



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 11:11 AM EDT

PDB ID : 5DL1  
Title : ClpP from Staphylococcus aureus in complex with AV145  
Authors : Vielberg, M.-T.; Groll, M.  
Deposited on : 2015-09-04  
Resolution : 3.00 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.

The types of validation reports are described at

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

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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 : 2.37.1  
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) : 2.37.1

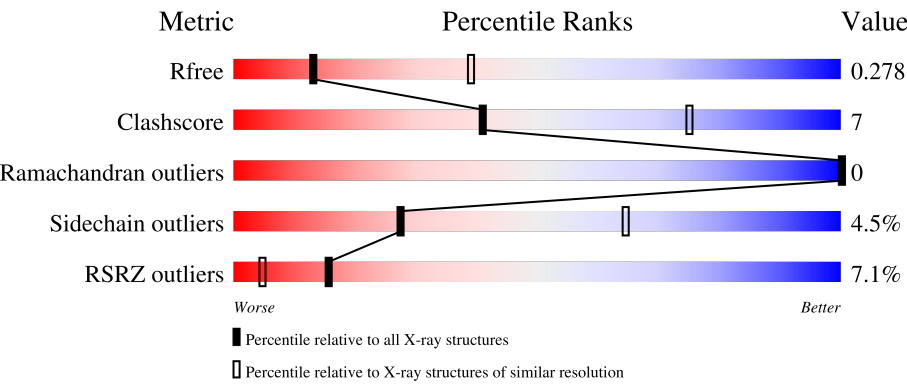
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.






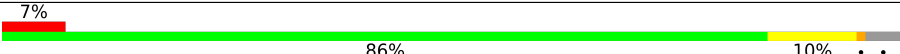
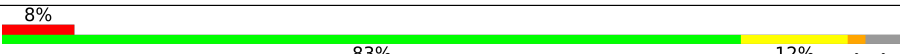
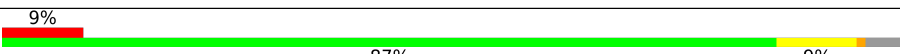
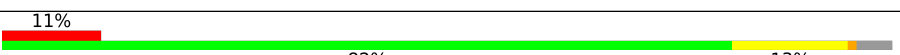
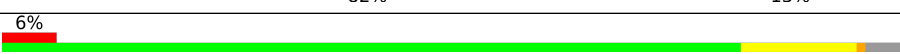

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	195	<div><div>3%</div><div>84%</div><div>11%</div><div>..</div></div>
1	B	195	<div><div>6%</div><div>83%</div><div>12%</div><div>..</div></div>
1	C	195	<div><div>8%</div><div>81%</div><div>14%</div><div>..</div></div>
1	D	195	<div><div>9%</div><div>83%</div><div>13%</div><div>..</div></div>
1	E	195	<div><div>8%</div><div>84%</div><div>11%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain	
1	F	195		..
1	G	195		..
1	H	195		..
1	I	195		..
1	J	195		..
1	K	195		..
1	L	195		..
1	M	195		..
1	N	195		..

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
2	5C2	A	201	-	-	X	-
2	5C2	C	201	-	-	X	-

## 2 Entry composition

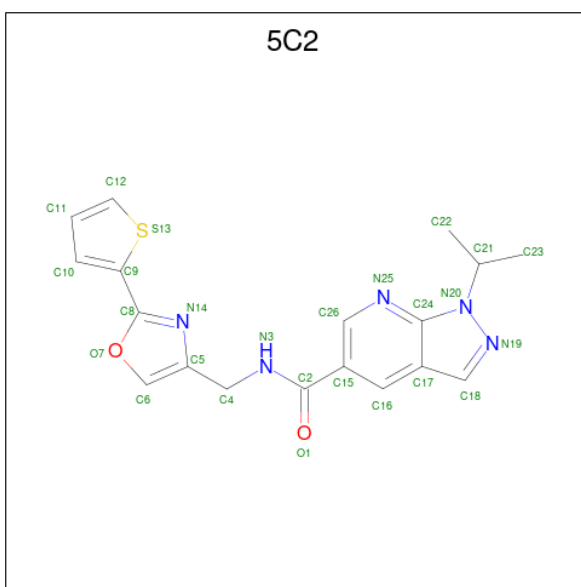
There are 2 unique types of molecules in this entry. The entry contains 20706 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	B	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	C	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	D	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	E	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	F	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	G	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	H	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	I	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	J	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	K	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	L	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	M	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			
1	N	188	Total	C	N	O	S	0	0	0
			1453	915	246	286	6			

- Molecule 2 is 1-(propan-2-yl)-N-{[2-(thiophen-2-yl)-1,3-oxazol-4-yl]methyl}-1H-pyrazolo[3,4-b]pyridine-5-carboxamide (three-letter code: 5C2) (formula: C<sub>18</sub>H<sub>17</sub>N<sub>5</sub>O<sub>2</sub>S).

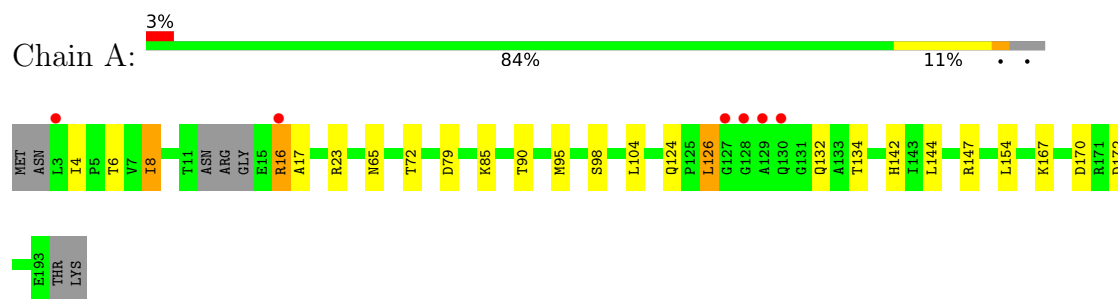


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	B	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	C	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	D	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	E	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	F	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	G	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	H	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	I	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	J	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	K	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	L	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	M	1	Total 26	C 18	N 5	O 2	S 1	0	0
2	N	1	Total 26	C 18	N 5	O 2	S 1	0	0

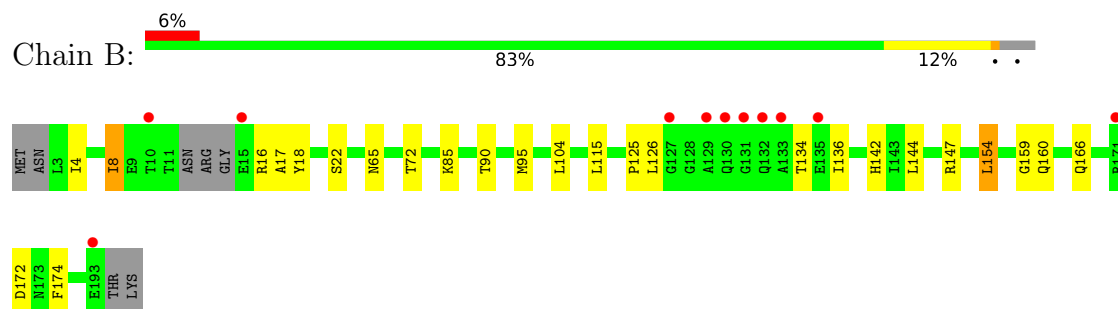
### 3 Residue-property plots [i](#)

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.

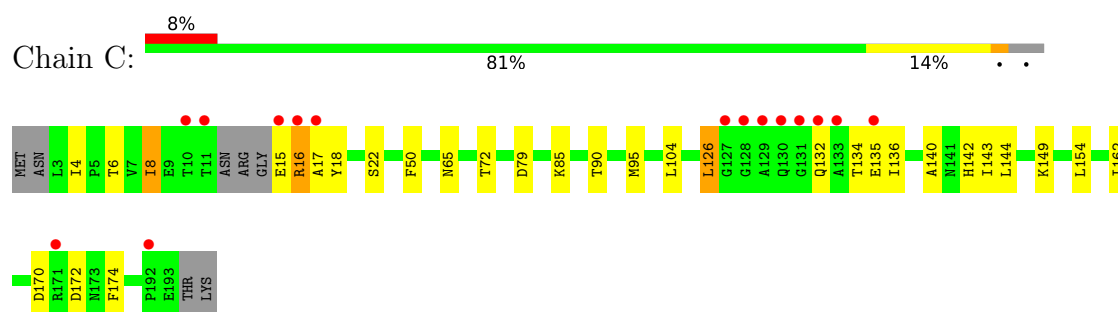
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



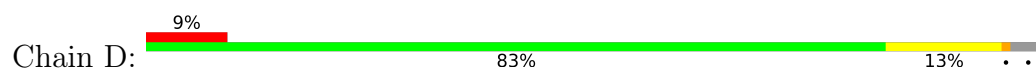
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

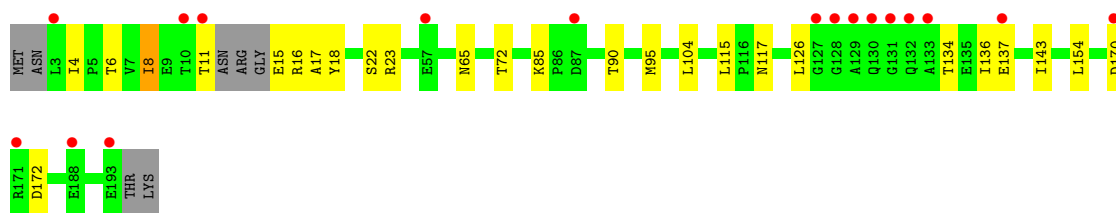


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

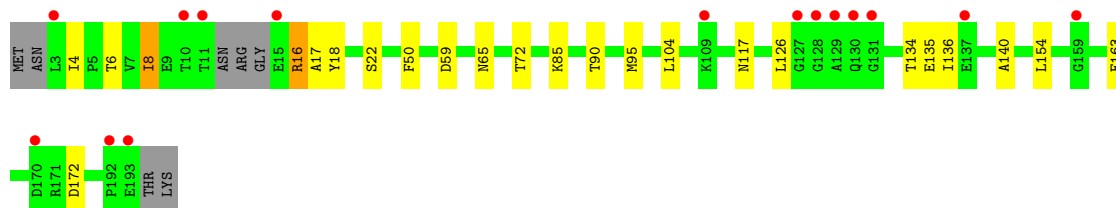
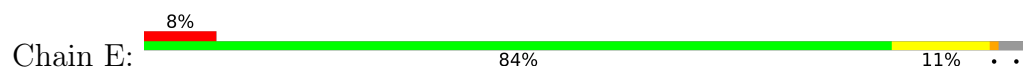


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

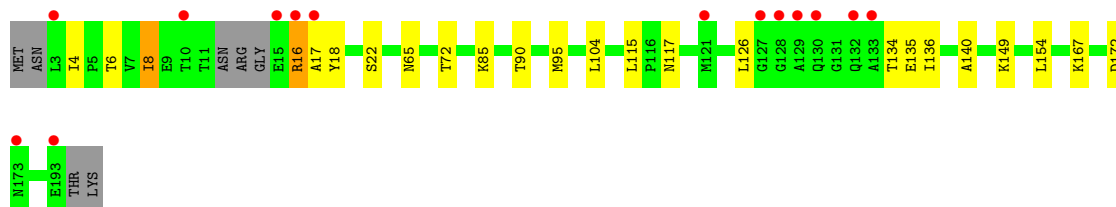
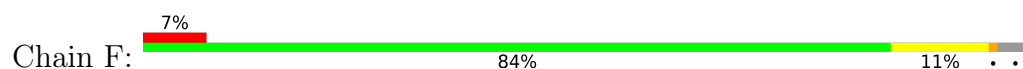




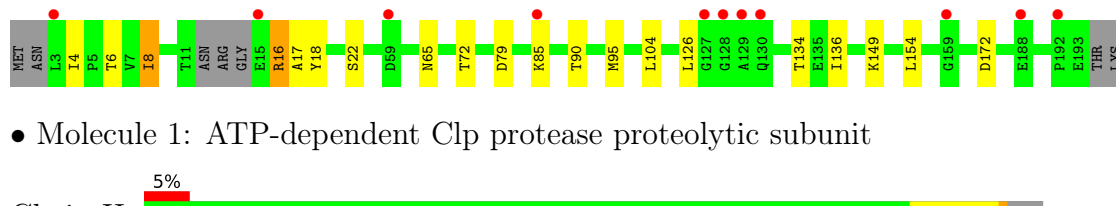
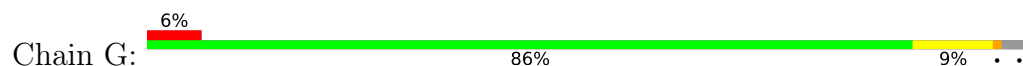
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



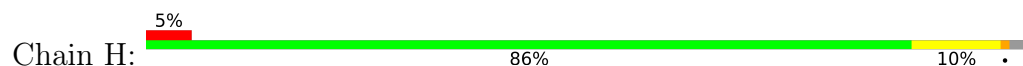
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



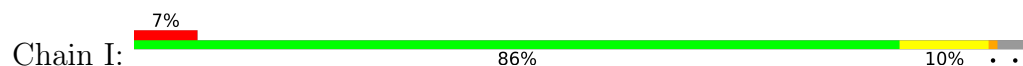
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



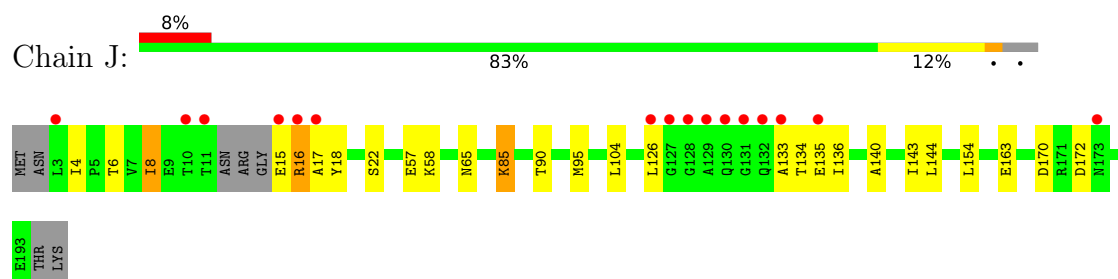
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



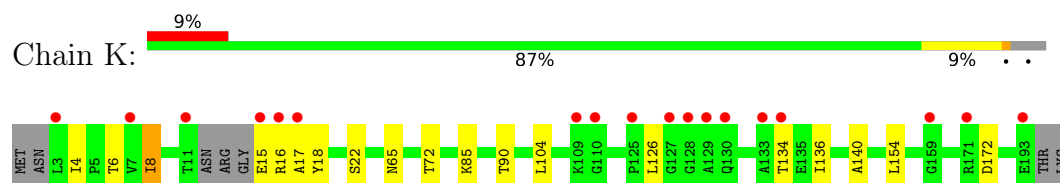
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



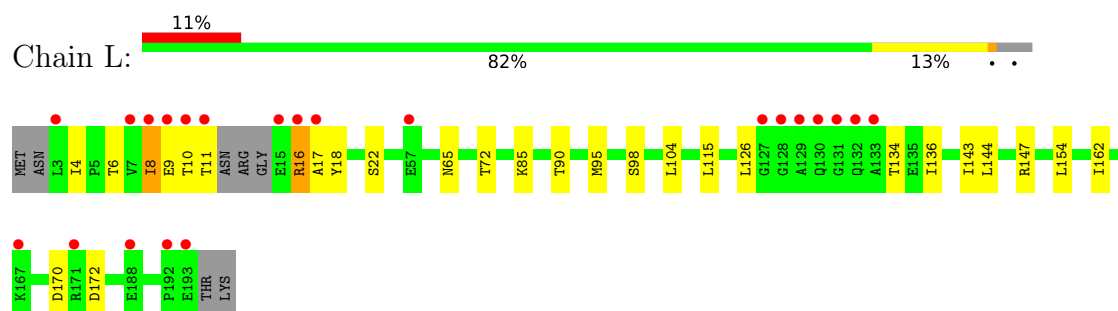
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



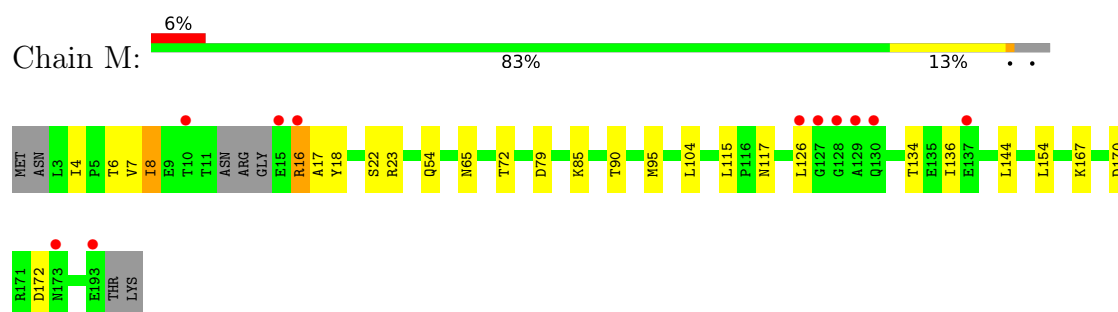
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



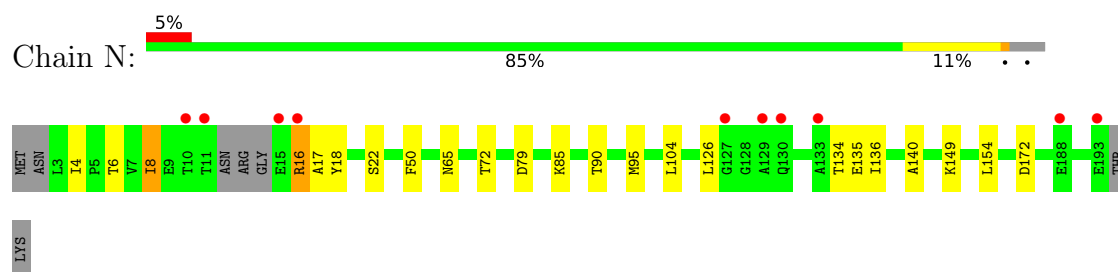
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.82Å 97.75Å 131.95Å 90.00° 95.49° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 14.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-3.00) 99.3 (14.99-3.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.252 , 0.274 0.243 , 0.278	Depositor DCC
$R_{free}$ test set	2828 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.4	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.68% 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: 5C2

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	0.27	0/1471	0.45	0/1986
1	B	0.28	0/1471	0.46	0/1986
1	C	0.27	0/1471	0.45	0/1986
1	D	0.27	0/1471	0.45	0/1986
1	E	0.28	0/1471	0.46	0/1986
1	F	0.27	0/1471	0.45	0/1986
1	G	0.26	0/1471	0.45	0/1986
1	H	0.27	0/1471	0.45	0/1986
1	I	0.28	0/1471	0.45	0/1986
1	J	0.35	0/1471	0.46	0/1986
1	K	0.27	0/1471	0.45	0/1986
1	L	0.35	0/1471	0.47	0/1986
1	M	0.28	0/1471	0.45	0/1986
1	N	0.27	0/1471	0.45	0/1986
All	All	0.28	0/20594	0.45	0/27804

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	1453	0	1468	42	1
1	B	1453	0	1468	28	8
1	C	1453	0	1468	67	2
1	D	1453	0	1468	28	4
1	E	1453	0	1468	37	5
1	F	1453	0	1468	32	3
1	G	1453	0	1468	20	0
1	H	1453	0	1468	25	2
1	I	1453	0	1468	27	4
1	J	1453	0	1468	66	34
1	K	1453	0	1468	23	0
1	L	1453	0	1468	35	33
1	M	1453	0	1468	41	8
1	N	1453	0	1468	42	0
2	A	26	0	17	11	0
2	B	26	0	17	3	0
2	C	26	0	17	14	0
2	D	26	0	17	3	0
2	E	26	0	17	3	0
2	F	26	0	17	1	0
2	G	26	0	17	0	0
2	H	26	0	17	0	0
2	I	26	0	17	2	0
2	J	26	0	17	4	0
2	K	26	0	17	1	0
2	L	26	0	17	3	0
2	M	26	0	17	3	0
2	N	26	0	17	0	0
All	All	20706	0	20790	296	52

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 7.

