



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 3, 2025 – 04:10 PM EDT

PDB ID : 9OIO / pdb\_00009oio  
Title : The von Hippel Lindau-ElonginB-ElonginC (VCB) complex with fragments 9 and 14  
Authors : Amporndanai, K.; Katinas, J.M.; Chopra, A.; Fesik, S.W.  
Deposited on : 2025-05-06  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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>.

---

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

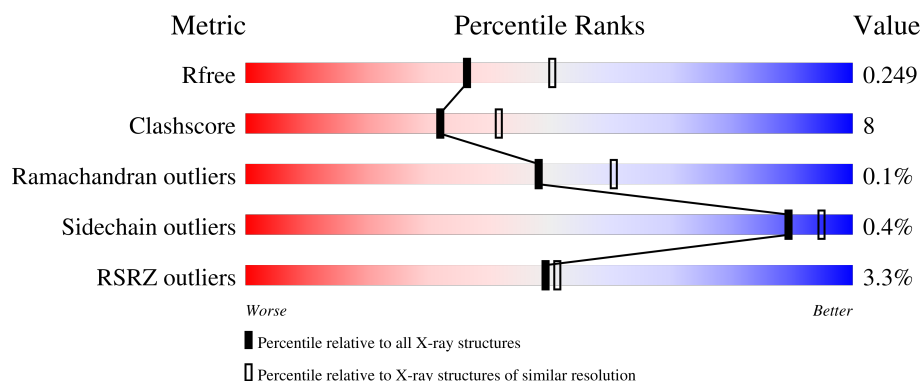
# 1 Overall quality at a glance

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))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (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	104	<div> <div>2%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	D	104	<div> <div>4%</div> <div>78%</div> <div>16%</div> <div>6%</div> <div>.</div> </div>
1	G	104	<div> <div>2%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
1	J	104	<div> <div>88%</div> <div>12%</div> <div>.</div> </div>
2	B	98	<div> <div>2%</div> <div>73%</div> <div>14%</div> <div>12%</div> <div>.</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	E	98	
2	H	98	
2	K	98	
3	C	180	
3	F	180	
3	L	180	
4	I	180	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DMS	H	202	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10766 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 Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			794	506	133	150	5			
1	D	98	Total	C	N	O	S	0	0	0
			751	482	121	143	5			
1	G	103	Total	C	N	O	S	0	0	0
			803	508	135	156	4			
1	J	103	Total	C	N	O	S	0	0	0
			807	512	136	154	5			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			682	440	109	127	6			
2	E	88	Total	C	N	O	S	0	0	0
			687	444	109	128	6			
2	H	88	Total	C	N	O	S	0	0	0
			686	444	111	125	6			
2	K	82	Total	C	N	O	S	0	1	0
			654	427	105	116	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	MET	-	initiating methionine	UNP Q15369
B	16	GLY	-	expression tag	UNP Q15369
E	15	MET	-	initiating methionine	UNP Q15369
E	16	GLY	-	expression tag	UNP Q15369
H	15	MET	-	initiating methionine	UNP Q15369
H	16	GLY	-	expression tag	UNP Q15369
K	15	MET	-	initiating methionine	UNP Q15369
K	16	GLY	-	expression tag	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	141	Total	As	C	N	O	S	0	1	0
			1125	1	717	200	205	2			
3	F	144	Total	As	C	N	O	S	0	0	0
			1122	1	718	198	203	2			
3	L	143	Total	As	C	N	O	S	0	0	0
			1147	1	732	206	206	2			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	34	MET	-	initiating methionine	UNP P40337
C	35	GLY	-	expression tag	UNP P40337
C	36	SER	-	expression tag	UNP P40337
C	37	SER	-	expression tag	UNP P40337
C	38	HIS	-	expression tag	UNP P40337
C	39	HIS	-	expression tag	UNP P40337
C	40	HIS	-	expression tag	UNP P40337
C	41	HIS	-	expression tag	UNP P40337
C	42	HIS	-	expression tag	UNP P40337
C	43	HIS	-	expression tag	UNP P40337
C	44	SER	-	expression tag	UNP P40337
C	45	SER	-	expression tag	UNP P40337
C	46	GLY	-	expression tag	UNP P40337
C	47	LEU	-	expression tag	UNP P40337
C	48	VAL	-	expression tag	UNP P40337
C	49	PRO	-	expression tag	UNP P40337
C	50	ARG	-	expression tag	UNP P40337
C	51	GLY	-	expression tag	UNP P40337
C	52	SER	-	expression tag	UNP P40337
C	53	HIS	-	expression tag	UNP P40337
F	34	MET	-	initiating methionine	UNP P40337
F	35	GLY	-	expression tag	UNP P40337
F	36	SER	-	expression tag	UNP P40337
F	37	SER	-	expression tag	UNP P40337
F	38	HIS	-	expression tag	UNP P40337
F	39	HIS	-	expression tag	UNP P40337
F	40	HIS	-	expression tag	UNP P40337
F	41	HIS	-	expression tag	UNP P40337
F	42	HIS	-	expression tag	UNP P40337
F	43	HIS	-	expression tag	UNP P40337
F	44	SER	-	expression tag	UNP P40337
F	45	SER	-	expression tag	UNP P40337

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	GLY	-	expression tag	UNP P40337
F	47	LEU	-	expression tag	UNP P40337
F	48	VAL	-	expression tag	UNP P40337
F	49	PRO	-	expression tag	UNP P40337
F	50	ARG	-	expression tag	UNP P40337
F	51	GLY	-	expression tag	UNP P40337
F	52	SER	-	expression tag	UNP P40337
F	53	HIS	-	expression tag	UNP P40337
L	34	MET	-	initiating methionine	UNP P40337
L	35	GLY	-	expression tag	UNP P40337
L	36	SER	-	expression tag	UNP P40337
L	37	SER	-	expression tag	UNP P40337
L	38	HIS	-	expression tag	UNP P40337
L	39	HIS	-	expression tag	UNP P40337
L	40	HIS	-	expression tag	UNP P40337
L	41	HIS	-	expression tag	UNP P40337
L	42	HIS	-	expression tag	UNP P40337
L	43	HIS	-	expression tag	UNP P40337
L	44	SER	-	expression tag	UNP P40337
L	45	SER	-	expression tag	UNP P40337
L	46	GLY	-	expression tag	UNP P40337
L	47	LEU	-	expression tag	UNP P40337
L	48	VAL	-	expression tag	UNP P40337
L	49	PRO	-	expression tag	UNP P40337
L	50	ARG	-	expression tag	UNP P40337
L	51	GLY	-	expression tag	UNP P40337
L	52	SER	-	expression tag	UNP P40337
L	53	HIS	-	expression tag	UNP P40337

- Molecule 4 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	143	Total	C	N	O	S	0	0	0
			1138	727	206	203	2			

There are 20 discrepancies between the modelled and reference sequences:

