



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 06:42 am BST

PDB ID : 4U01  
Title : HCV NS3/4A serine protease in complex with 6570  
Authors : Parsy, C.C.; Alexandre, F.-R.; Brandt, G.; Caillet, C.; Chaves, D.; Derock, M.; Gloux, D.; Griffon, Y.; Lallo, L.B.; Leroy, F.; Liuzzi, M.; Loi, A.-G.; Mayes, B.; Moulat, L.; Moussa, A.; Chiara, M.; Roques, V.; Rosinovsky, E.; Seifer, M.; Stewart, A.; Wang, J.; Standing, D.; Surleraux, D.  
Deposited on : 2014-07-11  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

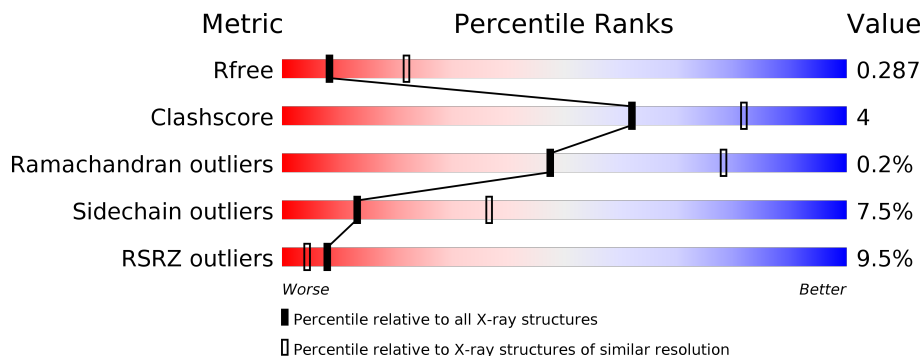
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



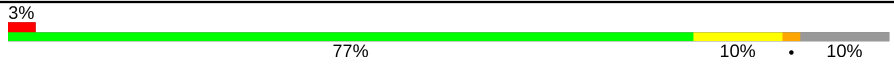




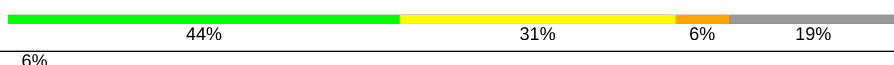
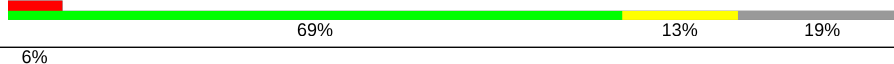

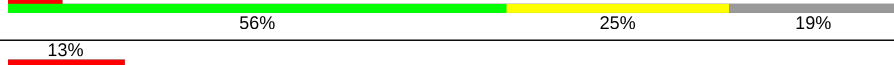


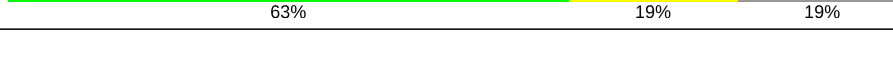
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	203	
1	B	203	
1	C	203	
1	D	203	
1	E	203	
1	F	203	

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Mol	Chain	Length	Quality of chain
1	G	203	
1	H	203	
1	J	203	
2	K	16	
2	L	16	
2	M	16	
2	N	16	
2	O	16	
2	P	16	
2	Q	16	
2	T	16	
2	U	16	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	G	302	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13360 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 Non-structural 3 protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	182	1337	829	244	254	10	0	0	0
1	B	182	1337	829	244	254	10	0	0	0
1	C	182	1337	829	244	254	10	0	0	0
1	D	182	1337	829	244	254	10	0	0	0
1	E	182	1337	829	244	254	10	0	0	0
1	F	182	1337	829	244	254	10	0	0	0
1	G	182	1337	829	244	254	10	0	0	0
1	H	182	1337	829	244	254	10	0	0	0
1	J	182	1337	829	244	254	10	0	0	0

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A6N4J4
A	26	ARG	LYS	conflict	UNP A6N4J4
A	181	ALA	-	expression tag	UNP A6N4J4
A	182	SER	-	expression tag	UNP A6N4J4
A	183	LYS	-	expression tag	UNP A6N4J4
A	184	LYS	-	expression tag	UNP A6N4J4
A	185	LYS	-	expression tag	UNP A6N4J4
A	186	LYS	-	expression tag	UNP A6N4J4
A	187	LYS	-	expression tag	UNP A6N4J4
A	188	GLY	-	expression tag	UNP A6N4J4
A	189	SER	-	expression tag	UNP A6N4J4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	190	VAL	-	expression tag	UNP A6N4J4
A	191	VAL	-	expression tag	UNP A6N4J4
A	192	ILE	-	expression tag	UNP A6N4J4
A	193	VAL	-	expression tag	UNP A6N4J4
A	194	GLY	-	expression tag	UNP A6N4J4
A	195	ARG	-	expression tag	UNP A6N4J4
A	196	ILE	-	expression tag	UNP A6N4J4
A	197	ILE	-	expression tag	UNP A6N4J4
A	198	LEU	-	expression tag	UNP A6N4J4
A	199	SER	-	expression tag	UNP A6N4J4
A	200	GLY	-	expression tag	UNP A6N4J4
A	201	ARG	-	expression tag	UNP A6N4J4
A	202	LYS	-	expression tag	UNP A6N4J4
B	0	MET	-	initiating methionine	UNP A6N4J4
B	26	ARG	LYS	conflict	UNP A6N4J4
B	181	ALA	-	expression tag	UNP A6N4J4
B	182	SER	-	expression tag	UNP A6N4J4
B	183	LYS	-	expression tag	UNP A6N4J4
B	184	LYS	-	expression tag	UNP A6N4J4
B	185	LYS	-	expression tag	UNP A6N4J4
B	186	LYS	-	expression tag	UNP A6N4J4
B	187	LYS	-	expression tag	UNP A6N4J4
B	188	GLY	-	expression tag	UNP A6N4J4
B	189	SER	-	expression tag	UNP A6N4J4
B	190	VAL	-	expression tag	UNP A6N4J4
B	191	VAL	-	expression tag	UNP A6N4J4
B	192	ILE	-	expression tag	UNP A6N4J4
B	193	VAL	-	expression tag	UNP A6N4J4
B	194	GLY	-	expression tag	UNP A6N4J4
B	195	ARG	-	expression tag	UNP A6N4J4
B	196	ILE	-	expression tag	UNP A6N4J4
B	197	ILE	-	expression tag	UNP A6N4J4
B	198	LEU	-	expression tag	UNP A6N4J4
B	199	SER	-	expression tag	UNP A6N4J4
B	200	GLY	-	expression tag	UNP A6N4J4
B	201	ARG	-	expression tag	UNP A6N4J4
B	202	LYS	-	expression tag	UNP A6N4J4
C	0	MET	-	initiating methionine	UNP A6N4J4
C	26	ARG	LYS	conflict	UNP A6N4J4
C	181	ALA	-	expression tag	UNP A6N4J4
C	182	SER	-	expression tag	UNP A6N4J4
C	183	LYS	-	expression tag	UNP A6N4J4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	184	LYS	-	expression tag	UNP A6N4J4
C	185	LYS	-	expression tag	UNP A6N4J4
C	186	LYS	-	expression tag	UNP A6N4J4
C	187	LYS	-	expression tag	UNP A6N4J4
C	188	GLY	-	expression tag	UNP A6N4J4
C	189	SER	-	expression tag	UNP A6N4J4
C	190	VAL	-	expression tag	UNP A6N4J4
C	191	VAL	-	expression tag	UNP A6N4J4
C	192	ILE	-	expression tag	UNP A6N4J4
C	193	VAL	-	expression tag	UNP A6N4J4
C	194	GLY	-	expression tag	UNP A6N4J4
C	195	ARG	-	expression tag	UNP A6N4J4
C	196	ILE	-	expression tag	UNP A6N4J4
C	197	ILE	-	expression tag	UNP A6N4J4
C	198	LEU	-	expression tag	UNP A6N4J4
C	199	SER	-	expression tag	UNP A6N4J4
C	200	GLY	-	expression tag	UNP A6N4J4
C	201	ARG	-	expression tag	UNP A6N4J4
C	202	LYS	-	expression tag	UNP A6N4J4
D	0	MET	-	initiating methionine	UNP A6N4J4
D	26	ARG	LYS	conflict	UNP A6N4J4
D	181	ALA	-	expression tag	UNP A6N4J4
D	182	SER	-	expression tag	UNP A6N4J4
D	183	LYS	-	expression tag	UNP A6N4J4
D	184	LYS	-	expression tag	UNP A6N4J4
D	185	LYS	-	expression tag	UNP A6N4J4
D	186	LYS	-	expression tag	UNP A6N4J4
D	187	LYS	-	expression tag	UNP A6N4J4
D	188	GLY	-	expression tag	UNP A6N4J4
D	189	SER	-	expression tag	UNP A6N4J4
D	190	VAL	-	expression tag	UNP A6N4J4
D	191	VAL	-	expression tag	UNP A6N4J4
D	192	ILE	-	expression tag	UNP A6N4J4
D	193	VAL	-	expression tag	UNP A6N4J4
D	194	GLY	-	expression tag	UNP A6N4J4
D	195	ARG	-	expression tag	UNP A6N4J4
D	196	ILE	-	expression tag	UNP A6N4J4
D	197	ILE	-	expression tag	UNP A6N4J4
D	198	LEU	-	expression tag	UNP A6N4J4
D	199	SER	-	expression tag	UNP A6N4J4
D	200	GLY	-	expression tag	UNP A6N4J4
D	201	ARG	-	expression tag	UNP A6N4J4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	202	LYS	-	expression tag	UNP A6N4J4
E	0	MET	-	initiating methionine	UNP A6N4J4
E	26	ARG	LYS	conflict	UNP A6N4J4
E	181	ALA	-	expression tag	UNP A6N4J4
E	182	SER	-	expression tag	UNP A6N4J4
E	183	LYS	-	expression tag	UNP A6N4J4
E	184	LYS	-	expression tag	UNP A6N4J4
E	185	LYS	-	expression tag	UNP A6N4J4
E	186	LYS	-	expression tag	UNP A6N4J4
E	187	LYS	-	expression tag	UNP A6N4J4
E	188	GLY	-	expression tag	UNP A6N4J4
E	189	SER	-	expression tag	UNP A6N4J4
E	190	VAL	-	expression tag	UNP A6N4J4
E	191	VAL	-	expression tag	UNP A6N4J4
E	192	ILE	-	expression tag	UNP A6N4J4
E	193	VAL	-	expression tag	UNP A6N4J4
E	194	GLY	-	expression tag	UNP A6N4J4
E	195	ARG	-	expression tag	UNP A6N4J4
E	196	ILE	-	expression tag	UNP A6N4J4
E	197	ILE	-	expression tag	UNP A6N4J4
E	198	LEU	-	expression tag	UNP A6N4J4
E	199	SER	-	expression tag	UNP A6N4J4
E	200	GLY	-	expression tag	UNP A6N4J4
E	201	ARG	-	expression tag	UNP A6N4J4
E	202	LYS	-	expression tag	UNP A6N4J4
F	0	MET	-	initiating methionine	UNP A6N4J4
F	26	ARG	LYS	conflict	UNP A6N4J4
F	181	ALA	-	expression tag	UNP A6N4J4
F	182	SER	-	expression tag	UNP A6N4J4
F	183	LYS	-	expression tag	UNP A6N4J4
F	184	LYS	-	expression tag	UNP A6N4J4
F	185	LYS	-	expression tag	UNP A6N4J4
F	186	LYS	-	expression tag	UNP A6N4J4
F	187	LYS	-	expression tag	UNP A6N4J4
F	188	GLY	-	expression tag	UNP A6N4J4
F	189	SER	-	expression tag	UNP A6N4J4
F	190	VAL	-	expression tag	UNP A6N4J4
F	191	VAL	-	expression tag	UNP A6N4J4
F	192	ILE	-	expression tag	UNP A6N4J4
F	193	VAL	-	expression tag	UNP A6N4J4
F	194	GLY	-	expression tag	UNP A6N4J4
F	195	ARG	-	expression tag	UNP A6N4J4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	196	ILE	-	expression tag	UNP A6N4J4
F	197	ILE	-	expression tag	UNP A6N4J4
F	198	LEU	-	expression tag	UNP A6N4J4
F	199	SER	-	expression tag	UNP A6N4J4
F	200	GLY	-	expression tag	UNP A6N4J4
F	201	ARG	-	expression tag	UNP A6N4J4
F	202	LYS	-	expression tag	UNP A6N4J4
G	0	MET	-	initiating methionine	UNP A6N4J4
G	26	ARG	LYS	conflict	UNP A6N4J4
G	181	ALA	-	expression tag	UNP A6N4J4
G	182	SER	-	expression tag	UNP A6N4J4
G	183	LYS	-	expression tag	UNP A6N4J4
G	184	LYS	-	expression tag	UNP A6N4J4
G	185	LYS	-	expression tag	UNP A6N4J4
G	186	LYS	-	expression tag	UNP A6N4J4
G	187	LYS	-	expression tag	UNP A6N4J4
G	188	GLY	-	expression tag	UNP A6N4J4
G	189	SER	-	expression tag	UNP A6N4J4
G	190	VAL	-	expression tag	UNP A6N4J4
G	191	VAL	-	expression tag	UNP A6N4J4
G	192	ILE	-	expression tag	UNP A6N4J4
G	193	VAL	-	expression tag	UNP A6N4J4
G	194	GLY	-	expression tag	UNP A6N4J4
G	195	ARG	-	expression tag	UNP A6N4J4
G	196	ILE	-	expression tag	UNP A6N4J4
G	197	ILE	-	expression tag	UNP A6N4J4
G	198	LEU	-	expression tag	UNP A6N4J4
G	199	SER	-	expression tag	UNP A6N4J4
G	200	GLY	-	expression tag	UNP A6N4J4
G	201	ARG	-	expression tag	UNP A6N4J4
G	202	LYS	-	expression tag	UNP A6N4J4
H	0	MET	-	initiating methionine	UNP A6N4J4
H	26	ARG	LYS	conflict	UNP A6N4J4
H	181	ALA	-	expression tag	UNP A6N4J4
H	182	SER	-	expression tag	UNP A6N4J4
H	183	LYS	-	expression tag	UNP A6N4J4
H	184	LYS	-	expression tag	UNP A6N4J4
H	185	LYS	-	expression tag	UNP A6N4J4
H	186	LYS	-	expression tag	UNP A6N4J4
H	187	LYS	-	expression tag	UNP A6N4J4
H	188	GLY	-	expression tag	UNP A6N4J4
H	189	SER	-	expression tag	UNP A6N4J4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	190	VAL	-	expression tag	UNP A6N4J4
H	191	VAL	-	expression tag	UNP A6N4J4
H	192	ILE	-	expression tag	UNP A6N4J4
H	193	VAL	-	expression tag	UNP A6N4J4
H	194	GLY	-	expression tag	UNP A6N4J4
H	195	ARG	-	expression tag	UNP A6N4J4
H	196	ILE	-	expression tag	UNP A6N4J4
H	197	ILE	-	expression tag	UNP A6N4J4
H	198	LEU	-	expression tag	UNP A6N4J4
H	199	SER	-	expression tag	UNP A6N4J4
H	200	GLY	-	expression tag	UNP A6N4J4
H	201	ARG	-	expression tag	UNP A6N4J4
H	202	LYS	-	expression tag	UNP A6N4J4
J	0	MET	-	initiating methionine	UNP A6N4J4
J	26	ARG	LYS	conflict	UNP A6N4J4
J	181	ALA	-	expression tag	UNP A6N4J4
J	182	SER	-	expression tag	UNP A6N4J4
J	183	LYS	-	expression tag	UNP A6N4J4
J	184	LYS	-	expression tag	UNP A6N4J4
J	185	LYS	-	expression tag	UNP A6N4J4
J	186	LYS	-	expression tag	UNP A6N4J4
J	187	LYS	-	expression tag	UNP A6N4J4
J	188	GLY	-	expression tag	UNP A6N4J4
J	189	SER	-	expression tag	UNP A6N4J4
J	190	VAL	-	expression tag	UNP A6N4J4
J	191	VAL	-	expression tag	UNP A6N4J4
J	192	ILE	-	expression tag	UNP A6N4J4
J	193	VAL	-	expression tag	UNP A6N4J4
J	194	GLY	-	expression tag	UNP A6N4J4
J	195	ARG	-	expression tag	UNP A6N4J4
J	196	ILE	-	expression tag	UNP A6N4J4
J	197	ILE	-	expression tag	UNP A6N4J4
J	198	LEU	-	expression tag	UNP A6N4J4
J	199	SER	-	expression tag	UNP A6N4J4
J	200	GLY	-	expression tag	UNP A6N4J4
J	201	ARG	-	expression tag	UNP A6N4J4
J	202	LYS	-	expression tag	UNP A6N4J4

