



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2025 – 10:17 AM EDT

PDB ID : 9PGS / pdb\_00009pgs  
Title : HIV Capsid Hexamer bound to Compound 6  
Authors : Somoza, J.R.; Anderson, R.L.; Villasenor, A.G.; Ferrao, R.D.  
Deposited on : 2025-07-08  
Resolution : 2.40 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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

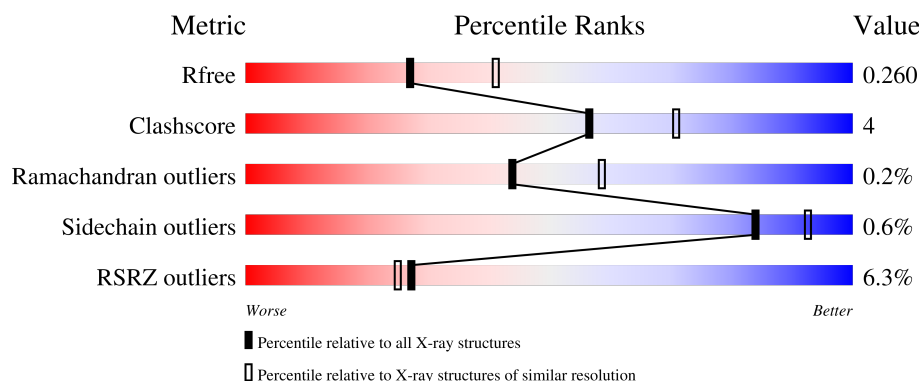
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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>12%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>9%</div> </div> </div>
1	B	232	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>9%</div> </div> </div>
1	C	232	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>
1	D	232	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>10%</div> </div> </div>
1	E	232	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	232	<p>2% 83% 12% 5%</p>
1	G	232	<p>5% 81% 9% 10%</p>
1	H	232	<p>6% 81% 13% 6%</p>
1	I	232	<p>6% 82% 10% 8%</p>
1	J	232	<p>3% 82% 12% 6%</p>
1	K	232	<p>7% 80% 11% 9%</p>
1	L	232	<p>9% 82% 11% 7%</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20550 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	212	Total	C	N	O	S	0	0	0
			1629	1025	284	307	13			
1	B	212	Total	C	N	O	S	0	0	0
			1639	1028	286	311	14			
1	C	208	Total	C	N	O	S	0	0	0
			1615	1015	283	303	14			
1	D	209	Total	C	N	O	S	0	0	0
			1613	1013	281	305	14			
1	E	218	Total	C	N	O	S	0	0	0
			1672	1050	293	315	14			
1	F	220	Total	C	N	O	S	0	0	0
			1690	1061	296	319	14			
1	G	208	Total	C	N	O	S	0	0	0
			1614	1016	281	303	14			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1047	292	314	14			
1	I	213	Total	C	N	O	S	0	0	0
			1634	1029	285	306	14			
1	J	218	Total	C	N	O	S	0	0	0
			1672	1050	293	315	14			
1	K	212	Total	C	N	O	S	0	0	0
			1631	1024	286	307	14			
1	L	216	Total	C	N	O	S	0	0	0
			1659	1043	290	312	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	engineered mutation	UNP B6DRA0
A	45	CYS	GLU	engineered mutation	UNP B6DRA0
A	184	ALA	TRP	engineered mutation	UNP B6DRA0
A	185	ALA	MET	engineered mutation	UNP B6DRA0

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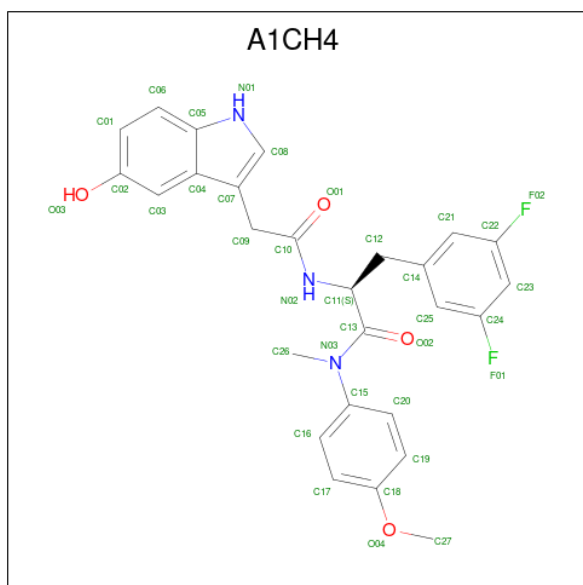
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP B6DRA0
B	14	CYS	ALA	engineered mutation	UNP B6DRA0
B	45	CYS	GLU	engineered mutation	UNP B6DRA0
B	184	ALA	TRP	engineered mutation	UNP B6DRA0
B	185	ALA	MET	engineered mutation	UNP B6DRA0
C	0	MET	-	initiating methionine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

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

- Molecule 2 is 3,5-difluoro-Nalpa-[(5-hydroxy-1H-indol-3-yl)acetyl]-N-(4-methoxyphenyl)-N-methyl-L-phenylalaninamide (CCD ID: A1CH4) (formula:  $C_{27}H_{25}F_2N_3O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 27	F 2	N 3	O 4	0	0
2	B	1	Total 36	C 27	F 2	N 3	O 4	0	0
2	C	1	Total 36	C 27	F 2	N 3	O 4	0	0
2	D	1	Total 36	C 27	F 2	N 3	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total 36	C 27	F 2	N 3	O 4	0	0
2	F	1	Total 36	C 27	F 2	N 3	O 4	0	0
2	G	1	Total 36	C 27	F 2	N 3	O 4	0	0
2	H	1	Total 36	C 27	F 2	N 3	O 4	0	0
2	I	1	Total 36	C 27	F 2	N 3	O 4	0	0
2	J	1	Total 36	C 27	F 2	N 3	O 4	0	0
2	K	1	Total 36	C 27	F 2	N 3	O 4	0	0
2	L	1	Total 36	C 27	F 2	N 3	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	32	Total 32	O 32	0	0
3	C	44	Total 44	O 44	0	0
3	D	45	Total 45	O 45	0	0
3	E	46	Total 46	O 46	0	0
3	F	50	Total 50	O 50	0	0
3	G	29	Total 29	O 29	0	0
3	H	25	Total 25	O 25	0	0
3	I	23	Total 23	O 23	0	0
3	J	20	Total 20	O 20	0	0
3	K	18	Total 18	O 18	0	0

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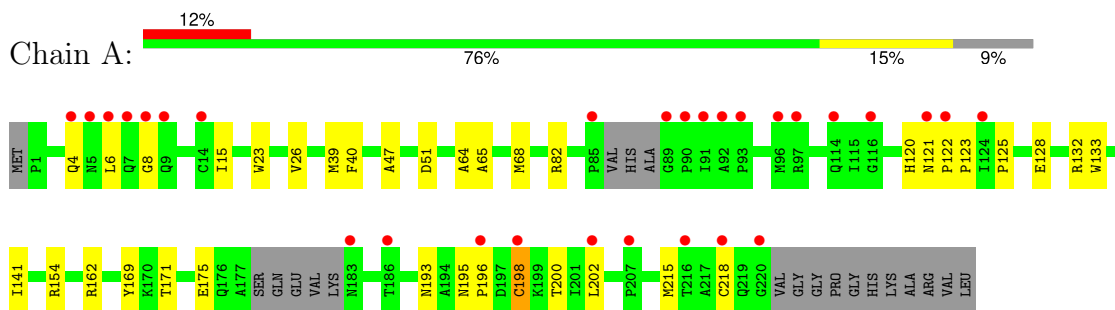
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	23	Total	O	0	0
			23	23		



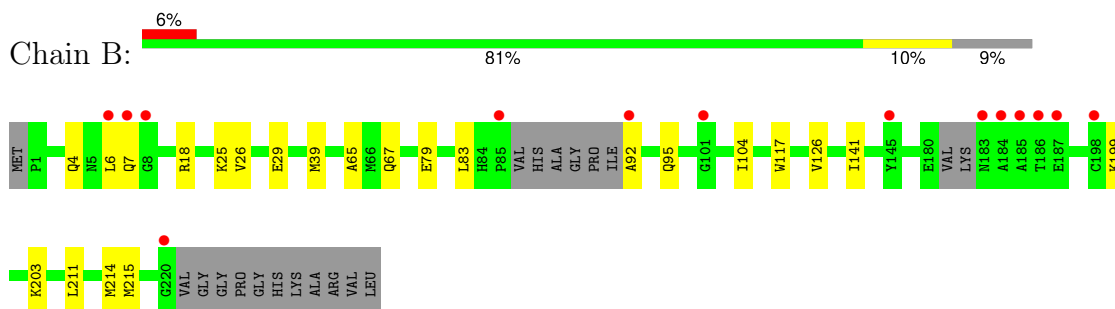
### 3 Residue-property plots [i](#)

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.

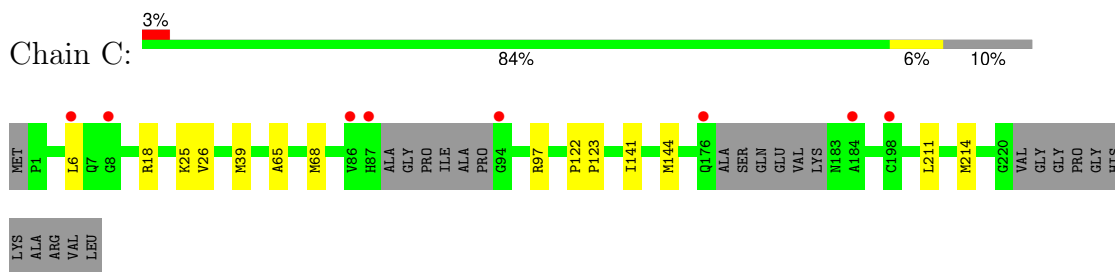
- Molecule 1: HIV-1 capsid



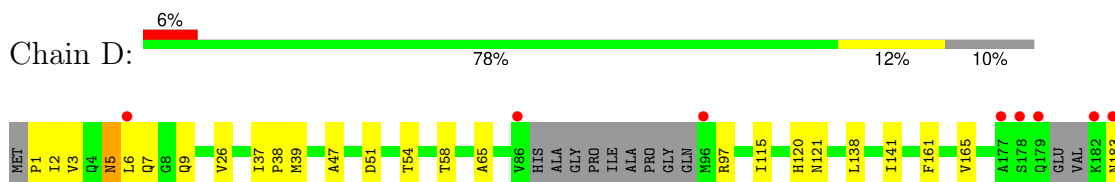
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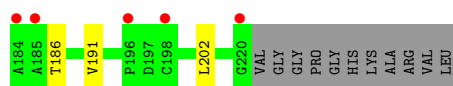


- Molecule 1: HIV-1 capsid

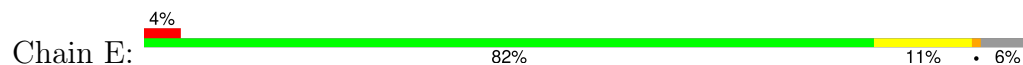


- Molecule 1: HIV-1 capsid

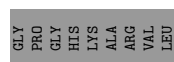
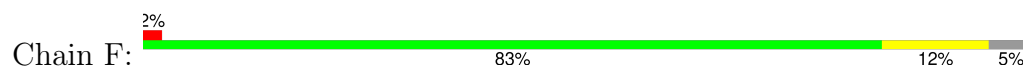




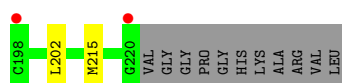
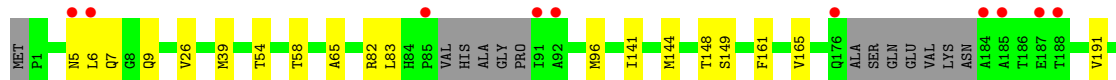
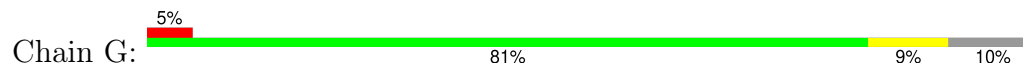
- Molecule 1: HIV-1 capsid



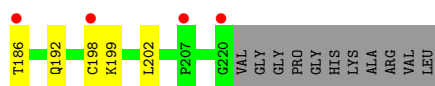
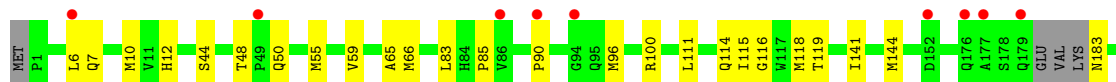
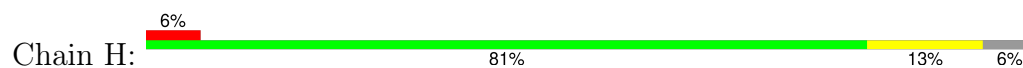
- Molecule 1: HIV-1 capsid



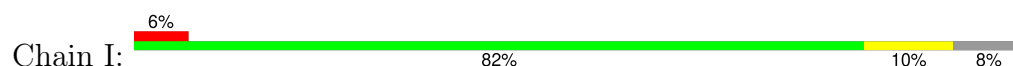
- Molecule 1: HIV-1 capsid

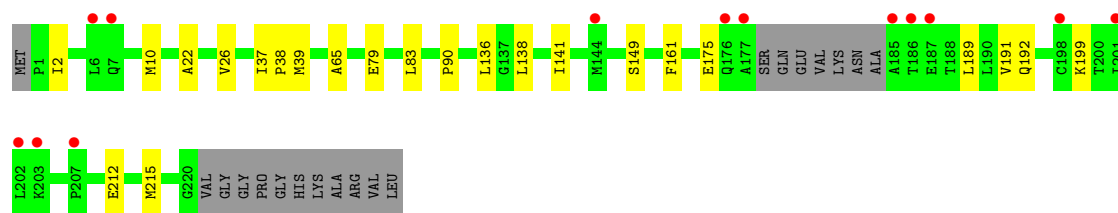


- Molecule 1: HIV-1 capsid

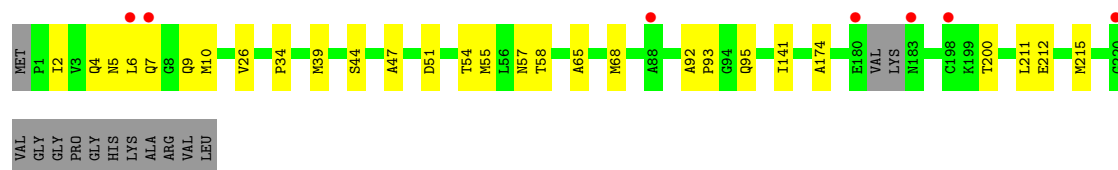
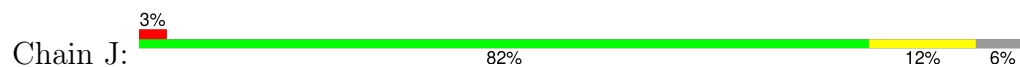


- Molecule 1: HIV-1 capsid

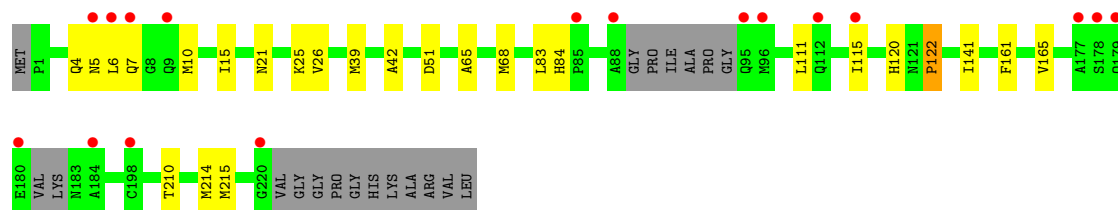
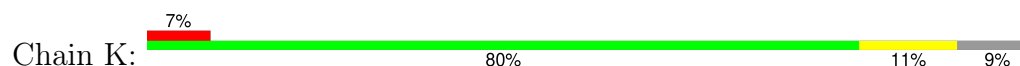




