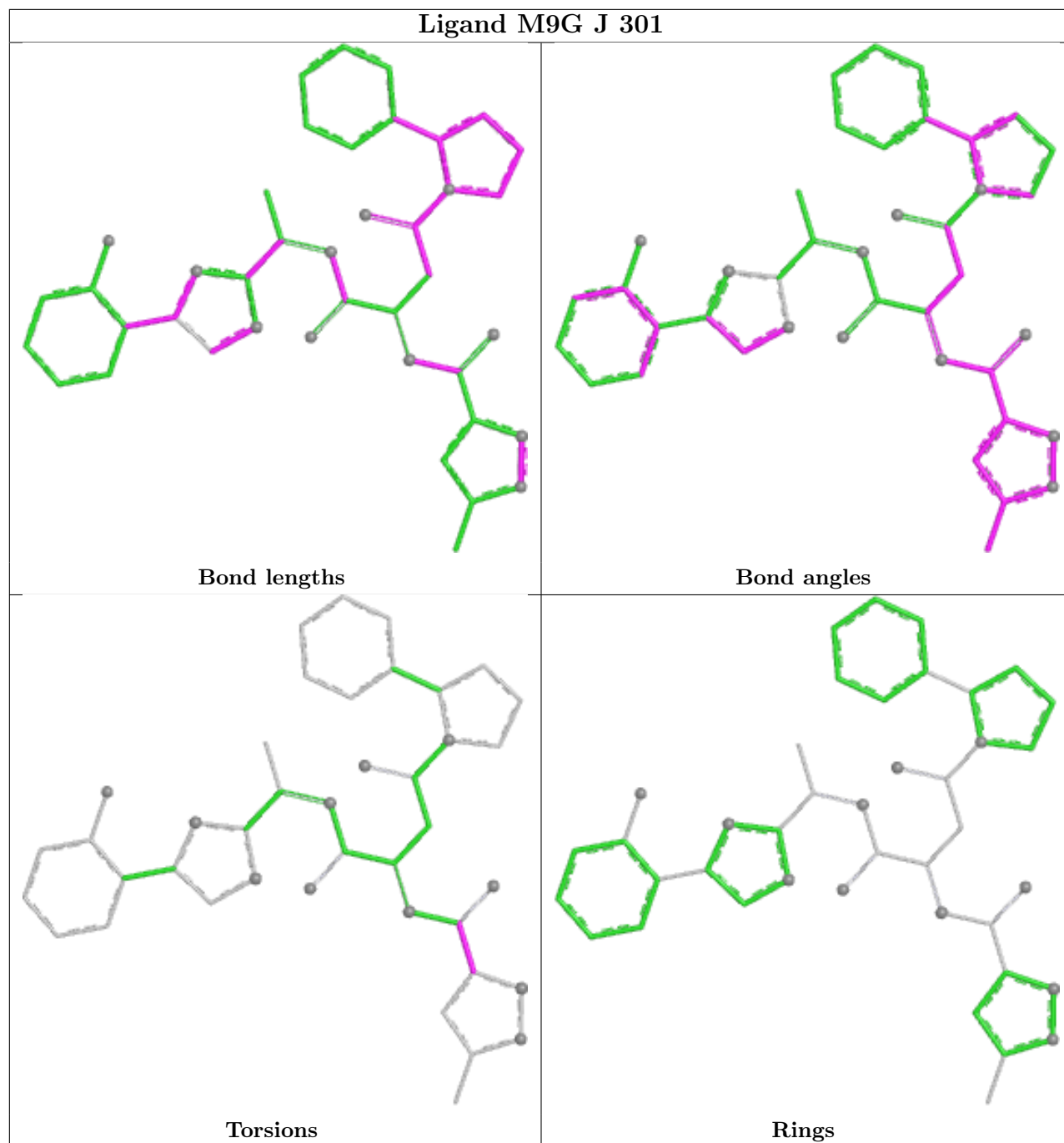


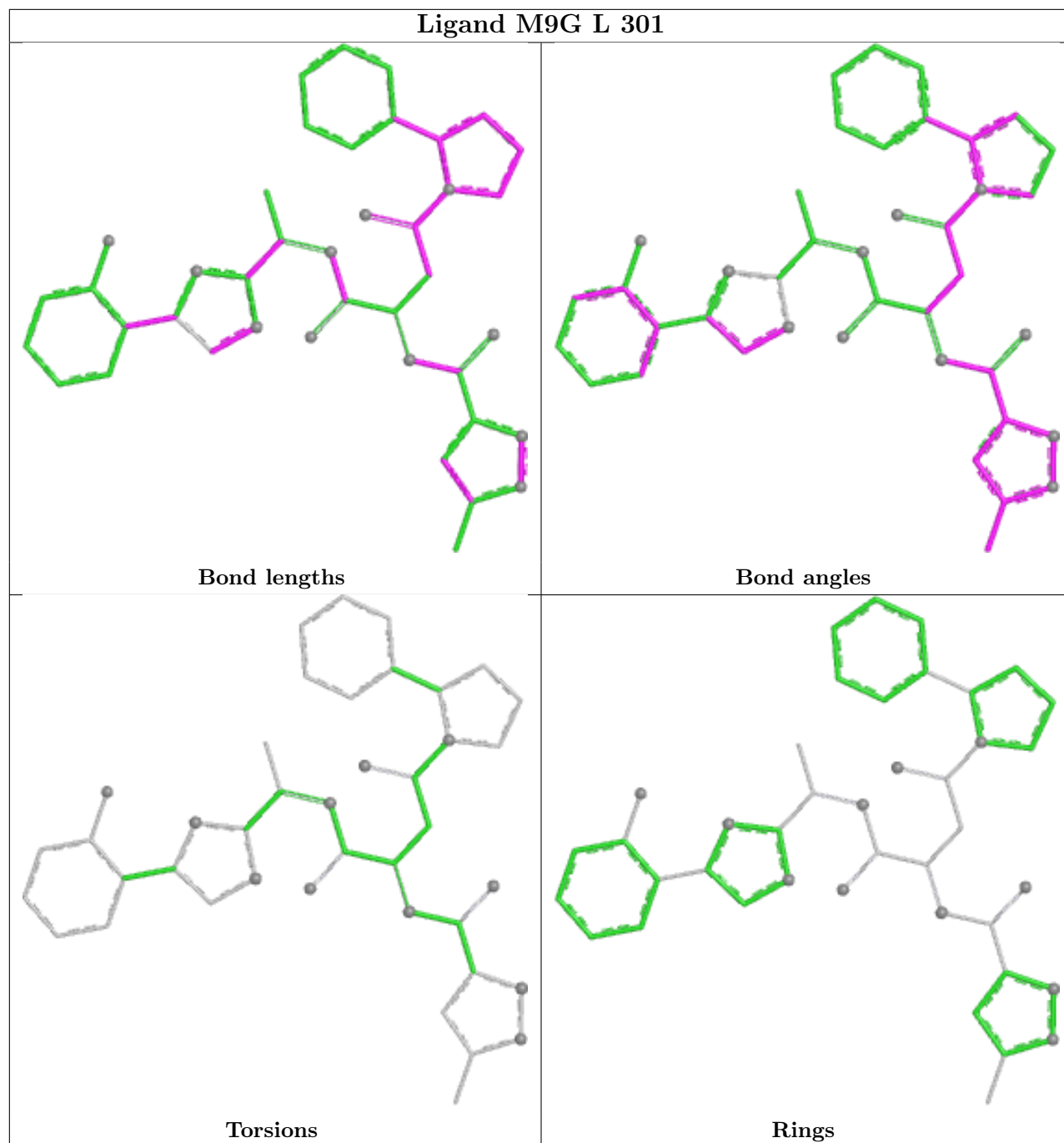


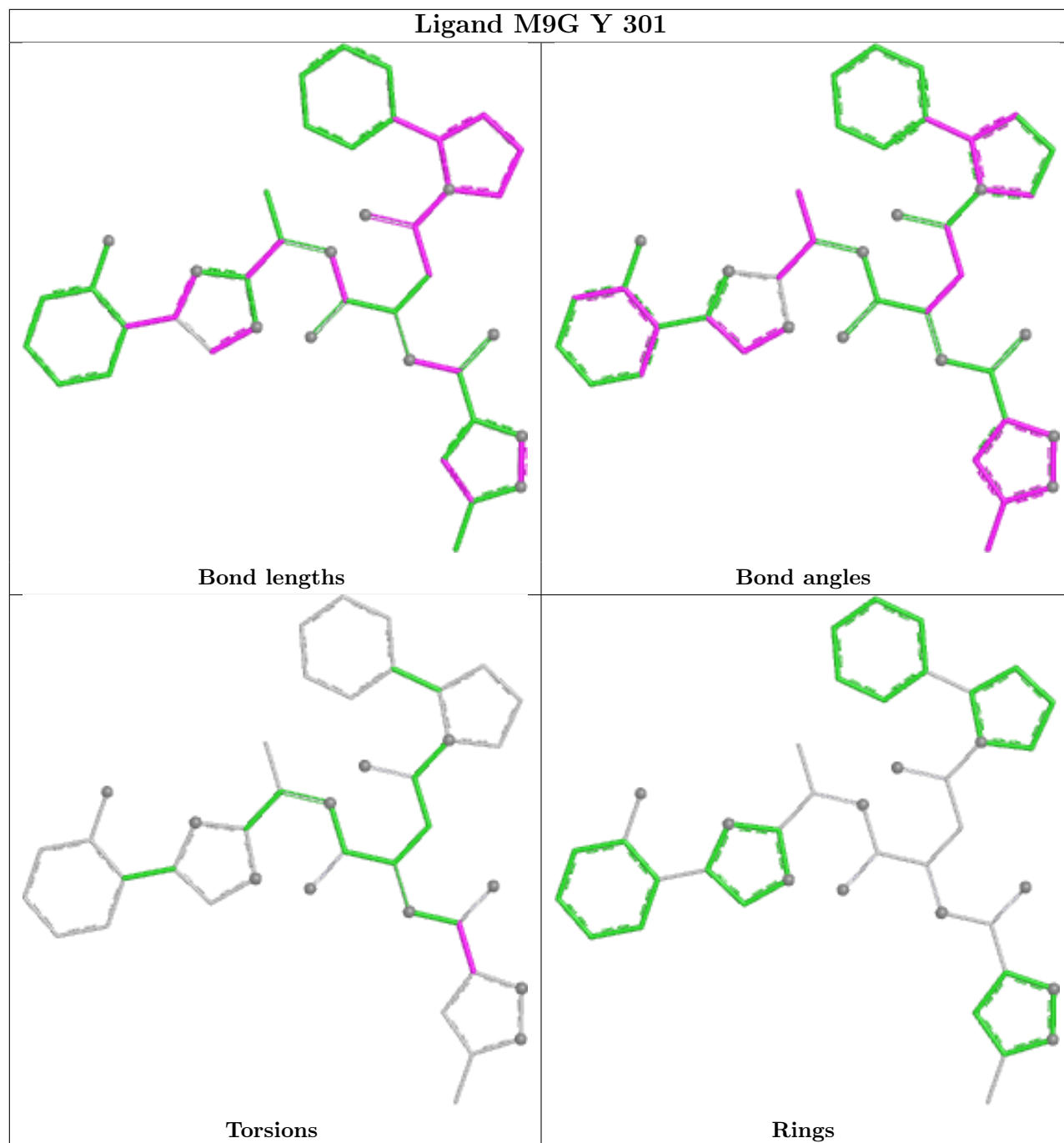


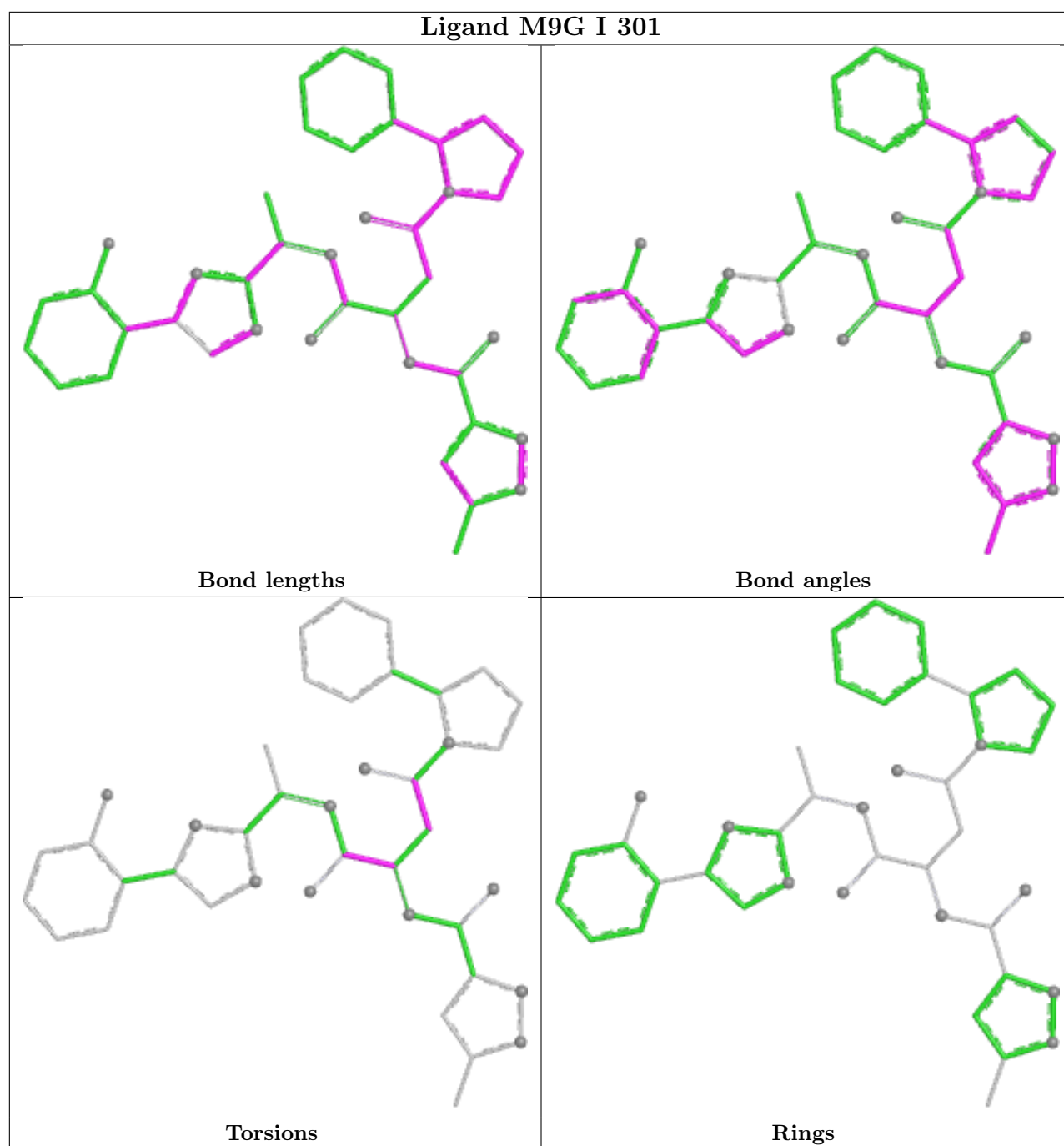












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/240 (90%)	-0.07	2 (0%) 81 75	18, 33, 55, 81	0
1	B	215/240 (89%)	0.35	8 (3%) 45 37	20, 42, 71, 90	0
1	C	216/240 (90%)	0.55	16 (7%) 20 17	21, 46, 75, 89	0
1	D	214/240 (89%)	0.31	7 (3%) 49 40	23, 44, 68, 84	0
1	E	217/240 (90%)	0.26	6 (2%) 55 46	21, 42, 68, 83	0
1	F	214/240 (89%)	0.33	3 (1%) 73 65	18, 44, 71, 81	0
1	G	216/240 (90%)	0.07	3 (1%) 73 65	17, 36, 64, 78	0
1	O	216/240 (90%)	0.43	8 (3%) 45 37	22, 46, 74, 87	0
1	P	219/240 (91%)	0.22	2 (0%) 81 75	19, 40, 67, 86	0
1	Q	215/240 (89%)	0.15	2 (0%) 81 75	20, 39, 61, 75	0
1	R	215/240 (89%)	0.11	2 (0%) 81 75	17, 38, 58, 66	0
1	S	218/240 (90%)	0.06	6 (2%) 55 46	18, 34, 59, 76	0
1	T	217/240 (90%)	0.34	6 (2%) 55 46	22, 45, 69, 100	0
1	U	216/240 (90%)	0.23	7 (3%) 50 41	19, 38, 66, 84	0
2	H	222/234 (94%)	-0.29	1 (0%) 87 83	15, 24, 42, 67	0
2	I	222/234 (94%)	-0.36	0 100 100	15, 23, 41, 61	0
