



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:09 PM UTC

PDB ID : 9PGV / pdb\_00009pgv  
Title : HIV Capsid Hexamer bound to Compound 24  
Authors : Somoza, J.R.; Anderson, R.L.; Villasenor, A.G.; Ferrao, R.D.  
Deposited on : 2025-07-08  
Resolution : 2.30 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

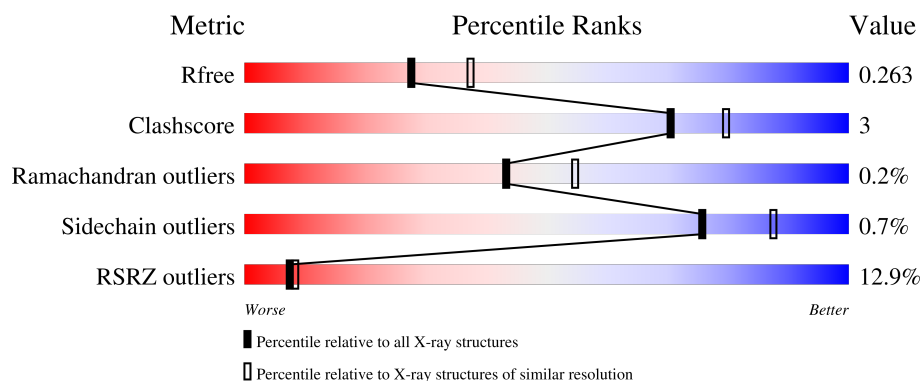
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	232	<div> <div>19%</div> <div> <div>75%</div> <div>16%</div> <div>9%</div> </div> </div>
1	B	232	<div> <div>8%</div> <div> <div>80%</div> <div>9%</div> <div>10%</div> </div> </div>
1	C	232	<div> <div>6%</div> <div> <div>85%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	232	<div> <div>6%</div> <div> <div>80%</div> <div>7%</div> <div>13%</div> </div> </div>
1	E	232	<div> <div>19%</div> <div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	232	
1	G	232	
1	H	232	
1	I	232	
1	J	232	
1	K	232	
1	L	232	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20187 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 HIV-1 capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1621	1022	281	304	14			
1	B	208	Total	C	N	O	S	0	0	0
			1602	1007	280	301	14			
1	C	207	Total	C	N	O	S	0	0	0
			1605	1009	280	302	14			
1	D	202	Total	C	N	O	S	0	0	0
			1567	988	272	293	14			
1	E	211	Total	C	N	O	S	0	0	0
			1619	1021	281	303	14			
1	F	218	Total	C	N	O	S	0	0	0
			1674	1051	293	316	14			
1	G	203	Total	C	N	O	S	0	0	0
			1580	995	276	295	14			
1	H	213	Total	C	N	O	S	0	0	0
			1640	1031	287	308	14			
1	I	211	Total	C	N	O	S	0	0	0
			1621	1022	282	303	14			
1	J	213	Total	C	N	O	S	0	0	0
			1639	1032	286	307	14			
1	K	204	Total	C	N	O	S	0	0	0
			1578	994	274	296	14			
1	L	212	Total	C	N	O	S	0	0	0
			1629	1026	283	306	14			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP B6DRA0
A	14	CYS	ALA	conflict	UNP B6DRA0
A	45	CYS	GLU	conflict	UNP B6DRA0
A	184	ALA	TRP	conflict	UNP B6DRA0
A	185	ALA	MET	conflict	UNP B6DRA0

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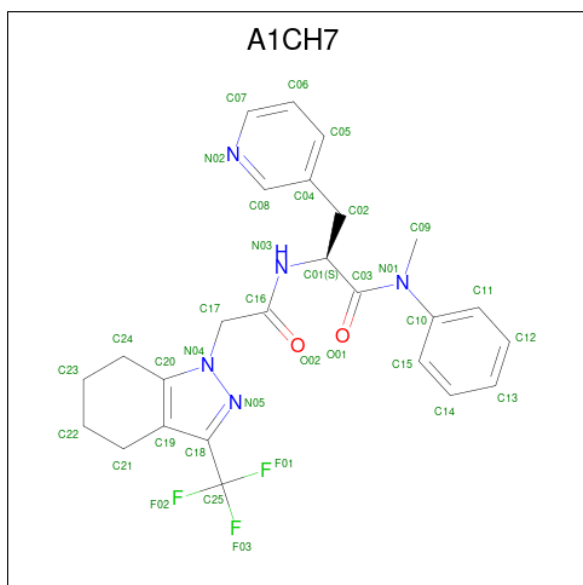
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP B6DRA0
B	14	CYS	ALA	conflict	UNP B6DRA0
B	45	CYS	GLU	conflict	UNP B6DRA0
B	184	ALA	TRP	conflict	UNP B6DRA0
B	185	ALA	MET	conflict	UNP B6DRA0
C	0	MET	-	initiating methionine	UNP B6DRA0
C	14	CYS	ALA	conflict	UNP B6DRA0
C	45	CYS	GLU	conflict	UNP B6DRA0
C	184	ALA	TRP	conflict	UNP B6DRA0
C	185	ALA	MET	conflict	UNP B6DRA0
D	0	MET	-	initiating methionine	UNP B6DRA0
D	14	CYS	ALA	conflict	UNP B6DRA0
D	45	CYS	GLU	conflict	UNP B6DRA0
D	184	ALA	TRP	conflict	UNP B6DRA0
D	185	ALA	MET	conflict	UNP B6DRA0
E	0	MET	-	initiating methionine	UNP B6DRA0
E	14	CYS	ALA	conflict	UNP B6DRA0
E	45	CYS	GLU	conflict	UNP B6DRA0
E	184	ALA	TRP	conflict	UNP B6DRA0
E	185	ALA	MET	conflict	UNP B6DRA0
F	0	MET	-	initiating methionine	UNP B6DRA0
F	14	CYS	ALA	conflict	UNP B6DRA0
F	45	CYS	GLU	conflict	UNP B6DRA0
F	184	ALA	TRP	conflict	UNP B6DRA0
F	185	ALA	MET	conflict	UNP B6DRA0
G	0	MET	-	initiating methionine	UNP B6DRA0
G	14	CYS	ALA	conflict	UNP B6DRA0
G	45	CYS	GLU	conflict	UNP B6DRA0
G	184	ALA	TRP	conflict	UNP B6DRA0
G	185	ALA	MET	conflict	UNP B6DRA0
H	0	MET	-	initiating methionine	UNP B6DRA0
H	14	CYS	ALA	conflict	UNP B6DRA0
H	45	CYS	GLU	conflict	UNP B6DRA0
H	184	ALA	TRP	conflict	UNP B6DRA0
H	185	ALA	MET	conflict	UNP B6DRA0
I	0	MET	-	initiating methionine	UNP B6DRA0
I	14	CYS	ALA	conflict	UNP B6DRA0
I	45	CYS	GLU	conflict	UNP B6DRA0
I	184	ALA	TRP	conflict	UNP B6DRA0
I	185	ALA	MET	conflict	UNP B6DRA0
J	0	MET	-	initiating methionine	UNP B6DRA0
J	14	CYS	ALA	conflict	UNP B6DRA0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	45	CYS	GLU	conflict	UNP B6DRA0
J	184	ALA	TRP	conflict	UNP B6DRA0
J	185	ALA	MET	conflict	UNP B6DRA0
K	0	MET	-	initiating methionine	UNP B6DRA0
K	14	CYS	ALA	conflict	UNP B6DRA0
K	45	CYS	GLU	conflict	UNP B6DRA0
K	184	ALA	TRP	conflict	UNP B6DRA0
K	185	ALA	MET	conflict	UNP B6DRA0
L	0	MET	-	initiating methionine	UNP B6DRA0
L	14	CYS	ALA	conflict	UNP B6DRA0
L	45	CYS	GLU	conflict	UNP B6DRA0
L	184	ALA	TRP	conflict	UNP B6DRA0
L	185	ALA	MET	conflict	UNP B6DRA0

- Molecule 2 is N-methyl-N-phenyl-3-(pyridin-3-yl)-N 2 -{[3-(trifluoromethyl)-4,5,6,7-tetrahydro-1H-indazol-1-yl]acetyl}-L-alaninamide (CCD ID: A1CH7) (formula: C<sub>25</sub>H<sub>26</sub>F<sub>3</sub>N<sub>5</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			35	25	3	5	2		
2	B	1	Total	C	F	N	O	0	0
			35	25	3	5	2		
2	C	1	Total	C	F	N	O	0	0
			35	25	3	5	2		
2	D	1	Total	C	F	N	O	0	0
			35	25	3	5	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	F	N	O	0	0
			35	25	3	5	2		
2	F	1	Total	C	F	N	O	0	0
			35	25	3	5	2		
2	G	1	Total	C	F	N	O	0	0
			35	25	3	5	2		
2	H	1	Total	C	F	N	O	0	0
			35	25	3	5	2		
2	I	1	Total	C	F	N	O	0	0
			35	25	3	5	2		
2	J	1	Total	C	F	N	O	0	0
			35	25	3	5	2		
2	K	1	Total	C	F	N	O	0	0
			35	25	3	5	2		
2	L	1	Total	C	F	N	O	0	0
			35	25	3	5	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	37	Total	O	0	0
			37	37		
3	C	32	Total	O	0	0
			32	32		
3	D	51	Total	O	0	0
			51	51		
3	E	35	Total	O	0	0
			35	35		
3	F	47	Total	O	0	0
			47	47		
3	G	30	Total	O	0	0
			30	30		
3	H	38	Total	O	0	0
			38	38		
3	I	25	Total	O	0	0
			25	25		
3	J	21	Total	O	0	0
			21	21		
3	K	17	Total	O	0	0
			17	17		

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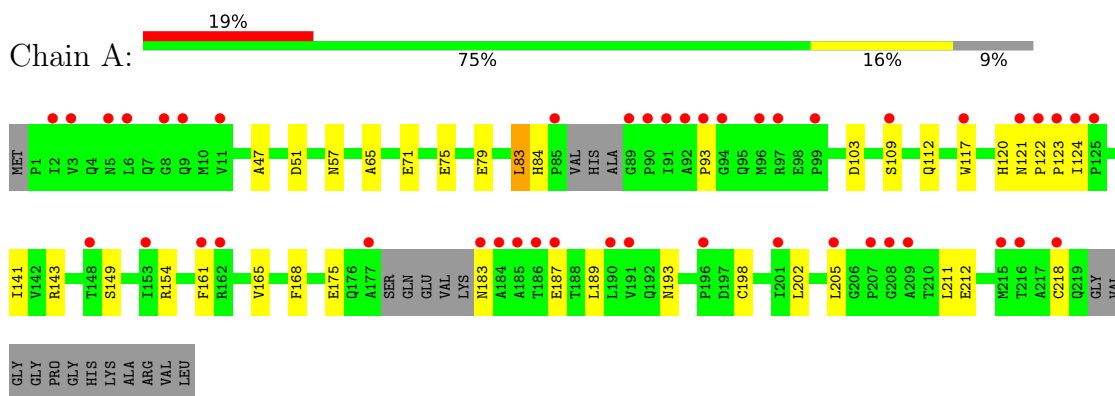
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	31	Total	O	0	0
			31	31		

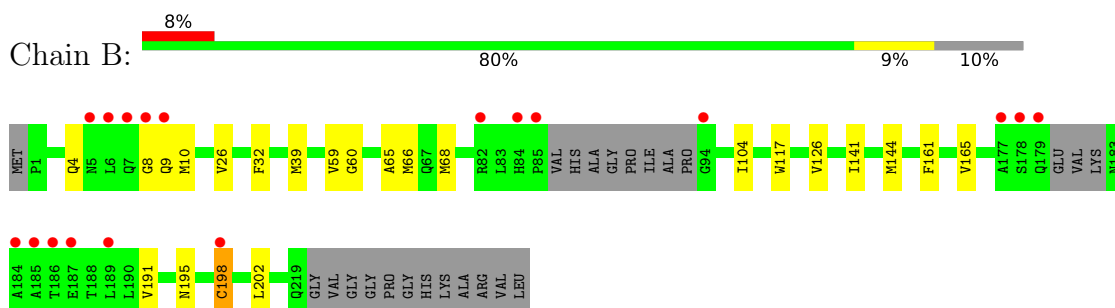
### 3 Residue-property plots [i](#)

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.

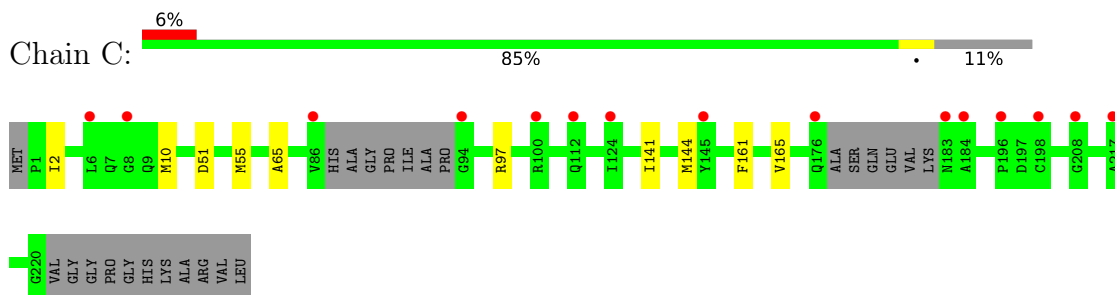
- Molecule 1: HIV-1 capsid



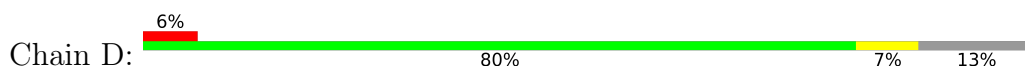
- Molecule 1: HIV-1 capsid

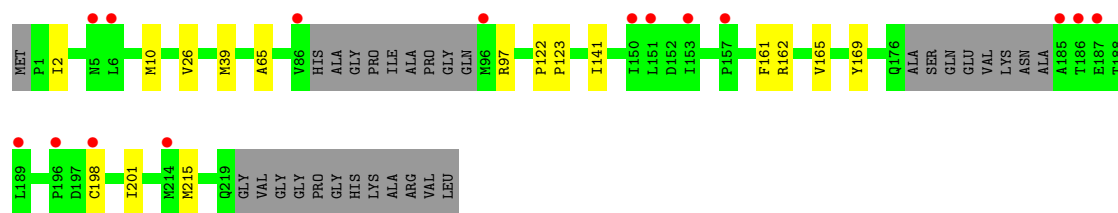


- Molecule 1: HIV-1 capsid

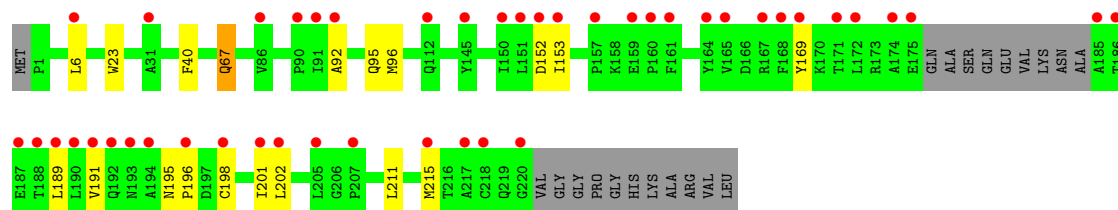
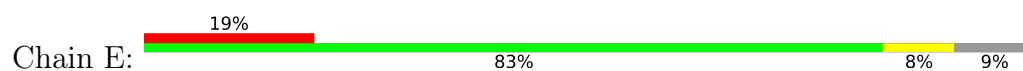


