



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:44 pm BST

PDB ID : 6G6U  
Title : The dynamic nature of the VDAC1 channels in bilayers: human VDAC1 at 2.7 Angstrom resolution  
Authors : Razeto, A.; Gribbon, P.; Loew, C.  
Deposited on : 2018-04-03  
Resolution : 2.74 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	:	2.11
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)	:	2.11

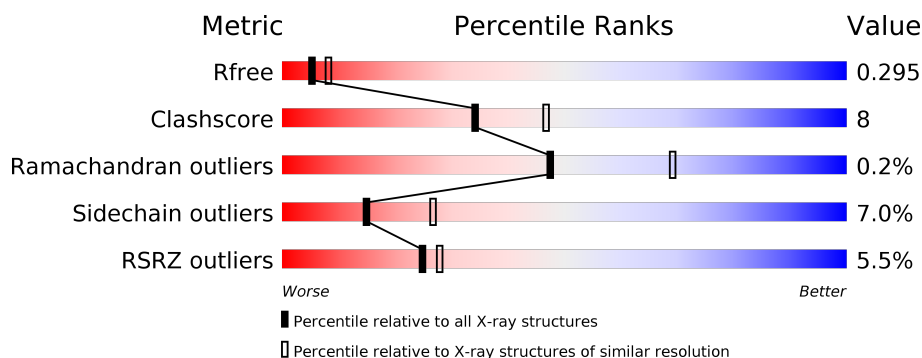
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	291	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	291	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>

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
2	MC3	B	302	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4411 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.

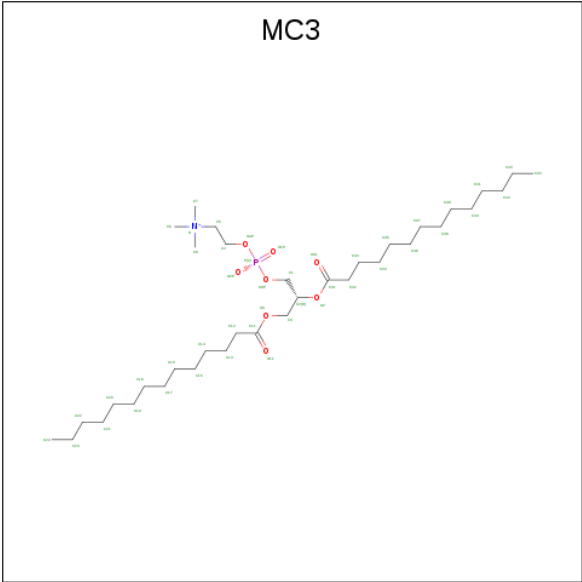
- Molecule 1 is a protein called Voltage-dependent anion-selective channel protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	101	0	0
			2162	1367	365	426	4			
1	B	282	Total	C	N	O	S	128	0	0
			2162	1367	365	426	4			

There are 16 discrepancies between the modelled and reference sequences:

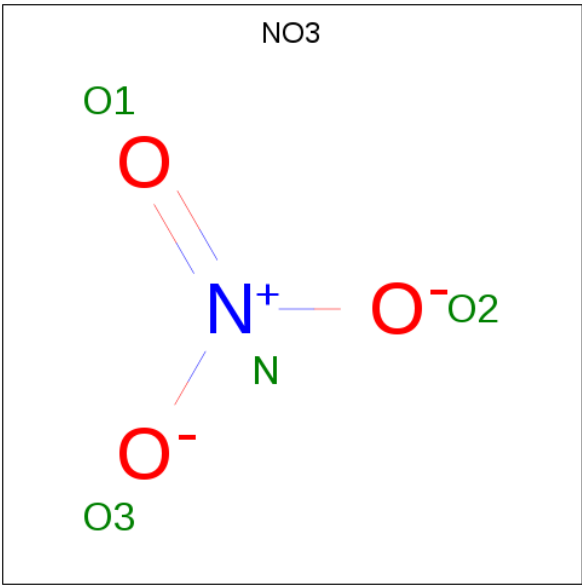
Chain	Residue	Modelled	Actual	Comment	Reference
A	284	LEU	-	expression tag	UNP P21796
A	285	GLU	-	expression tag	UNP P21796
A	286	HIS	-	expression tag	UNP P21796
A	287	HIS	-	expression tag	UNP P21796
A	288	HIS	-	expression tag	UNP P21796
A	289	HIS	-	expression tag	UNP P21796
A	290	HIS	-	expression tag	UNP P21796
A	291	HIS	-	expression tag	UNP P21796
B	284	LEU	-	expression tag	UNP P21796
B	285	GLU	-	expression tag	UNP P21796
B	286	HIS	-	expression tag	UNP P21796
B	287	HIS	-	expression tag	UNP P21796
B	288	HIS	-	expression tag	UNP P21796
B	289	HIS	-	expression tag	UNP P21796
B	290	HIS	-	expression tag	UNP P21796
B	291	HIS	-	expression tag	UNP P21796