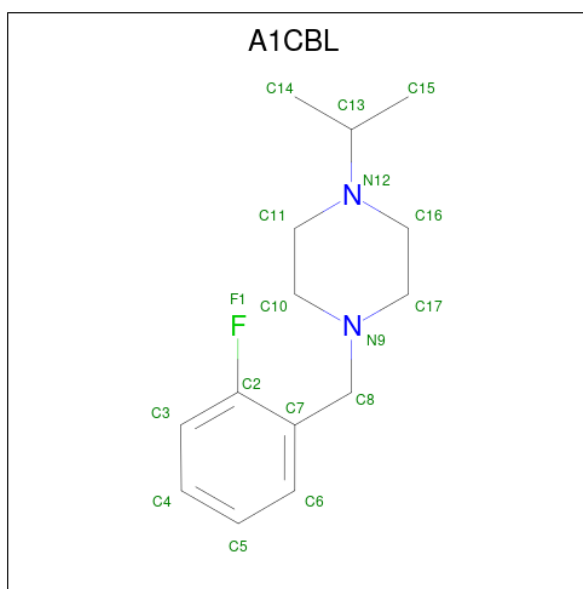
Chain	Residue	Modelled	Actual	Comment	Reference
I	34	MET	-	expression tag	UNP P40337
I	35	GLY	-	expression tag	UNP P40337
I	36	SER	-	expression tag	UNP P40337
I	37	SER	-	expression tag	UNP P40337

*Continued on next page...*

Continued from previous page...

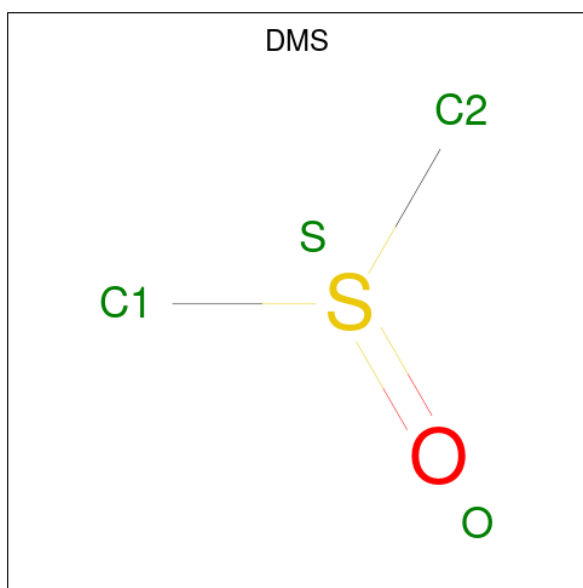
Chain	Residue	Modelled	Actual	Comment	Reference
I	38	HIS	-	expression tag	UNP P40337
I	39	HIS	-	expression tag	UNP P40337
I	40	HIS	-	expression tag	UNP P40337
I	41	HIS	-	expression tag	UNP P40337
I	42	HIS	-	expression tag	UNP P40337
I	43	HIS	-	expression tag	UNP P40337
I	44	SER	-	expression tag	UNP P40337
I	45	SER	-	expression tag	UNP P40337
I	46	GLY	-	expression tag	UNP P40337
I	47	LEU	-	expression tag	UNP P40337
I	48	VAL	-	expression tag	UNP P40337
I	49	PRO	-	expression tag	UNP P40337
I	50	ARG	-	expression tag	UNP P40337
I	51	GLY	-	expression tag	UNP P40337
I	52	SER	-	expression tag	UNP P40337
I	53	HIS	-	expression tag	UNP P40337

- Molecule 5 is 1-[(2-fluorophenyl)methyl]-4-(propan-2-yl)piperazine (CCD ID: A1CBL) (formula: C<sub>14</sub>H<sub>21</sub>FN<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	F	N	0	0
			17	14	1	2		
5	F	1	Total	C	F	N	0	0
			17	14	1	2		
5	L	1	Total	C	F	N	0	0
			17	14	1	2		

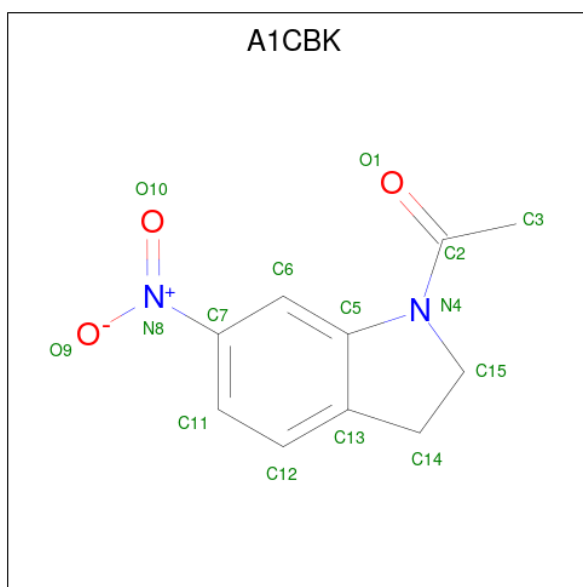
- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	O	S	0	0
			4	2	1	1		
6	F	1	Total	C	O	S	0	0
			4	2	1	1		
6	F	1	Total	C	O	S	0	0
			4	2	1	1		
6	H	1	Total	C	O	S	0	0
			4	2	1	1		
6	I	1	Total	C	O	S	0	0
			4	2	1	1		
6	L	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is 1-[6-[oxidanyl(oxidanylidene)- $l^{\{4\}}$ -azanyl]-2,3-dihydroindol-1-yl]ethanone (CCD ID: A1CBK) (formula:  $C_{10}H_{10}N_2O_3$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			15	10	2	3		
7	H	1	Total	C	N	O	0	0
			15	10	2	3		
7	K	1	Total	C	N	O	0	0
			15	10	2	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	34	Total	O	0	0
			34	34		
8	B	14	Total	O	0	0
			14	14		
8	C	18	Total	O	0	0
			18	18		
8	D	10	Total	O	0	0
			10	10		
8	E	10	Total	O	0	0
			10	10		
8	F	29	Total	O	0	0
			29	29		
8	G	12	Total	O	0	0
			12	12		
8	H	13	Total	O	0	0
			13	13		
8	I	29	Total	O	0	0
			29	29		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	29	Total	O	0	0
			29	29		
8	K	21	Total	O	0	0
			21	21		
8	L	31	Total	O	0	0
			31	31		

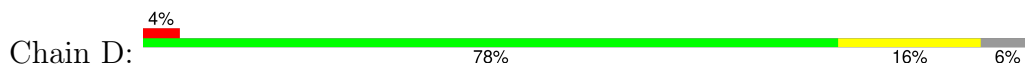
### 3 Residue-property plots [i](#)

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: Elongin-B



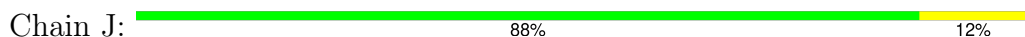
- Molecule 1: Elongin-B



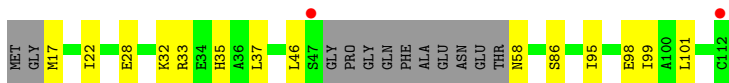
- Molecule 1: Elongin-B



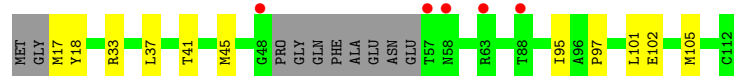
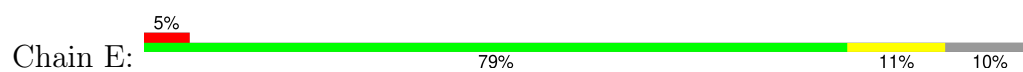
- Molecule 1: Elongin-B