- Molecule 2 is a protein called NS4A protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
2	K	13	93	61	17	15	0	0	0

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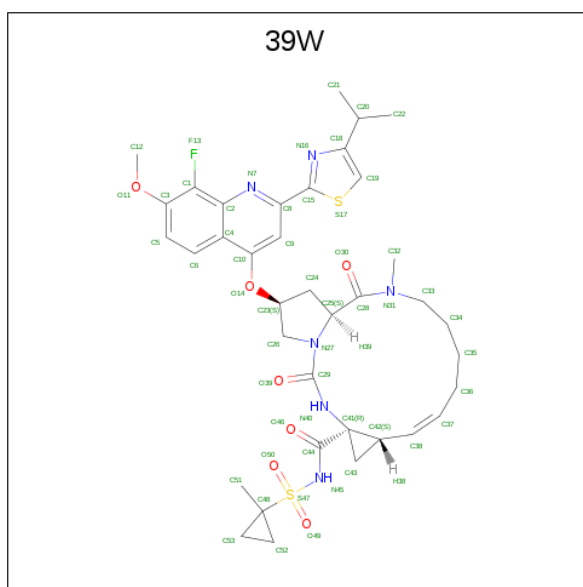
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	L	13	93	61	17	15	0	0	0
2	M	13	93	61	17	15	0	0	0
2	N	13	93	61	17	15	0	0	0
2	O	13	93	61	17	15	0	0	0
2	P	13	93	61	17	15	0	0	0
2	Q	13	93	61	17	15	0	0	0
2	T	13	93	61	17	15	0	0	0
2	U	13	93	61	17	15	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	220	LYS	-	expression tag	UNP F0UY39
K	235	LYS	-	expression tag	UNP F0UY39
L	220	LYS	-	expression tag	UNP F0UY39
L	235	LYS	-	expression tag	UNP F0UY39
M	220	LYS	-	expression tag	UNP F0UY39
M	235	LYS	-	expression tag	UNP F0UY39
N	220	LYS	-	expression tag	UNP F0UY39
N	235	LYS	-	expression tag	UNP F0UY39
O	220	LYS	-	expression tag	UNP F0UY39
O	235	LYS	-	expression tag	UNP F0UY39
P	220	LYS	-	expression tag	UNP F0UY39
P	235	LYS	-	expression tag	UNP F0UY39
Q	220	LYS	-	expression tag	UNP F0UY39
Q	235	LYS	-	expression tag	UNP F0UY39
T	220	LYS	-	expression tag	UNP F0UY39
T	235	LYS	-	expression tag	UNP F0UY39
U	220	LYS	-	expression tag	UNP F0UY39
U	235	LYS	-	expression tag	UNP F0UY39

- Molecule 3 is (2S,3aS,10Z,11aS,12aR)-2-({8-fluoro-7-methoxy-2-[4-(propan-2-yl)-1,3-thiazol-2-yl]quinolin-4-yl}oxy)-5-methyl-N-[(1-methylcyclopropyl)sulfonyl]-4,14-dioxo-1,2,3,3a,4,5,6,7,8,9,11a,12,13,14-tetradecahydro-12aH-cyclopropa[m]pyrrolo[1,2-c][1,3,6]triazacyclotetradecine-12a-carboxamide (three-letter code: 39W) (formula: C<sub>37</sub>H<sub>45</sub>FN<sub>6</sub>O<sub>7</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
3	A	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	B	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	C	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	D	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	E	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	F	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	G	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	H	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	J	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Zn 1	0	0
4	J	1	Total 1	Zn 1	0	0
4	D	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Zn 1	0	0
4	H	1	Total 1	Zn 1	0	0
4	B	1	Total 1	Zn 1	0	0
4	C	1	Total 1	Zn 1	0	0
4	A	1	Total 1	Zn 1	0	0
4	F	1	Total 1	Zn 1	0	0

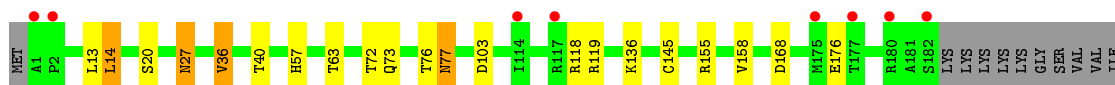
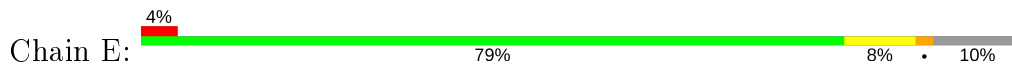
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0
5	D	1	Total 1	Cl 1	0	0
5	E	1	Total 1	Cl 1	0	0



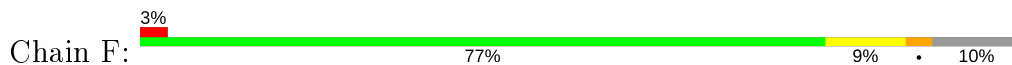
VAL  
GLY  
ARG  
ILE  
ILE  
LEU  
SER  
GLY  
ARG  
LYS

• Molecule 1: Non-structural 3 protease



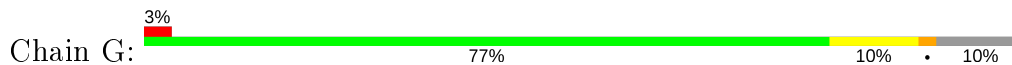
VAL  
GLY  
ARG  
ILE  
ILE  
LEU  
SER  
GLY  
ARG  
LYS

• Molecule 1: Non-structural 3 protease



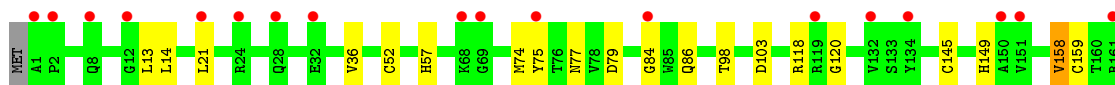
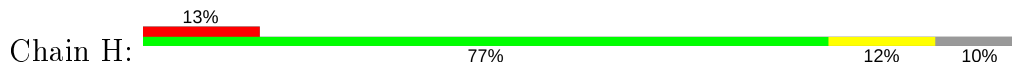
LYS  
LYS  
LYS  
GLY  
SER  
VAL  
VAL  
VAL  
ARG  
GLY  
ILE  
ILE  
LEU  
SER  
GLY  
ARG  
LYS

• Molecule 1: Non-structural 3 protease

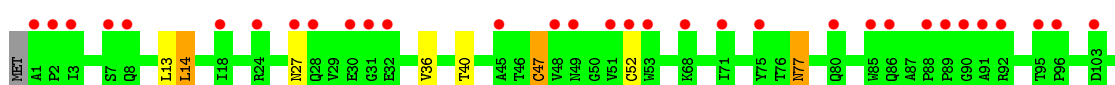
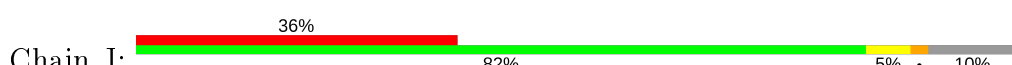


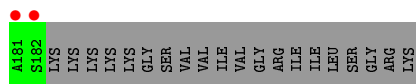
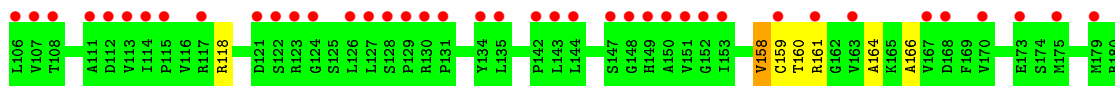
VAL  
VAL  
ILE  
VAL  
VAL  
ARG  
GLY  
ILE  
ILE  
LEU  
SER  
SER  
ARG  
LYS

• Molecule 1: Non-structural 3 protease



• Molecule 1: Non-structural 3 protease





- Molecule 2: NS4A protein



- Molecule 2: NS4A protein



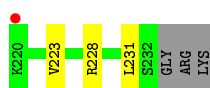
- Molecule 2: NS4A protein



- Molecule 2: NS4A protein



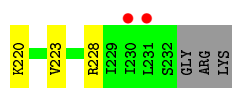
- Molecule 2: NS4A protein



- Molecule 2: NS4A protein



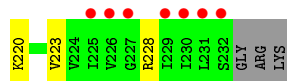
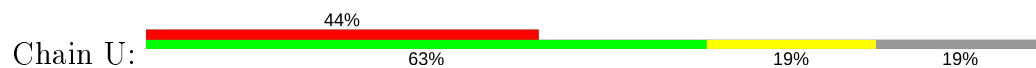
## ● Molecule 2: NS4A protein



## ● Molecule 2: NS4A protein



## ● Molecule 2: NS4A protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.03Å 174.36Å 133.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.23 – 2.80 43.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.23-2.80) 97.0 (43.22-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.233 , 0.290 0.234 , 0.287	Depositor DCC
$R_{free}$ test set	2088 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.3	Xtrriage
Anisotropy	0.245	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, 39W, CL

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	0.47	0/1363	0.63	0/1857
1	B	0.38	0/1363	0.58	0/1857
1	C	0.42	0/1363	0.59	0/1857
1	D	0.42	0/1363	0.61	0/1857
1	E	0.40	0/1363	0.57	0/1857
1	F	0.41	0/1363	0.56	0/1857
1	G	0.40	0/1363	0.58	0/1857
1	H	0.37	0/1363	0.54	0/1857
1	J	0.35	0/1363	0.50	0/1857
2	K	0.40	0/92	0.72	0/122
2	L	0.52	0/92	0.66	0/122
2	M	0.45	0/92	0.71	0/122
2	N	0.57	0/92	0.71	0/122
2	O	0.46	0/92	0.67	0/122
2	P	0.41	0/92	0.64	0/122
2	Q	0.45	0/92	0.57	0/122
2	T	0.43	0/92	0.75	0/122
2	U	0.39	0/92	0.65	0/122
All	All	0.41	0/13095	0.58	0/17811

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1337	0	1344	14	0
1	B	1337	0	1345	13	0
1	C	1337	0	1344	13	0
1	D	1337	0	1344	12	0
1	E	1337	0	1344	11	0
1	F	1337	0	1345	14	0
1	G	1337	0	1346	15	0
1	H	1337	0	1344	12	0
1	J	1337	0	1344	6	0
2	K	93	0	112	3	0
2	L	93	0	112	1	0
2	M	93	0	112	5	0
2	N	93	0	112	2	0
2	O	93	0	112	2	0
2	P	93	0	112	2	0
2	Q	93	0	112	4	0
2	T	93	0	112	4	0
2	U	93	0	112	4	0
3	A	53	0	44	4	0
3	B	53	0	44	0	0
3	C	53	0	44	2	0
3	D	53	0	44	6	0
3	E	53	0	44	3	0
3	F	53	0	44	1	0
3	G	53	0	44	0	0
3	H	53	0	44	3	0
3	J	53	0	44	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	2	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
All	All	13360	0	13504	119	0

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

All (119) 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:G:97:CYS:SG	4:G:302:ZN:ZN	1.57	0.92
1:A:159:CYS:HB3	1:A:164:ALA:HA	1.57	0.86
1:D:36:VAL:HG13	2:N:223:VAL:CG1	2.20	0.71
1:H:159:CYS:HB3	1:H:164:ALA:HA	1.76	0.68
1:D:159:CYS:HB3	1:D:164:ALA:HA	1.76	0.68
1:G:176:GLU:O	1:G:180:ARG:HG3	1.95	0.66
1:C:99:CYS:SG	4:C:302:ZN:ZN	1.84	0.64
1:H:57:HIS:HB2	3:H:301:39W:H10	1.80	0.63
1:G:97:CYS:HG	4:G:302:ZN:ZN	0.39	0.62
1:G:159:CYS:HB3	1:G:164:ALA:HA	1.81	0.60
1:E:27:ASN:HD22	1:G:27:ASN:HD22	1.50	0.59
1:J:77:ASN:C	1:J:77:ASN:HD22	2.06	0.58
1:A:158:VAL:HG13	1:A:166:ALA:HB3	1.85	0.58
1:G:115:PRO:HB2	1:G:127:LEU:HD12	1.86	0.58
1:F:75:TYR:CE1	1:F:179:MET:HA	2.40	0.56
1:G:158:VAL:HG13	1:G:166:ALA:HB3	1.88	0.56
1:C:36:VAL:HG13	2:M:223:VAL:CG1	2.37	0.55
1:B:36:VAL:HG13	2:L:223:VAL:CG1	2.37	0.55
1:C:77:ASN:C	1:C:77:ASN:HD22	2.10	0.55
1:J:36:VAL:HG13	2:U:223:VAL:CG1	2.37	0.55
1:A:77:ASN:C	1:A:77:ASN:HD22	2.09	0.54
1:G:118:ARG:HD2	1:G:120:GLY:O	2.08	0.54
1:H:118:ARG:HD2	1:H:120:GLY:O	2.08	0.54
1:J:158:VAL:HG13	1:J:166:ALA:HB3	1.90	0.53
1:A:114:ILE:HG22	1:A:130:ARG:NH2	2.23	0.53
3:A:301:39W:H17	1:D:79:ASP:HB3	1.91	0.53
1:B:97:CYS:HB3	1:B:151:VAL:HG12	1.92	0.52
1:D:158:VAL:HG13	1:D:166:ALA:HB3	1.92	0.52
1:J:159:CYS:HB3	1:J:164:ALA:HA	1.90	0.52
1:C:36:VAL:HG13	2:M:223:VAL:HG13	1.91	0.52
1:C:63:THR:HG22	1:C:72:THR:HA	1.90	0.52
1:F:36:VAL:HG13	2:P:223:VAL:HG13	1.91	0.52
2:T:220:LYS:HZ3	2:U:220:LYS:HB3	1.74	0.52
1:G:77:ASN:C	1:G:77:ASN:HD22	2.13	0.51
1:D:155:ARG:HD3	3:D:301:39W:C5	2.40	0.51
1:H:36:VAL:HG13	2:T:223:VAL:CG1	2.40	0.51
3:D:301:39W:C28	3:D:301:39W:O39	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:VAL:HG13	2:Q:223:VAL:CG1	2.41	0.50
1:E:36:VAL:HG13	2:O:223:VAL:CG1	2.41	0.50
1:D:18:ILE:HD11	1:F:14:LEU:HG	1.94	0.50
1:H:75:TYR:CE1	1:H:179:MET:HA	2.47	0.49
2:Q:220:LYS:HG2	2:U:220:LYS:NZ	2.28	0.49
2:T:220:LYS:HZ1	2:U:220:LYS:HG2	1.78	0.49
2:Q:220:LYS:HD3	2:T:220:LYS:HG2	1.94	0.49
1:F:36:VAL:HG13	2:P:223:VAL:CG1	2.43	0.48
1:B:158:VAL:HG13	1:B:166:ALA:HB3	1.94	0.48
3:H:301:39W:C28	3:H:301:39W:O39	2.61	0.48
1:A:59:ALA:O	1:A:60:GLY:C	2.51	0.48
1:F:47:CYS:SG	1:F:52:CYS:SG	3.11	0.47
3:A:301:39W:H14	3:D:301:39W:H5	1.97	0.47
1:G:36:VAL:HG13	2:Q:223:VAL:HG13	1.97	0.47
1:B:159:CYS:HB3	1:B:164:ALA:HA	1.96	0.47
1:A:47:CYS:SG	1:A:52:CYS:SG	3.04	0.47
1:B:115:PRO:HB2	1:B:127:LEU:HD12	1.97	0.47
1:E:63:THR:HG22	1:E:72:THR:HA	1.97	0.46
1:G:75:TYR:CE1	1:G:179:MET:HA	2.49	0.46
1:F:14:LEU:HD13	1:H:14:LEU:HD13	1.96	0.46
1:A:115:PRO:HB2	1:A:127:LEU:HD12	1.97	0.46
2:K:220:LYS:HB3	2:M:220:LYS:NZ	2.30	0.46
2:K:220:LYS:HB3	2:M:220:LYS:HZ3	1.80	0.46
1:H:158:VAL:HG13	1:H:166:ALA:HB3	1.98	0.46
1:F:176:GLU:O	1:F:180:ARG:HG3	2.17	0.46
1:E:57:HIS:HB2	3:E:301:39W:H10	1.98	0.45
1:B:104:LEU:HD13	1:B:151:VAL:HG21	1.97	0.45
1:F:118:ARG:HD2	1:F:120:GLY:O	2.17	0.45
1:B:176:GLU:HA	1:B:179:MET:HE2	1.99	0.45
1:E:77:ASN:C	1:E:77:ASN:HD22	2.19	0.45
1:D:77:ASN:C	1:D:77:ASN:HD22	2.21	0.44
3:A:301:39W:O39	3:A:301:39W:C28	2.64	0.44
1:B:55:VAL:HG21	1:B:57:HIS:CE1	2.52	0.44
1:F:158:VAL:HG13	1:F:166:ALA:HB3	1.97	0.44
1:A:73:GLN:NE2	1:A:76:THR:OG1	2.48	0.44
3:C:301:39W:C28	3:C:301:39W:O39	2.65	0.44
1:E:136:LYS:HA	3:E:301:39W:H27	1.99	0.44
1:G:17:ILE:HG21	1:H:21:LEU:HD13	1.99	0.43
1:D:52:CYS:O	1:D:84:GLY:HA2	2.18	0.43
1:A:32:GLU:HA	1:A:92:ARG:O	2.18	0.43
1:E:155:ARG:HD3	3:E:301:39W:C5	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:MET:O	1:C:179:MET:HG3	2.19	0.43
1:C:159:CYS:HB3	1:C:164:ALA:HA	2.00	0.43
1:C:52:CYS:O	1:C:84:GLY:HA2	2.19	0.43
1:D:80:GLN:HA	3:D:301:39W:H4	2.00	0.43
1:E:14:LEU:HD12	1:J:14:LEU:CD1	2.48	0.43
1:C:46:THR:HG21	1:C:142:PRO:HB3	2.00	0.42
1:D:14:LEU:HD22	1:D:18:ILE:HD12	2.01	0.42
1:F:77:ASN:C	1:F:77:ASN:HD22	2.22	0.42
1:B:43:PHE:HA	1:B:137:GLY:O	2.19	0.42
1:F:43:PHE:HA	1:F:137:GLY:O	2.20	0.42
1:F:63:THR:HG22	1:F:72:THR:HA	2.00	0.42
1:A:22:THR:CG2	1:C:17:ILE:HD11	2.50	0.42
3:D:301:39W:H23	3:D:301:39W:O39	2.20	0.42
1:G:57:HIS:N	1:G:81:ASP:OD1	2.52	0.42
1:A:34:GLN:HE21	2:K:225:ILE:HG21	1.84	0.42
1:H:52:CYS:O	1:H:84:GLY:HA2	2.20	0.42
1:E:73:GLN:NE2	1:E:76:THR:OG1	2.53	0.42
1:E:155:ARG:HD2	1:E:168:ASP:OD2	2.20	0.42
1:H:74:MET:SD	1:H:86:GLN:HG3	2.60	0.42
1:F:32:GLU:HA	1:F:92:ARG:O	2.21	0.41
1:E:36:VAL:HG13	2:O:223:VAL:HG13	2.01	0.41
1:A:52:CYS:O	1:A:84:GLY:HA2	2.21	0.41
1:H:172:VAL:HA	1:H:175:MET:SD	2.60	0.41
1:A:114:ILE:HA	1:A:115:PRO:HD3	1.92	0.41
1:B:46:THR:HG21	1:B:142:PRO:HB3	2.01	0.41
1:A:56:TYR:CD1	1:A:60:GLY:HA2	2.55	0.41
3:F:301:39W:O39	3:F:301:39W:C28	2.69	0.41
1:B:25:ASP:OD1	1:B:27:ASN:HB2	2.21	0.41
1:C:156:ALA:HB2	3:C:301:39W:H42	2.03	0.41
3:A:301:39W:H15	3:A:301:39W:H39	1.83	0.41
1:H:145:CYS:SG	1:H:149:HIS:HB2	2.61	0.41
1:J:47:CYS:HG	1:J:52:CYS:HG	1.64	0.41
1:D:36:VAL:CG1	2:N:223:VAL:CG1	2.95	0.41
1:B:75:TYR:O	1:B:84:GLY:N	2.54	0.40
1:D:136:LYS:HA	3:D:301:39W:H27	2.02	0.40
1:B:155:ARG:HD2	1:B:168:ASP:OD2	2.21	0.40
1:C:5:ALA:HB2	2:M:231:LEU:HD12	2.03	0.40
1:C:105:TYR:HB3	1:C:113:VAL:CG1	2.51	0.40
1:F:102:SER:HA	1:F:118:ARG:HB3	2.03	0.40
3:H:301:39W:H39	3:H:301:39W:H15	1.91	0.40
1:G:130:ARG:HG2	1:G:134:TYR:CD2	2.57	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	180/203 (89%)	174 (97%)	5 (3%)	1 (1%)	25	56
1	B	180/203 (89%)	172 (96%)	8 (4%)	0	100	100
1	C	180/203 (89%)	170 (94%)	10 (6%)	0	100	100
1	D	180/203 (89%)	171 (95%)	8 (4%)	1 (1%)	25	56
1	E	180/203 (89%)	173 (96%)	7 (4%)	0	100	100
1	F	180/203 (89%)	170 (94%)	10 (6%)	0	100	100
1	G	180/203 (89%)	174 (97%)	6 (3%)	0	100	100
1	H	180/203 (89%)	170 (94%)	10 (6%)	0	100	100
1	J	180/203 (89%)	173 (96%)	6 (3%)	1 (1%)	25	56
2	K	11/16 (69%)	11 (100%)	0	0	100	100
2	L	11/16 (69%)	11 (100%)	0	0	100	100
2	M	11/16 (69%)	11 (100%)	0	0	100	100
2	N	11/16 (69%)	11 (100%)	0	0	100	100
2	O	11/16 (69%)	11 (100%)	0	0	100	100
2	P	11/16 (69%)	11 (100%)	0	0	100	100
2	Q	11/16 (69%)	11 (100%)	0	0	100	100
2	T	11/16 (69%)	11 (100%)	0	0	100	100
2	U	11/16 (69%)	11 (100%)	0	0	100	100
All	All	1719/1971 (87%)	1646 (96%)	70 (4%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLY