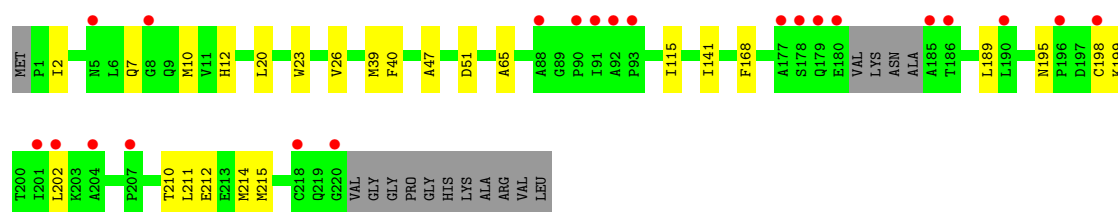
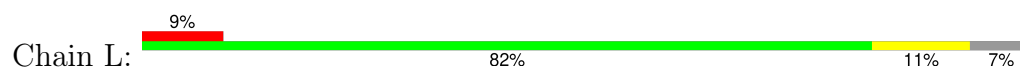
● Molecule 1: HIV-1 capsid



● Molecule 1: HIV-1 capsid



● Molecule 1: HIV-1 capsid



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.87Å 156.56Å 118.92Å 90.00° 97.82° 90.00°	Depositor
Resolution (Å)	47.72 – 2.40 47.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.72-2.40) 88.9 (47.72-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.63 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.219 , 0.261 0.218 , 0.260	Depositor DCC
$R_{free}$ test set	2000 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 34.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1CH4

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	0.14	0/1663	0.31	0/2261
1	B	0.14	0/1672	0.31	0/2270
1	C	0.12	0/1648	0.28	0/2237
1	D	0.12	0/1645	0.27	0/2234
1	E	0.12	0/1708	0.27	0/2323
1	F	0.12	0/1727	0.29	0/2350
1	G	0.11	0/1647	0.27	0/2236
1	H	0.11	0/1703	0.26	0/2316
1	I	0.11	0/1670	0.28	0/2272
1	J	0.11	0/1708	0.28	0/2323
1	K	0.12	0/1664	0.27	0/2260
1	L	0.11	0/1695	0.29	0/2305
All	All	0.12	0/20150	0.28	0/27387

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

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	1629	0	1609	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1639	0	1621	16	0
1	C	1615	0	1601	10	0
1	D	1613	0	1589	18	0
1	E	1672	0	1646	20	0
1	F	1690	0	1669	21	0
1	G	1614	0	1609	15	0
1	H	1667	0	1645	19	0
1	I	1634	0	1612	14	0
1	J	1672	0	1646	17	0
1	K	1631	0	1604	17	0
1	L	1659	0	1635	15	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
2	C	36	0	0	0	0
2	D	36	0	0	0	0
2	E	36	0	0	0	0
2	F	36	0	0	0	0
2	G	36	0	0	0	0
2	H	36	0	0	0	0
2	I	36	0	0	0	0
2	J	36	0	0	0	0
2	K	36	0	0	0	0
2	L	36	0	0	0	0
3	A	28	0	0	0	0
3	B	32	0	0	0	0
3	C	44	0	0	0	0
3	D	45	0	0	0	0
3	E	46	0	0	0	0
3	F	50	0	0	0	0
3	G	29	0	0	0	0
3	H	25	0	0	0	0
3	I	23	0	0	0	0
3	J	20	0	0	0	0
3	K	18	0	0	0	0
3	L	23	0	0	0	0
All	All	20550	0	19486	177	0

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

All (177) 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:E:191:VAL:HG12	1:E:202:LEU:HD13	1.69	0.73
1:E:6:LEU:HD11	1:F:6:LEU:HD23	1.76	0.67
1:D:6:LEU:HB3	1:E:6:LEU:HD23	1.75	0.66
1:H:59:VAL:HG11	1:H:66:MET:HE3	1.79	0.64
1:J:26:VAL:HG21	1:J:39:MET:HG2	1.79	0.63
1:H:85:PRO:HA	1:H:100:ARG:HH12	1.64	0.63
1:G:144:MET:HE1	1:L:212:GLU:HG3	1.80	0.63
1:K:120:HIS:CD2	1:K:122:PRO:HD2	2.34	0.62
1:G:5:ASN:HD22	1:G:9:GLN:HE21	1.49	0.61
1:B:211:LEU:HA	1:B:214:MET:HE3	1.82	0.60
1:A:132:ARG:NH2	1:A:133:TRP:HE1	2.00	0.60
1:I:189:LEU:HA	1:I:192:GLN:HG2	1.82	0.60
1:F:7:GLN:HE21	1:L:7:GLN:HG3	1.67	0.59
1:C:211:LEU:HA	1:C:214:MET:HE3	1.85	0.59
1:B:26:VAL:HG21	1:B:39:MET:HG2	1.85	0.58
1:H:111:LEU:O	1:H:115:ILE:HG12	2.04	0.58
1:H:183:ASN:HB3	1:H:186:THR:HG23	1.86	0.58
1:D:5:ASN:HD22	1:D:9:GLN:HE21	1.51	0.57
1:J:65:ALA:HB1	1:J:141:ILE:HD13	1.85	0.57
1:J:92:ALA:HB3	1:J:95:GLN:HG3	1.85	0.56
1:C:65:ALA:HB1	1:C:141:ILE:HD13	1.88	0.56
1:I:212:GLU:HB2	1:J:68:MET:HE3	1.86	0.56
1:J:2:ILE:HG22	1:J:10:MET:HE3	1.88	0.56
1:A:65:ALA:HB1	1:A:141:ILE:HD13	1.88	0.56
1:H:44:SER:HB3	1:H:55:MET:HE1	1.88	0.55
1:B:65:ALA:HB1	1:B:141:ILE:HD13	1.88	0.55
1:F:211:LEU:HA	1:F:214:MET:HE3	1.88	0.55
1:K:15:ILE:HD11	1:K:51:ASP:HB3	1.88	0.55
1:K:111:LEU:O	1:K:115:ILE:HG13	2.07	0.55
1:E:168:PHE:HE1	1:E:189:LEU:HD12	1.71	0.54
1:A:154:ARG:HG2	1:A:193:ASN:HD22	1.72	0.54
1:L:26:VAL:HG21	1:L:39:MET:HG2	1.88	0.54
1:F:92:ALA:HB3	1:F:95:GLN:HG3	1.90	0.54
1:K:83:LEU:HD22	1:K:84:HIS:CE1	2.42	0.54
1:E:154:ARG:HG2	1:E:193:ASN:HB3	1.90	0.54
1:D:97:ARG:HB2	1:H:90:PRO:HB2	1.90	0.54
1:E:65:ALA:HB1	1:E:141:ILE:HD13	1.90	0.54
1:L:199:LYS:HA	1:L:202:LEU:HD23	1.90	0.53
1:J:34:PRO:HG3	1:J:174:ALA:HA	1.90	0.53
1:H:12:HIS:HB2	1:H:115:ILE:HD12	1.89	0.53
1:D:191:VAL:HG22	1:D:202:LEU:HD13	1.91	0.53
1:D:54:THR:O	1:D:58:THR:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:215:MET:HE2	1:H:144:MET:HE1	1.92	0.52
1:I:2:ILE:HG22	1:I:10:MET:HE3	1.91	0.52
1:F:144:MET:HE2	1:F:145:TYR:CE1	2.44	0.52
1:K:65:ALA:HB1	1:K:141:ILE:HD13	1.91	0.52
1:L:65:ALA:HB1	1:L:141:ILE:HD13	1.90	0.52
1:D:2:ILE:HD11	1:D:115:ILE:HG12	1.91	0.52
1:E:2:ILE:HG22	1:E:10:MET:HE3	1.90	0.52
1:D:65:ALA:HB1	1:D:141:ILE:HD13	1.92	0.52
1:G:82:ARG:NH1	1:G:83:LEU:HD12	2.24	0.52
1:D:37:ILE:HD12	1:D:138:LEU:HB3	1.92	0.52
1:G:65:ALA:HB1	1:G:141:ILE:HD13	1.92	0.51
1:A:121:ASN:HB2	1:A:122:PRO:HD3	1.93	0.51
1:D:47:ALA:HB1	1:D:51:ASP:HB2	1.91	0.51
1:D:120:HIS:CD2	1:D:121:ASN:H	2.29	0.51
1:A:26:VAL:HG21	1:A:39:MET:HG2	1.93	0.51
1:B:117:TRP:CE2	1:J:93:PRO:HG3	2.46	0.51
1:G:5:ASN:HD22	1:G:9:GLN:NE2	2.09	0.50
1:E:168:PHE:CE1	1:E:189:LEU:HD12	2.46	0.50
1:K:4:GLN:HG2	1:K:10:MET:SD	2.52	0.50
1:H:114:GLN:O	1:H:118:MET:HE3	2.11	0.50
1:D:5:ASN:HB2	1:D:9:GLN:O	2.12	0.50
1:G:6:LEU:HB3	1:H:6:LEU:HD23	1.93	0.50
1:G:191:VAL:HG22	1:G:202:LEU:HD13	1.94	0.50
1:J:44:SER:HA	1:J:55:MET:HE1	1.94	0.50
1:A:120:HIS:CG	1:A:122:PRO:HD2	2.47	0.49
1:I:149:SER:HA	1:I:175:GLU:OE2	2.12	0.49
1:L:168:PHE:HE2	1:L:189:LEU:HD12	1.78	0.49
1:B:104:ILE:HG12	1:B:126:VAL:HG12	1.95	0.49
1:E:22:ALA:O	1:E:26:VAL:HG13	2.12	0.49
1:F:184:ALA:O	1:F:188:THR:HG23	2.13	0.49
1:A:4:GLN:NE2	1:A:8:GLY:HA2	2.28	0.49
1:A:64:ALA:HB1	1:F:215:MET:HE1	1.94	0.49
1:E:165:VAL:HG22	1:E:190:LEU:HD11	1.95	0.48
1:I:161:PHE:CD2	1:I:215:MET:HG2	2.48	0.48
1:L:2:ILE:HD11	1:L:115:ILE:HG12	1.94	0.48
1:I:65:ALA:HB1	1:I:141:ILE:HD13	1.94	0.48
1:A:195:ASN:OD1	1:A:198:CYS:HB2	2.13	0.48
1:C:26:VAL:HG21	1:C:39:MET:HG2	1.96	0.47
1:D:26:VAL:HG21	1:D:39:MET:HG2	1.96	0.47
1:F:37:ILE:HD12	1:F:138:LEU:HB3	1.95	0.47
1:J:211:LEU:O	1:J:215:MET:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLU:O	1:B:83:LEU:HG	2.14	0.47
1:I:37:ILE:HD11	1:I:138:LEU:HB3	1.97	0.47
1:J:5:ASN:HB2	1:J:9:GLN:O	2.15	0.47
1:H:198:CYS:O	1:H:202:LEU:HG	2.15	0.47
1:K:26:VAL:HG21	1:K:39:MET:HG2	1.97	0.47
1:J:6:LEU:HD12	1:K:7:GLN:HG2	1.98	0.46
1:K:25:LYS:HA	1:K:25:LYS:HD3	1.83	0.46
1:B:117:TRP:CZ2	1:J:93:PRO:HG3	2.51	0.46
1:F:26:VAL:HG21	1:F:39:MET:HG2	1.97	0.46
1:G:144:MET:HE3	1:G:144:MET:HB2	1.84	0.46
1:A:6:LEU:HD13	1:B:6:LEU:HD12	1.98	0.46
1:D:5:ASN:ND2	1:D:9:GLN:HE21	2.13	0.46
1:B:7:GLN:HB2	1:J:7:GLN:OE1	2.16	0.46
1:D:1:PRO:HB2	1:D:3:VAL:HG13	1.97	0.46
1:A:125:PRO:HB2	1:A:128:GLU:HB2	1.97	0.45
1:F:4:GLN:OE1	1:F:8:GLY:HA2	2.16	0.45
1:B:18:ARG:HH21	1:C:18:ARG:NH1	2.14	0.45
1:F:47:ALA:HB1	1:F:51:ASP:HB2	1.99	0.45
1:L:2:ILE:HG22	1:L:10:MET:HE3	1.98	0.45
1:I:38:PRO:HG3	1:J:57:ASN:HB3	1.98	0.45
1:D:38:PRO:HG3	1:E:57:ASN:HB3	1.99	0.45
1:H:65:ALA:HB1	1:H:141:ILE:HD13	1.99	0.45
1:K:42:ALA:HB1	1:L:20:LEU:HD11	1.99	0.44
1:B:6:LEU:HD13	1:C:6:LEU:HD22	1.99	0.44
1:B:92:ALA:HB3	1:B:95:GLN:HB2	1.99	0.44
1:B:199:LYS:O	1:B:203:LYS:HG2	2.17	0.44
1:E:191:VAL:O	1:E:199:LYS:HD3	2.17	0.44
1:F:161:PHE:O	1:F:165:VAL:HG23	2.16	0.44
1:G:96:MET:HE2	1:G:96:MET:HB3	1.81	0.44
1:L:210:THR:O	1:L:214:MET:HG3	2.17	0.44
1:E:26:VAL:HG11	1:E:39:MET:HG2	1.99	0.44
1:A:171:THR:O	1:A:175:GLU:HG2	2.18	0.44
1:E:18:ARG:CZ	1:E:18:ARG:HB2	2.47	0.44
1:L:47:ALA:HB1	1:L:51:ASP:HB2	2.00	0.44
1:A:47:ALA:HB1	1:A:51:ASP:HB2	2.00	0.44
1:E:6:LEU:HD13	1:E:6:LEU:HA	1.74	0.44
1:K:210:THR:O	1:K:214:MET:HG3	2.18	0.44
1:F:144:MET:HE2	1:F:145:TYR:HE1	1.82	0.44
1:K:5:ASN:HD22	1:K:6:LEU:H	1.66	0.44
1:A:82:ARG:HE	1:A:82:ARG:HB3	1.53	0.43
1:A:195:ASN:HB2	1:A:196:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:212:GLU:HB2	1:K:68:MET:HE3	2.00	0.43
1:A:121:ASN:O	1:A:123:PRO:HD3	2.18	0.43
1:C:97:ARG:HB2	1:I:90:PRO:HB2	1.99	0.43
1:G:26:VAL:HG21	1:G:39:MET:HG2	1.99	0.43
1:H:10:MET:HB2	1:H:119:THR:HG22	2.00	0.43
1:G:148:THR:HG22	1:G:149:SER:O	2.19	0.43
1:A:169:TYR:CZ	1:B:67:GLN:HG2	2.54	0.43
1:I:79:GLU:O	1:I:83:LEU:HG	2.19	0.43
1:F:4:GLN:HG2	1:F:10:MET:SD	2.58	0.43
1:G:7:GLN:HE21	1:G:9:GLN:NE2	2.17	0.43
1:I:26:VAL:HG11	1:I:39:MET:HG2	2.01	0.43
1:B:25:LYS:O	1:B:29:GLU:HG3	2.19	0.43
1:L:23:TRP:CZ3	1:L:40:PHE:HB2	2.54	0.43
1:D:183:ASN:HB3	1:D:186:THR:HG23	2.02	0.42
1:E:96:MET:HE3	1:E:96:MET:HB3	1.82	0.42
1:G:54:THR:O	1:G:58:THR:HG23	2.20	0.42
1:H:83:LEU:C	1:H:85:PRO:HD3	2.44	0.42
1:L:211:LEU:O	1:L:215:MET:HG3	2.20	0.42
1:A:15:ILE:HD11	1:A:51:ASP:HB3	2.00	0.42
1:F:211:LEU:HG	1:F:215:MET:HE2	2.01	0.42
1:L:2:ILE:HD13	1:L:12:HIS:HA	2.01	0.42
1:C:25:LYS:HA	1:C:25:LYS:HD3	1.89	0.42
1:C:122:PRO:HA	1:C:123:PRO:HD3	1.91	0.42
1:F:37:ILE:CD1	1:F:138:LEU:HB3	2.50	0.42
1:F:191:VAL:HG22	1:F:202:LEU:HD13	2.02	0.42
1:H:192:GLN:HA	1:H:199:LYS:HE3	2.02	0.42
1:K:5:ASN:ND2	1:K:6:LEU:H	2.18	0.42
1:K:21:ASN:O	1:K:25:LYS:HG2	2.20	0.42
1:J:54:THR:O	1:J:58:THR:HG23	2.20	0.41
1:D:161:PHE:O	1:D:165:VAL:HG23	2.19	0.41
1:J:47:ALA:HB1	1:J:51:ASP:HB2	2.03	0.41
1:K:161:PHE:CE2	1:K:215:MET:HG2	2.56	0.41
1:E:146:SER:HA	1:E:147:PRO:HD3	1.93	0.41
1:F:199:LYS:O	1:F:203:LYS:HG2	2.20	0.41
1:E:54:THR:O	1:E:58:THR:HG23	2.20	0.41
1:H:96:MET:HE1	1:H:116:GLY:C	2.46	0.41
1:E:68:MET:HE2	1:E:68:MET:HB3	1.85	0.41
1:A:68:MET:SD	1:F:215:MET:HE3	2.60	0.41
1:B:215:MET:HE2	1:C:68:MET:SD	2.61	0.41
1:D:7:GLN:HB3	1:H:7:GLN:NE2	2.35	0.41
1:G:161:PHE:O	1:G:165:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:191:VAL:O	1:I:199:LYS:HG3	2.20	0.41
1:F:202:LEU:HD22	1:F:214:MET:HG2	2.01	0.41
1:A:23:TRP:CZ3	1:A:40:PHE:HB2	2.56	0.41
1:I:192:GLN:HA	1:I:199:LYS:HE2	2.03	0.41
1:L:195:ASN:OD1	1:L:198:CYS:HB3	2.20	0.41
1:H:55:MET:HB2	1:H:55:MET:HE3	1.86	0.40
1:I:22:ALA:O	1:I:26:VAL:HG13	2.21	0.40
1:A:162:ARG:HA	1:A:215:MET:HE3	2.04	0.40
1:C:144:MET:HB2	1:C:144:MET:HE2	1.80	0.40
1:E:38:PRO:HG3	1:F:57:ASN:HB3	2.04	0.40
1:H:48:THR:C	1:H:50:GLN:H	2.30	0.40
1:K:161:PHE:O	1:K:165:VAL:HG23	2.21	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	206/232 (89%)	200 (97%)	6 (3%)	0	100	100
1	B	206/232 (89%)	202 (98%)	4 (2%)	0	100	100
1	C	202/232 (87%)	200 (99%)	2 (1%)	0	100	100
1	D	203/232 (88%)	199 (98%)	3 (2%)	1 (0%)	25	38
1	E	214/232 (92%)	209 (98%)	3 (1%)	2 (1%)	14	22
1	F	218/232 (94%)	217 (100%)	1 (0%)	0	100	100
1	G	202/232 (87%)	198 (98%)	4 (2%)	0	100	100
1	H	213/232 (92%)	208 (98%)	5 (2%)	0	100	100
1	I	209/232 (90%)	201 (96%)	8 (4%)	0	100	100
1	J	214/232 (92%)	210 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	206/232 (89%)	200 (97%)	5 (2%)	1 (0%)	25	38
1	L	212/232 (91%)	208 (98%)	4 (2%)	0	100	100
All	All	2505/2784 (90%)	2452 (98%)	49 (2%)	4 (0%)	44	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	147	PRO
1	E	157	PRO
1	D	5	ASN
1	K	122	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/194 (90%)	171 (98%)	4 (2%)	45	66
1	B	178/194 (92%)	177 (99%)	1 (1%)	84	92
1	C	176/194 (91%)	176 (100%)	0	100	100
1	D	174/194 (90%)	174 (100%)	0	100	100
1	E	179/194 (92%)	177 (99%)	2 (1%)	70	84
1	F	182/194 (94%)	180 (99%)	2 (1%)	70	84
1	G	176/194 (91%)	176 (100%)	0	100	100
1	H	179/194 (92%)	179 (100%)	0	100	100
1	I	175/194 (90%)	174 (99%)	1 (1%)	84	92
1	J	179/194 (92%)	177 (99%)	2 (1%)	70	84
1	K	175/194 (90%)	175 (100%)	0	100	100
1	L	178/194 (92%)	178 (100%)	0	100	100
All	All	2126/2328 (91%)	2114 (99%)	12 (1%)	84	92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	CYS
1	A	200	THR
1	A	202	LEU
1	A	218	CYS
1	B	4	GLN
1	E	6	LEU
1	E	131	LYS
1	F	7	GLN
1	F	16	SER
1	I	136	LEU
1	J	4	GLN
1	J	200	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	7	GLN
1	A	114	GLN
1	A	193	ASN
1	B	84	HIS
1	B	192	GLN
1	C	7	GLN
1	C	50	GLN
1	D	5	ASN
1	D	114	GLN
1	D	120	HIS
1	E	4	GLN
1	E	84	HIS
1	E	112	GLN
1	F	21	ASN
1	F	67	GLN
1	F	84	HIS
1	G	7	GLN
1	G	9	GLN
1	J	120	HIS
1	J	193	ASN
1	J	219	GLN
1	K	5	ASN
1	K	12	HIS
1	K	120	HIS
1	K	121	ASN
1	L	4	GLN

