



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:01 PM BST

PDB ID : 6RV2  
Title : Crystal structure of the human two pore domain potassium ion channel TASK-1 (K2P3.1) in a closed conformation  
Authors : Rodstrom, K.E.J.; Pike, A.C.W.; Zhang, W.; Quigley, A.; Speedman, D.; Mukhopadhyay, S.M.M.; Shrestha, L.; Chalk, R.; Venkaya, S.; Bushell, S.R.; Tessitore, A.; Burgess-Brown, N.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Carpenter, E.P.; Structural Genomics Consortium (SGC)  
Deposited on : 2019-05-30  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

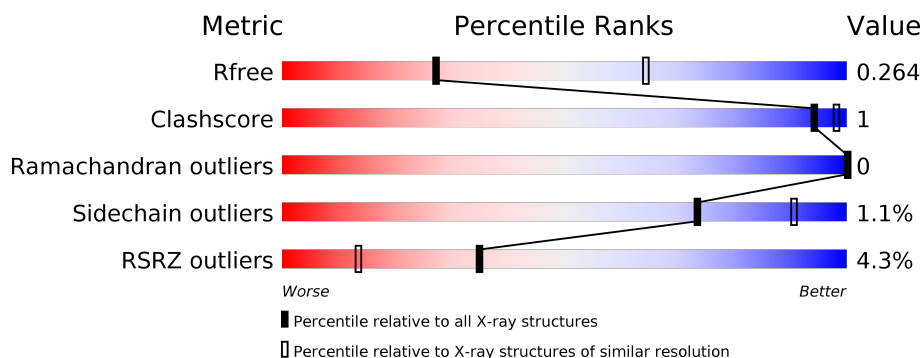
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	264	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> <div></div> </div>
1	B	264	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> <div></div> </div>
1	C	264	<div> <div>8%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> <div></div> </div>
1	D	264	<div> <div>5%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> <div></div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8466 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 Potassium channel subfamily K member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1987	1300	325	350	12			
1	B	258	Total	C	N	O	S	0	0	0
			2019	1317	333	357	12			
1	C	257	Total	C	N	O	S	0	0	0
			1999	1311	325	350	13			
1	D	261	Total	C	N	O	S	0	0	0
			2004	1309	328	355	12			

There are 20 discrepancies between the modelled and reference sequences:

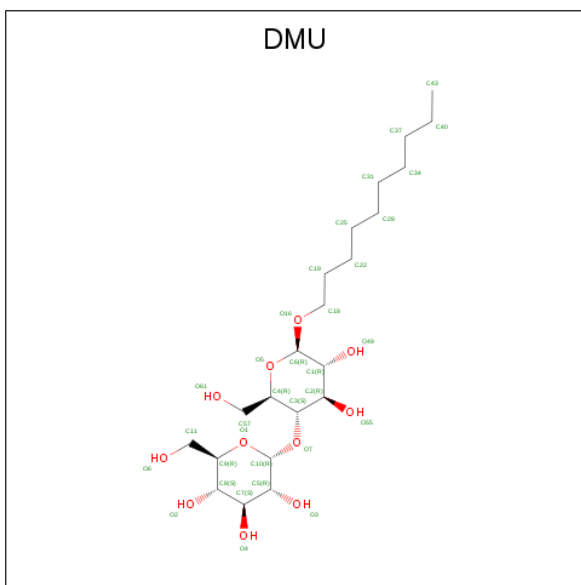
Chain	Residue	Modelled	Actual	Comment	Reference
A	260	ASN	-	expression tag	UNP O14649
A	261	LEU	-	expression tag	UNP O14649
A	262	TYR	-	expression tag	UNP O14649
A	263	PHE	-	expression tag	UNP O14649
A	264	GLN	-	expression tag	UNP O14649
B	260	ASN	-	expression tag	UNP O14649
B	261	LEU	-	expression tag	UNP O14649
B	262	TYR	-	expression tag	UNP O14649
B	263	PHE	-	expression tag	UNP O14649
B	264	GLN	-	expression tag	UNP O14649
C	260	ASN	-	expression tag	UNP O14649
C	261	LEU	-	expression tag	UNP O14649
C	262	TYR	-	expression tag	UNP O14649
C	263	PHE	-	expression tag	UNP O14649
C	264	GLN	-	expression tag	UNP O14649
D	260	ASN	-	expression tag	UNP O14649
D	261	LEU	-	expression tag	UNP O14649
D	262	TYR	-	expression tag	UNP O14649
D	263	PHE	-	expression tag	UNP O14649
D	264	GLN	-	expression tag	UNP O14649

- | Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 2   | A     | 4        | Total K<br>4 4 | 0       | 0       |
| 2   | C     | 4        | Total K<br>4 4 | 0       | 0       |

- # Y01

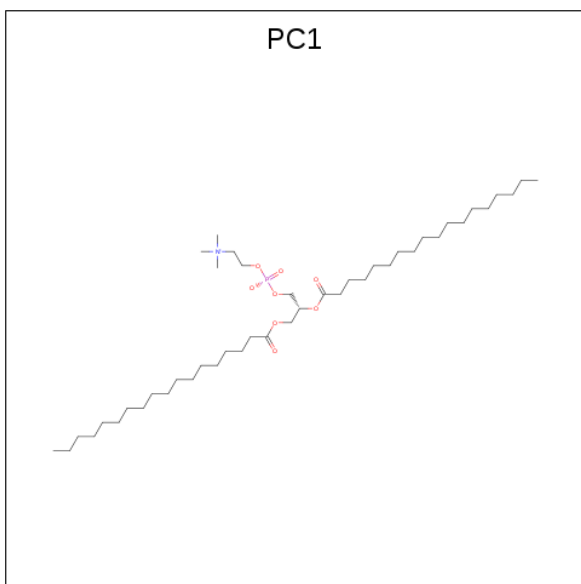
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 35	C 31	O 4	0	0
3	A	1	Total 35	C 31	O 4	0	0
3	A	1	Total 35	C 31	O 4	0	0
3	B	1	Total 35	C 31	O 4	0	0
3	C	1	Total 35	C 31	O 4	0	0
3	D	1	Total 35	C 31	O 4	0	0
3	D	1	Total 35	C 31	O 4	0	0

- 
- WORLD WIDE  
PDB  
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	16	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			22	16	6		

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			32	28	4		
5	B	1	Total	C	O	0	0
			18	16	2		
5	D	1	Total	C	O	0	0
			38	34	4		
5	D	1	Total	C	O	0	0
			21	19	2		

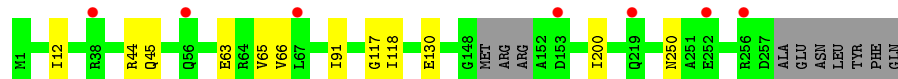
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	6	Total	O	0	0
			6	6		
6	C	12	Total	O	0	0
			12	12		
6	D	4	Total	O	0	0
			4	4		

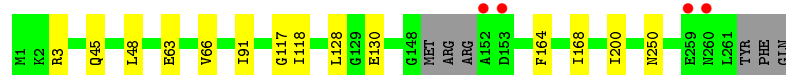
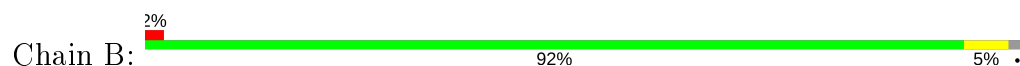
### 3 Residue-property plots [i](#)

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: Potassium channel subfamily K member 3



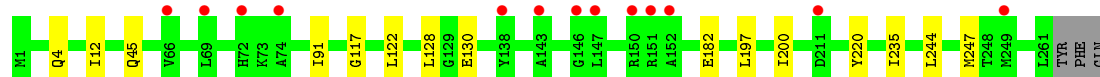
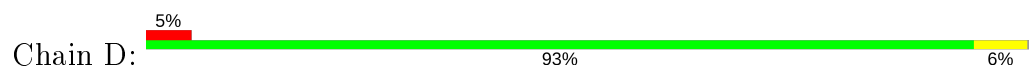
- Molecule 1: Potassium channel subfamily K member 3



- Molecule 1: Potassium channel subfamily K member 3



- Molecule 1: Potassium channel subfamily K member 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.14Å 204.79Å 238.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.04 – 3.00 47.04 – 3.00	Depositor EDS
% Data completeness (in resolution range)	79.7 (47.04-3.00) 79.7 (47.04-3.00)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.253 , 0.257 0.263 , 0.264	Depositor DCC
$R_{free}$ test set	1756 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	8466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	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 20.70 % 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 8.2129e-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: K, Y01, DMU, PC1

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	0.43	0/2031	0.58	0/2754
1	B	0.43	0/2064	0.58	0/2798
1	C	0.41	0/2045	0.57	0/2774
1	D	0.41	0/2048	0.57	0/2783
All	All	0.42	0/8188	0.57	0/11109

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	1987	0	1966	9	0
1	B	2019	0	1993	10	0
1	C	1999	0	1970	8	0
1	D	2004	0	1948	9	0
2	A	4	0	0	0	0
2	C	4	0	0	0	0
3	A	105	0	147	0	0
3	B	35	0	49	0	0
3	C	35	0	49	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	70	0	98	0	0
4	A	22	0	31	0	0
4	B	20	0	24	0	0
4	C	22	0	31	0	0
5	A	32	0	45	0	0
5	B	18	0	26	0	0
5	D	59	0	95	0	0
6	A	9	0	0	0	0
6	B	6	0	0	0	0
6	C	12	0	0	0	0
6	D	4	0	0	0	0
All	All	8466	0	8472	22	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 1.