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: MC3) (formula: C<sub>36</sub>H<sub>72</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			23	17	5	1		
2	B	1	Total	C	O	P	0	0
			23	17	5	1		
2	B	1	Total	C	O	P	0	0
			23	17	5	1		

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	N	O	0	0
			4	1	3		

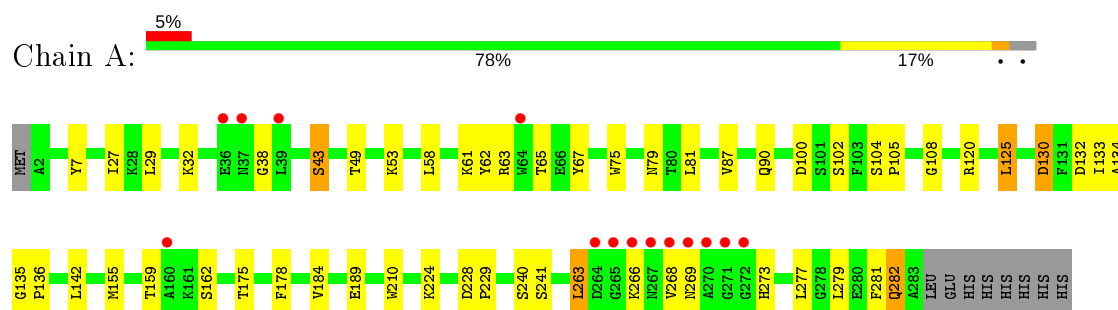
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	4	Total	O	0	0
			4	4		

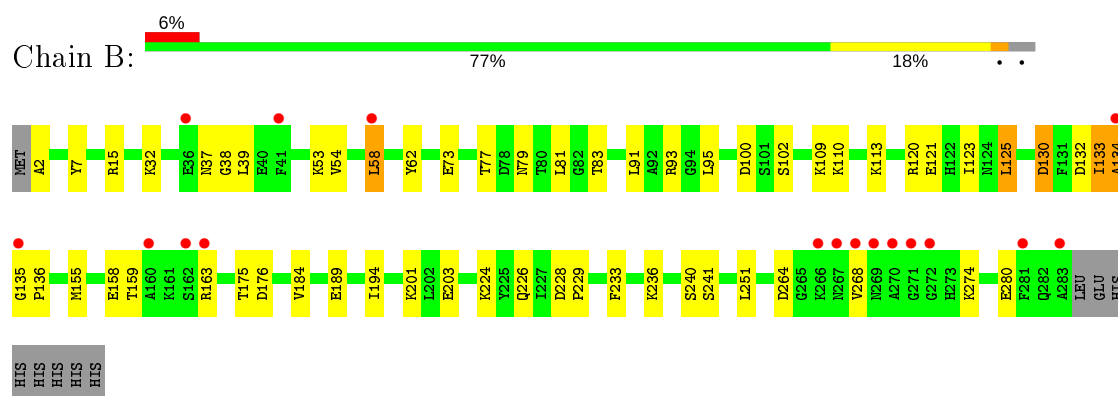
### 3 Residue-property plots [i](#)

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 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: Voltage-dependent anion-selective channel protein 1