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Mol	Chain	Res	Type
1	L	13	GLN
1	L	50	GLN
1	L	63	GLN
1	L	95	GLN
1	L	219	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	A1CH4	G	301	-	38,39,39	0.83	0	48,55,55	1.38	6 (12%)
2	A1CH4	C	301	-	38,39,39	0.84	0	48,55,55	1.34	7 (14%)
2	A1CH4	E	301	-	38,39,39	0.81	0	48,55,55	1.35	6 (12%)
2	A1CH4	L	301	-	38,39,39	0.81	0	48,55,55	1.37	7 (14%)
2	A1CH4	H	301	-	38,39,39	0.81	0	48,55,55	1.38	8 (16%)
2	A1CH4	A	301	-	38,39,39	0.83	0	48,55,55	1.36	6 (12%)
2	A1CH4	F	301	-	38,39,39	0.84	0	48,55,55	1.36	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A1CH4	D	301	-	38,39,39	0.82	0	48,55,55	1.39	7 (14%)
2	A1CH4	I	301	-	38,39,39	0.84	0	48,55,55	1.30	6 (12%)
2	A1CH4	K	301	-	38,39,39	0.84	0	48,55,55	1.40	9 (18%)
2	A1CH4	B	301	-	38,39,39	0.79	0	48,55,55	1.30	5 (10%)
2	A1CH4	J	301	-	38,39,39	0.83	0	48,55,55	1.35	6 (12%)

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	A1CH4	G	301	-	-	0/26/26/26	0/4/4/4
2	A1CH4	C	301	-	-	0/26/26/26	0/4/4/4
2	A1CH4	E	301	-	-	0/26/26/26	0/4/4/4
2	A1CH4	L	301	-	-	0/26/26/26	0/4/4/4
2	A1CH4	H	301	-	-	0/26/26/26	0/4/4/4
2	A1CH4	A	301	-	-	0/26/26/26	0/4/4/4
2	A1CH4	F	301	-	-	2/26/26/26	0/4/4/4
2	A1CH4	D	301	-	-	0/26/26/26	0/4/4/4
2	A1CH4	I	301	-	-	0/26/26/26	0/4/4/4
2	A1CH4	K	301	-	-	0/26/26/26	0/4/4/4
2	A1CH4	B	301	-	-	2/26/26/26	0/4/4/4
2	A1CH4	J	301	-	-	0/26/26/26	0/4/4/4

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	301	A1CH4	C26-N03-C13	3.66	123.33	118.81
2	D	301	A1CH4	C01-C06-C05	-3.46	116.67	120.80
2	E	301	A1CH4	C15-N03-C13	-3.40	119.58	124.26
2	J	301	A1CH4	C01-C06-C05	-3.32	116.83	120.80
2	B	301	A1CH4	C01-C06-C05	-3.31	116.84	120.80
2	L	301	A1CH4	C26-N03-C13	3.30	122.89	118.81
2	H	301	A1CH4	C26-N03-C13	3.29	122.88	118.81
2	C	301	A1CH4	C01-C06-C05	-3.27	116.89	120.80
2	K	301	A1CH4	C15-N03-C13	-3.27	119.76	124.26
2	A	301	A1CH4	C01-C06-C05	-3.25	116.91	120.80
2	D	301	A1CH4	C26-N03-C13	3.24	122.82	118.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	A1CH4	C01-C06-C05	-3.23	116.94	120.80
2	H	301	A1CH4	C01-C06-C05	-3.22	116.95	120.80
2	F	301	A1CH4	C26-N03-C13	3.21	122.78	118.81
2	G	301	A1CH4	C15-N03-C13	-3.18	119.88	124.26
2	G	301	A1CH4	C26-N03-C13	3.18	122.75	118.81
2	F	301	A1CH4	C01-C06-C05	-3.15	117.03	120.80
2	G	301	A1CH4	C01-C06-C05	-3.15	117.04	120.80
2	L	301	A1CH4	C01-C06-C05	-3.14	117.04	120.80
2	H	301	A1CH4	C15-N03-C13	-3.13	119.95	124.26
2	K	301	A1CH4	C01-C06-C05	-3.09	117.10	120.80
2	G	301	A1CH4	C23-C22-C21	-3.07	119.77	123.50
2	I	301	A1CH4	C01-C06-C05	-3.05	117.15	120.80
2	L	301	A1CH4	C23-C22-C21	-3.02	119.83	123.50
2	B	301	A1CH4	C23-C22-C21	-2.99	119.86	123.50
2	C	301	A1CH4	C23-C22-C21	-2.99	119.87	123.50
2	C	301	A1CH4	C15-N03-C13	-2.99	120.15	124.26
2	F	301	A1CH4	C23-C22-C21	-2.96	119.90	123.50
2	J	301	A1CH4	C26-N03-C13	2.95	122.46	118.81
2	A	301	A1CH4	C23-C22-C21	-2.93	119.94	123.50
2	I	301	A1CH4	C26-N03-C13	2.92	122.42	118.81
2	A	301	A1CH4	C26-N03-C13	2.89	122.39	118.81
2	A	301	A1CH4	C15-N03-C13	-2.89	120.28	124.26
2	L	301	A1CH4	C25-C24-C23	-2.89	119.99	123.50
2	J	301	A1CH4	C25-C24-C23	-2.88	120.00	123.50
2	J	301	A1CH4	C23-C22-C21	-2.88	120.00	123.50
2	D	301	A1CH4	C25-C24-C23	-2.87	120.01	123.50
2	E	301	A1CH4	C23-C22-C21	-2.86	120.03	123.50
2	I	301	A1CH4	C25-C24-C23	-2.85	120.04	123.50
2	K	301	A1CH4	C25-C24-C23	-2.83	120.06	123.50
2	B	301	A1CH4	C25-C24-C23	-2.83	120.07	123.50
2	F	301	A1CH4	C15-N03-C13	-2.82	120.38	124.26
2	E	301	A1CH4	C25-C24-C23	-2.80	120.09	123.50
2	L	301	A1CH4	C15-N03-C13	-2.80	120.41	124.26
2	I	301	A1CH4	C15-N03-C13	-2.79	120.42	124.26
2	D	301	A1CH4	C23-C22-C21	-2.79	120.11	123.50
2	H	301	A1CH4	C23-C22-C21	-2.78	120.12	123.50
2	L	301	A1CH4	C24-C23-C22	2.77	120.12	116.08
2	E	301	A1CH4	C26-N03-C13	2.76	122.22	118.81
2	F	301	A1CH4	C25-C24-C23	-2.75	120.15	123.50
2	B	301	A1CH4	C24-C23-C22	2.74	120.07	116.08
2	I	301	A1CH4	C23-C22-C21	-2.73	120.18	123.50
2	F	301	A1CH4	C24-C23-C22	2.73	120.06	116.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	A1CH4	C25-C24-C23	-2.72	120.20	123.50
2	J	301	A1CH4	C24-C23-C22	2.71	120.02	116.08
2	D	301	A1CH4	C24-C23-C22	2.69	120.00	116.08
2	G	301	A1CH4	C24-C23-C22	2.67	119.97	116.08
2	A	301	A1CH4	C24-C23-C22	2.67	119.97	116.08
2	H	301	A1CH4	C25-C24-C23	-2.67	120.26	123.50
2	G	301	A1CH4	C25-C24-C23	-2.66	120.27	123.50
2	C	301	A1CH4	C26-N03-C13	2.64	122.08	118.81
2	B	301	A1CH4	C15-N03-C13	-2.63	120.64	124.26
2	E	301	A1CH4	C24-C23-C22	2.62	119.90	116.08
2	D	301	A1CH4	C15-N03-C13	-2.61	120.67	124.26
2	H	301	A1CH4	C24-C23-C22	2.60	119.87	116.08
2	K	301	A1CH4	C23-C22-C21	-2.55	120.40	123.50
2	I	301	A1CH4	C24-C23-C22	2.55	119.79	116.08
2	C	301	A1CH4	C25-C24-C23	-2.51	120.45	123.50
2	C	301	A1CH4	C24-C23-C22	2.50	119.73	116.08
2	K	301	A1CH4	C24-C23-C22	2.41	119.59	116.08
2	K	301	A1CH4	O02-C13-N03	2.31	124.39	121.48
2	J	301	A1CH4	C15-N03-C13	-2.16	121.29	124.26
2	D	301	A1CH4	C02-C03-C04	-2.12	119.06	120.47
2	K	301	A1CH4	O02-C13-C11	-2.12	115.74	119.61
2	H	301	A1CH4	O02-C13-N03	2.11	124.15	121.48
2	L	301	A1CH4	C14-C21-C22	2.09	120.57	118.75
2	K	301	A1CH4	C14-C25-C24	2.07	120.56	118.75
2	C	301	A1CH4	C11-N02-C10	2.06	126.84	121.68
2	H	301	A1CH4	C02-C03-C04	-2.05	119.11	120.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

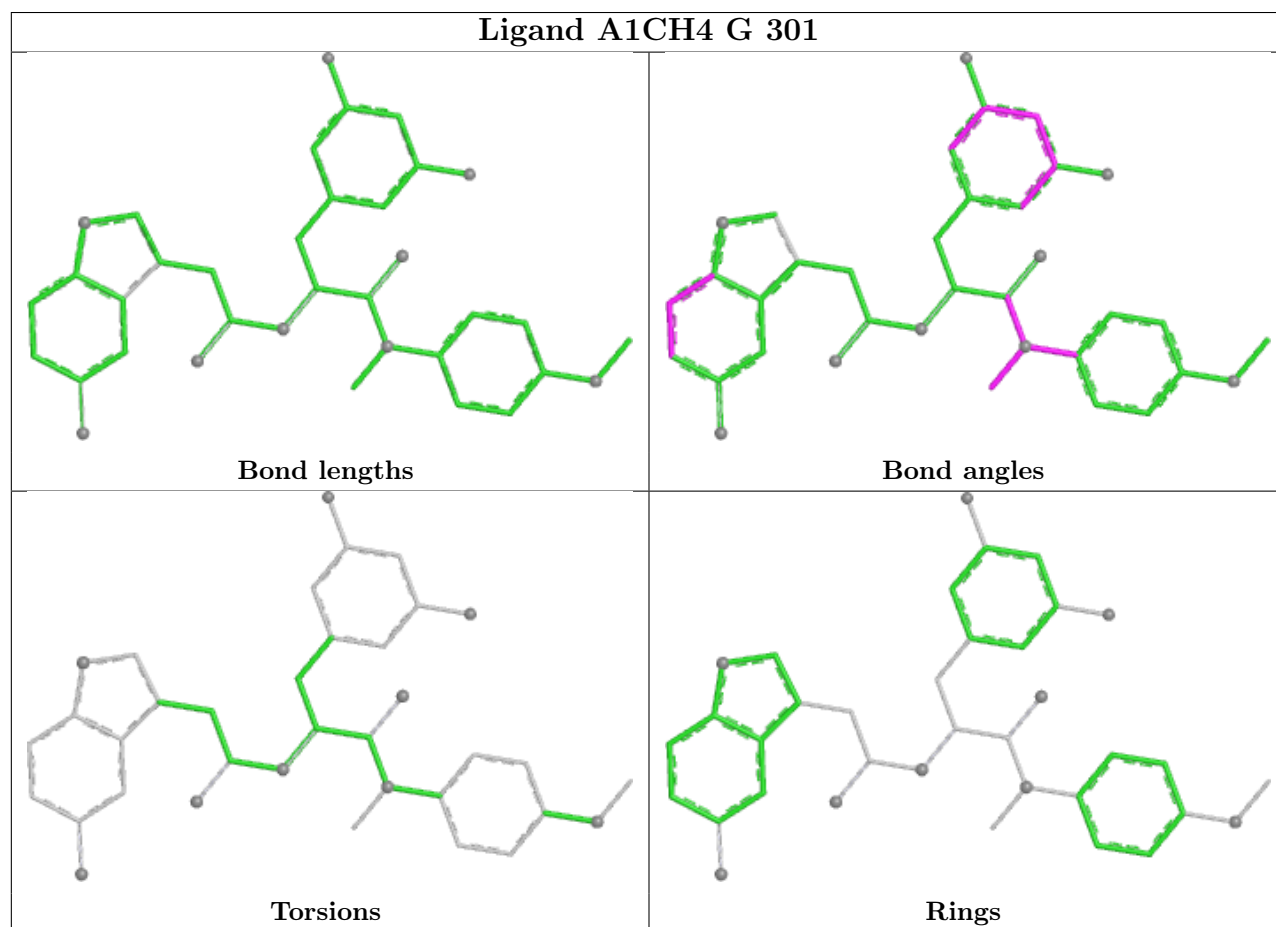
Mol	Chain	Res	Type	Atoms
2	F	301	A1CH4	C19-C18-O04-C27
2	F	301	A1CH4	C17-C18-O04-C27
2	B	301	A1CH4	C19-C18-O04-C27
2	B	301	A1CH4	C17-C18-O04-C27

There are no ring outliers.