All (22) 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:A:250:ASN:HD22	1:B:130:GLU:HB3	1.71	0.56
1:A:12:ILE:HD11	1:B:128:LEU:HD13	1.93	0.51
1:A:66:VAL:HG13	1:B:63:GLU:HG3	1.96	0.48
1:A:63:GLU:HG3	1:B:66:VAL:HG13	1.95	0.48
1:C:247:MET:HE1	1:D:122:LEU:HB3	1.97	0.46
1:C:250:ASN:HD22	1:D:130:GLU:HB3	1.80	0.45
1:A:200:ILE:HD11	1:B:118:ILE:HD11	1.97	0.45
1:D:197:LEU:HB3	1:D:235:ILE:HG13	1.97	0.45
1:A:118:ILE:HD11	1:B:200:ILE:HD11	1.99	0.45
1:A:130:GLU:HB3	1:B:250:ASN:HD22	1.83	0.44
1:D:182:GLU:HG2	1:D:220:TYR:OH	2.17	0.44
1:A:91:ILE:HG22	1:A:117:GLY:HA3	1.99	0.44
1:B:91:ILE:HG22	1:B:117:GLY:HA3	2.01	0.43
1:C:118:ILE:HD11	1:D:200:ILE:HD11	2.00	0.43
1:C:91:ILE:HG22	1:C:117:GLY:HA3	2.01	0.42
1:C:12:ILE:HD11	1:D:128:LEU:HD13	2.02	0.42
1:A:65:VAL:HG21	1:B:48:LEU:HD12	2.02	0.42
1:C:122:LEU:HB3	1:D:247:MET:HE1	2.01	0.42
1:C:164:PHE:CE2	1:C:168:ILE:HD11	2.54	0.41
1:D:91:ILE:HG22	1:D:117:GLY:HA3	2.02	0.41
1:C:128:LEU:HD13	1:D:12:ILE:HD11	2.02	0.41
1:B:164:PHE:CE2	1:B:168:ILE:HD11	2.56	0.40

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 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	250/264 (95%)	245 (98%)	5 (2%)	0	100	100
1	B	254/264 (96%)	248 (98%)	6 (2%)	0	100	100
1	C	255/264 (97%)	249 (98%)	6 (2%)	0	100	100
1	D	259/264 (98%)	253 (98%)	6 (2%)	0	100	100
All	All	1018/1056 (96%)	995 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	201/221 (91%)	199 (99%)	2 (1%)	76	91
1	B	205/221 (93%)	203 (99%)	2 (1%)	76	91
1	C	200/221 (90%)	198 (99%)	2 (1%)	76	91
1	D	196/221 (89%)	193 (98%)	3 (2%)	65	87
All	All	802/884 (91%)	793 (99%)	9 (1%)	73	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	45	GLN
1	B	3	ARG
1	B	45	GLN
1	C	45	GLN
1	C	244	LEU
1	D	4	GLN
1	D	45	GLN
1	D	244	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	ASN
1	C	250	ASN
1	D	250	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 for Mogul analysis.

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	Y01	D	602	-	35,38,38	0.36	0	54,57,57	0.48	0
4	DMU	A	307	-	22,22,34	0.26	0	27,27,45	0.48	0
4	DMU	B	303	-	20,20,34	0.30	0	25,25,45	0.48	0
5	PC1	D	601	-	37,37,53	0.27	0	39,39,61	0.37	0
3	Y01	A	306	-	35,38,38	0.34	0	54,57,57	0.52	0
3	Y01	C	305	-	35,38,38	0.35	0	54,57,57	0.48	0
5	PC1	D	604	-	20,20,53	0.33	0	20,20,61	0.28	0
3	Y01	A	305	-	35,38,38	0.36	0	54,57,57	0.50	0
3	Y01	D	603	-	35,38,38	0.32	0	54,57,57	0.48	0
3	Y01	A	301	-	35,38,38	0.37	0	54,57,57	0.45	0
4	DMU	C	306	-	22,22,34	0.27	0	27,27,45	0.45	0
5	PC1	A	308	-	31,31,53	0.25	0	33,33,61	0.36	0
3	Y01	B	302	-	35,38,38	0.34	0	54,57,57	0.51	0
5	PC1	B	304	-	17,17,53	0.26	0	17,17,61	0.26	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	Y01	D	602	-	-	5/17/77/77	0/4/4/4
4	DMU	A	307	-	-	7/13/33/59	0/1/1/2
4	DMU	B	303	-	-	6/11/31/59	0/1/1/2
5	PC1	D	601	-	-	10/38/38/57	-
3	Y01	A	306	-	-	4/17/77/77	0/4/4/4
3	Y01	C	305	-	-	5/17/77/77	0/4/4/4
5	PC1	D	604	-	-	3/19/19/57	-
3	Y01	A	305	-	-	5/17/77/77	0/4/4/4
3	Y01	D	603	-	-	5/17/77/77	0/4/4/4
3	Y01	A	301	-	-	5/17/77/77	0/4/4/4
4	DMU	C	306	-	-	8/13/33/59	0/1/1/2
5	PC1	A	308	-	-	7/32/32/57	-
3	Y01	B	302	-	-	5/17/77/77	0/4/4/4
5	PC1	B	304	-	-	3/16/16/57	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	307	DMU	C1-C6-O16-C18
4	A	307	DMU	O5-C6-O16-C18
4	B	303	DMU	C1-C6-O16-C18
4	B	303	DMU	O5-C6-O16-C18
4	C	306	DMU	C1-C6-O16-C18
4	C	306	DMU	O5-C6-O16-C18
3	B	302	Y01	CAJ-CAO-CBB-CBE
3	D	602	Y01	CAJ-CAO-CBB-CBE
3	C	305	Y01	CAJ-CAO-CBB-CBE
3	A	305	Y01	CAJ-CAO-CBB-CBE
3	A	306	Y01	CAJ-CAO-CBB-CAC
3	B	302	Y01	CAJ-CAO-CBB-CAC
3	D	603	Y01	CAJ-CAO-CBB-CAC
3	A	306	Y01	CAJ-CAO-CBB-CBE
3	D	603	Y01	CAJ-CAO-CBB-CBE
3	A	301	Y01	CAJ-CAO-CBB-CBE
3	D	602	Y01	CAJ-CAO-CBB-CAC
3	C	305	Y01	CAJ-CAO-CBB-CAC
3	A	305	Y01	CAJ-CAO-CBB-CAC
3	D	602	Y01	CAN-CAJ-CAO-CBB
3	A	305	Y01	CAN-CAJ-CAO-CBB
3	C	305	Y01	CAN-CAJ-CAO-CBB
3	B	302	Y01	CAJ-CAN-CBA-CAA
4	B	303	DMU	C22-C25-C28-C31
3	A	301	Y01	CAN-CAJ-CAO-CBB
3	C	305	Y01	CAJ-CAN-CBA-CAA
3	A	301	Y01	CAJ-CAN-CBA-CAA
3	A	301	Y01	CAJ-CAO-CBB-CAC
3	D	602	Y01	CAJ-CAN-CBA-CAA
3	D	602	Y01	CAJ-CAN-CBA-CAB
3	A	305	Y01	CAJ-CAN-CBA-CAA
3	A	305	Y01	CAJ-CAN-CBA-CAB
3	C	305	Y01	CAJ-CAN-CBA-CAB
3	A	301	Y01	CAJ-CAN-CBA-CAB
4	C	306	DMU	C31-C34-C37-C40
5	B	304	PC1	C21-C22-C23-C24
4	C	306	DMU	O5-C4-C57-O61
5	D	601	PC1	C37-C38-C39-C3A
5	D	604	PC1	C27-C28-C29-C2A
3	B	302	Y01	CAJ-CAN-CBA-CAB
5	B	304	PC1	C23-C24-C25-C26
5	A	308	PC1	C31-C32-C33-C34