All (296) 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)
2:C:201:5C2:C4	1:J:136:ILE:HG13	1.80	1.10
1:C:132:GLN:HE22	2:C:201:5C2:H8	1.11	1.08
2:C:201:5C2:N3	1:J:136:ILE:HG13	1.68	1.07
1:C:18:TYR:CZ	1:D:8:ILE:HD13	1.90	1.05
1:F:172:ASP:OD2	1:G:134:THR:OG1	1.74	1.04
1:M:8:ILE:HD13	1:N:18:TYR:CZ	1.95	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:ASP:OD2	1:F:134:THR:OG1	1.80	0.99
1:A:8:ILE:HD13	1:E:18:TYR:CZ	1.97	0.98
1:A:134:THR:OG1	1:B:172:ASP:OD2	1.81	0.98
1:L:172:ASP:OD2	1:M:134:THR:OG1	1.85	0.94
1:M:172:ASP:OD2	1:N:134:THR:OG1	1.84	0.94
1:J:18:TYR:CZ	1:K:8:ILE:HD13	2.05	0.92
1:C:136:ILE:HG13	2:J:201:5C2:N3	1.86	0.90
1:B:72:THR:HG21	1:C:95:MET:HE1	1.53	0.89
1:H:134:THR:OG1	1:I:172:ASP:OD2	1.91	0.88
1:D:134:THR:OG1	1:G:172:ASP:OD2	1.93	0.87
1:M:8:ILE:CD1	1:N:18:TYR:CZ	2.58	0.86
1:C:140:ALA:HB1	1:J:140:ALA:O	1.78	0.84
1:C:18:TYR:CZ	1:D:8:ILE:CD1	2.60	0.84
2:C:201:5C2:H2	1:J:136:ILE:HG13	1.59	0.84
1:E:8:ILE:HD13	1:F:18:TYR:CZ	2.14	0.82
1:M:6:THR:N	1:N:22:SER:OG	2.11	0.82
1:I:134:THR:OG1	1:J:172:ASP:OD2	1.98	0.82
1:C:22:SER:OG	1:D:6:THR:N	2.13	0.81
1:A:8:ILE:CD1	1:E:18:TYR:CZ	2.64	0.81
1:C:170:ASP:OD2	1:J:135:GLU:HG3	1.81	0.81
2:C:201:5C2:N3	1:J:136:ILE:CG1	2.44	0.81
1:K:134:THR:OG1	1:N:172:ASP:OD2	1.98	0.80
1:C:140:ALA:O	1:J:140:ALA:HB1	1.81	0.80
1:B:72:THR:HG21	1:C:95:MET:CE	2.12	0.79
1:A:172:ASP:OD2	1:E:134:THR:OG1	2.01	0.79
1:C:18:TYR:CE2	1:D:8:ILE:HD11	2.17	0.79
2:A:201:5C2:C4	1:N:136:ILE:HG13	2.15	0.77
1:C:132:GLN:NE2	2:C:201:5C2:H8	1.96	0.77
1:E:136:ILE:HG13	2:M:201:5C2:C4	2.15	0.77
1:C:18:TYR:CE1	1:D:8:ILE:HD13	2.20	0.76
1:H:172:ASP:OD2	1:L:134:THR:OG1	2.01	0.76
1:I:18:TYR:CZ	1:J:8:ILE:HD13	2.19	0.76
1:J:16:ARG:HG2	1:K:8:ILE:HG13	1.67	0.76
1:A:6:THR:N	1:E:22:SER:OG	2.13	0.75
2:E:201:5C2:C4	1:M:136:ILE:HG13	2.17	0.75
1:H:6:THR:H	1:L:22:SER:HG	1.35	0.75
1:A:6:THR:H	1:E:22:SER:HG	1.31	0.75
1:M:6:THR:H	1:N:22:SER:HG	1.28	0.75
1:C:136:ILE:HG13	2:J:201:5C2:C4	2.16	0.74
1:B:134:THR:OG1	1:C:172:ASP:OD2	2.04	0.74
1:J:22:SER:OG	1:K:6:THR:N	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:SER:O	2:A:201:5C2:H16	1.88	0.74
1:H:8:ILE:HD13	1:L:18:TYR:CZ	2.23	0.74
1:A:147:ARG:HD3	1:N:136:ILE:CG2	2.19	0.73
1:C:18:TYR:CE2	1:D:8:ILE:CD1	2.70	0.73
1:E:6:THR:H	1:F:22:SER:HG	1.37	0.72
1:C:144:LEU:HD13	1:J:140:ALA:CB	2.20	0.71
1:C:136:ILE:HG23	1:J:143:ILE:HG23	1.72	0.71
1:C:134:THR:OG1	1:D:172:ASP:OD2	2.07	0.71
2:C:201:5C2:C4	1:J:136:ILE:CG1	2.65	0.71
1:C:140:ALA:HB2	1:J:143:ILE:HB	1.73	0.70
1:C:22:SER:HB3	1:D:6:THR:O	1.91	0.69
1:M:8:ILE:HD13	1:N:18:TYR:OH	1.90	0.69
1:C:16:ARG:HG2	1:D:8:ILE:HG13	1.74	0.69
1:E:8:ILE:CD1	1:F:18:TYR:CZ	2.76	0.69
1:C:143:ILE:HG23	1:J:136:ILE:HG23	1.75	0.69
1:J:16:ARG:HG2	1:K:8:ILE:CG1	2.24	0.68
1:C:143:ILE:CG2	1:J:136:ILE:HG23	2.24	0.68
1:F:8:ILE:HD13	1:G:18:TYR:CZ	2.27	0.68
1:I:22:SER:HG	1:J:6:THR:H	1.41	0.68
2:D:201:5C2:C4	1:I:136:ILE:HG13	2.24	0.68
1:A:8:ILE:HG13	1:E:16:ARG:HG2	1.75	0.67
1:A:72:THR:HG21	1:B:95:MET:CE	2.24	0.67
1:J:18:TYR:CZ	1:K:8:ILE:CD1	2.77	0.66
1:B:18:TYR:CZ	1:C:8:ILE:HD13	2.31	0.66
1:C:144:LEU:CD1	1:J:140:ALA:HB3	2.26	0.66
1:L:8:ILE:HD13	1:M:18:TYR:CZ	2.30	0.66
1:B:136:ILE:HG13	2:K:201:5C2:C4	2.26	0.65
1:A:124:GLN:N	2:A:201:5C2:S13	2.70	0.65
1:J:22:SER:HB3	1:K:6:THR:O	1.96	0.65
1:M:8:ILE:CD1	1:N:18:TYR:CE2	2.80	0.65
1:C:135:GLU:HG3	1:J:170:ASP:OD2	1.97	0.65
1:A:147:ARG:HD3	1:N:136:ILE:HG21	1.79	0.65
1:A:8:ILE:HD11	1:E:18:TYR:CE2	2.32	0.64
2:A:201:5C2:H2	1:N:136:ILE:HG13	1.79	0.64
1:J:134:THR:OG1	1:K:172:ASP:OD2	2.15	0.64
1:A:8:ILE:CD1	1:E:18:TYR:CE2	2.81	0.64
1:C:142:HIS:CD2	2:C:201:5C2:H13	2.32	0.64
1:C:144:LEU:HD13	1:J:140:ALA:HB3	1.77	0.64
1:B:22:SER:HG	1:C:6:THR:H	1.42	0.64
1:J:18:TYR:CE2	1:K:8:ILE:HD11	2.33	0.63
2:C:201:5C2:N3	1:J:136:ILE:CD1	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:18:TYR:CE2	1:K:8:ILE:CD1	2.82	0.63
1:M:8:ILE:HG13	1:N:16:ARG:HG2	1.80	0.62
1:M:23:ARG:HG2	1:N:50:PHE:CE1	2.35	0.61
1:H:72:THR:HG21	1:I:95:MET:CE	2.30	0.61
1:C:136:ILE:HG13	2:J:201:5C2:C2	2.31	0.61
1:I:18:TYR:CZ	1:J:8:ILE:CD1	2.84	0.61
1:A:72:THR:HG21	1:B:95:MET:HE1	1.81	0.61
1:C:136:ILE:HG23	1:J:143:ILE:CG2	2.31	0.61
1:C:140:ALA:O	1:J:140:ALA:CB	2.49	0.61
1:E:136:ILE:HG13	2:M:201:5C2:H2	1.83	0.60
1:C:136:ILE:CG2	1:J:143:ILE:CG2	2.80	0.59
1:M:8:ILE:HD11	1:N:18:TYR:CE2	2.37	0.59
2:D:201:5C2:H2	1:I:136:ILE:HG13	1.85	0.59
1:H:6:THR:N	1:L:22:SER:OG	2.25	0.59
1:C:135:GLU:OE1	1:J:170:ASP:OD1	2.22	0.58
1:L:95:MET:CE	1:M:72:THR:HG21	2.34	0.58
1:M:95:MET:CE	1:N:72:THR:HG21	2.33	0.57
1:M:95:MET:HE1	1:N:72:THR:HG21	1.85	0.57
1:C:143:ILE:CG2	1:J:136:ILE:CG2	2.82	0.57
1:I:22:SER:OG	1:J:6:THR:N	2.29	0.57
1:C:143:ILE:HB	1:J:140:ALA:HB2	1.87	0.57
1:F:8:ILE:CD1	1:G:18:TYR:CZ	2.87	0.57
1:A:72:THR:OG1	1:B:95:MET:HB3	2.05	0.56
1:C:126:LEU:HD21	1:J:133:ALA:HA	1.87	0.56
2:E:201:5C2:H2	1:M:136:ILE:HG13	1.87	0.56
1:C:142:HIS:HD2	2:C:201:5C2:H13	1.71	0.56
2:C:201:5C2:H1	1:J:136:ILE:HD11	1.71	0.56
2:C:201:5C2:C2	1:J:136:ILE:HG13	2.34	0.56
1:A:16:ARG:HG2	1:B:8:ILE:HD11	1.89	0.55
1:C:15:GLU:O	1:D:15:GLU:HG2	2.06	0.55
2:F:201:5C2:C4	1:L:136:ILE:HG13	2.37	0.55
1:C:136:ILE:HG22	1:J:143:ILE:HG22	1.89	0.55
1:C:170:ASP:OD1	1:J:135:GLU:OE1	2.25	0.55
1:A:147:ARG:HD3	1:N:136:ILE:HG22	1.89	0.55
2:C:201:5C2:H1	1:J:136:ILE:CD1	2.20	0.55
1:A:142:HIS:CE1	1:B:174:PHE:CD1	2.95	0.54
1:E:136:ILE:HG13	2:M:201:5C2:N3	2.23	0.54
1:E:8:ILE:HD11	1:F:18:TYR:CE2	2.43	0.54
1:G:136:ILE:HG21	1:H:147:ARG:HD3	1.88	0.54
1:H:8:ILE:HG13	1:L:16:ARG:HG2	1.88	0.54
1:C:143:ILE:HG22	1:J:136:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:5C2:N3	1:M:136:ILE:HG13	2.22	0.54
1:F:6:THR:H	1:G:22:SER:HG	1.52	0.54
1:L:6:THR:N	1:M:22:SER:OG	2.35	0.54
1:A:6:THR:O	1:E:22:SER:HB3	2.08	0.54
1:C:16:ARG:HG2	1:D:8:ILE:CG1	2.37	0.54
1:F:136:ILE:HG13	2:L:201:5C2:C4	2.38	0.54
1:H:8:ILE:CD1	1:L:18:TYR:CZ	2.90	0.54
1:C:140:ALA:CB	1:J:140:ALA:O	2.53	0.53
1:H:95:MET:CE	1:L:72:THR:HG21	2.37	0.53
1:L:95:MET:HE1	1:M:72:THR:HG21	1.89	0.53
1:D:170:ASP:OD2	1:I:135:GLU:HG3	2.09	0.53
1:H:18:TYR:CZ	1:I:8:ILE:HD13	2.42	0.53
1:H:72:THR:HG21	1:I:95:MET:HE1	1.90	0.53
1:D:18:TYR:CZ	1:G:8:ILE:HD13	2.42	0.53
1:A:8:ILE:CG1	1:E:16:ARG:HG2	2.39	0.53
1:E:8:ILE:HD13	1:F:18:TYR:CE1	2.43	0.53
1:G:136:ILE:CG2	1:H:147:ARG:HD3	2.39	0.53
1:K:72:THR:HG21	1:N:95:MET:CE	2.39	0.53
1:D:22:SER:HG	1:G:6:THR:H	1.58	0.52
1:J:18:TYR:CE1	1:K:8:ILE:HD13	2.42	0.52
1:I:72:THR:HG21	1:J:95:MET:CE	2.40	0.52
1:A:147:ARG:CD	1:N:136:ILE:HG21	2.39	0.52
1:D:136:ILE:HG13	2:I:201:5C2:C4	2.40	0.52
1:A:126:LEU:HA	2:A:201:5C2:C18	2.40	0.52
1:A:8:ILE:HD13	1:E:18:TYR:CE1	2.43	0.52
1:A:72:THR:HG21	1:B:95:MET:HE2	1.92	0.51
1:B:18:TYR:CZ	1:C:8:ILE:CD1	2.93	0.51
1:H:8:ILE:CG1	1:L:16:ARG:HG2	2.40	0.51
1:A:95:MET:CE	1:E:72:THR:HG21	2.41	0.50
2:D:201:5C2:N3	1:I:136:ILE:HG13	2.27	0.50
1:C:22:SER:CB	1:D:6:THR:O	2.57	0.50
1:A:144:LEU:CD1	1:N:140:ALA:CB	2.90	0.50
1:H:72:THR:HG21	1:I:95:MET:HE2	1.92	0.50
1:L:95:MET:HB3	1:M:72:THR:OG1	2.12	0.50
1:M:115:LEU:HD13	1:N:79:ASP:HB3	1.93	0.50
1:C:143:ILE:HG22	1:J:136:ILE:CG2	2.42	0.49
1:E:95:MET:CE	1:F:72:THR:HG21	2.42	0.49
1:I:72:THR:HG21	1:J:95:MET:HE1	1.94	0.49
1:F:95:MET:CE	1:G:72:THR:HG21	2.42	0.49
1:F:135:GLU:HG3	1:L:170:ASP:OD2	2.13	0.49
1:A:126:LEU:HA	2:A:201:5C2:H14	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:5C2:H11	2:C:201:5C2:N25	2.27	0.49
1:L:8:ILE:CG1	1:M:16:ARG:HG2	2.44	0.48
1:E:6:THR:N	1:F:22:SER:OG	2.29	0.48
1:I:18:TYR:CE2	1:J:8:ILE:HD11	2.49	0.48
2:B:201:5C2:C4	1:K:136:ILE:HG13	2.44	0.48
1:K:22:SER:HG	1:N:6:THR:H	1.62	0.48
1:K:72:THR:HG21	1:N:95:MET:HE1	1.94	0.48
1:B:142:HIS:CE1	1:C:174:PHE:CD1	3.02	0.48
1:E:135:GLU:OE1	1:M:170:ASP:OD1	2.32	0.48
1:A:79:ASP:HB3	1:B:115:LEU:HD13	1.95	0.48
1:M:117:ASN:HB3	1:N:149:LYS:HE2	1.95	0.48
1:B:147:ARG:HD3	1:K:136:ILE:CG2	2.45	0.47
1:L:6:THR:O	1:M:22:SER:HB3	2.13	0.47
1:C:136:ILE:HG22	1:J:143:ILE:CG2	2.44	0.47
1:C:140:ALA:CB	1:J:144:LEU:HD13	2.44	0.47
1:I:18:TYR:CE1	1:J:8:ILE:HD13	2.48	0.47
1:M:6:THR:N	1:N:22:SER:HG	2.02	0.47
1:M:7:VAL:HG11	1:N:50:PHE:CZ	2.50	0.47
1:E:8:ILE:CD1	1:F:18:TYR:CE2	2.98	0.47
1:E:95:MET:HE1	1:F:72:THR:HG21	1.95	0.47
1:H:95:MET:HE1	1:L:72:THR:HG21	1.95	0.47
1:K:18:TYR:CZ	1:N:8:ILE:HD13	2.48	0.47
1:C:136:ILE:HG13	2:J:201:5C2:H2	1.95	0.46
1:E:140:ALA:CB	1:M:144:LEU:HD13	2.45	0.46
1:F:140:ALA:CB	1:L:144:LEU:HD13	2.45	0.46
1:M:95:MET:HB3	1:N:72:THR:OG1	2.16	0.46
1:L:8:ILE:CD1	1:M:18:TYR:CZ	2.98	0.46
1:C:136:ILE:CG2	1:J:143:ILE:HG23	2.43	0.46
1:A:8:ILE:HD13	1:E:18:TYR:OH	2.15	0.46
1:A:147:ARG:CD	1:N:136:ILE:CG2	2.92	0.46
1:L:98:SER:O	2:L:201:5C2:H16	2.15	0.46
1:A:170:ASP:OD1	1:N:135:GLU:HG3	2.16	0.46
1:B:144:LEU:CD1	1:K:140:ALA:CB	2.94	0.46
1:L:8:ILE:HG13	1:M:16:ARG:HG2	1.98	0.46
1:H:8:ILE:HD11	1:L:16:ARG:HG2	1.98	0.45
1:B:8:ILE:HG22	1:B:17:ALA:HA	1.99	0.45
1:C:170:ASP:OD2	1:J:135:GLU:CG	2.60	0.45
1:C:140:ALA:HB3	1:J:144:LEU:HD13	1.99	0.45
1:A:23:ARG:HG2	1:E:50:PHE:CE1	2.52	0.45
1:A:95:MET:HE2	1:E:72:THR:HG21	1.99	0.45
1:A:8:ILE:HG22	1:A:17:ALA:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:ILE:CG2	1:I:136:ILE:HG23	2.47	0.45
1:C:79:ASP:HB3	1:D:115:LEU:HD13	1.99	0.44
2:A:201:5C2:N3	1:N:136:ILE:HG13	2.32	0.44
1:E:8:ILE:HG22	1:E:17:ALA:HA	2.00	0.44
1:F:8:ILE:HG22	1:F:17:ALA:HA	1.99	0.44
1:M:8:ILE:CG1	1:N:16:ARG:HG2	2.47	0.44
1:C:140:ALA:HB3	1:J:144:LEU:CD1	2.47	0.44
1:L:8:ILE:HG22	1:L:17:ALA:HA	1.99	0.44
1:F:136:ILE:HG13	2:L:201:5C2:N3	2.32	0.44
1:G:8:ILE:HG22	1:G:17:ALA:HA	2.00	0.44
1:I:22:SER:HB3	1:J:6:THR:O	2.18	0.44
1:M:6:THR:O	1:N:22:SER:HB3	2.18	0.44
1:B:72:THR:HG21	1:C:95:MET:HE2	1.97	0.44
1:C:8:ILE:HG22	1:C:17:ALA:HA	1.99	0.44
1:E:6:THR:O	1:F:22:SER:HB3	2.17	0.44
1:N:8:ILE:HG22	1:N:17:ALA:HA	2.00	0.44
1:E:8:ILE:HG13	1:F:16:ARG:HG2	2.00	0.44
1:I:16:ARG:HG2	1:J:8:ILE:HG13	1.99	0.44
1:J:8:ILE:HG22	1:J:17:ALA:HA	2.00	0.44
1:J:22:SER:CB	1:K:6:THR:O	2.66	0.44
1:D:136:ILE:HG13	2:I:201:5C2:H2	2.00	0.43
1:A:170:ASP:CG	1:N:135:GLU:HG3	2.38	0.43
1:E:135:GLU:HG3	1:M:170:ASP:OD2	2.18	0.43
1:H:18:TYR:CZ	1:I:8:ILE:CD1	3.01	0.43
1:I:8:ILE:HG22	1:I:17:ALA:HA	2.00	0.43
1:K:8:ILE:HG22	1:K:17:ALA:HA	2.00	0.43
1:M:8:ILE:HG22	1:M:17:ALA:HA	2.00	0.43
1:B:147:ARG:HD3	1:K:136:ILE:HG22	2.00	0.43
1:C:72:THR:HG21	1:D:95:MET:CE	2.48	0.43
1:C:90:THR:HG21	1:C:104:LEU:HA	2.00	0.43
1:A:144:LEU:HD13	1:N:140:ALA:CB	2.48	0.43
1:J:15:GLU:O	1:K:15:GLU:HG2	2.17	0.43
1:B:72:THR:OG1	1:C:95:MET:HB3	2.19	0.43
1:D:90:THR:HG21	1:D:104:LEU:HA	2.00	0.43
1:C:126:LEU:CD2	1:J:133:ALA:O	2.67	0.43
1:D:8:ILE:HG22	1:D:17:ALA:HA	1.99	0.43
1:E:117:ASN:HB3	1:F:149:LYS:HE2	2.00	0.43
1:F:90:THR:HG21	1:F:104:LEU:HA	2.01	0.43
1:H:95:MET:HE2	1:L:72:THR:HG21	2.01	0.42
1:J:90:THR:HG21	1:J:104:LEU:HA	2.01	0.42
1:A:90:THR:HG21	1:A:104:LEU:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:THR:HG21	1:G:104:LEU:HA	2.01	0.42
2:A:201:5C2:H1	1:N:136:ILE:HD11	1.83	0.42
1:F:136:ILE:CG2	1:L:147:ARG:HD3	2.49	0.42
1:F:117:ASN:HB3	1:G:149:LYS:HE2	2.01	0.42
1:L:115:LEU:HB3	1:M:79:ASP:HB3	2.02	0.42
1:H:8:ILE:HG22	1:H:17:ALA:HA	2.00	0.42
1:L:11:THR:HG23	1:L:16:ARG:HD2	2.02	0.42
1:D:72:THR:HG21	1:G:95:MET:CE	2.49	0.42
1:E:90:THR:HG21	1:E:104:LEU:HA	2.01	0.42
1:F:8:ILE:HD11	1:G:16:ARG:HG2	2.02	0.42
1:H:90:THR:HG21	1:H:104:LEU:HA	2.02	0.42
1:K:90:THR:HG21	1:K:104:LEU:HA	2.01	0.42
1:M:115:LEU:CD1	1:N:79:ASP:HB3	2.49	0.42
1:A:132:GLN:HG2	1:B:174:PHE:CE2	2.53	0.42
1:F:95:MET:HE1	1:G:72:THR:HG21	2.01	0.42
1:D:170:ASP:OD1	1:I:135:GLU:OE1	2.38	0.42
1:I:18:TYR:CE2	1:J:8:ILE:CD1	3.03	0.42
1:F:95:MET:HB3	1:G:72:THR:OG1	2.20	0.42
1:B:90:THR:HG21	1:B:104:LEU:HA	2.01	0.41
1:C:50:PHE:CE1	1:D:23:ARG:HG2	2.55	0.41
1:C:149:LYS:HE2	1:D:117:ASN:HB3	2.01	0.41
1:N:90:THR:HG21	1:N:104:LEU:HA	2.01	0.41
1:A:144:LEU:HD11	1:N:140:ALA:HB3	2.03	0.41
1:H:6:THR:O	1:L:22:SER:HB3	2.20	0.41
1:L:8:ILE:HD11	1:M:16:ARG:HG2	2.01	0.41
1:B:125:PRO:O	2:B:201:5C2:H14	2.20	0.41
1:A:124:GLN:HB2	2:A:201:5C2:S13	2.61	0.41
1:F:115:LEU:HD13	1:G:79:ASP:HB3	2.02	0.41
1:M:90:THR:HG21	1:M:104:LEU:HA	2.02	0.41
1:A:79:ASP:HB3	1:B:115:LEU:CD1	2.50	0.41
1:B:154:LEU:HD12	2:B:201:5C2:H5	2.02	0.41
1:H:79:ASP:HB3	1:I:115:LEU:HD13	2.03	0.41
1:L:90:THR:HG21	1:L:104:LEU:HA	2.02	0.41
1:F:136:ILE:HG23	1:L:143:ILE:CG2	2.51	0.40
2:A:201:5C2:O1	2:A:201:5C2:C6	2.69	0.40
1:D:18:TYR:CZ	1:G:8:ILE:CD1	3.05	0.40
2:A:201:5C2:N3	1:N:136:ILE:CD1	2.85	0.40
1:B:22:SER:OG	1:C:6:THR:N	2.34	0.40
1:E:140:ALA:HB3	1:M:144:LEU:CD1	2.51	0.40
1:H:8:ILE:CD1	1:L:16:ARG:HG2	2.51	0.40
1:I:90:THR:HG21	1:I:104:LEU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLU:CG	1:J:170:ASP:OD2	2.68	0.40
1:F:8:ILE:HG13	1:G:16:ARG:HG2	2.02	0.40
1:H:8:ILE:HD11	1:L:18:TYR:CE2	2.57	0.40