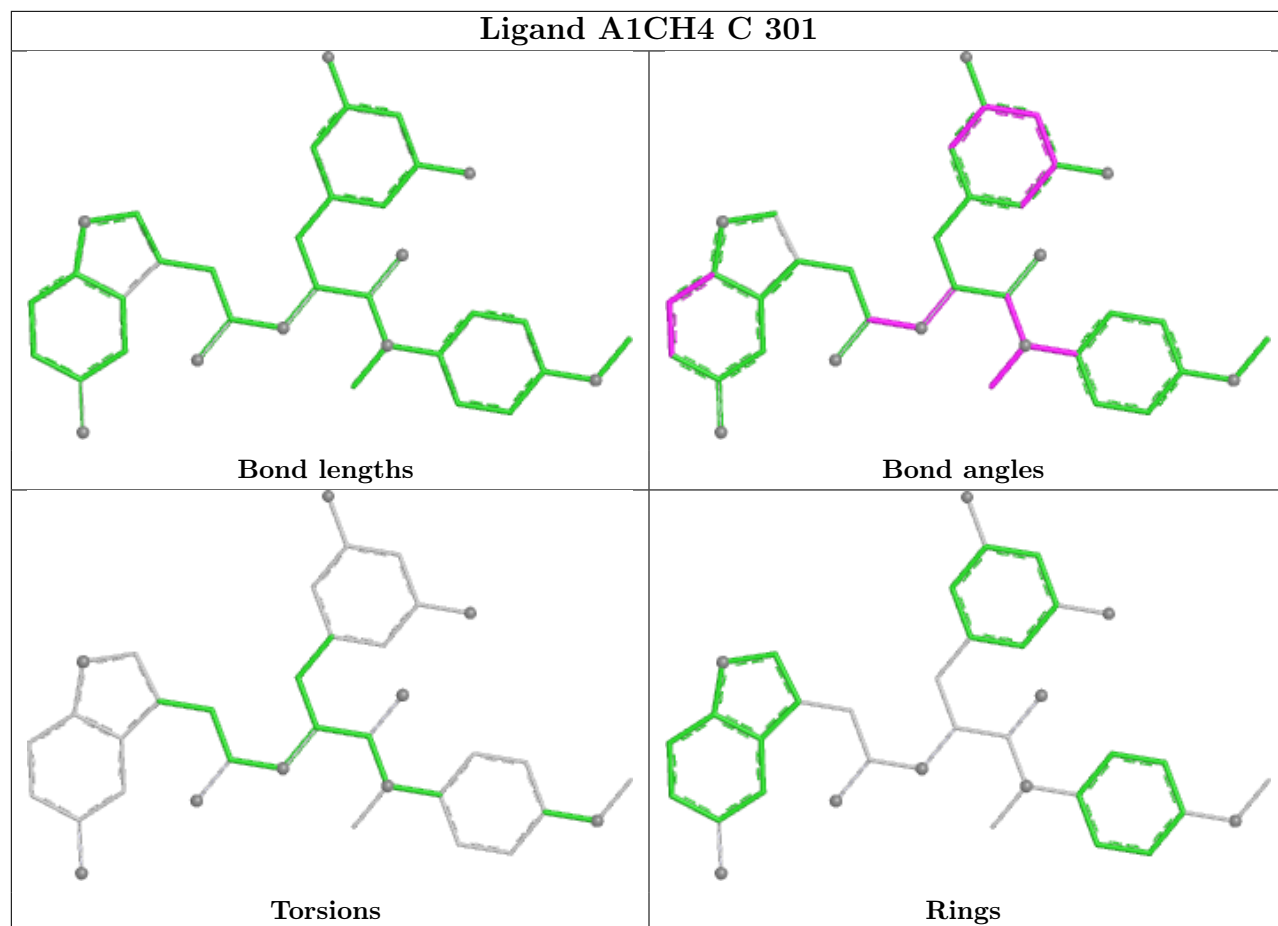
No monomer is involved in short contacts.

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

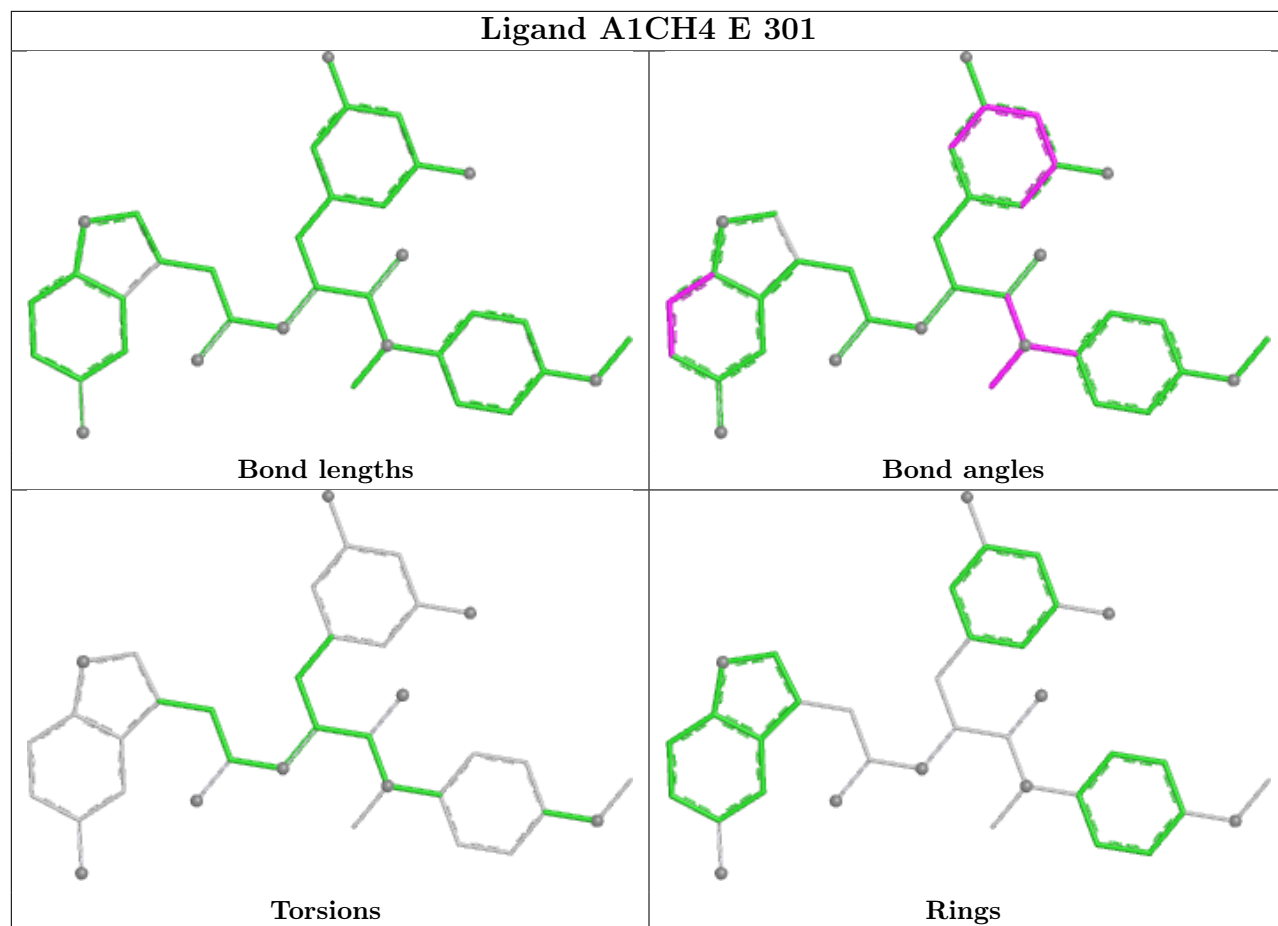
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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