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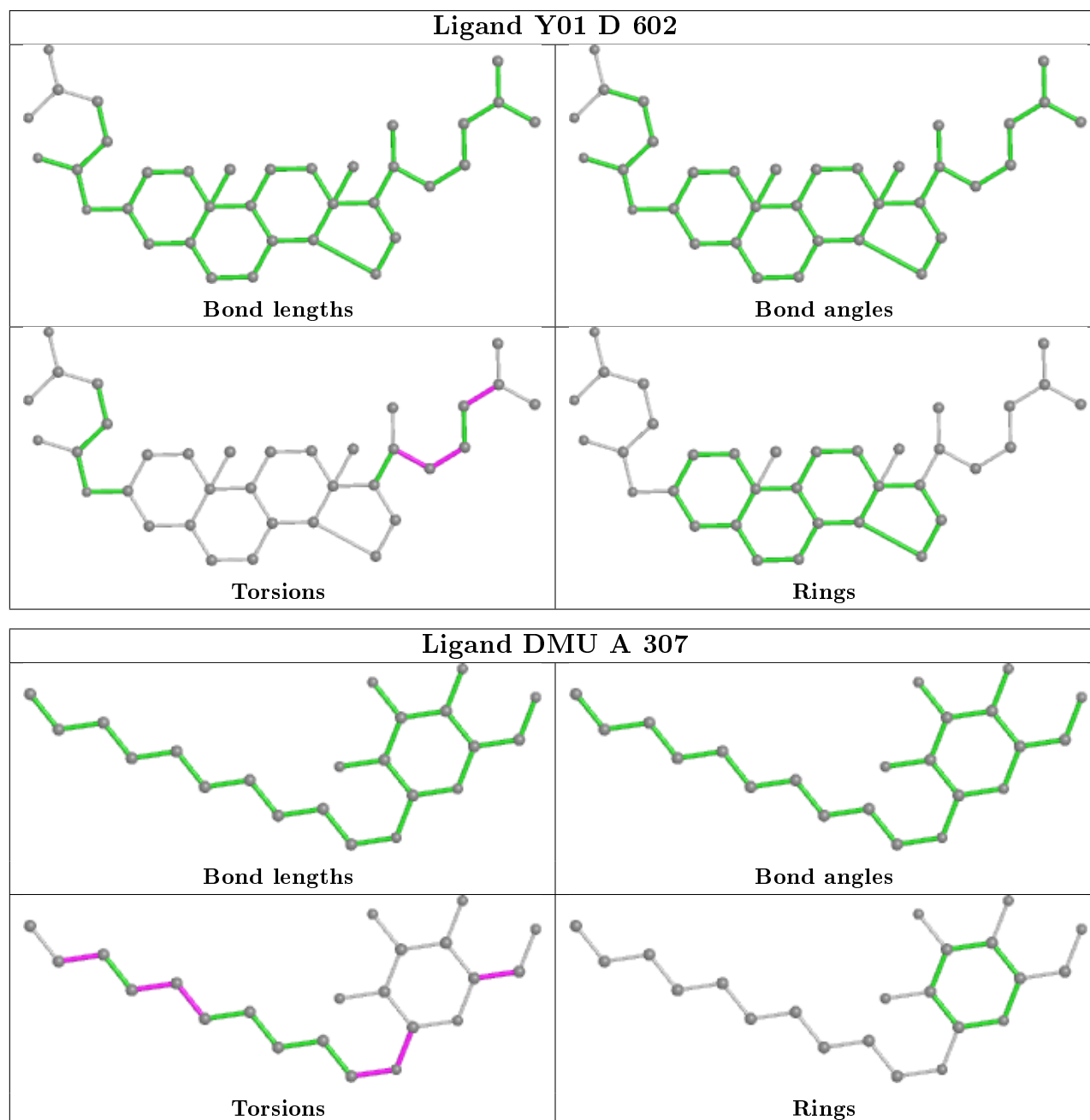
Mol	Chain	Res	Type	Atoms
5	D	601	PC1	C21-C22-C23-C24
4	A	307	DMU	O5-C4-C57-O61
4	B	303	DMU	O5-C4-C57-O61
5	B	304	PC1	C27-C28-C29-C2A
4	A	307	DMU	C28-C31-C34-C37
4	C	306	DMU	C28-C31-C34-C37
4	B	303	DMU	C28-C31-C34-C37
5	A	308	PC1	C37-C38-C39-C3A
4	A	307	DMU	C19-C18-O16-C6
4	B	303	DMU	C19-C18-O16-C6
4	C	306	DMU	C19-C18-O16-C6
5	D	601	PC1	C22-C23-C24-C25
5	A	308	PC1	C21-C22-C23-C24
5	A	308	PC1	C22-C23-C24-C25
5	D	604	PC1	C21-C22-C23-C24
5	D	601	PC1	C31-C32-C33-C34
5	D	601	PC1	C2A-C2B-C2C-C2D
3	D	603	Y01	CAJ-CAN-CBA-CAA
4	A	307	DMU	C34-C37-C40-C43
3	A	306	Y01	CAN-CAJ-CAO-CBB
5	A	308	PC1	C33-C34-C35-C36
4	C	306	DMU	C34-C37-C40-C43
5	D	604	PC1	C2D-C2E-C2F-C2G
5	D	601	PC1	C33-C34-C35-C36
5	D	601	PC1	C26-C27-C28-C29
3	D	603	Y01	CAN-CAJ-CAO-CBB
3	A	306	Y01	CAJ-CAN-CBA-CAB
5	D	601	PC1	C3D-C3E-C3F-C3G
3	B	302	Y01	CAN-CAJ-CAO-CBB
3	D	603	Y01	CAJ-CAN-CBA-CAB
4	C	306	DMU	C25-C28-C31-C34
4	A	307	DMU	C25-C28-C31-C34
5	A	308	PC1	C26-C27-C28-C29
5	D	601	PC1	O21-C21-C22-C23
5	A	308	PC1	O21-C21-C22-C23
5	D	601	PC1	O22-C21-C22-C23

There are no ring outliers.

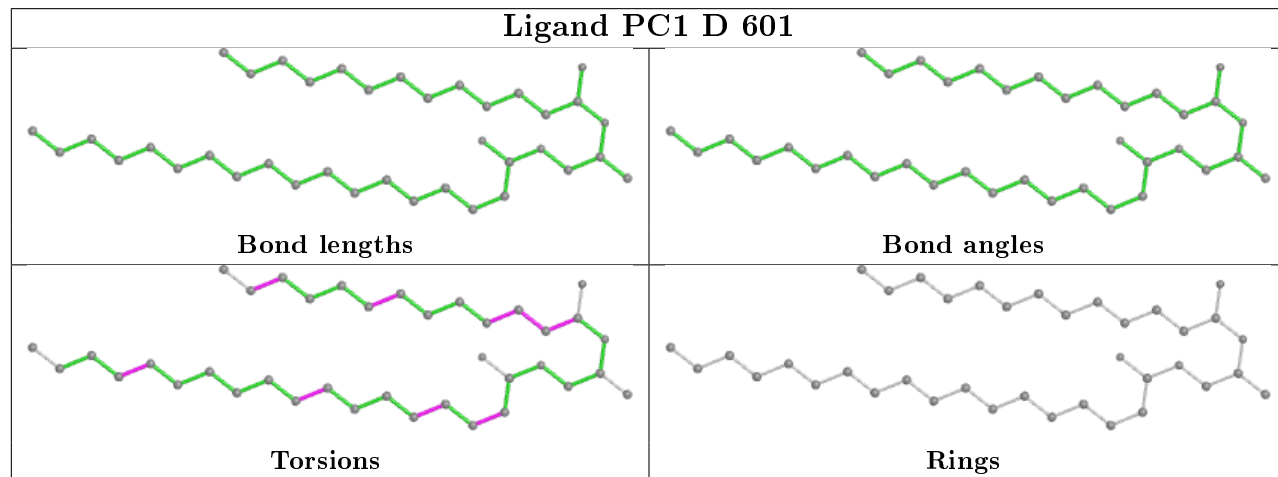
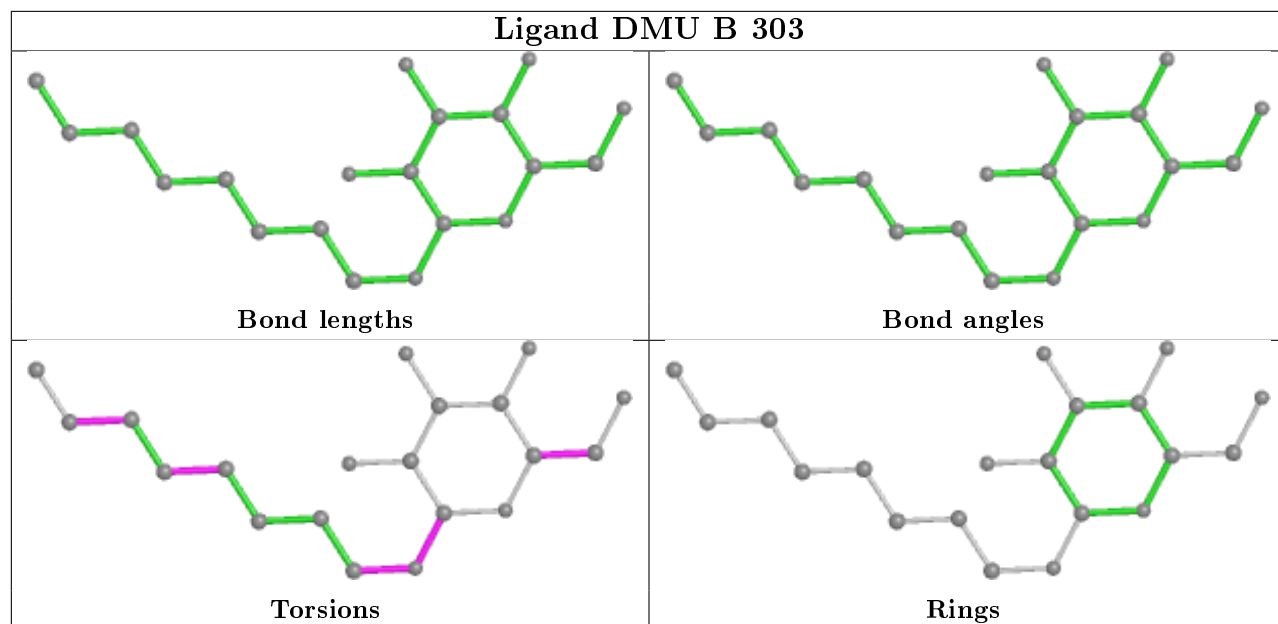
No monomer is involved in short contacts.

