



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 2, 2019 – 09:52 PM EDT

PDB ID : 6E30
EMDB ID: : EMD-8972
Title : Mechanism of cellular recognition by PCV2
Authors : Khayat, R.; Dhindwal, S.
Deposited on : 2018-07-12
Resolution : 3.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

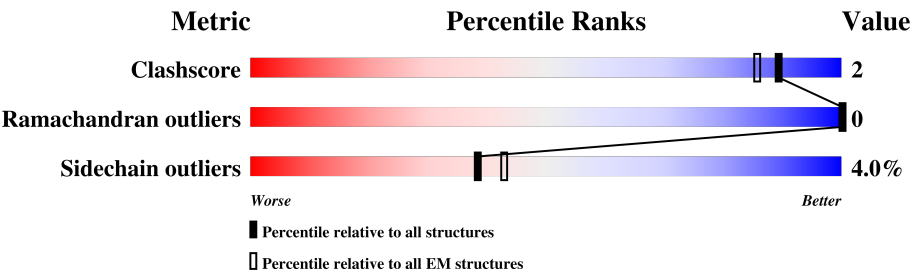
MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.
















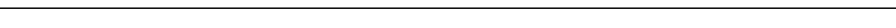











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A1	233	72% 9% 19%
1	A2	233	73% 7% 19%
1	A3	233	73% 7% 19%
1	A4	233	74% 7% 19%
1	A5	233	73% 8% 19%
1	A6	233	73% 7% 19%
1	A7	233	73% 7% 19%
1	A8	233	73% 8% 19%
1	A9	233	73% 7% 19%


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AA	233	 73% 7% 19%
1	AB	233	 73% 7% 19%
1	AC	233	 73% 7% 19%
1	AD	233	 71% 9% 19%
1	AE	233	 73% 8% 19%
1	AF	233	 74% 6% 19%
1	AG	233	 73% 7% 19%
1	AH	233	 73% 8% 19%
1	AI	233	 71% 9% 19%
1	AJ	233	 72% 9% 19%
1	AK	233	 72% 9% 19%
1	AL	233	 72% 9% 19%
1	AM	233	 73% 7% 19%
1	AN	233	 73% 8% 19%
1	AO	233	 73% 7% 19%
1	AP	233	 73% 8% 19%
1	AQ	233	 72% 9% 19%
1	AR	233	 72% 8% 19%
1	AS	233	 73% 7% 19%
1	AT	233	 73% 7% 19%
1	AU	233	 73% 7% 19%
1	AV	233	 72% 9% 19%
1	AW	233	 73% 7% 19%
1	AX	233	 73% 7% 19%
1	AY	233	 72% 8% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AZ	233	 73%7%19%
1	Aa	233	 78%1%19%
1	Ab	233	 78%1%19%
1	Ac	233	 78%1%19%
1	Ad	233	 78%1%19%
1	Ae	233	 78%1%19%
1	Af	233	 78%1%19%
1	Ag	233	 78%1%19%
1	Ah	233	 78%1%19%
1	Ai	233	 78%1%19%
1	Aj	233	 78%1%19%
1	Ak	233	 78%1%19%
1	Al	233	 78%1%19%
1	Am	233	 78%1%19%
1	An	233	 78%1%19%
1	Ao	233	 78%1%19%
1	Ap	233	 78%1%19%
1	Aq	233	 78%1%19%
1	Ar	233	 78%1%19%
1	As	233	 78%1%19%
1	At	233	 78%1%19%
1	Au	233	 78%1%19%
1	Av	233	 78%1%19%
1	Aw	233	 78%1%19%
1	Ax	233	 78%1%19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Ay	233	<div><div></div><div>78%</div><div></div><div>•</div><div>19%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 183270 atoms, of which 90180 are hydrogens and 0 are deuteriums.

In the tables below, 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 Capsid protein of PCV2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A2	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A3	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A4	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A5	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A6	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A7	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A8	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A9	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AA	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AB	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AC	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AD	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AE	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AF	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AG	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AH	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
1	AI	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AJ	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AK	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AL	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AM	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AN	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AO	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AP	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AQ	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AR	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AS	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AT	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AU	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AV	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AW	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AX	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AY	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AZ	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Aa	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ab	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ac	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		

Continued on next page...

Continued from previous page...

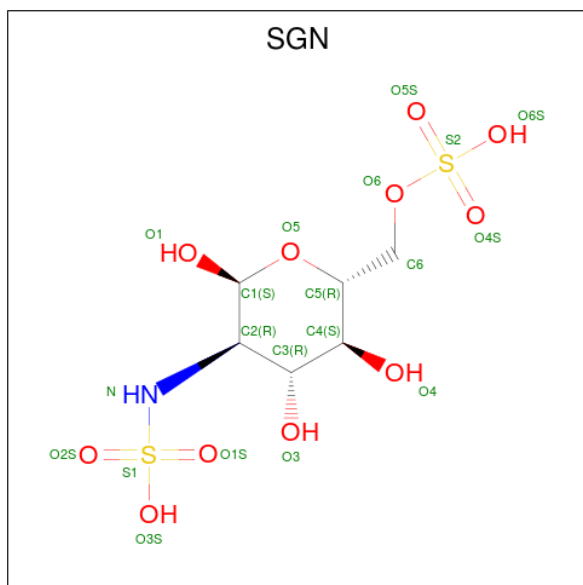
Mol	Chain	Residues	Atoms						AltConf	Trace
1	Ad	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ae	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Af	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ag	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ah	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ai	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Aj	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ak	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Al	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Am	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	An	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ao	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ap	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Aq	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ar	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	As	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	At	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Au	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Av	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Aw	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ax	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		

Continued on next page...

Continued from previous page...

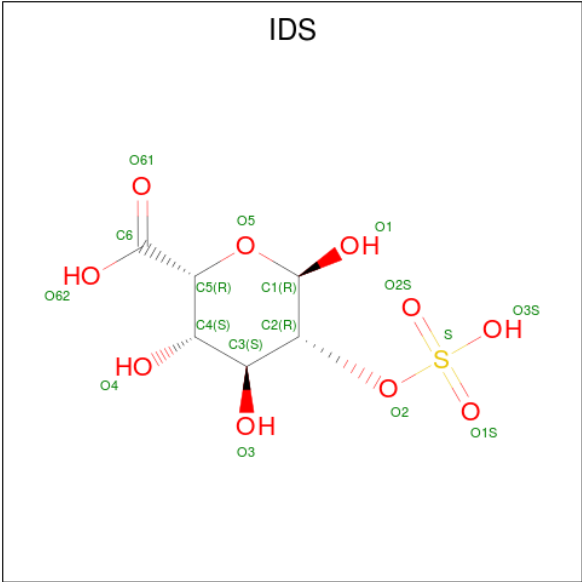
Mol	Chain	Residues	Atoms						AltConf	Trace
1	Ay	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		

- Molecule 2 is N,O6-DISULFO-GLUCOSAMINE (three-letter code: SGN) (formula: $C_6H_{13}NO_{11}S_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						AltConf
2	A1	1	Total	C	N	O	S		0
			58	18	3	31	6		
2	A1	1	Total	C	N	O	S		0
			58	18	3	31	6		
2	A1	1	Total	C	N	O	S		0
			58	18	3	31	6		

- Molecule 3 is 2-O-sulfo-alpha-L-idopyranuronic acid (three-letter code: IDS) (formula: $C_6H_{10}O_{10}S$) (labeled as "Ligand of Interest" by author).

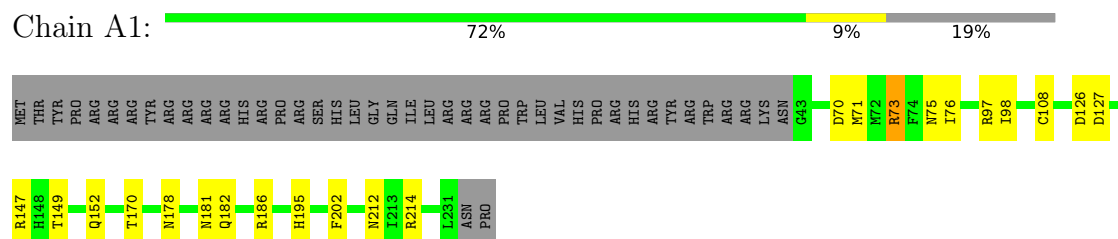


Mol	Chain	Residues	Atoms				AltConf
3	A1	1	Total	C	O	S	0
			32	12	18	2	
3	A1	1	Total	C	O	S	0
			32	12	18	2	

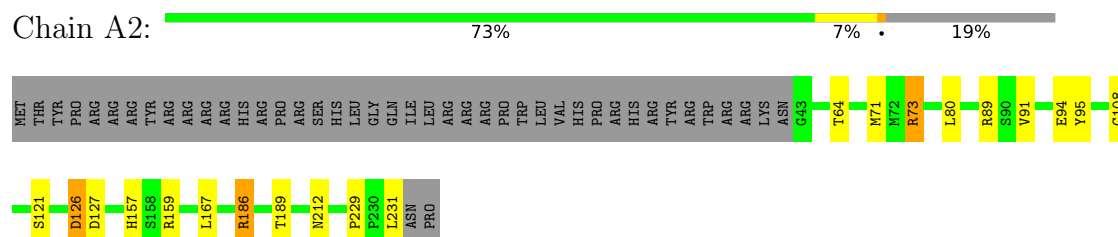
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