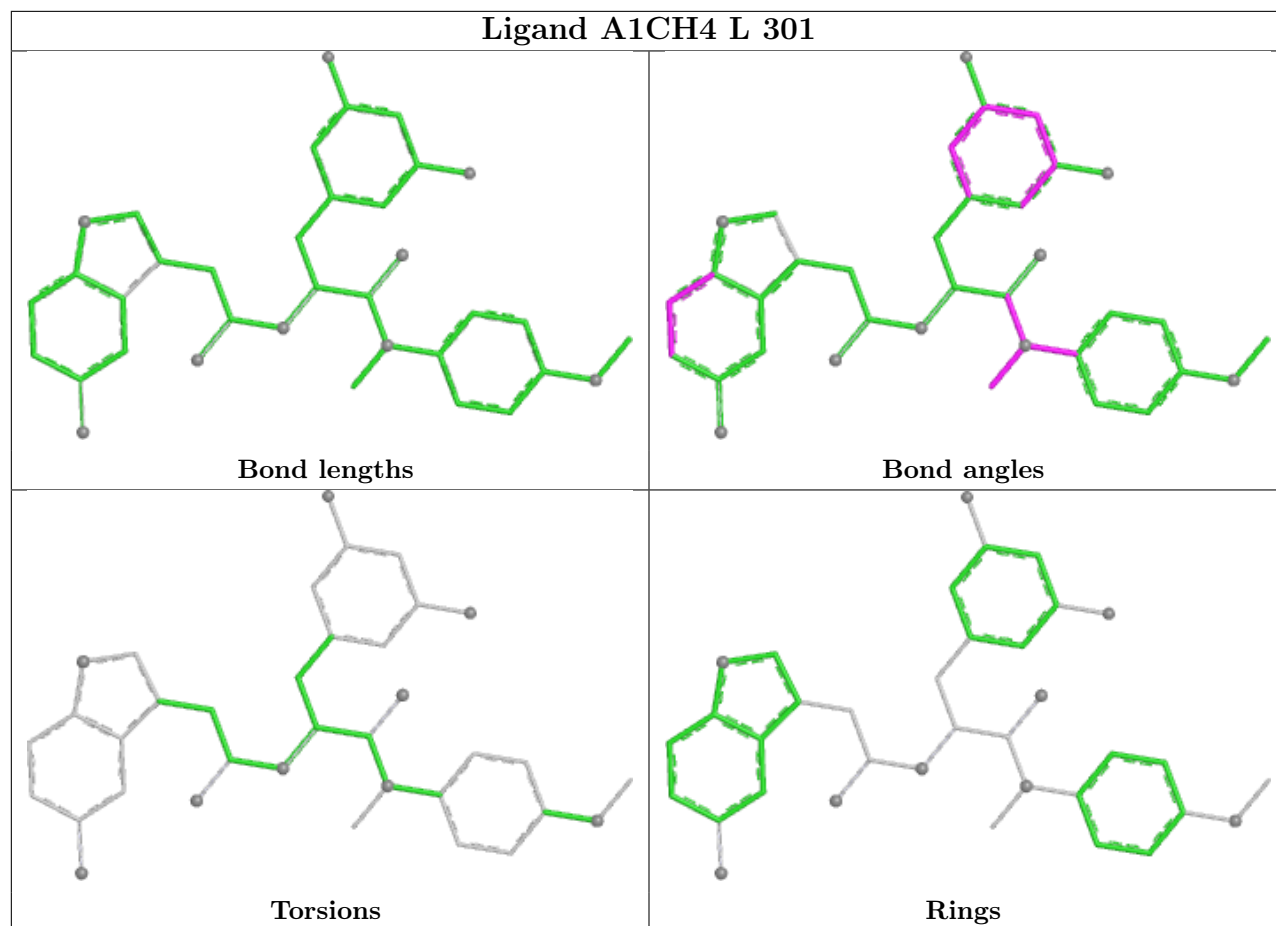
## Ligand A1CH4 C 301



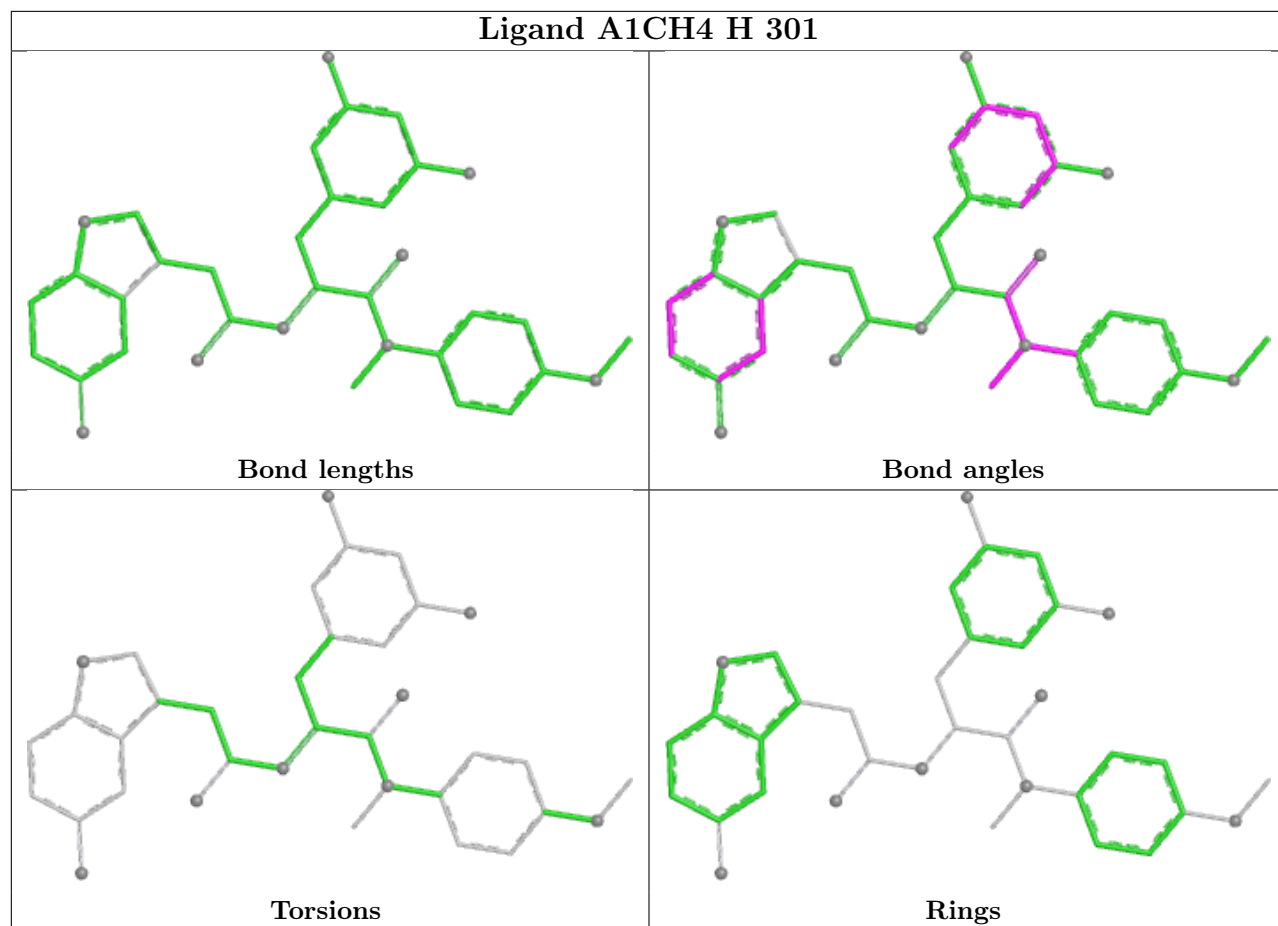
## Ligand A1CH4 E 301



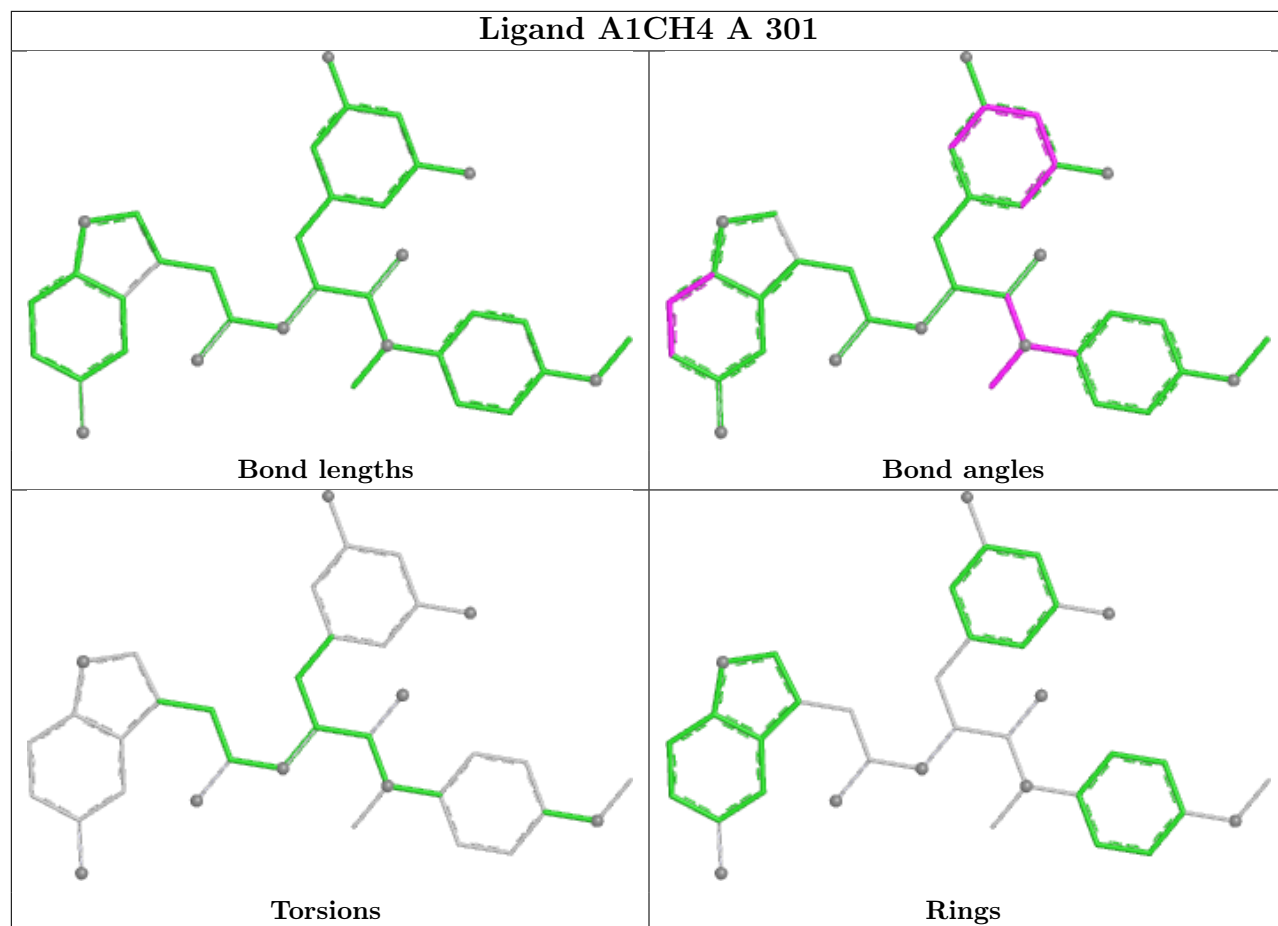
## Ligand A1CH4 L 301



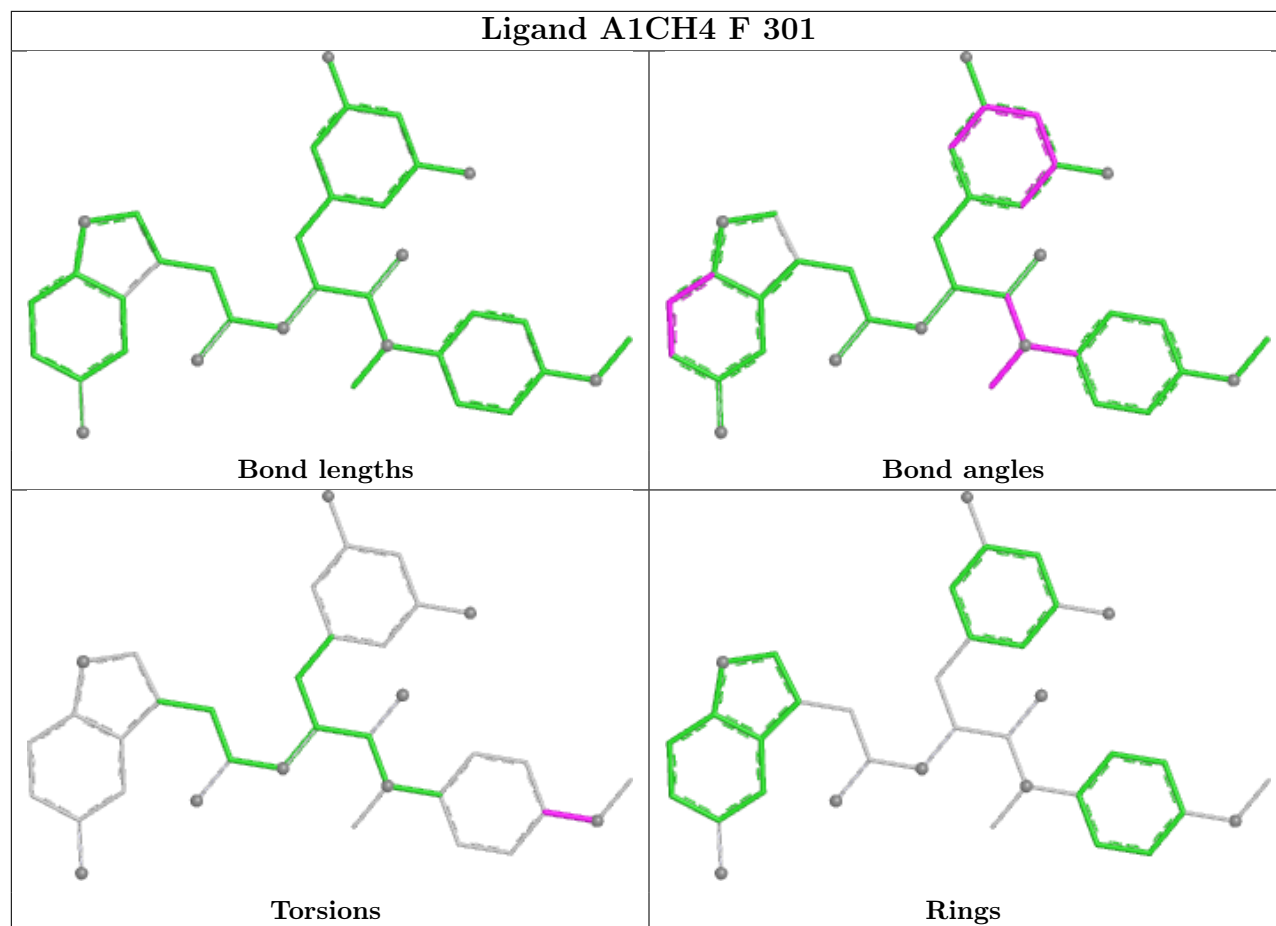
## Ligand A1CH4 H 301



## Ligand A1CH4 A 301

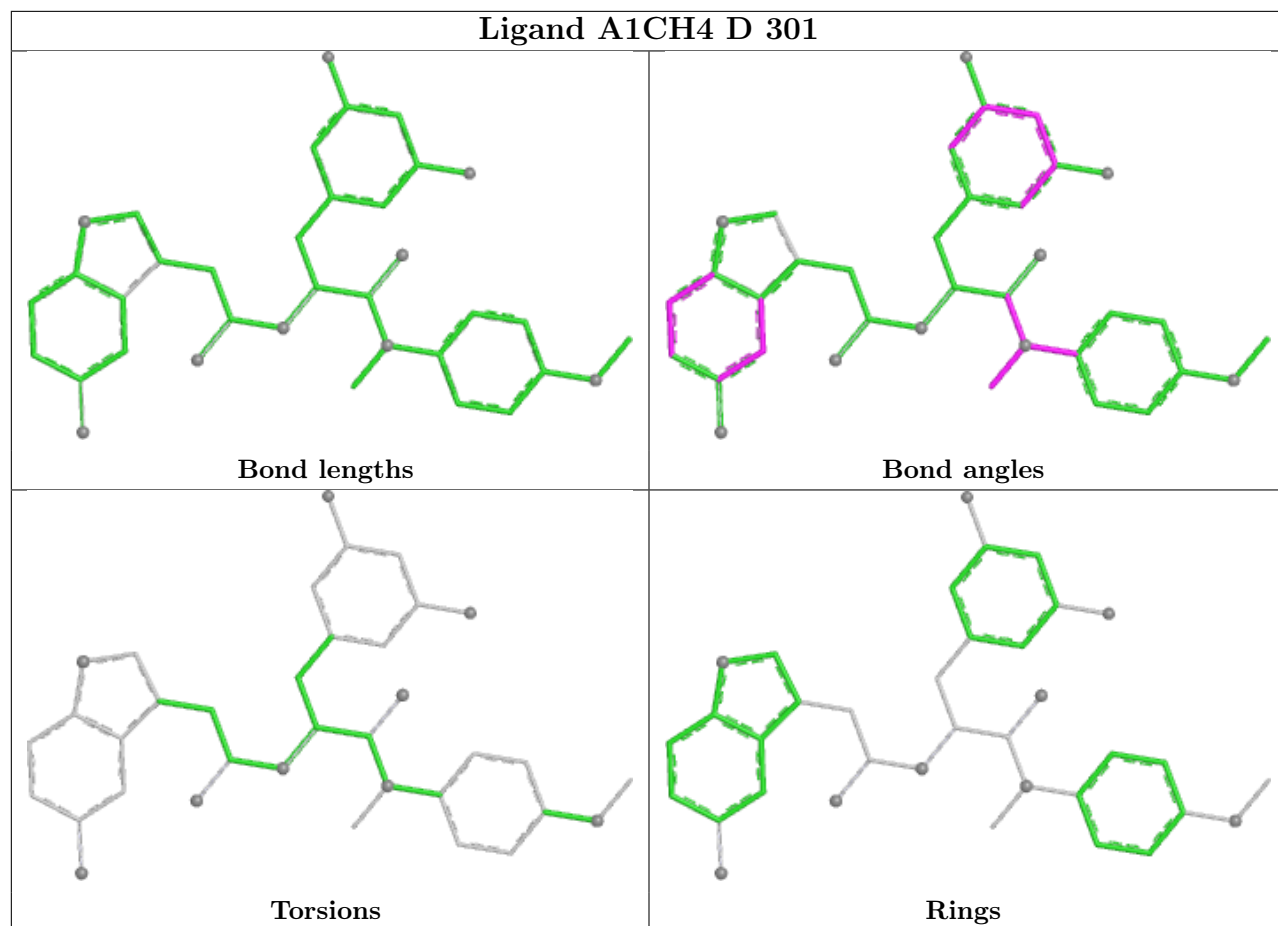


## Ligand A1CH4 F 301

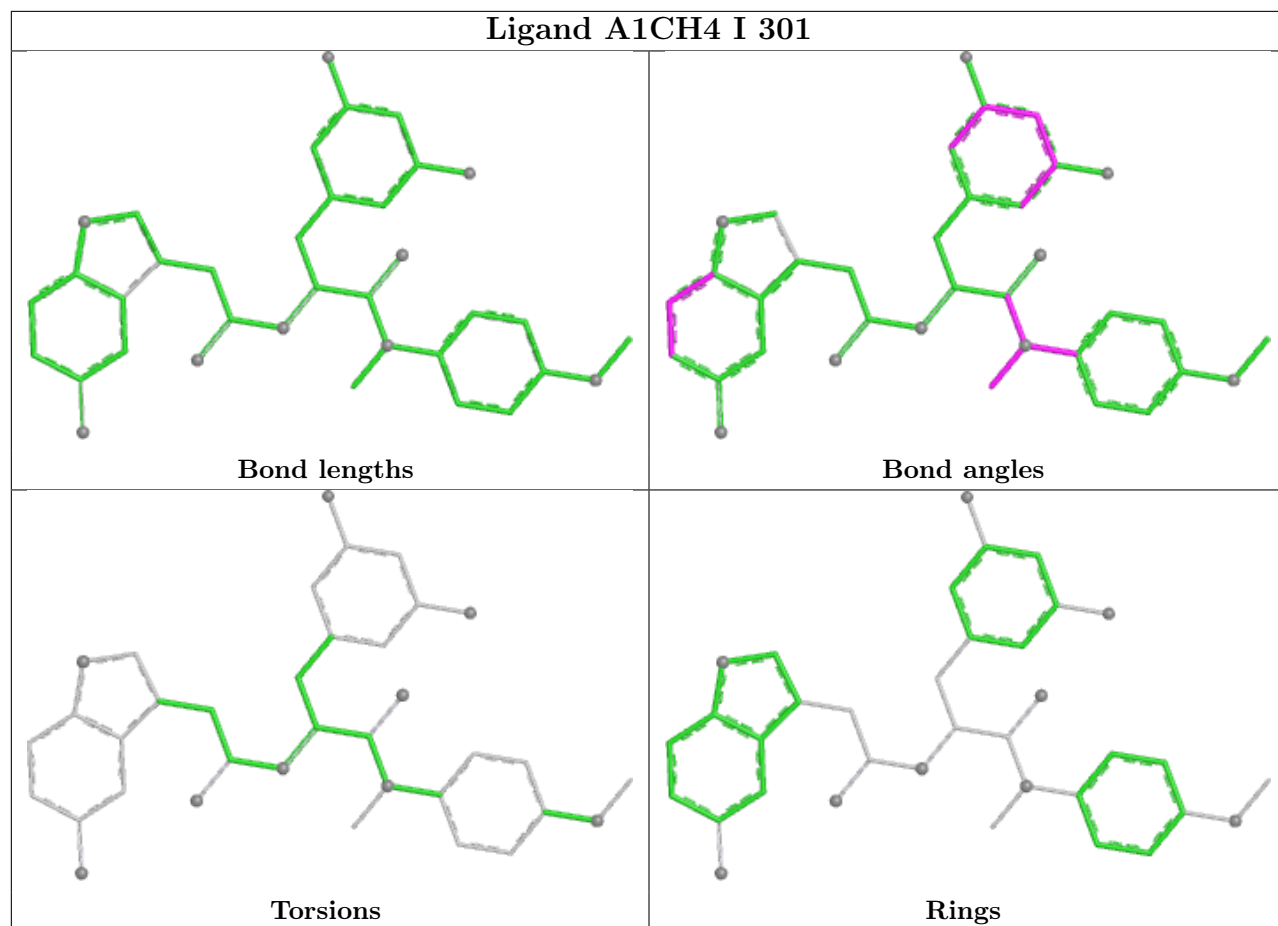




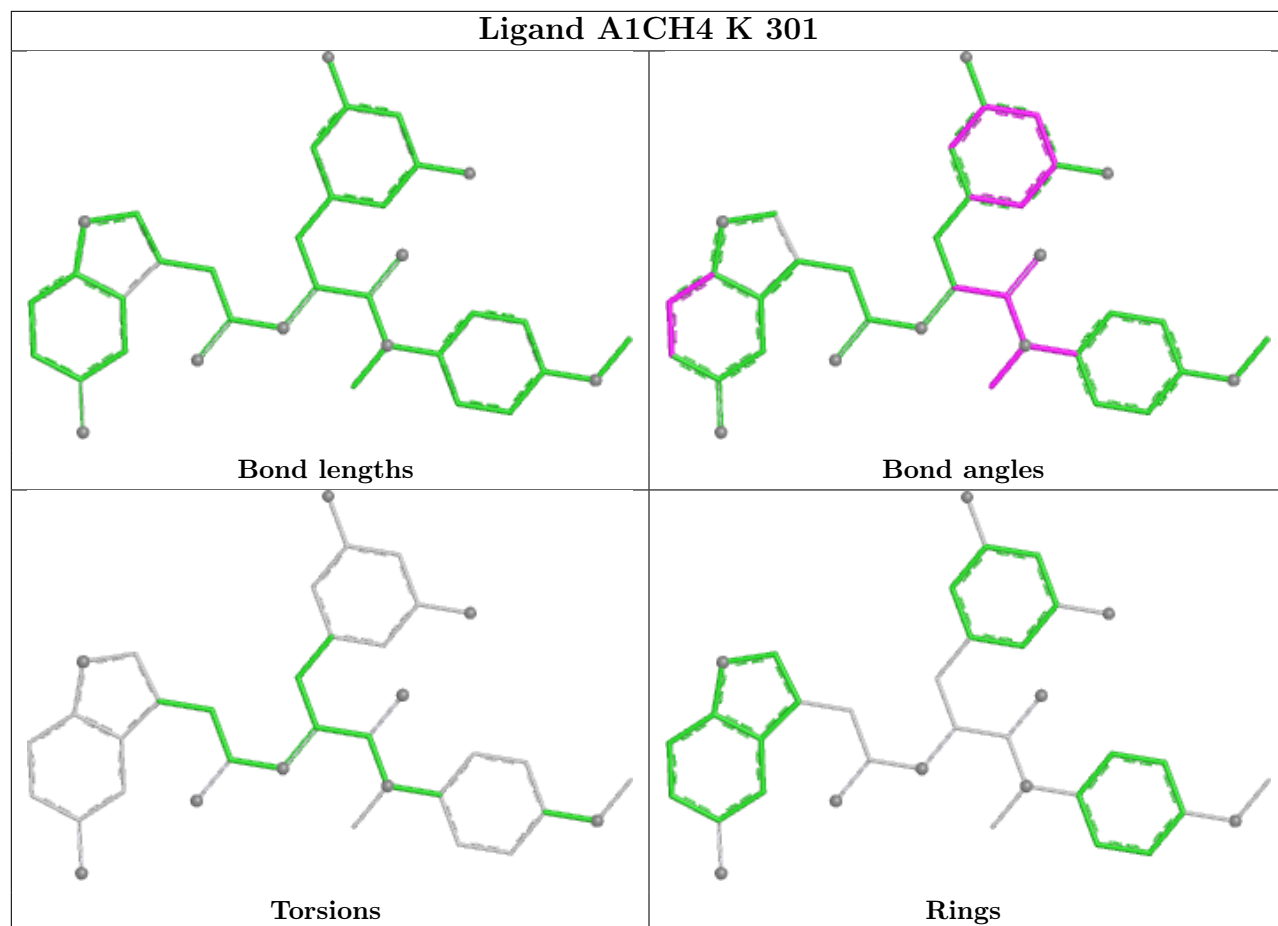
## Ligand A1CH4 D 301



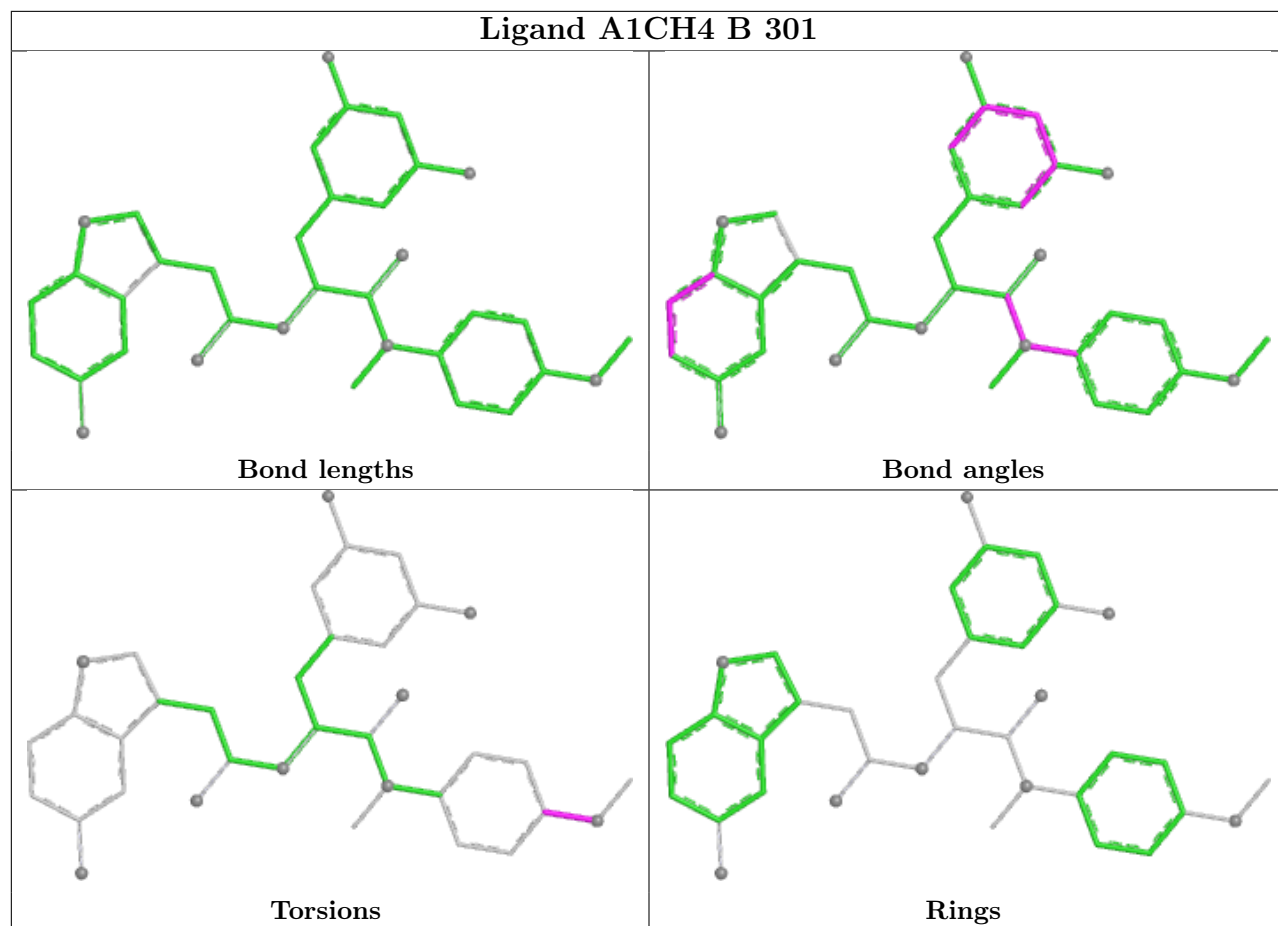
## Ligand A1CH4 I 301

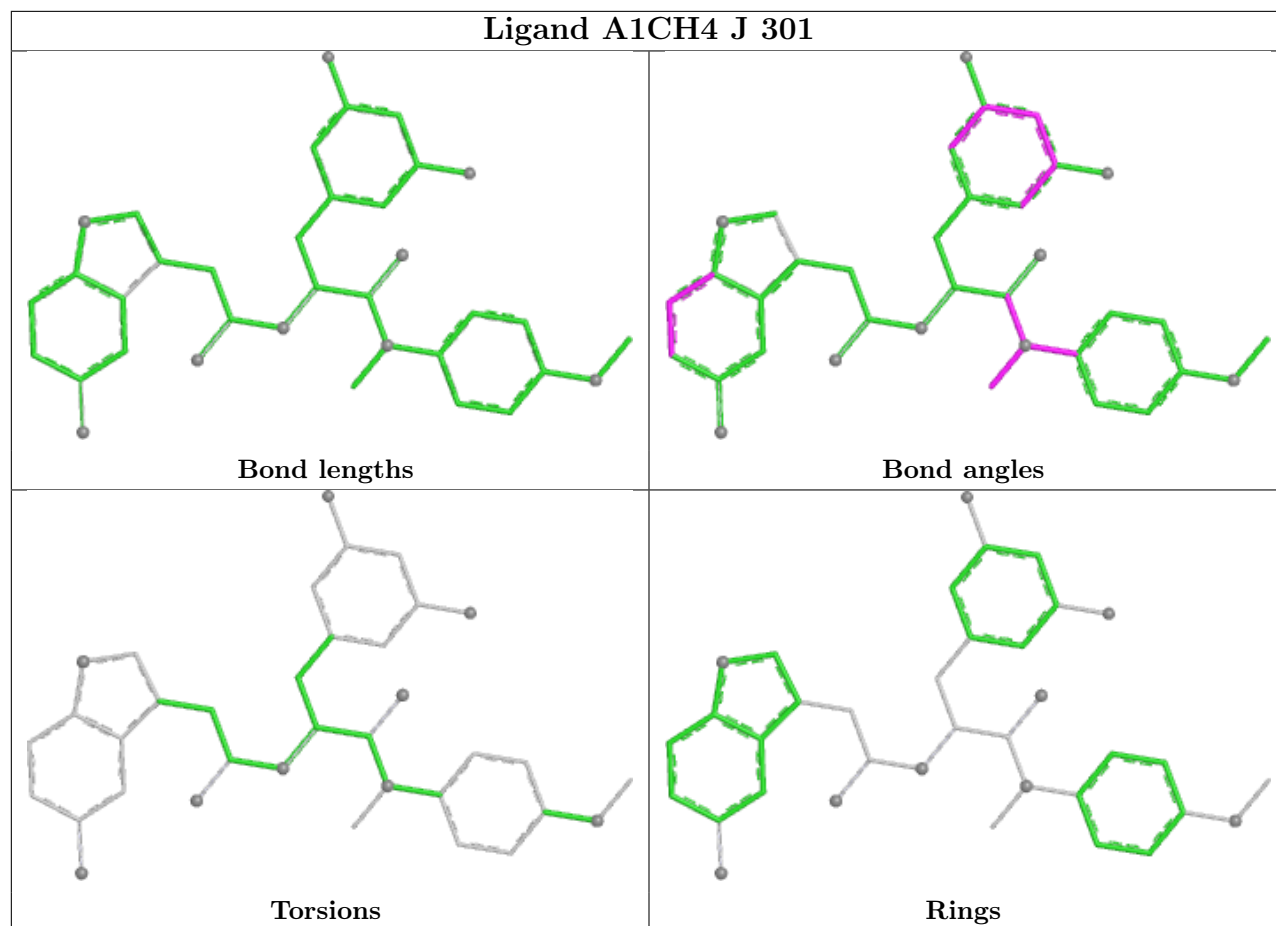


## Ligand A1CH4 K 301



## Ligand A1CH4 B 301





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	212/232 (91%)	0.71	29 (13%) 8 7	34, 66, 109, 123	0
1	B	212/232 (91%)	0.22	14 (6%) 26 23	36, 54, 88, 105	0
1	C	208/232 (89%)	0.06	8 (3%) 44 42	32, 51, 78, 113	0
1	D	209/232 (90%)	0.27	13 (6%) 28 25	32, 56, 89, 110	0
1	E	218/232 (93%)	0.32	9 (4%) 42 39	36, 56, 101, 115	0
1	F	220/232 (94%)	0.06	5 (2%) 61 58	33, 50, 81, 105	0
1	G	208/232 (89%)	0.18	12 (5%) 30 27	37, 55, 84, 100	0
1	H	217/232 (93%)	0.51	13 (5%) 29 26	41, 64, 96, 109	0
1	I	213/232 (91%)	0.33	13 (6%) 28 26	40, 59, 102, 125	0
1	J	218/232 (93%)	0.41	7 (3%) 50 47	48, 65, 91, 109	0
1	K	212/232 (91%)	0.46	17 (8%) 20 18	41, 59, 96, 113	0
1	L	216/232 (93%)	0.44	22 (10%) 13 12	37, 61, 103, 126	0
All	All	2563/2784 (92%)	0.33	162 (6%) 27 25	32, 58, 97, 126	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	198	CYS	5.4
1	G	198	CYS	4.8
1	I	177	ALA	4.8
1	G	91	ILE	4.6
1	L	185	ALA	4.5
1	C	198	CYS	4.5
1	A	92	ALA	4.3
1	F	6	LEU	4.3
1	L	178	SER	4.3
1	K	180	GLU	4.2
1	L	92	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	6	LEU	3.9
1	J	180	GLU	3.9
1	I	7	GLN	3.8
1	F	198	CYS	3.8
1	I	185	ALA	3.8
1	L	180	GLU	3.8
1	H	6	LEU	3.7
1	K	184	ALA	3.7
1	A	90	PRO	3.6
1	A	220	GLY	3.6
1	B	8	GLY	3.6
1	I	202	LEU	3.5
1	E	180	GLU	3.5
1	B	185	ALA	3.5
1	A	6	LEU	3.5
1	A	91	ILE	3.5
1	I	6	LEU	3.3
1	B	198	CYS	3.3
1	B	92	ALA	3.3
1	D	96	MET	3.3
1	C	8	GLY	3.3
1	B	184	ALA	3.3
1	E	178	SER	3.2
1	I	198	CYS	3.2
1	B	220	GLY	3.2
1	D	86	VAL	3.2
1	A	97	ARG	3.2
1	J	198	CYS	3.2