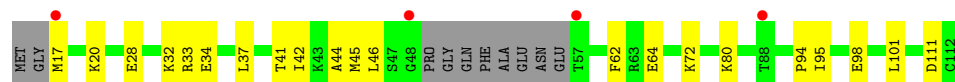
- Molecule 2: Elongin-C



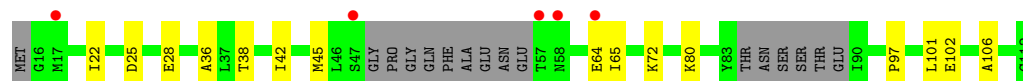
- Molecule 2: Elongin-C



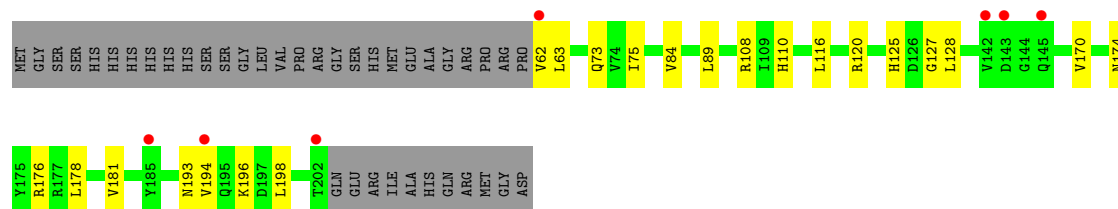
• Molecule 2: Elongin-C



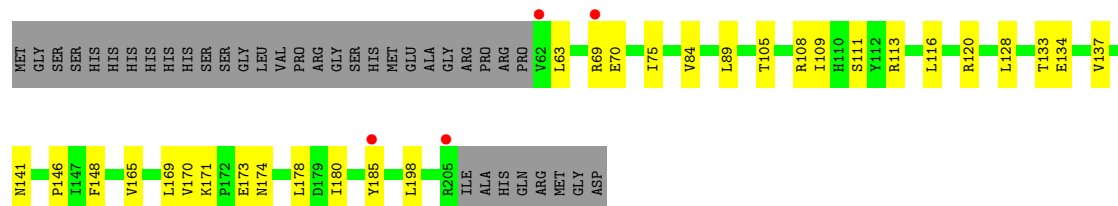
• Molecule 2: Elongin-C



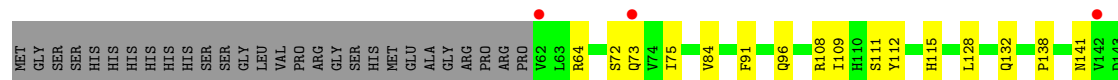
• Molecule 3: von Hippel-Lindau disease tumor suppressor

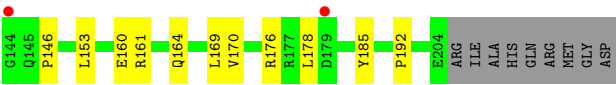


• Molecule 3: von Hippel-Lindau disease tumor suppressor

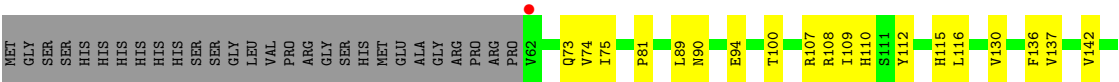


• Molecule 3: von Hippel-Lindau disease tumor suppressor





● Molecule 4: von Hippel-Lindau disease tumor suppressor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.90Å 92.90Å 359.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.49 – 2.30 48.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.49-2.30) 96.3 (48.49-2.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.211 , 0.249 0.211 , 0.249	Depositor DCC
$R_{free}$ test set	3597 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4812e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CAS, DMS, A1CBK, A1CBL

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	0.38	0/810	0.66	0/1097
1	D	0.37	0/766	0.62	0/1036
1	G	0.38	0/819	0.60	0/1110
1	J	0.43	0/823	0.66	0/1113
2	B	0.44	0/696	0.58	0/940
2	E	0.35	0/701	0.60	0/946
2	H	0.40	0/700	0.55	0/944
2	K	0.42	0/667	0.62	0/897
3	C	0.39	0/1147	0.60	0/1568
3	F	0.40	0/1142	0.59	0/1567
3	L	0.44	0/1167	0.63	0/1595
4	I	0.43	0/1168	0.61	0/1598
All	All	0.40	0/10606	0.61	0/14411

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	794	0	790	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	751	0	740	9	0
1	G	803	0	791	12	1
1	J	807	0	807	10	0
2	B	682	0	674	14	0
2	E	687	0	674	11	0
2	H	686	0	677	20	0
2	K	654	0	650	13	0
3	C	1125	0	1094	14	0
3	F	1122	0	1069	30	0
3	L	1147	0	1120	24	0
4	I	1138	0	1119	23	0
5	C	17	0	0	0	0
5	F	17	0	0	0	0
5	L	17	0	0	0	0
6	C	4	0	6	0	0
6	F	8	0	12	1	0
6	H	4	0	6	4	0
6	I	4	0	6	1	0
6	L	4	0	6	2	0
7	E	15	0	0	1	0
7	H	15	0	0	0	0
7	K	15	0	0	3	0
8	A	34	0	0	0	0
8	B	14	0	0	1	0
8	C	18	0	0	0	0
8	D	10	0	0	0	0
8	E	10	0	0	0	0
8	F	29	0	0	1	0
8	G	12	0	0	0	0
8	H	13	0	0	1	0
8	I	29	0	0	0	0
8	J	29	0	0	1	0
8	K	21	0	0	1	0
8	L	31	0	0	3	0
All	All	10766	0	10241	163	1

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 8.

The worst 5 of 163 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)
3:L:161:ARG:HH22	6:L:302:DMS:H13	1.41	0.85
4:I:89:LEU:HD12	4:I:116:LEU:HD23	1.57	0.84
4:I:176:ARG:NH2	4:I:189:GLU:OE2	2.12	0.81
2:H:64:GLU:H	6:H:202:DMS:H13	1.45	0.81
2:E:97:PRO:HB3	3:F:169:LEU:HD21	1.66	0.77

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:GLN:OE1	1:G:68:ARG:NH2[7_644]	2.19	0.01

## 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	101/104 (97%)	95 (94%)	5 (5%)	1 (1%)	13	15
1	D	94/104 (90%)	90 (96%)	4 (4%)	0	100	100
1	G	101/104 (97%)	95 (94%)	6 (6%)	0	100	100
1	J	101/104 (97%)	95 (94%)	6 (6%)	0	100	100
2	B	82/98 (84%)	82 (100%)	0	0	100	100
2	E	84/98 (86%)	83 (99%)	1 (1%)	0	100	100
2	H	84/98 (86%)	84 (100%)	0	0	100	100
2	K	77/98 (79%)	76 (99%)	1 (1%)	0	100	100
3	C	139/180 (77%)	136 (98%)	3 (2%)	0	100	100
3	F	141/180 (78%)	138 (98%)	3 (2%)	0	100	100
3	L	140/180 (78%)	136 (97%)	4 (3%)	0	100	100
4	I	141/180 (78%)	135 (96%)	6 (4%)	0	100	100
All	All	1285/1528 (84%)	1245 (97%)	39 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ALA