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Mol	Chain	Res	Type
1	D	109	ARG
1	J	161	ARG

### 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	147/165 (89%)	135 (92%)	12 (8%)	11	33
1	B	147/165 (89%)	140 (95%)	7 (5%)	25	58
1	C	147/165 (89%)	141 (96%)	6 (4%)	30	64
1	D	147/165 (89%)	134 (91%)	13 (9%)	10	29
1	E	147/165 (89%)	134 (91%)	13 (9%)	10	29
1	F	147/165 (89%)	134 (91%)	13 (9%)	10	29
1	G	147/165 (89%)	138 (94%)	9 (6%)	18	48
1	H	147/165 (89%)	140 (95%)	7 (5%)	25	58
1	J	147/165 (89%)	138 (94%)	9 (6%)	18	48
2	K	11/13 (85%)	9 (82%)	2 (18%)	1	5
2	L	11/13 (85%)	10 (91%)	1 (9%)	9	27
2	M	11/13 (85%)	7 (64%)	4 (36%)	0	0
2	N	11/13 (85%)	10 (91%)	1 (9%)	9	27
2	O	11/13 (85%)	9 (82%)	2 (18%)	1	5
2	P	11/13 (85%)	8 (73%)	3 (27%)	0	1
2	Q	11/13 (85%)	10 (91%)	1 (9%)	9	27
2	T	11/13 (85%)	9 (82%)	2 (18%)	1	5
2	U	11/13 (85%)	10 (91%)	1 (9%)	9	27
All	All	1422/1602 (89%)	1316 (92%)	106 (8%)	13	37

All (106) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	13	LEU
1	A	14	LEU
1	A	61	SER
1	A	74	MET
1	A	77	ASN
1	A	95	THR
1	A	98	THR
1	A	109	ARG
1	A	118	ARG
1	A	122	SER
1	A	158	VAL
1	A	159	CYS
1	B	13	LEU
1	B	14	LEU
1	B	36	VAL
1	B	95	THR
1	B	118	ARG
1	B	158	VAL
1	B	176	GLU
1	C	13	LEU
1	C	14	LEU
1	C	77	ASN
1	C	118	ARG
1	C	145	CYS
1	C	158	VAL
1	D	13	LEU
1	D	14	LEU
1	D	77	ASN
1	D	93	SER
1	D	109	ARG
1	D	118	ARG
1	D	121	ASP
1	D	128	SER
1	D	136	LYS
1	D	158	VAL
1	D	159	CYS
1	D	175	MET
1	D	176	GLU
1	E	13	LEU
1	E	14	LEU
1	E	20	SER
1	E	27	ASN
1	E	36	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	40	THR
1	E	77	ASN
1	E	103	ASP
1	E	118	ARG
1	E	119	ARG
1	E	145	CYS
1	E	158	VAL
1	E	176	GLU
1	F	13	LEU
1	F	36	VAL
1	F	40	THR
1	F	52	CYS
1	F	77	ASN
1	F	95	THR
1	F	98	THR
1	F	102	SER
1	F	118	ARG
1	F	128	SER
1	F	151	VAL
1	F	158	VAL
1	F	176	GLU
1	G	13	LEU
1	G	26	ARG
1	G	27	ASN
1	G	77	ASN
1	G	98	THR
1	G	118	ARG
1	G	145	CYS
1	G	158	VAL
1	G	176	GLU
1	H	13	LEU
1	H	77	ASN
1	H	79	ASP
1	H	98	THR
1	H	103	ASP
1	H	158	VAL
1	H	163	VAL
1	J	13	LEU
1	J	14	LEU
1	J	27	ASN
1	J	40	THR
1	J	47	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	J	77	ASN
1	J	118	ARG
1	J	158	VAL
1	J	160	THR
2	K	228	ARG
2	K	231	LEU
2	L	228	ARG
2	M	222	SER
2	M	228	ARG
2	M	231	LEU
2	M	232	SER
2	N	228	ARG
2	O	228	ARG
2	O	231	LEU
2	P	220	LYS
2	P	228	ARG
2	P	231	LEU
2	Q	228	ARG
2	T	228	ARG
2	T	232	SER
2	U	228	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	8	GLN
1	A	27	ASN
1	A	34	GLN
1	A	73	GLN
1	A	77	ASN
1	B	8	GLN
1	B	9	GLN
1	B	27	ASN
1	B	34	GLN
1	C	8	GLN
1	C	27	ASN
1	C	28	GLN
1	C	34	GLN
1	C	73	GLN
1	C	77	ASN
1	D	8	GLN
1	D	9	GLN

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Mol	Chain	Res	Type
1	D	27	ASN
1	D	34	GLN
1	D	73	GLN
1	D	77	ASN
1	D	80	GLN
1	E	8	GLN
1	E	9	GLN
1	E	27	ASN
1	E	34	GLN
1	E	73	GLN
1	E	77	ASN
1	F	8	GLN
1	F	9	GLN
1	F	27	ASN
1	F	34	GLN
1	F	73	GLN
1	F	77	ASN
1	G	8	GLN
1	G	9	GLN
1	G	27	ASN
1	G	34	GLN
1	G	77	ASN
1	H	8	GLN
1	H	77	ASN
1	J	8	GLN
1	J	34	GLN
1	J	73	GLN
1	J	77	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 22 ligands modelled in this entry, 13 are monoatomic - leaving 9 for Mogul analysis.

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	39W	H	301	-	54,59,59	2.14	8 (14%)	70,91,91	2.53	19 (27%)
3	39W	B	301	-	54,59,59	2.18	8 (14%)	70,91,91	2.54	20 (28%)
3	39W	A	301	-	54,59,59	2.17	8 (14%)	70,91,91	2.52	16 (22%)
3	39W	C	301	-	54,59,59	2.01	9 (16%)	70,91,91	2.57	18 (25%)
3	39W	J	301	-	54,59,59	2.12	9 (16%)	70,91,91	2.23	19 (27%)
3	39W	E	301	-	54,59,59	2.05	9 (16%)	70,91,91	2.32	20 (28%)
3	39W	G	301	-	54,59,59	2.03	9 (16%)	70,91,91	2.56	21 (30%)
3	39W	F	301	-	54,59,59	2.11	8 (14%)	70,91,91	2.35	19 (27%)
3	39W	D	301	-	54,59,59	2.21	7 (12%)	70,91,91	2.81	23 (32%)

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	39W	H	301	-	-	11/48/84/84	0/6/7/7
3	39W	B	301	-	-	11/48/84/84	0/6/7/7
3	39W	A	301	-	-	12/48/84/84	0/6/7/7
3	39W	C	301	-	-	13/48/84/84	0/6/7/7
3	39W	J	301	-	-	12/48/84/84	0/6/7/7
3	39W	E	301	-	-	11/48/84/84	0/6/7/7
3	39W	G	301	-	-	12/48/84/84	0/6/7/7
3	39W	F	301	-	-	10/48/84/84	0/6/7/7
3	39W	D	301	-	-	13/48/84/84	0/6/7/7

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	39W	C15-S17	-10.88	1.58	1.73
3	D	301	39W	C15-S17	-10.67	1.58	1.73
3	A	301	39W	C15-S17	-10.50	1.59	1.73
3	F	301	39W	C15-S17	-10.17	1.59	1.73
3	H	301	39W	C15-S17	-10.08	1.59	1.73
3	E	301	39W	C15-S17	-9.52	1.60	1.73
3	J	301	39W	C15-S17	-9.24	1.60	1.73
3	G	301	39W	C15-S17	-9.22	1.60	1.73
3	C	301	39W	C15-S17	-9.12	1.61	1.73
3	A	301	39W	C19-S17	-7.34	1.59	1.70
3	D	301	39W	C19-S17	-7.15	1.59	1.70
3	B	301	39W	C19-S17	-7.11	1.59	1.70
3	J	301	39W	C19-S17	-7.09	1.59	1.70
3	F	301	39W	C19-S17	-6.98	1.59	1.70
3	G	301	39W	C19-S17	-6.90	1.59	1.70
3	H	301	39W	C19-S17	-6.89	1.59	1.70
3	E	301	39W	C19-S17	-6.84	1.59	1.70
3	C	301	39W	C19-S17	-6.77	1.59	1.70
3	J	301	39W	C8-N7	4.35	1.39	1.33
3	H	301	39W	C8-N7	4.24	1.39	1.33
3	D	301	39W	C43-C41	-3.96	1.46	1.51
3	J	301	39W	C43-C41	-3.89	1.46	1.51
3	G	301	39W	C8-N7	3.88	1.39	1.33
3	C	301	39W	C8-N7	3.87	1.39	1.33
3	H	301	39W	C43-C41	-3.74	1.47	1.51
3	J	301	39W	C42-C38	3.72	1.54	1.49
3	G	301	39W	C43-C41	-3.69	1.47	1.51
3	D	301	39W	C8-N7	3.68	1.38	1.33
3	F	301	39W	C43-C41	-3.67	1.47	1.51
3	D	301	39W	C42-C38	3.65	1.53	1.49
3	B	301	39W	C8-N7	3.58	1.38	1.33
3	A	301	39W	C42-C38	3.54	1.53	1.49
3	E	301	39W	C8-N7	3.50	1.38	1.33
3	B	301	39W	C43-C41	-3.49	1.47	1.51
3	A	301	39W	C8-N7	3.44	1.38	1.33
3	B	301	39W	C42-C38	3.43	1.53	1.49
3	E	301	39W	C43-C41	-3.42	1.47	1.51
3	F	301	39W	C8-N7	3.38	1.38	1.33
3	J	301	39W	C28-N31	3.38	1.41	1.35
3	A	301	39W	C43-C41	-3.32	1.47	1.51
3	E	301	39W	C52-C53	3.30	1.58	1.50
3	J	301	39W	C52-C53	3.27	1.58	1.50
3	B	301	39W	C52-C53	3.26	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	39W	C28-N31	3.26	1.40	1.35
3	H	301	39W	C52-C53	3.25	1.58	1.50
3	G	301	39W	C28-N31	3.21	1.40	1.35
3	F	301	39W	C52-C53	3.17	1.58	1.50
3	A	301	39W	C52-C53	3.15	1.57	1.50
3	E	301	39W	C42-C38	3.15	1.53	1.49
3	C	301	39W	C52-C53	3.14	1.57	1.50
3	G	301	39W	C42-C38	3.12	1.53	1.49
3	D	301	39W	C52-C53	3.12	1.57	1.50
3	F	301	39W	C42-C38	3.10	1.53	1.49
3	G	301	39W	C52-C53	3.09	1.57	1.50
3	C	301	39W	C43-C41	-3.04	1.47	1.51
3	H	301	39W	C28-N31	3.04	1.40	1.35
3	E	301	39W	C28-N31	3.01	1.40	1.35
3	C	301	39W	C28-N31	2.92	1.40	1.35
3	C	301	39W	C42-C38	2.91	1.53	1.49
3	F	301	39W	C28-N31	2.87	1.40	1.35
3	H	301	39W	C42-C38	2.84	1.53	1.49
3	B	301	39W	C28-N31	2.79	1.40	1.35
3	D	301	39W	C28-N31	2.79	1.40	1.35
3	J	301	39W	S47-N45	2.75	1.64	1.60
3	J	301	39W	C15-N16	2.74	1.35	1.31
3	E	301	39W	C15-N16	2.67	1.35	1.31
3	F	301	39W	C15-N16	2.59	1.35	1.31
3	C	301	39W	C15-N16	2.58	1.35	1.31
3	C	301	39W	S47-N45	2.51	1.64	1.60
3	H	301	39W	C15-N16	2.50	1.35	1.31
3	A	301	39W	S47-N45	2.12	1.63	1.60
3	G	301	39W	C48-S47	-2.09	1.79	1.81
3	G	301	39W	C15-N16	2.02	1.34	1.31
3	B	301	39W	C15-N16	2.01	1.34	1.31
3	E	301	39W	C48-S47	-2.01	1.80	1.81