1	L	220	GLY	3.2
1	D	184	ALA	3.2
1	A	121	ASN	3.2
1	K	177	ALA	3.2
1	I	176	GLN	3.2
1	K	5	ASN	3.1
1	D	198	CYS	3.1
1	D	6	LEU	3.1
1	E	161	PHE	3.1
1	E	198	CYS	3.1
1	K	95	GLN	3.1
1	L	88	ALA	3.0
1	K	9	GLN	3.0
1	K	179	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	88	ALA	3.0
1	L	91	ILE	3.0
1	H	90	PRO	3.0
1	K	6	LEU	3.0
1	B	6	LEU	2.9
1	H	198	CYS	2.9
1	A	89	GLY	2.9
1	D	183	ASN	2.9
1	K	178	SER	2.9
1	L	8	GLY	2.9
1	L	207	PRO	2.9
1	A	7	GLN	2.9
1	E	6	LEU	2.8
1	G	6	LEU	2.8
1	A	85	PRO	2.8
1	A	196	PRO	2.8
1	L	218	CYS	2.8
1	A	93	PRO	2.8
1	G	92	ALA	2.8
1	C	184	ALA	2.8
1	L	179	GLN	2.8
1	H	177	ALA	2.8
1	K	88	ALA	2.8
1	B	183	ASN	2.7
1	D	182	LYS	2.7
1	K	7	GLN	2.7
1	A	122	PRO	2.7
1	G	176	GLN	2.7
1	A	114	GLN	2.6
1	J	6	LEU	2.6
1	D	177	ALA	2.6
1	I	186	THR	2.6
1	A	183	ASN	2.6
1	H	179	GLN	2.6
1	J	220	GLY	2.6
1	K	85	PRO	2.6
1	A	124	ILE	2.6
1	A	186	THR	2.5
1	B	186	THR	2.5
1	D	179	GLN	2.5
1	L	93	PRO	2.5
1	I	203	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	92	ALA	2.5
1	A	9	GLN	2.5
1	A	216	THR	2.5
1	I	201	ILE	2.5
1	C	176	GLN	2.5
1	A	8	GLY	2.5
1	E	220	GLY	2.5
1	L	5	ASN	2.5
1	B	7	GLN	2.4
1	L	90	PRO	2.4
1	J	7	GLN	2.4
1	K	112	GLN	2.4
1	A	207	PRO	2.4
1	D	178	SER	2.4
1	F	5	ASN	2.4
1	A	14	CYS	2.4
1	L	196	PRO	2.4
1	E	177	ALA	2.4
1	L	177	ALA	2.4
1	H	152	ASP	2.3
1	G	5	ASN	2.3
1	G	187	GLU	2.3
1	C	94	GLY	2.3
1	D	185	ALA	2.3
1	E	202	LEU	2.3
1	L	186	THR	2.3
1	J	183	ASN	2.3
1	B	187	GLU	2.3
1	H	220	GLY	2.3
1	A	5	ASN	2.3
1	K	96	MET	2.3
1	E	207	PRO	2.3
1	H	49	PRO	2.3
1	I	207	PRO	2.3
1	A	4	GLN	2.3
1	K	220	GLY	2.2
1	B	101	GLY	2.2
1	F	208	GLY	2.2
1	H	94	GLY	2.2
1	H	176	GLN	2.2
1	L	190	LEU	2.2
1	A	96	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	198	CYS	2.2
1	I	144	MET	2.2
1	H	86	VAL	2.2
1	G	184	ALA	2.2
1	A	218	CYS	2.2
1	D	196	PRO	2.2
1	D	220	GLY	2.1
1	G	188	THR	2.1
1	K	115	ILE	2.1
1	L	201	ILE	2.1
1	B	85	PRO	2.1
1	C	87	HIS	2.1
1	L	202	LEU	2.1
1	B	145	TYR	2.1
1	G	85	PRO	2.1
1	A	202	LEU	2.0
1	C	86	VAL	2.0
1	A	116	GLY	2.0
1	G	220	GLY	2.0
1	H	186	THR	2.0
1	I	187	GLU	2.0
1	L	198	CYS	2.0
1	G	185	ALA	2.0
1	L	204	ALA	2.0
1	H	207	PRO	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