- Molecule 1: HIV-1 capsid

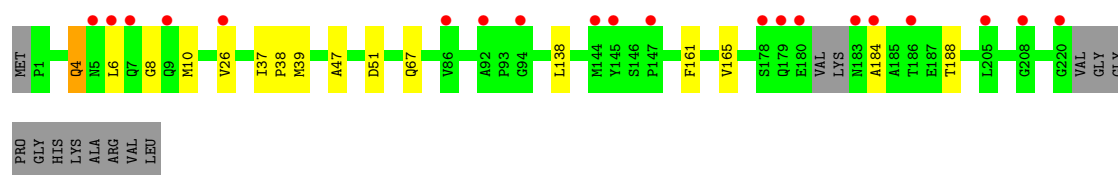
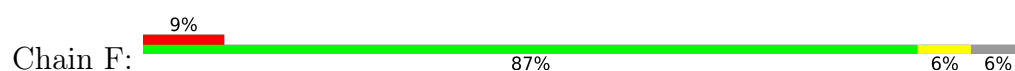




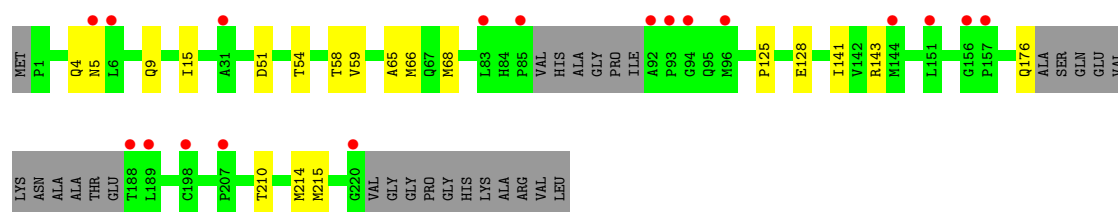
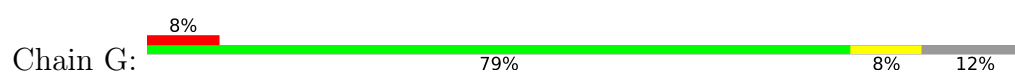
● Molecule 1: HIV-1 capsid



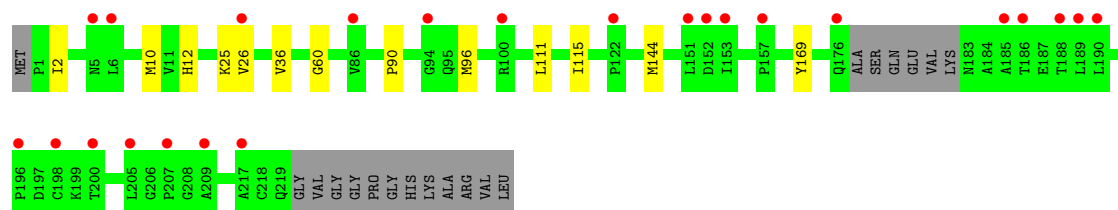
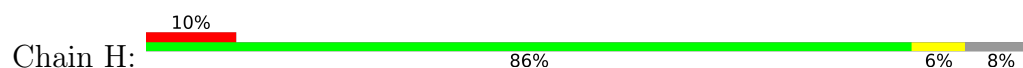
● Molecule 1: HIV-1 capsid




● Molecule 1: HIV-1 capsid

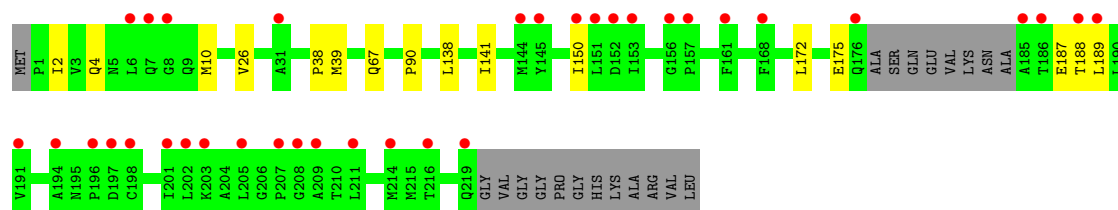


● Molecule 1: HIV-1 capsid




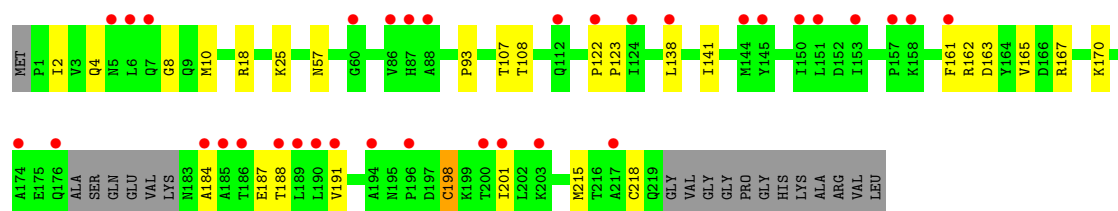
- Molecule 1: HIV-1 capsid

Chain I: 




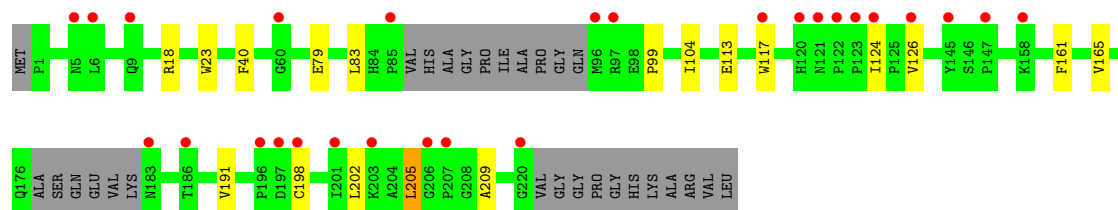
- Molecule 1: HIV-1 capsid

Chain J: 




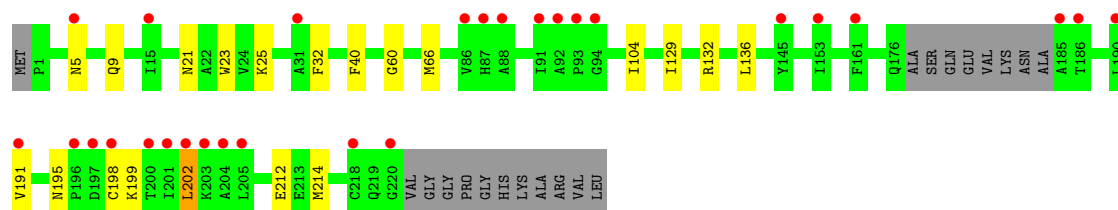
- Molecule 1: HIV-1 capsid

Chain K: 



- Molecule 1: HIV-1 capsid

Chain L: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.74Å 156.55Å 119.23Å 90.00° 97.05° 90.00°	Depositor
Resolution (Å)	47.51 – 2.30 47.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.51-2.30) 91.2 (47.51-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.60 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.232 , 0.263 0.232 , 0.263	Depositor DCC
$R_{free}$ test set	2000 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: A1CH7

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.15	0/1655	0.33	0/2250
1	B	0.12	0/1634	0.30	0/2219
1	C	0.08	0/1637	0.22	0/2222
1	D	0.09	0/1599	0.24	0/2172
1	E	0.10	0/1655	0.26	0/2252
1	F	0.11	0/1710	0.25	0/2325
1	G	0.10	0/1613	0.25	0/2189
1	H	0.10	0/1676	0.24	0/2280
1	I	0.08	0/1657	0.22	0/2255
1	J	0.09	0/1675	0.23	0/2279
1	K	0.09	0/1610	0.25	0/2186
1	L	0.09	0/1664	0.25	0/2263
All	All	0.10	0/19785	0.26	0/26892

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	1621	0	1603	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1602	0	1586	15	0
1	C	1605	0	1594	6	0
1	D	1567	0	1551	10	0
1	E	1619	0	1598	12	0
1	F	1674	0	1653	10	0
1	G	1580	0	1577	12	0
1	H	1640	0	1615	11	0
1	I	1621	0	1598	10	0
1	J	1639	0	1617	17	0
1	K	1578	0	1564	12	0
1	L	1629	0	1610	12	0
2	A	35	0	0	0	0
2	B	35	0	0	0	0
2	C	35	0	0	0	0
2	D	70	0	0	0	0
2	F	35	0	0	0	0
2	G	35	0	0	0	0
2	H	35	0	0	0	0
2	I	35	0	0	0	0
2	J	35	0	0	0	0
2	K	35	0	0	0	0
2	L	35	0	0	0	0
3	A	28	0	0	0	0
3	B	37	0	0	0	0
3	C	32	0	0	0	0
3	D	51	0	0	0	0
3	E	35	0	0	0	0
3	F	47	0	0	0	0
3	G	30	0	0	0	0
3	H	38	0	0	0	0
3	I	25	0	0	0	0
3	J	21	0	0	0	0
3	K	17	0	0	0	0
3	L	31	0	0	0	0
All	All	20187	0	19166	132	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 3.

All (132) 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:59:VAL:HG11	1:G:66:MET:HE3	1.67	0.76
1:A:212:GLU:HG3	1:B:144:MET:HE1	1.68	0.75
1:G:5:ASN:HD22	1:G:9:GLN:HE21	1.35	0.75
1:G:143:ARG:HD3	1:G:176:GLN:HE22	1.55	0.72
1:B:59:VAL:HG11	1:B:66:MET:HE3	1.72	0.72
1:B:26:VAL:HG21	1:B:39:MET:HG2	1.75	0.69
1:L:202:LEU:HD11	1:L:214:MET:HG3	1.74	0.69
1:A:83:LEU:HD12	1:A:84:HIS:CE1	2.33	0.63
1:J:138:LEU:HD23	1:J:141:ILE:HD12	1.79	0.62
1:F:37:ILE:HD12	1:F:138:LEU:HB3	1.80	0.62
1:G:143:ARG:HH11	1:G:176:GLN:HE22	1.46	0.61
1:G:215:MET:HE2	1:H:144:MET:HE1	1.83	0.61
1:A:211:LEU:HD22	1:B:68:MET:HG3	1.82	0.60
1:D:2:ILE:HG22	1:D:10:MET:HE3	1.84	0.59
1:D:198:CYS:HA	1:D:201:ILE:HD12	1.84	0.59
1:E:6:LEU:HD11	1:F:6:LEU:HB2	1.83	0.59
1:D:26:VAL:HG21	1:D:39:MET:HG2	1.83	0.58
1:A:168:PHE:HE1	1:A:189:LEU:HD12	1.68	0.57
1:H:111:LEU:O	1:H:115:ILE:HG12	2.06	0.56
1:D:97:ARG:HB2	1:H:90:PRO:HB2	1.89	0.55
1:B:4:GLN:HB3	1:B:10:MET:SD	2.46	0.55
1:E:92:ALA:HB3	1:E:95:GLN:HG3	1.88	0.54
1:A:112:GLN:H	1:A:112:GLN:CD	2.16	0.54
1:A:161:PHE:O	1:A:165:VAL:HG23	2.09	0.53
1:H:26:VAL:HG12	1:H:36:VAL:HG23	1.91	0.53
1:G:143:ARG:HH11	1:G:176:GLN:NE2	2.08	0.51
1:J:2:ILE:HG22	1:J:10:MET:HE3	1.92	0.51
1:A:93:PRO:HG2	1:K:113:GLU:HG2	1.92	0.51
1:A:93:PRO:HG3	1:K:117:TRP:CZ2	2.46	0.51
1:C:2:ILE:HG22	1:C:10:MET:HE3	1.93	0.51
1:L:191:VAL:O	1:L:199:LYS:HD3	2.11	0.50
1:I:2:ILE:HG22	1:I:10:MET:HE3	1.94	0.50
1:J:198:CYS:HA	1:J:201:ILE:HD12	1.92	0.50
1:C:65:ALA:HB1	1:C:141:ILE:HD13	1.93	0.50
1:G:125:PRO:HB2	1:G:128:GLU:HB2	1.93	0.50
1:F:161:PHE:O	1:F:165:VAL:HG23	2.12	0.48
1:F:26:VAL:HG21	1:F:39:MET:HG2	1.94	0.48
1:J:18:ARG:NE	1:K:18:ARG:HH21	2.10	0.48
1:J:107:THR:HG23	1:J:108:THR:HG23	1.94	0.48
1:E:198:CYS:HA	1:E:201:ILE:HD12	1.96	0.48
1:F:4:GLN:HG2	1:F:10:MET:SD	2.55	0.47
1:A:183:ASN:O	1:A:187:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:162:ARG:HA	1:J:215:MET:HE3	1.97	0.47
1:B:195:ASN:OD1	1:B:198:CYS:HB3	2.15	0.47
1:D:162:ARG:HB2	1:D:215:MET:HE3	1.97	0.47
1:I:150:ILE:HD12	1:I:172:LEU:HB2	1.97	0.47
1:K:79:GLU:O	1:K:83:LEU:HG	2.16	0.46
1:K:124:ILE:HG22	1:K:126:VAL:HG13	1.98	0.46
1:G:210:THR:O	1:G:214:MET:HG3	2.15	0.46
1:A:117:TRP:CD1	1:A:124:ILE:HD12	2.51	0.46
1:F:184:ALA:O	1:F:188:THR:HG23	2.16	0.46
1:G:65:ALA:HB1	1:G:141:ILE:HD13	1.98	0.46
1:L:202:LEU:CD1	1:L:214:MET:HG3	2.46	0.46
1:A:71:GLU:O	1:A:75:GLU:HG3	2.16	0.46
1:K:205:LEU:HD12	1:K:209:ALA:HB2	1.98	0.46
1:K:99:PRO:HG3	1:K:124:ILE:HG21	1.96	0.45
1:H:2:ILE:HG22	1:H:10:MET:HE3	1.98	0.45
1:A:154:ARG:HA	1:A:193:ASN:HB3	1.99	0.45
1:B:161:PHE:O	1:B:165:VAL:HG23	2.17	0.45
1:H:12:HIS:HB2	1:H:115:ILE:HD12	1.99	0.45
1:I:187:GLU:OE2	1:I:188:THR:HG23	2.17	0.45
1:C:97:ARG:HB2	1:I:90:PRO:HB2	1.98	0.44
1:K:198:CYS:O	1:K:202:LEU:HG	2.17	0.44
1:J:122:PRO:HA	1:J:123:PRO:HD3	1.89	0.44
1:L:195:ASN:OD1	1:L:198:CYS:HB3	2.17	0.44
1:A:120:HIS:ND1	1:A:122:PRO:HD2	2.33	0.44
1:H:25:LYS:HD3	1:H:25:LYS:HA	1.68	0.44
1:A:47:ALA:HB1	1:A:51:ASP:HB2	1.99	0.44
1:D:161:PHE:O	1:D:165:VAL:HG23	2.17	0.44
1:G:68:MET:HE3	1:L:212:GLU:HB2	2.00	0.44
1:J:4:GLN:HE21	1:J:8:GLY:HA2	1.82	0.44
1:K:23:TRP:CZ3	1:K:40:PHE:HB2	2.53	0.43
1:C:144:MET:HE2	1:C:144:MET:HB2	1.64	0.43
1:E:96:MET:HE3	1:E:96:MET:HB3	1.85	0.43
1:A:79:GLU:HG3	1:A:83:LEU:HD21	2.00	0.43
1:A:198:CYS:O	1:A:202:LEU:HG	2.18	0.43
1:F:4:GLN:OE1	1:F:8:GLY:HA2	2.18	0.43
1:B:191:VAL:HG22	1:B:202:LEU:HD13	2.00	0.43
1:C:161:PHE:O	1:C:165:VAL:HG23	2.19	0.43
1:J:163:ASP:O	1:J:167:ARG:HG3	2.19	0.43
1:D:65:ALA:HB1	1:D:141:ILE:HD13	2.01	0.43
1:E:191:VAL:HG22	1:E:202:LEU:HD13	2.00	0.43
1:L:5:ASN:HB2	1:L:9:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:TRP:CZ2	1:J:93:PRO:HG3	2.54	0.43
1:G:54:THR:O	1:G:58:THR:HG23	2.19	0.43
1:H:144:MET:HE2	1:H:144:MET:HB3	1.78	0.43
1:K:161:PHE:O	1:K:165:VAL:HG23	2.19	0.43
1:I:38:PRO:HG3	1:J:57:ASN:HB3	2.00	0.43
1:B:117:TRP:CE2	1:J:93:PRO:HG3	2.54	0.42
1:H:26:VAL:CG1	1:H:36:VAL:HG23	2.50	0.42
1:H:96:MET:HE3	1:H:96:MET:HB2	1.70	0.42
1:B:65:ALA:HB1	1:B:141:ILE:HD13	2.01	0.42
1:I:138:LEU:HD23	1:I:141:ILE:HD12	2.00	0.42
1:B:104:ILE:HG12	1:B:126:VAL:HG12	2.01	0.42
1:K:191:VAL:HG22	1:K:202:LEU:HD13	1.99	0.42
1:A:57:ASN:HB3	1:F:38:PRO:HG3	2.02	0.42
1:E:211:LEU:O	1:E:215:MET:HG3	2.20	0.42
1:D:169:TYR:CE2	1:E:67:GLN:HG3	2.54	0.42
1:D:169:TYR:CZ	1:E:67:GLN:HG3	2.54	0.42
1:E:23:TRP:CZ3	1:E:40:PHE:HB2	2.54	0.42
1:E:169:TYR:CZ	1:F:67:GLN:HG2	2.55	0.42
1:G:15:ILE:HD11	1:G:51:ASP:HB3	2.00	0.42
1:A:121:ASN:O	1:A:123:PRO:HD3	2.20	0.42
1:J:187:GLU:O	1:J:191:VAL:HG23	2.20	0.42
1:E:198:CYS:O	1:E:202:LEU:HG	2.20	0.42
1:J:161:PHE:O	1:J:165:VAL:HG23	2.19	0.42
1:L:21:ASN:O	1:L:25:LYS:HG2	2.20	0.41
1:L:132:ARG:O	1:L:136:LEU:HD23	2.20	0.41
1:A:103:ASP:HA	1:A:109:SER:HB3	2.02	0.41
1:B:4:GLN:HA	1:B:9:GLN:O	2.21	0.41
1:D:122:PRO:HA	1:D:123:PRO:HD3	1.92	0.41
1:H:169:TYR:CE2	1:I:67:GLN:HG3	2.55	0.41
1:A:65:ALA:HB1	1:A:141:ILE:HD13	2.01	0.41
1:E:195:ASN:HB2	1:E:196:PRO:HD2	2.03	0.41
1:J:170:LYS:HE2	1:J:170:LYS:HB3	1.93	0.41
1:L:214:MET:HE3	1:L:214:MET:HB2	1.86	0.41
1:F:47:ALA:HB1	1:F:51:ASP:HB2	2.02	0.41
1:A:149:SER:HA	1:A:175:GLU:OE2	2.20	0.41
1:K:104:ILE:HG12	1:K:126:VAL:HG12	2.02	0.41
1:B:144:MET:HE3	1:B:144:MET:HB2	1.83	0.41
1:I:26:VAL:HG21	1:I:39:MET:HG2	2.03	0.40
1:I:150:ILE:HG12	1:I:189:LEU:HD23	2.03	0.40
1:J:25:LYS:HD3	1:J:25:LYS:HA	1.91	0.40
1:L:32:PHE:HZ	1:L:66:MET:HE3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:HIS:CE1	1:A:122:PRO:HD2	2.56	0.40
1:B:32:PHE:HZ	1:B:66:MET:HE2	1.87	0.40
1:A:143:ARG:HG2	1:A:175:GLU:HA	2.02	0.40
1:C:51:ASP:O	1:C:55:MET:HG3	2.22	0.40
1:I:4:GLN:HB3	1:I:10:MET:SD	2.62	0.40
1:J:184:ALA:O	1:J:188:THR:HG23	2.22	0.40
1:L:23:TRP:CZ3	1:L:40:PHE:HB2	2.57	0.40
1:L:104:ILE:HD13	1:L:129:ILE:HG21	2.04	0.40