### 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	86/92 (94%)	86 (100%)	0	100	100
1	D	81/92 (88%)	81 (100%)	0	100	100
1	G	88/92 (96%)	88 (100%)	0	100	100
1	J	89/92 (97%)	89 (100%)	0	100	100
2	B	76/86 (88%)	75 (99%)	1 (1%)	65	79
2	E	75/86 (87%)	75 (100%)	0	100	100
2	H	74/86 (86%)	74 (100%)	0	100	100
2	K	70/86 (81%)	70 (100%)	0	100	100
3	C	124/163 (76%)	121 (98%)	3 (2%)	44	61
3	F	120/163 (74%)	120 (100%)	0	100	100
3	L	126/163 (77%)	125 (99%)	1 (1%)	79	89
4	I	126/164 (77%)	126 (100%)	0	100	100
All	All	1135/1365 (83%)	1130 (100%)	5 (0%)	89	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	86	SER
3	C	62	VAL
3	C	181	VAL
3	C	194	VAL
3	L	153	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
4	I	73	GLN
2	K	61	ASN
3	L	191	HIS
3	L	132	GLN
3	L	141	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	CAS	F	77	3	5,8,9	0.57	0	1,9,11	0.03	0
3	CAS	L	77	3	5,8,9	0.71	0	1,9,11	0.15	0
3	CAS	C	77	3	5,8,9	0.83	0	1,9,11	0.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAS	F	77	3	-	0/0/7/9	-
3	CAS	L	77	3	-	0/0/7/9	-
3	CAS	C	77	3	-	0/0/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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$
6	DMS	I	301	-	3,3,3	0.58	0	3,3,3	0.45	0
5	A1CBL	L	301	-	18,18,18	1.03	2 (11%)	24,24,24	0.83	1 (4%)
6	DMS	C	302	-	3,3,3	0.66	0	3,3,3	0.47	0
7	A1CBK	K	201	-	16,16,16	0.54	0	21,23,23	0.74	1 (4%)
7	A1CBK	E	201	-	16,16,16	0.56	0	21,23,23	0.80	0
6	DMS	F	303	-	3,3,3	0.61	0	3,3,3	0.20	0
6	DMS	H	202	-	3,3,3	0.57	0	3,3,3	0.37	0
6	DMS	L	302	-	3,3,3	0.76	0	3,3,3	0.55	0
5	A1CBL	C	301	-	18,18,18	1.06	1 (5%)	24,24,24	0.66	0
5	A1CBL	F	301	-	18,18,18	1.94	3 (16%)	24,24,24	1.31	4 (16%)
7	A1CBK	H	201	-	16,16,16	0.52	0	21,23,23	0.72	1 (4%)
6	DMS	F	302	-	3,3,3	0.68	0	3,3,3	0.25	0

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
5	A1CBL	L	301	-	-	0/8/18/18	1/2/2/2
7	A1CBK	K	201	-	-	0/6/17/17	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	A1CBK	E	201	-	-	0/6/17/17	0/2/2/2
5	A1CBL	C	301	-	-	4/8/18/18	1/2/2/2
5	A1CBL	F	301	-	-	5/8/18/18	1/2/2/2
7	A1CBK	H	201	-	-	2/6/17/17	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	301	A1CBL	C13-N12	6.96	1.61	1.48
5	F	301	A1CBL	C8-N9	2.35	1.52	1.47
5	C	301	A1CBL	C8-N9	2.22	1.51	1.47
5	L	301	A1CBL	C8-N9	2.20	1.51	1.47
5	F	301	A1CBL	C16-N12	2.18	1.51	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	301	A1CBL	C11-N12-C13	2.98	117.76	113.01
5	F	301	A1CBL	C15-C13-N12	2.97	119.00	112.26
5	F	301	A1CBL	C16-N12-C13	2.97	117.74	113.01
5	F	301	A1CBL	C8-C7-C2	2.46	126.71	120.89
5	L	301	A1CBL	C8-C7-C2	2.18	126.02	120.89

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	A1CBL	C15-C13-N12-C16
5	F	301	A1CBL	C15-C13-N12-C11
5	F	301	A1CBL	C7-C8-N9-C10
5	F	301	A1CBL	C7-C8-N9-C17
7	H	201	A1CBK	O1-C2-N4-C5

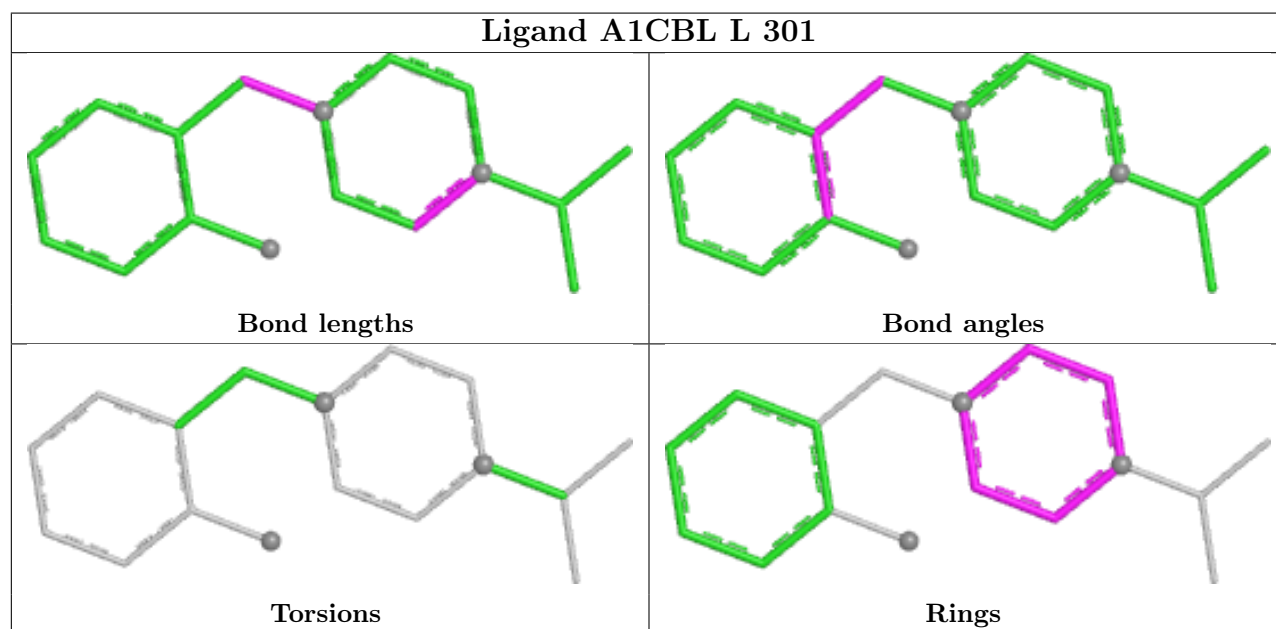
All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	301	A1CBL	C10-C11-C16-C17-N12-N9
5	F	301	A1CBL	C10-C11-C16-C17-N12-N9
5	C	301	A1CBL	C10-C11-C16-C17-N12-N9