- Molecule 1: Voltage-dependent anion-selective channel protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.40 Å 58.15 Å 122.72 Å 90.00° 94.03° 90.00°	Depositor
Resolution (Å)	122.42 – 2.74 122.42 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.1 (122.42-2.74) 99.1 (122.42-2.74)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.73 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.256 , 0.287 0.258 , 0.295	Depositor DCC
$R_{free}$ test set	960 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4411	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	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 41.08 % 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 2.4873e-04. 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: MC3, NO3

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	1.02	2/2203 (0.1%)	1.03	3/2976 (0.1%)
1	B	1.01	3/2203 (0.1%)	1.02	10/2976 (0.3%)
All	All	1.02	5/4406 (0.1%)	1.03	13/5952 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	GLU	CD-OE1	5.76	1.31	1.25
1	B	158	GLU	CA-CB	5.54	1.66	1.53
1	A	279	LEU	CB-CG	-5.51	1.36	1.52
1	A	100	ASP	CB-CG	5.44	1.63	1.51
1	B	233	PHE	CG-CD2	5.09	1.46	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	LEU	CA-CB-CG	7.13	131.71	115.30
1	B	264	ASP	CB-CA-C	6.60	123.60	110.40
1	B	201	LYS	CD-CE-NZ	6.25	126.07	111.70
1	B	132	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	130	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	B	58	LEU	CA-CB-CG	6.08	129.29	115.30
1	B	132	ASP	CB-CG-OD1	-5.85	113.04	118.30
1	B	58	LEU	CB-CG-CD1	-5.82	101.11	111.00
1	B	109	LYS	CB-CG-CD	5.52	125.95	111.60
1	B	130	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	277	LEU	CB-CG-CD2	5.29	119.99	111.00
1	B	53	LYS	CD-CE-NZ	5.18	123.61	111.70
1	B	236	LYS	CD-CE-NZ	-5.01	100.18	111.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2162	0	2133	37	0
1	B	2162	0	2133	31	0
2	A	23	0	30	3	0
2	B	46	0	60	6	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	6	0	0	0	0
4	B	4	0	0	0	0
All	All	4411	0	4356	69	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 8.