There are no symmetry-related clashes.

## 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	205/232 (88%)	198 (97%)	7 (3%)	0	100	100
1	B	202/232 (87%)	198 (98%)	2 (1%)	2 (1%)	12	15
1	C	201/232 (87%)	197 (98%)	4 (2%)	0	100	100
1	D	196/232 (84%)	192 (98%)	4 (2%)	0	100	100
1	E	207/232 (89%)	198 (96%)	9 (4%)	0	100	100
1	F	214/232 (92%)	213 (100%)	1 (0%)	0	100	100
1	G	197/232 (85%)	195 (99%)	2 (1%)	0	100	100
1	H	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	24	31
1	I	207/232 (89%)	203 (98%)	4 (2%)	0	100	100
1	J	209/232 (90%)	206 (99%)	3 (1%)	0	100	100
1	K	198/232 (85%)	191 (96%)	7 (4%)	0	100	100
1	L	208/232 (90%)	203 (98%)	4 (2%)	1 (0%)	24	31
All	All	2453/2784 (88%)	2399 (98%)	50 (2%)	4 (0%)	43	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	60	GLY
1	H	60	GLY
1	B	60	GLY
1	B	8	GLY

### 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	174/194 (90%)	171 (98%)	3 (2%)	53	72
1	B	173/194 (89%)	172 (99%)	1 (1%)	78	89
1	C	175/194 (90%)	175 (100%)	0	100	100
1	D	170/194 (88%)	170 (100%)	0	100	100
1	E	174/194 (90%)	170 (98%)	4 (2%)	44	63
1	F	180/194 (93%)	179 (99%)	1 (1%)	78	89
1	G	173/194 (89%)	172 (99%)	1 (1%)	78	89
1	H	176/194 (91%)	176 (100%)	0	100	100
1	I	174/194 (90%)	173 (99%)	1 (1%)	78	89
1	J	176/194 (91%)	174 (99%)	2 (1%)	65	81
1	K	171/194 (88%)	170 (99%)	1 (1%)	78	89
1	L	175/194 (90%)	174 (99%)	1 (1%)	78	89
All	All	2091/2328 (90%)	2076 (99%)	15 (1%)	76	87

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LEU
1	A	205	LEU
1	A	218	CYS
1	B	198	CYS
1	E	67	GLN

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Mol	Chain	Res	Type
1	E	152	ASP
1	E	153	ILE
1	E	189	LEU
1	F	4	GLN
1	G	4	GLN
1	I	175	GLU
1	J	198	CYS
1	J	218	CYS
1	K	205	LEU
1	L	202	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	B	50	GLN
1	B	67	GLN
1	B	95	GLN
1	D	219	GLN
1	E	7	GLN
1	E	9	GLN
1	E	84	HIS
1	E	95	GLN
1	F	21	ASN
1	F	50	GLN
1	F	63	GLN
1	F	84	HIS
1	F	95	GLN
1	G	9	GLN
1	G	176	GLN
1	H	21	ASN
1	H	50	GLN
1	H	112	GLN
1	H	121	ASN
1	I	12	HIS
1	I	67	GLN
1	I	84	HIS
1	I	95	GLN
1	J	67	GLN
1	J	112	GLN
1	L	12	HIS
1	L	50	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

12 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	A1CH7	A	301	-	38,38,38	0.92	0	50,54,54	0.80	1 (2%)
2	A1CH7	F	301	-	38,38,38	0.93	0	50,54,54	0.87	2 (4%)
2	A1CH7	J	301	-	38,38,38	0.93	0	50,54,54	0.82	1 (2%)
2	A1CH7	G	301	-	38,38,38	0.94	0	50,54,54	0.82	1 (2%)
2	A1CH7	I	301	-	38,38,38	0.92	0	50,54,54	0.86	1 (2%)
2	A1CH7	L	301	-	38,38,38	0.94	0	50,54,54	0.84	1 (2%)
2	A1CH7	B	301	-	38,38,38	0.93	1 (2%)	50,54,54	0.82	1 (2%)
2	A1CH7	K	301	-	38,38,38	0.92	0	50,54,54	0.81	1 (2%)
2	A1CH7	C	301	-	38,38,38	0.93	0	50,54,54	0.82	1 (2%)
2	A1CH7	D	301	-	38,38,38	0.91	0	50,54,54	0.81	1 (2%)
2	A1CH7	D	302	-	38,38,38	0.92	0	50,54,54	0.82	1 (2%)
2	A1CH7	H	301	-	38,38,38	0.93	0	50,54,54	0.87	2 (4%)

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	A1CH7	A	301	-	-	0/30/37/37	0/4/4/4
2	A1CH7	F	301	-	-	0/30/37/37	0/4/4/4
2	A1CH7	J	301	-	-	6/30/37/37	0/4/4/4
2	A1CH7	G	301	-	-	6/30/37/37	0/4/4/4
2	A1CH7	I	301	-	-	6/30/37/37	0/4/4/4
2	A1CH7	L	301	-	-	6/30/37/37	0/4/4/4
2	A1CH7	B	301	-	-	6/30/37/37	0/4/4/4
2	A1CH7	K	301	-	-	0/30/37/37	0/4/4/4
2	A1CH7	C	301	-	-	6/30/37/37	0/4/4/4
2	A1CH7	D	301	-	-	0/30/37/37	0/4/4/4
2	A1CH7	D	302	-	-	0/30/37/37	0/4/4/4
2	A1CH7	H	301	-	-	6/30/37/37	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	A1CH7	C20-N04	2.01	1.37	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	A1CH7	C16-C17-N04	2.72	116.97	111.89
2	I	301	A1CH7	C02-C01-C03	2.54	115.27	109.94
2	F	301	A1CH7	C02-C01-C03	2.54	115.25	109.94
2	L	301	A1CH7	C02-C01-C03	2.48	115.14	109.94
2	D	302	A1CH7	C02-C01-C03	2.47	115.10	109.94
2	B	301	A1CH7	C02-C01-C03	2.41	114.99	109.94
2	G	301	A1CH7	C02-C01-C03	2.41	114.98	109.94
2	H	301	A1CH7	C02-C01-C03	2.36	114.88	109.94
2	K	301	A1CH7	C02-C01-C03	2.35	114.87	109.94
2	J	301	A1CH7	C02-C01-C03	2.32	114.79	109.94
2	D	301	A1CH7	C02-C01-C03	2.28	114.72	109.94
2	C	301	A1CH7	C02-C01-C03	2.26	114.67	109.94
2	A	301	A1CH7	C02-C01-C03	2.26	114.67	109.94
2	F	301	A1CH7	C16-C17-N04	2.24	116.08	111.89

There are no chirality outliers.

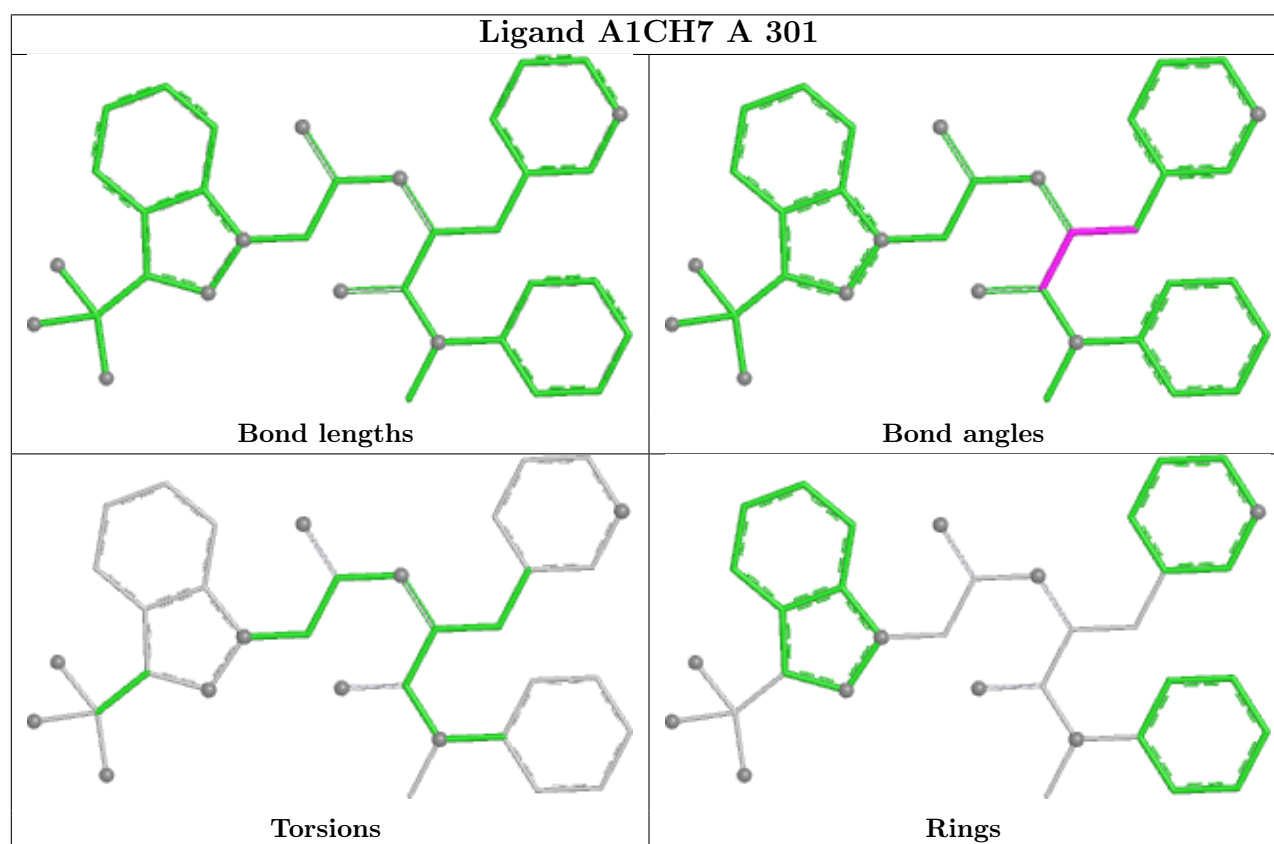
All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	A1CH7	C19-C18-C25-F03
2	H	301	A1CH7	C19-C18-C25-F03
2	B	301	A1CH7	C19-C18-C25-F02
2	C	301	A1CH7	C19-C18-C25-F02
2	H	301	A1CH7	C19-C18-C25-F02
2	B	301	A1CH7	C19-C18-C25-F01
2	C	301	A1CH7	C19-C18-C25-F01
2	C	301	A1CH7	C19-C18-C25-F03
2	H	301	A1CH7	C19-C18-C25-F01
2	I	301	A1CH7	C19-C18-C25-F01
2	I	301	A1CH7	C19-C18-C25-F02
2	I	301	A1CH7	C19-C18-C25-F03
2	B	301	A1CH7	N05-C18-C25-F02
2	B	301	A1CH7	N05-C18-C25-F03
2	H	301	A1CH7	N05-C18-C25-F02
2	H	301	A1CH7	N05-C18-C25-F03
2	C	301	A1CH7	N05-C18-C25-F02
2	H	301	A1CH7	N05-C18-C25-F01
2	B	301	A1CH7	N05-C18-C25-F01
2	C	301	A1CH7	N05-C18-C25-F01
2	C	301	A1CH7	N05-C18-C25-F03
2	I	301	A1CH7	N05-C18-C25-F01
2	I	301	A1CH7	N05-C18-C25-F03
2	J	301	A1CH7	N05-C18-C25-F01
2	J	301	A1CH7	N05-C18-C25-F03
2	L	301	A1CH7	N05-C18-C25-F01
2	L	301	A1CH7	N05-C18-C25-F03
2	J	301	A1CH7	C19-C18-C25-F02
2	J	301	A1CH7	C19-C18-C25-F03
2	G	301	A1CH7	N05-C18-C25-F01
2	I	301	A1CH7	N05-C18-C25-F02
2	L	301	A1CH7	N05-C18-C25-F02
2	J	301	A1CH7	C19-C18-C25-F01
2	L	301	A1CH7	C19-C18-C25-F01
2	L	301	A1CH7	C19-C18-C25-F02
2	L	301	A1CH7	C19-C18-C25-F03
2	G	301	A1CH7	N05-C18-C25-F02
2	G	301	A1CH7	N05-C18-C25-F03
2	J	301	A1CH7	N05-C18-C25-F02
2	G	301	A1CH7	C19-C18-C25-F01
2	G	301	A1CH7	C19-C18-C25-F03
2	G	301	A1CH7	C19-C18-C25-F02