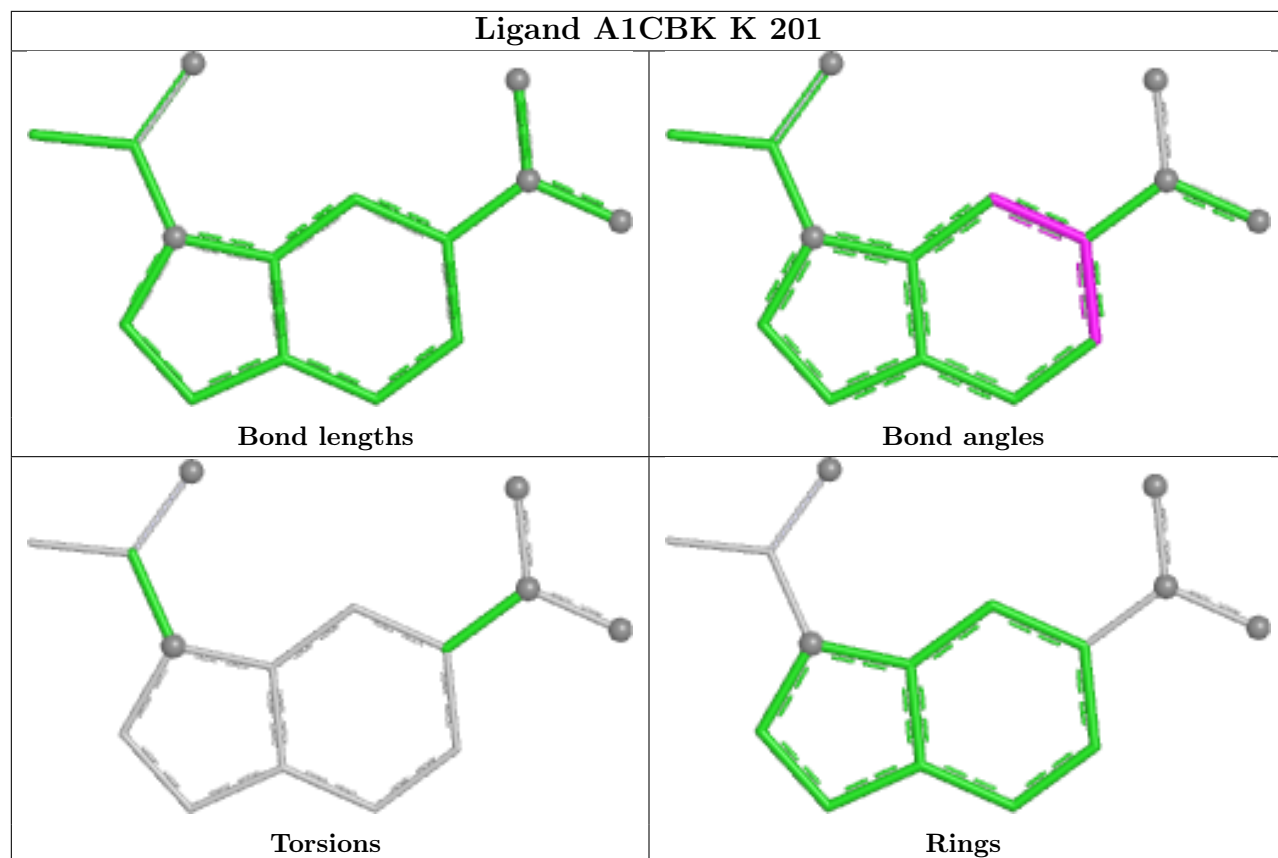
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	301	DMS	1	0
7	K	201	A1CBK	3	0
7	E	201	A1CBK	1	0
6	F	303	DMS	1	0
6	H	202	DMS	4	0
6	L	302	DMS	2	0

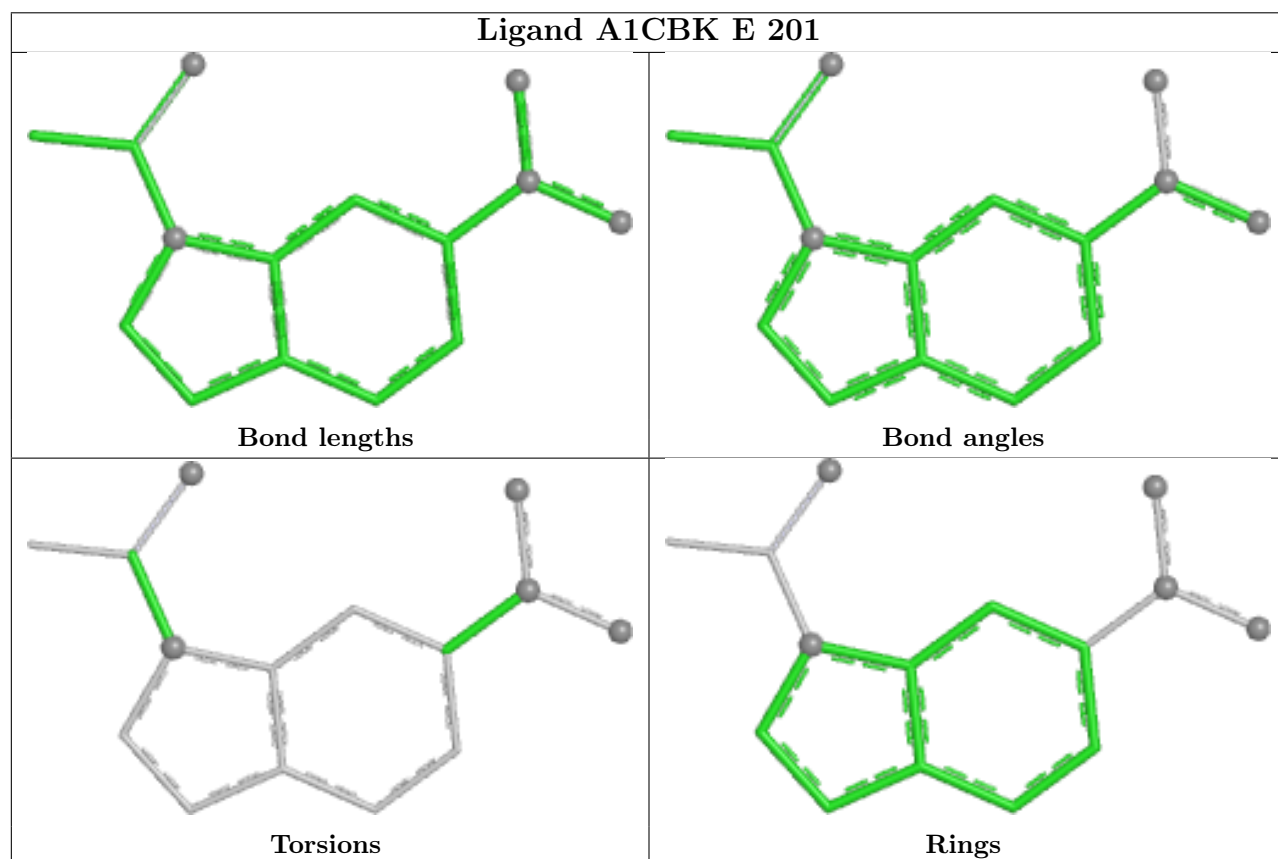
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