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	39W	O11-C3-C1	13.45	125.83	116.27
3	B	301	39W	O11-C3-C1	11.69	124.58	116.27
3	G	301	39W	O11-C3-C1	10.95	124.05	116.27
3	C	301	39W	O11-C3-C1	10.63	123.82	116.27
3	A	301	39W	O11-C3-C1	10.04	123.41	116.27
3	H	301	39W	O11-C3-C1	9.72	123.18	116.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	39W	O11-C3-C1	8.81	122.53	116.27
3	E	301	39W	O11-C3-C1	8.25	122.14	116.27
3	J	301	39W	O11-C3-C1	7.57	121.65	116.27
3	D	301	39W	C12-O11-C3	7.34	128.61	117.53
3	H	301	39W	C52-C48-C53	6.87	63.13	59.54
3	A	301	39W	C52-C48-C53	6.73	63.06	59.54
3	D	301	39W	C52-C48-C53	6.72	63.05	59.54
3	B	301	39W	C52-C48-C53	6.72	63.05	59.54
3	A	301	39W	C12-O11-C3	6.69	127.63	117.53
3	F	301	39W	C52-C48-C53	6.60	62.99	59.54
3	J	301	39W	C52-C48-C53	6.59	62.99	59.54
3	E	301	39W	C52-C48-C53	6.58	62.98	59.54
3	C	301	39W	C12-O11-C3	6.51	127.36	117.53
3	A	301	39W	O49-S47-O50	-6.51	107.36	120.57
3	G	301	39W	C52-C48-C53	6.49	62.94	59.54
3	H	301	39W	O50-S47-C48	6.47	112.79	107.60
3	C	301	39W	C52-C48-C53	6.22	62.79	59.54
3	G	301	39W	C12-O11-C3	6.21	126.91	117.53
3	C	301	39W	C41-C44-N45	5.79	125.72	115.70
3	G	301	39W	O49-S47-O50	-5.73	108.94	120.57
3	H	301	39W	O49-S47-O50	-5.57	109.27	120.57
3	D	301	39W	O49-S47-O50	-5.44	109.52	120.57
3	F	301	39W	C41-C44-N45	5.38	125.01	115.70
3	A	301	39W	C41-C44-N45	5.30	124.87	115.70
3	B	301	39W	C12-O11-C3	5.28	125.51	117.53
3	D	301	39W	O11-C3-C5	-5.25	115.38	124.37
3	F	301	39W	O49-S47-O50	-5.23	109.96	120.57
3	B	301	39W	O11-C3-C5	-5.20	115.46	124.37
3	E	301	39W	O14-C10-C4	5.08	120.91	114.22
3	J	301	39W	C41-C44-N45	5.08	124.48	115.70
3	D	301	39W	O50-S47-C48	4.98	111.59	107.60
3	J	301	39W	O49-S47-O50	-4.95	110.53	120.57
3	C	301	39W	O49-S47-O50	-4.90	110.62	120.57
3	H	301	39W	C12-O11-C3	4.83	124.82	117.53
3	E	301	39W	C12-O11-C3	4.80	124.77	117.53
3	B	301	39W	C41-C44-N45	4.76	123.94	115.70
3	H	301	39W	C41-C44-N45	4.75	123.92	115.70
3	C	301	39W	C43-C42-C38	4.75	132.04	120.03
3	J	301	39W	C12-O11-C3	4.74	124.69	117.53
3	A	301	39W	O11-C3-C5	-4.72	116.28	124.37
3	F	301	39W	C12-O11-C3	4.67	124.58	117.53
3	A	301	39W	C19-C18-C20	-4.66	122.08	129.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	39W	O11-C3-C5	-4.64	116.43	124.37
3	J	301	39W	C43-C42-C38	4.50	131.41	120.03
3	B	301	39W	O14-C10-C4	4.47	120.10	114.22
3	E	301	39W	O49-S47-O50	-4.42	111.59	120.57
3	F	301	39W	C43-C42-C38	4.42	131.19	120.03
3	H	301	39W	C19-C18-C20	-4.41	122.47	129.25
3	G	301	39W	O14-C10-C4	4.40	120.01	114.22
3	F	301	39W	C19-C18-C20	-4.38	122.51	129.25
3	H	301	39W	C15-C8-N7	4.38	121.91	117.28
3	B	301	39W	C43-C42-C38	4.34	131.00	120.03
3	B	301	39W	O49-S47-O50	-4.28	111.88	120.57
3	E	301	39W	C43-C42-C38	4.28	130.84	120.03
3	C	301	39W	O11-C3-C5	-4.26	117.07	124.37
3	C	301	39W	O46-C44-C41	-4.23	115.70	120.74
3	J	301	39W	C19-C18-C20	-4.22	122.76	129.25
3	G	301	39W	C41-C44-N45	4.19	122.94	115.70
3	H	301	39W	C43-C42-C38	4.13	130.48	120.03
3	C	301	39W	C8-N7-C2	4.04	121.36	118.26
3	H	301	39W	O11-C3-C5	-4.00	117.52	124.37
3	A	301	39W	C43-C42-C38	3.97	130.06	120.03
3	H	301	39W	O14-C10-C4	3.95	119.42	114.22
3	F	301	39W	O14-C10-C4	3.95	119.41	114.22
3	D	301	39W	C43-C42-C38	3.94	129.99	120.03
3	G	301	39W	C15-C8-N7	3.92	121.43	117.28
3	E	301	39W	O50-S47-C48	3.88	110.71	107.60
3	C	301	39W	C19-C18-C20	-3.83	123.35	129.25
3	E	301	39W	C41-C44-N45	3.81	122.29	115.70
3	D	301	39W	C43-C42-C41	-3.78	56.82	59.09
3	C	301	39W	C9-C8-N7	-3.76	118.80	122.23
3	D	301	39W	C15-C8-N7	3.71	121.20	117.28
3	J	301	39W	C43-C42-C41	-3.64	56.90	59.09
3	E	301	39W	C19-C18-C20	-3.55	123.80	129.25
3	G	301	39W	C19-C18-C20	-3.48	123.90	129.25
3	F	301	39W	O11-C3-C5	-3.46	118.45	124.37
3	G	301	39W	C43-C42-C38	3.45	128.75	120.03
3	B	301	39W	C43-C42-C41	-3.44	57.02	59.09
3	D	301	39W	C44-C41-N40	-3.37	112.43	116.06
3	E	301	39W	C8-N7-C2	3.34	120.82	118.26
3	D	301	39W	C19-C18-C20	-3.34	124.12	129.25
3	D	301	39W	C25-C28-N31	3.32	126.25	119.40
3	H	301	39W	C43-C42-C41	-3.32	57.10	59.09
3	F	301	39W	C43-C42-C41	-3.29	57.11	59.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	39W	O14-C10-C4	3.29	118.55	114.22
3	J	301	39W	O11-C3-C5	-3.27	118.76	124.37
3	B	301	39W	C19-C18-C20	-3.25	124.26	129.25
3	E	301	39W	C9-C8-N7	-3.23	119.28	122.23
3	G	301	39W	C43-C42-C41	-3.19	57.17	59.09
3	F	301	39W	O49-S47-C48	3.17	110.14	107.60
3	A	301	39W	O50-S47-C48	3.15	110.13	107.60
3	E	301	39W	C43-C42-C41	-3.15	57.20	59.09
3	J	301	39W	O50-S47-C48	3.13	110.11	107.60
3	G	301	39W	O50-S47-C48	3.12	110.11	107.60
3	A	301	39W	C43-C42-C41	-3.12	57.21	59.09
3	B	301	39W	C25-C28-N31	3.12	125.84	119.40
3	E	301	39W	C23-C26-N27	3.10	106.88	102.62
3	E	301	39W	O11-C3-C5	-3.06	119.12	124.37
3	D	301	39W	C41-C44-N45	3.03	120.94	115.70
3	D	301	39W	C44-N45-S47	-2.99	119.25	124.08
3	D	301	39W	C9-C8-N7	-2.97	119.53	122.23
3	C	301	39W	C43-C42-C41	-2.96	57.31	59.09
3	D	301	39W	O14-C10-C4	2.95	118.10	114.22
3	F	301	39W	C23-C26-N27	2.91	106.61	102.62
3	J	301	39W	O14-C10-C4	2.86	117.98	114.22
3	H	301	39W	C8-N7-C2	2.82	120.42	118.26
3	A	301	39W	C32-N31-C33	-2.81	110.19	115.89
3	H	301	39W	C25-C28-N31	2.75	125.08	119.40
3	G	301	39W	C41-N40-C29	-2.74	117.68	123.89
3	J	301	39W	O46-C44-C41	-2.73	117.49	120.74
3	H	301	39W	C9-C8-N7	-2.72	119.75	122.23
3	C	301	39W	C32-N31-C33	-2.70	110.40	115.89
3	A	301	39W	O46-C44-C41	-2.68	117.55	120.74
3	B	301	39W	C28-C25-N27	-2.68	104.72	111.03
3	B	301	39W	C15-C8-N7	2.66	120.09	117.28
3	G	301	39W	C44-C41-N40	-2.63	113.22	116.06
3	D	301	39W	O49-S47-C48	2.62	109.70	107.60
3	J	301	39W	C25-C28-N31	2.59	124.75	119.40
3	D	301	39W	F13-C1-C3	2.59	122.79	119.16
3	G	301	39W	C8-N7-C2	2.59	120.24	118.26
3	D	301	39W	C43-C41-N40	2.56	121.24	117.80
3	E	301	39W	C32-N31-C33	-2.55	110.71	115.89
3	J	301	39W	C32-N31-C33	-2.54	110.73	115.89
3	C	301	39W	C15-C8-N7	2.53	119.96	117.28
3	B	301	39W	O50-S47-C48	2.52	109.63	107.60
3	J	301	39W	C43-C41-N40	2.52	121.18	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	39W	C43-C41-N40	2.51	121.17	117.80
3	J	301	39W	C8-N7-C2	2.49	120.17	118.26
3	A	301	39W	C51-C48-C53	-2.47	110.68	117.35
3	H	301	39W	C43-C41-N40	2.47	121.11	117.80
3	D	301	39W	C41-C43-C42	2.45	63.83	61.56
3	H	301	39W	C32-N31-C33	-2.44	110.94	115.89
3	E	301	39W	C51-C48-C52	2.38	123.77	117.35
3	F	301	39W	C43-C41-N40	2.38	120.99	117.80
3	B	301	39W	C41-C43-C42	2.38	63.77	61.56
3	E	301	39W	C25-C28-N31	2.38	124.31	119.40
3	C	301	39W	C25-C28-N31	2.38	124.31	119.40
3	G	301	39W	C32-N31-C33	-2.36	111.09	115.89
3	G	301	39W	C25-C28-N31	2.35	124.26	119.40
3	E	301	39W	C24-C25-N27	2.34	106.19	103.10
3	H	301	39W	C20-C18-N16	2.32	124.08	120.30
3	D	301	39W	C8-N7-C2	2.30	120.03	118.26
3	C	301	39W	C41-C43-C42	2.30	63.69	61.56
3	F	301	39W	C51-C48-C53	-2.29	111.18	117.35
3	A	301	39W	O49-S47-C48	2.27	109.42	107.60
3	J	301	39W	O14-C23-C26	2.25	113.67	108.19
3	F	301	39W	C32-N31-C33	-2.25	111.32	115.89
3	B	301	39W	O30-C28-C25	-2.25	115.52	120.22
3	F	301	39W	C44-N45-S47	-2.25	120.45	124.08
3	E	301	39W	C1-C2-C4	2.22	121.61	117.13
3	A	301	39W	C42-C41-C44	2.22	121.51	116.80
3	J	301	39W	C9-C8-N7	-2.22	120.21	122.23
3	F	301	39W	C9-C8-N7	-2.21	120.21	122.23
3	G	301	39W	C34-C35-C36	-2.19	104.26	113.79
3	A	301	39W	O14-C10-C4	2.18	117.09	114.22
3	H	301	39W	C41-C43-C42	2.16	63.57	61.56
3	J	301	39W	C20-C18-N16	2.16	123.81	120.30
3	G	301	39W	C51-C48-C52	2.13	123.09	117.35
3	E	301	39W	C20-C18-N16	2.12	123.75	120.30
3	C	301	39W	C42-C41-C44	2.12	121.30	116.80
3	B	301	39W	C8-N7-C2	2.11	119.88	118.26
3	D	301	39W	C32-N31-C33	-2.10	111.62	115.89
3	F	301	39W	C51-C48-C52	2.08	122.97	117.35
3	G	301	39W	C23-C26-N27	2.06	105.45	102.62
3	G	301	39W	C44-N45-S47	-2.03	120.79	124.08
3	B	301	39W	C32-N31-C33	-2.03	111.77	115.89
3	F	301	39W	O46-C44-C41	-2.03	118.33	120.74
3	B	301	39W	C51-C48-C53	-2.03	111.89	117.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	39W	C23-C26-N27	2.01	105.38	102.62

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	39W	C1-C3-O11-C12
3	B	301	39W	C24-C23-O14-C10
3	B	301	39W	C26-C23-O14-C10
3	B	301	39W	C34-C33-N31-C32
3	B	301	39W	C34-C33-N31-C28
3	B	301	39W	C44-N45-S47-C48
3	B	301	39W	C43-C41-N40-C29
3	E	301	39W	C1-C3-O11-C12
3	E	301	39W	C24-C23-O14-C10
3	E	301	39W	C34-C33-N31-C28
3	E	301	39W	C44-N45-S47-C48
3	E	301	39W	C43-C41-N40-C29
3	E	301	39W	C42-C41-N40-C29
3	G	301	39W	C1-C3-O11-C12
3	G	301	39W	C24-C23-O14-C10
3	G	301	39W	C44-N45-S47-C48
3	G	301	39W	C43-C41-N40-C29
3	G	301	39W	C42-C41-N40-C29
3	D	301	39W	C1-C3-O11-C12
3	D	301	39W	C24-C23-O14-C10
3	D	301	39W	C44-N45-S47-C48
3	C	301	39W	C1-C3-O11-C12
3	C	301	39W	C34-C33-N31-C28
3	C	301	39W	C44-N45-S47-C48
3	C	301	39W	C43-C41-N40-C29
3	C	301	39W	C42-C41-N40-C29
3	J	301	39W	C1-C3-O11-C12
3	J	301	39W	N16-C15-C8-N7
3	J	301	39W	C44-N45-S47-C48
3	J	301	39W	C43-C41-N40-C29
3	H	301	39W	C1-C3-O11-C12
3	H	301	39W	C24-C23-O14-C10
3	H	301	39W	C44-N45-S47-C48
3	A	301	39W	C1-C3-O11-C12
3	A	301	39W	C24-C23-O14-C10
3	A	301	39W	C44-N45-S47-C48

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Mol	Chain	Res	Type	Atoms
3	F	301	39W	C1-C3-O11-C12
3	F	301	39W	C34-C33-N31-C28
3	F	301	39W	C44-N45-S47-C48
3	C	301	39W	C5-C3-O11-C12
3	G	301	39W	C5-C3-O11-C12
3	D	301	39W	C5-C3-O11-C12
3	B	301	39W	C5-C3-O11-C12
3	E	301	39W	C5-C3-O11-C12
3	H	301	39W	C5-C3-O11-C12
3	F	301	39W	C5-C3-O11-C12
3	A	301	39W	C5-C3-O11-C12
3	J	301	39W	C5-C3-O11-C12
3	B	301	39W	C44-N45-S47-O50
3	C	301	39W	C44-N45-S47-O50
3	J	301	39W	C44-N45-S47-O50
3	A	301	39W	C44-N45-S47-O50
3	E	301	39W	C34-C33-N31-C32
3	C	301	39W	C34-C33-N31-C32
3	E	301	39W	C44-N45-S47-O50
3	D	301	39W	C26-C23-O14-C10
3	C	301	39W	C33-C34-C35-C36
3	C	301	39W	N31-C33-C34-C35
3	G	301	39W	C34-C33-N31-C28
3	J	301	39W	C34-C33-N31-C28
3	H	301	39W	C34-C33-N31-C28
3	A	301	39W	C34-C33-N31-C28
3	A	301	39W	N31-C33-C34-C35
3	A	301	39W	C33-C34-C35-C36
3	E	301	39W	C26-C23-O14-C10
3	G	301	39W	C26-C23-O14-C10
3	A	301	39W	C26-C23-O14-C10
3	H	301	39W	C33-C34-C35-C36
3	J	301	39W	C33-C34-C35-C36
3	F	301	39W	N31-C33-C34-C35
3	F	301	39W	C33-C34-C35-C36
3	C	301	39W	C24-C23-O14-C10
3	J	301	39W	C24-C23-O14-C10
3	J	301	39W	N31-C33-C34-C35
3	D	301	39W	C44-C41-N40-C29
3	H	301	39W	N31-C33-C34-C35
3	D	301	39W	C43-C41-N40-C29
3	D	301	39W	C42-C41-N40-C29