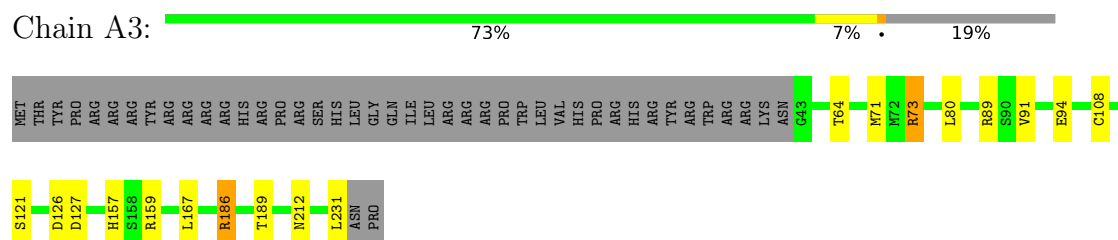
- Molecule 1: Capsid protein of PCV2



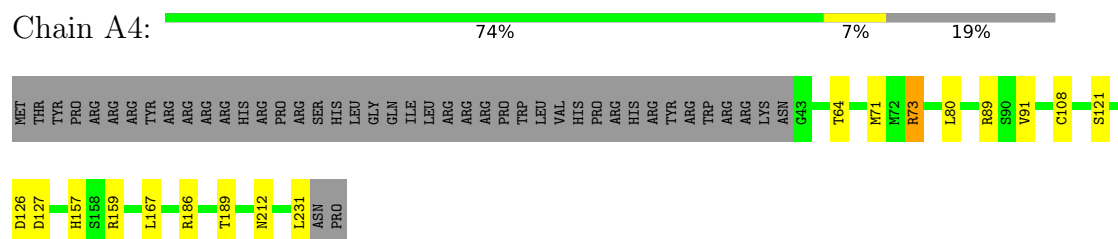
- Molecule 1: Capsid protein of PCV2



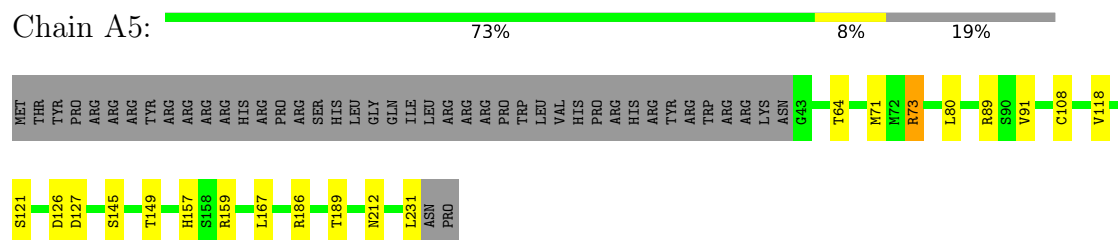
- Molecule 1: Capsid protein of PCV2



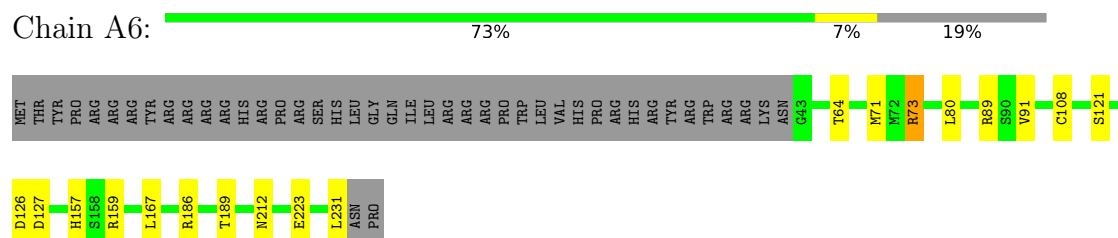
- Molecule 1: Capsid protein of PCV2



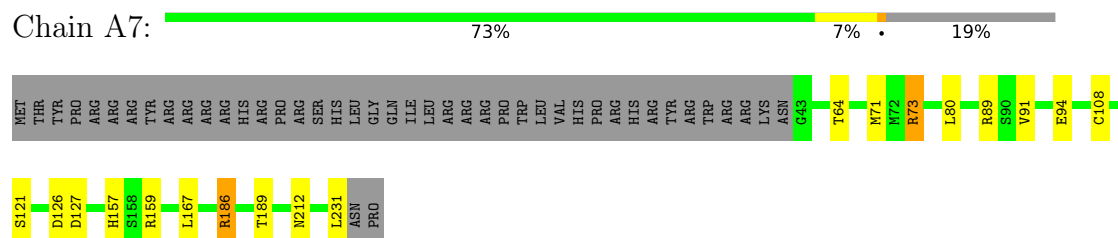
- Molecule 1: Capsid protein of PCV2



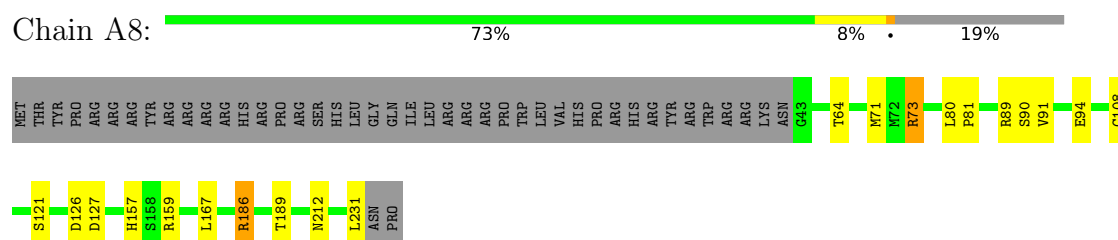
- Molecule 1: Capsid protein of PCV2



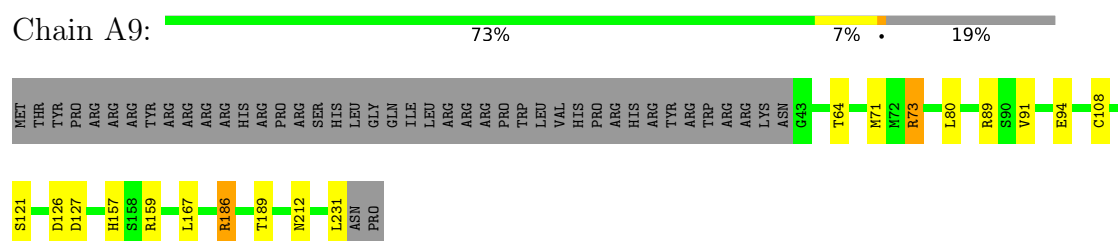
- Molecule 1: Capsid protein of PCV2



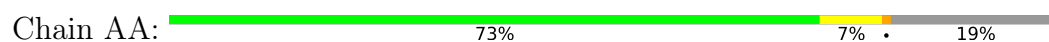
- Molecule 1: Capsid protein of PCV2

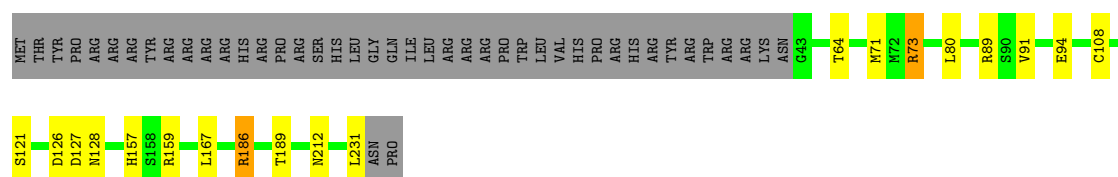


- Molecule 1: Capsid protein of PCV2



- Molecule 1: Capsid protein of PCV2





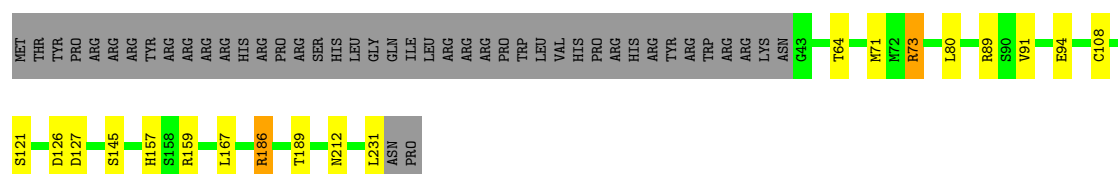
- Molecule 1: Capsid protein of PCV2

Chain AB: 73% 7% 19%



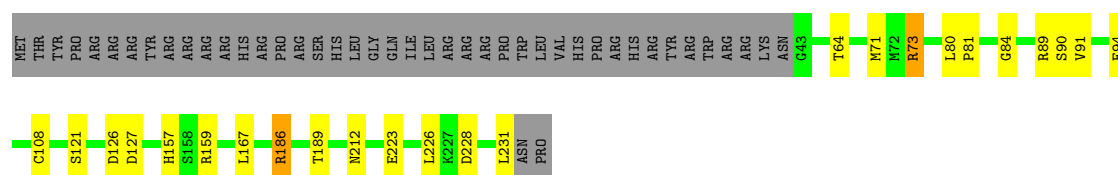
- Molecule 1: Capsid protein of PCV2

Chain AC: 73% 7% 19%



- Molecule 1: Capsid protein of PCV2

Chain AD: 71% 9% 19%



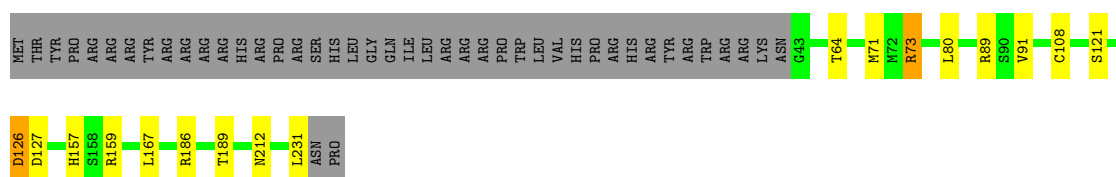
- Molecule 1: Capsid protein of PCV2

Chain AE: 73% 8% 19%



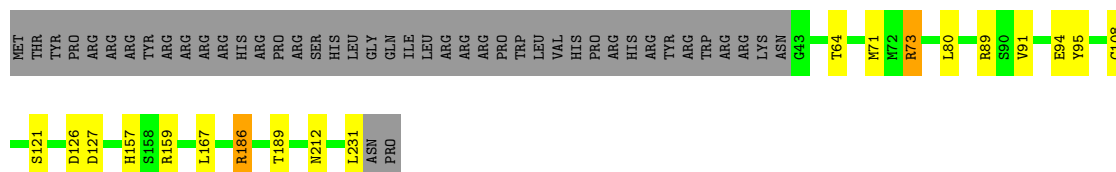
- Molecule 1: Capsid protein of PCV2