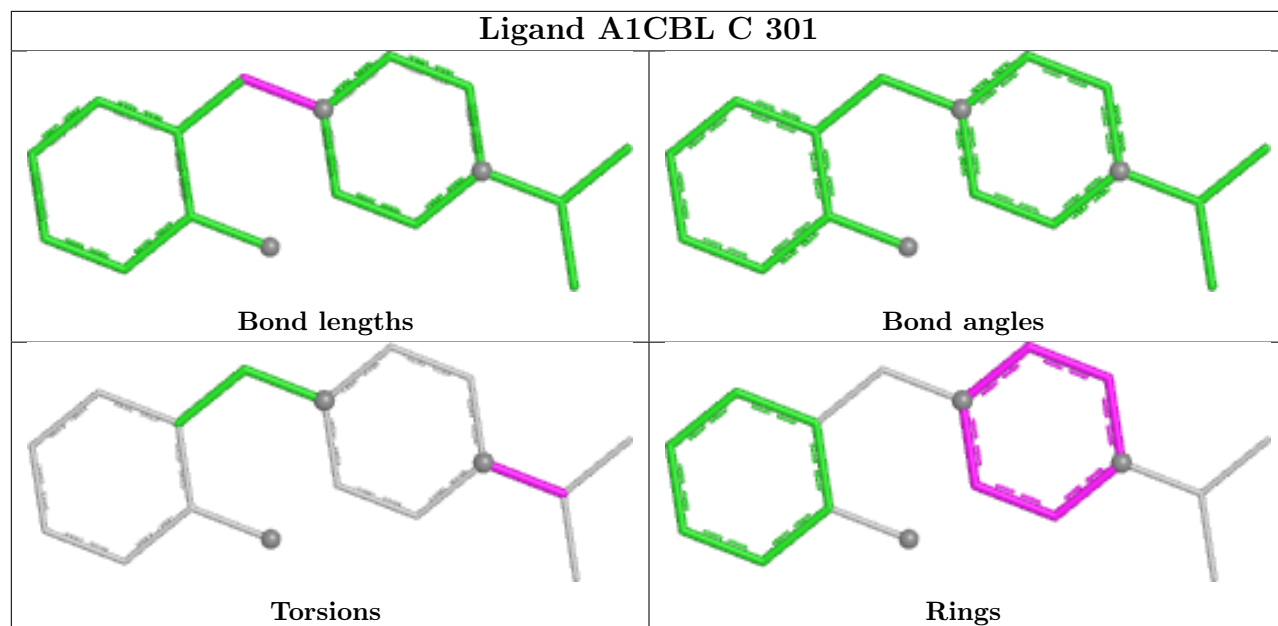
## Ligand A1CBK K 201



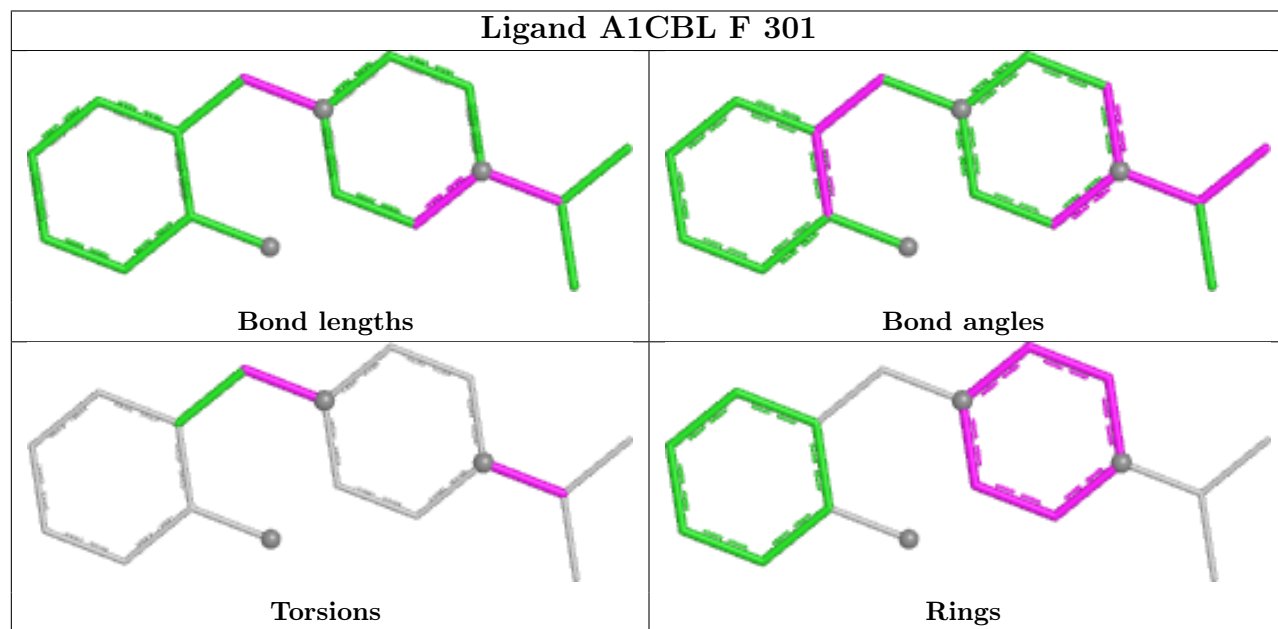
## Ligand A1CBK E 201



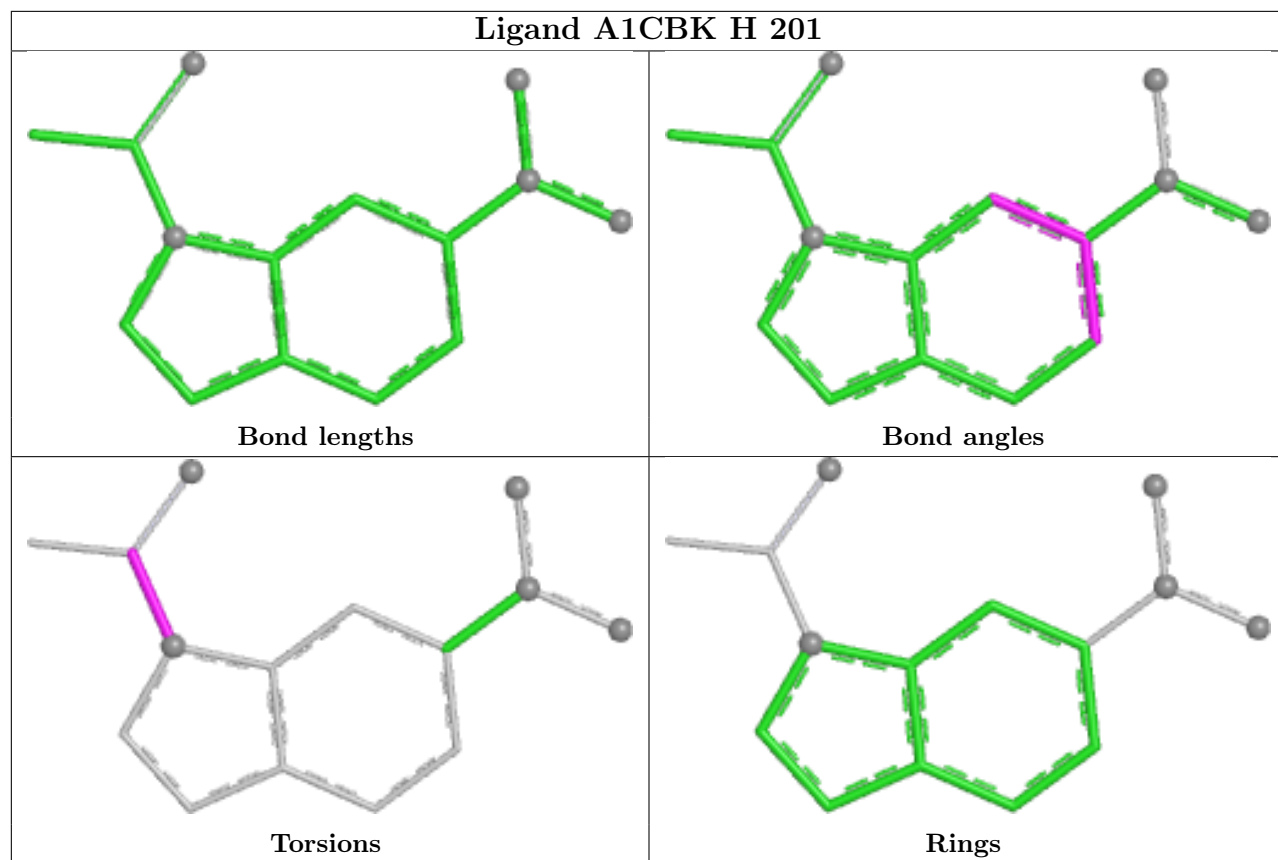
## Ligand A1CBL C 301



## Ligand A1CBL F 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	103/104 (99%)	0.03	2 (1%) 66 67	41, 52, 76, 94	0
1	D	98/104 (94%)	0.60	4 (4%) 42 43	47, 69, 93, 99	0
1	G	103/104 (99%)	0.19	2 (1%) 66 67	45, 62, 79, 93	0
1	J	103/104 (99%)	-0.10	0 100 100	39, 50, 74, 86	0
2	B	86/98 (87%)	0.16	2 (2%) 61 62	41, 50, 70, 107	0
2	E	88/98 (89%)	0.44	5 (5%) 30 32	45, 64, 84, 101	0
2	H	88/98 (89%)	0.30	4 (4%) 39 40	44, 56, 92, 107	0
2	K	82/98 (83%)	0.21	5 (6%) 28 30	31, 50, 74, 92	1 (1%)
3	C	140/180 (77%)	0.31	7 (5%) 35 36	41, 56, 91, 128	1 (0%)
3	F	143/180 (79%)	0.32	4 (2%) 55 56	43, 57, 91, 104	0
3	L	142/180 (78%)	0.13	5 (3%) 47 49	39, 53, 75, 101	0
4	I	143/180 (79%)	0.28	4 (2%) 55 56	43, 56, 86, 107	0
All	All	1319/1528 (86%)	0.24	44 (3%) 49 51	31, 56, 87, 128	2 (0%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	48	GLY	5.1