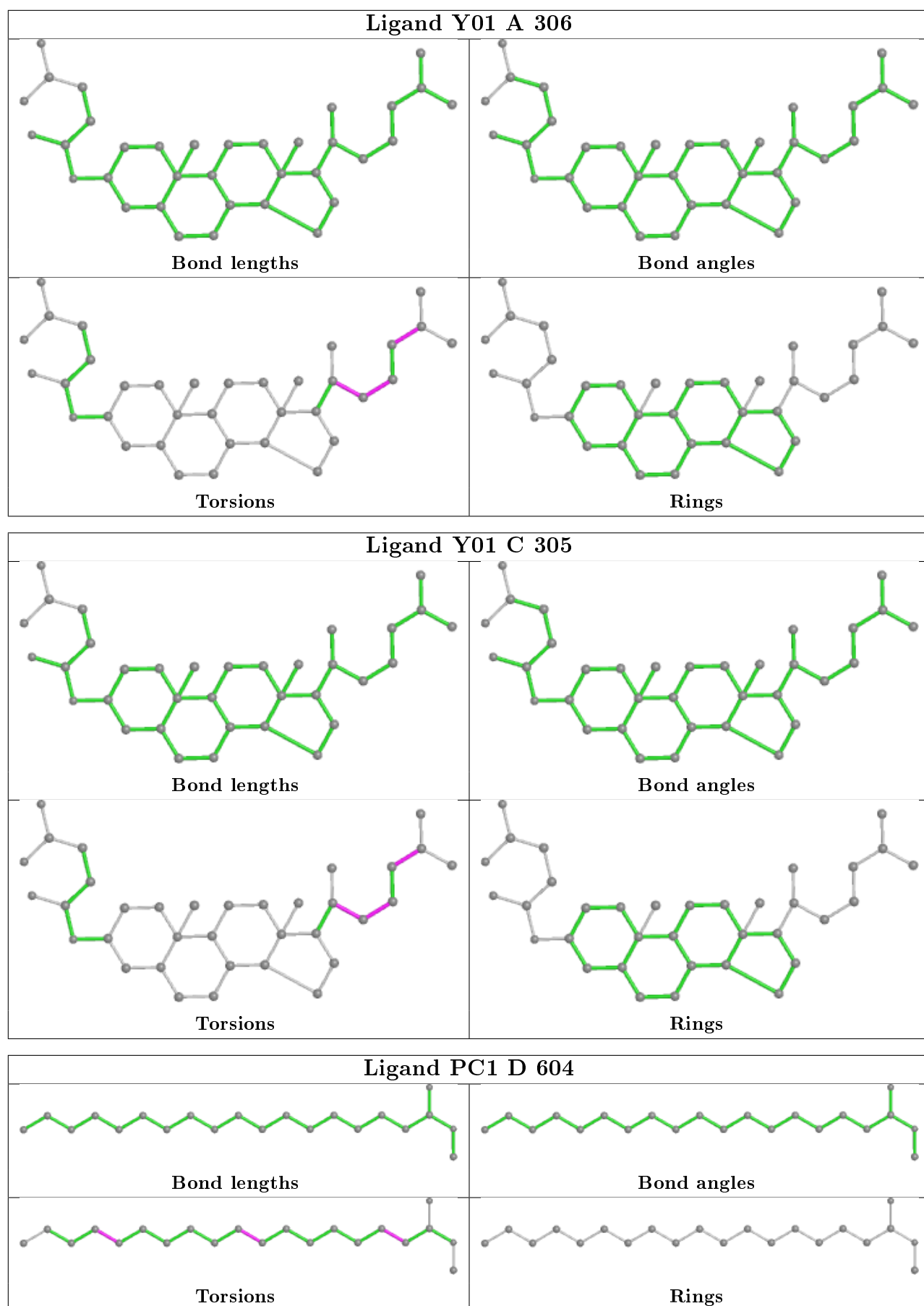
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