All (69) 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)
2:A:301:MC3:H332	2:A:301:MC3:C3	1.54	1.36
2:A:301:MC3:C33	2:A:301:MC3:C3	2.48	0.88
1:B:123:ILE:HG22	1:B:125:LEU:CD2	2.07	0.84
1:A:58:LEU:HD13	1:B:58:LEU:HD11	1.64	0.80
1:B:123:ILE:CG2	1:B:125:LEU:CD2	2.64	0.76
1:A:61:LYS:HE3	1:A:63:ARG:NH2	2.03	0.73
1:B:91:LEU:HB2	1:B:95:LEU:HD23	1.75	0.69
2:B:302:MC3:O3P	2:B:302:MC3:H321	1.95	0.66
1:B:130:ASP:O	1:B:136:PRO:HA	1.94	0.65
1:A:130:ASP:O	1:A:136:PRO:HA	1.95	0.65
1:B:73:GLU:HG3	1:B:83:THR:HG22	1.79	0.63
1:B:123:ILE:HG22	1:B:125:LEU:HD23	1.79	0.63
1:B:73:GLU:CG	1:B:83:THR:HG22	2.30	0.62
1:A:268:VAL:HG22	1:A:268:VAL:O	2.00	0.61
1:B:268:VAL:O	1:B:268:VAL:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:MC3:H321	2:B:302:MC3:C1	2.31	0.59
1:A:27:ILE:HD12	1:A:49:THR:HG22	1.86	0.57
1:A:61:LYS:HE3	1:A:63:ARG:CZ	2.34	0.57
1:A:61:LYS:CE	1:A:63:ARG:NH2	2.66	0.57
1:A:125:LEU:HD12	1:A:142:LEU:CD1	2.35	0.57
1:A:58:LEU:HD13	1:B:58:LEU:CD1	2.34	0.57
1:A:210:TRP:HE1	2:A:301:MC3:H322	1.69	0.57
2:B:302:MC3:C32	2:B:302:MC3:H11	2.37	0.54
2:B:302:MC3:C32	2:B:302:MC3:C1	2.86	0.53
1:A:38:GLY:HA2	1:A:62:TYR:HE1	1.74	0.53
1:A:32:LYS:HB3	1:A:282:GLN:HG3	1.90	0.52
1:A:125:LEU:HD12	1:A:142:LEU:HD13	1.90	0.52
1:A:240:SER:O	1:A:241:SER:HB2	2.11	0.51
1:A:125:LEU:CD1	1:A:142:LEU:HD13	2.42	0.50
1:A:43:SER:OG	1:B:58:LEU:HD21	2.12	0.50
1:B:133:ILE:O	1:B:134:ALA:C	2.49	0.50
1:A:281:PHE:HE2	1:B:54:VAL:O	1.95	0.50
1:B:136:PRO:HG2	1:B:159:THR:HB	1.95	0.49
1:A:263:LEU:HD23	1:A:273:HIS:HB2	1.95	0.48
1:B:2:ALA:N	1:B:121:GLU:OE2	2.46	0.48
1:A:61:LYS:CE	1:A:63:ARG:HH21	2.27	0.48
1:B:123:ILE:CG2	1:B:125:LEU:HD22	2.41	0.48
1:B:133:ILE:O	1:B:135:GLY:N	2.46	0.48
1:A:228:ASP:HB2	1:A:229:PRO:CD	2.44	0.48
1:A:136:PRO:HG2	1:A:159:THR:HB	1.95	0.47
1:A:184:VAL:HA	1:A:189:GLU:O	2.16	0.46
1:A:132:ASP:HB3	1:A:135:GLY:H	1.81	0.46
1:B:184:VAL:HA	1:B:189:GLU:O	2.16	0.46
1:A:87:VAL:HG12	1:A:90:GLN:HB2	1.97	0.46
1:B:7:TYR:CD1	1:B:7:TYR:C	2.89	0.46
1:A:7:TYR:C	1:A:7:TYR:CD1	2.89	0.46
1:A:175:THR:HG22	1:A:178:PHE:HB3	1.99	0.45
1:B:228:ASP:HB2	1:B:229:PRO:CD	2.47	0.45
1:B:125:LEU:N	1:B:125:LEU:HD23	2.31	0.45
1:A:61:LYS:HE3	1:A:63:ARG:HH21	1.80	0.44
1:B:100:ASP:HB3	1:B:113:LYS:HB2	2.00	0.43
1:A:27:ILE:HD12	1:A:49:THR:CG2	2.49	0.43
1:B:240:SER:O	1:B:241:SER:HB2	2.17	0.43
1:B:73:GLU:HG2	1:B:83:THR:HG22	2.00	0.43
1:A:125:LEU:CD1	1:A:142:LEU:CD1	2.96	0.43
1:B:194:ILE:HG13	2:B:301:MC3:H441	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ASP:HB2	1:B:229:PRO:HD3	2.01	0.42
1:A:228:ASP:HB2	1:A:229:PRO:HD3	2.02	0.42
2:B:302:MC3:H371	2:B:302:MC3:H342	1.23	0.41
1:B:203:GLU:OE2	1:B:224:LYS:HD2	2.20	0.41
1:A:79:ASN:O	1:A:105:PRO:HD2	2.21	0.41
1:A:175:THR:CG2	1:A:178:PHE:HB3	2.51	0.41
1:A:281:PHE:CE2	1:B:54:VAL:O	2.74	0.41
1:A:104:SER:O	1:A:108:GLY:N	2.53	0.41
1:A:75:TRP:HZ2	1:B:39:LEU:HD13	1.85	0.41
1:A:224:LYS:HB2	1:A:224:LYS:HE2	1.76	0.41
1:B:38:GLY:HA2	1:B:62:TYR:HE1	1.86	0.41
1:B:77:THR:C	1:B:79:ASN:H	2.25	0.40
1:A:133:ILE:O	1:A:134:ALA:C	2.60	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	280/291 (96%)	269 (96%)	11 (4%)	0	100	100
1	B	280/291 (96%)	265 (95%)	14 (5%)	1 (0%)	34	55
All	All	560/582 (96%)	534 (95%)	25 (4%)	1 (0%)	47	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	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	229/238 (96%)	214 (93%)	15 (7%)	16	29
1	B	229/238 (96%)	212 (93%)	17 (7%)	13	24
All	All	458/476 (96%)	426 (93%)	32 (7%)	15	27