All (52) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:85:LYS:CD	1:L:11:THR:CA[2_456]	0.72	1.48
1:J:163:GLU:CD	1:L:162:ILE:CD1[1_565]	0.74	1.46
1:J:85:LYS:CD	1:L:11:THR:C[2_456]	1.13	1.07
1:J:163:GLU:OE1	1:L:162:ILE:CD1[1_565]	1.21	0.99
1:D:11:THR:OG1	1:E:59:ASP:OD2[2_555]	1.23	0.97
1:J:85:LYS:CG	1:L:11:THR:OG1[2_456]	1.23	0.97
1:J:85:LYS:CG	1:L:11:THR:CB[2_456]	1.34	0.86
1:J:57:GLU:CD	1:L:9:GLU:CB[2_456]	1.36	0.84
1:J:85:LYS:CE	1:L:11:THR:CA[2_456]	1.39	0.81
1:J:57:GLU:CG	1:L:9:GLU:CD[2_456]	1.42	0.78
1:B:160:GLN:CA	1:M:167:LYS:CE[2_455]	1.44	0.76
1:J:85:LYS:CB	1:L:11:THR:CB[2_456]	1.46	0.74
1:J:57:GLU:OE2	1:L:9:GLU:CB[2_456]	1.47	0.73
1:J:85:LYS:CG	1:L:11:THR:CA[2_456]	1.47	0.73
1:J:57:GLU:CD	1:L:9:GLU:CG[2_456]	1.49	0.71
1:J:85:LYS:CB	1:L:11:THR:OG1[2_456]	1.49	0.71
1:J:57:GLU:CG	1:L:9:GLU:OE2[2_456]	1.50	0.70
1:D:11:THR:OG1	1:E:59:ASP:CG[2_555]	1.52	0.68
1:J:85:LYS:CE	1:L:11:THR:N[2_456]	1.52	0.68
1:B:159:GLY:O	1:M:167:LYS:NZ[2_455]	1.54	0.66
1:J:163:GLU:CG	1:L:162:ILE:CD1[1_565]	1.54	0.66
1:C:162:ILE:CD1	1:E:163:GLU:OE1[1_565]	1.59	0.61
1:D:137:GLU:OE2	1:H:161:SER:OG[2_556]	1.59	0.61
1:J:57:GLU:CG	1:L:9:GLU:CG[2_456]	1.61	0.59
1:C:162:ILE:CG1	1:E:163:GLU:OE1[1_565]	1.64	0.56
1:J:85:LYS:CD	1:L:11:THR:N[2_456]	1.66	0.54
1:J:57:GLU:OE1	1:L:9:GLU:CG[2_456]	1.69	0.51
1:J:57:GLU:OE2	1:L:9:GLU:CA[2_456]	1.73	0.47
1:J:85:LYS:NZ	1:L:11:THR:N[2_456]	1.75	0.45
1:J:57:GLU:CG	1:L:9:GLU:CB[2_456]	1.76	0.44
1:J:57:GLU:OE2	1:L:9:GLU:C[2_456]	1.77	0.43
1:D:11:THR:OG1	1:E:59:ASP:OD1[2_555]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:85:LYS:CD	1:L:11:THR:CB[2_456]	1.82	0.38
1:J:163:GLU:OE1	1:L:162:ILE:CG1[1_565]	1.84	0.36
1:J:163:GLU:OE2	1:L:162:ILE:CD1[1_565]	1.84	0.36
1:J:85:LYS:CG	1:L:11:THR:C[2_456]	1.86	0.34
1:B:159:GLY:C	1:M:167:LYS:NZ[2_455]	1.89	0.31
1:F:167:LYS:NZ	1:I:159:GLY:C[2_546]	1.89	0.31
1:J:57:GLU:OE2	1:L:10:THR:N[2_456]	1.92	0.28
1:H:167:LYS:NZ	1:I:166:GLN:OE1[2_546]	1.95	0.25
1:J:85:LYS:CE	1:L:11:THR:C[2_456]	1.96	0.24
1:F:167:LYS:NZ	1:I:159:GLY:O[2_546]	1.98	0.22
1:A:167:LYS:NZ	1:B:166:GLN:OE1[2_445]	2.00	0.20
1:F:167:LYS:NZ	1:I:159:GLY:CA[2_546]	2.04	0.16
1:J:57:GLU:CB	1:L:9:GLU:OE2[2_456]	2.07	0.13
1:B:159:GLY:O	1:M:167:LYS:CE[2_455]	2.12	0.08
1:B:160:GLN:N	1:M:167:LYS:CE[2_455]	2.14	0.06
1:J:58:LYS:NZ	1:M:54:GLN:O[2_456]	2.14	0.06
1:B:160:GLN:CA	1:M:167:LYS:CD[2_455]	2.15	0.05
1:J:85:LYS:CB	1:L:11:THR:CA[2_456]	2.16	0.04
1:B:159:GLY:O	1:M:167:LYS:CD[2_455]	2.18	0.02
1:J:163:GLU:CD	1:L:162:ILE:CG1[1_565]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
1	B	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
1	C	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
1	D	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
1	E	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
1	F	184/195 (94%)	176 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
1	H	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
1	I	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
1	J	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
1	K	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
1	L	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
1	M	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
1	N	184/195 (94%)	176 (96%)	8 (4%)	0	100	100
All	All	2576/2730 (94%)	2464 (96%)	112 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	157/163 (96%)	150 (96%)	7 (4%)	27	64
1	B	157/163 (96%)	150 (96%)	7 (4%)	27	64
1	C	157/163 (96%)	150 (96%)	7 (4%)	27	64
1	D	157/163 (96%)	150 (96%)	7 (4%)	27	64
1	E	157/163 (96%)	150 (96%)	7 (4%)	27	64
1	F	157/163 (96%)	150 (96%)	7 (4%)	27	64
1	G	157/163 (96%)	150 (96%)	7 (4%)	27	64
1	H	157/163 (96%)	150 (96%)	7 (4%)	27	64
1	I	157/163 (96%)	150 (96%)	7 (4%)	27	64
1	J	157/163 (96%)	150 (96%)	7 (4%)	27	64
1	K	157/163 (96%)	150 (96%)	7 (4%)	27	64
1	L	157/163 (96%)	150 (96%)	7 (4%)	27	64
1	M	157/163 (96%)	150 (96%)	7 (4%)	27	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	157/163 (96%)	150 (96%)	7 (4%)	27	64
All	All	2198/2282 (96%)	2100 (96%)	98 (4%)	27	64

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	8	ILE
1	A	16	ARG
1	A	65	ASN
1	A	85	LYS
1	A	126	LEU
1	A	154	LEU
1	B	4	ILE
1	B	8	ILE
1	B	16	ARG
1	B	65	ASN
1	B	85	LYS
1	B	126	LEU
1	B	154	LEU
1	C	4	ILE
1	C	8	ILE
1	C	16	ARG
1	C	65	ASN
1	C	85	LYS
1	C	126	LEU
1	C	154	LEU
1	D	4	ILE
1	D	8	ILE
1	D	16	ARG
1	D	65	ASN
1	D	85	LYS
1	D	126	LEU
1	D	154	LEU
1	E	4	ILE
1	E	8	ILE
1	E	16	ARG
1	E	65	ASN
1	E	85	LYS
1	E	126	LEU
1	E	154	LEU
1	F	4	ILE

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Mol	Chain	Res	Type
1	F	8	ILE
1	F	16	ARG
1	F	65	ASN
1	F	85	LYS
1	F	126	LEU
1	F	154	LEU
1	G	4	ILE
1	G	8	ILE
1	G	16	ARG
1	G	65	ASN
1	G	85	LYS
1	G	126	LEU
1	G	154	LEU
1	H	4	ILE
1	H	8	ILE
1	H	16	ARG
1	H	65	ASN
1	H	85	LYS
1	H	126	LEU
1	H	154	LEU
1	I	4	ILE
1	I	8	ILE
1	I	16	ARG
1	I	65	ASN
1	I	85	LYS
1	I	126	LEU
1	I	154	LEU
1	J	4	ILE
1	J	8	ILE
1	J	16	ARG
1	J	65	ASN
1	J	85	LYS
1	J	126	LEU
1	J	154	LEU
1	K	4	ILE
1	K	8	ILE
1	K	16	ARG
1	K	65	ASN
1	K	85	LYS
1	K	126	LEU
1	K	154	LEU
1	L	4	ILE

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Mol	Chain	Res	Type
1	L	8	ILE
1	L	16	ARG
1	L	65	ASN
1	L	85	LYS
1	L	126	LEU
1	L	154	LEU
1	M	4	ILE
1	M	8	ILE
1	M	16	ARG
1	M	65	ASN
1	M	85	LYS
1	M	126	LEU
1	M	154	LEU
1	N	4	ILE
1	N	8	ILE
1	N	16	ARG
1	N	65	ASN
1	N	85	LYS
1	N	126	LEU
1	N	154	LEU

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

Mol	Chain	Res	Type
1	A	65	ASN
1	A	82	GLN
1	A	166	GLN
1	B	65	ASN
1	B	82	GLN
1	B	117	ASN
1	B	166	GLN
1	C	65	ASN
1	C	82	GLN
1	C	132	GLN
1	C	142	HIS
1	C	166	GLN
1	D	65	ASN
1	D	82	GLN
1	D	166	GLN
1	E	65	ASN
1	E	82	GLN
1	E	166	GLN