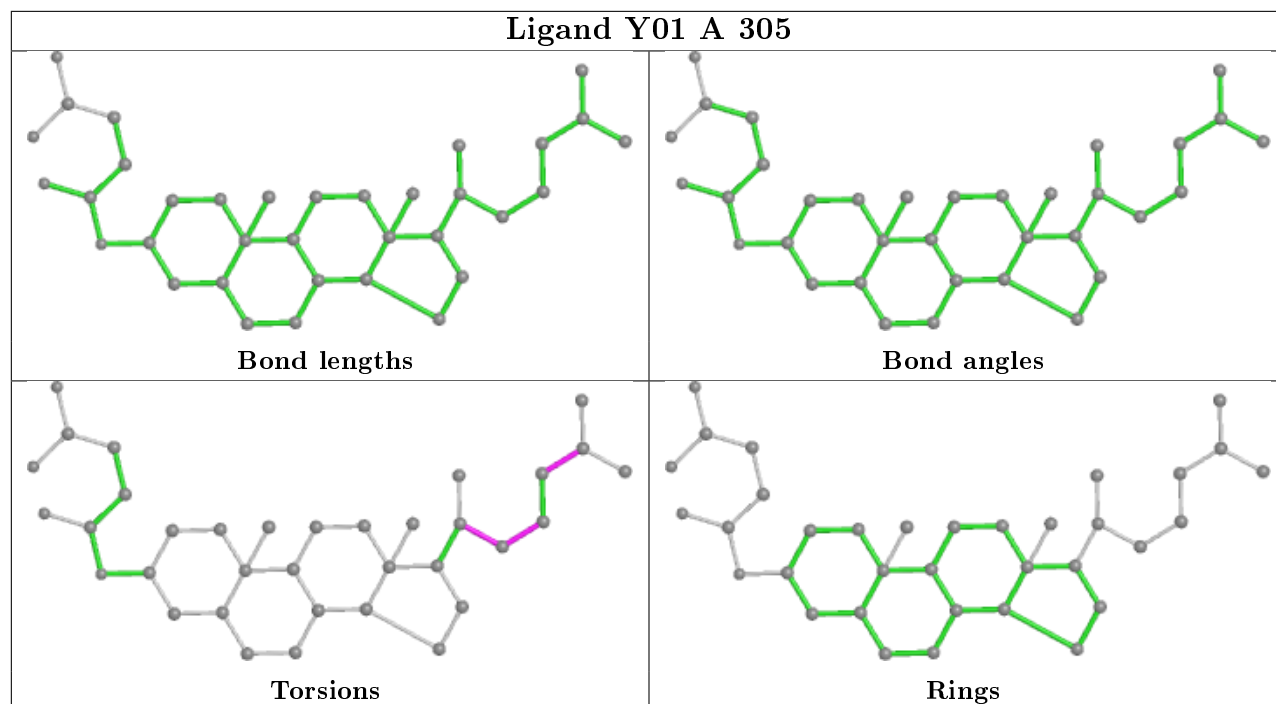




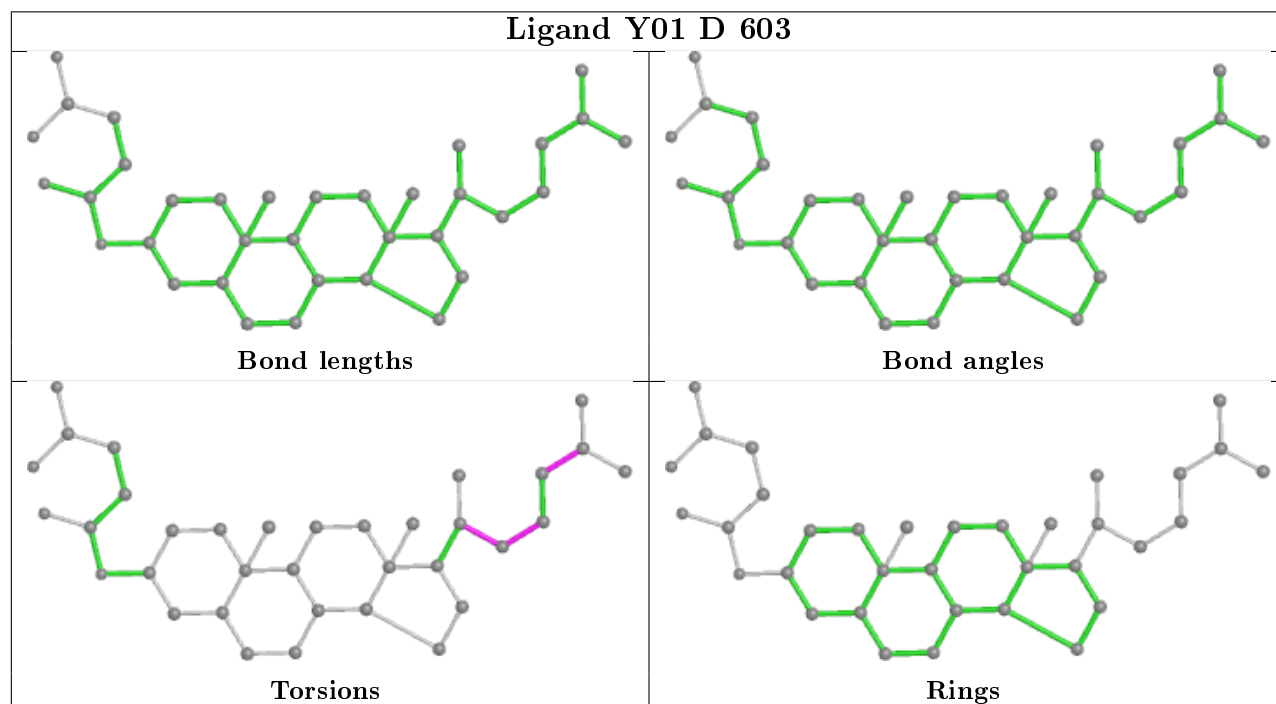




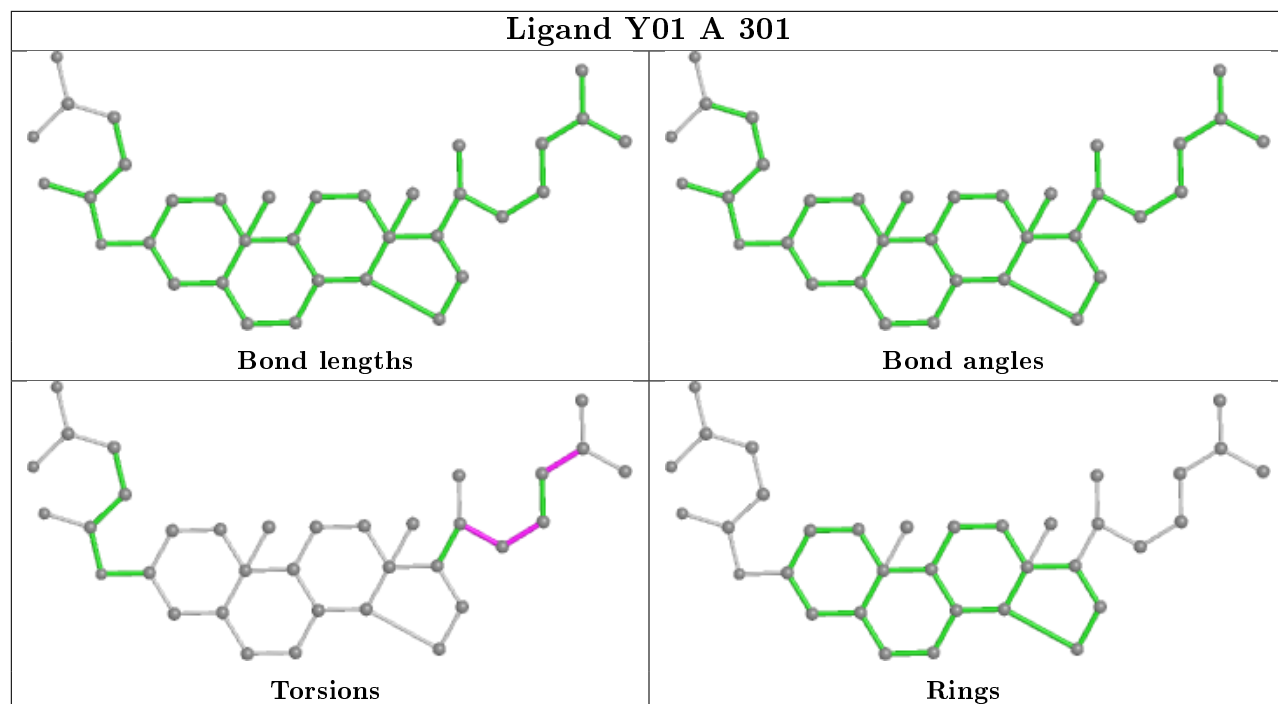
## Ligand Y01 A 305



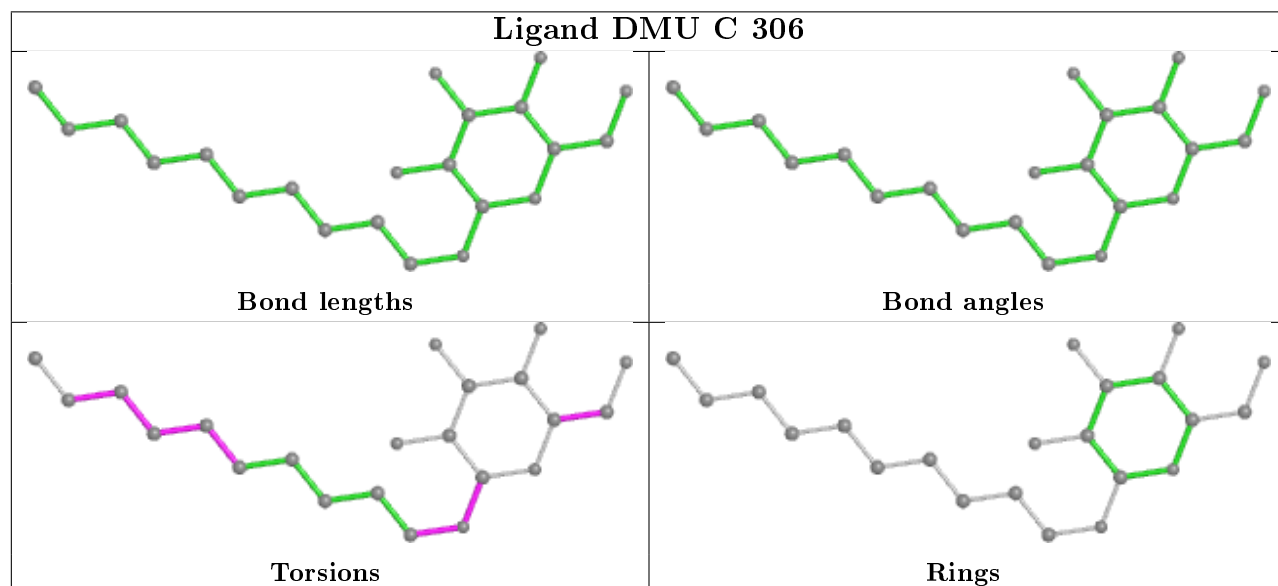
## Ligand Y01 D 603

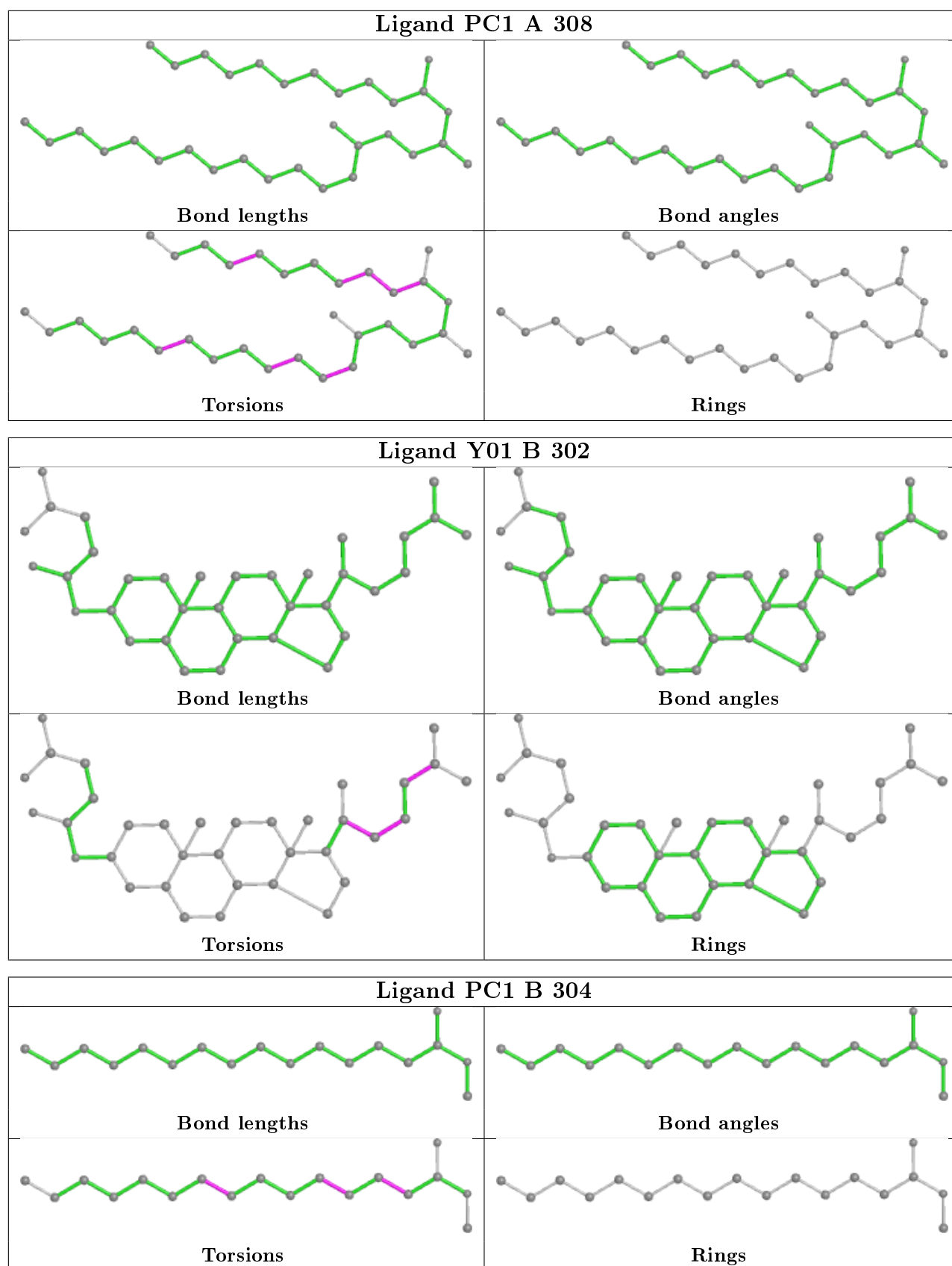


## Ligand Y01 A 301



## Ligand DMU C 306





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	254/264 (96%)	-0.15	7 (2%)	53 25	30, 56, 107, 141	0
1	B	258/264 (97%)	-0.23	4 (1%)	72 44	31, 59, 104, 145	0
1	C	257/264 (97%)	0.09	20 (7%)	13 4	38, 61, 102, 119	0
1	D	261/264 (98%)	-0.01	13 (4%)	28 10	38, 61, 110, 125	0
All	All	1030/1056 (97%)	-0.08	44 (4%)	35 13	30, 59, 107, 145	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	150	ARG	5.4
1	D	151	ARG	4.6
1	D	152	ALA	4.6
1	A	219	GLN	4.5
1	C	38	ARG	4.3
1	C	59	TYR	4.2
1	C	6	VAL	3.8
1	C	4	GLN	3.7
1	D	211	ASP	3.4
1	C	253	ASP	3.3
1	B	259	GLU	3.3
1	B	152	ALA	3.1
1	B	260	ASN	3.1
1	C	5	ASN	3.1
1	C	39	GLN	3.1
1	A	252	GLU	3.0
1	A	38	ARG	3.0
1	C	36	ILE	2.8
1	B	153	ASP	2.8
1	D	74	ALA	2.7
1	C	257	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	256	ARG	2.7
1	A	153	ASP	2.6
1	A	56	GLN	2.6
1	C	41	LEU	2.6
1	D	138	TYR	2.5
1	C	1	MET	2.5
1	D	72	HIS	2.4
1	D	146	GLY	2.4
1	C	40	ARG	2.4
1	C	42	GLU	2.3
1	C	48	LEU	2.3
1	D	143	ALA	2.3
1	D	147	LEU	2.3
1	D	69	LEU	2.2
1	C	254	GLU	2.2
1	C	2	LYS	2.2
1	C	43	LEU	2.2
1	D	249	MET	2.2
1	C	256	ARG	2.1
1	C	67	LEU	2.1
1	C	3	ARG	2.1
1	A	67	LEU	2.0
1	D	66	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