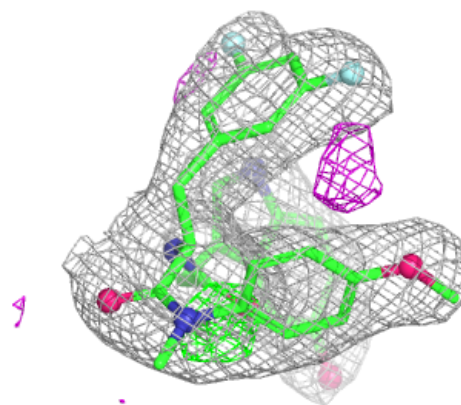
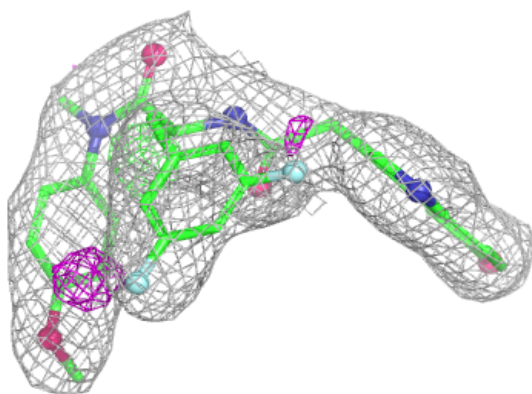
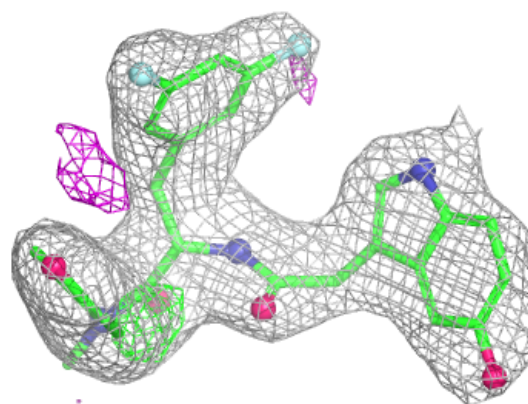
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1CH4	H	301	36/36	0.91	0.12	40,51,59,67	0
2	A1CH4	G	301	36/36	0.92	0.10	31,44,60,76	0
2	A1CH4	A	301	36/36	0.92	0.10	28,42,52,56	0
2	A1CH4	F	301	36/36	0.93	0.11	38,48,59,63	0
2	A1CH4	J	301	36/36	0.93	0.10	46,57,65,65	0
2	A1CH4	K	301	36/36	0.93	0.09	34,48,58,61	0
2	A1CH4	C	301	36/36	0.94	0.09	29,41,47,48	0
2	A1CH4	L	301	36/36	0.94	0.09	28,45,64,74	0
2	A1CH4	B	301	36/36	0.95	0.09	30,44,54,56	0
2	A1CH4	D	301	36/36	0.95	0.08	26,39,51,59	0
2	A1CH4	E	301	36/36	0.95	0.09	27,42,50,56	0
2	A1CH4	I	301	36/36	0.96	0.07	32,46,58,61	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.

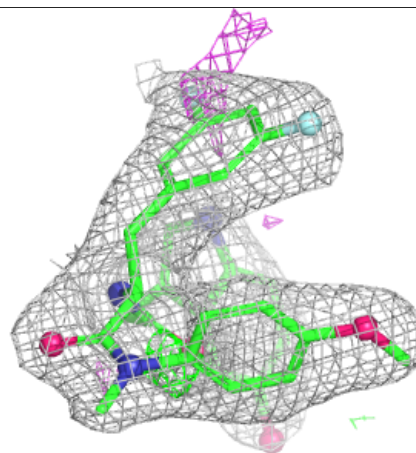
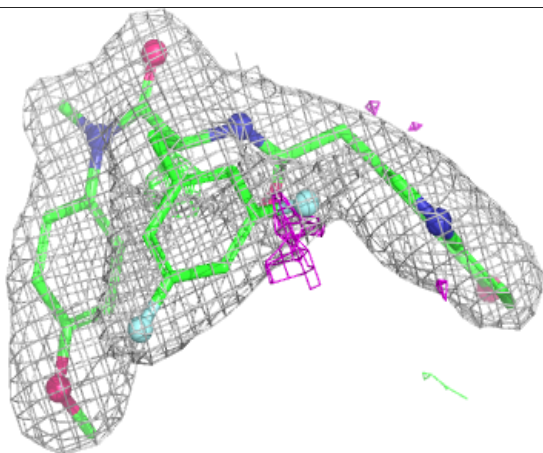
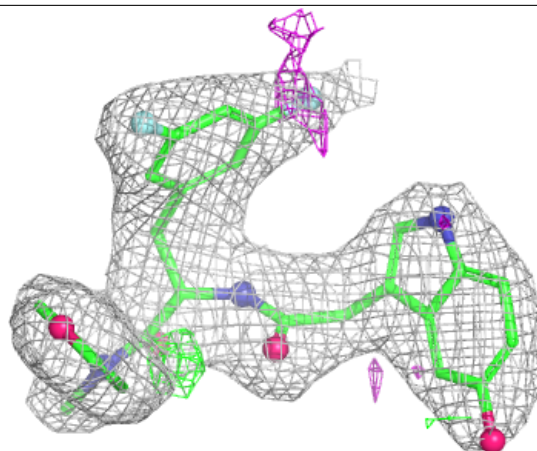
**Electron density around A1CH4 H 301:**

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)



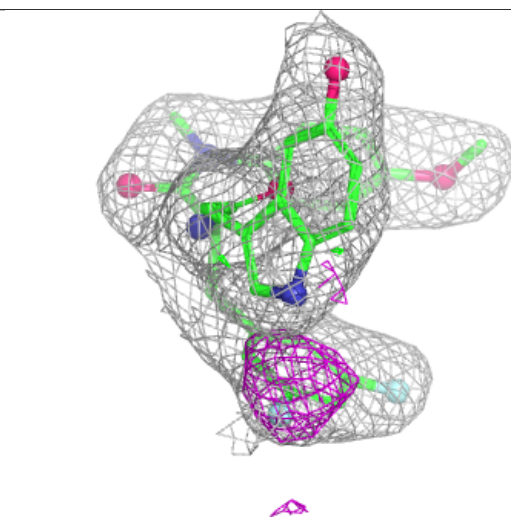
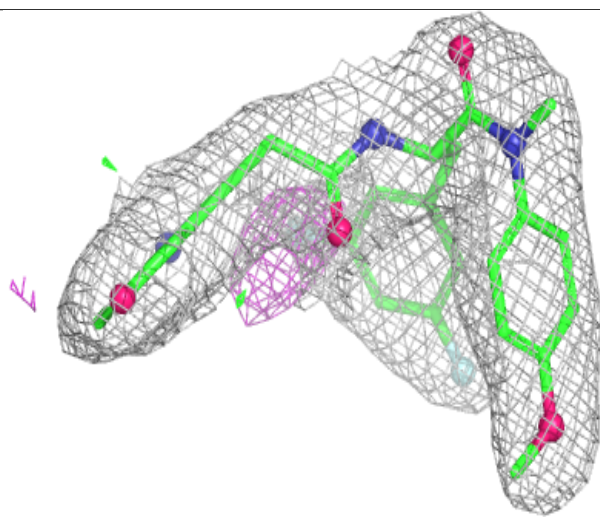
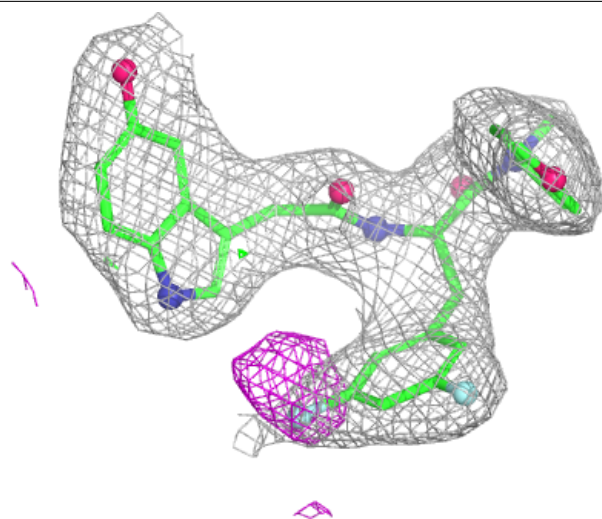
**Electron density around A1CH4 G 301:**

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



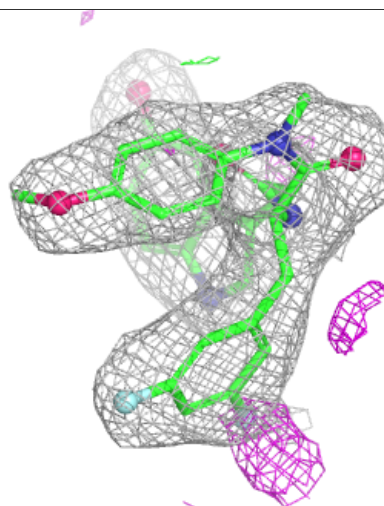
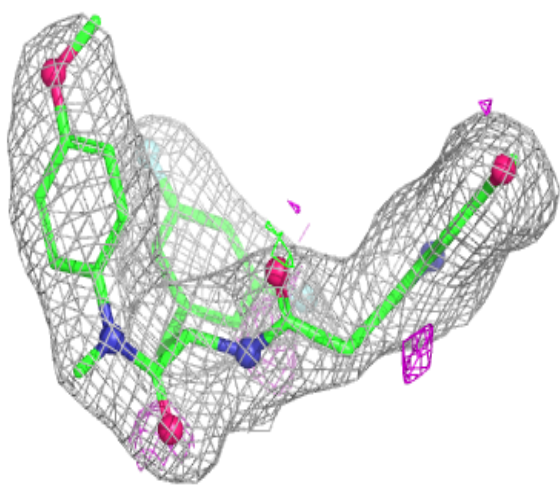
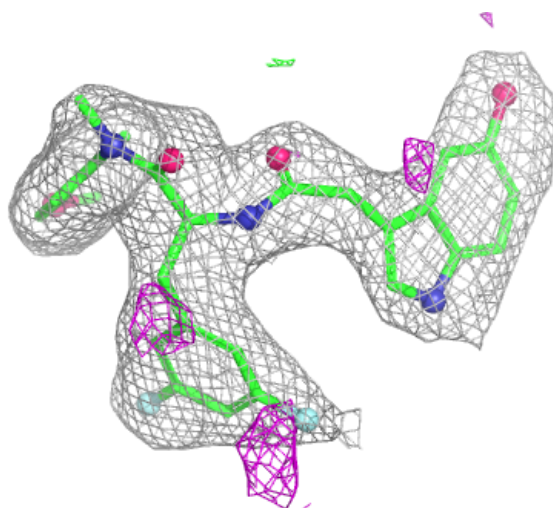
**Electron density around A1CH4 A 301:**

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



**Electron density around A1CH4 F 301:**

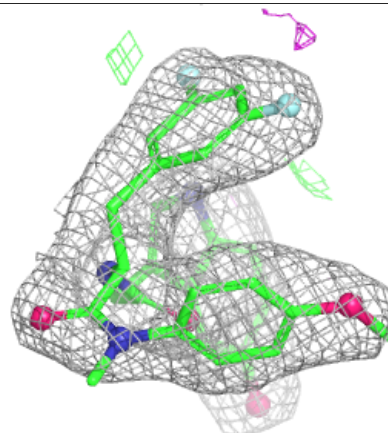
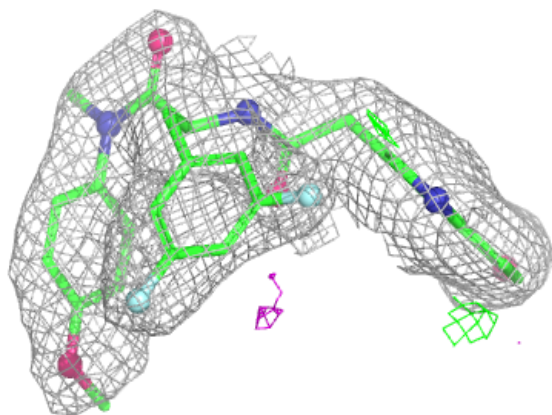
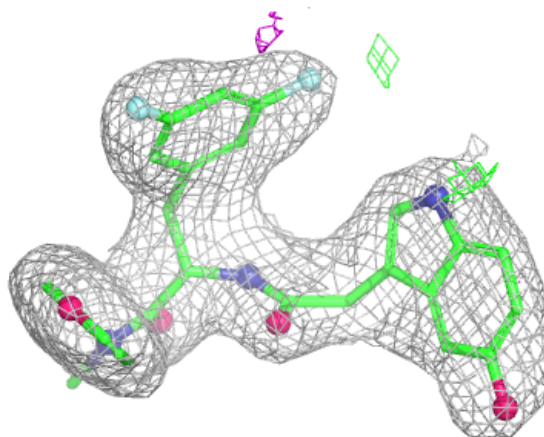
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