2	J	222/234 (94%)	-0.28	0 100 100	15, 25, 42, 59	0
2	K	223/234 (95%)	-0.31	0 100 100	11, 23, 40, 54	0
2	L	223/234 (95%)	-0.31	0 100 100	16, 24, 41, 58	0
2	M	222/234 (94%)	-0.22	0 100 100	17, 27, 47, 63	0
2	N	223/234 (95%)	-0.18	0 100 100	16, 28, 49, 64	0
2	V	223/234 (95%)	-0.30	0 100 100	14, 24, 40, 54	0
2	W	223/234 (95%)	-0.31	1 (0%) 88 85	16, 25, 42, 56	0
2	X	222/234 (94%)	-0.29	0 100 100	16, 25, 42, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	Y	223/234 (95%)	-0.25	2 (0%) 81 75	14, 24, 41, 66	0
2	Z	223/234 (95%)	-0.21	1 (0%) 88 85	15, 26, 46, 60	0
2	a	223/234 (95%)	-0.14	0 100 100	19, 28, 48, 66	0
2	b	223/234 (95%)	-0.20	0 100 100	17, 27, 45, 64	0
All	All	6143/6636 (92%)	-0.02	83 (1%) 73 65	11, 30, 64, 100	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	235	VAL	4.7
1	B	235	VAL	4.1
1	C	10	GLU	3.7
1	C	9	MET	3.6
1	C	203	LEU	3.5
1	S	9	MET	3.4
1	D	233	LEU	3.4
1	C	163	ILE	3.3
1	T	235	VAL	3.3
1	U	234	LEU	3.2
1	B	9	MET	3.1
1	O	153	PHE	3.1
1	C	12	ALA	3.0
1	D	191	GLY	3.0
1	C	13	MET	3.0
1	C	171	TYR	2.9
1	D	203	LEU	2.8
1	P	191	GLY	2.8
1	S	192	SER	2.7
1	C	11	GLN	2.7
1	T	202	THR	2.7
1	C	14	ARG	2.7