Chain AF: 74% 6% 19%



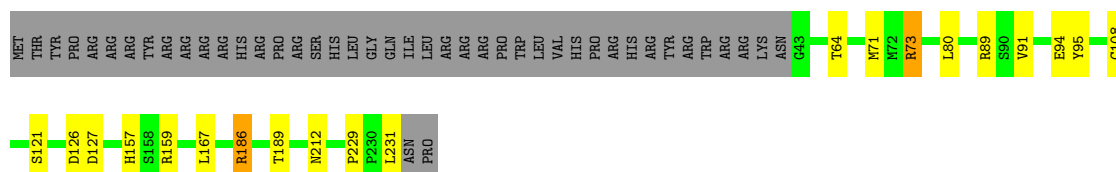
- Molecule 1: Capsid protein of PCV2

Chain AG: 73% 7% 19%



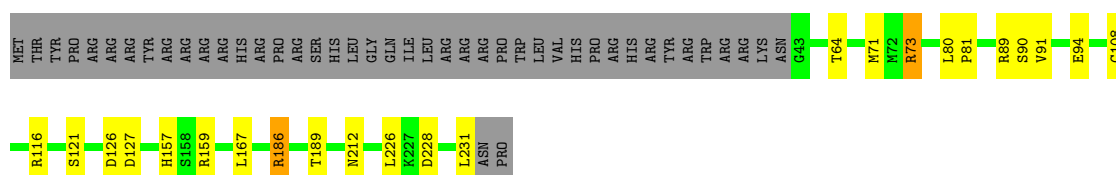
- Molecule 1: Capsid protein of PCV2

Chain AH: 73% 8% 19%



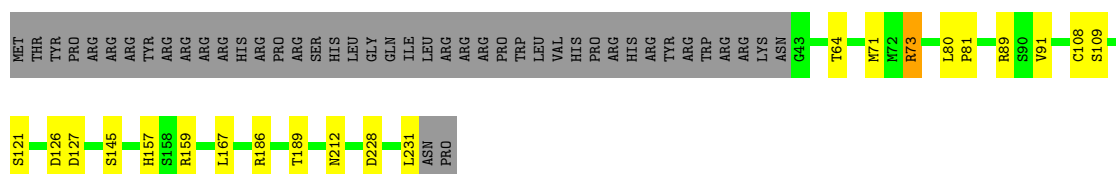
- Molecule 1: Capsid protein of PCV2

Chain AI: 71% 9% 19%



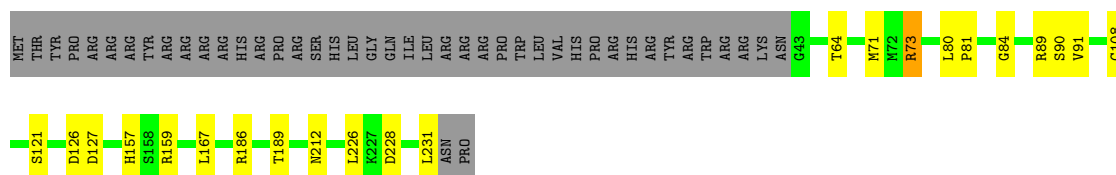
- Molecule 1: Capsid protein of PCV2

Chain AJ: 72% 9% 19%



- Molecule 1: Capsid protein of PCV2

Chain AK: 72% 9% 19%



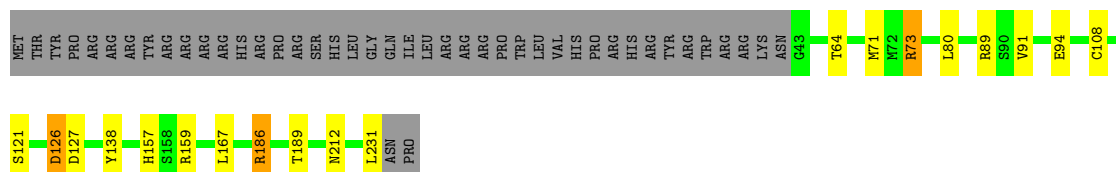
- Molecule 1: Capsid protein of PCV2

Chain AL: 72% 9% 19%



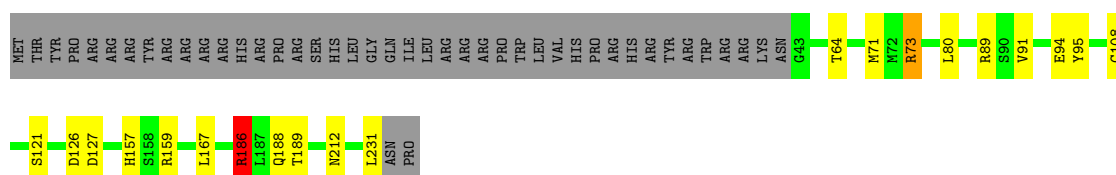
- Molecule 1: Capsid protein of PCV2

Chain AM: 73% 7% 19%



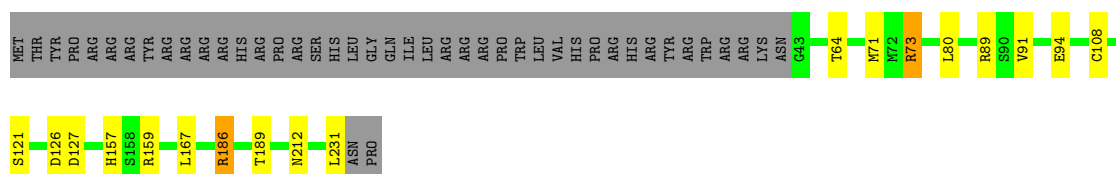
- Molecule 1: Capsid protein of PCV2

Chain AN: 73% 8% 19%



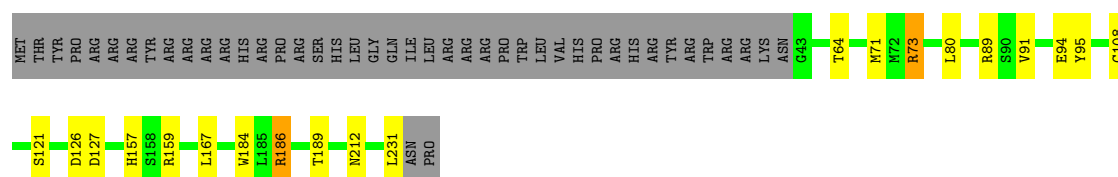
- Molecule 1: Capsid protein of PCV2

Chain AO: 73% 7% 19%

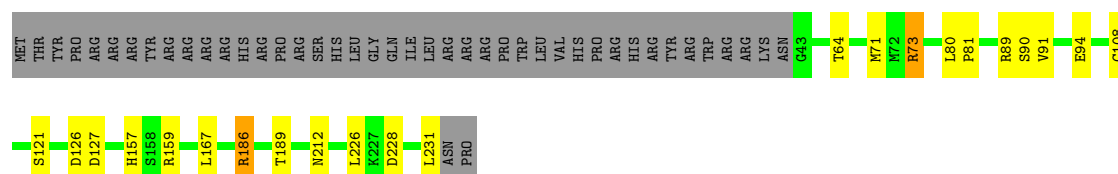


- Molecule 1: Capsid protein of PCV2

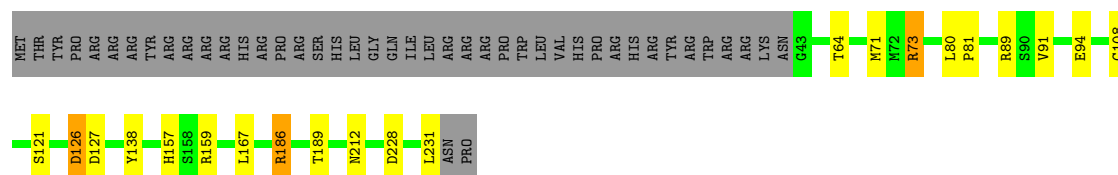
Chain AP: 73% 8% 19%



- Molecule 1: Capsid protein of PCV2



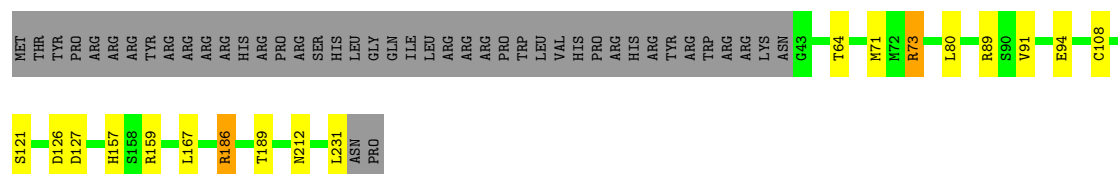
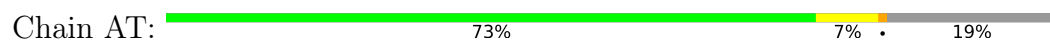
- Molecule 1: Capsid protein of PCV2