2	H	57	THR	4.3
3	F	205	ARG	4.2
4	I	204	GLU	4.2
2	K	47	SER	4.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
3	CAS	F	77	9/10	0.74	0.20	47,49,79,116	9
3	CAS	C	77	9/10	0.83	0.17	49,52,86,151	0
3	CAS	L	77	9/10	0.84	0.17	43,48,81,122	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

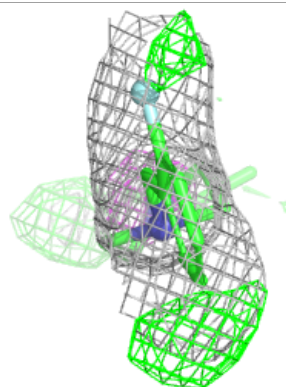
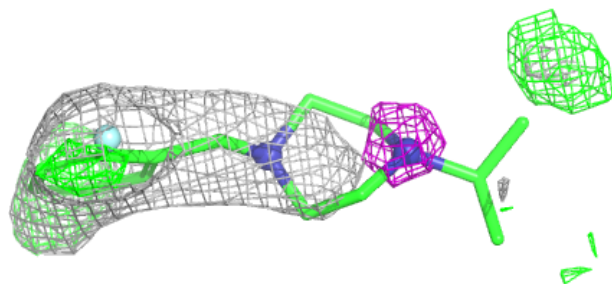
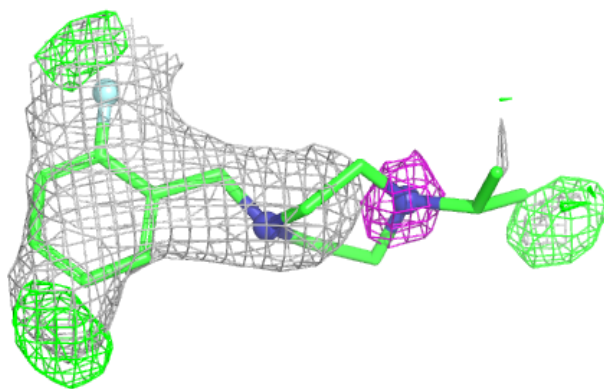
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	A1CBL	F	301	17/17	0.65	0.25	71,83,102,102	0
5	A1CBL	C	301	17/17	0.71	0.26	69,79,102,107	0
6	DMS	F	303	4/4	0.71	0.17	92,96,96,114	0
7	A1CBK	E	201	15/15	0.71	0.29	112,116,119,119	15
6	DMS	H	202	4/4	0.74	0.23	83,84,96,113	0
6	DMS	C	302	4/4	0.77	0.19	60,64,75,90	0
5	A1CBL	L	301	17/17	0.78	0.24	62,75,86,88	0
7	A1CBK	K	201	15/15	0.78	0.22	62,67,70,70	15
6	DMS	I	301	4/4	0.82	0.19	63,70,79,92	0
6	DMS	L	302	4/4	0.82	0.18	53,58,61,91	0
7	A1CBK	H	201	15/15	0.83	0.22	64,71,74,75	15
6	DMS	F	302	4/4	0.84	0.20	71,73,84,101	0