1	C	235	VAL	2.7
1	U	191	GLY	2.7
1	E	202	THR	2.7
1	S	172	ALA	2.6
1	P	203	LEU	2.6
1	E	169	GLU	2.6
1	Q	235	VAL	2.6
1	S	191	GLY	2.6
1	A	235	VAL	2.5
1	Q	149	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	190	ALA	2.5
1	T	203	LEU	2.5
1	F	234	LEU	2.4
1	U	9	MET	2.4
1	U	29	SER	2.4
1	D	219	ARG	2.4
1	U	10	GLU	2.4
1	B	172	ALA	2.4
1	C	206	ALA	2.4
1	O	33	LEU	2.4
1	G	48	ARG	2.3
1	T	133	THR	2.3
1	C	191	GLY	2.3
1	D	232	ALA	2.3
1	G	234	LEU	2.3
1	C	159	THR	2.3
1	C	162	PRO	2.3
1	E	235	VAL	2.3
1	C	15	GLU	2.2
1	S	171	TYR	2.2
1	G	10	GLU	2.2
1	E	174	ASN	2.2
2	Y	113	ASP	2.2
1	D	207	SER	2.2
1	F	11	GLN	2.2
1	T	191	GLY	2.2
2	W	223	GLY	2.2
1	D	190	ALA	2.2
1	U	190	ALA	2.2
1	O	152	HIS	2.2
1	O	190	ALA	2.2
2	H	38	ASP	2.1
1	B	227	GLY	2.1
1	B	10	GLU	2.1
1	E	11	GLN	2.1
1	O	206	ALA	2.1
1	B	231	GLN	2.1
1	F	205	VAL	2.1
1	B	178	THR	2.1
1	C	160	THR	2.1
1	O	175	ALA	2.1
1	R	171	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	Y	112	SER	2.1
1	O	205	VAL	2.1
1	T	205	VAL	2.1
1	E	162	PRO	2.1
1	A	11	GLN	2.0
2	Z	96	GLN	2.0
1	S	235	VAL	2.0
1	O	203	LEU	2.0
1	R	172	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