- Molecule 1: Capsid protein of PCV2

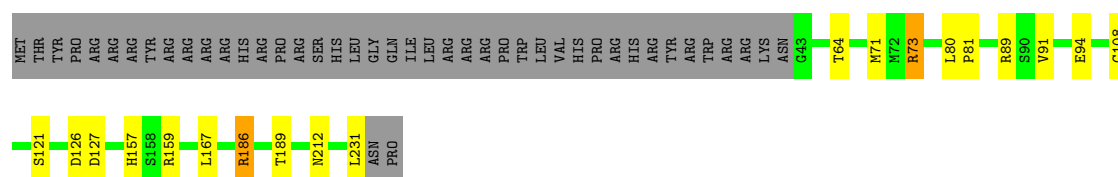


- Molecule 1: Capsid protein of PCV2



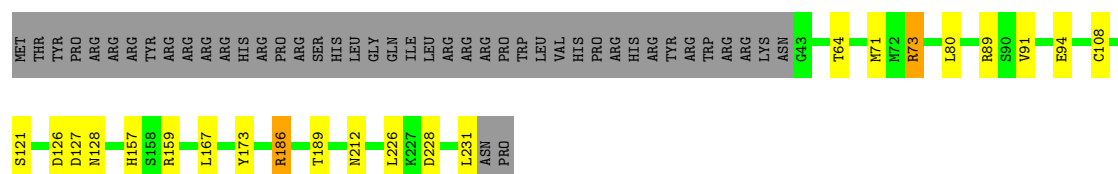
- Molecule 1: Capsid protein of PCV2





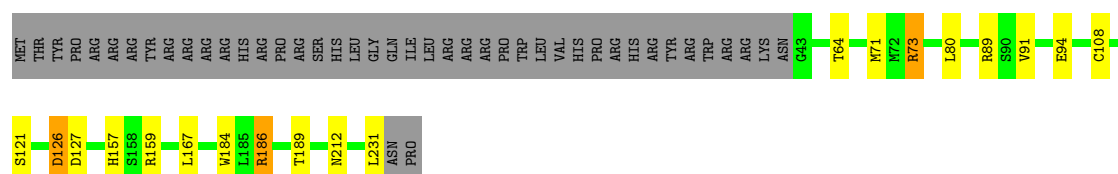
- Molecule 1: Capsid protein of PCV2

Chain AV: 72% 9% 19%



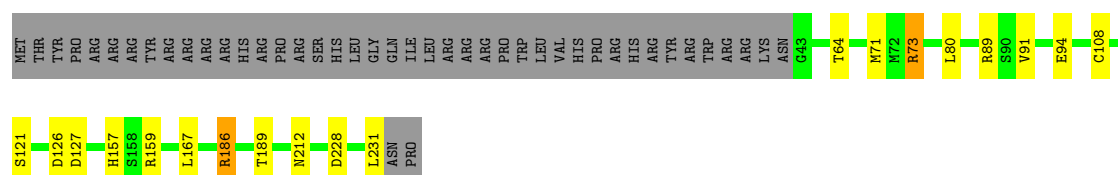
- Molecule 1: Capsid protein of PCV2

Chain AW: 73% 7% 19%



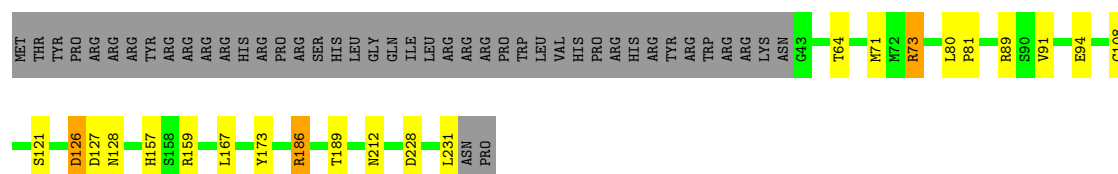
- Molecule 1: Capsid protein of PCV2

Chain AX: 73% 7% 19%



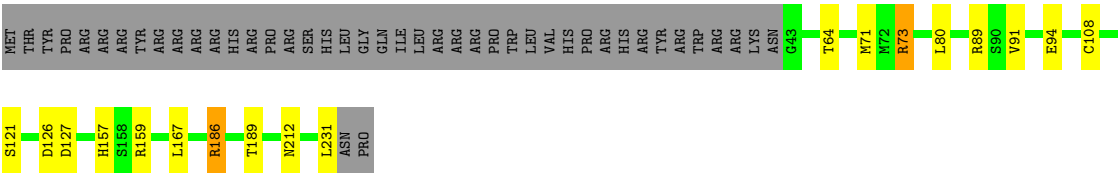
- Molecule 1: Capsid protein of PCV2

Chain AY: 72% 8% 19%



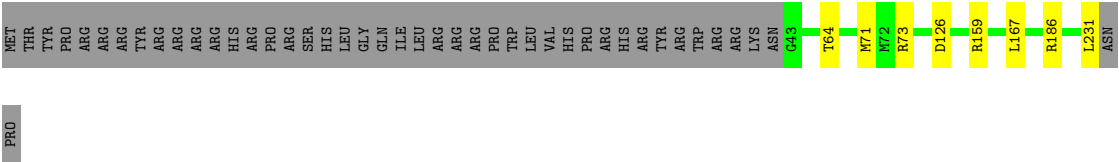
- Molecule 1: Capsid protein of PCV2

Chain AZ: 73% 7% 19%



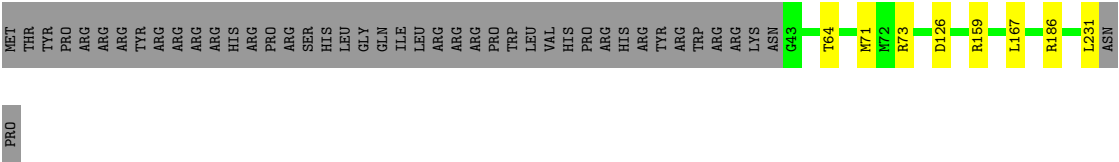
● Molecule 1: Capsid protein of PCV2

Chain Aa: 78% 19%



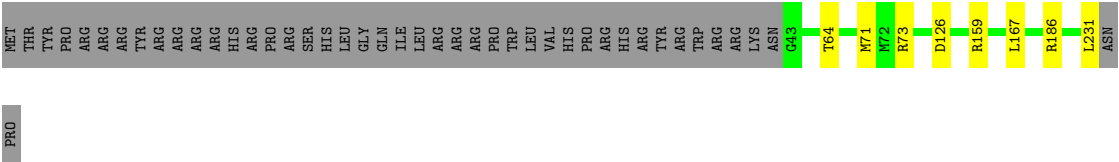
● Molecule 1: Capsid protein of PCV2

Chain Ab: 78% 19%



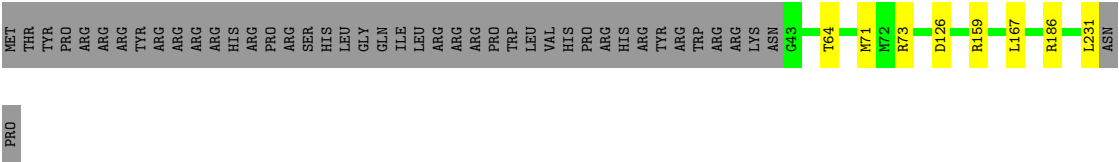
● Molecule 1: Capsid protein of PCV2

Chain Ac: 78% 19%



● Molecule 1: Capsid protein of PCV2

Chain Ad: 78% 19%




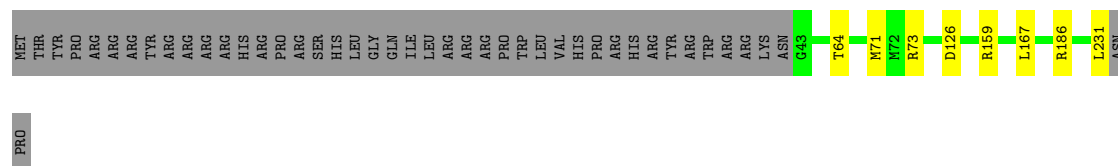
● Molecule 1: Capsid protein of PCV2

Chain Ae: 78% 19%

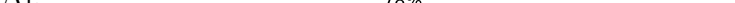


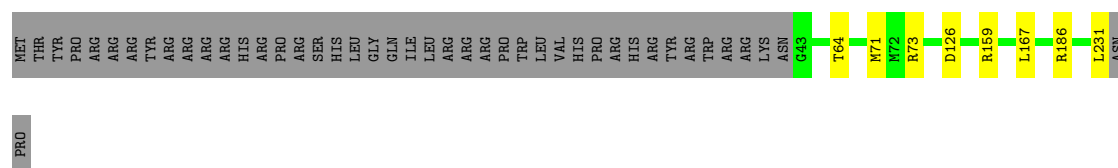
- Molecule 1: Capsid protein of PCV2

Chain Ak:  78% 19%



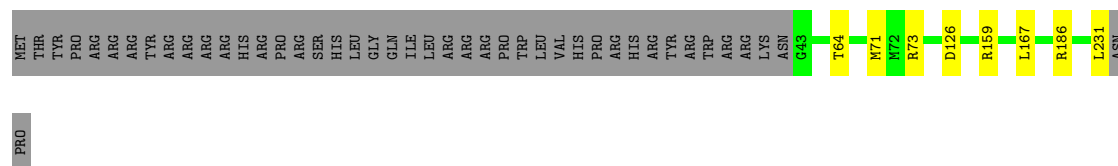