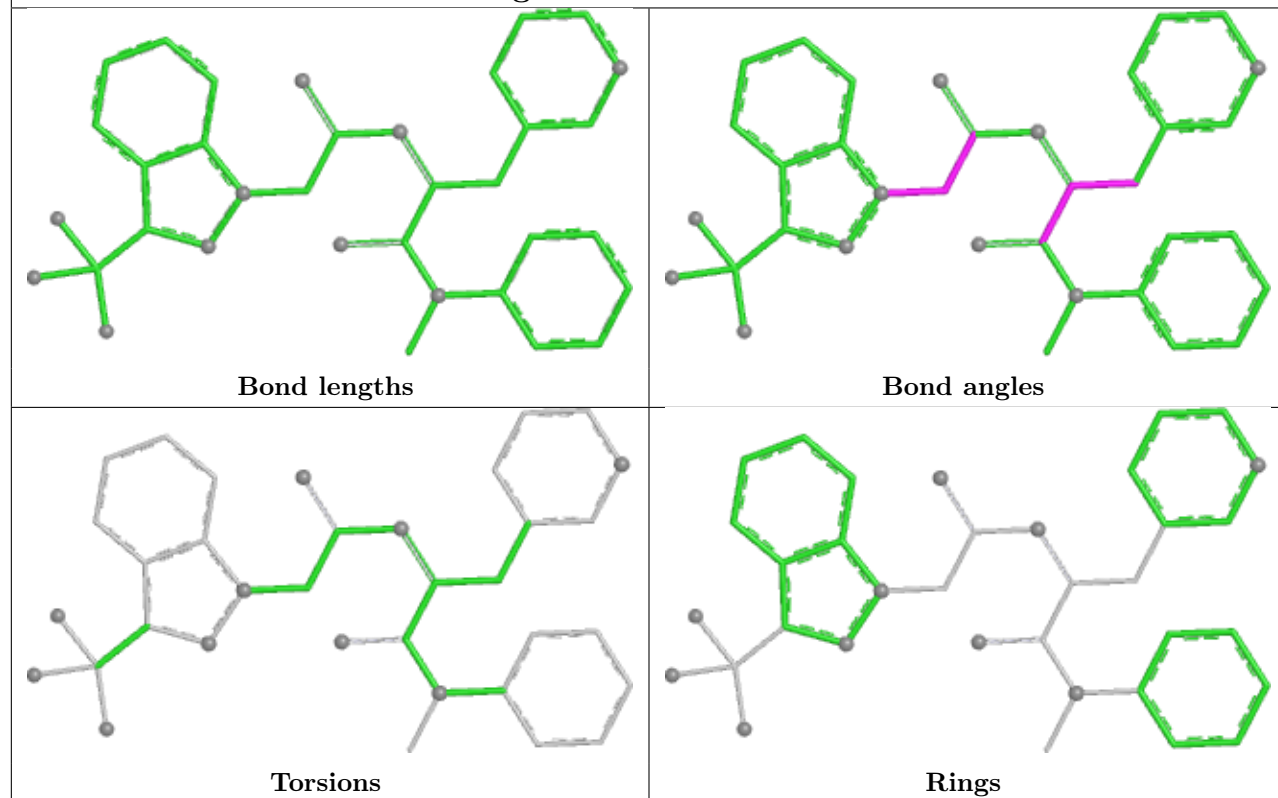
There are no ring outliers.

No monomer is involved in short contacts.

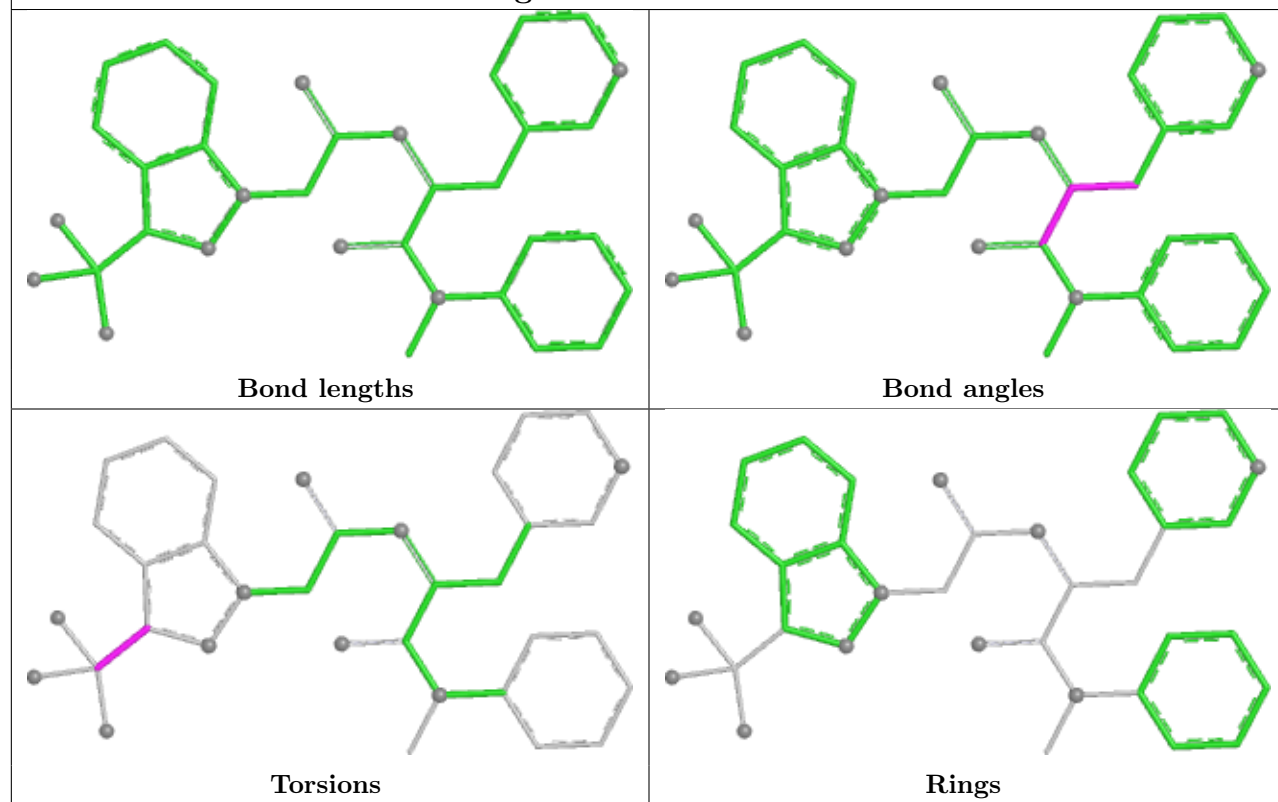
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