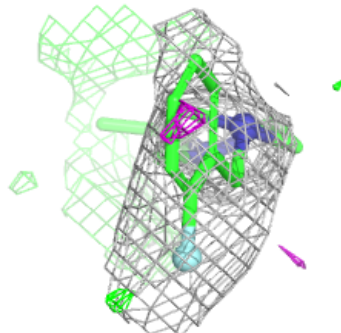
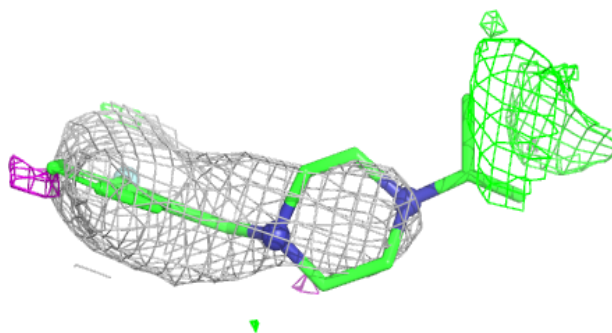
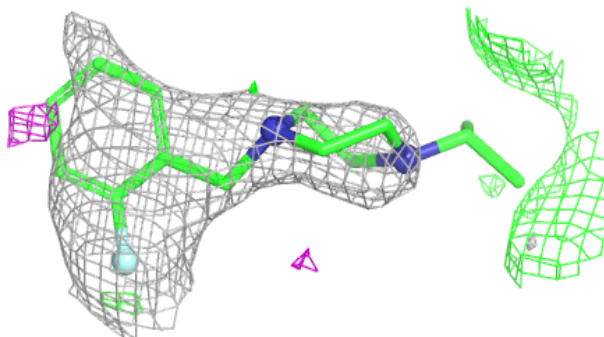
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around A1CBL 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)

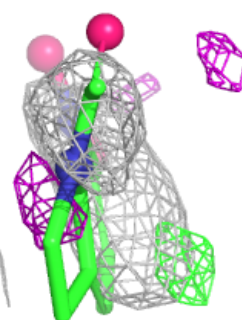
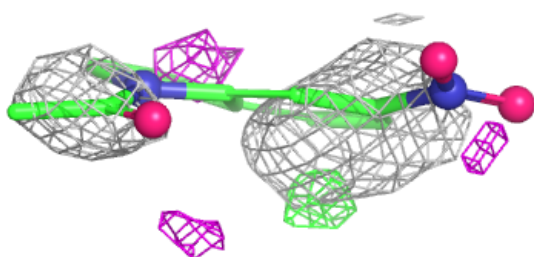
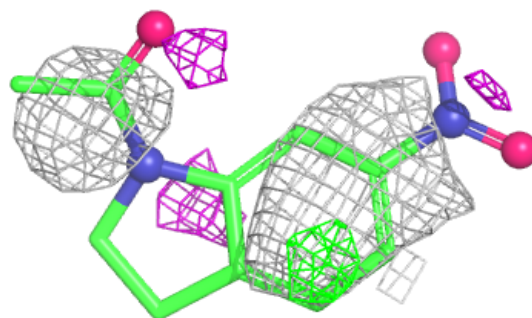
**Electron density around A1CBL C 301:**

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

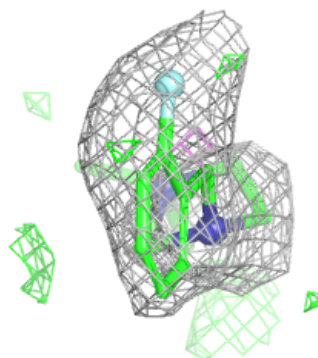
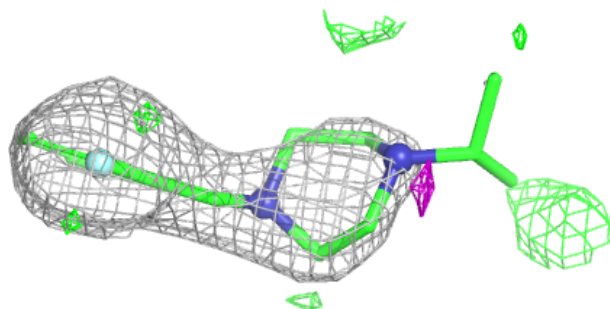
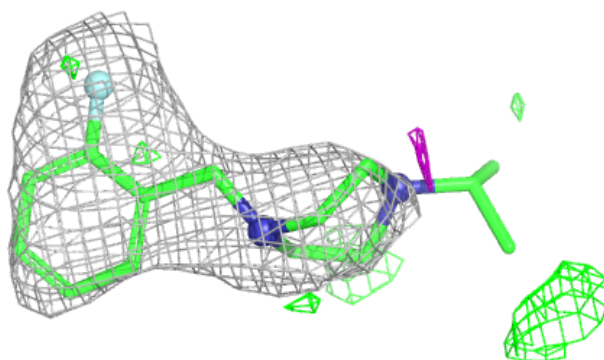


**Electron density around A1CBK E 201:**

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

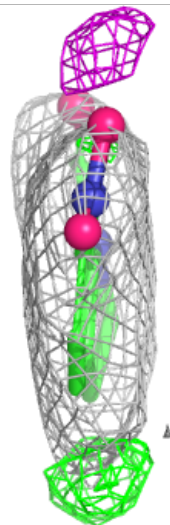
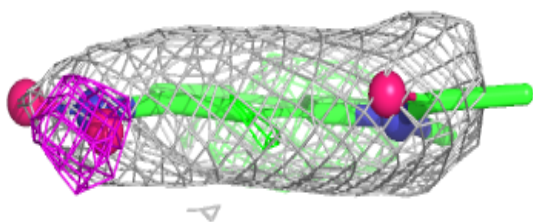
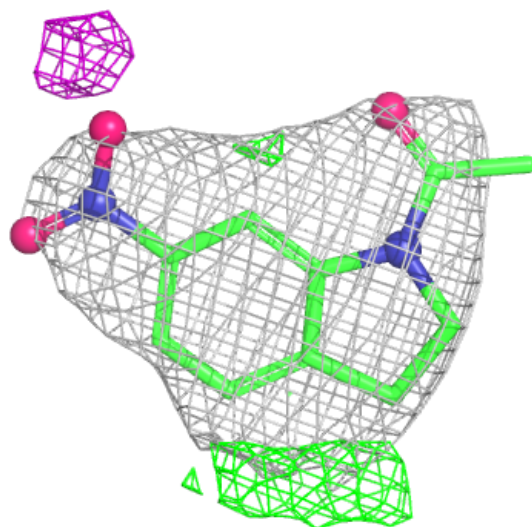
**Electron density around A1CBL L 301:**

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



**Electron density around A1CBK K 201:**

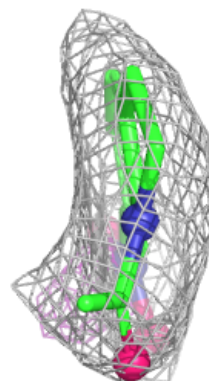
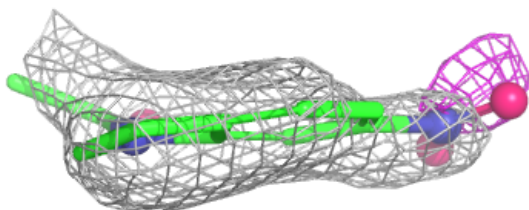
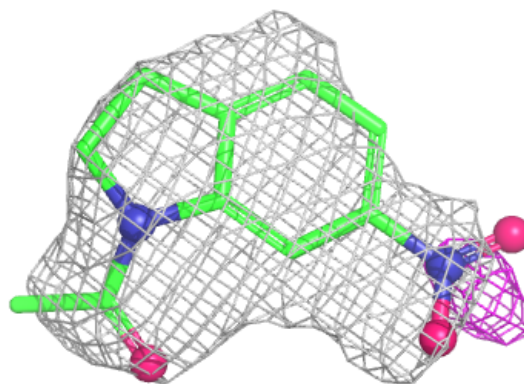
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around A1CBK H 201:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.