- Molecule 1: Capsid protein of PCV2

Chain AI:  78% 19%




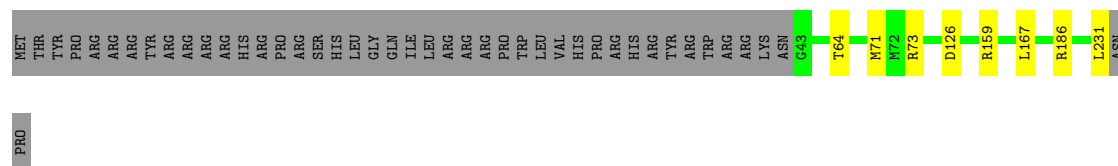
- Molecule 1: Capsid protein of PCV2

Chain Am: 78% • 19%




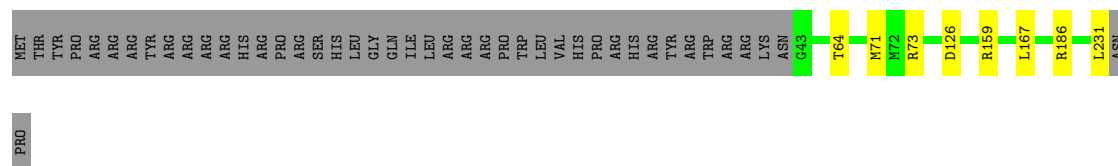
- Molecule 1: Capsid protein of PCV2

Chain An:  78% • 19%




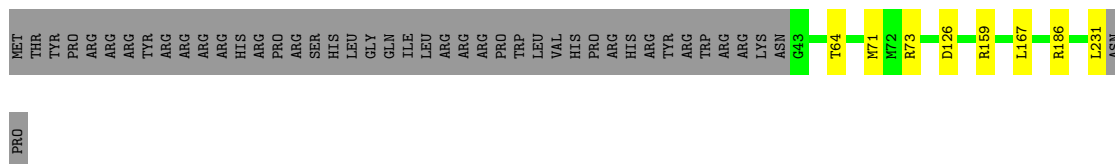
- Molecule 1: Capsid protein of PCV2

Chain Ao:  78% 19%




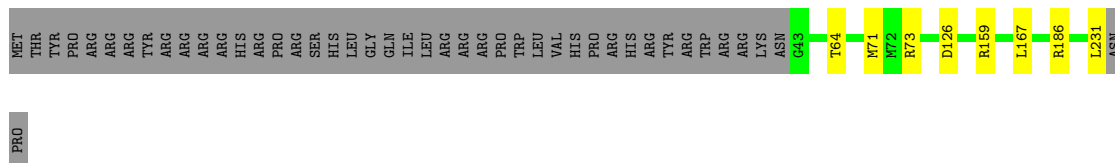
- Molecule 1: Capsid protein of PCV2

Chain Ap:  78% 19%




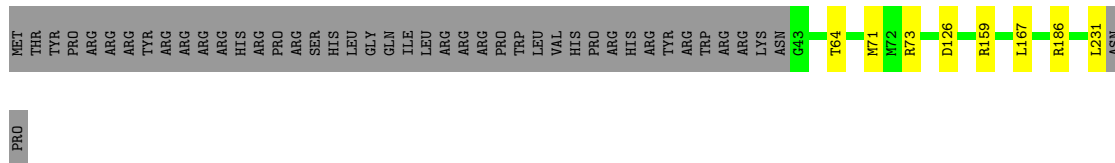
- Molecule 1: Capsid protein of PCV2

Chain Aq:  78% 19%




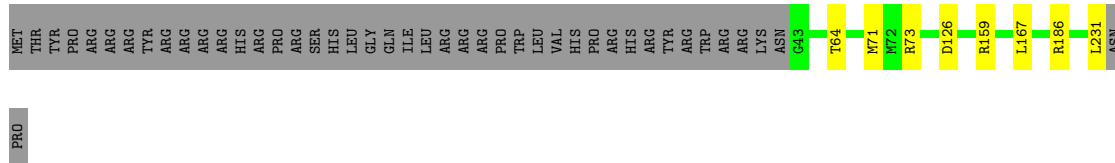
- Molecule 1: Capsid protein of PCV2

Chain Ar:  78% 19%




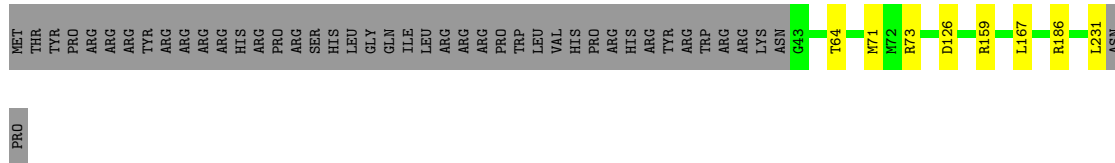
- Molecule 1: Capsid protein of PCV2

Chain As:  78% 19%




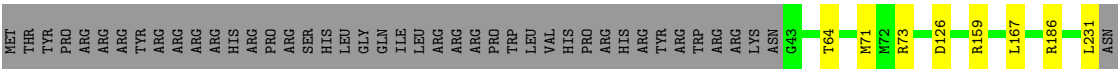
- Molecule 1: Capsid protein of PCV2

Chain At:  78% 19%



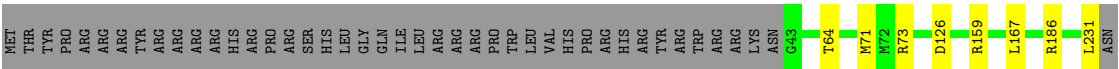
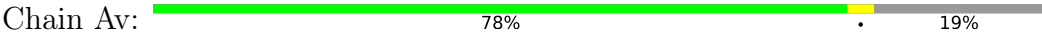
- Molecule 1: Capsid protein of PCV2

Chain Au:  78% 19%



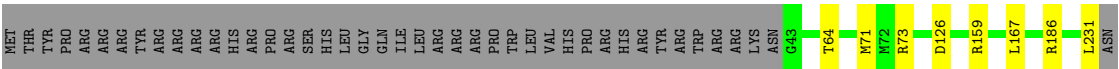
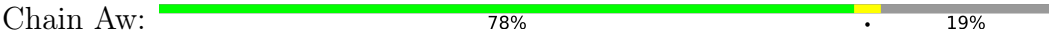
PRO

• Molecule 1: Capsid protein of PCV2



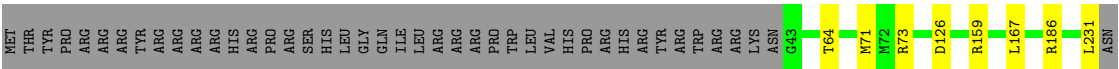
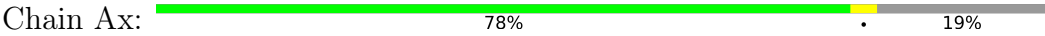
PRO

• Molecule 1: Capsid protein of PCV2



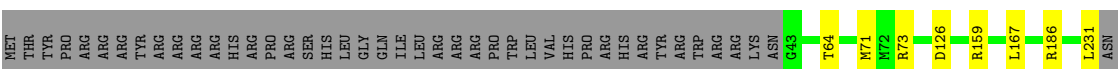
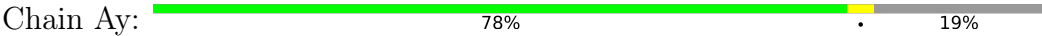
PRO