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	43	SER
1	A	53	LYS
1	A	65	THR
1	A	67	TYR
1	A	81	LEU
1	A	102	SER
1	A	120	ARG
1	A	125	LEU
1	A	155	MET
1	A	162	SER
1	A	263	LEU
1	A	266	LYS
1	A	269	ASN
1	A	282	GLN
1	B	15	ARG
1	B	32	LYS
1	B	37	ASN
1	B	81	LEU
1	B	93	ARG
1	B	102	SER
1	B	110	LYS
1	B	120	ARG
1	B	125	LEU
1	B	133	ILE
1	B	155	MET
1	B	163	ARG

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Mol	Chain	Res	Type
1	B	175	THR
1	B	176	ASP
1	B	226	GLN
1	B	251	LEU
1	B	274	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	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	$\# Z  > 2$
3	NO3	B	303	-	1,3,3	0.40	0	0,3,3	0.00	-
3	NO3	A	302	-	1,3,3	0.41	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MC3	B	301	-	19,22,45	1.55	3 (15%)	19,24,53	2.47	7 (36%)
2	MC3	A	301	-	19,22,45	1.31	2 (10%)	19,24,53	1.56	3 (15%)
2	MC3	B	302	-	19,22,45	1.12	1 (5%)	19,24,53	1.78	3 (15%)

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	MC3	B	301	-	-	11/20/22/49	-
2	MC3	A	301	-	-	13/20/22/49	-
2	MC3	B	302	-	-	12/20/22/49	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	MC3	O2-C31	5.47	1.49	1.34
2	A	301	MC3	O2-C31	5.04	1.48	1.34
2	B	302	MC3	O2-C31	4.29	1.46	1.34
2	B	301	MC3	O3P-C1	2.25	1.50	1.44
2	B	301	MC3	C34-C33	2.17	1.63	1.51
2	A	301	MC3	O2-C2	-2.11	1.43	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	MC3	C34-C33-C32	-6.68	89.18	113.19
2	B	302	MC3	O2-C31-C32	4.69	121.61	111.50
2	B	301	MC3	O2-C31-C32	4.69	121.61	111.50
2	A	301	MC3	O2-C31-C32	4.34	120.85	111.50
2	B	301	MC3	O2-C2-C3	4.16	117.44	107.93
2	B	302	MC3	C2-O2-C31	-4.02	112.71	117.88
2	B	301	MC3	C33-C32-C31	-3.08	102.41	113.62
2	A	301	MC3	C2-O2-C31	-2.71	114.40	117.88
2	B	301	MC3	O31-C31-C32	-2.50	113.98	123.73
2	A	301	MC3	C3-C2-C1	-2.45	105.58	112.63
2	B	301	MC3	C3-C2-C1	-2.34	105.90	112.63
2	B	301	MC3	O2-C2-C1	2.08	110.95	106.13
2	B	302	MC3	C33-C32-C31	-2.04	106.19	113.62