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Mol	Chain	Res	Type
1	F	65	ASN
1	F	82	GLN
1	F	166	GLN
1	G	65	ASN
1	G	82	GLN
1	G	166	GLN
1	H	65	ASN
1	H	82	GLN
1	H	166	GLN
1	I	65	ASN
1	I	82	GLN
1	I	166	GLN
1	J	65	ASN
1	J	82	GLN
1	J	166	GLN
1	K	65	ASN
1	K	82	GLN
1	K	166	GLN
1	L	65	ASN
1	L	82	GLN
1	L	166	GLN
1	M	65	ASN
1	M	82	GLN
1	M	166	GLN
1	N	65	ASN
1	N	82	GLN
1	N	166	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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
2	5C2	G	201	-	22,29,29	3.43	6 (27%)	18,41,41	2.78	5 (27%)
2	5C2	J	201	-	22,29,29	3.28	6 (27%)	18,41,41	2.73	5 (27%)
2	5C2	C	201	-	22,29,29	6.55	9 (40%)	18,41,41	3.40	5 (27%)
2	5C2	M	201	-	22,29,29	3.34	6 (27%)	18,41,41	2.71	5 (27%)
2	5C2	N	201	-	22,29,29	3.21	6 (27%)	18,41,41	2.67	5 (27%)
2	5C2	B	201	-	22,29,29	6.42	7 (31%)	18,41,41	3.41	6 (33%)
2	5C2	H	201	-	22,29,29	3.50	6 (27%)	18,41,41	2.74	5 (27%)
2	5C2	F	201	-	22,29,29	3.25	6 (27%)	18,41,41	2.73	5 (27%)
2	5C2	E	201	-	22,29,29	3.48	6 (27%)	18,41,41	2.75	5 (27%)
2	5C2	K	201	-	22,29,29	3.42	6 (27%)	18,41,41	2.76	5 (27%)
2	5C2	D	201	-	22,29,29	3.25	6 (27%)	18,41,41	2.74	5 (27%)
2	5C2	A	201	-	22,29,29	4.91	9 (40%)	18,41,41	3.03	6 (33%)
2	5C2	L	201	-	22,29,29	6.78	9 (40%)	18,41,41	3.31	6 (33%)
2	5C2	I	201	-	22,29,29	3.38	6 (27%)	18,41,41	2.72	5 (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
2	5C2	G	201	-	-	2/11/17/17	0/4/4/4
2	5C2	J	201	-	-	2/11/17/17	0/4/4/4
2	5C2	C	201	-	-	6/11/17/17	0/4/4/4
2	5C2	M	201	-	-	2/11/17/17	0/4/4/4
2	5C2	N	201	-	-	2/11/17/17	0/4/4/4
2	5C2	B	201	-	-	2/11/17/17	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5C2	H	201	-	-	2/11/17/17	0/4/4/4
2	5C2	F	201	-	-	2/11/17/17	0/4/4/4
2	5C2	E	201	-	-	2/11/17/17	0/4/4/4
2	5C2	K	201	-	-	2/11/17/17	0/4/4/4
2	5C2	D	201	-	-	2/11/17/17	0/4/4/4
2	5C2	A	201	-	-	5/11/17/17	0/4/4/4
2	5C2	L	201	-	-	2/11/17/17	0/4/4/4
2	5C2	I	201	-	-	2/11/17/17	0/4/4/4

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	201	5C2	C9-S13	-29.79	1.43	1.72
2	C	201	5C2	C9-S13	-28.69	1.44	1.72
2	B	201	5C2	C9-S13	-27.90	1.45	1.72
2	A	201	5C2	C9-S13	-19.66	1.53	1.72
2	H	201	5C2	C9-S13	-13.08	1.59	1.72
2	E	201	5C2	C9-S13	-12.99	1.59	1.72
2	G	201	5C2	C9-S13	-12.58	1.60	1.72
2	K	201	5C2	C9-S13	-12.57	1.60	1.72
2	I	201	5C2	C9-S13	-12.42	1.60	1.72
2	M	201	5C2	C9-S13	-12.22	1.60	1.72
2	J	201	5C2	C9-S13	-11.85	1.61	1.72
2	F	201	5C2	C9-S13	-11.60	1.61	1.72
2	D	201	5C2	C9-S13	-11.54	1.61	1.72
2	N	201	5C2	C9-S13	-11.37	1.61	1.72
2	A	201	5C2	C15-C2	-5.60	1.38	1.50
2	C	201	5C2	C15-C2	-5.33	1.39	1.50
2	B	201	5C2	C15-C2	-5.25	1.39	1.50
2	K	201	5C2	C26-N25	5.02	1.39	1.31
2	M	201	5C2	C26-N25	4.98	1.39	1.31
2	H	201	5C2	C26-N25	4.96	1.39	1.31
2	F	201	5C2	C26-N25	4.95	1.39	1.31
2	B	201	5C2	C26-N25	4.95	1.39	1.31
2	L	201	5C2	C15-C2	-4.94	1.39	1.50
2	E	201	5C2	C26-N25	4.94	1.39	1.31
2	J	201	5C2	C26-N25	4.93	1.39	1.31
2	I	201	5C2	C26-N25	4.93	1.39	1.31
2	N	201	5C2	C26-N25	4.93	1.39	1.31
2	D	201	5C2	C26-N25	4.91	1.39	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	201	5C2	C26-N25	4.87	1.39	1.31
2	A	201	5C2	C18-C17	-4.77	1.30	1.40
2	A	201	5C2	C17-C24	-4.66	1.30	1.43
2	D	201	5C2	C15-C2	-4.66	1.40	1.50
2	L	201	5C2	C26-N25	4.65	1.39	1.31
2	L	201	5C2	C18-C17	-4.63	1.31	1.40
2	B	201	5C2	C18-C17	-4.60	1.31	1.40
2	K	201	5C2	C15-C2	-4.60	1.40	1.50
2	F	201	5C2	C15-C2	-4.58	1.40	1.50
2	G	201	5C2	C15-C2	-4.58	1.40	1.50
2	N	201	5C2	C15-C2	-4.46	1.40	1.50
2	E	201	5C2	C15-C2	-4.46	1.40	1.50
2	H	201	5C2	C15-C2	-4.45	1.40	1.50
2	J	201	5C2	C15-C2	-4.45	1.40	1.50
2	I	201	5C2	C15-C2	-4.42	1.41	1.50
2	M	201	5C2	C15-C2	-4.38	1.41	1.50
2	C	201	5C2	C17-C24	-4.35	1.31	1.43
2	L	201	5C2	C17-C24	-4.21	1.31	1.43
2	C	201	5C2	C18-C17	-4.20	1.32	1.40
2	C	201	5C2	C26-N25	4.19	1.38	1.31
2	B	201	5C2	C17-C24	-4.18	1.31	1.43
2	L	201	5C2	C16-C17	-3.99	1.32	1.42
2	C	201	5C2	C16-C17	-3.99	1.32	1.42
2	A	201	5C2	C16-C17	-3.98	1.33	1.42
2	A	201	5C2	C26-N25	3.97	1.38	1.31
2	G	201	5C2	C18-C17	-3.93	1.32	1.40
2	E	201	5C2	C18-C17	-3.87	1.32	1.40
2	B	201	5C2	C16-C17	-3.86	1.33	1.42
2	K	201	5C2	C18-C17	-3.86	1.32	1.40
2	F	201	5C2	C18-C17	-3.83	1.32	1.40
2	J	201	5C2	C18-C17	-3.82	1.32	1.40
2	N	201	5C2	C18-C17	-3.81	1.32	1.40
2	M	201	5C2	C18-C17	-3.80	1.32	1.40
2	D	201	5C2	C18-C17	-3.80	1.32	1.40
2	I	201	5C2	C18-C17	-3.79	1.32	1.40
2	H	201	5C2	C18-C17	-3.74	1.33	1.40
2	G	201	5C2	C16-C17	-3.66	1.33	1.42
2	E	201	5C2	C16-C17	-3.63	1.33	1.42
2	D	201	5C2	C16-C17	-3.61	1.33	1.42
2	K	201	5C2	C17-C24	-3.59	1.33	1.43
2	F	201	5C2	C16-C17	-3.59	1.33	1.42
2	K	201	5C2	C16-C17	-3.59	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	201	5C2	C16-C17	-3.59	1.33	1.42
2	N	201	5C2	C17-C24	-3.58	1.33	1.43
2	G	201	5C2	C17-C24	-3.58	1.33	1.43
2	I	201	5C2	C16-C17	-3.58	1.33	1.42
2	M	201	5C2	C16-C17	-3.58	1.33	1.42
2	I	201	5C2	C17-C24	-3.58	1.33	1.43
2	H	201	5C2	C16-C17	-3.58	1.33	1.42
2	N	201	5C2	C16-C17	-3.57	1.33	1.42
2	E	201	5C2	C17-C24	-3.55	1.33	1.43
2	M	201	5C2	C17-C24	-3.55	1.33	1.43
2	F	201	5C2	C17-C24	-3.55	1.33	1.43
2	H	201	5C2	C17-C24	-3.54	1.33	1.43
2	D	201	5C2	C17-C24	-3.53	1.33	1.43
2	A	201	5C2	C21-N20	-3.53	1.44	1.49
2	J	201	5C2	C17-C24	-3.52	1.33	1.43
2	B	201	5C2	C12-S13	-2.71	1.58	1.71
2	A	201	5C2	C24-N25	-2.53	1.32	1.35
2	C	201	5C2	C24-N25	-2.35	1.32	1.35
2	A	201	5C2	C12-S13	-2.33	1.59	1.71
2	L	201	5C2	C12-S13	-2.33	1.59	1.71
2	C	201	5C2	C12-S13	-2.07	1.61	1.71
2	C	201	5C2	C21-N20	-2.03	1.46	1.49
2	L	201	5C2	C11-C10	-2.01	1.33	1.39
2	L	201	5C2	C21-N20	-2.01	1.46	1.49

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	5C2	C11-C12-S13	-10.37	104.56	112.98
2	B	201	5C2	C11-C12-S13	-10.22	104.69	112.98
2	L	201	5C2	C11-C12-S13	-9.90	104.95	112.98
2	A	201	5C2	C11-C12-S13	-8.18	106.34	112.98
2	K	201	5C2	C15-C26-N25	-7.50	119.23	125.19
2	D	201	5C2	C15-C26-N25	-7.44	119.29	125.19
2	G	201	5C2	C15-C26-N25	-7.41	119.31	125.19
2	F	201	5C2	C15-C26-N25	-7.39	119.33	125.19
2	A	201	5C2	C15-C26-N25	-7.33	119.37	125.19
2	E	201	5C2	C15-C26-N25	-7.32	119.38	125.19
2	N	201	5C2	C15-C26-N25	-7.32	119.38	125.19
2	J	201	5C2	C15-C26-N25	-7.31	119.39	125.19
2	I	201	5C2	C15-C26-N25	-7.30	119.39	125.19
2	H	201	5C2	C15-C26-N25	-7.26	119.43	125.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	5C2	C15-C26-N25	-7.22	119.46	125.19
2	M	201	5C2	C15-C26-N25	-7.18	119.49	125.19
2	B	201	5C2	C15-C26-N25	-7.09	119.56	125.19
2	G	201	5C2	C11-C12-S13	-6.83	107.44	112.98
2	H	201	5C2	C11-C12-S13	-6.74	107.51	112.98
2	E	201	5C2	C11-C12-S13	-6.62	107.61	112.98
2	K	201	5C2	C11-C12-S13	-6.54	107.67	112.98
2	I	201	5C2	C11-C12-S13	-6.44	107.76	112.98
2	D	201	5C2	C11-C12-S13	-6.43	107.76	112.98
2	M	201	5C2	C11-C12-S13	-6.39	107.80	112.98
2	F	201	5C2	C11-C12-S13	-6.35	107.83	112.98
2	J	201	5C2	C11-C12-S13	-6.33	107.84	112.98
2	L	201	5C2	C15-C26-N25	-6.19	120.27	125.19
2	N	201	5C2	C11-C12-S13	-6.06	108.06	112.98
2	B	201	5C2	C5-C4-N3	-4.76	102.41	112.71
2	L	201	5C2	C5-C4-N3	-4.53	102.89	112.71
2	C	201	5C2	C4-C5-C6	-4.51	123.27	129.63
2	M	201	5C2	C4-C5-C6	-4.49	123.30	129.63
2	E	201	5C2	C4-C5-C6	-4.33	123.53	129.63
2	N	201	5C2	C4-C5-C6	-4.25	123.65	129.63
2	J	201	5C2	C4-C5-C6	-4.24	123.65	129.63
2	H	201	5C2	C4-C5-C6	-4.20	123.71	129.63
2	K	201	5C2	C4-C5-C6	-4.20	123.72	129.63
2	F	201	5C2	C4-C5-C6	-4.19	123.72	129.63
2	I	201	5C2	C4-C5-C6	-4.17	123.75	129.63
2	D	201	5C2	C4-C5-C6	-4.16	123.77	129.63
2	L	201	5C2	C4-C5-C6	-4.08	123.89	129.63
2	G	201	5C2	C4-C5-C6	-4.04	123.94	129.63
2	B	201	5C2	C4-C5-C6	-3.32	124.95	129.63
2	A	201	5C2	C18-C17-C24	-3.24	102.20	105.20
2	J	201	5C2	C5-C4-N3	-3.18	105.82	112.71
2	C	201	5C2	C5-C4-N3	-3.10	105.99	112.71
2	K	201	5C2	C26-N25-C24	2.90	120.43	116.73
2	I	201	5C2	C5-C4-N3	-2.84	106.56	112.71
2	D	201	5C2	C26-N25-C24	2.80	120.31	116.73
2	I	201	5C2	C26-N25-C24	2.80	120.31	116.73
2	N	201	5C2	C26-N25-C24	2.79	120.29	116.73
2	E	201	5C2	C5-C4-N3	-2.76	106.74	112.71
2	F	201	5C2	C5-C4-N3	-2.76	106.74	112.71
2	G	201	5C2	C5-C4-N3	-2.73	106.80	112.71
2	M	201	5C2	C26-N25-C24	2.73	120.21	116.73
2	F	201	5C2	C26-N25-C24	2.72	120.21	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	5C2	C26-N25-C24	2.71	120.20	116.73
2	G	201	5C2	C26-N25-C24	2.71	120.19	116.73
2	J	201	5C2	C26-N25-C24	2.70	120.18	116.73
2	M	201	5C2	C5-C4-N3	-2.69	106.89	112.71
2	N	201	5C2	C5-C4-N3	-2.64	106.99	112.71
2	E	201	5C2	C26-N25-C24	2.64	120.10	116.73
2	D	201	5C2	C5-C4-N3	-2.63	107.01	112.71
2	H	201	5C2	C5-C4-N3	-2.61	107.06	112.71
2	A	201	5C2	C26-N25-C24	2.60	120.05	116.73
2	L	201	5C2	C18-C17-C24	-2.52	102.86	105.20
2	K	201	5C2	C5-C4-N3	-2.51	107.27	112.71
2	C	201	5C2	C26-N25-C24	2.43	119.84	116.73
2	B	201	5C2	C26-N25-C24	2.33	119.70	116.73
2	L	201	5C2	C26-N25-C24	2.29	119.66	116.73
2	A	201	5C2	C17-C18-N19	-2.19	105.70	111.30
2	A	201	5C2	O1-C2-C15	-2.07	117.24	120.94
2	B	201	5C2	C17-C18-N19	-2.02	106.12	111.30

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	5C2	C23-C21-N20-N19
2	B	201	5C2	C23-C21-N20-C24
2	B	201	5C2	C23-C21-N20-N19
2	C	201	5C2	C23-C21-N20-N19
2	D	201	5C2	C23-C21-N20-N19
2	E	201	5C2	C23-C21-N20-N19
2	F	201	5C2	C23-C21-N20-N19
2	G	201	5C2	C23-C21-N20-N19
2	H	201	5C2	C23-C21-N20-N19
2	I	201	5C2	C23-C21-N20-N19
2	J	201	5C2	C23-C21-N20-N19
2	K	201	5C2	C23-C21-N20-N19
2	L	201	5C2	C23-C21-N20-C24
2	L	201	5C2	C23-C21-N20-N19
2	M	201	5C2	C23-C21-N20-N19
2	N	201	5C2	C23-C21-N20-N19
2	C	201	5C2	C22-C21-N20-C24
2	A	201	5C2	C16-C15-C2-O1
2	C	201	5C2	C26-C15-C2-O1
2	C	201	5C2	C26-C15-C2-N3

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Mol	Chain	Res	Type	Atoms
2	A	201	5C2	C5-C4-N3-C2
2	D	201	5C2	C23-C21-N20-C24
2	E	201	5C2	C23-C21-N20-C24
2	F	201	5C2	C23-C21-N20-C24
2	G	201	5C2	C23-C21-N20-C24
2	H	201	5C2	C23-C21-N20-C24
2	I	201	5C2	C23-C21-N20-C24
2	J	201	5C2	C23-C21-N20-C24
2	K	201	5C2	C23-C21-N20-C24
2	M	201	5C2	C23-C21-N20-C24
2	N	201	5C2	C23-C21-N20-C24
2	A	201	5C2	C16-C15-C2-N3
2	C	201	5C2	C16-C15-C2-O1
2	A	201	5C2	C26-C15-C2-O1
2	C	201	5C2	C16-C15-C2-N3

There are no ring outliers.