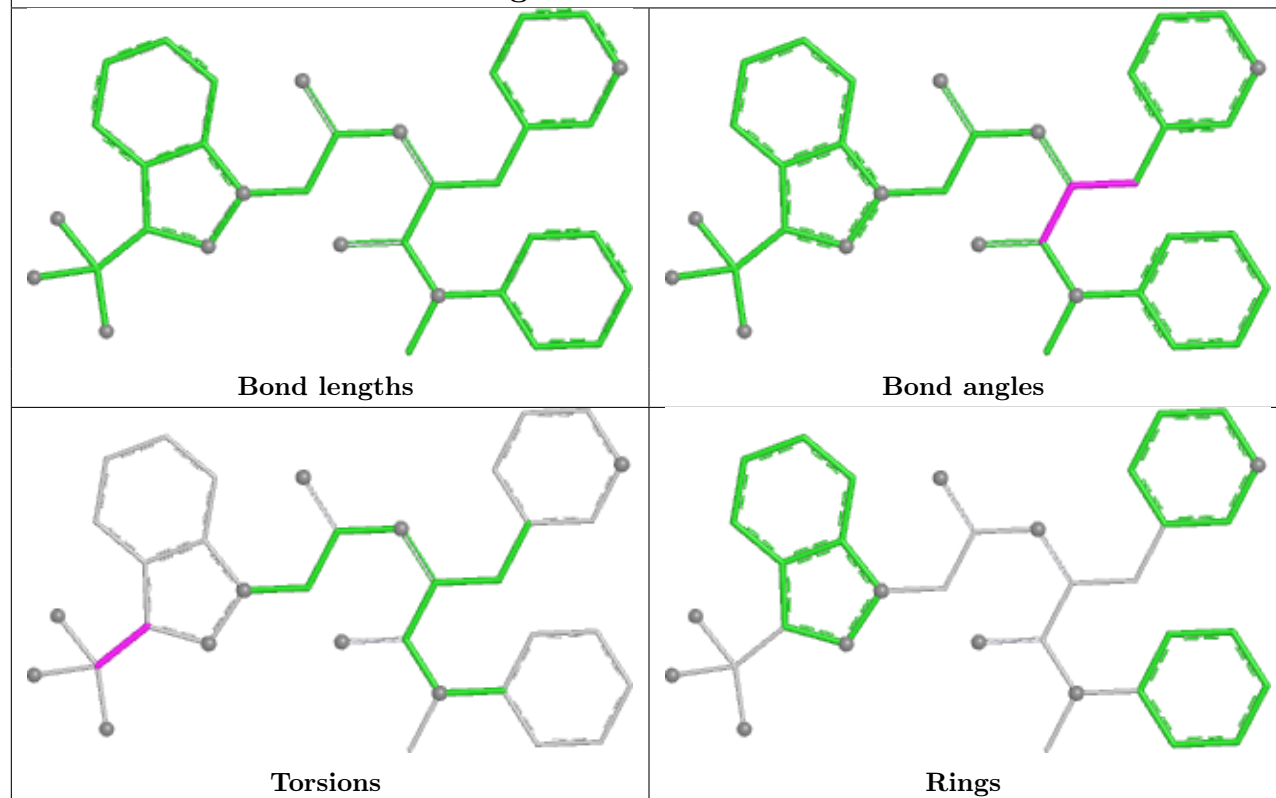
## Ligand A1CH7 F 301



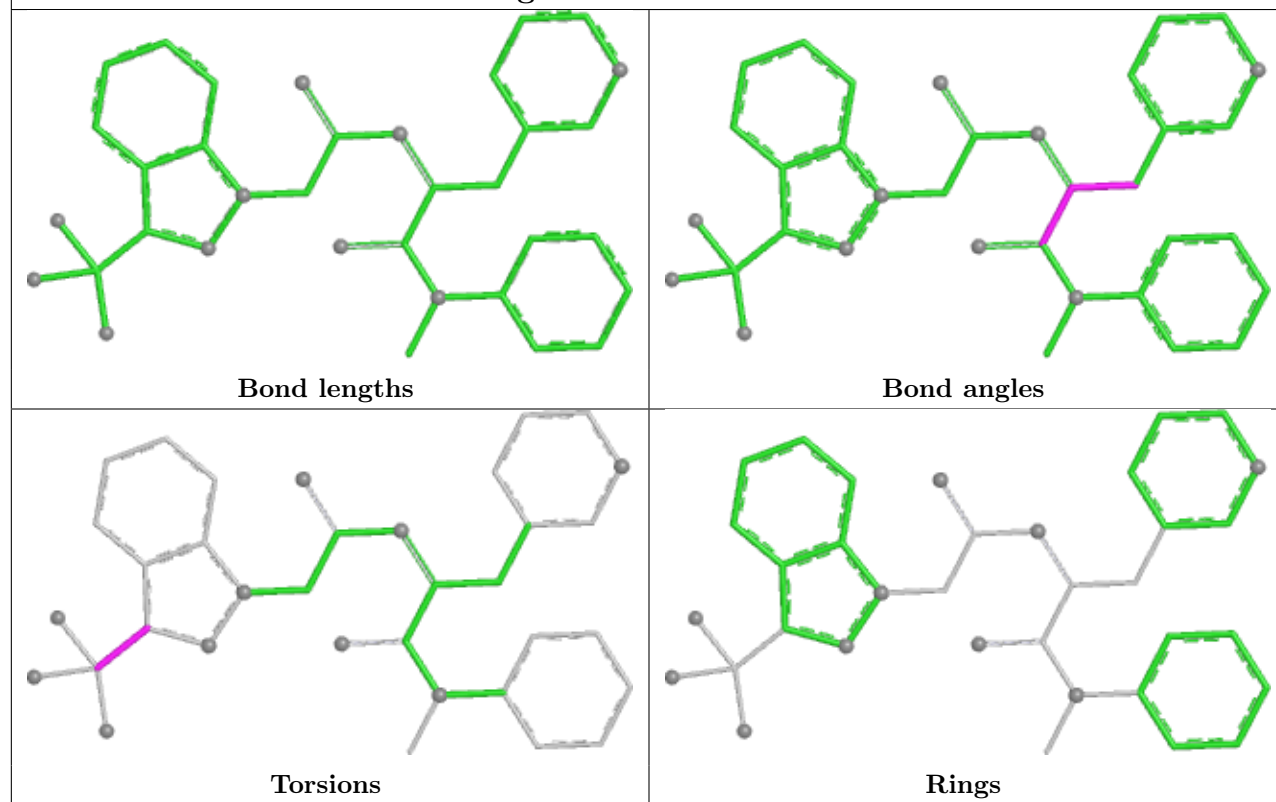
## Ligand A1CH7 J 301



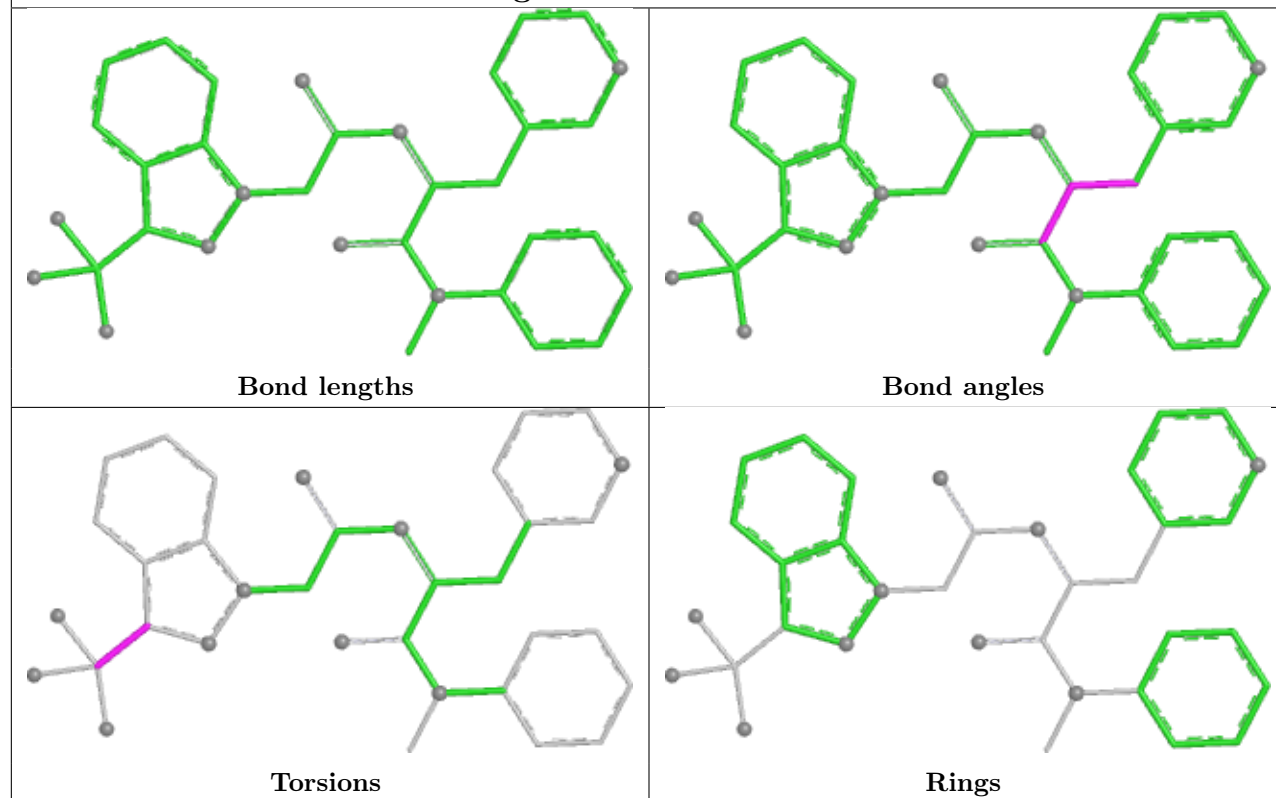
## Ligand A1CH7 G 301



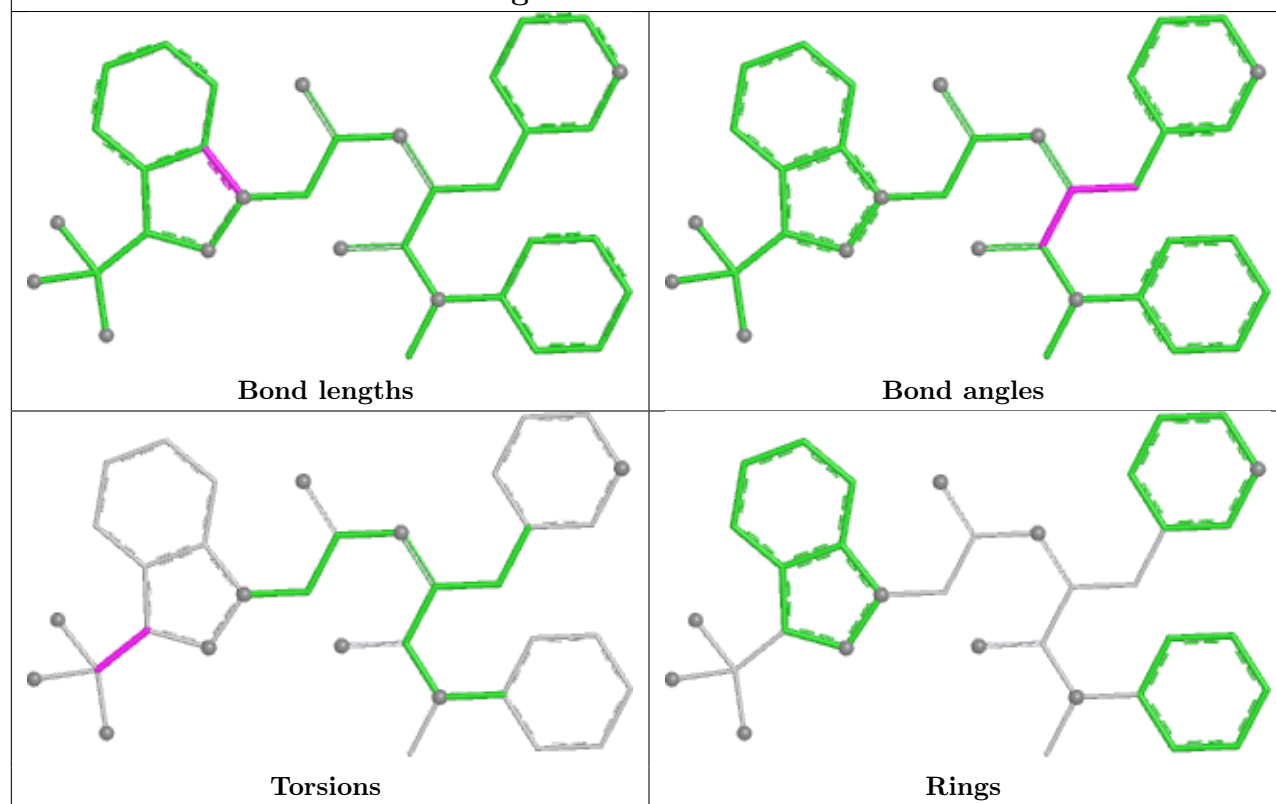
## Ligand A1CH7 I 301



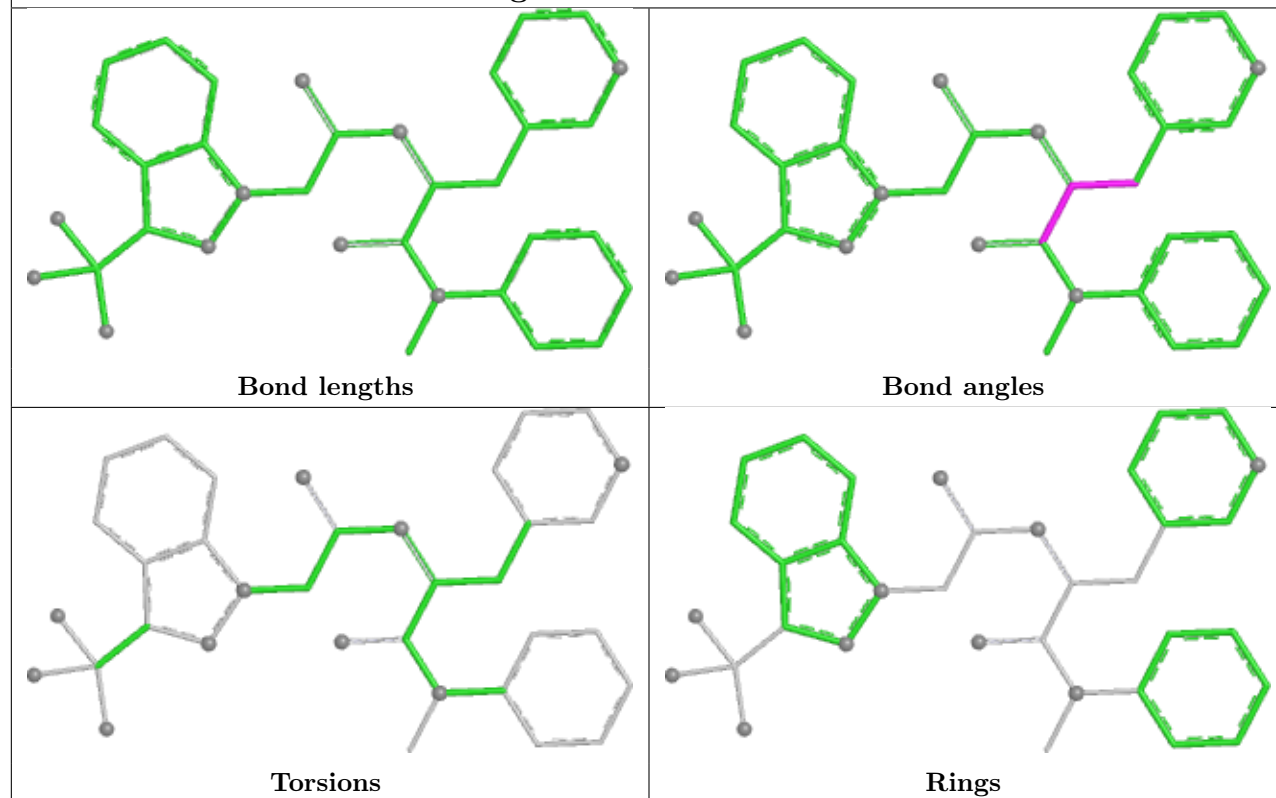
## Ligand A1CH7 L 301



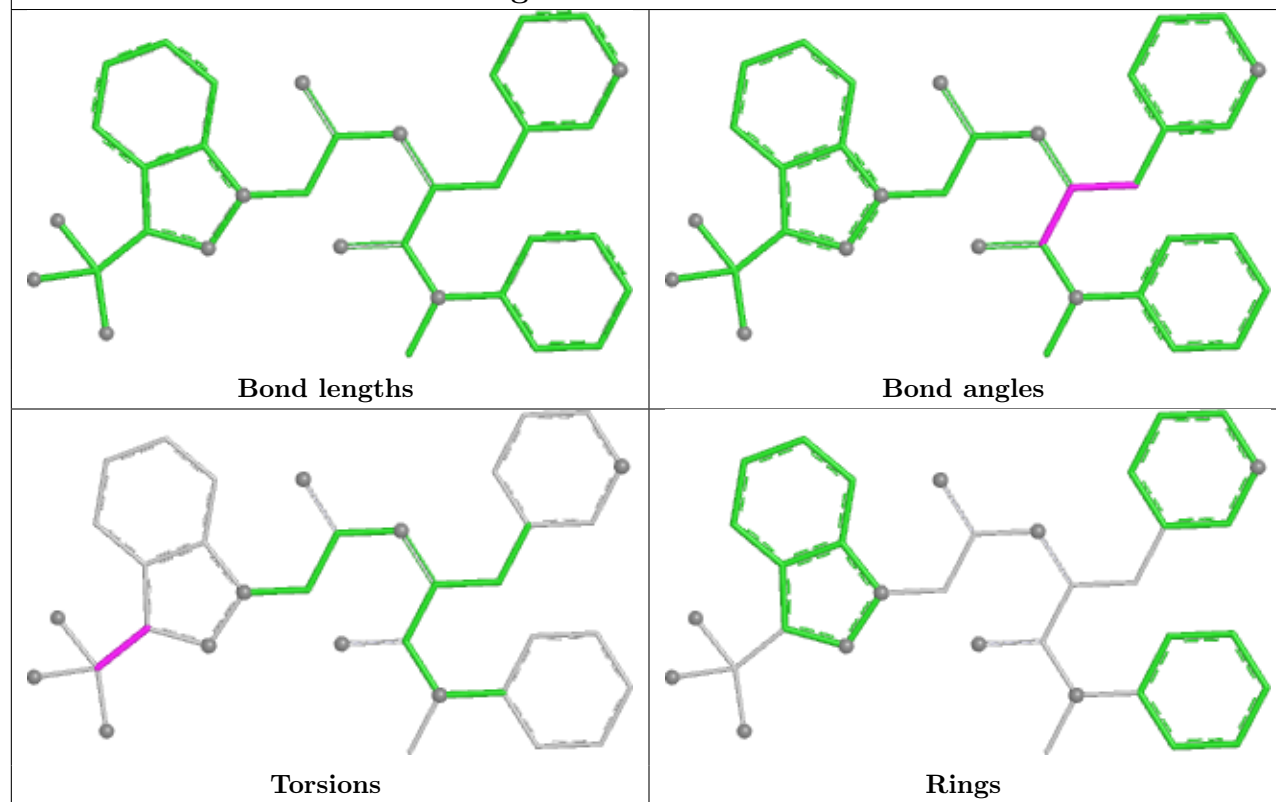
## Ligand A1CH7 B 301



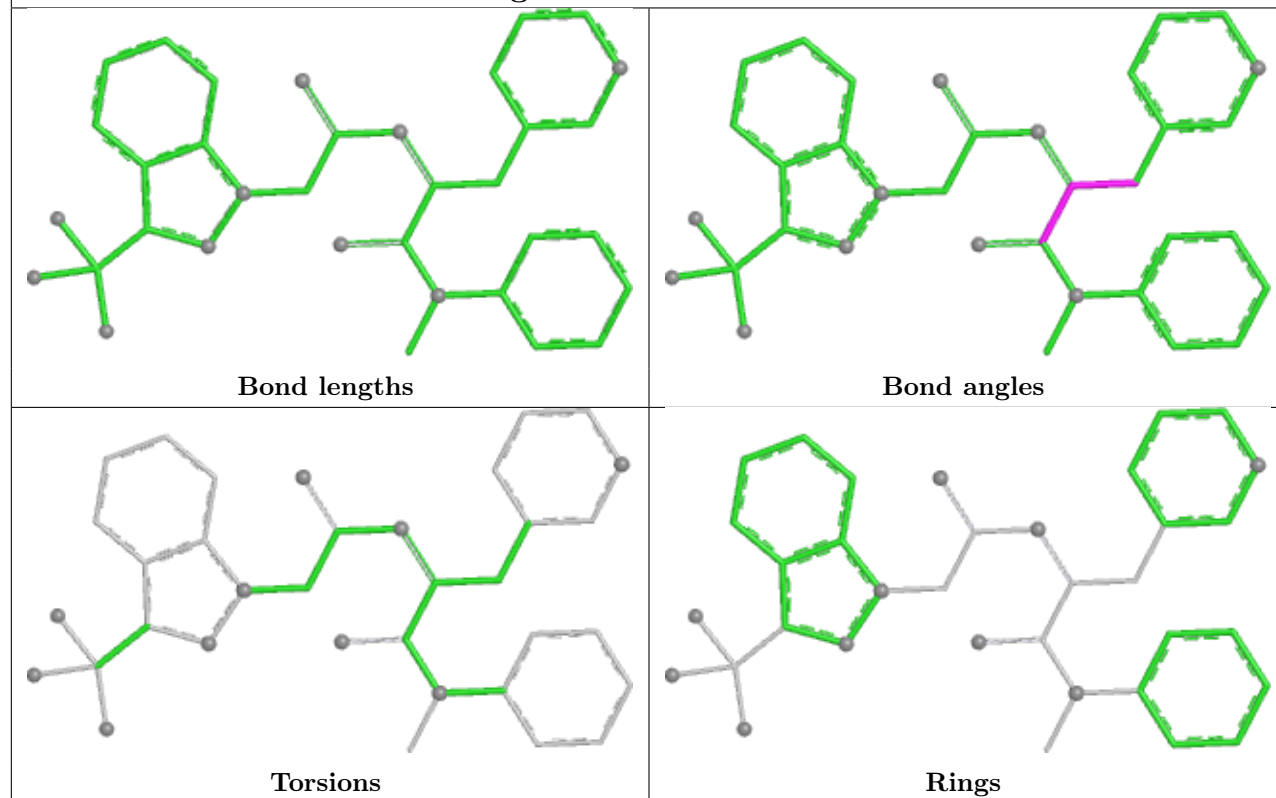
## Ligand A1CH7 K 301



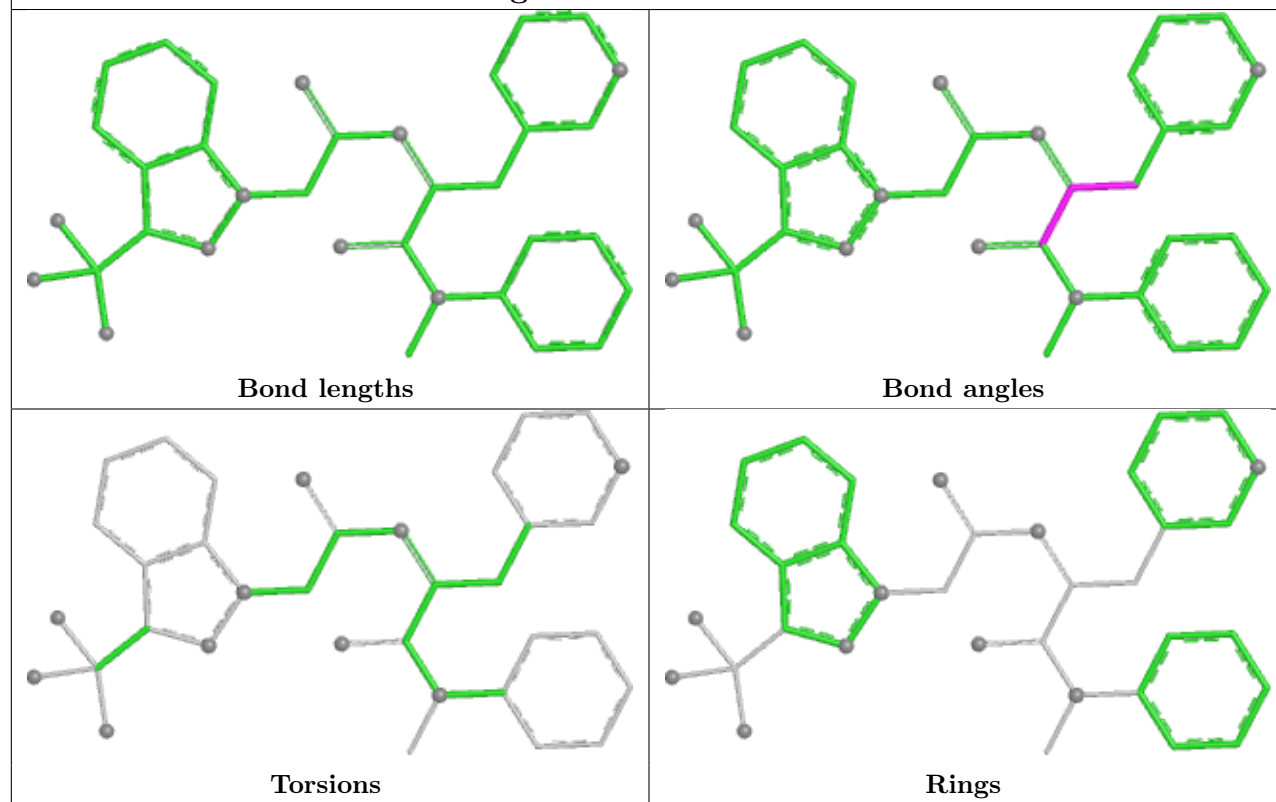
## Ligand A1CH7 C 301

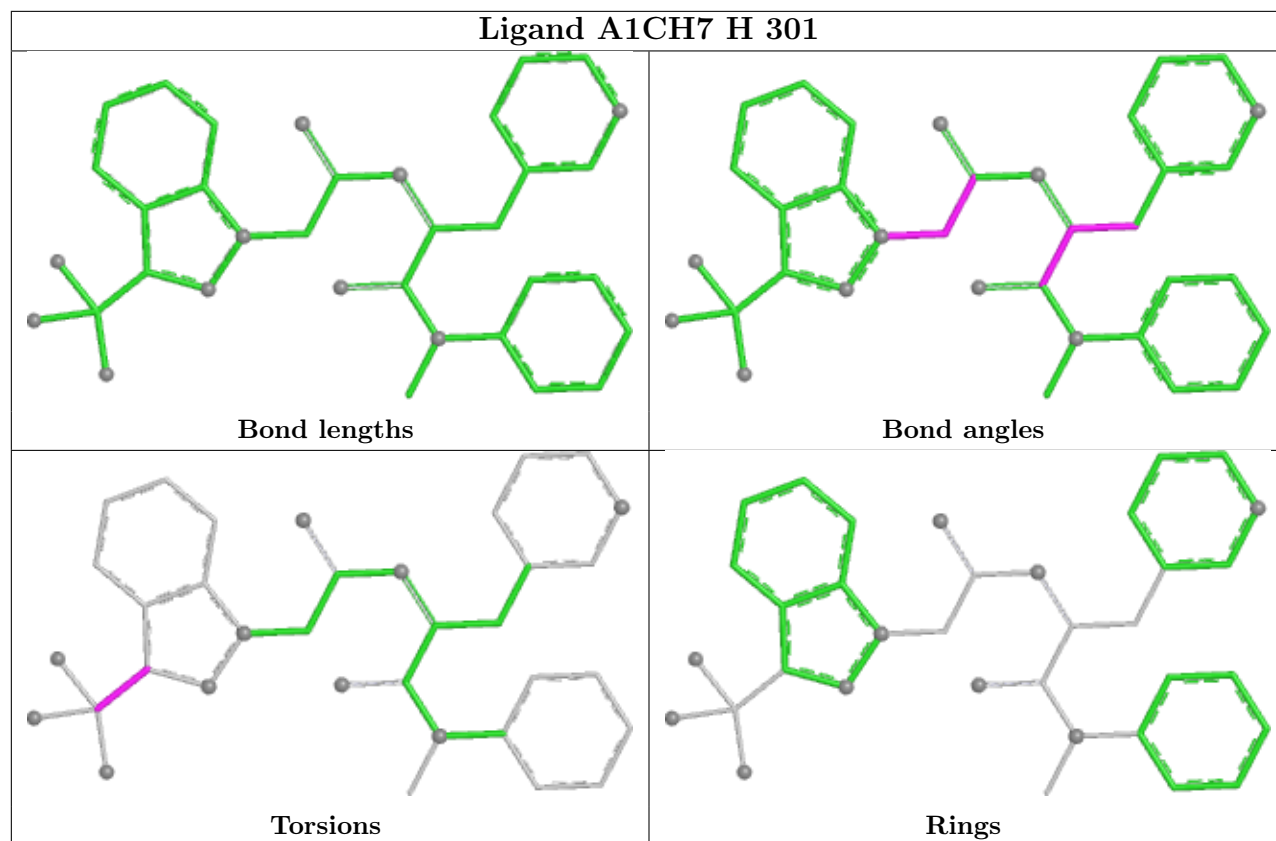


## Ligand A1CH7 D 301



## Ligand A1CH7 D 302





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	211/232 (90%)	1.25	45 (21%) <b>2</b> <b>3</b>	41, 71, 104, 112	0
1	B	208/232 (89%)	0.78	18 (8%) <b>16</b> <b>17</b>	45, 62, 85, 106	0
1	C	207/232 (89%)	0.65	15 (7%) <b>21</b> <b>23</b>	43, 59, 81, 94	0
1	D	202/232 (87%)	0.63	15 (7%) <b>20</b> <b>22</b>	37, 56, 90, 106	0
1	E	211/232 (90%)	1.05	45 (21%) <b>2</b> <b>3</b>	39, 63, 111, 120	0
1	F	218/232 (93%)	0.65	20 (9%) <b>14</b> <b>16</b>	41, 58, 86, 101	0
1	G	203/232 (87%)	0.77	18 (8%) <b>15</b> <b>17</b>	42, 62, 88, 105	0
1	H	213/232 (91%)	0.94	24 (11%) <b>10</b> <b>11</b>	45, 65, 108, 115	0
1	I	211/232 (90%)	1.00	35 (16%) <b>4</b> <b>5</b>	47, 69, 105, 112	0
1	J	213/232 (91%)	1.08	34 (15%) <b>5</b> <b>5</b>	52, 73, 99, 109	0
1	K	204/232 (87%)	1.00	27 (13%) <b>7</b> <b>8</b>	49, 66, 90, 118	0
1	L	212/232 (91%)	0.90	28 (13%) <b>7</b> <b>8</b>	40, 61, 93, 123	0
All	All	2513/2784 (90%)	0.89	324 (12%) <b>7</b> <b>8</b>	37, 64, 100, 123	0

All (324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	6	LEU	6.5
1	E	189	LEU	5.2
1	E	190	LEU	5.1
1	E	191	VAL	5.0
1	B	177	ALA	4.9
1	D	185	ALA	4.8
1	A	124	ILE	4.7
1	E	153	ILE	4.7
1	E	198	CYS	4.7
1	J	145	TYR	4.7
1	E	185	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	198	CYS	4.5
1	K	198	CYS	4.4
1	A	93	PRO	4.4
1	L	200	THR	4.2
1	F	6	LEU	4.1
1	I	202	LEU	4.1
1	I	201	ILE	4.1
1	K	124	ILE	4.1
1	I	191	VAL	4.1
1	E	151	LEU	4.0
1	L	198	CYS	4.0
1	A	85	PRO	4.0
1	G	6	LEU	4.0
1	H	217	ALA	4.0
1	L	220	GLY	4.0
1	B	6	LEU	3.9
1	D	6	LEU	3.9
1	A	186	THR	3.9
1	D	186	THR	3.9
1	F	186	THR	3.9
1	L	91	ILE	3.9
1	E	186	THR	3.8
1	B	179	GLN	3.8
1	F	145	TYR	3.8
1	B	94	GLY	3.8
1	A	6	LEU	3.8
1	L	5	ASN	3.7
1	E	150	ILE	3.7
1	E	187	GLU	3.7
1	A	148	THR	3.6
1	J	185	ALA	3.6
1	B	178	SER	3.6
1	C	6	LEU	3.6
1	I	186	THR	3.6
1	D	157	PRO	3.6
1	A	89	GLY	3.5
1	G	220	GLY	3.5
1	L	218	CYS	3.5
1	I	151	LEU	3.5
1	E	86	VAL	3.5
1	A	96	MET	3.5
1	D	96	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	L	185	ALA	3.5
1	D	151	LEU	3.5
1	L	205	LEU	3.5
1	C	176	GLN	3.5
1	A	90	PRO	3.4
1	B	85	PRO	3.4
1	H	151	LEU	3.4
1	I	219	GLN	3.4
1	G	85	PRO	3.4
1	I	198	CYS	3.4
1	I	211	LEU	3.4
1	A	122	PRO	3.4
1	L	92	ALA	3.4
1	L	204	ALA	3.4
1	H	198	CYS	3.4
1	C	86	VAL	3.4
1	G	92	ALA	3.4
1	K	183	ASN	3.4
1	I	6	LEU	3.3
1	E	157	PRO	3.3
1	A	187	GLU	3.3
1	A	8	GLY	3.3
1	C	198	CYS	3.3
1	G	157	PRO	3.3
1	K	85	PRO	3.3
1	K	123	PRO	3.3
1	L	203	LYS	3.3
1	J	184	ALA	3.3
1	J	88	ALA	3.3
1	A	91	ILE	3.2
1	I	168	PHE	3.2
1	E	194	ALA	3.2
1	F	220	GLY	3.2
1	K	220	GLY	3.2
1	L	94	GLY	3.2
1	L	196	PRO	3.2
1	J	200	THR	3.2
1	I	203	LYS	3.2
1	A	2	ILE	3.2
1	G	188	THR	3.2
1	A	177	ALA	3.2
1	G	156	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	190	LEU	3.2
1	C	94	GLY	3.1
1	A	97	ARG	3.1
1	I	144	MET	3.1
1	H	185	ALA	3.1
1	J	191	VAL	3.1
1	E	160	PRO	3.1
1	E	164	TYR	3.1
1	A	117	TRP	3.1
1	J	186	THR	3.1
1	E	165	VAL	3.1
1	E	161	PHE	3.0
1	K	158	LYS	3.0
1	F	147	PRO	3.0
1	F	86	VAL	3.0
1	C	145	TYR	3.0
1	H	186	THR	3.0
1	F	7	GLN	3.0
1	E	220	GLY	3.0