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Mol	Chain	Res	Type	Atoms
3	J	301	39W	C42-C41-N40-C29
3	H	301	39W	C43-C41-N40-C29
3	H	301	39W	C42-C41-N40-C29
3	A	301	39W	C43-C41-N40-C29
3	A	301	39W	C42-C41-N40-C29
3	F	301	39W	C43-C41-N40-C29
3	F	301	39W	C42-C41-N40-C29
3	G	301	39W	C19-C18-C20-C21
3	G	301	39W	N31-C33-C34-C35
3	D	301	39W	N31-C33-C34-C35
3	G	301	39W	C33-C34-C35-C36
3	G	301	39W	C34-C33-N31-C32
3	F	301	39W	C34-C33-N31-C32
3	D	301	39W	C24-C25-C28-N31
3	H	301	39W	C26-C23-O14-C10
3	J	301	39W	C34-C33-N31-C32
3	H	301	39W	C34-C33-N31-C32
3	A	301	39W	C34-C33-N31-C32
3	B	301	39W	N31-C33-C34-C35
3	D	301	39W	C33-C34-C35-C36
3	C	301	39W	C44-N45-S47-O49
3	D	301	39W	C34-C33-N31-C32
3	B	301	39W	C33-C34-C35-C36
3	D	301	39W	N27-C25-C28-N31
3	E	301	39W	N40-C41-C44-O46
3	C	301	39W	C37-C38-C42-C41
3	F	301	39W	C37-C38-C42-C41

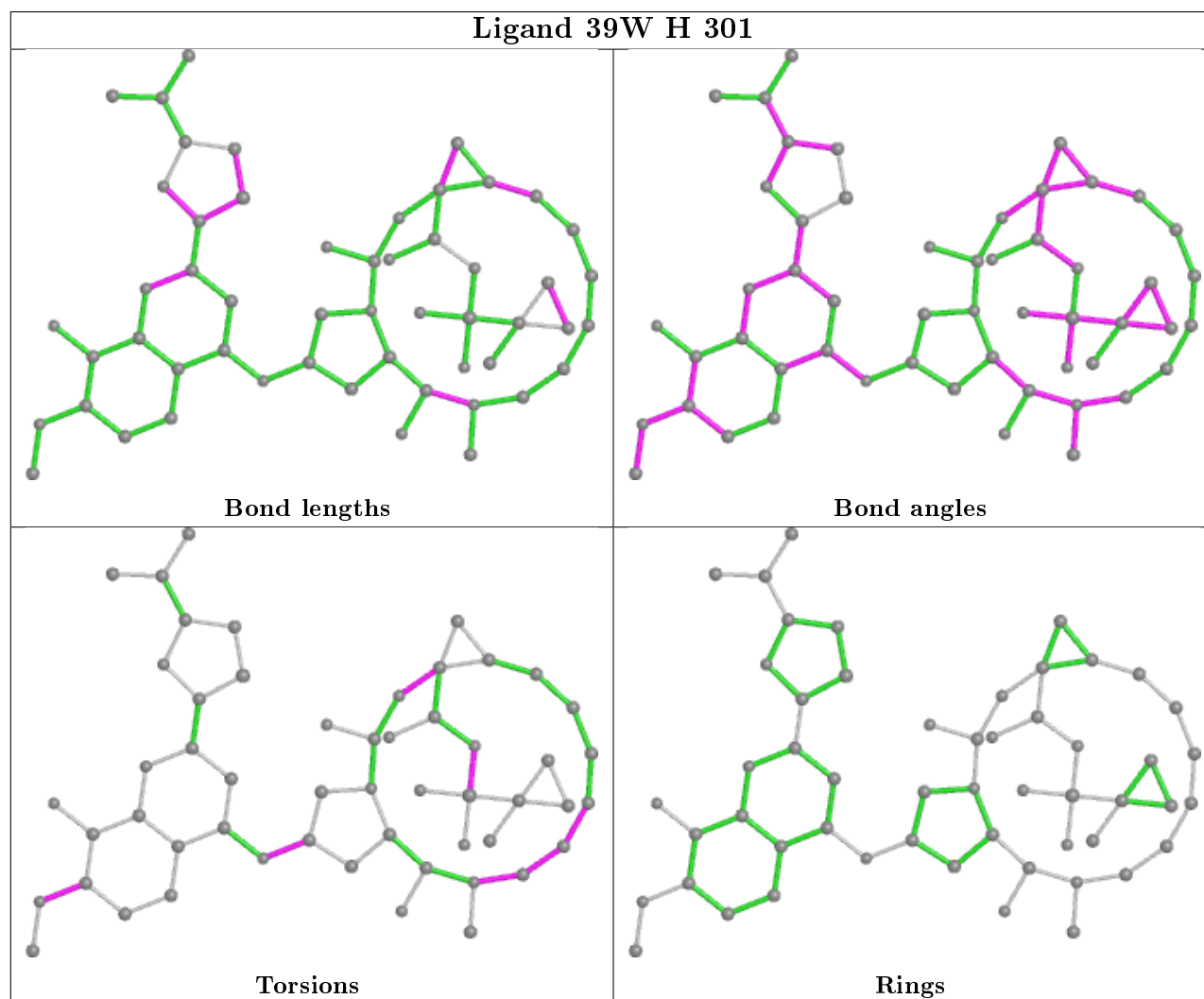
There are no ring outliers.

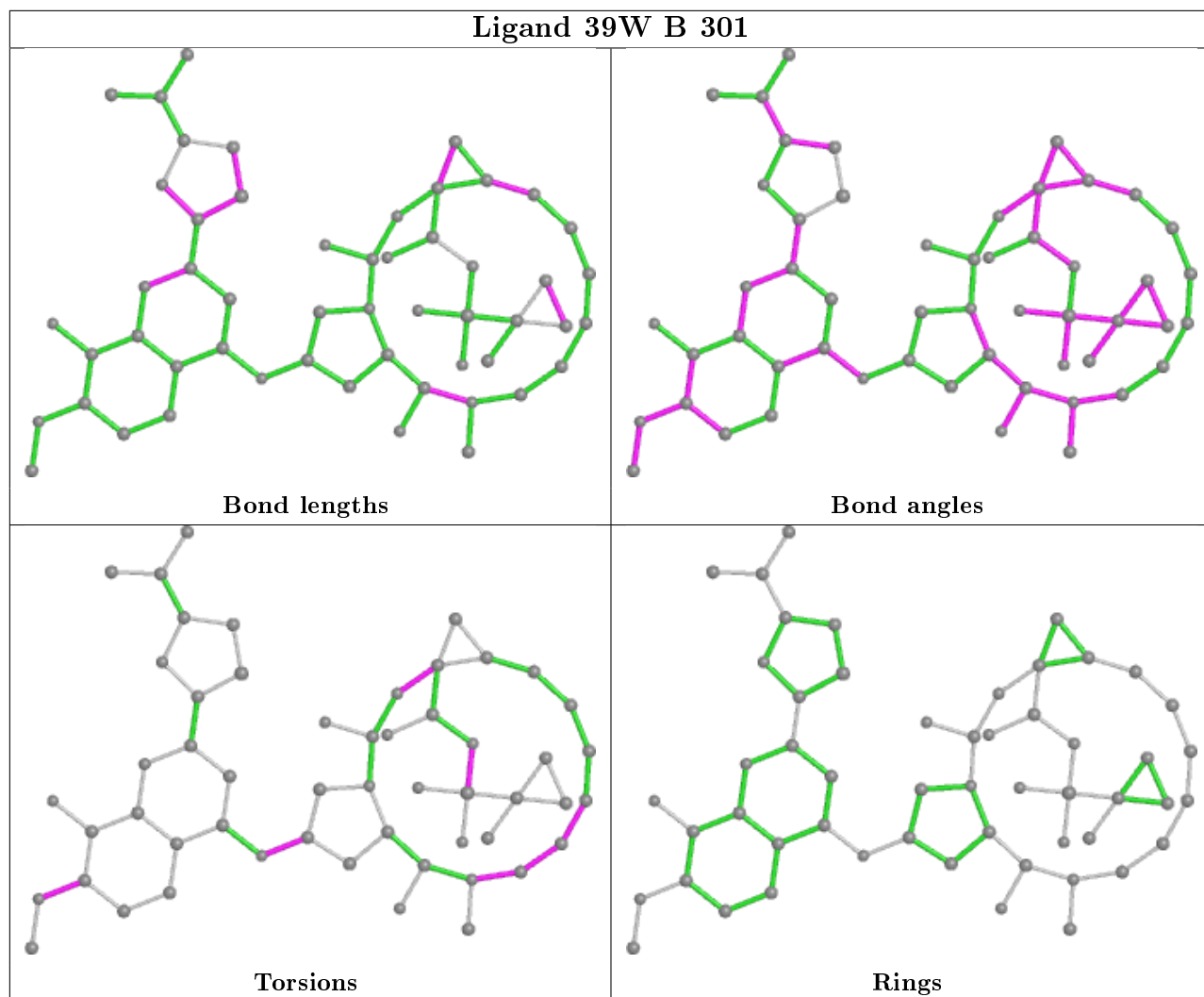
6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	301	39W	3	0
3	A	301	39W	4	0
3	C	301	39W	2	0
3	E	301	39W	3	0
3	F	301	39W	1	0
3	D	301	39W	6	0

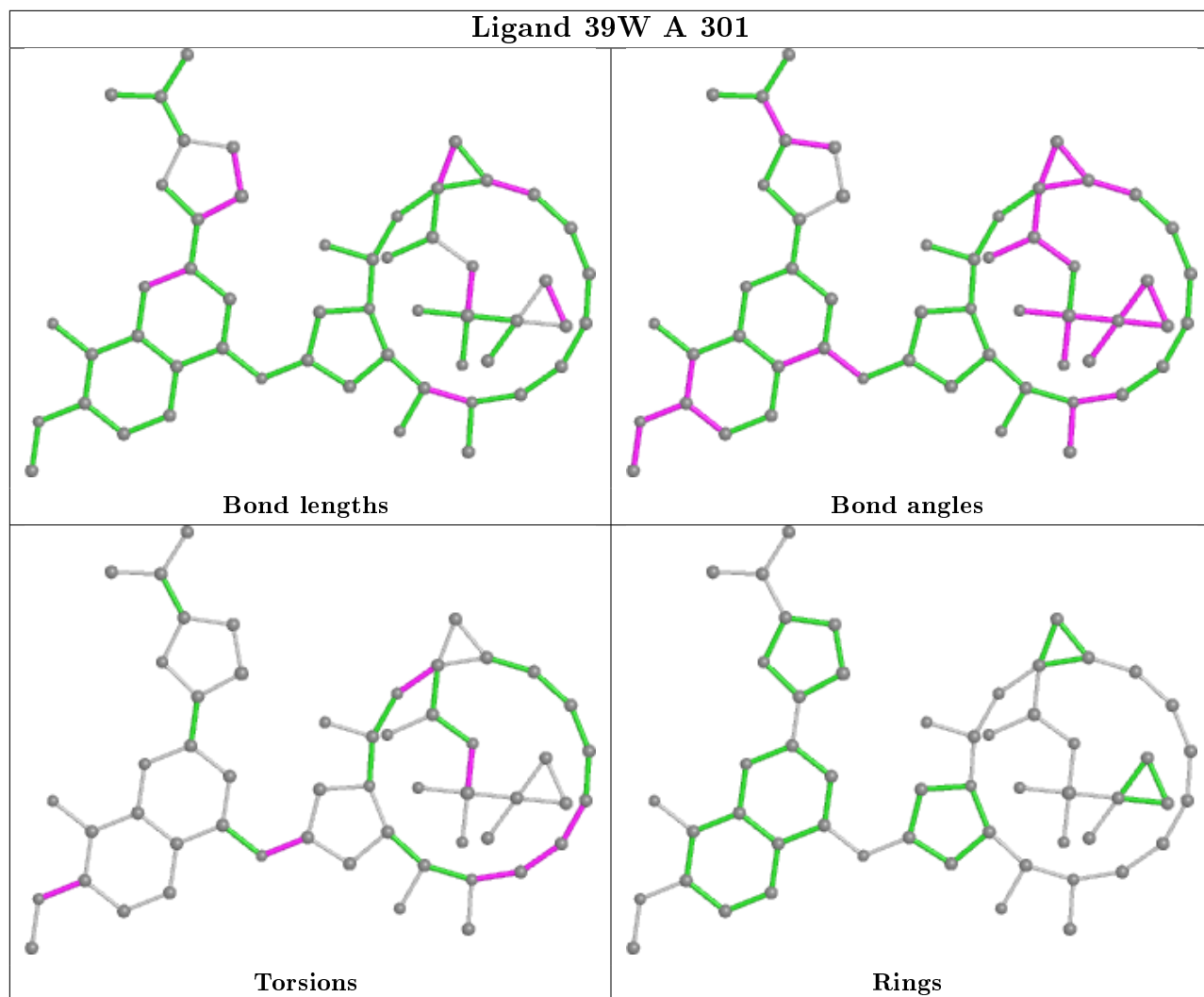
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

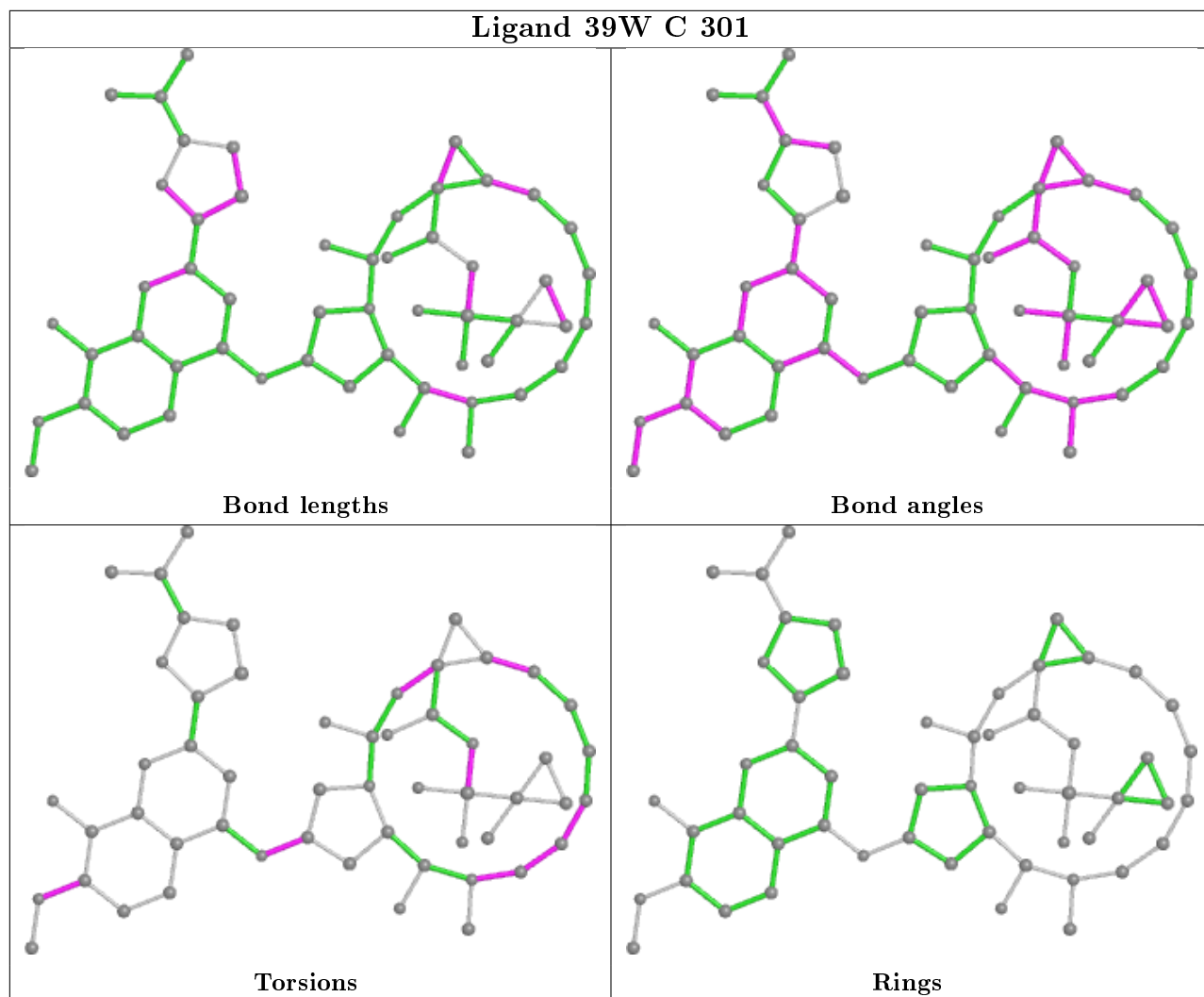
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