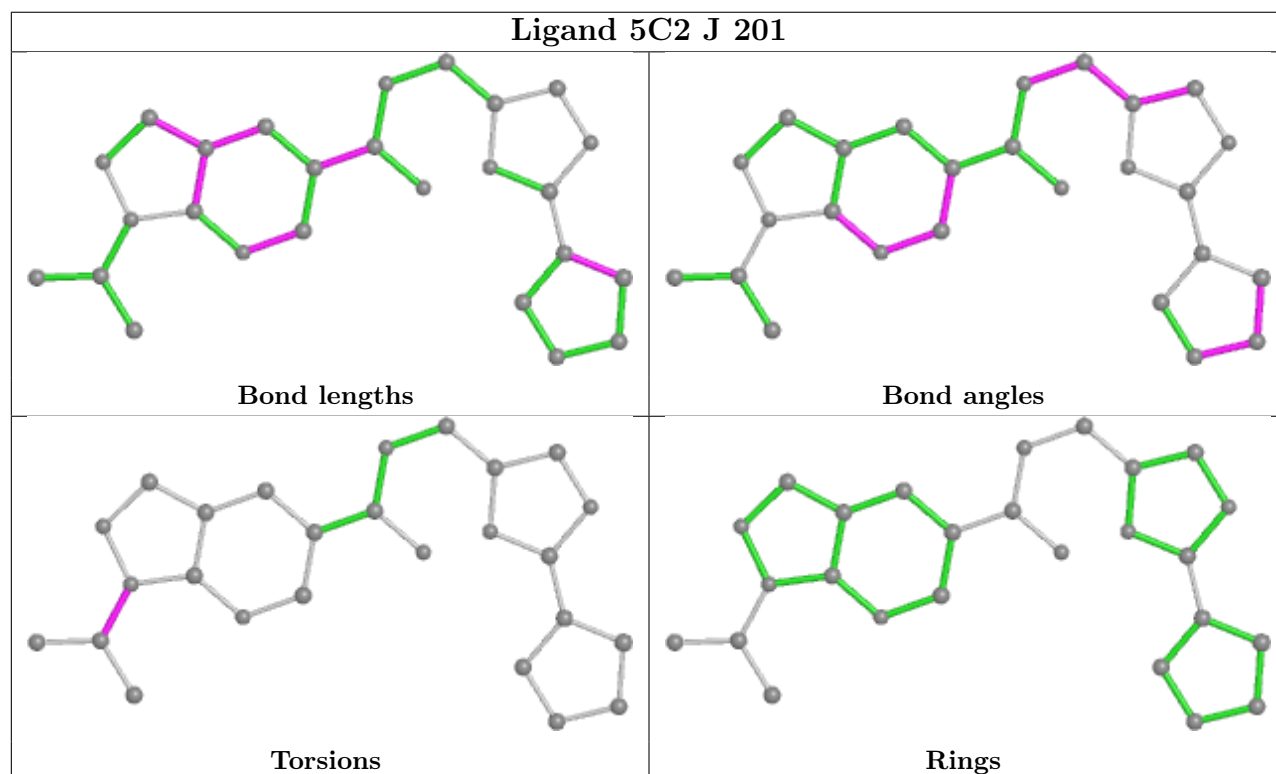
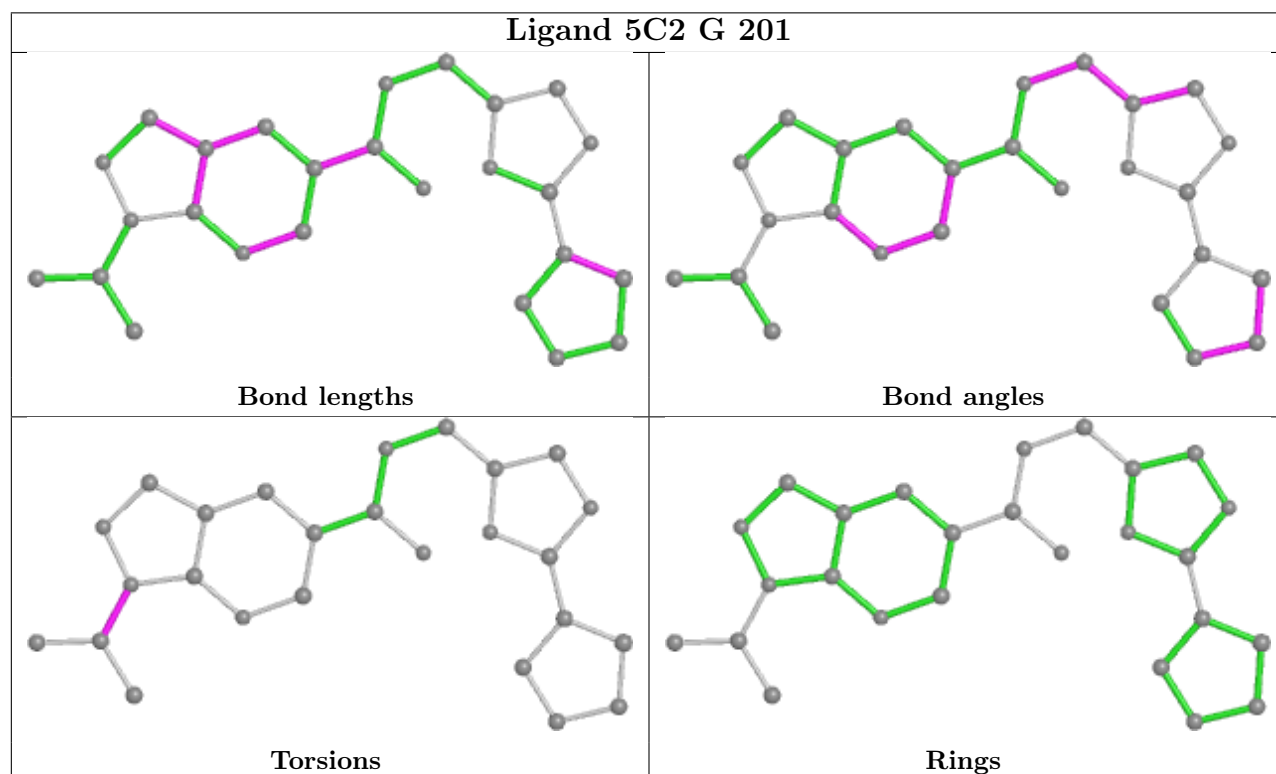
11 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	201	5C2	4	0
2	C	201	5C2	14	0
2	M	201	5C2	3	0
2	B	201	5C2	3	0
2	F	201	5C2	1	0
2	E	201	5C2	3	0
2	K	201	5C2	1	0
2	D	201	5C2	3	0
2	A	201	5C2	11	0
2	L	201	5C2	3	0
2	I	201	5C2	2	0

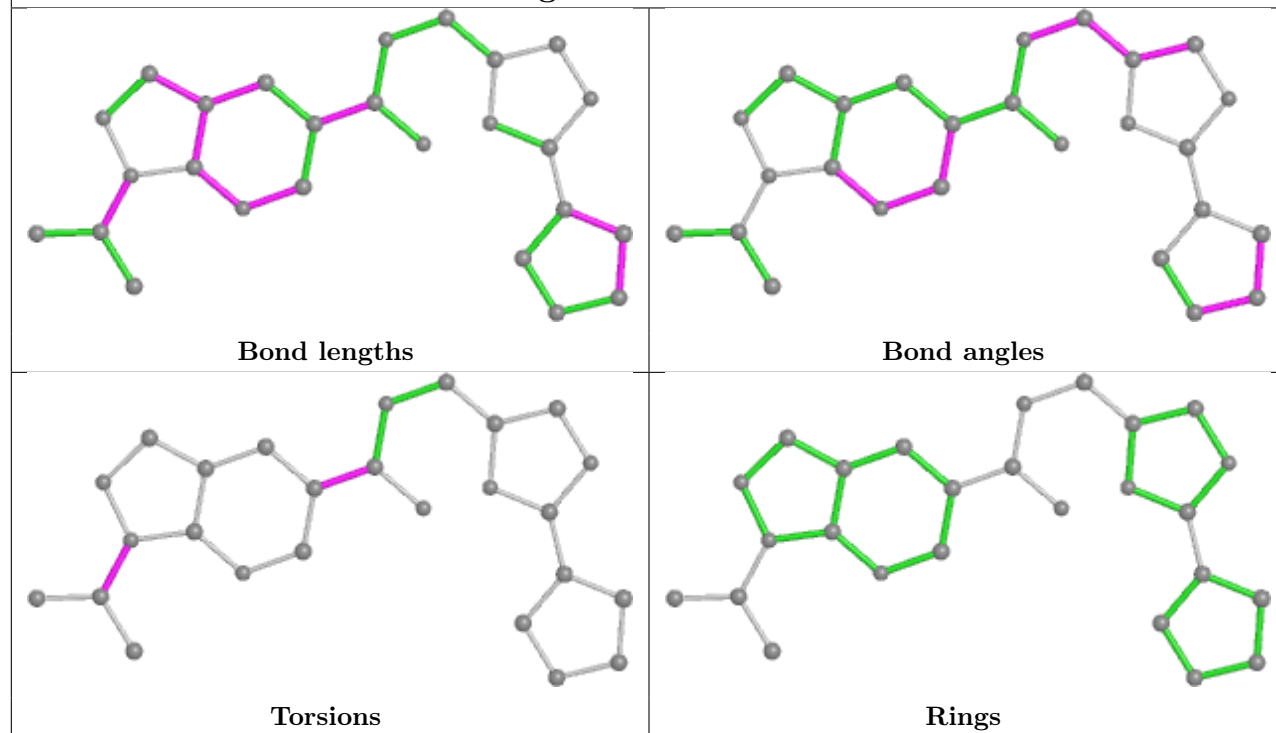
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.



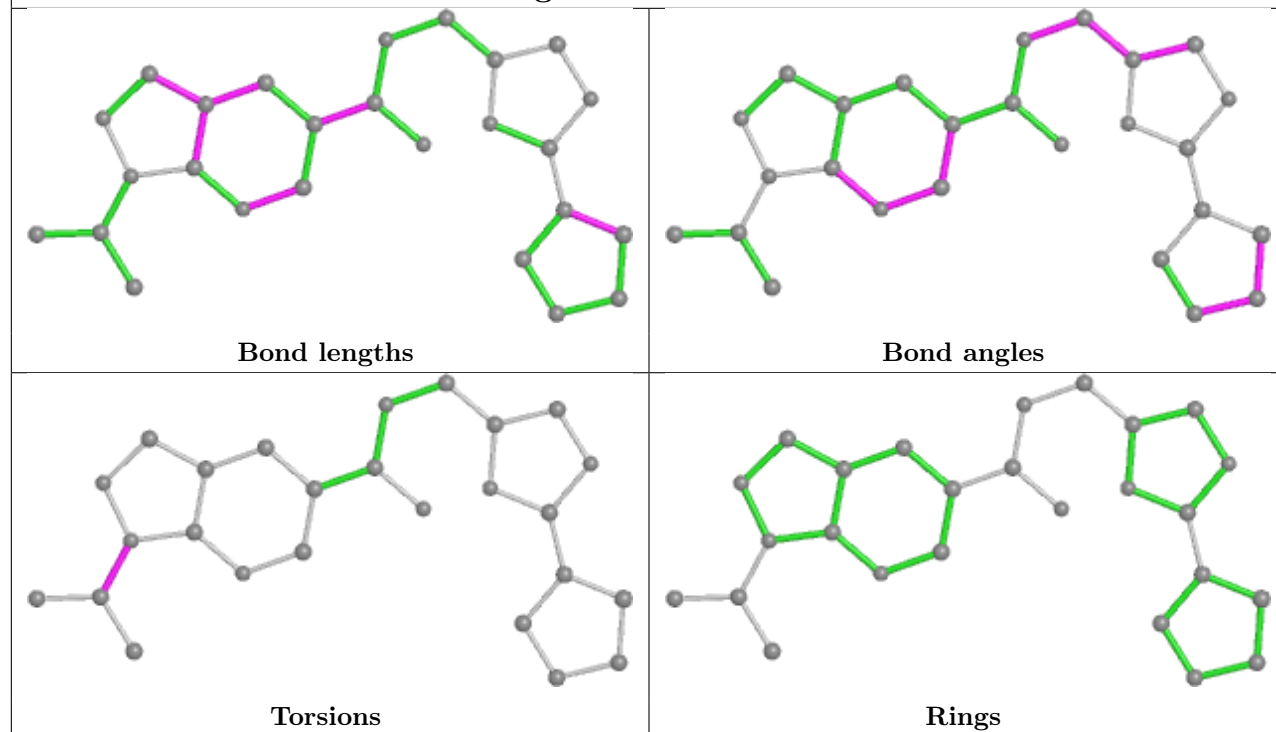
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