• Molecule 1: Capsid protein of PCV2



PRO

• Molecule 1: Capsid protein of PCV2



PRO

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	74170	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Per particle estimation	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A1	0.44	0/1597	0.57	0/2175
1	A2	0.76	0/1597	0.63	1/2175 (0.0%)
1	A3	0.76	0/1597	0.63	1/2175 (0.0%)
1	A4	0.76	0/1597	0.63	1/2175 (0.0%)
1	A5	0.76	0/1597	0.63	1/2175 (0.0%)
1	A6	0.76	0/1597	0.63	1/2175 (0.0%)
1	A7	0.76	0/1597	0.63	1/2175 (0.0%)
1	A8	0.76	0/1597	0.63	1/2175 (0.0%)
1	A9	0.76	0/1597	0.63	1/2175 (0.0%)
1	AA	0.76	0/1597	0.63	1/2175 (0.0%)
1	AB	0.76	0/1597	0.63	1/2175 (0.0%)
1	AC	0.76	0/1597	0.63	1/2175 (0.0%)
1	AD	0.76	0/1597	0.63	1/2175 (0.0%)
1	AE	0.76	0/1597	0.63	1/2175 (0.0%)
1	AF	0.76	0/1597	0.63	1/2175 (0.0%)
1	AG	0.76	0/1597	0.63	1/2175 (0.0%)
1	AH	0.76	0/1597	0.63	1/2175 (0.0%)
1	AI	0.76	0/1597	0.63	1/2175 (0.0%)
1	AJ	0.76	0/1597	0.63	1/2175 (0.0%)
1	AK	0.76	0/1597	0.63	1/2175 (0.0%)
1	AL	0.76	0/1597	0.63	1/2175 (0.0%)
1	AM	0.76	0/1597	0.63	1/2175 (0.0%)
1	AN	0.76	0/1597	0.63	1/2175 (0.0%)
1	AO	0.76	0/1597	0.63	1/2175 (0.0%)
1	AP	0.76	0/1597	0.63	1/2175 (0.0%)
1	AQ	0.76	0/1597	0.63	1/2175 (0.0%)
1	AR	0.76	0/1597	0.63	1/2175 (0.0%)
1	AS	0.76	0/1597	0.63	1/2175 (0.0%)
1	AT	0.76	0/1597	0.63	1/2175 (0.0%)
1	AU	0.76	0/1597	0.63	1/2175 (0.0%)
1	AV	0.76	0/1597	0.63	1/2175 (0.0%)
1	AW	0.76	0/1597	0.63	1/2175 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	AX	0.76	0/1597	0.63	1/2175 (0.0%)
1	AY	0.76	0/1597	0.63	1/2175 (0.0%)
1	AZ	0.76	0/1597	0.63	1/2175 (0.0%)
1	Aa	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ab	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ac	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ad	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ae	0.76	0/1597	0.63	1/2175 (0.0%)
1	Af	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ag	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ah	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ai	0.76	0/1597	0.63	1/2175 (0.0%)
1	Aj	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ak	0.76	0/1597	0.63	1/2175 (0.0%)
1	Al	0.76	0/1597	0.63	1/2175 (0.0%)
1	Am	0.76	0/1597	0.63	1/2175 (0.0%)
1	An	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ao	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ap	0.76	0/1597	0.63	1/2175 (0.0%)
1	Aq	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ar	0.76	0/1597	0.63	1/2175 (0.0%)
1	As	0.76	0/1597	0.63	1/2175 (0.0%)
1	At	0.76	0/1597	0.63	1/2175 (0.0%)
1	Au	0.76	0/1597	0.63	1/2175 (0.0%)
1	Av	0.76	0/1597	0.63	1/2175 (0.0%)
1	Aw	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ax	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ay	0.76	0/1597	0.63	1/2175 (0.0%)
All	All	0.76	0/95820	0.63	59/130500 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AN	0	1

There are no bond length outliers.

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AD	159	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	AI	159	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	AV	159	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	A3	159	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	Ak	159	ARG	NE-CZ-NH2	6.14	123.37	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AN	186	ARG	Sidechain

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	A1	1550	1503	1503	22	0
1	A2	1550	1503	1503	12	0
1	A3	1550	1503	1503	9	0
1	A4	1550	1503	1503	7	0
1	A5	1550	1503	1503	14	0
1	A6	1550	1503	1503	8	0
1	A7	1550	1503	1503	9	0
1	A8	1550	1503	1503	13	0
1	A9	1550	1503	1503	8	0
1	AA	1550	1503	1503	11	0
1	AB	1550	1503	1503	8	0
1	AC	1550	1503	1503	10	0
1	AD	1550	1503	1503	22	0
1	AE	1550	1503	1503	11	0
1	AF	1550	1503	1503	10	0
1	AG	1550	1503	1503	11	0
1	AH	1550	1503	1503	11	0
1	AI	1550	1503	1503	14	0
1	AJ	1550	1503	1503	11	0
1	AK	1550	1503	1503	14	0
1	AL	1550	1503	1503	14	0
1	AM	1550	1503	1503	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AN	1550	1503	1503	10	0
1	AO	1550	1503	1503	10	0
1	AP	1550	1503	1503	12	0
1	AQ	1550	1503	1503	12	0
1	AR	1550	1503	1503	12	0
1	AS	1550	1503	1503	8	0
1	AT	1550	1503	1503	9	0
1	AU	1550	1503	1503	9	0
1	AV	1550	1503	1503	16	0
1	AW	1550	1503	1503	11	0
1	AX	1550	1503	1503	10	0
1	AY	1550	1503	1503	14	0
1	AZ	1550	1503	1503	8	0
1	Aa	1550	1503	1503	0	0
1	Ab	1550	1503	1503	0	0
1	Ac	1550	1503	1503	0	0
1	Ad	1550	1503	1503	0	0
1	Ae	1550	1503	1503	0	0
1	Af	1550	1503	1503	0	0
1	Ag	1550	1503	1503	0	0
1	Ah	1550	1503	1503	0	0
1	Ai	1550	1503	1503	0	0
1	Aj	1550	1503	1503	0	0
1	Ak	1550	1503	1503	0	0
1	Al	1550	1503	1503	0	0
1	Am	1550	1503	1503	0	0
1	An	1550	1503	1503	0	0
1	Ao	1550	1503	1503	0	0
1	Ap	1550	1503	1503	0	0
1	Aq	1550	1503	1503	0	0
1	Ar	1550	1503	1503	0	0
1	As	1550	1503	1503	0	0
1	At	1550	1503	1503	0	0
1	Au	1550	1503	1503	0	0
1	Av	1550	1503	1503	0	0
1	Aw	1550	1503	1503	0	0
1	Ax	1550	1503	1503	0	0
1	Ay	1550	1503	1503	0	0
2	A1	58	0	27	1	0
3	A1	32	0	10	0	0
All	All	93090	90180	90217	346	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 2.

The worst 5 of 346 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:A1:186:ARG:HH12	1:AA:128:ASN:HB2	1.42	0.84
1:A1:71:MET:HG3	1:A1:73:ARG:HH21	1.43	0.83
1:A1:98:ILE:HD12	1:A1:195:HIS:CD2	2.18	0.78
1:AJ:80:LEU:O	1:AJ:89:ARG:NH1	2.22	0.73
1:AN:80:LEU:O	1:AN:89:ARG:NH1	2.22	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	A1	187/233 (80%)	177 (95%)	10 (5%)	0	100	100
1	A2	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	A3	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	A4	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	A5	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	A6	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	A7	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	A8	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	A9	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AA	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AB	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	AC	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AD	187/233 (80%)	181 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AE	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AF	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AG	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AH	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AI	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AJ	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AK	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AL	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	AM	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	AN	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AO	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AP	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	AQ	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AR	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	AS	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	AT	187/233 (80%)	179 (96%)	8 (4%)	0	100	100
1	AU	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AV	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AW	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AX	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AY	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AZ	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Aa	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ab	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ac	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ad	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ae	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Af	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Ag	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Ah	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ai	187/233 (80%)	180 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aj	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Ak	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Al	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Am	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	An	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ao	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ap	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Aq	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ar	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	As	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	At	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Au	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Av	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Aw	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ax	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ay	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
All	All	11220/13980 (80%)	10838 (97%)	382 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	A1	172/215 (80%)	171 (99%)	1 (1%)	87	95
1	A2	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	A3	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	A4	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	A5	172/215 (80%)	165 (96%)	7 (4%)	33	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A6	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	A7	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	A8	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	A9	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AA	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AB	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AC	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AD	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AE	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AF	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AG	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AH	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AI	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AJ	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AK	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AL	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AM	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AN	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AO	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AP	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AQ	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AR	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AS	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AT	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AU	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AV	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AW	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AX	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AY	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	AZ	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Aa	172/215 (80%)	165 (96%)	7 (4%)	33	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ab	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Ac	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Ad	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Ae	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Af	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Ag	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Ah	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Ai	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Aj	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Ak	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Al	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Am	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	An	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Ao	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Ap	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Aq	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Ar	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	As	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	At	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Au	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Av	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Aw	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Ax	172/215 (80%)	165 (96%)	7 (4%)	33	67
1	Ay	172/215 (80%)	165 (96%)	7 (4%)	33	67
All	All	10320/12900 (80%)	9906 (96%)	414 (4%)	38	67

5 of 414 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AS	167	LEU
1	AY	231	LEU
1	Au	126	ASP
1	AT	73	ARG
1	AV	231	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	AP	212	ASN
1	AX	212	ASN
1	Au	212	ASN
1	AQ	212	ASN
1	AT	212	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	SGN	A1	301	3	19,20,20	3.64	6 (31%)	24,31,31	2.55	6 (25%)
3	IDS	A1	302	2	13,16,17	1.23	1 (7%)	15,24,26	0.96	0
2	SGN	A1	303	3	18,19,20	3.68	5 (27%)	22,29,31	1.47	4 (18%)
3	IDS	A1	304	2	13,16,17	1.26	1 (7%)	15,24,26	1.10	0
2	SGN	A1	305	3	18,19,20	3.70	5 (27%)	22,29,31	1.73	5 (22%)

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	SGN	A1	301	3	-	5/11/31/31	0/1/1/1
3	IDS	A1	302	2	-	0/5/26/29	0/1/1/1
2	SGN	A1	303	3	-	4/11/28/31	0/1/1/1
3	IDS	A1	304	2	-	5/5/26/29	0/1/1/1
2	SGN	A1	305	3	-	5/11/28/31	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A1	303	SGN	S1-N	14.31	1.79	1.59
2	A1	305	SGN	S1-N	14.31	1.79	1.59
2	A1	301	SGN	S1-N	14.24	1.79	1.59
2	A1	301	SGN	O1S-S1	3.32	1.45	1.42
2	A1	305	SGN	O2S-S1	3.08	1.45	1.42

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A1	301	SGN	O1-C1-C2	-10.28	87.87	109.22
2	A1	305	SGN	O2S-S1-O1S	-3.76	110.57	120.11
2	A1	305	SGN	O2S-S1-N	-3.08	103.16	108.91
2	A1	301	SGN	O2S-S1-N	-3.02	103.28	108.91
2	A1	305	SGN	O1S-S1-N	-2.96	103.38	108.91