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	MC3	O3P-C1-C2-C3
2	B	301	MC3	C3-C2-O2-C31
2	B	301	MC3	C32-C31-O2-C2
2	B	301	MC3	O31-C31-O2-C2
2	A	301	MC3	O3P-C1-C2-C3
2	A	301	MC3	O3P-C1-C2-O2
2	A	301	MC3	O31-C31-O2-C2
2	B	302	MC3	C1-C2-O2-C31
2	B	302	MC3	C32-C31-O2-C2
2	B	302	MC3	O31-C31-O2-C2
2	A	301	MC3	C32-C31-O2-C2
2	B	302	MC3	C34-C35-C36-C37
2	B	302	MC3	C39-C40-C41-C42
2	B	302	MC3	C36-C37-C38-C39
2	A	301	MC3	C34-C35-C36-C37
2	B	302	MC3	C38-C39-C40-C41
2	B	302	MC3	C35-C36-C37-C38
2	A	301	MC3	C32-C33-C34-C35
2	A	301	MC3	C37-C38-C39-C40
2	B	302	MC3	C37-C38-C39-C40
2	B	301	MC3	C32-C33-C34-C35
2	B	301	MC3	C38-C39-C40-C41
2	B	301	MC3	C1-C2-O2-C31
2	A	301	MC3	C39-C40-C41-C42
2	B	301	MC3	C36-C37-C38-C39
2	B	302	MC3	C40-C41-C42-C43
2	B	301	MC3	C41-C42-C43-C44
2	A	301	MC3	C35-C36-C37-C38
2	A	301	MC3	C38-C39-C40-C41
2	A	301	MC3	C2-C1-O3P-P
2	B	301	MC3	C33-C34-C35-C36
2	A	301	MC3	O2-C31-C32-C33
2	B	302	MC3	C32-C33-C34-C35
2	A	301	MC3	C36-C37-C38-C39
2	B	301	MC3	O3P-C1-C2-O2
2	B	302	MC3	C33-C34-C35-C36

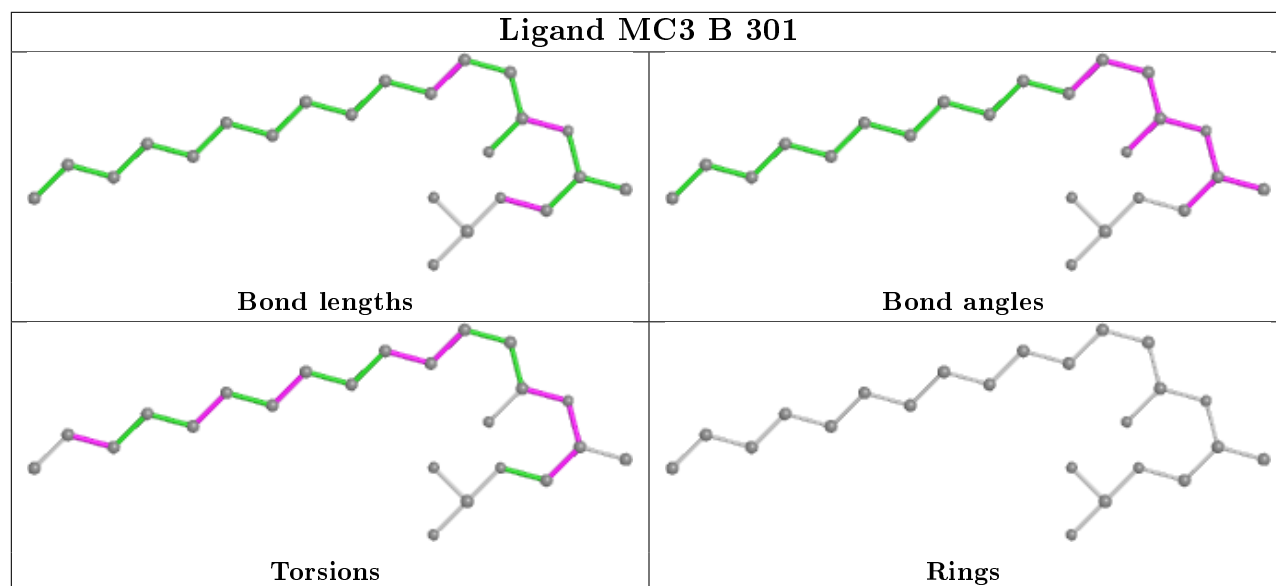
There are no ring outliers.