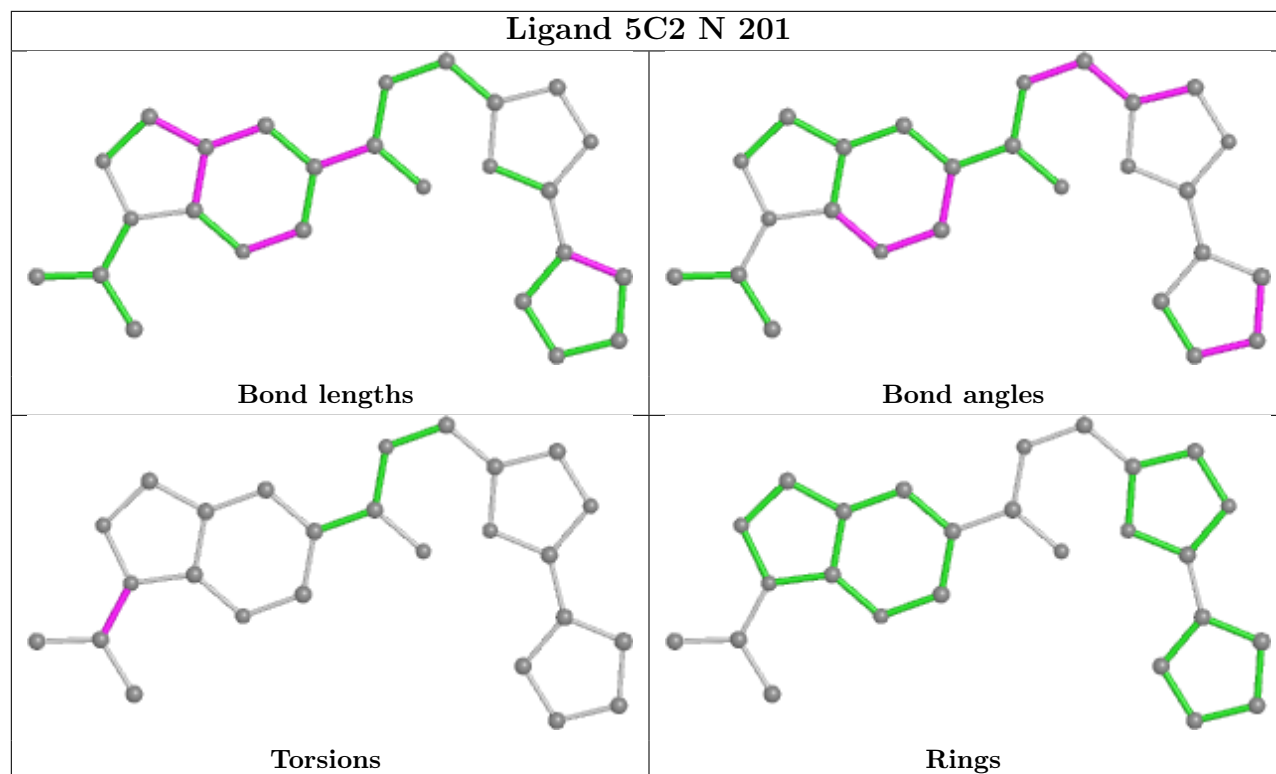
## Ligand 5C2 C 201



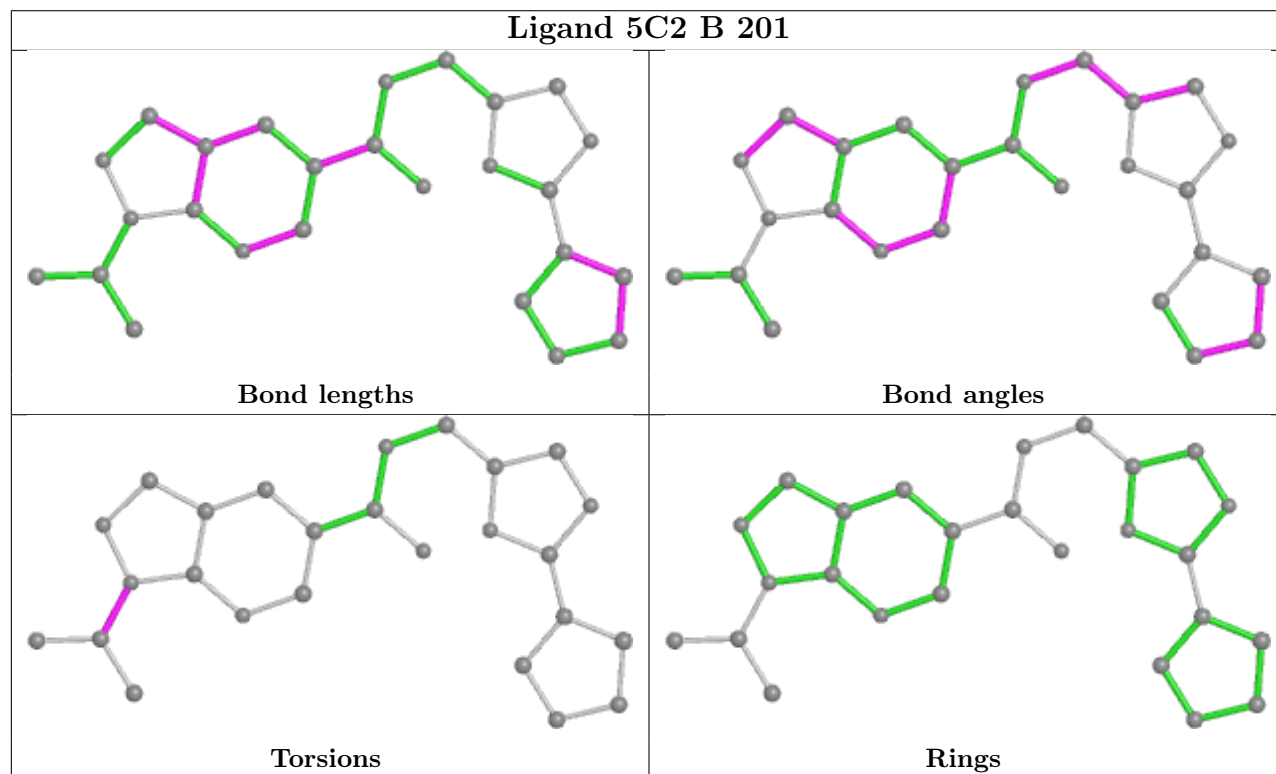
## Ligand 5C2 M 201



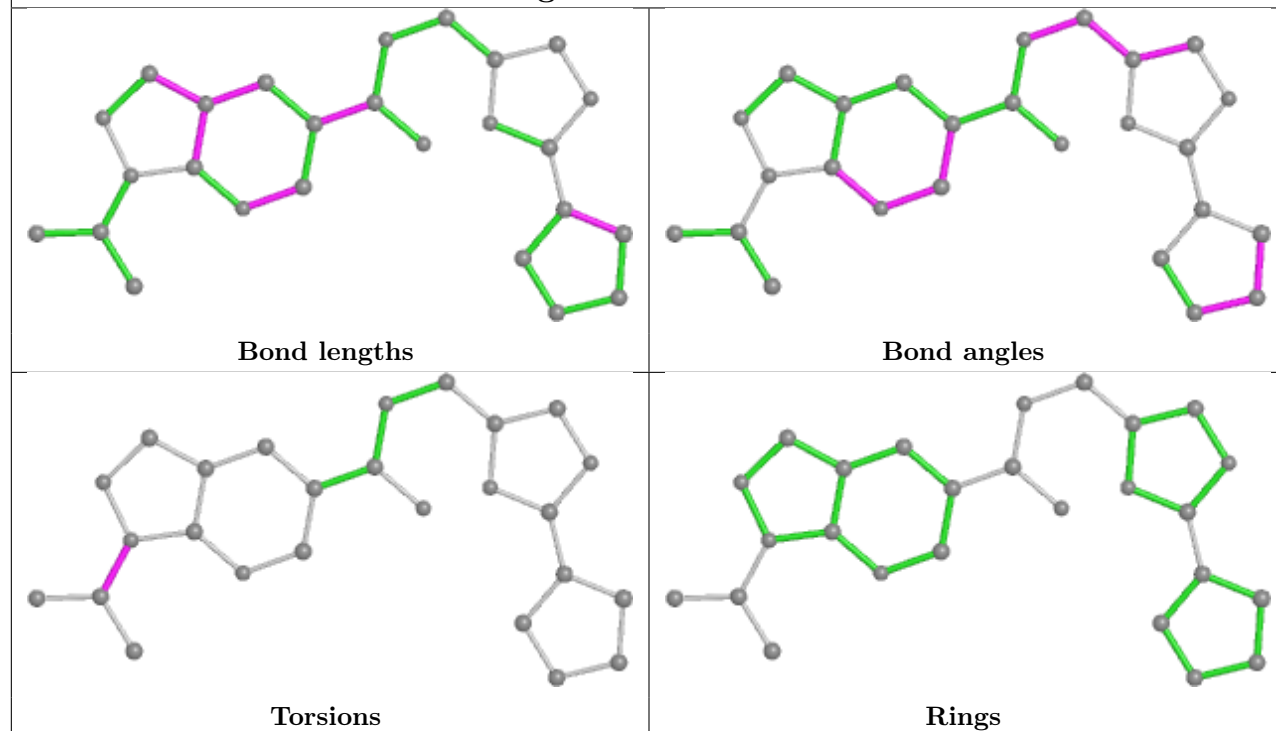
## Ligand 5C2 N 201



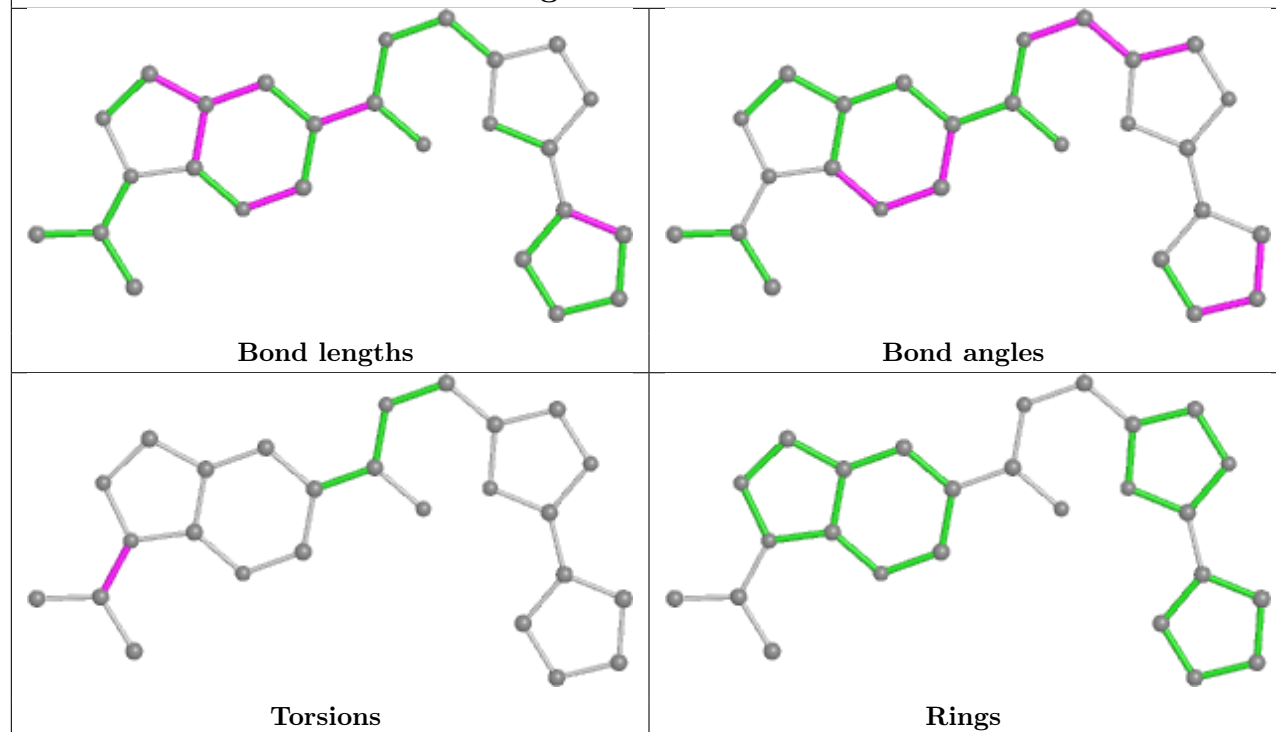
## Ligand 5C2 B 201



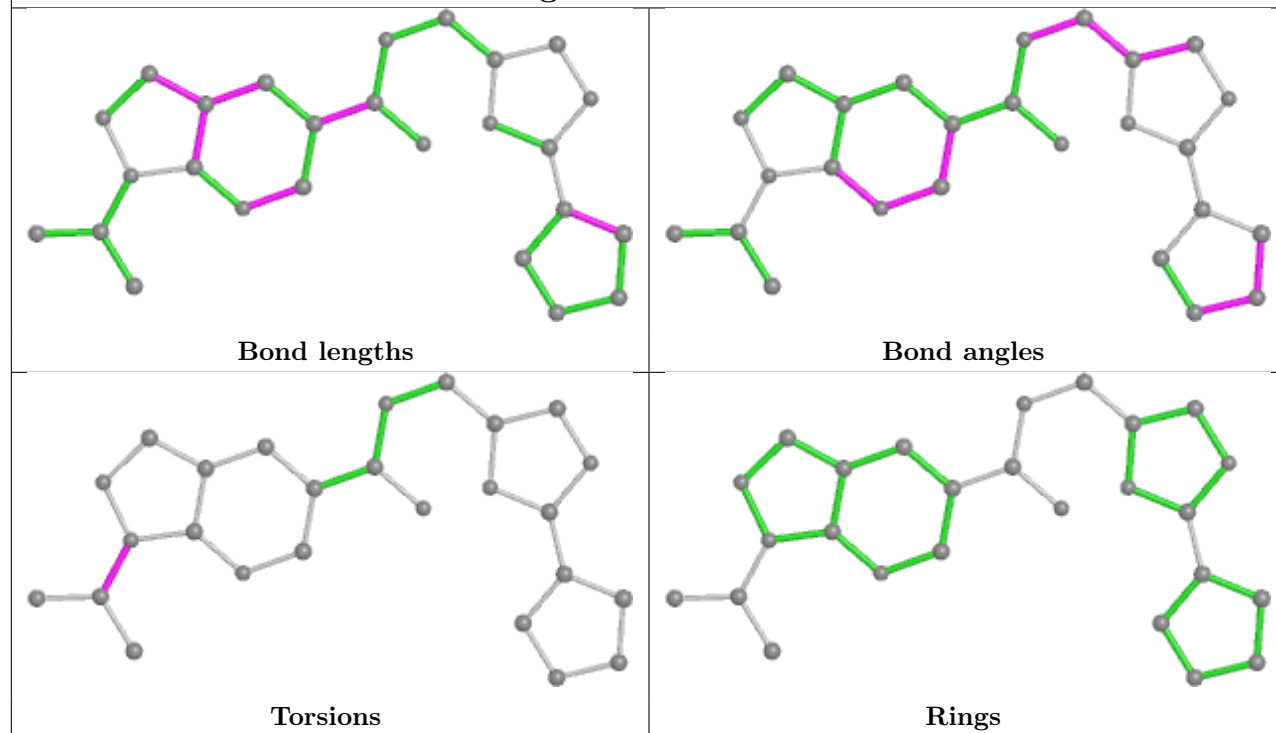
## Ligand 5C2 H 201



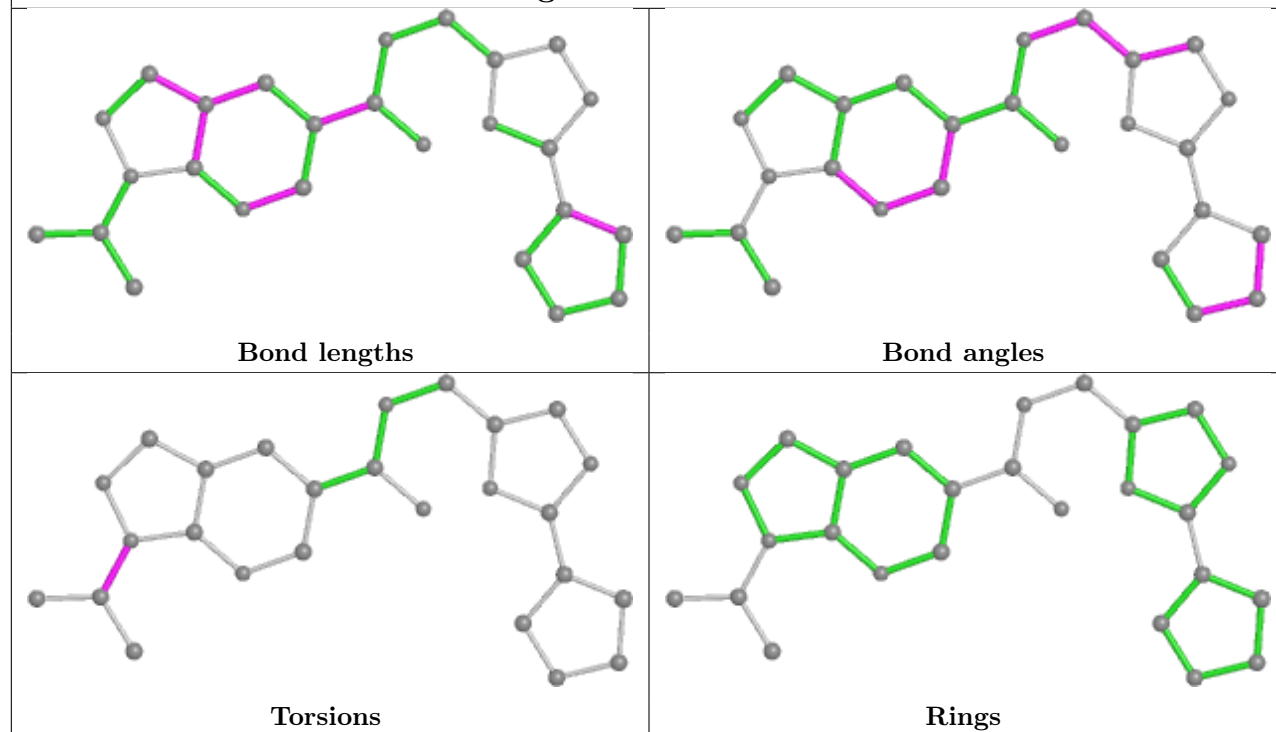
## Ligand 5C2 F 201



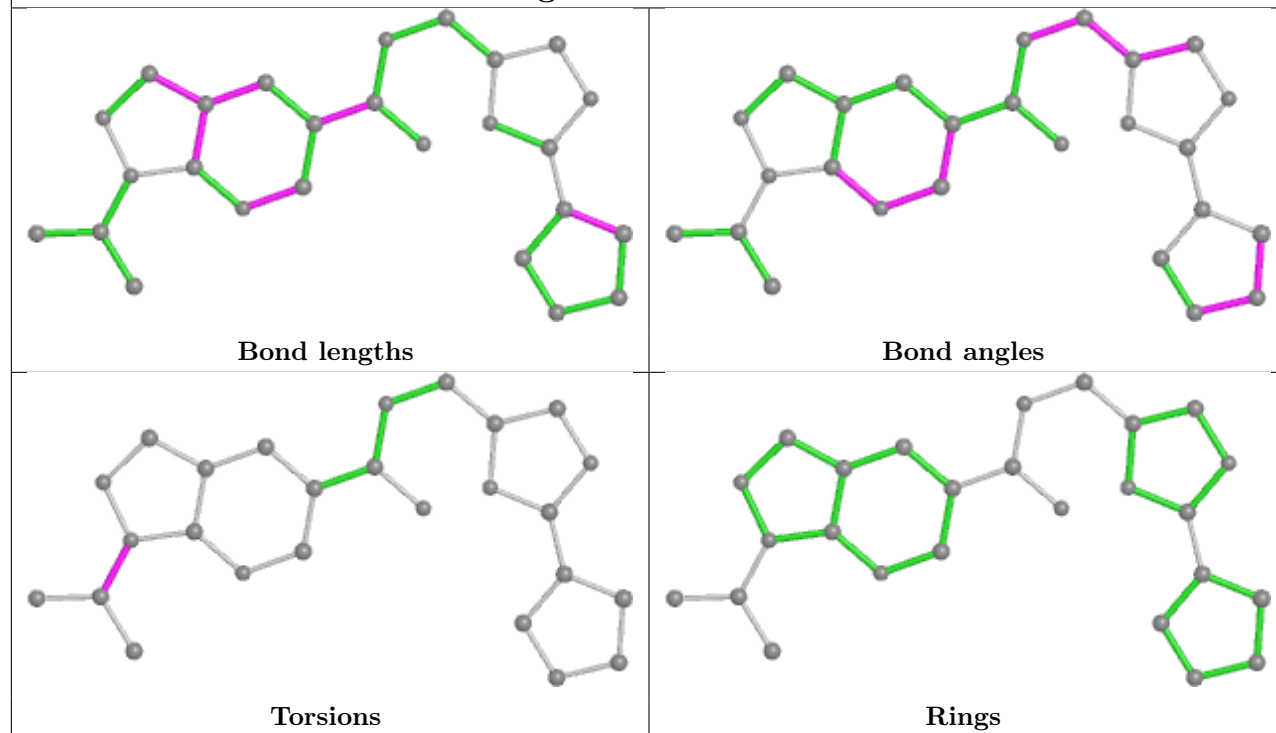
## Ligand 5C2 E 201



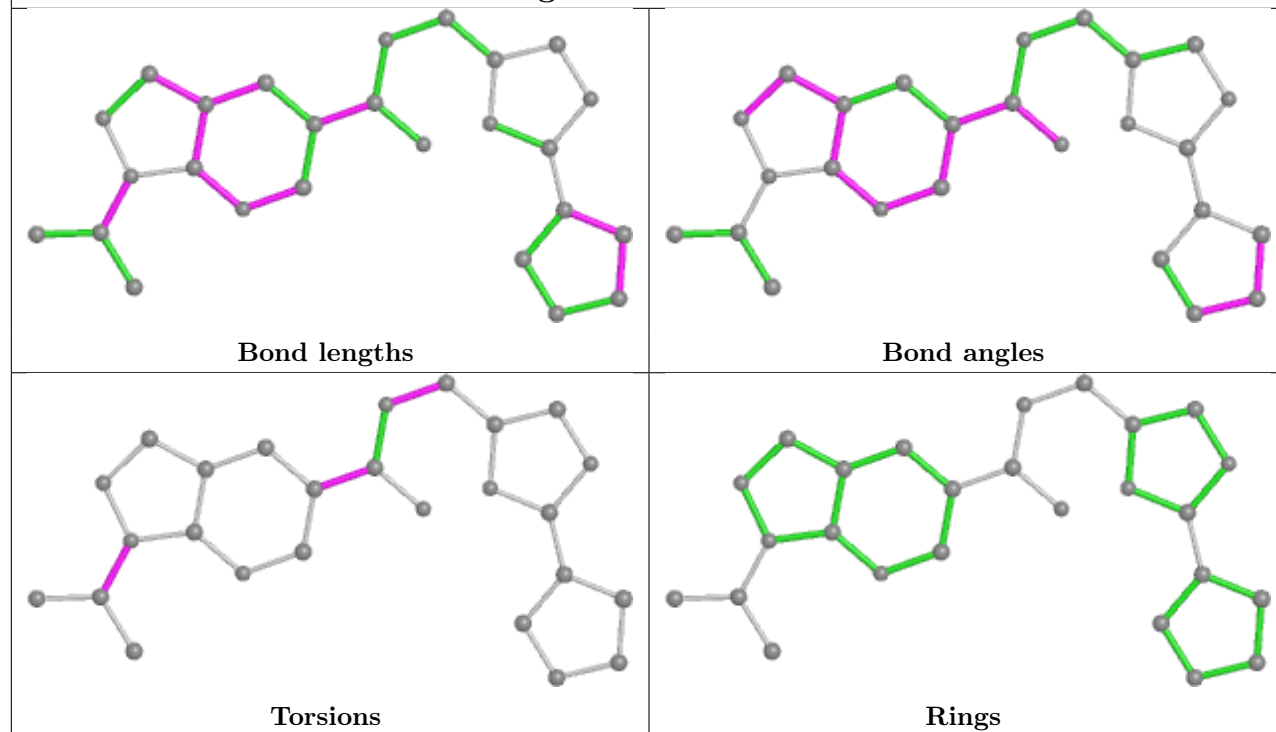
## Ligand 5C2 K 201

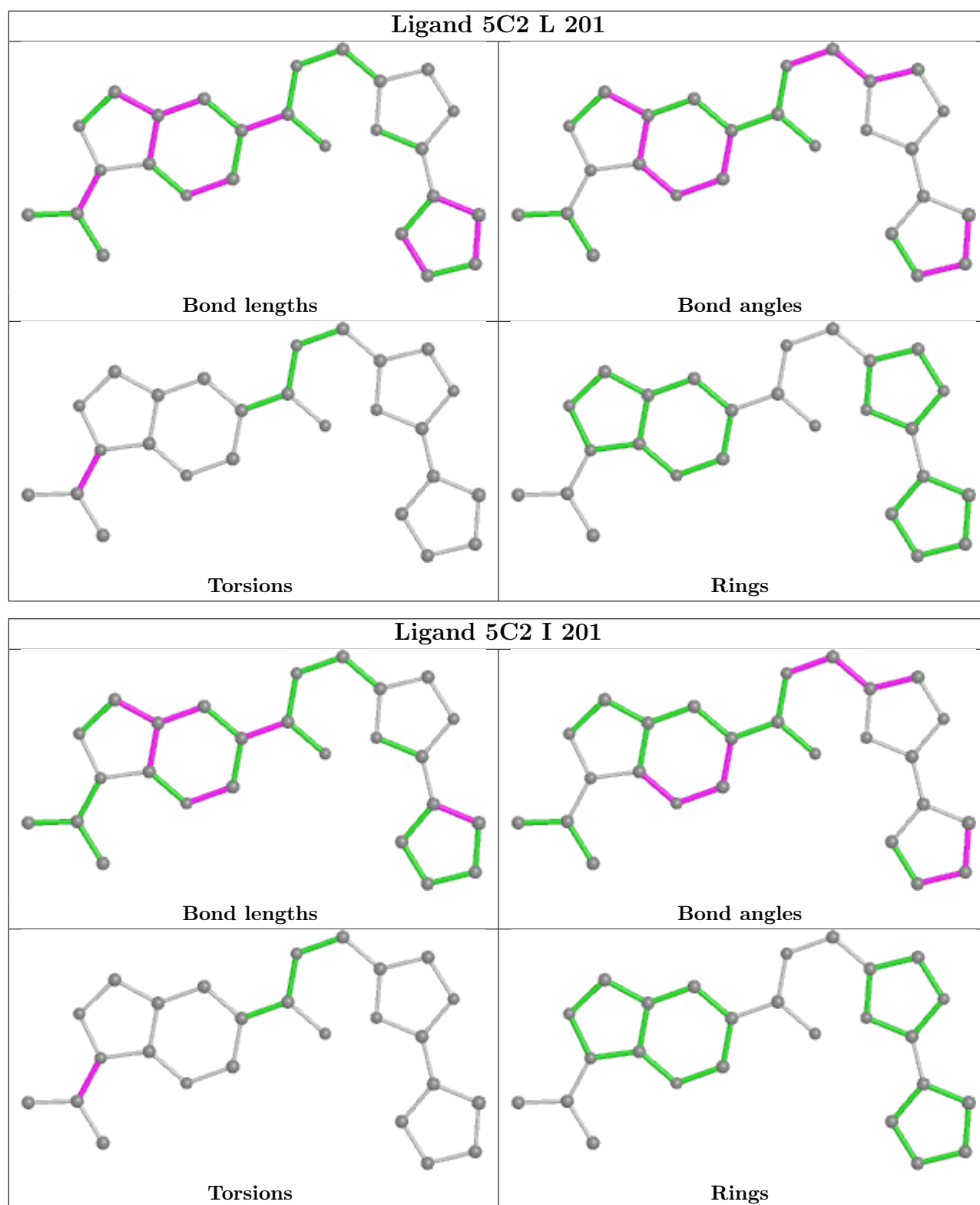


## Ligand 5C2 D 201



## Ligand 5C2 A 201





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	188/195 (96%)	-0.34	6 (3%)	47	20	58, 98, 167, 188	0
1	B	188/195 (96%)	-0.15	11 (5%)	22	7	57, 99, 179, 198	0
1	C	188/195 (96%)	0.14	15 (7%)	12	4	77, 119, 189, 208	0
1	D	188/195 (96%)	0.26	17 (9%)	9	3	82, 125, 201, 219	0
1	E	188/195 (96%)	0.14	15 (7%)	12	4	65, 113, 185, 203	0
1	F	188/195 (96%)	0.16	14 (7%)	14	4	76, 123, 194, 206	0
1	G	188/195 (96%)	0.14	11 (5%)	22	7	86, 131, 203, 215	0
1	H	188/195 (96%)	-0.23	9 (4%)	30	11	61, 103, 171, 195	0
1	I	188/195 (96%)	-0.04	13 (6%)	16	5	62, 106, 178, 200	0
1	J	188/195 (96%)	0.11	16 (8%)	10	3	65, 109, 189, 207	0
1	K	188/195 (96%)	0.13	18 (9%)	8	2	76, 117, 190, 204	0
1	L	188/195 (96%)	0.09	22 (11%)	4	1	62, 108, 190, 207	0
1	M	188/195 (96%)	-0.01	11 (5%)	22	7	70, 108, 187, 207	0
1	N	188/195 (96%)	0.01	10 (5%)	26	10	74, 113, 185, 203	0
All	All	2632/2730 (96%)	0.03	188 (7%)	16	5	57, 111, 188, 219	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	11	THR	10.1
1	D	133	ALA	7.6
1	K	193	GLU	7.1
1	F	15	GLU	6.9
1	E	10	THR	6.9
1	J	11	THR	6.5
1	L	129	ALA	6.1
1	C	127	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	127	GLY	6.1
1	M	127	GLY	5.9
1	I	130	GLN	5.8
1	C	15	GLU	5.7
1	J	130	GLN	5.5
1	E	127	GLY	5.5
1	N	15	GLU	5.5
1	I	15	GLU	5.4
1	J	10	THR	5.4
1	G	128	GLY	5.3
1	C	130	GLN	5.3
1	D	10	THR	5.1
1	E	129	ALA	5.1
1	K	129	ALA	5.0
1	J	15	GLU	5.0
1	M	130	GLN	5.0
1	J	129	ALA	4.9
1	D	132	GLN	4.9
1	L	132	GLN	4.8
1	F	193	GLU	4.8
1	N	133	ALA	4.8
1	M	129	ALA	4.7
1	B	130	GLN	4.6
1	L	11	THR	4.6
1	L	127	GLY	4.4
1	L	15	GLU	4.4
1	L	10	THR	4.4
1	C	132	GLN	4.4
1	F	10	THR	4.4
1	F	130	GLN	4.2
1	F	16	ARG	4.2
1	H	131	GLY	4.2
1	F	173	ASN	4.2
1	F	128	GLY	4.1
1	J	131	GLY	4.1
1	K	17	ALA	4.1
1	M	10	THR	4.1
1	D	128	GLY	4.1
1	A	127	GLY	4.1
1	E	15	GLU	4.0
1	N	127	GLY	4.0
1	K	127	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	129	ALA	3.9
1	D	3	LEU	3.8
1	L	128	GLY	3.8
1	E	130	GLN	3.8
1	I	131	GLY	3.7
1	I	129	ALA	3.7
1	B	10	THR	3.7
1	I	132	GLN	3.7
1	H	10	THR	3.6
1	D	170	ASP	3.6
1	I	135	GLU	3.6
1	C	128	GLY	3.6
1	B	193	GLU	3.6
1	E	192	PRO	3.5
1	D	130	GLN	3.5
1	D	193	GLU	3.5
1	L	9	GLU	3.5
1	G	127	GLY	3.5
1	E	131	GLY	3.5
1	L	130	GLN	3.5
1	H	132	GLN	3.4
1	N	130	GLN	3.4
1	D	129	ALA	3.4
1	J	3	LEU	3.4
1	J	126	LEU	3.4
1	M	137	GLU	3.4
1	N	16	ARG	3.4
1	M	15	GLU	3.3
1	A	129	ALA	3.3
1	F	127	GLY	3.3
1	I	173	ASN	3.3
1	L	188	GLU	3.3
1	L	17	ALA	3.2
1	J	133	ALA	3.2
1	F	17	ALA	3.2
1	H	130	GLN	3.2
1	C	10	THR	3.2
1	J	128	GLY	3.2
1	K	110	GLY	3.2
1	L	171	ARG	3.1
1	G	129	ALA	3.1
1	D	11	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	57	GLU	3.0
1	M	173	ASN	3.0
1	C	133	ALA	3.0
1	G	192	PRO	2.9
1	K	11	THR	2.9