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

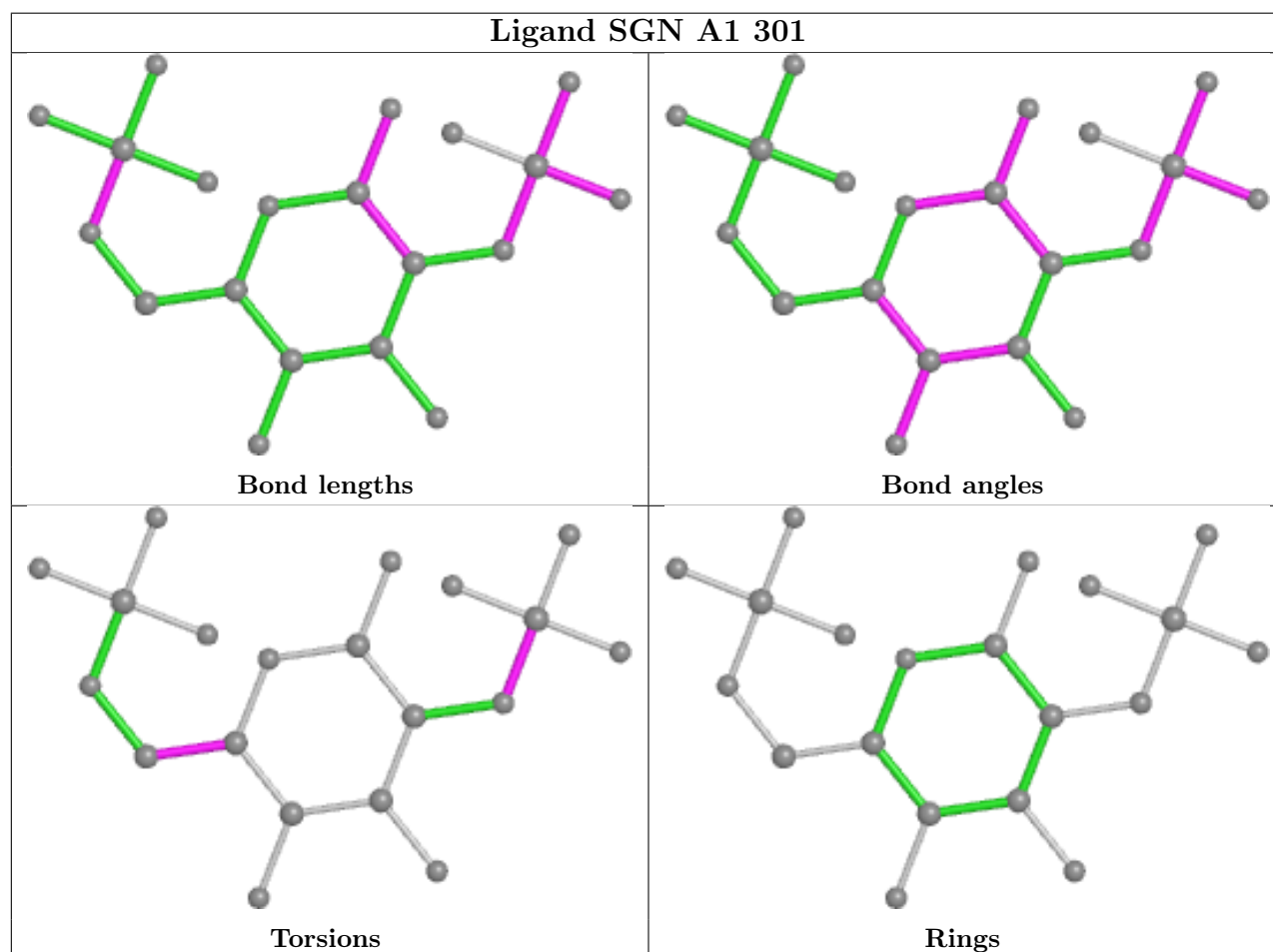
Mol	Chain	Res	Type	Atoms
2	A1	303	SGN	C2-N-S1-O3S
2	A1	305	SGN	C2-N-S1-O1S
2	A1	305	SGN	C2-N-S1-O2S
2	A1	305	SGN	C2-N-S1-O3S
2	A1	301	SGN	C4-C5-C6-O6

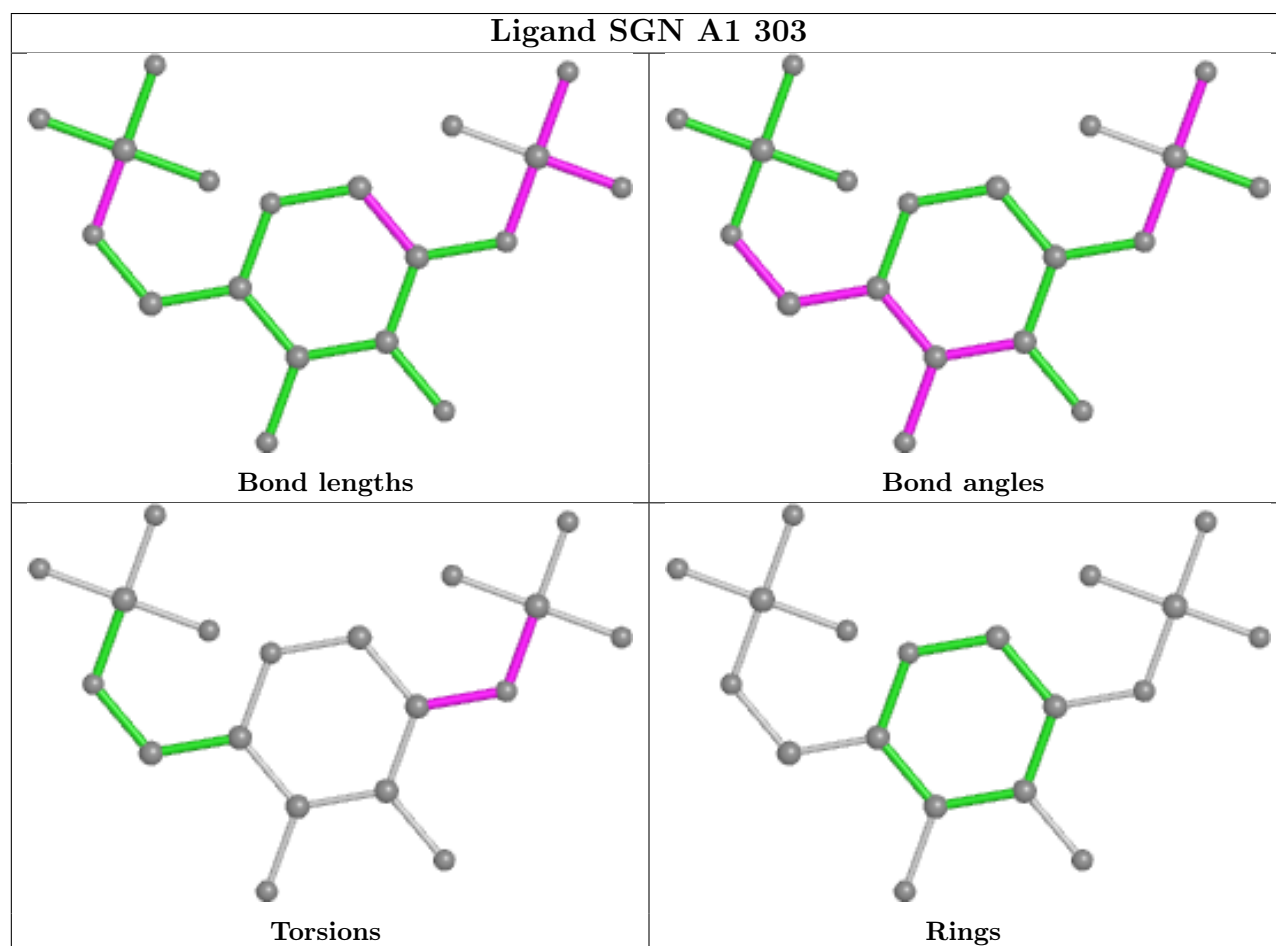
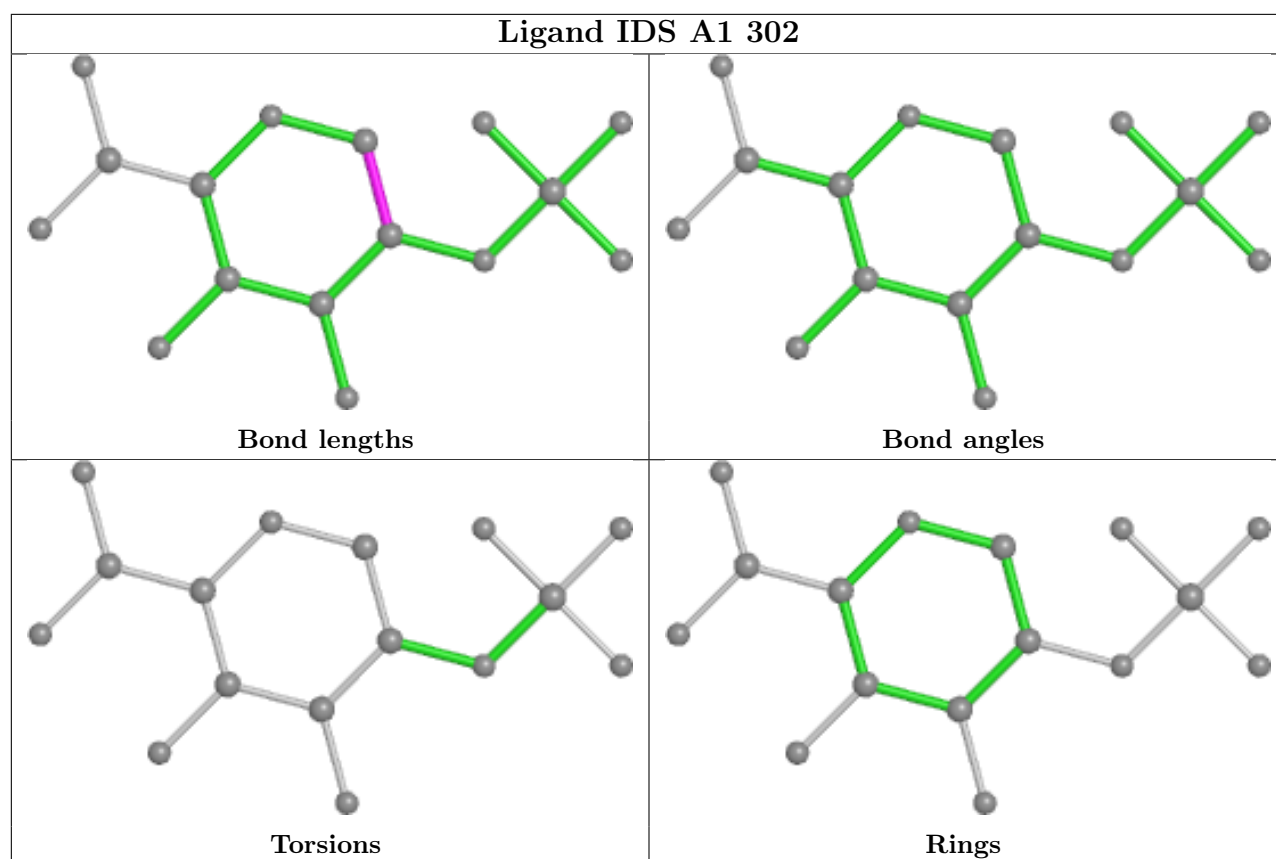
There are no ring outliers.