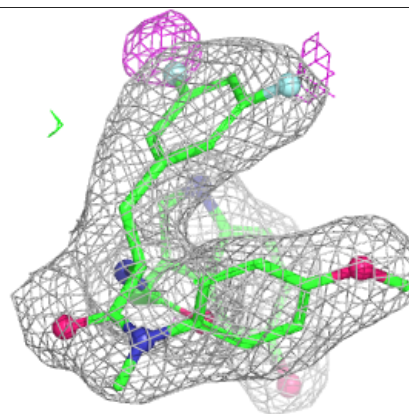
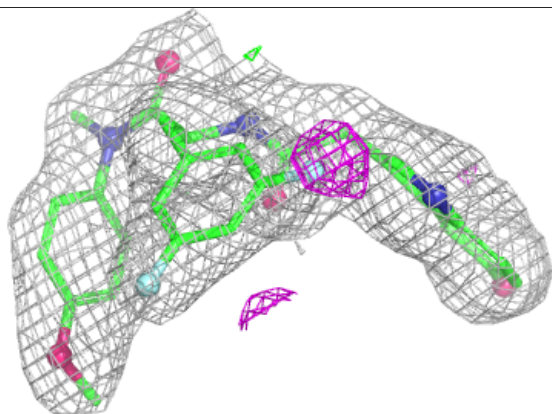
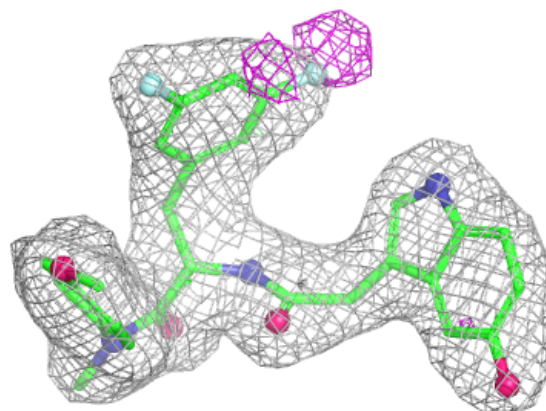
**Electron density around A1CH4 J 301:**

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



**Electron density around A1CH4 K 301:**

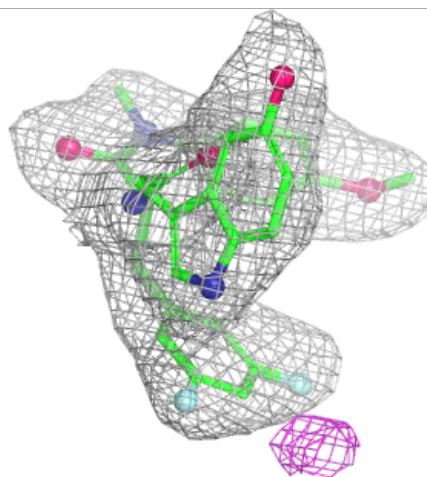
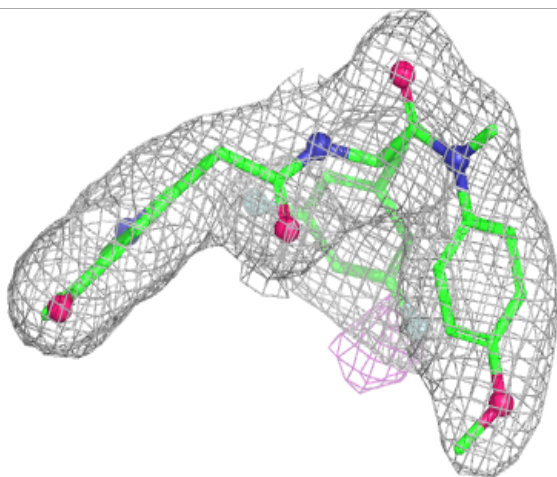
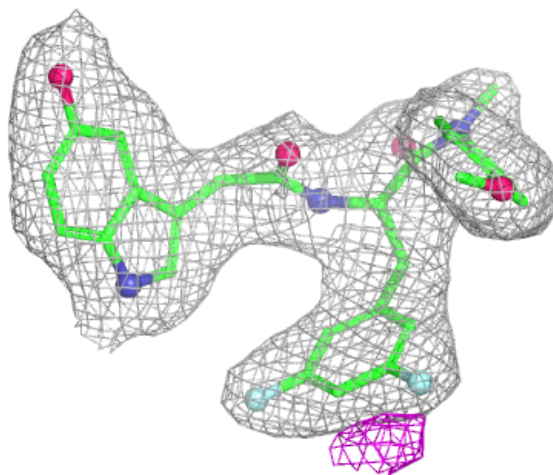
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





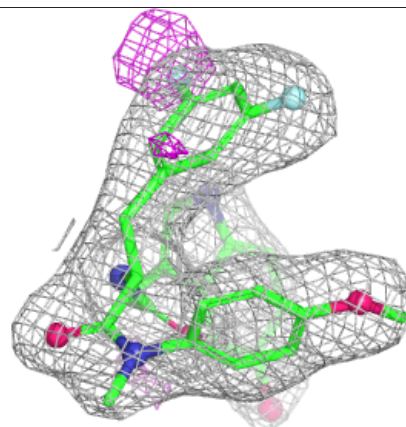
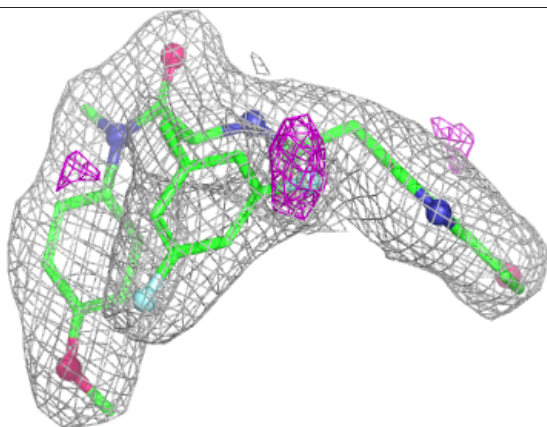
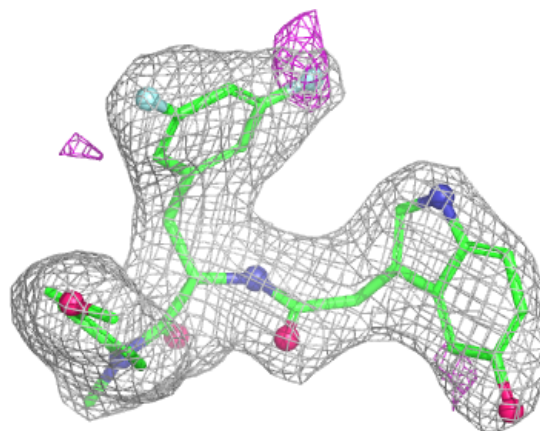
**Electron density around A1CH4 C 301:**

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



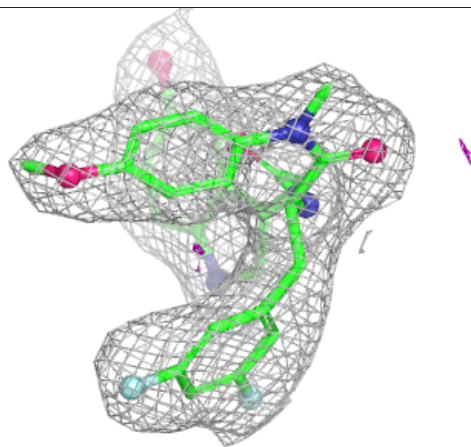
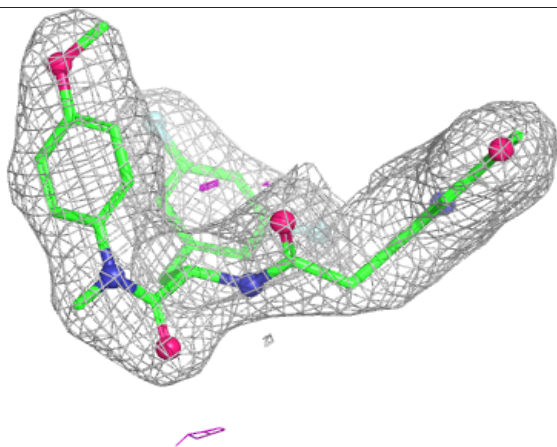
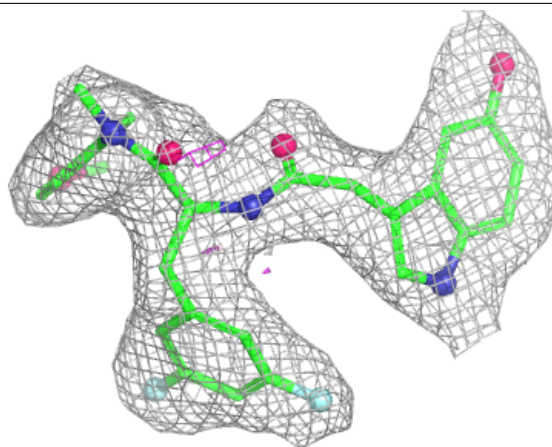
**Electron density around A1CH4 L 301:**

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



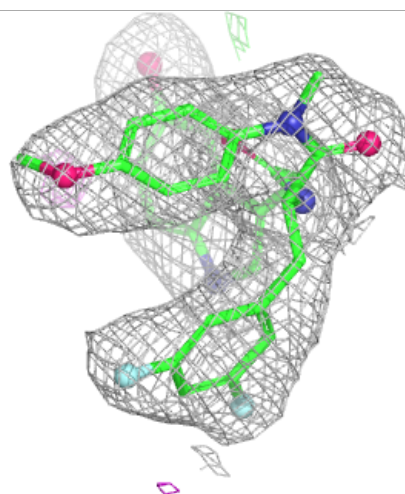
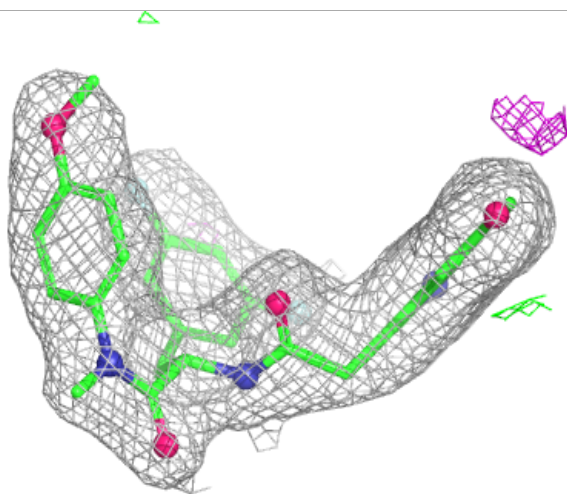
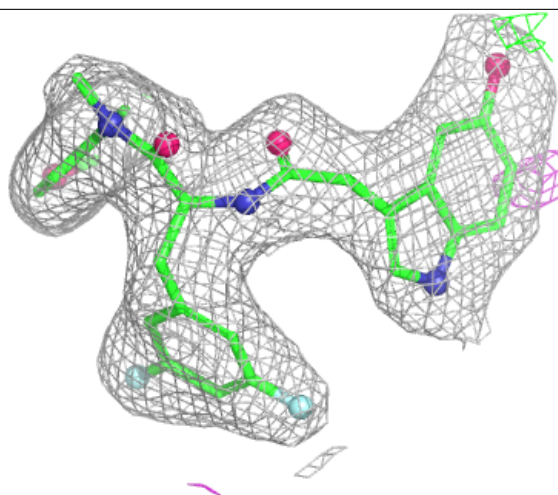
**Electron density around A1CH4 B 301:**

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



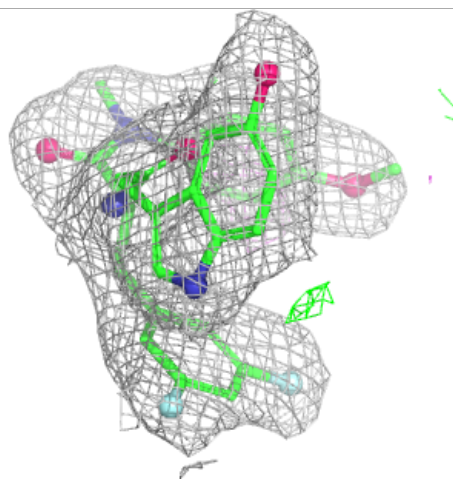
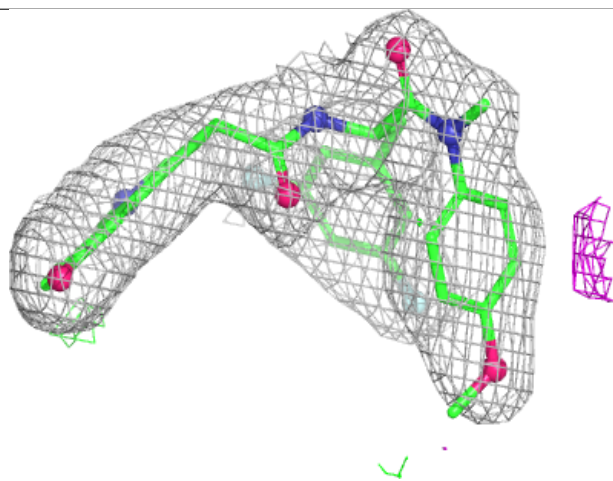
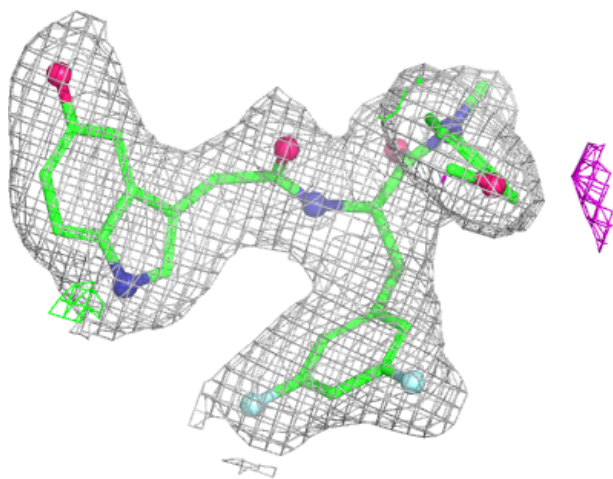
**Electron density around A1CH4 D 301:**

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



**Electron density around A1CH4 E 301:**

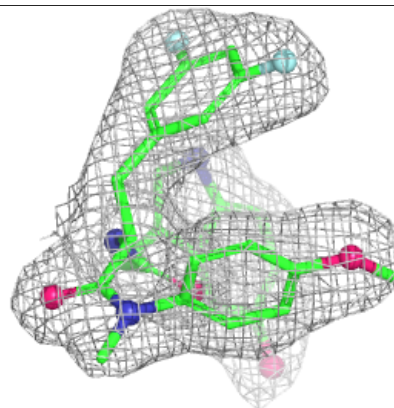
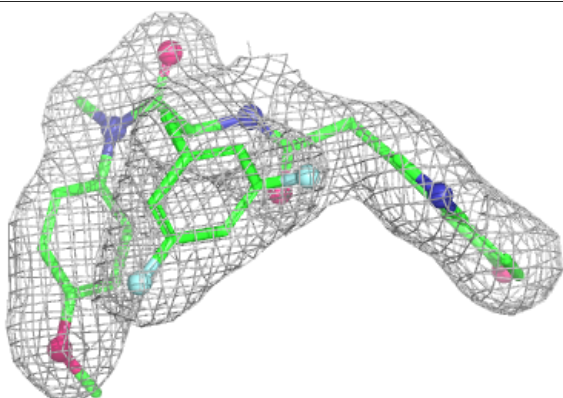
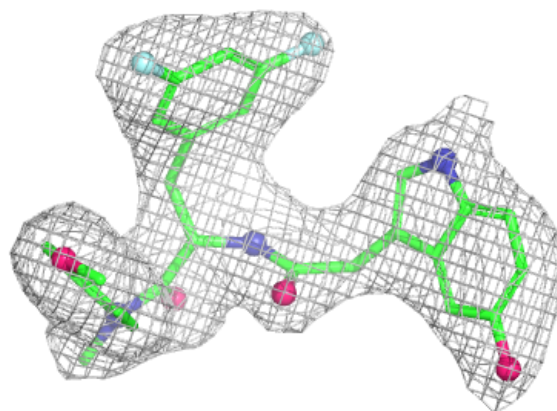
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around A1CH4 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.