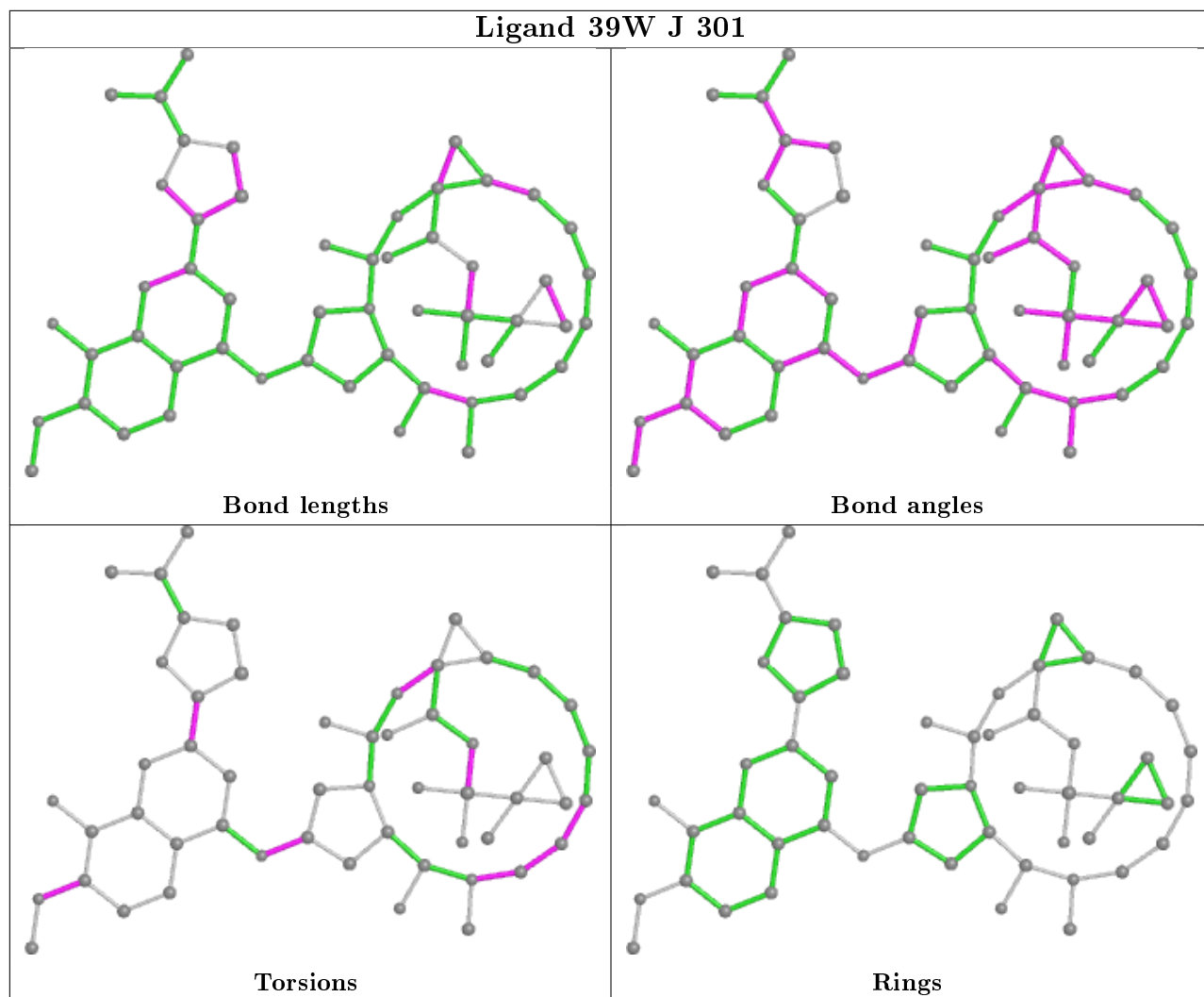


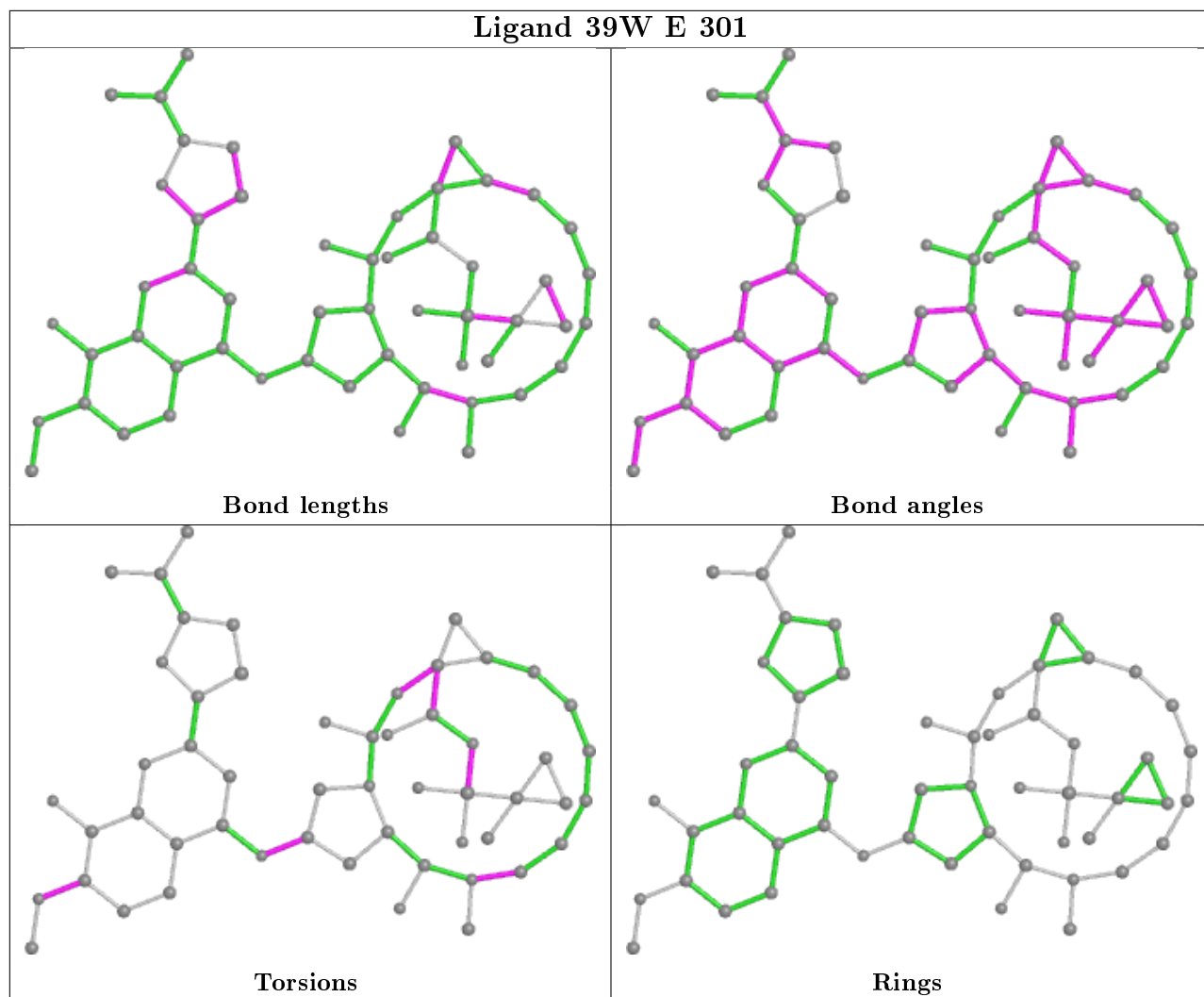


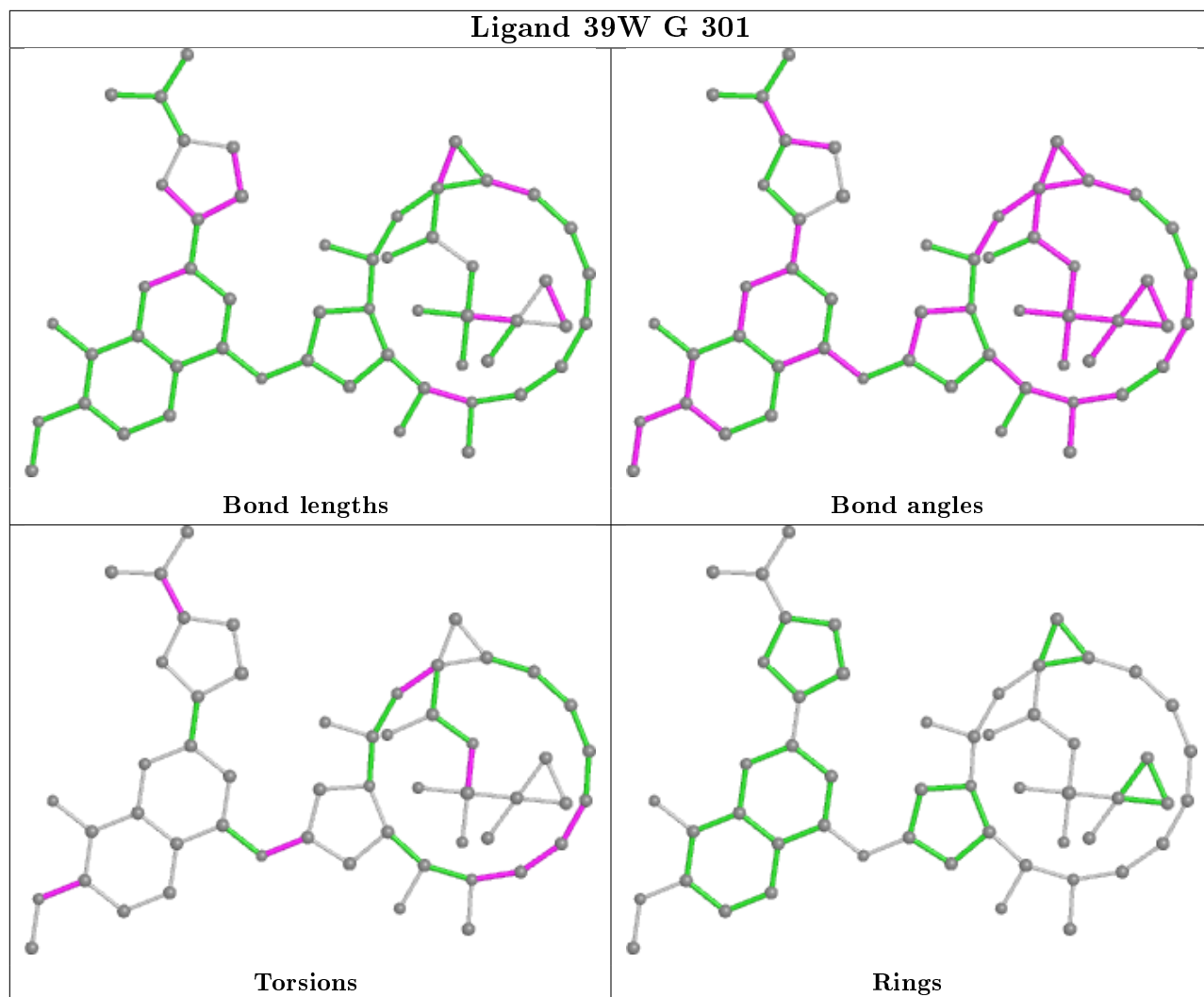


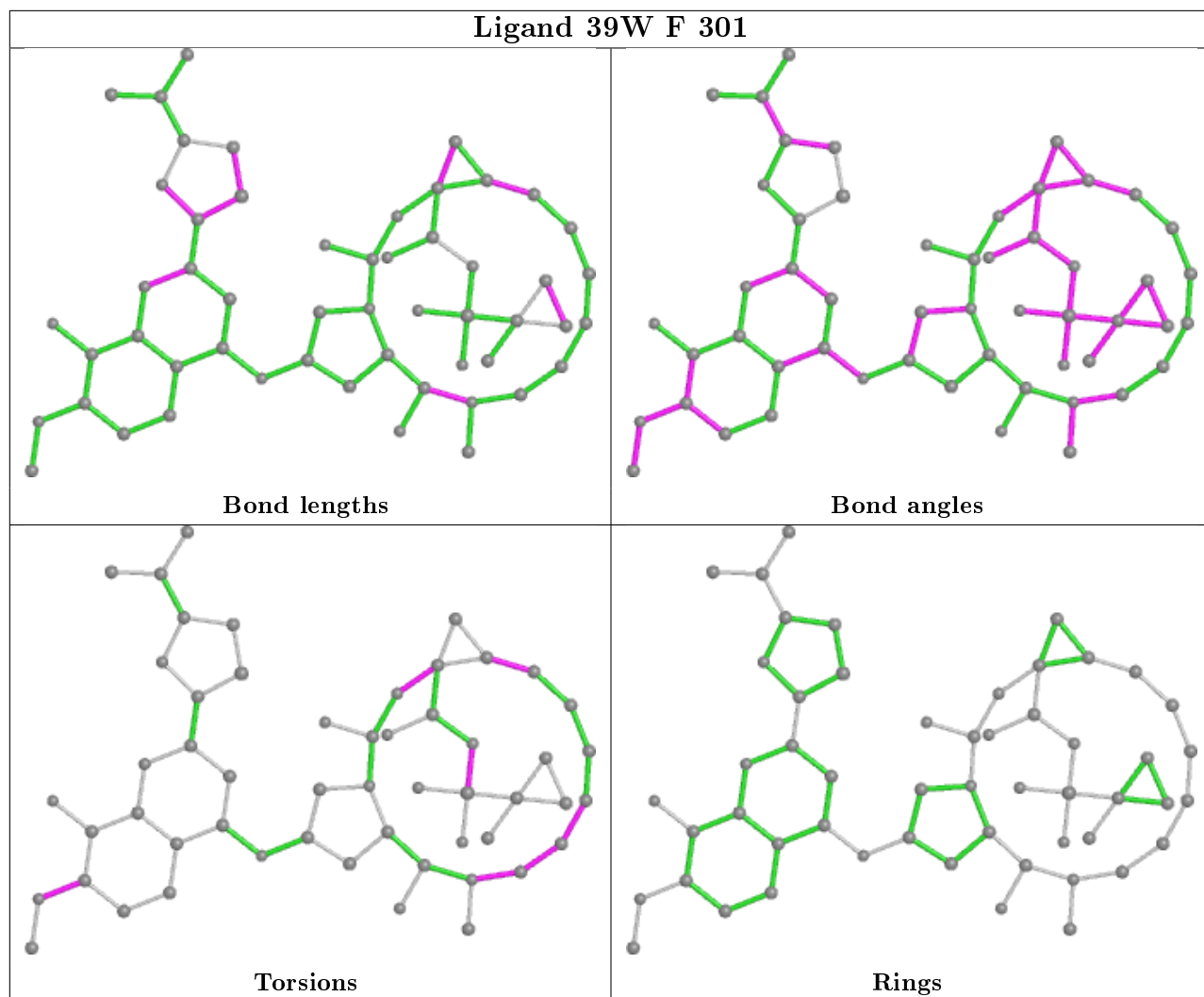


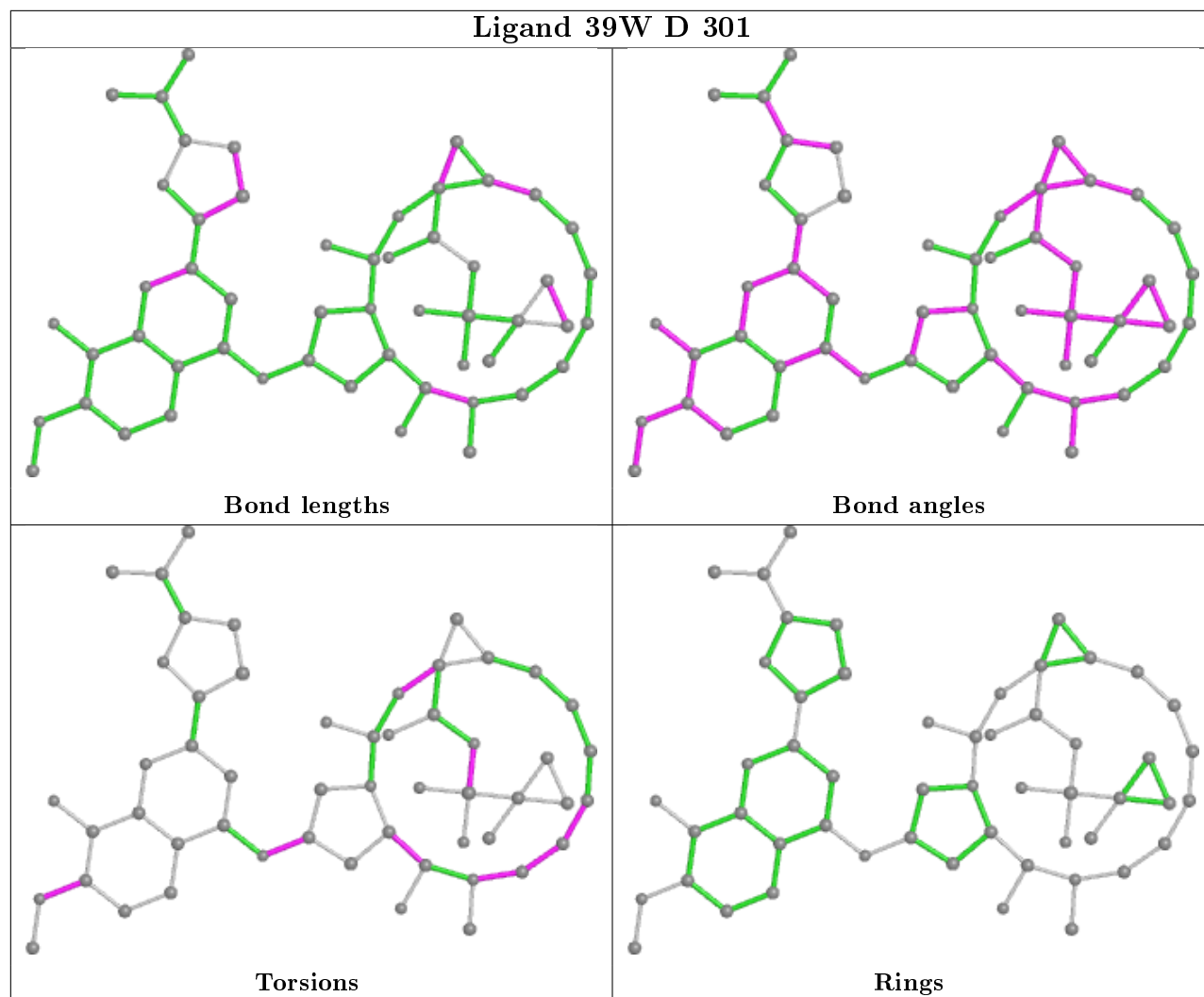












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	182/203 (89%)	0.13	3 (1%) 72 66	40, 63, 100, 127	1 (0%)
1	B	182/203 (89%)	0.42	17 (9%) 8 4	52, 89, 137, 173	0
1	C	182/203 (89%)	0.33	6 (3%) 46 36	51, 88, 123, 176	0
1	D	182/203 (89%)	0.16	6 (3%) 46 36	42, 76, 110, 155	1 (0%)
1	E	182/203 (89%)	0.21	8 (4%) 34 24	52, 81, 125, 147	0
1	F	182/203 (89%)	0.32	6 (3%) 46 36	47, 85, 125, 167	0
1	G	182/203 (89%)	0.16	6 (3%) 46 36	51, 84, 131, 173	0
1	H	182/203 (89%)	0.80	26 (14%) 2 1	70, 106, 146, 187	0
1	J	182/203 (89%)	1.91	74 (40%) 0 0	69, 143, 185, 215	0
2	K	13/16 (81%)	-0.01	0 100 100	45, 59, 79, 95	0
2	L	13/16 (81%)	0.34	0 100 100	50, 68, 99, 118	0
2	M	13/16 (81%)	0.17	0 100 100	57, 64, 104, 126	0
2	N	13/16 (81%)	0.30	1 (7%) 13 7	51, 61, 93, 103	0
2	O	13/16 (81%)	0.27	1 (7%) 13 7	57, 69, 98, 112	0
2	P	13/16 (81%)	0.81	1 (7%) 13 7	78, 95, 115, 118	0
2	Q	13/16 (81%)	0.54	2 (15%) 2 1	57, 67, 98, 121	0
2	T	13/16 (81%)	1.44	3 (23%) 0 0	98, 112, 139, 158	0
2	U	13/16 (81%)	2.41	7 (53%) 0 0	104, 110, 173, 195	0
All	All	1755/1971 (89%)	0.51	167 (9%) 8 4	40, 87, 153, 215	2 (0%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	152	GLY	13.6
1	J	124	GLY	10.9
1	J	113	VAL	10.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1	ALA	9.5
2	U	231	LEU	8.2
1	D	1	ALA	8.0
1	B	1	ALA	7.8
1	J	49	ASN	7.4
1	H	1	ALA	7.4
1	J	182	SER	6.9
1	J	88	PRO	6.8
1	J	106	LEU	6.7
1	H	182	SER	6.4
2	U	230	ILE	6.3
1	J	107	VAL	6.2
1	B	180	ARG	5.7
1	J	167	VAL	5.6
1	J	86	GLN	5.5
1	F	1	ALA	5.5
1	B	2	PRO	5.5
1	J	151	VAL	5.4
1	J	111	ALA	5.3
1	H	8	GLN	5.3
1	C	1	ALA	5.2
1	J	2	PRO	5.0
1	F	180	ARG	5.0
1	J	7	SER	4.9
1	J	95	THR	4.9
1	J	112	ASP	4.9
1	J	173	GLU	4.8
1	C	162	GLY	4.7
1	A	182	SER	4.7
1	J	3	ILE	4.6
1	J	149	HIS	4.4
1	H	164	ALA	4.2
1	J	181	ALA	4.2
1	H	180	ARG	4.2
1	J	142	PRO	4.1
1	J	1	ALA	4.0
1	J	128	SER	4.0
1	G	1	ALA	4.0
1	J	148	GLY	4.0
2	P	220	LYS	4.0
1	J	168	ASP	4.0
1	B	161	ARG	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	J	53	TRP	3.8
1	J	150	ALA	3.7
1	J	127	LEU	3.7
1	J	91	ALA	3.7
1	H	177	THR	3.7
1	J	45	ALA	3.6
1	H	24	ARG	3.6
1	H	132	VAL	3.5
1	B	113	VAL	3.5
1	D	182	SER	3.5
1	F	161	ARG	3.4
1	J	123	ARG	3.4
2	U	227	GLY	3.4
1	H	134	TYR	3.4
1	H	178	THR	3.4
1	J	108	THR	3.3
1	J	143	LEU	3.3
2	U	229	ILE	3.2
1	J	159	CYS	3.2
1	H	12	GLY	3.2
1	J	30	GLU	3.2
1	J	121	ASP	3.2
1	B	177	THR	3.2
1	H	161	ARG	3.2
1	H	163	VAL	3.2
1	E	175	MET	3.1
1	D	161	ARG	3.1
2	T	227	GLY	3.1
1	E	1	ALA	3.1
1	J	147	SER	3.0
1	B	162	GLY	3.0
1	J	170	VAL	3.0
1	J	129	PRO	3.0
1	J	52	CYS	3.0
1	J	18	ILE	3.0