1	C	131	GLY	2.9
1	H	133	ALA	2.9
1	I	10	THR	2.9
1	C	129	ALA	2.8
1	J	135	GLU	2.8
1	L	3	LEU	2.8
1	L	167	LYS	2.8
1	B	15	GLU	2.8
1	I	127	GLY	2.8
1	D	131	GLY	2.8
1	K	3	LEU	2.8
1	H	127	GLY	2.7
1	E	137	GLU	2.7
1	E	159	GLY	2.7
1	G	15	GLU	2.7
1	L	7	VAL	2.7
1	C	17	ALA	2.7
1	I	137	GLU	2.7
1	C	171	ARG	2.6
1	L	131	GLY	2.6
1	I	193	GLU	2.6
1	M	128	GLY	2.6
1	G	85	LYS	2.6
1	M	16	ARG	2.6
1	B	131	GLY	2.6
1	E	128	GLY	2.6
1	K	15	GLU	2.6
1	M	193	GLU	2.6
1	L	16	ARG	2.6
1	M	126	LEU	2.6
1	B	132	GLN	2.5
1	J	132	GLN	2.5
1	A	128	GLY	2.5
1	G	159	GLY	2.5
1	F	133	ALA	2.5
1	J	16	ARG	2.5
1	E	3	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	109	LYS	2.5
1	F	121	MET	2.5
1	K	125	PRO	2.5
1	B	129	ALA	2.5
1	I	134	THR	2.5
1	L	133	ALA	2.5
1	N	188	GLU	2.5
1	F	3	LEU	2.5
1	K	16	ARG	2.5
1	G	59	ASP	2.5
1	L	192	PRO	2.5
1	N	10	THR	2.5
1	N	11	THR	2.5
1	H	15	GLU	2.5
1	G	130	GLN	2.5
1	K	130	GLN	2.5
1	K	133	ALA	2.4
1	A	130	GLN	2.4
1	K	128	GLY	2.4
1	B	127	GLY	2.4
1	B	133	ALA	2.4
1	J	173	ASN	2.4
1	D	137	GLU	2.4
1	E	170	ASP	2.4
1	C	11	THR	2.4
1	J	127	GLY	2.4
1	A	16	ARG	2.3
1	L	8	ILE	2.3
1	D	87	ASP	2.3
1	F	132	GLN	2.3
1	D	171	ARG	2.2
1	H	128	GLY	2.2
1	N	129	ALA	2.2
1	A	3	LEU	2.2
1	N	193	GLU	2.2
1	E	109	LYS	2.2
1	C	135	GLU	2.2
1	L	57	GLU	2.2
1	C	192	PRO	2.1
1	K	171	ARG	2.1
1	B	171	ARG	2.1
1	I	11	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	17	ALA	2.1
1	E	193	GLU	2.1
1	D	188	GLU	2.1
1	G	3	LEU	2.1
1	G	188	GLU	2.1
1	K	159	GLY	2.1
1	L	193	GLU	2.0
1	J	17	ALA	2.0
1	K	134	THR	2.0
1	B	135	GLU	2.0
1	K	7	VAL	2.0
1	C	16	ARG	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 monosaccharides 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
2	5C2	D	201	26/26	0.82	0.33	116,126,137,138	0
2	5C2	E	201	26/26	0.83	0.37	111,116,127,132	0
2	5C2	H	201	26/26	0.83	0.29	97,109,121,123	0
2	5C2	M	201	26/26	0.83	0.44	103,115,129,132	0
2	5C2	J	201	26/26	0.84	0.32	110,119,131,134	0
2	5C2	G	201	26/26	0.86	0.26	118,127,137,141	0
2	5C2	C	201	26/26	0.87	0.28	112,123,133,136	0
2	5C2	K	201	26/26	0.87	0.24	109,117,128,130	0
2	5C2	F	201	26/26	0.87	0.33	116,126,133,135	0
2	5C2	L	201	26/26	0.90	0.21	101,106,119,124	0
2	5C2	I	201	26/26	0.91	0.20	108,113,121,125	0

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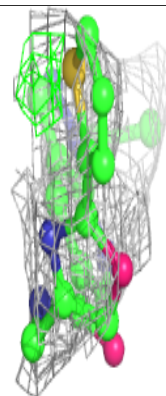
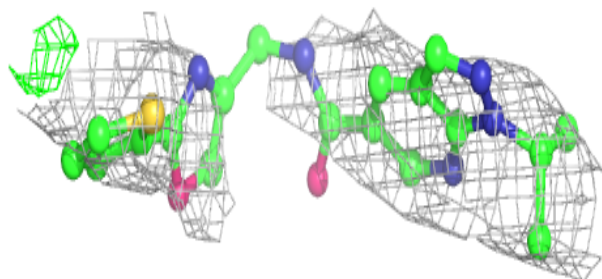
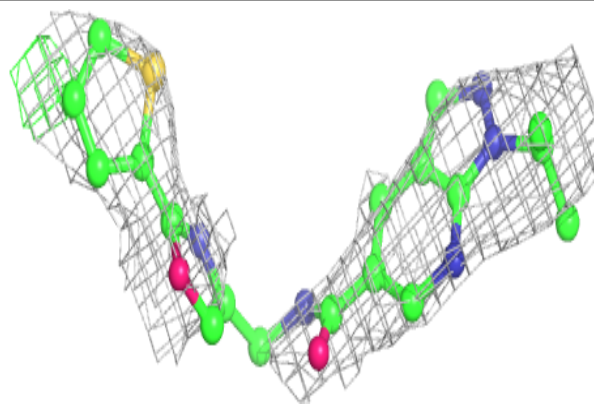
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	5C2	N	201	26/26	0.91	0.26	102,112,120,123	0
2	5C2	A	201	26/26	0.92	0.20	86,97,111,116	0
2	5C2	B	201	26/26	0.94	0.19	96,107,120,124	0

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.

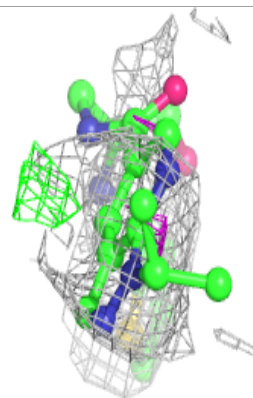
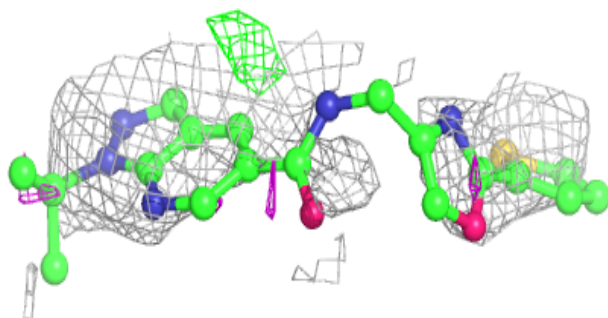
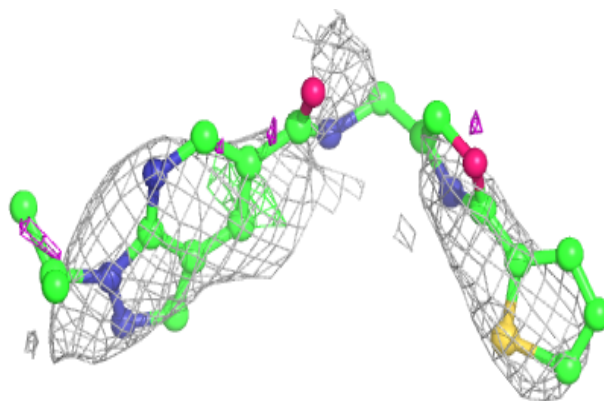
**Electron density around 5C2 D 201:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

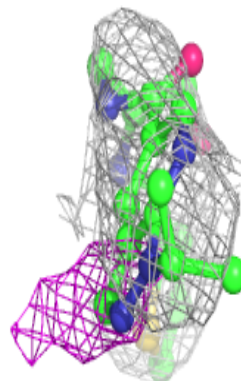
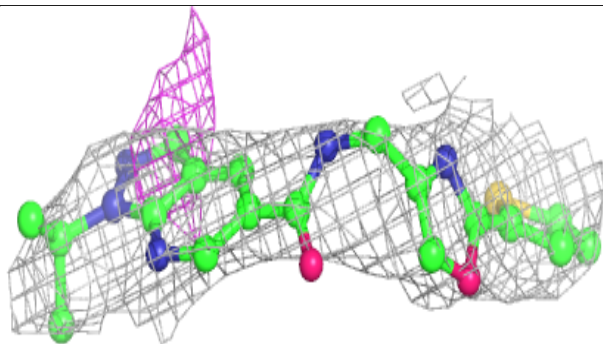
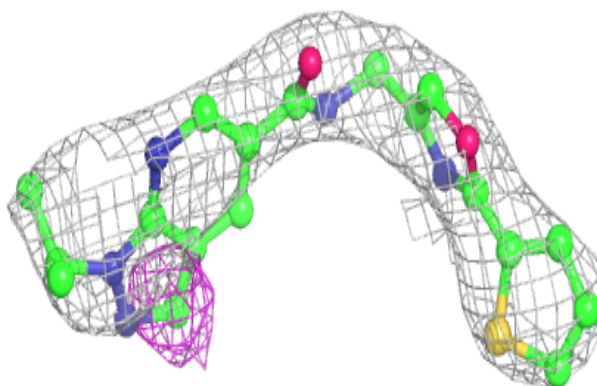


**Electron density around 5C2 E 201:**

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

**Electron density around 5C2 H 201:**

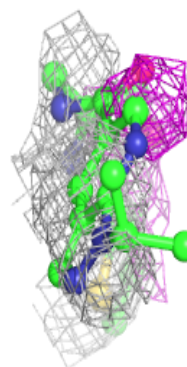
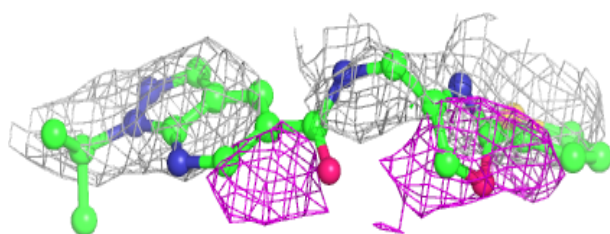
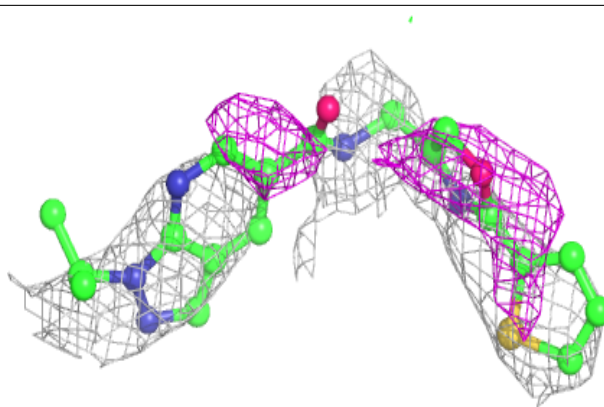
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