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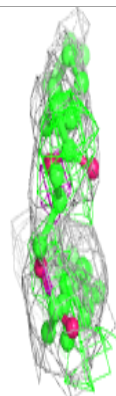
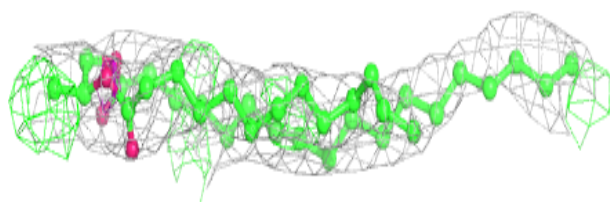
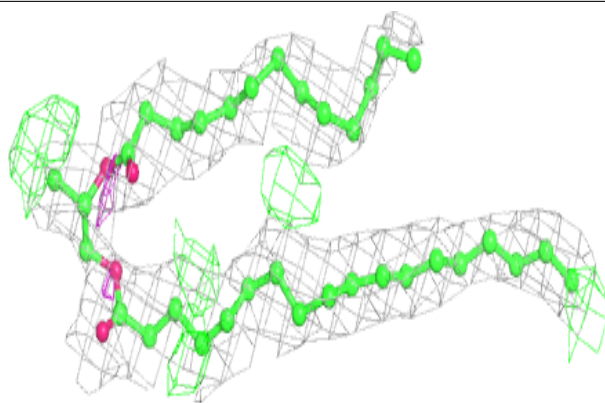
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PC1	D	601	38/54	0.71	0.32	56,64,79,80	0
5	PC1	A	308	32/54	0.72	0.33	59,75,94,95	0
5	PC1	D	604	21/54	0.73	0.30	39,56,68,68	0
4	DMU	B	303	20/33	0.74	0.28	126,134,136,137	0
5	PC1	B	304	18/54	0.77	0.36	74,79,90,90	0
3	Y01	C	305	35/35	0.83	0.27	51,58,72,73	0
4	DMU	A	307	22/33	0.85	0.18	144,155,156,156	0
3	Y01	D	603	35/35	0.85	0.53	83,88,95,96	0
3	Y01	A	306	35/35	0.86	0.55	86,89,95,96	0
4	DMU	C	306	22/33	0.87	0.18	77,100,102,103	0
3	Y01	B	302	35/35	0.88	0.51	100,105,112,113	0
3	Y01	A	305	35/35	0.90	0.21	45,50,72,73	0
3	Y01	D	602	35/35	0.91	0.23	48,61,81,83	0
3	Y01	A	301	35/35	0.91	0.21	53,59,66,67	0
2	K	C	302	1/1	0.92	0.15	114,114,114,114	0
2	K	C	301	1/1	0.93	0.12	40,40,40,40	0
2	K	A	302	1/1	0.94	0.11	43,43,43,43	0
2	K	A	304	1/1	0.94	0.08	40,40,40,40	0
2	K	A	303	1/1	0.95	0.07	33,33,33,33	0
2	K	C	303	1/1	0.96	0.05	37,37,37,37	0
2	K	A	309	1/1	0.97	0.12	33,33,33,33	0
2	K	C	304	1/1	0.98	0.08	44,44,44,44	0

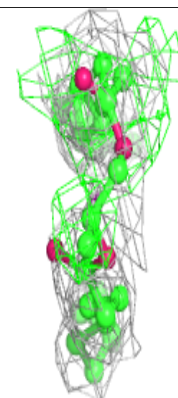
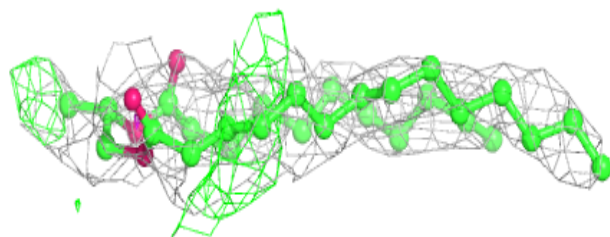
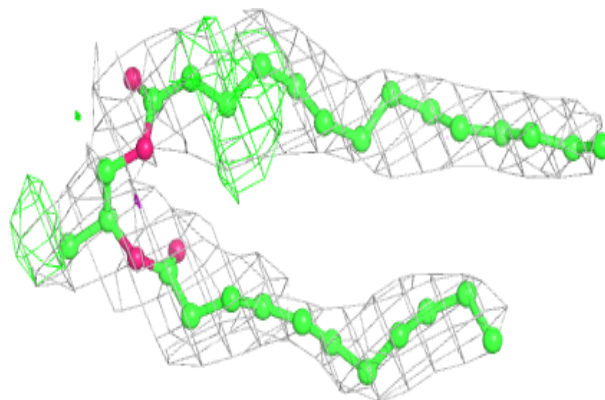
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PC1 D 601:**

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

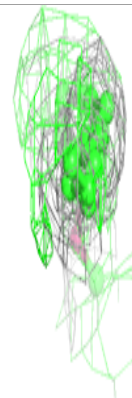
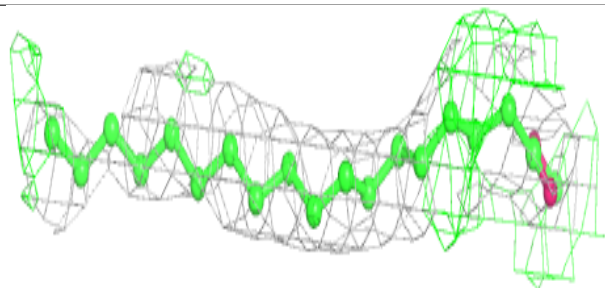
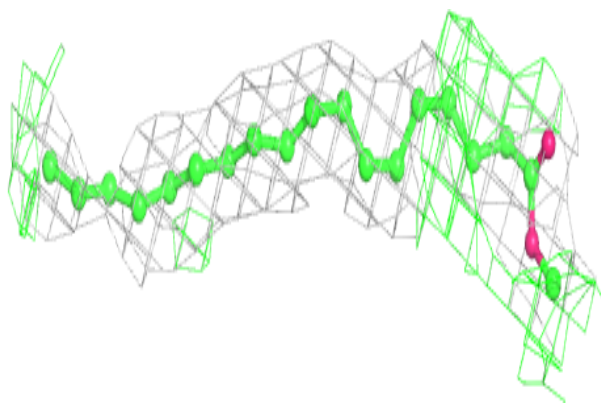
**Electron density around PC1 A 308:**