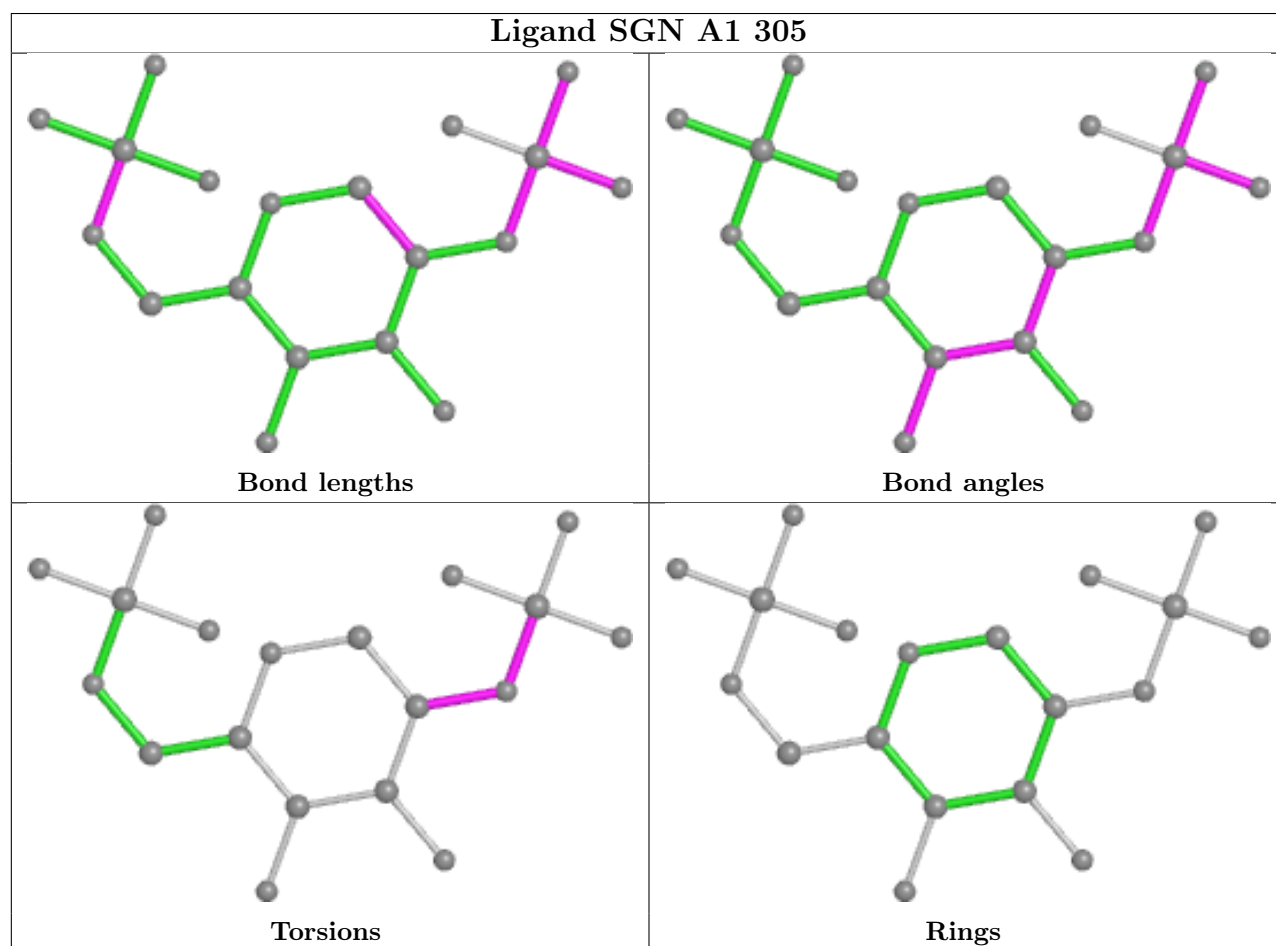
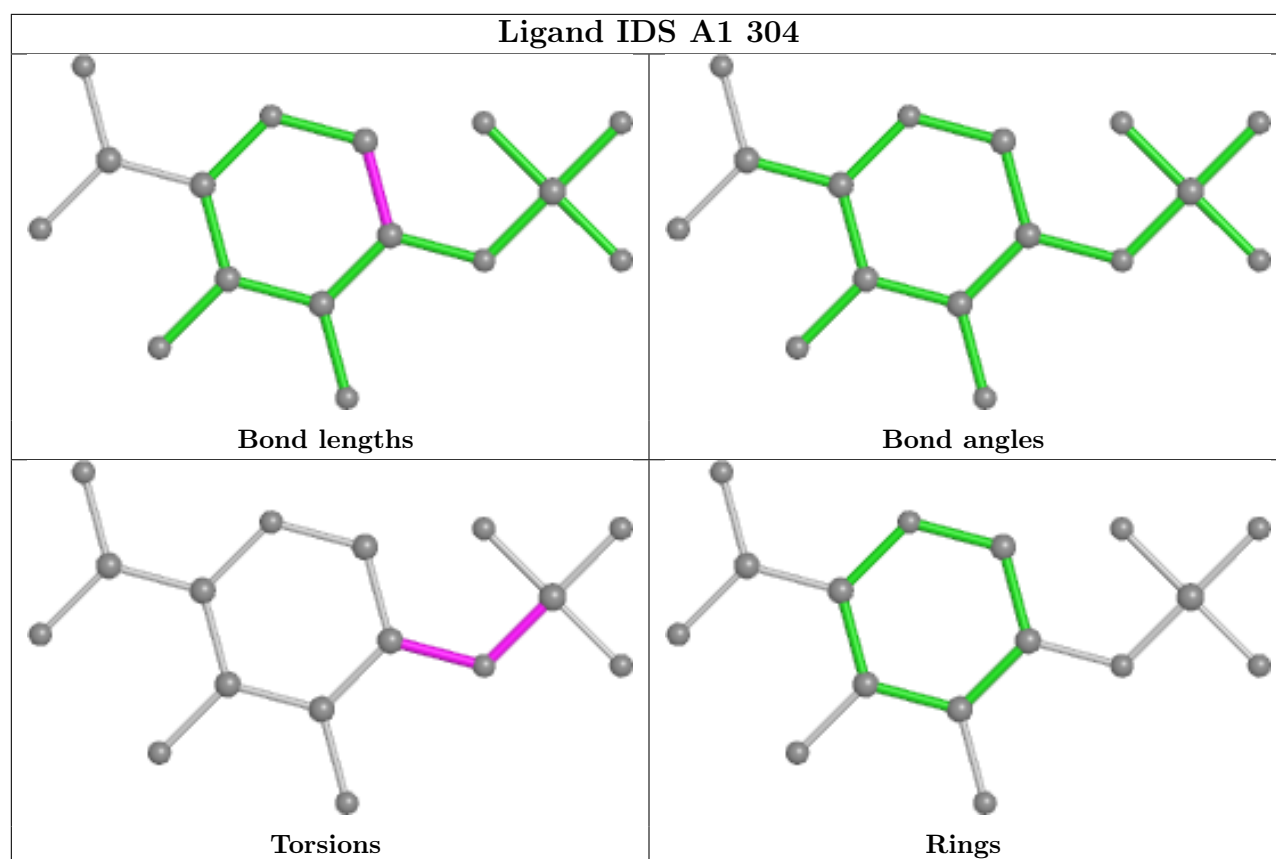
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A1	305	SGN	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.