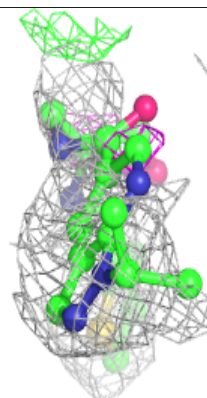
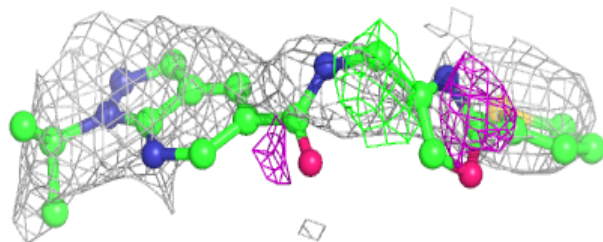
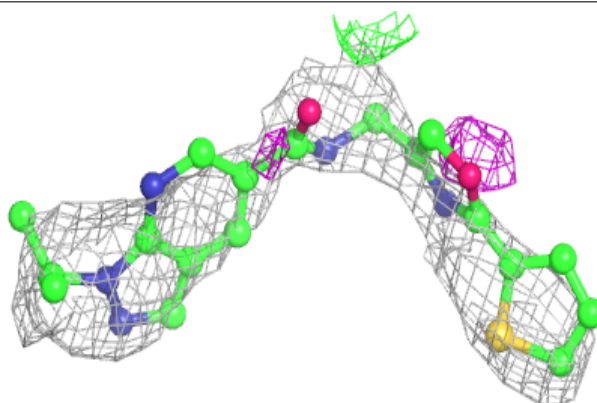


**Electron density around 5C2 M 201:**

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

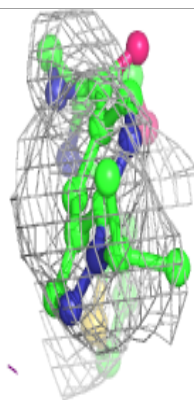
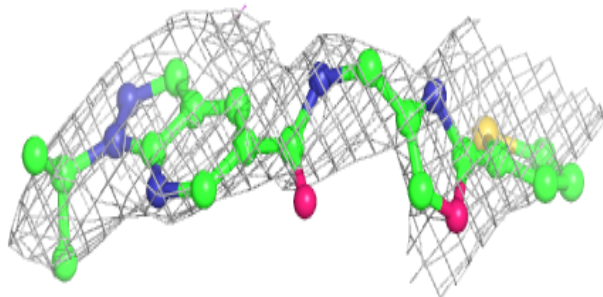
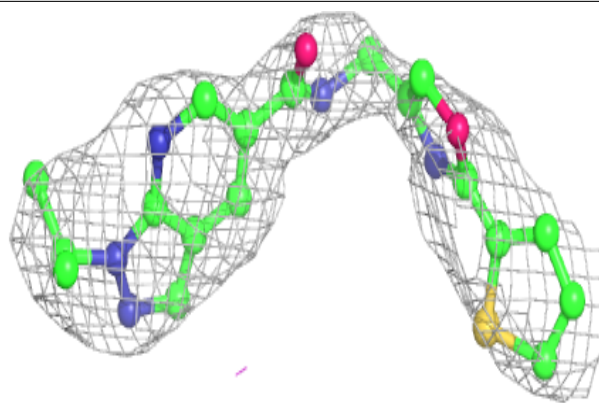
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and green (positive)

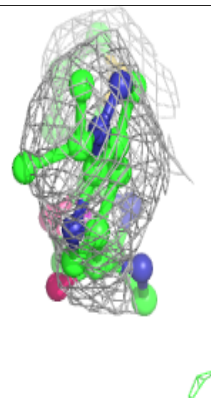
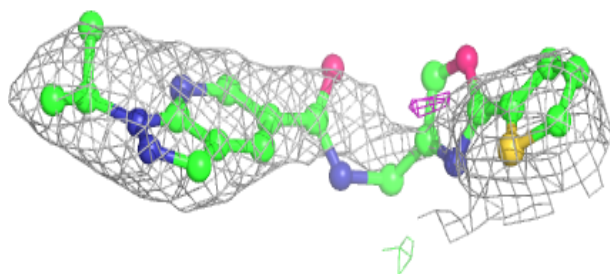
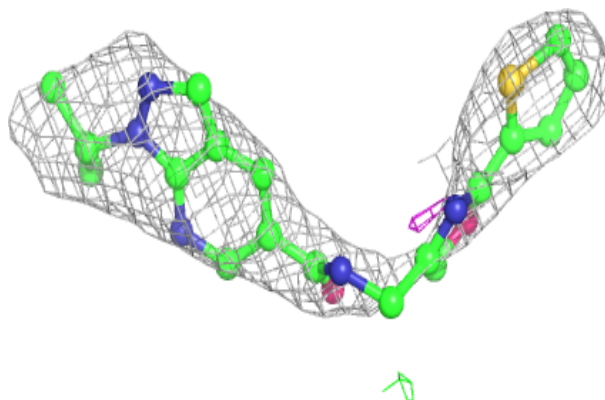


**Electron density around 5C2 G 201:**

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

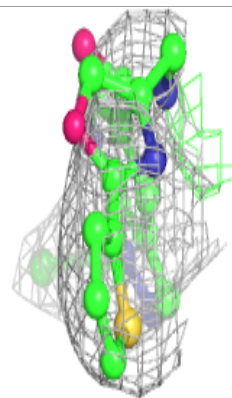
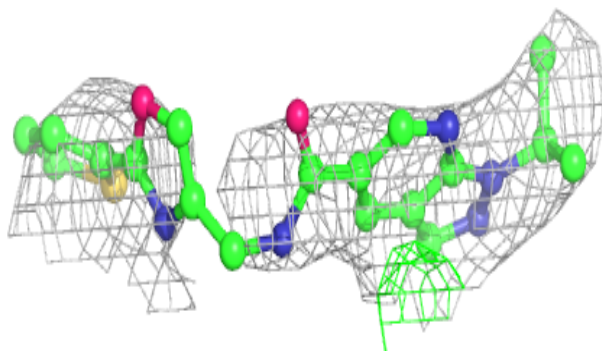
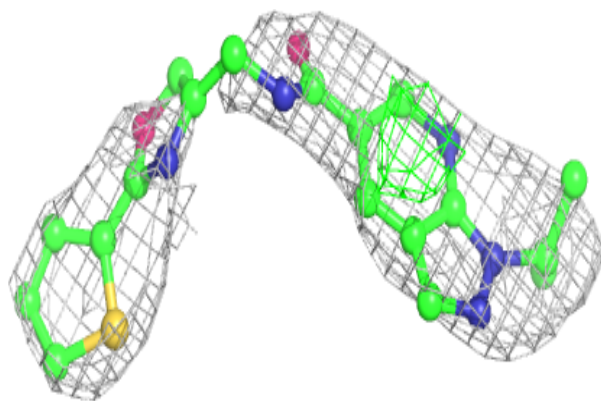
**Electron density around 5C2 C 201:**

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

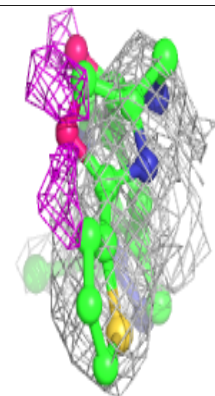
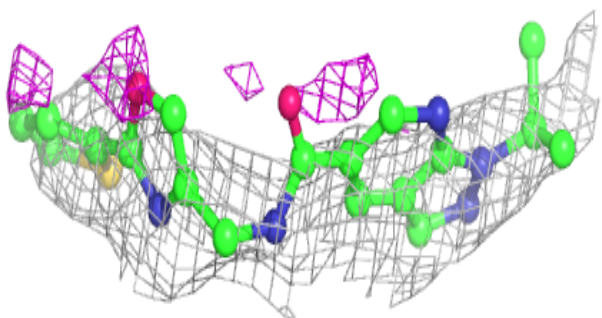
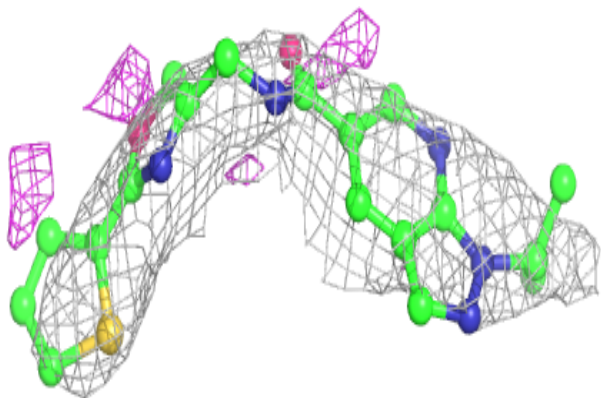


**Electron density around 5C2 K 201:**

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

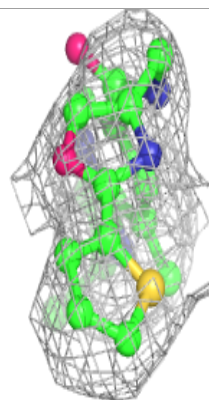
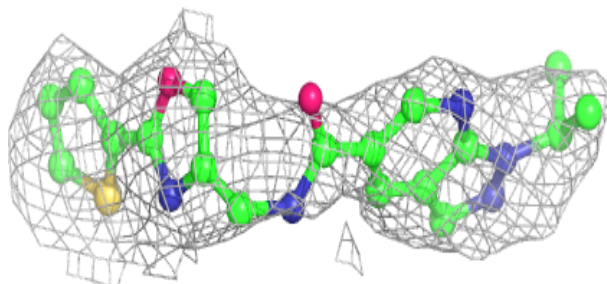
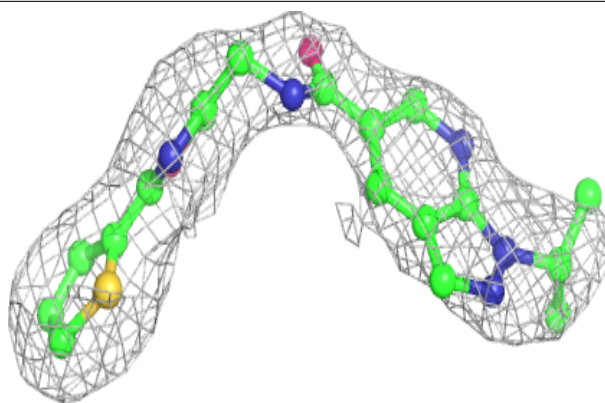
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and green (positive)

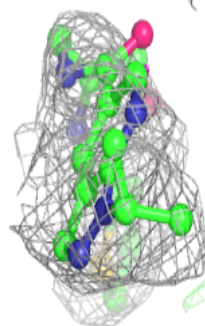
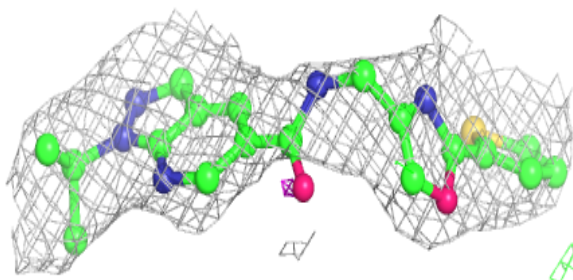
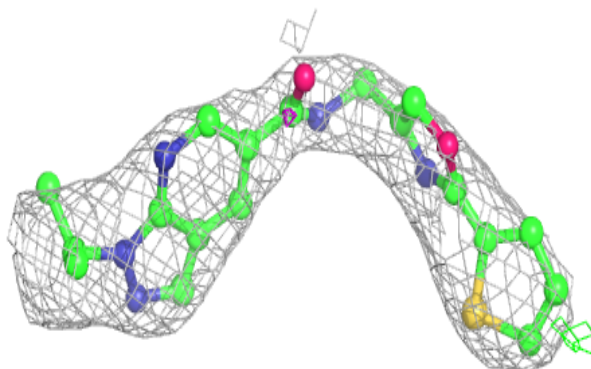


**Electron density around 5C2 L 201:**

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

**Electron density around 5C2 I 201:**

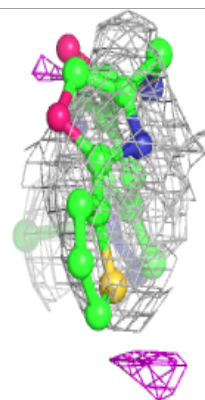
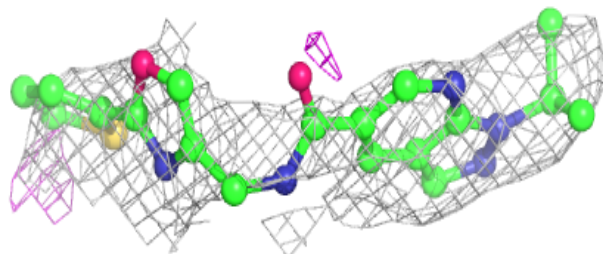
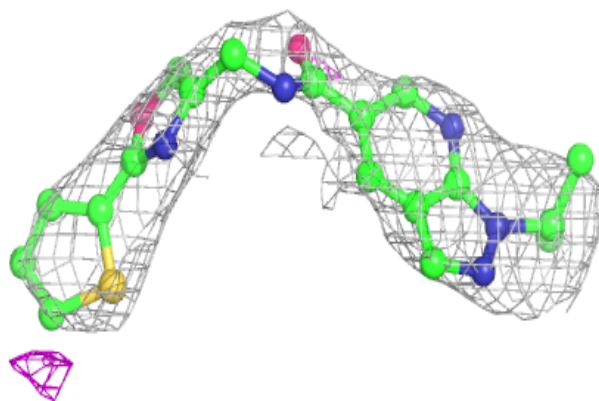
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



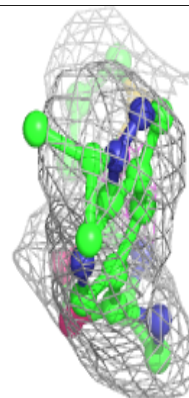
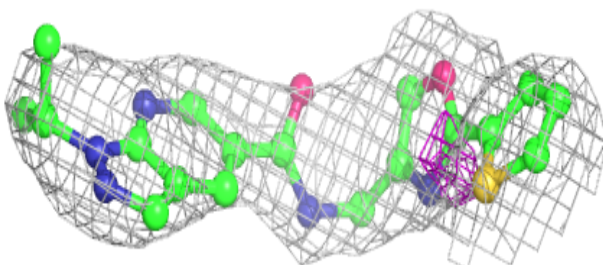
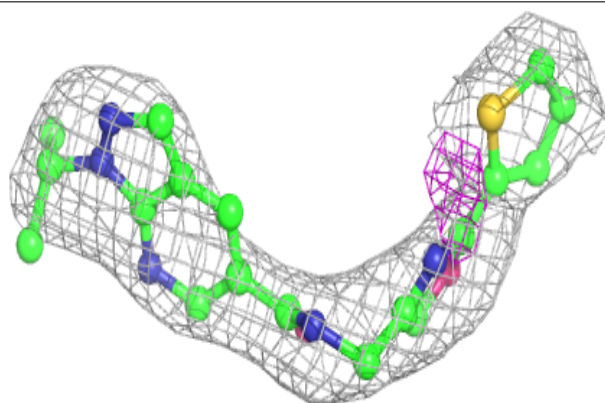


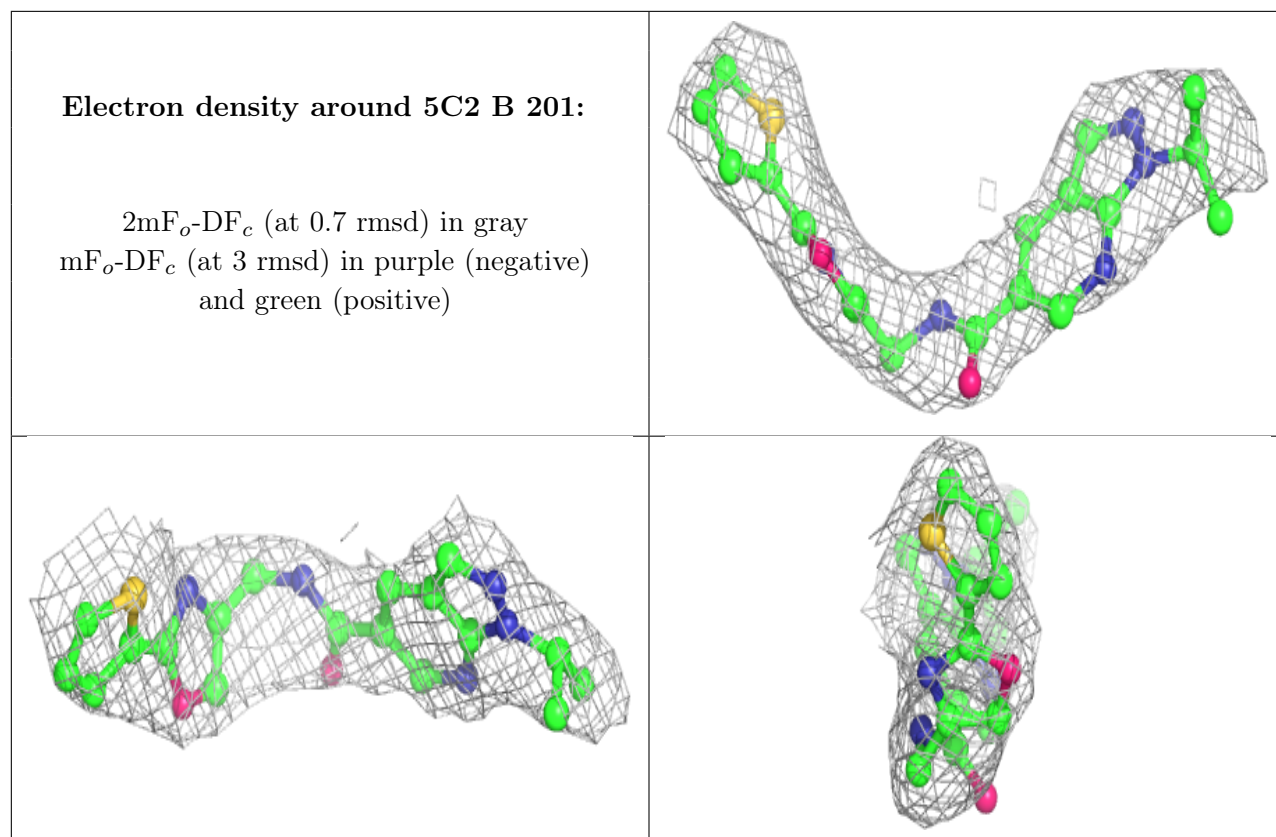
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and green (positive)

**Electron density around 5C2 A 201:**

$2mF_o-DF_c$  (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.