1	J	126	LEU	3.0
1	B	176	GLU	3.0
1	G	105	TYR	2.9
1	J	75	TYR	2.9
1	J	175	MET	2.9
1	J	90	GLY	2.9
1	J	131	PRO	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	T	231	LEU	2.9
1	J	92	ARG	2.8
1	J	32	GLU	2.8
1	F	176	GLU	2.8
1	H	75	TYR	2.8
1	H	32	GLU	2.8
1	H	69	GLY	2.8
1	J	153	ILE	2.8
1	J	27	ASN	2.8
1	B	182	SER	2.8
1	H	21	LEU	2.7
1	J	51	VAL	2.7
1	H	179	MET	2.7
1	J	130	ARG	2.7
1	C	161	ARG	2.7
1	F	98	THR	2.6
1	E	114	ILE	2.6
1	C	92	ARG	2.6
1	E	2	PRO	2.6
1	J	115	PRO	2.6
1	J	134	TYR	2.6
1	B	98	THR	2.5
1	J	163	VAL	2.5
1	E	117	ARG	2.5
1	J	103	ASP	2.5
2	N	220	LYS	2.5
1	J	135	LEU	2.5
1	B	164	ALA	2.5
1	D	162	GLY	2.5
1	H	162	GLY	2.5
2	U	226	VAL	2.5
1	J	114	ILE	2.5
1	H	151	VAL	2.5
1	J	161	ARG	2.5
2	O	220	LYS	2.5
2	Q	231	LEU	2.5
1	G	2	PRO	2.4
1	E	180	ARG	2.4
2	U	232	SER	2.4
1	J	48	VAL	2.4
1	H	84	GLY	2.3
1	H	2	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	117	ARG	2.3
1	G	98	THR	2.3
1	G	182	SER	2.3
1	H	119	ARG	2.3
1	H	150	ALA	2.3
1	J	24	ARG	2.3
1	J	68	LYS	2.3
1	E	182	SER	2.2
1	D	2	PRO	2.2
1	D	180	ARG	2.2
1	C	88	PRO	2.2
1	J	80	GLN	2.2
1	A	134	TYR	2.2
1	H	28	GLN	2.2
1	B	150	ALA	2.2
1	G	179	MET	2.2
2	T	221	GLY	2.1
1	H	68	LYS	2.1
1	J	179	MET	2.1
1	B	75	TYR	2.1
1	J	144	LEU	2.1
1	B	123	ARG	2.1
1	J	8	GLN	2.1
1	C	182	SER	2.1
1	J	71	ILE	2.1
1	B	117	ARG	2.1
1	J	96	PRO	2.1
1	J	31	GLY	2.1
1	F	30	GLU	2.1
1	E	177	THR	2.1
2	Q	230	ILE	2.1
1	J	122	SER	2.0
2	U	225	ILE	2.0
1	B	97	CYS	2.0
1	J	89	PRO	2.0
1	B	99	CYS	2.0
1	J	28	GLN	2.0
1	J	85	TRP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

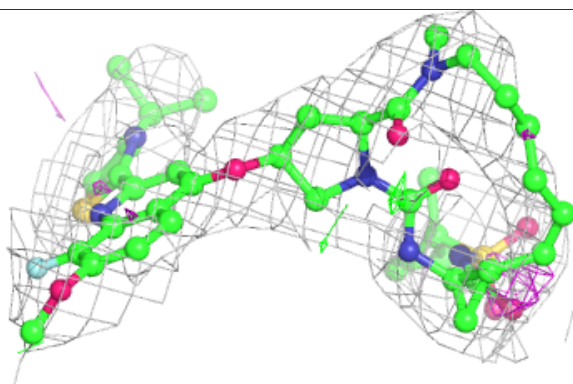
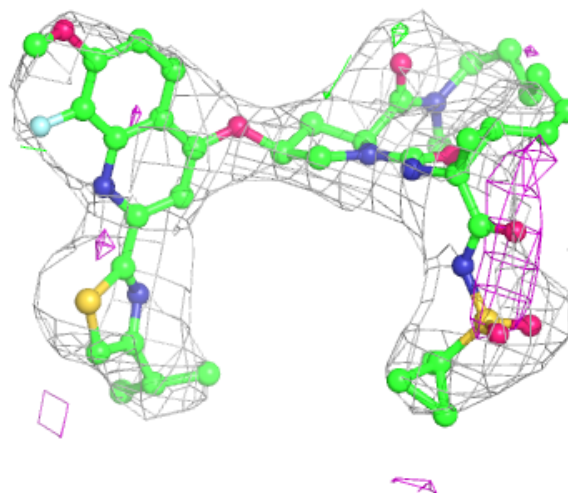
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

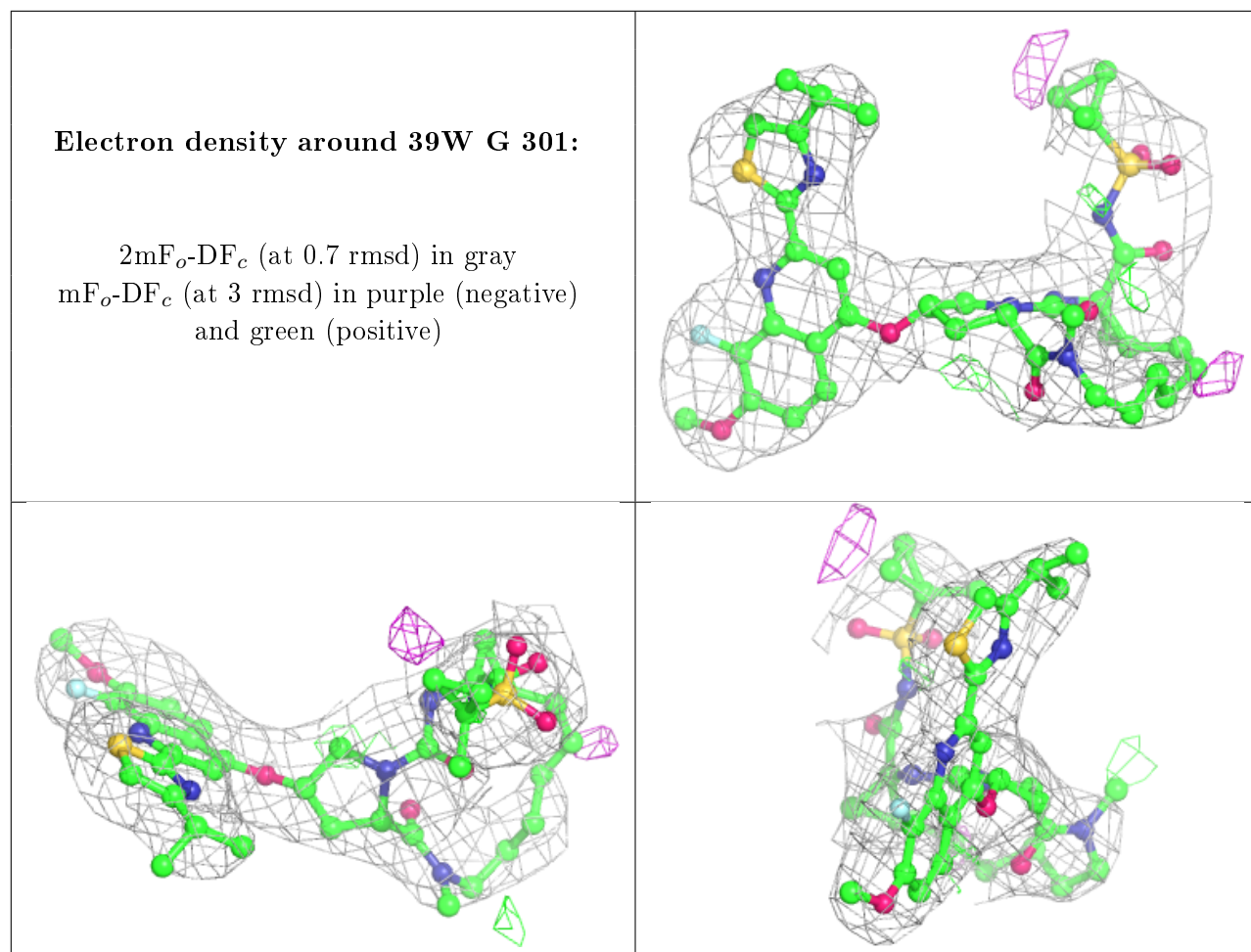
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	CL	D	303	1/1	0.42	0.27	97,97,97,97	0
4	ZN	J	302	1/1	0.67	0.07	314,314,314,314	0
5	CL	G	303	1/1	0.82	0.27	81,81,81,81	0
4	ZN	C	302	1/1	0.82	0.16	127,127,127,127	0
5	CL	B	303	1/1	0.85	0.17	76,76,76,76	0
4	ZN	D	302	1/1	0.86	0.14	87,87,87,87	0
4	ZN	H	302	1/1	0.87	0.14	114,114,114,114	0
4	ZN	B	302	1/1	0.89	0.13	117,117,117,117	0
3	39W	J	301	53/53	0.91	0.20	67,74,77,79	0
5	CL	E	303	1/1	0.92	0.25	91,91,91,91	0
4	ZN	E	302	1/1	0.93	0.10	141,141,141,141	0
3	39W	G	301	53/53	0.95	0.20	57,62,66,70	0
3	39W	H	301	53/53	0.96	0.20	55,62,67,70	0
3	39W	A	301	53/53	0.96	0.21	47,54,63,64	0
3	39W	B	301	53/53	0.96	0.17	56,62,65,68	0
3	39W	E	301	53/53	0.96	0.20	48,63,65,67	0
4	ZN	A	302	1/1	0.96	0.18	89,89,89,89	0
3	39W	F	301	53/53	0.96	0.20	54,59,64,66	0
4	ZN	F	302	1/1	0.97	0.18	93,93,93,93	0
3	39W	C	301	53/53	0.97	0.18	53,60,63,66	0
4	ZN	G	302	1/1	0.97	0.16	115,115,115,115	0
3	39W	D	301	53/53	0.98	0.20	47,55,62,65	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 39W J 301:**