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

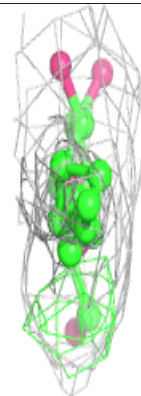
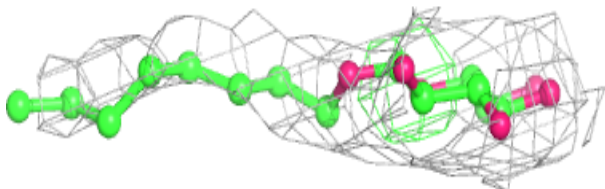
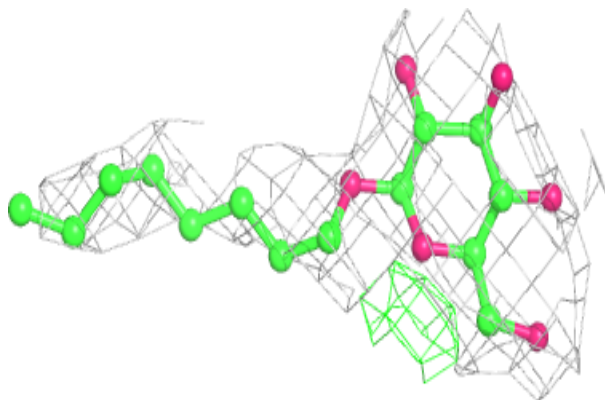


**Electron density around PC1 D 604:**

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

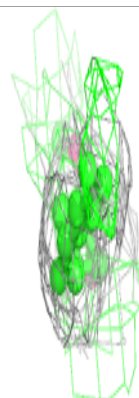
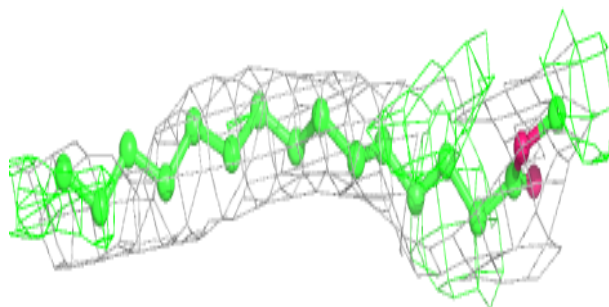
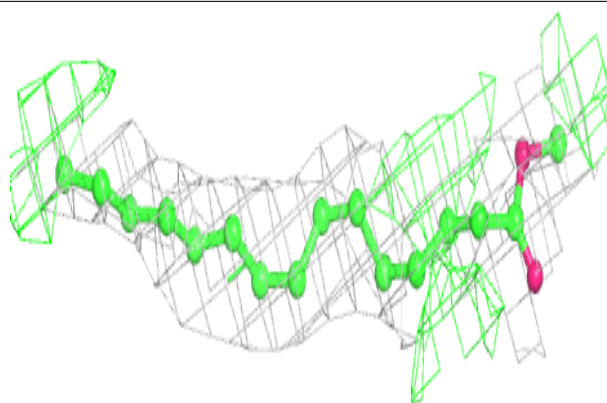
**Electron density around DMU B 303:**

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

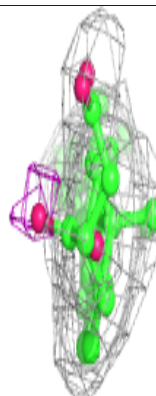
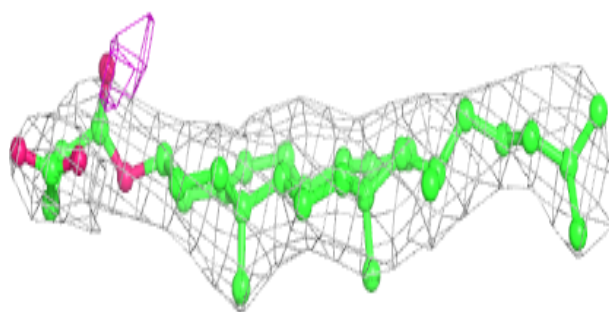
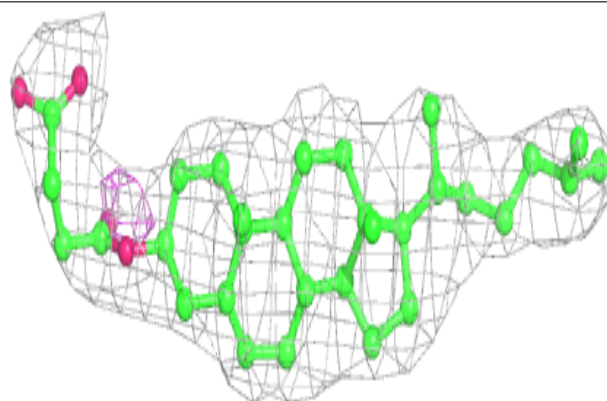


**Electron density around PC1 B 304:**

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

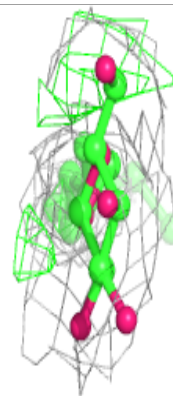
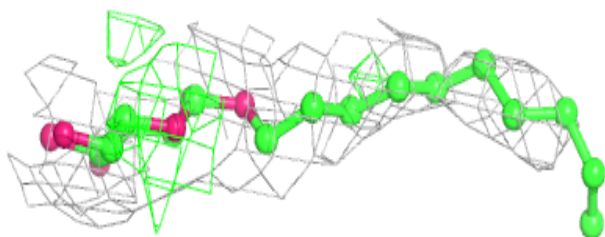
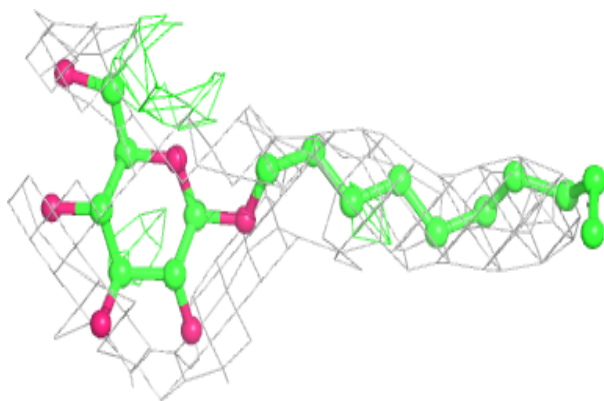
**Electron density around Y01 C 305:**

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

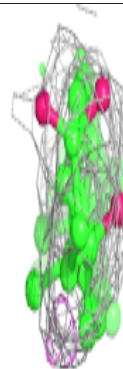
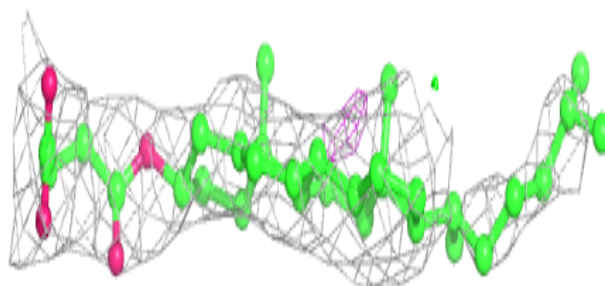
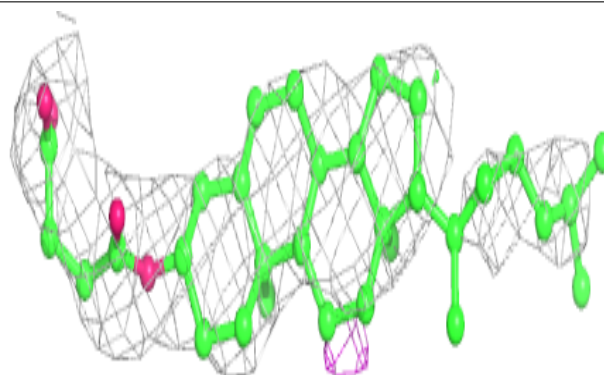