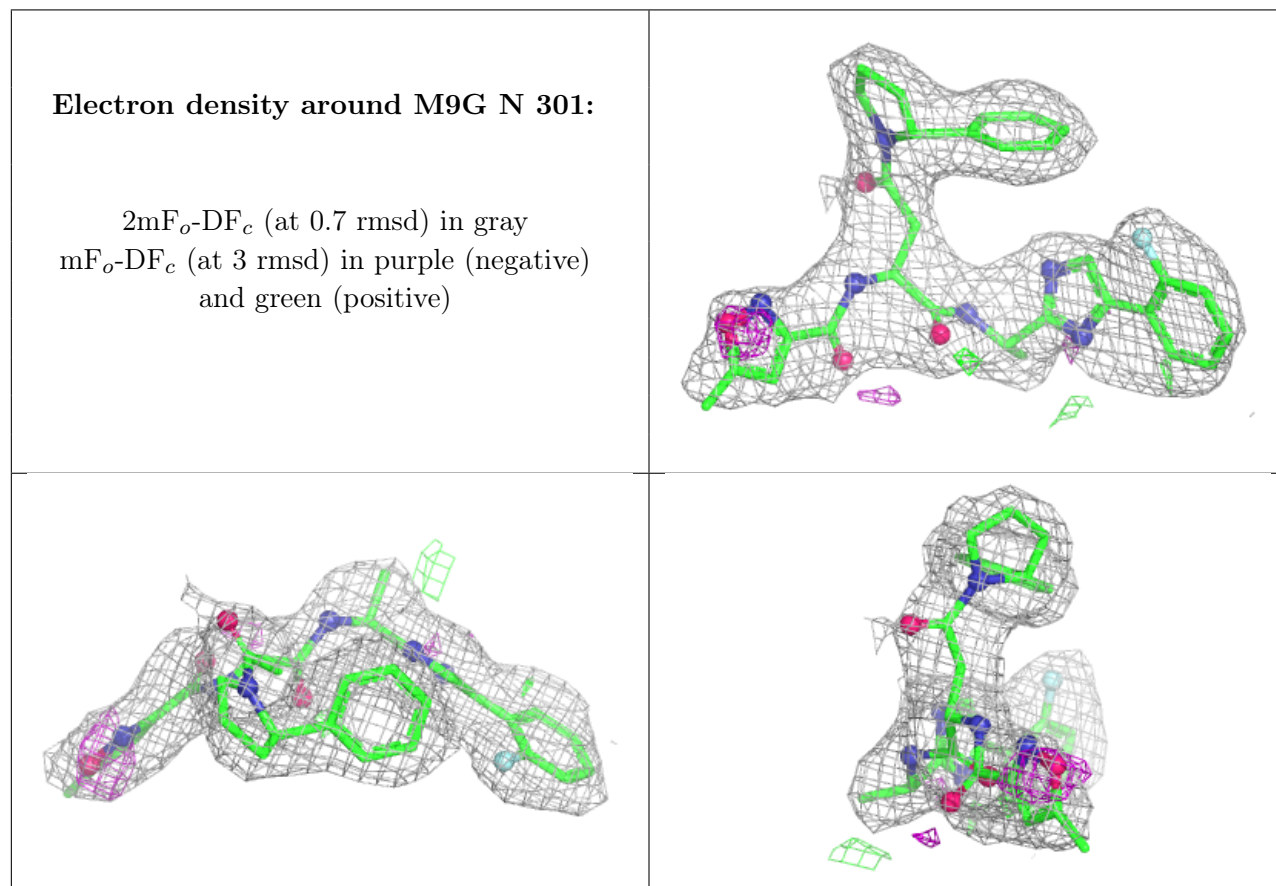
There are no oligosaccharides in this entry.

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.