1	H	189	LEU	3.0
1	J	153	ILE	3.0
1	L	153	ILE	3.0
1	J	158	LYS	3.0
1	K	206	GLY	3.0
1	I	185	ALA	3.0
1	D	86	VAL	3.0
1	I	7	GLN	3.0
1	J	144	MET	3.0
1	I	157	PRO	3.0
1	E	201	ILE	2.9
1	H	157	PRO	2.9
1	A	92	ALA	2.9
1	A	153	ILE	2.9
1	E	171	THR	2.9
1	A	207	PRO	2.9
1	I	196	PRO	2.9
1	B	82	ARG	2.9
1	E	217	ALA	2.9
1	J	5	ASN	2.9
1	B	7	GLN	2.9
1	H	176	GLN	2.9
1	L	93	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	192	GLN	2.8
1	K	117	TRP	2.8
1	L	186	THR	2.8
1	G	93	PRO	2.8
1	H	196	PRO	2.8
1	I	207	PRO	2.8
1	J	157	PRO	2.8
1	K	196	PRO	2.8
1	A	11	VAL	2.8
1	J	86	VAL	2.8
1	D	198	CYS	2.8
1	B	8	GLY	2.8
1	L	202	LEU	2.8
1	I	194	ALA	2.8
1	K	186	THR	2.8
1	E	193	ASN	2.8
1	J	201	ILE	2.7
1	B	9	GLN	2.7
1	D	189	LEU	2.7
1	E	92	ALA	2.7
1	A	121	ASN	2.7
1	E	188	THR	2.7
1	G	207	PRO	2.7
1	K	147	PRO	2.7
1	I	205	LEU	2.7
1	J	6	LEU	2.7
1	J	112	GLN	2.7
1	J	161	PHE	2.7
1	F	183	ASN	2.7
1	L	201	ILE	2.7
1	A	196	PRO	2.7
1	L	161	PHE	2.6
1	A	191	VAL	2.6
1	I	216	THR	2.6
1	C	8	GLY	2.6
1	I	150	ILE	2.6
1	E	202	LEU	2.6
1	I	31	ALA	2.6
1	F	180	GLU	2.6
1	I	153	ILE	2.6
1	G	5	ASN	2.6
1	J	124	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	145	TYR	2.6
1	E	172	LEU	2.5
1	H	6	LEU	2.5
1	B	5	ASN	2.5
1	K	5	ASN	2.5
1	K	122	PRO	2.5
1	L	145	TYR	2.5
1	J	151	LEU	2.5
1	H	152	ASP	2.5
1	J	217	ALA	2.5
1	H	207	PRO	2.5
1	J	87	HIS	2.5
1	B	187	GLU	2.5
1	K	97	ARG	2.5
1	F	205	LEU	2.5
1	F	5	ASN	2.5
1	F	208	GLY	2.5
1	K	126	VAL	2.5
1	C	184	ALA	2.5
1	I	176	GLN	2.5
1	A	201	ILE	2.4
1	E	169	TYR	2.4
1	K	9	GLN	2.4
1	C	217	ALA	2.4
1	C	208	GLY	2.4
1	I	156	GLY	2.4
1	A	161	PHE	2.4
1	H	205	LEU	2.4
1	K	120	HIS	2.4
1	A	183	ASN	2.4
1	J	122	PRO	2.4
1	G	94	GLY	2.4
1	J	150	ILE	2.4
1	A	215	MET	2.4
1	E	205	LEU	2.4
1	D	187	GLU	2.4
1	E	175	GLU	2.4
1	K	121	ASN	2.4
1	A	9	GLN	2.4
1	E	145	TYR	2.3
1	I	208	GLY	2.3
1	A	209	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	92	ALA	2.3
1	I	214	MET	2.3
1	A	3	VAL	2.3
1	L	15	ILE	2.3
1	A	205	LEU	2.3
1	H	190	LEU	2.3
1	I	189	LEU	2.3
1	A	94	GLY	2.3
1	E	167	ARG	2.3
1	B	189	LEU	2.3
1	G	189	LEU	2.3
1	I	8	GLY	2.3
1	K	96	MET	2.3
1	J	7	GLN	2.3
1	H	26	VAL	2.3
1	G	151	LEU	2.3
1	H	94	GLY	2.3
1	B	185	ALA	2.3
1	E	174	ALA	2.3
1	J	176	GLN	2.3
1	E	91	ILE	2.3
1	I	161	PHE	2.2
1	J	60	GLY	2.2
1	A	184	ALA	2.2
1	E	31	ALA	2.2
1	J	203	LYS	2.2
1	C	124	ILE	2.2
1	E	6	LEU	2.2
1	F	26	VAL	2.2
1	G	83	LEU	2.2
1	L	86	VAL	2.2
1	D	5	ASN	2.2
1	K	197	ASP	2.2
1	A	125	PRO	2.2
1	D	196	PRO	2.2
1	E	90	PRO	2.2
1	E	215	MET	2.2
1	I	209	ALA	2.2
1	A	109	SER	2.2
1	I	145	TYR	2.2
1	A	162	ARG	2.2
1	F	94	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	185	ALA	2.2
1	G	31	ALA	2.2
1	H	188	THR	2.2
1	I	188	THR	2.2
1	L	88	ALA	2.2
1	A	190	LEU	2.2
1	J	138	LEU	2.2
1	E	168	PHE	2.2
1	I	152	ASP	2.2
1	K	207	PRO	2.2
1	K	60	GLY	2.2
1	G	198	CYS	2.2
1	F	178	SER	2.2
1	E	196	PRO	2.1
1	E	218	CYS	2.1
1	A	216	THR	2.1
1	F	184	ALA	2.1
1	J	194	ALA	2.1
1	L	31	ALA	2.1
1	G	96	MET	2.1
1	L	197	ASP	2.1
1	B	84	HIS	2.1
1	A	218	CYS	2.1
1	H	200	THR	2.1
1	B	184	ALA	2.1
1	H	209	ALA	2.1
1	J	174	ALA	2.1
1	D	214	MET	2.1
1	G	144	MET	2.1
1	E	159	GLU	2.1
1	J	189	LEU	2.1
1	I	197	ASP	2.1
1	K	201	ILE	2.1
1	F	9	GLN	2.1
1	A	99	PRO	2.1
1	C	196	PRO	2.1
1	J	196	PRO	2.1
1	K	203	LYS	2.1
1	A	5	ASN	2.1
1	H	5	ASN	2.1
1	L	87	HIS	2.1
1	E	207	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	86	VAL	2.1
1	L	191	VAL	2.1
1	A	208	GLY	2.1
1	J	188	THR	2.0
1	C	183	ASN	2.0
1	E	152	ASP	2.0
1	L	190	LEU	2.0
1	A	123	PRO	2.0
1	F	144	MET	2.0
1	B	186	THR	2.0
1	C	112	GLN	2.0
1	E	112	GLN	2.0
1	F	179	GLN	2.0
1	C	100	ARG	2.0
1	D	150	ILE	2.0
1	D	153	ILE	2.0
1	H	100	ARG	2.0
1	H	122	PRO	2.0
1	H	153	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