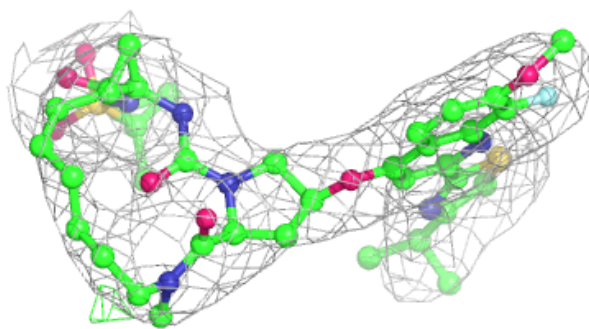
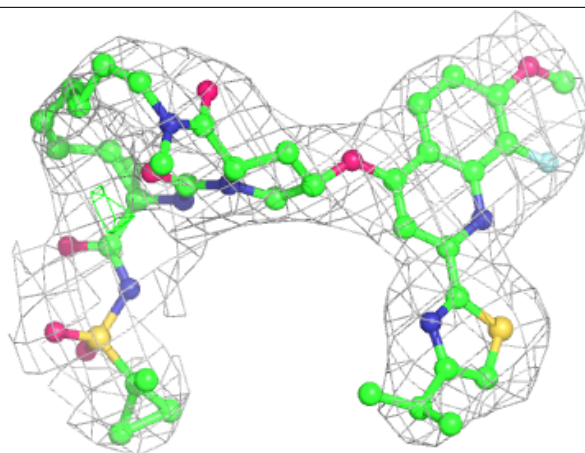
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around 39W H 301:**

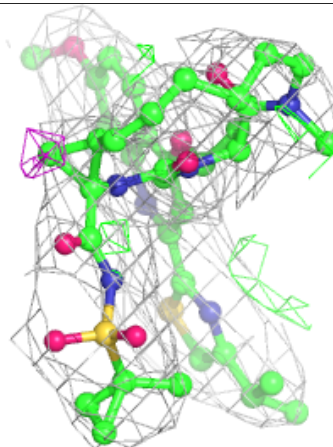
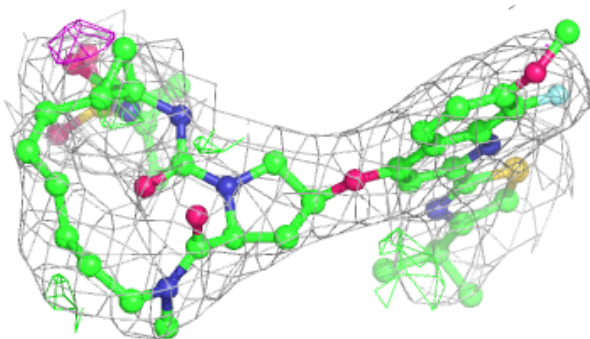
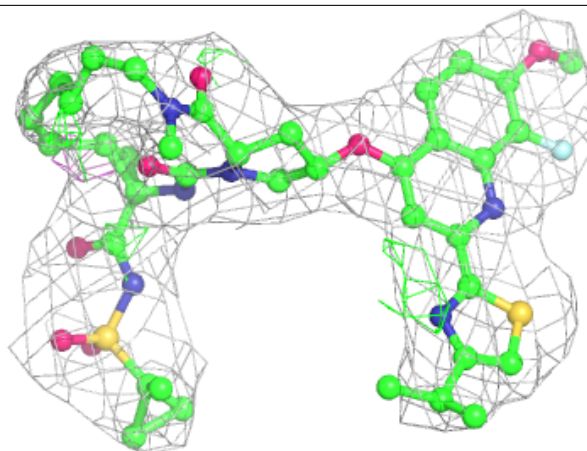
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





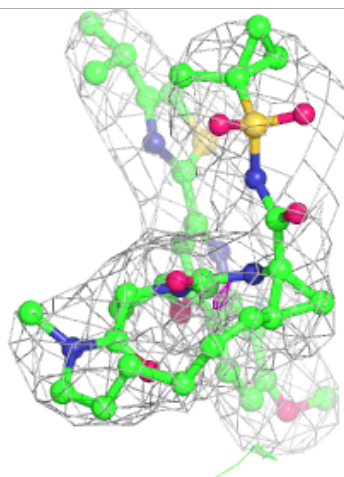
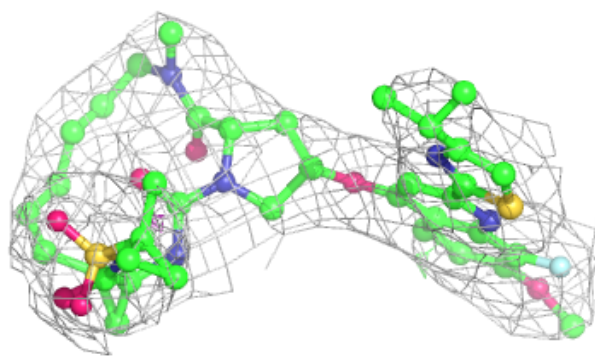
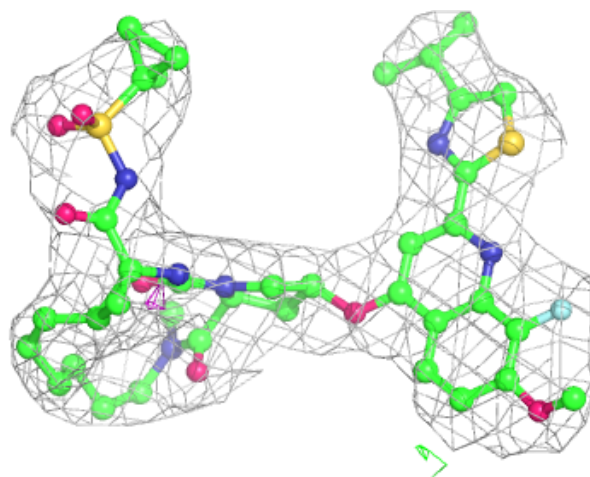
**Electron density around 39W A 301:**

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



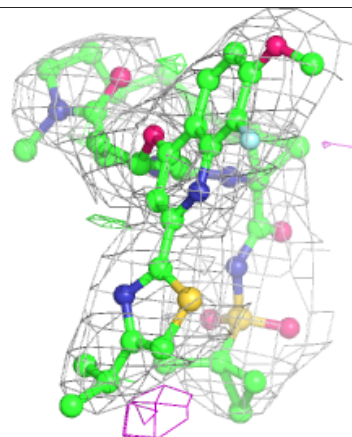
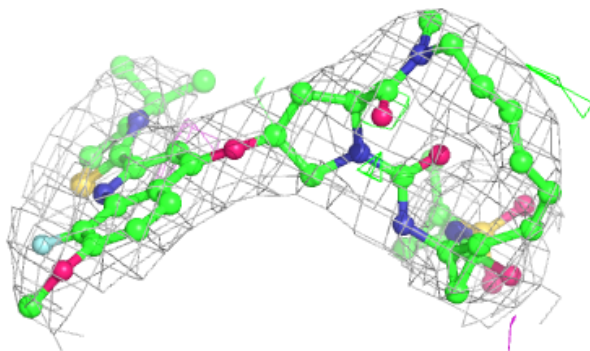
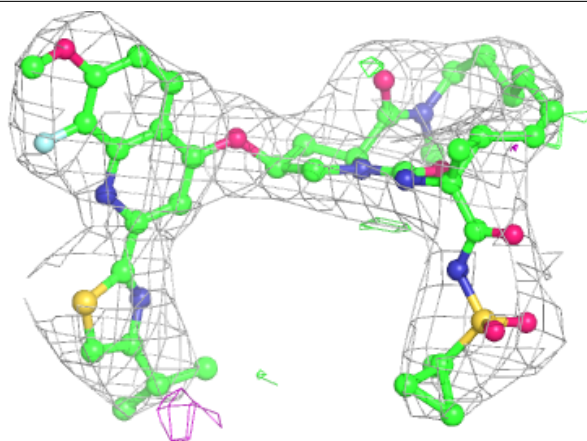
**Electron density around 39W B 301:**

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



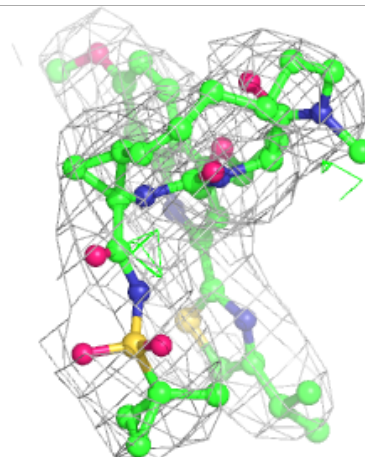
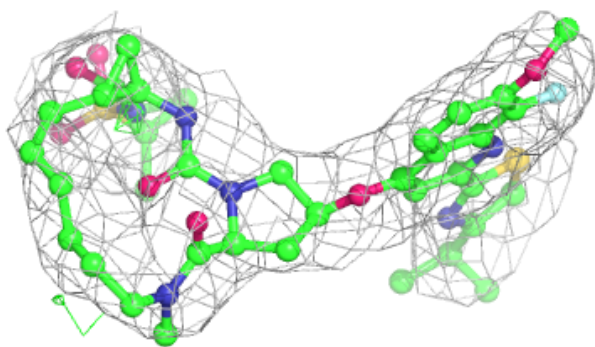
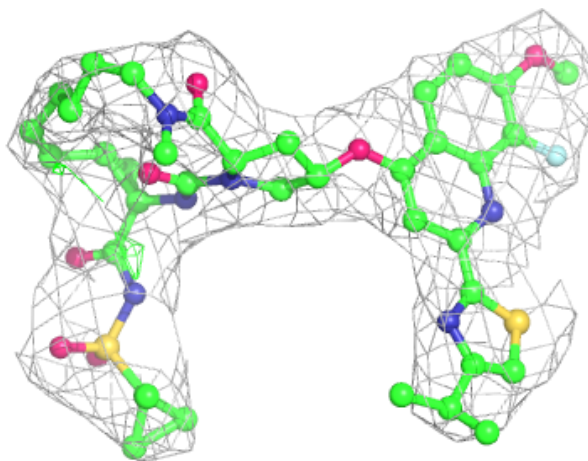
**Electron density around 39W E 301:**

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



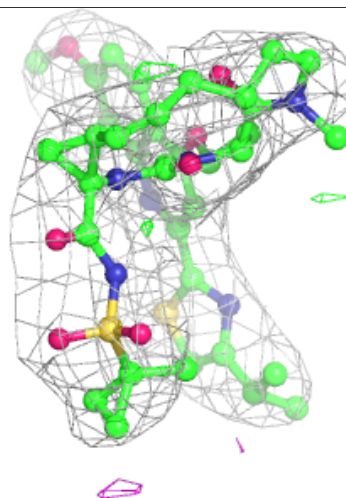
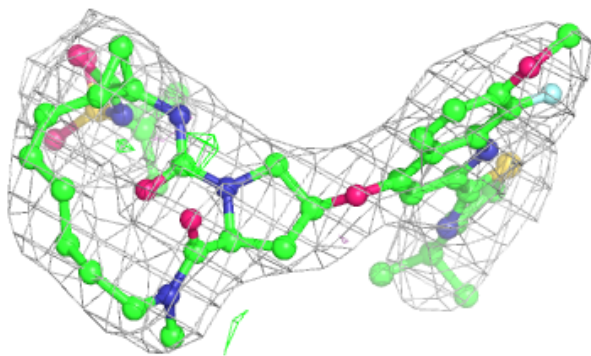
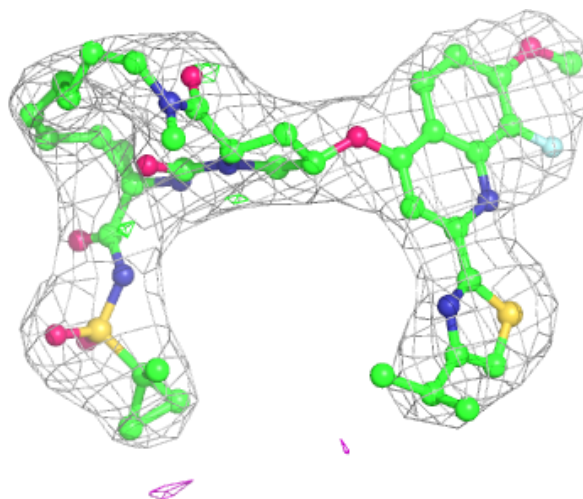
**Electron density around 39W F 301:**

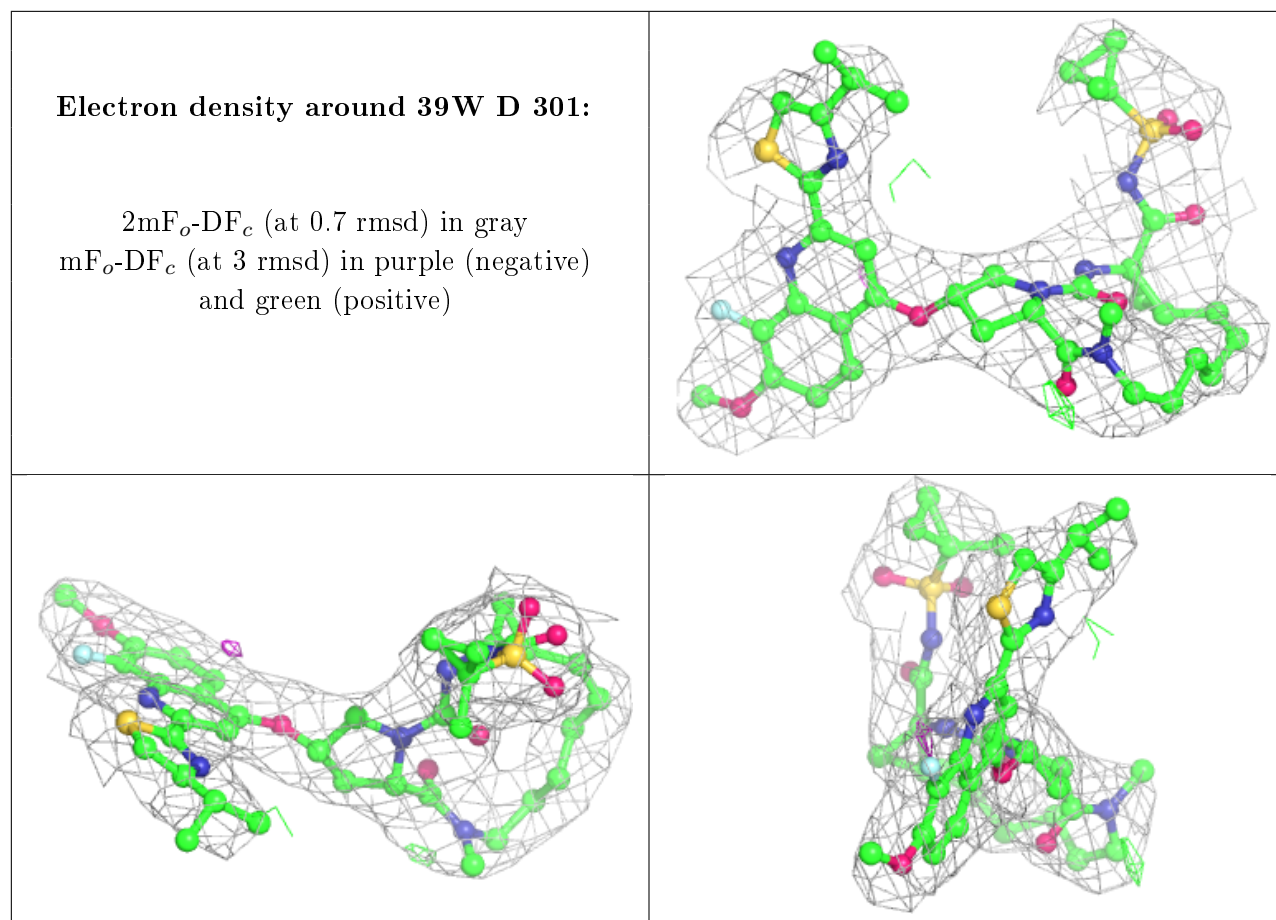
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 39W C 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.