**Electron density around DMU A 307:**

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

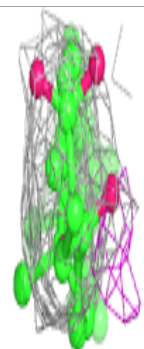
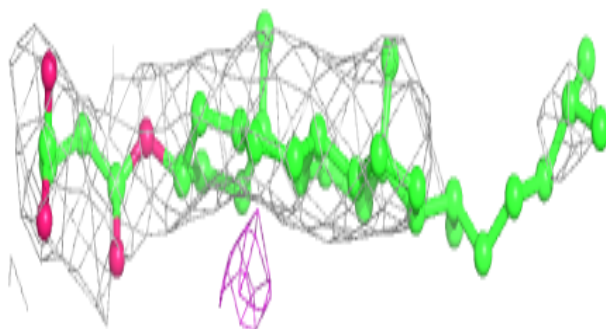
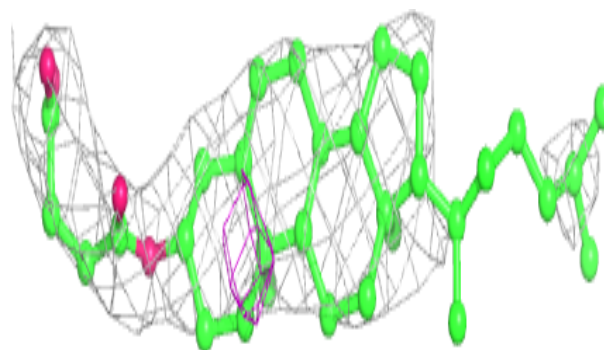
**Electron density around Y01 D 603:**

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

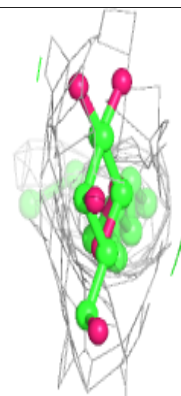
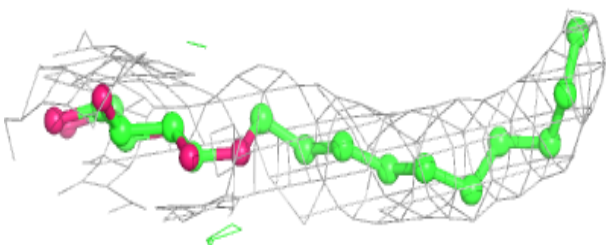
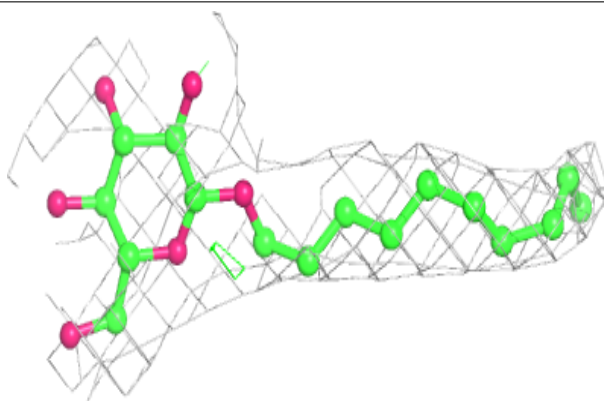


**Electron density around Y01 A 306:**

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

**Electron density around DMU C 306:**

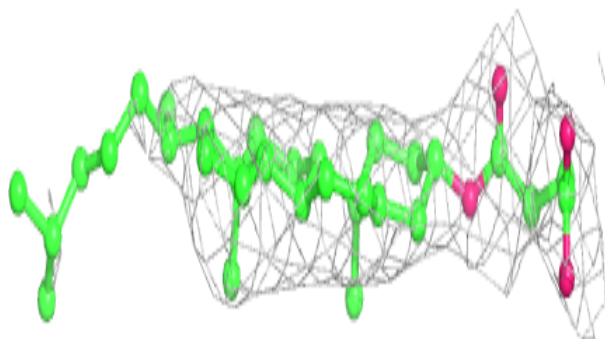
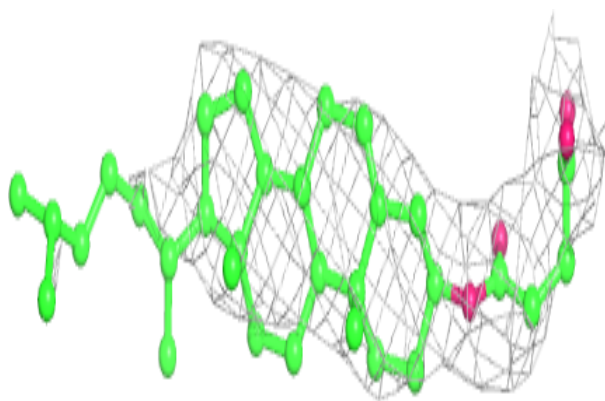
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



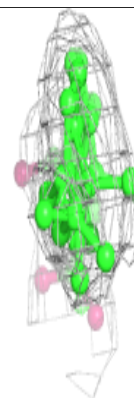
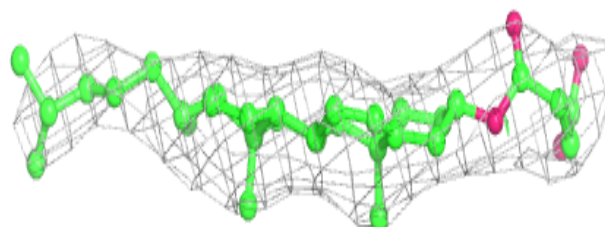
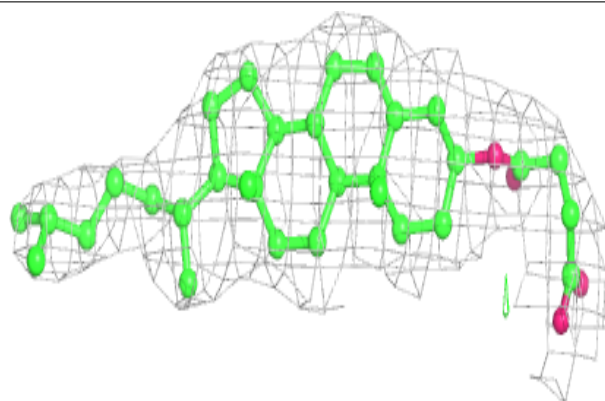


**Electron density around Y01 B 302:**

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

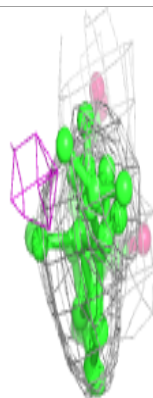
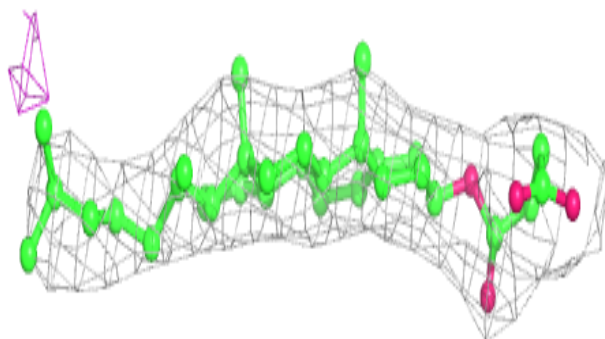
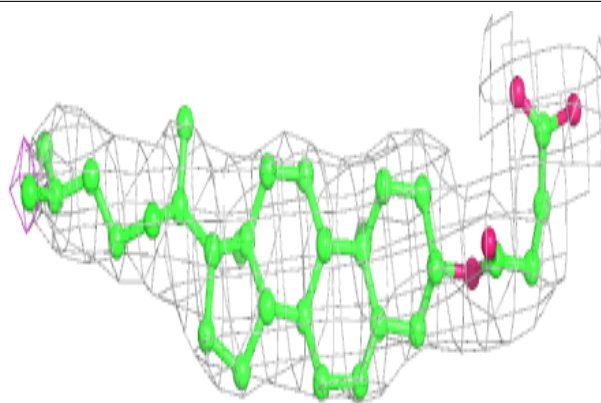
**Electron density around Y01 A 305:**

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

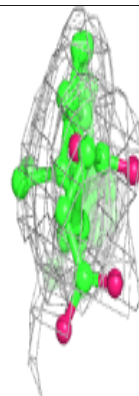
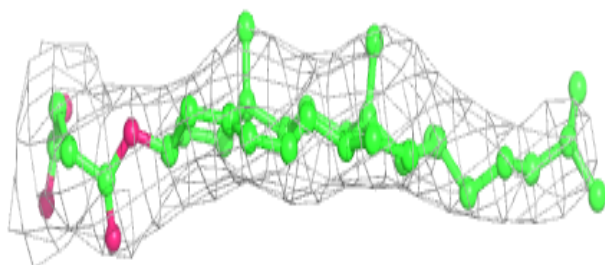
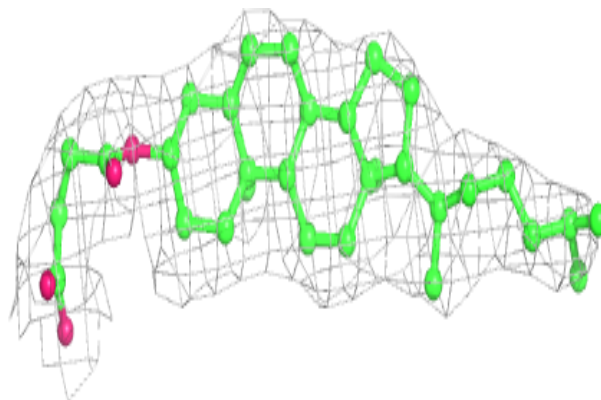


**Electron density around Y01 D 602:**

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

**Electron density around Y01 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)





## 6.5 Other polymers

There are no such residues in this entry.