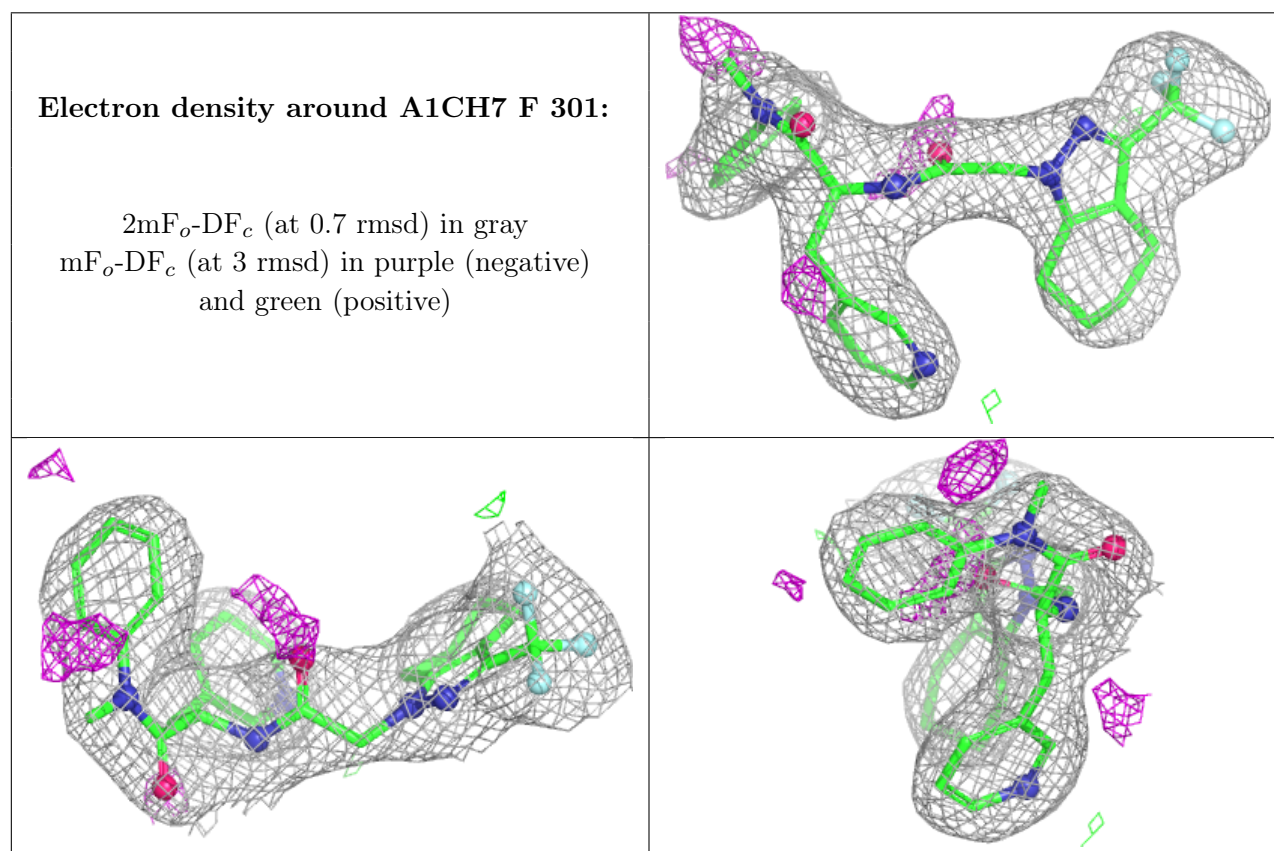
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	A1CH7	F	301	35/35	0.93	0.12	48,55,72,74	0
2	A1CH7	H	301	35/35	0.93	0.10	42,51,59,63	0
2	A1CH7	G	301	35/35	0.94	0.09	36,51,57,61	0
2	A1CH7	B	301	35/35	0.94	0.10	42,57,67,69	0

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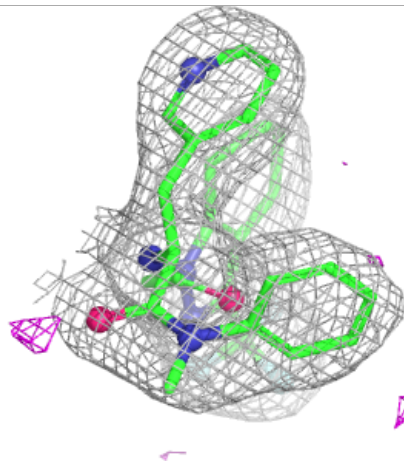
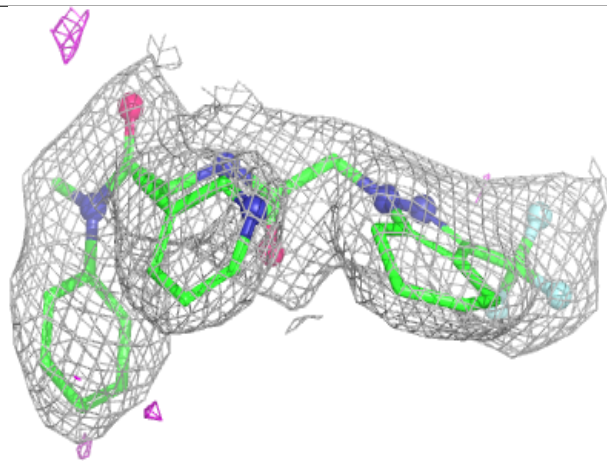
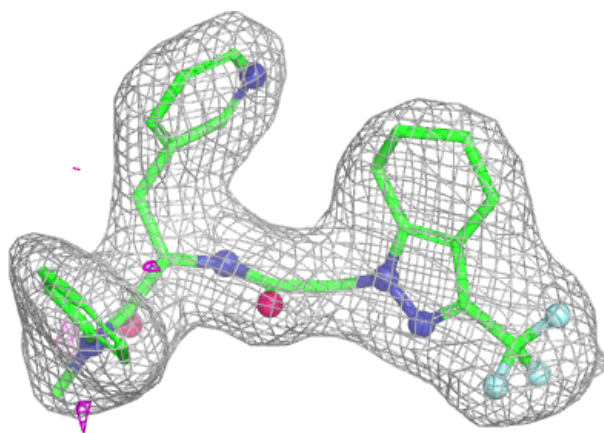
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1CH7	J	301	35/35	0.94	0.10	52,61,70,77	0
2	A1CH7	C	301	35/35	0.95	0.09	41,48,58,61	0
2	A1CH7	D	302	35/35	0.95	0.09	38,47,57,64	0
2	A1CH7	I	301	35/35	0.95	0.08	47,55,70,75	0
2	A1CH7	A	301	35/35	0.95	0.10	39,46,53,55	0
2	A1CH7	K	301	35/35	0.95	0.10	47,59,72,76	0
2	A1CH7	L	301	35/35	0.95	0.08	36,48,56,60	0
2	A1CH7	D	301	35/35	0.96	0.08	35,43,48,53	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.



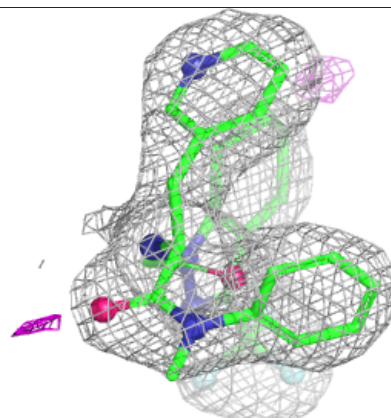
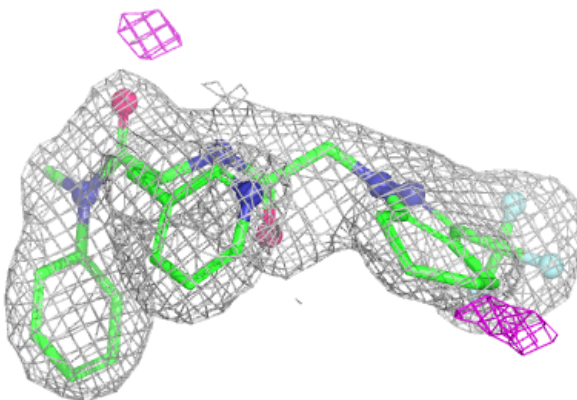
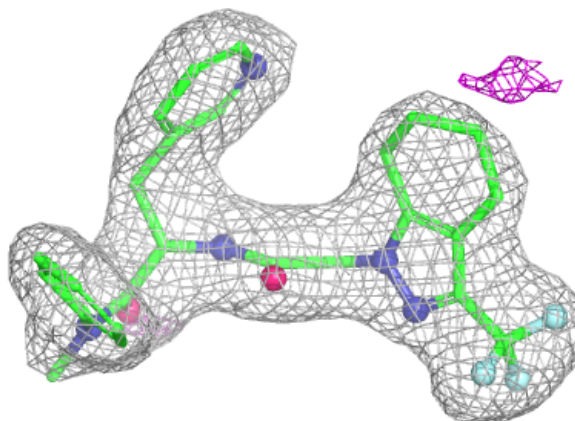
**Electron density around A1CH7 H 301:**

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



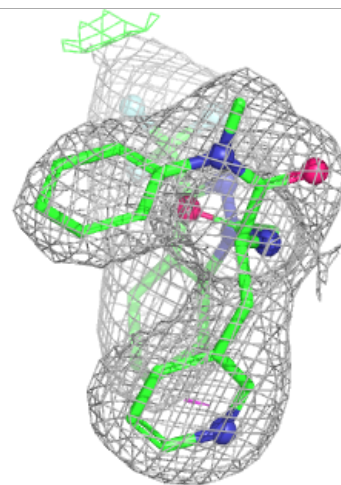
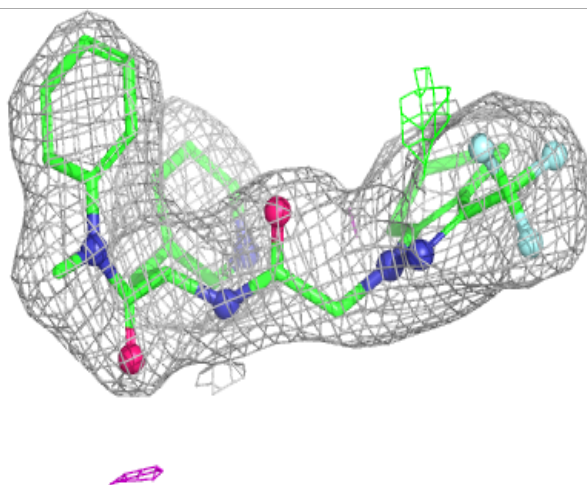
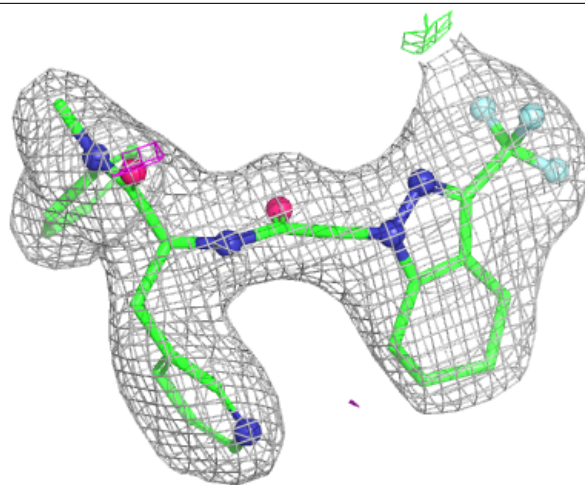
**Electron density around A1CH7 G 301:**

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



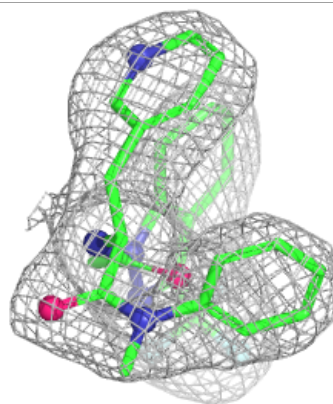
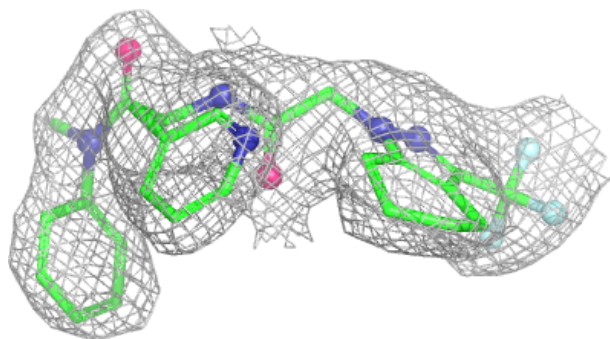
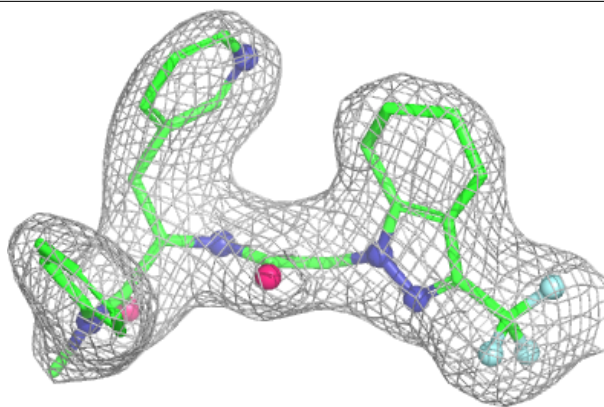
**Electron density around A1CH7 B 301:**