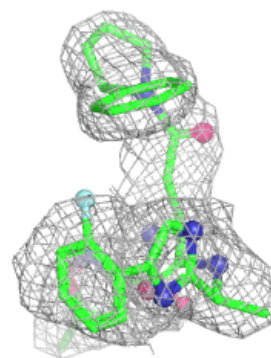
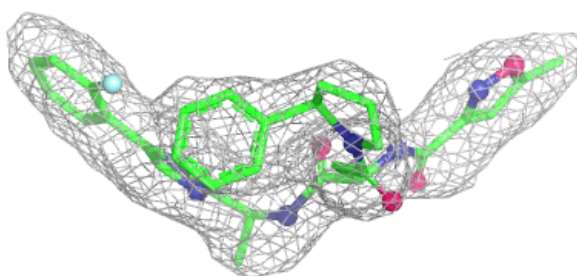
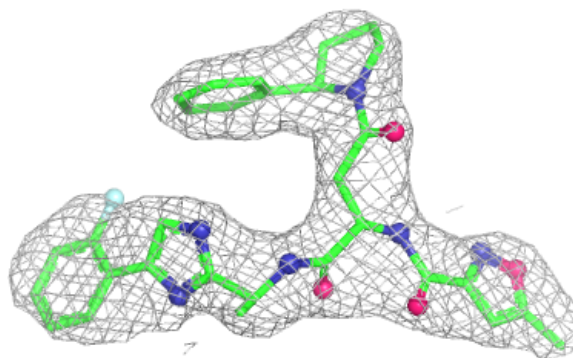
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	M9G	N	301	41/41	0.92	0.11	13,24,36,49	0
3	M9G	M	301	41/41	0.93	0.11	18,26,40,51	0
3	M9G	H	301	41/41	0.93	0.10	17,24,36,50	0
3	M9G	W	301	41/41	0.93	0.10	19,28,38,48	0
3	M9G	J	301	41/41	0.94	0.10	18,27,38,42	0
3	M9G	L	301	41/41	0.94	0.10	15,25,43,51	0
3	M9G	V	301	41/41	0.94	0.10	19,24,41,53	0
3	M9G	L	302	41/41	0.94	0.09	17,26,36,48	0
3	M9G	Z	301	41/41	0.94	0.09	17,26,37,49	0
3	M9G	X	301	41/41	0.95	0.09	18,26,39,45	0
3	M9G	Y	301	41/41	0.95	0.09	13,24,35,45	0
3	M9G	I	301	41/41	0.95	0.09	15,24,40,45	0
3	M9G	a	301	41/41	0.95	0.08	19,27,36,45	0
3	M9G	b	301	41/41	0.96	0.08	15,24,35,40	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.

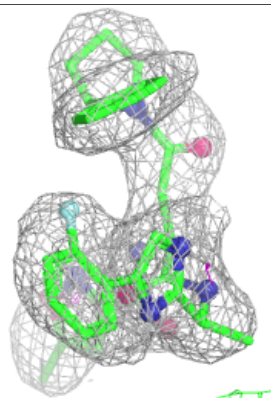
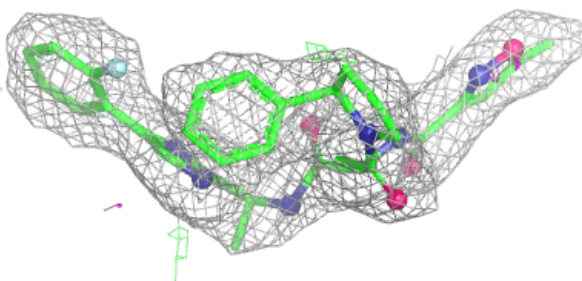
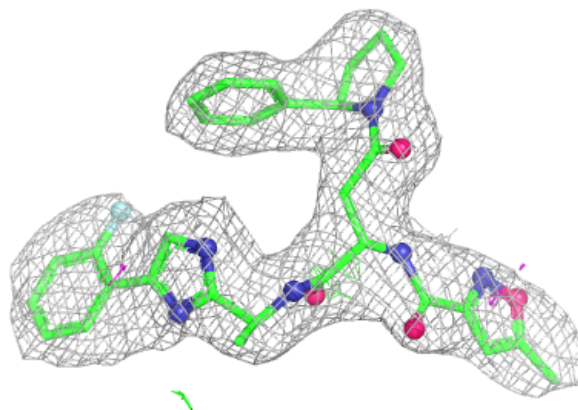


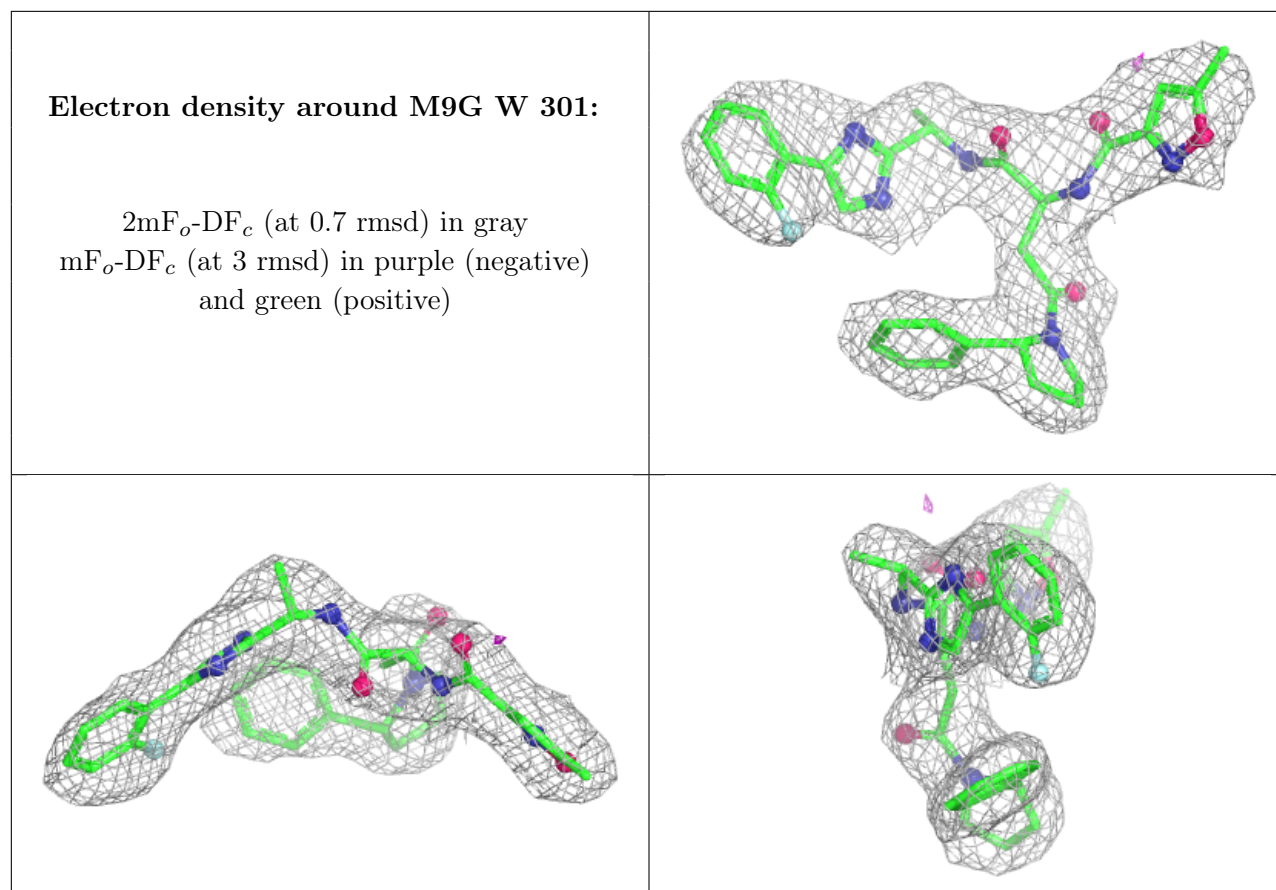
Electron density around M9G M 301:

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

**Electron density around M9G H 301:**

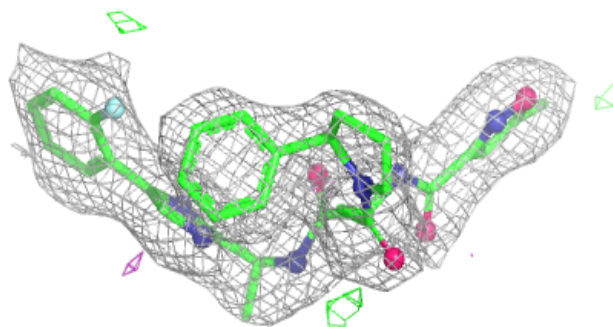
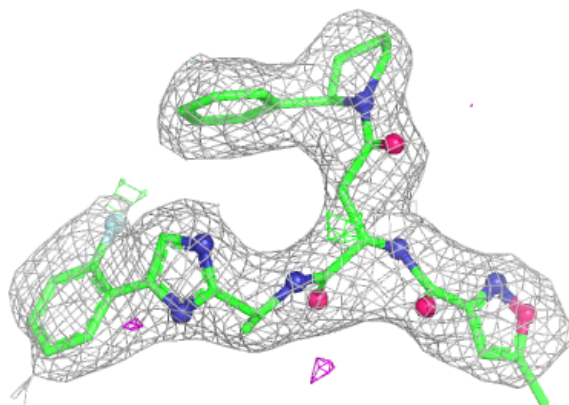
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





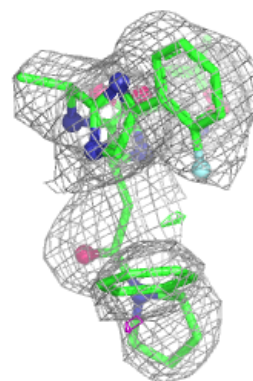
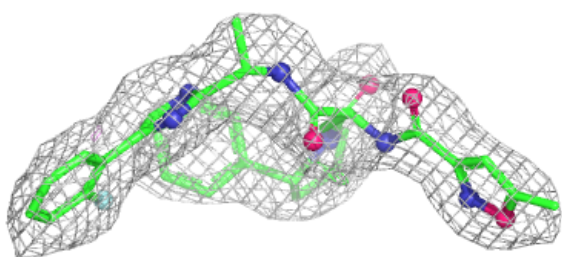
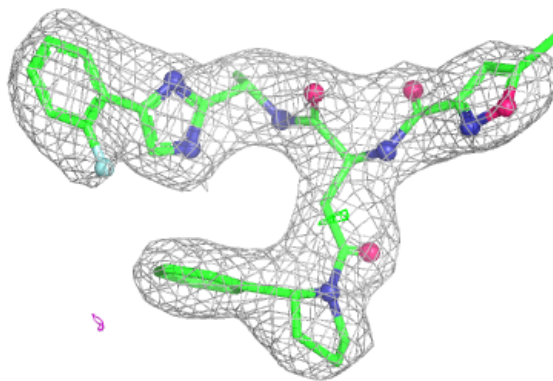
Electron density around M9G J 301:

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

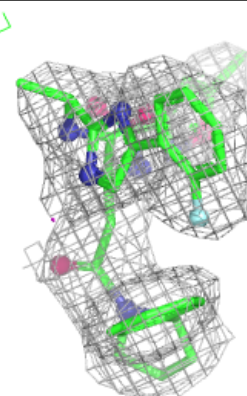
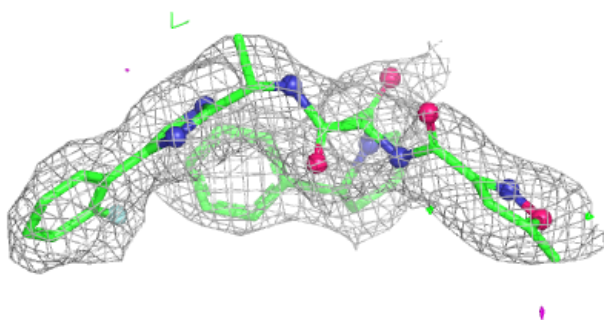
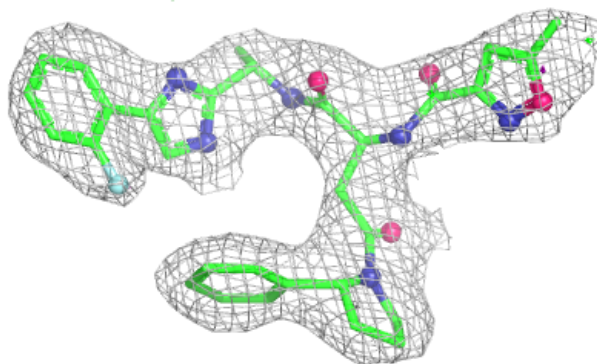


Electron density around M9G L 301:

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

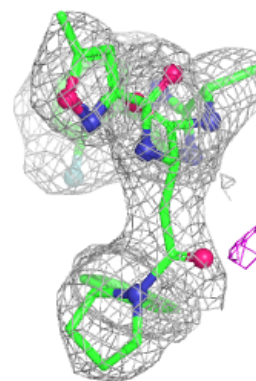
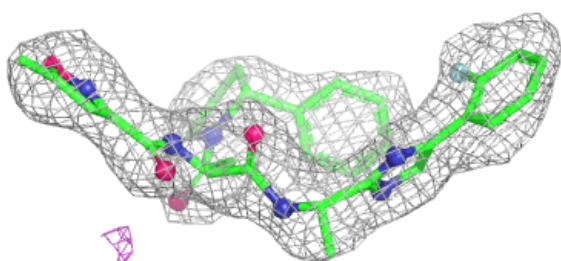
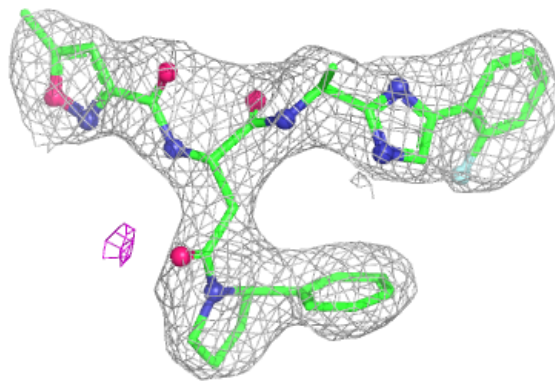
**Electron density around M9G V 301:**

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

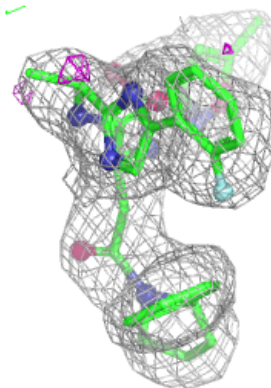
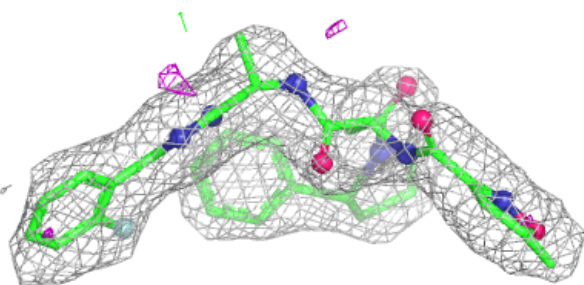
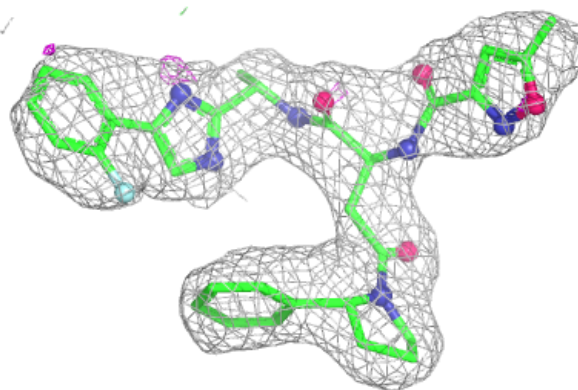


Electron density around M9G L 302:

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

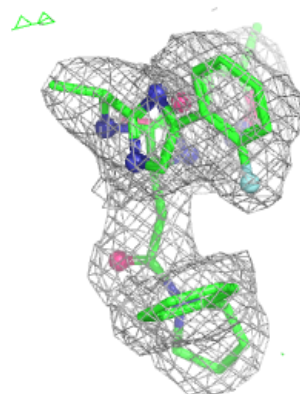
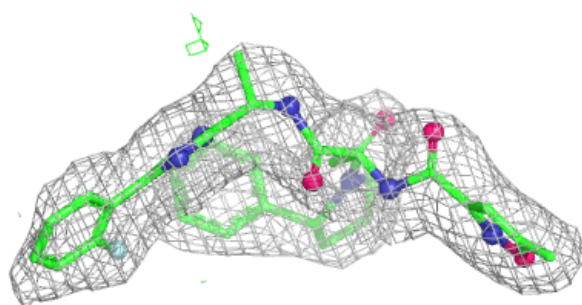
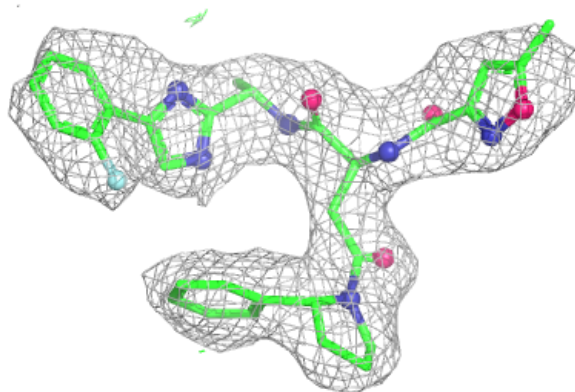
**Electron density around M9G Z 301:**

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

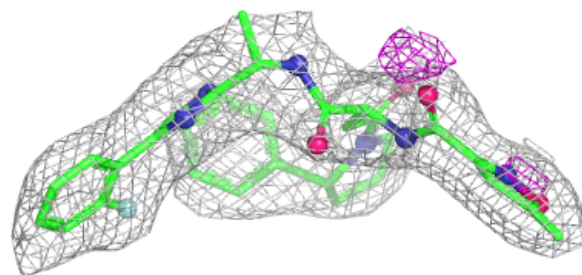
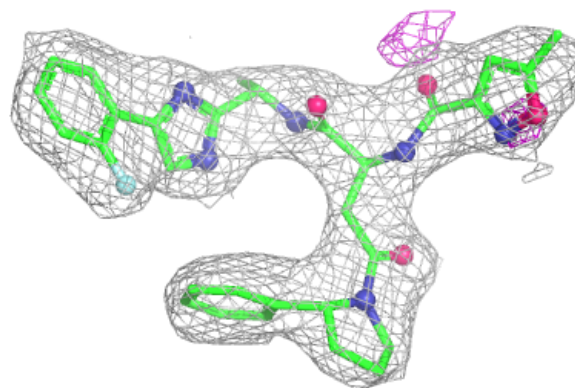


Electron density around M9G X 301:

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

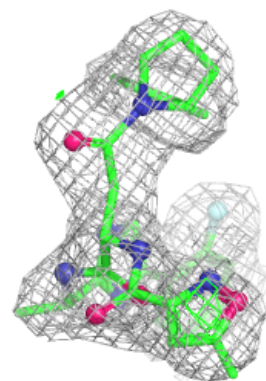
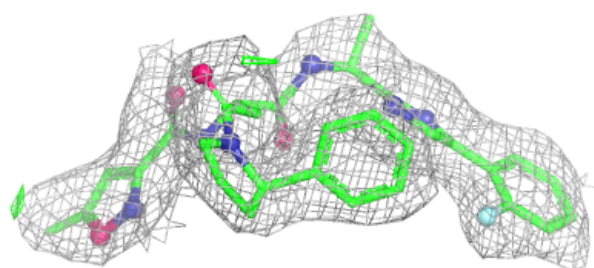
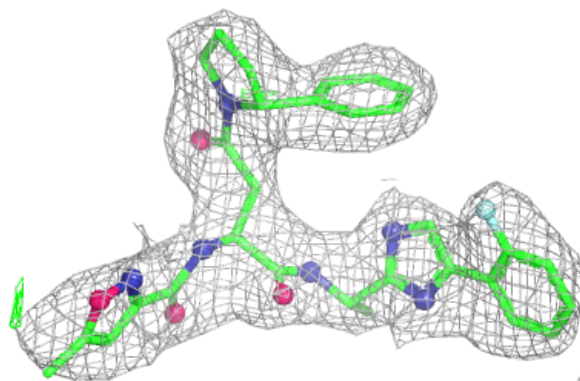
**Electron density around M9G Y 301:**

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

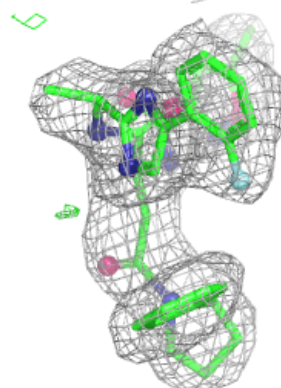
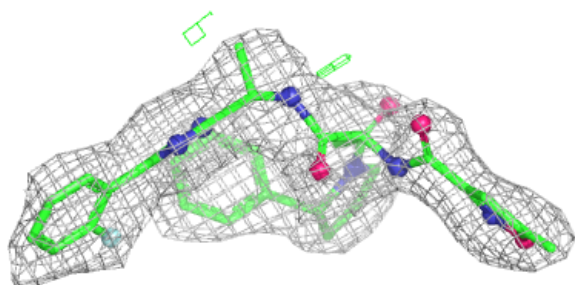
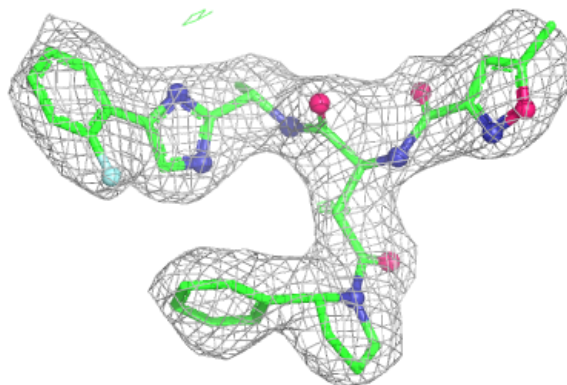


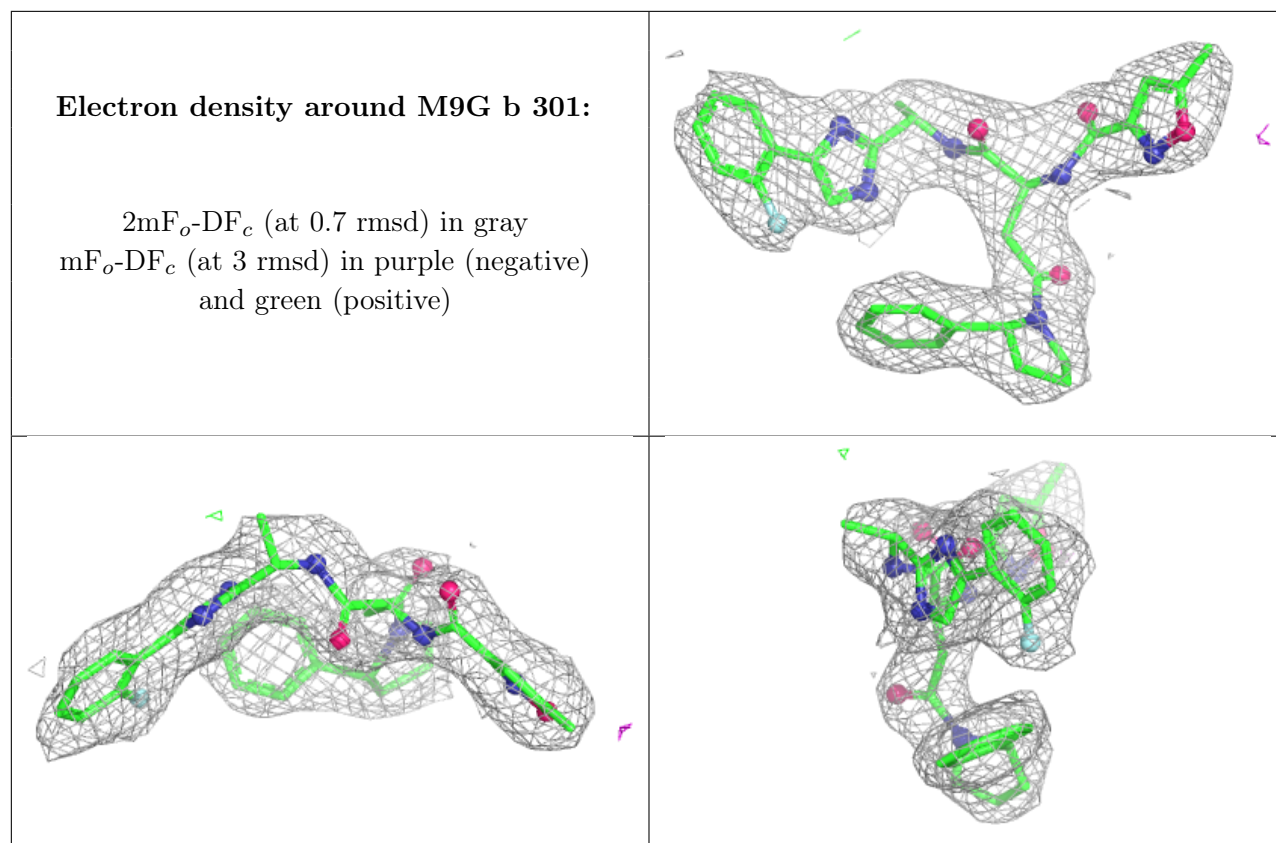
Electron density around M9G I 301:

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

**Electron density around M9G 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.