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

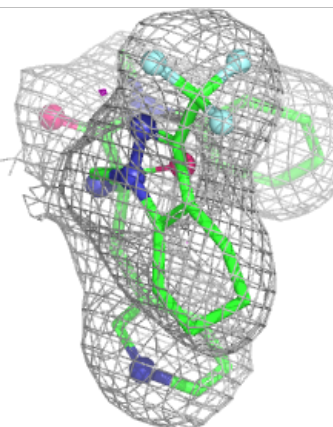
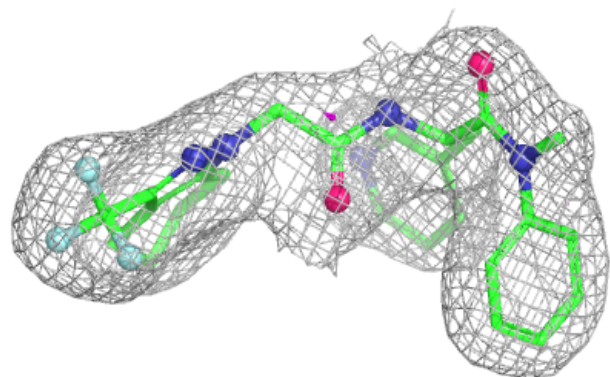
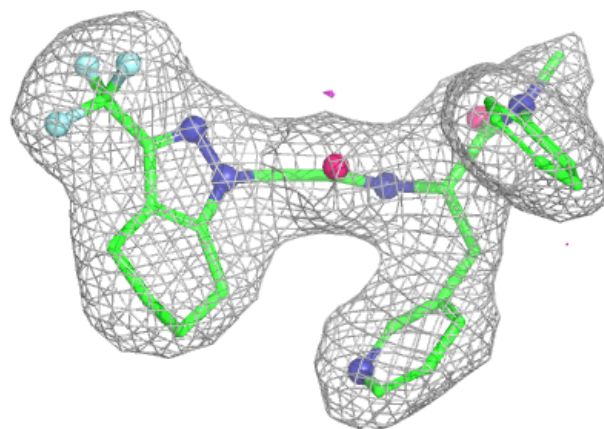


**Electron density around A1CH7 J 301:**

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

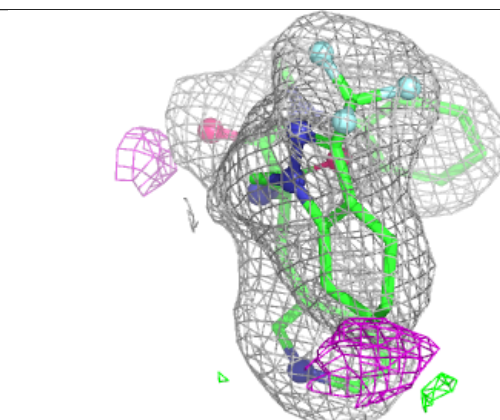
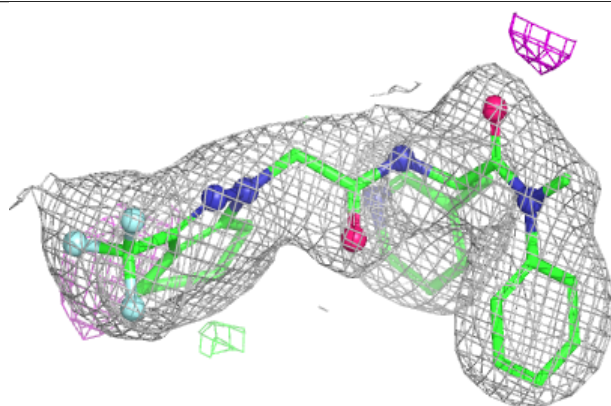
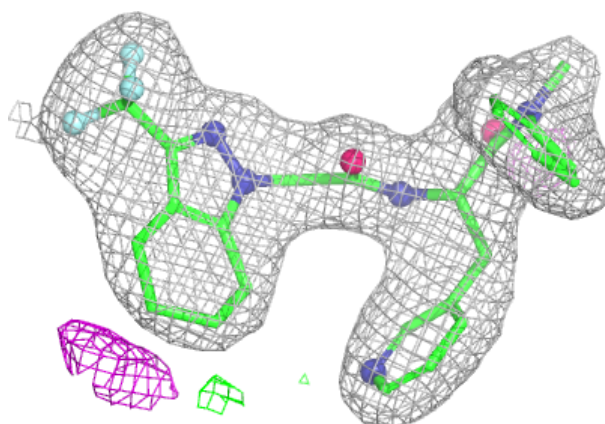
**Electron density around A1CH7 C 301:**

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

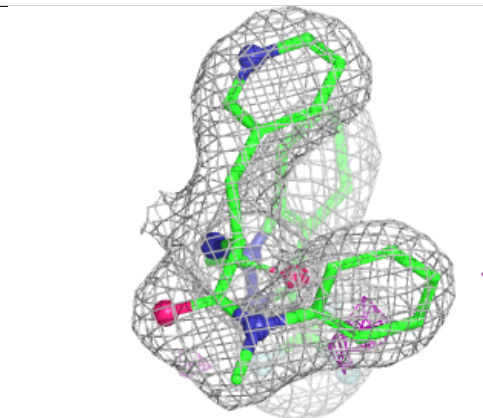
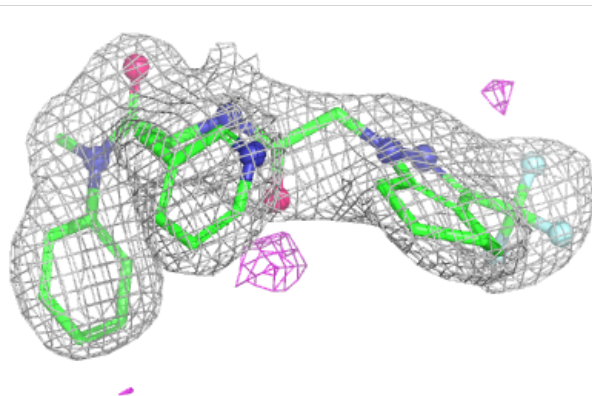
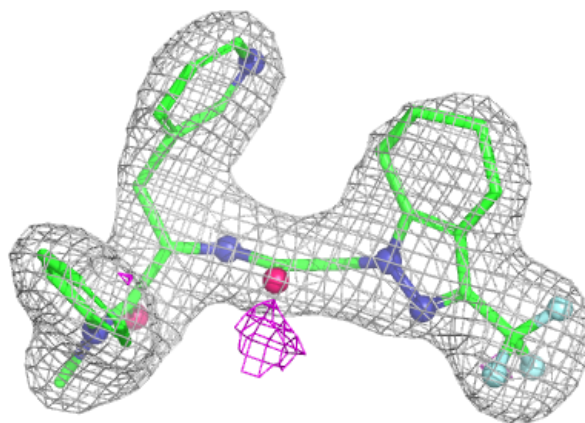


**Electron density around A1CH7 D 302:**

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

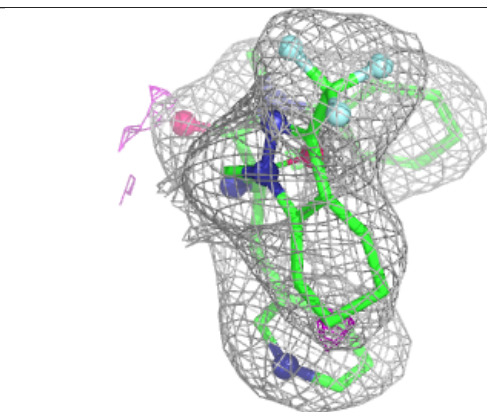
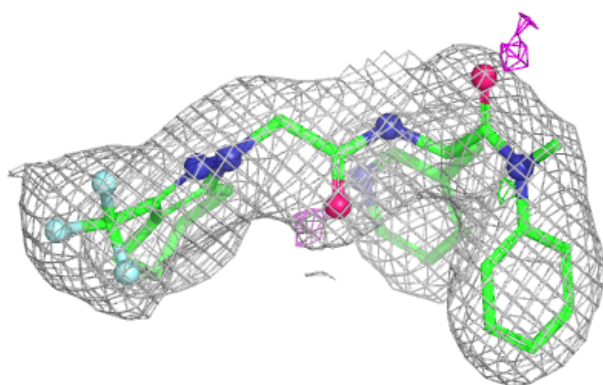
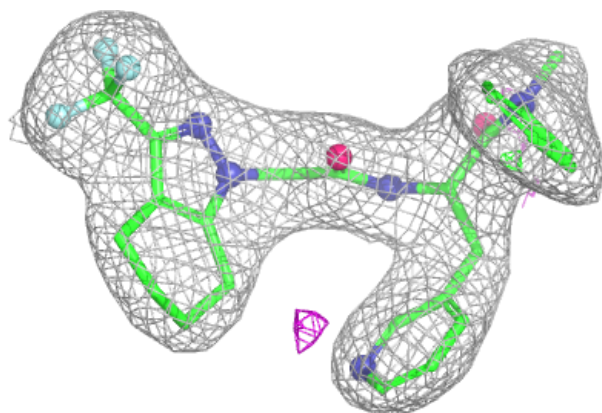
**Electron density around A1CH7 I 301:**

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

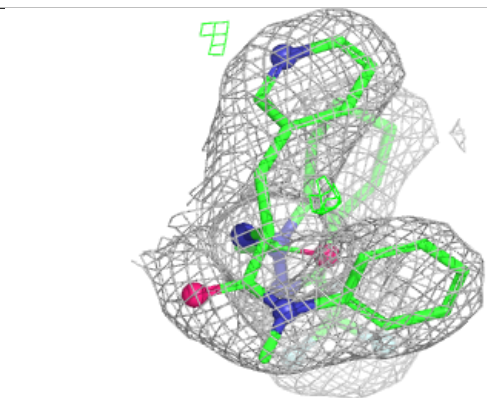
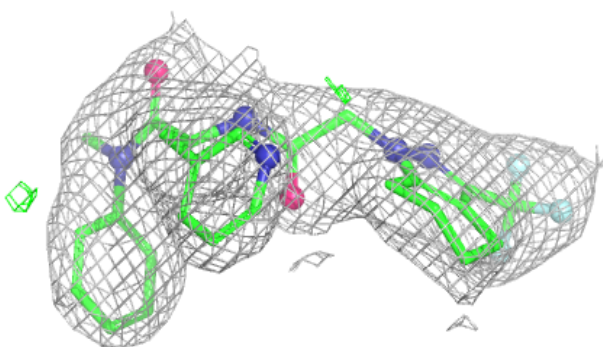
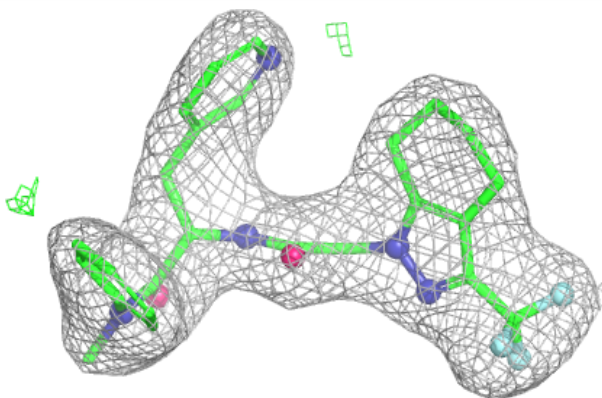


**Electron density around A1CH7 A 301:**

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

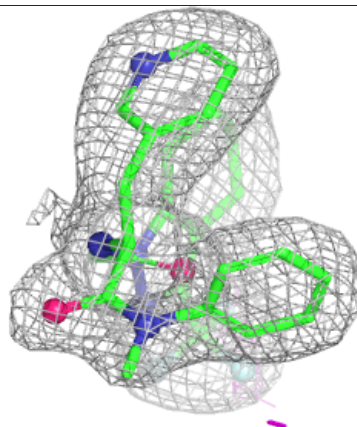
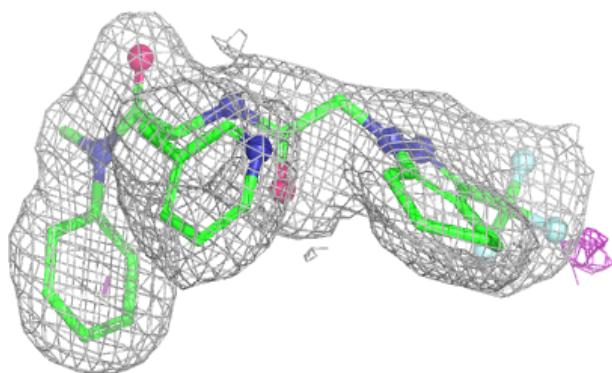
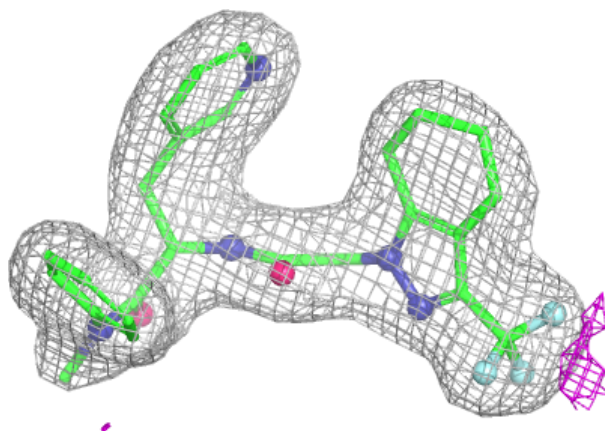
**Electron density around A1CH7 K 301:**

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



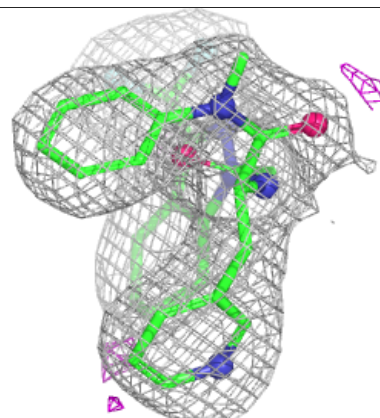
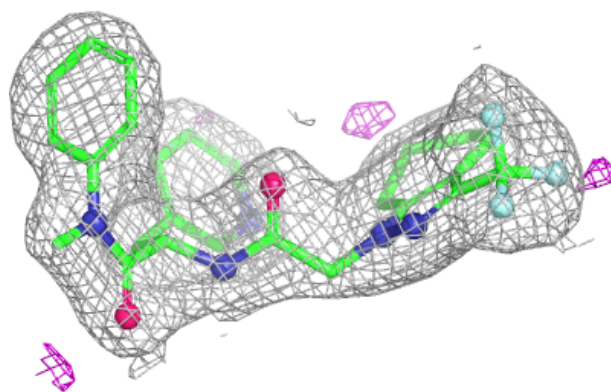
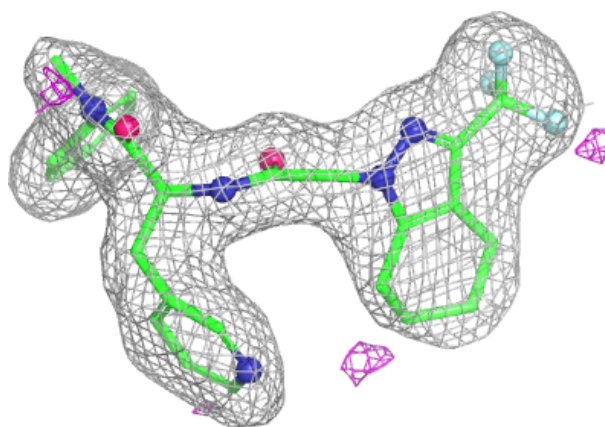
**Electron density around A1CH7 L 301:**

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



**Electron density around A1CH7 D 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.