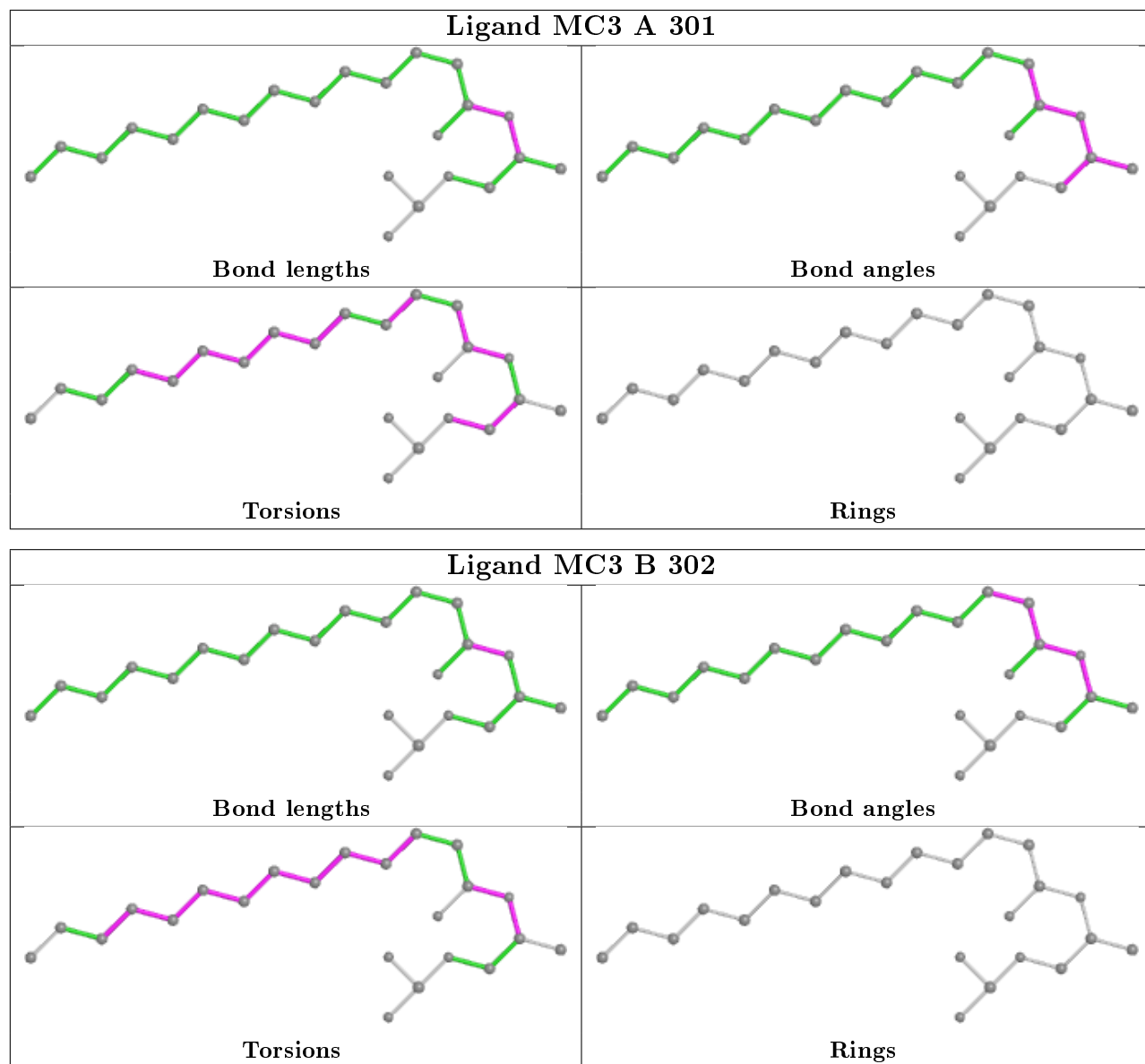
3 monomers are involved in 9 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	MC3	1	0
2	A	301	MC3	3	0
2	B	302	MC3	5	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.

## 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	282/291 (96%)	0.35	14 (4%) 28 32	32, 57, 88, 189	38 (13%)
1	B	282/291 (96%)	0.35	17 (6%) 21 24	33, 62, 102, 189	39 (13%)
All	All	564/582 (96%)	0.35	31 (5%) 25 28	32, 59, 95, 189	77 (13%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	ASN	9.3
1	B	272	GLY	9.3
1	B	266	LYS	6.6
1	A	36	GLU	6.3
1	A	272	GLY	5.8
1	A	266	LYS	5.1
1	B	134	ALA	5.0
1	B	270	ALA	4.6
1	B	271	GLY	4.5
1	B	36	GLU	4.5
1	B	160	ALA	4.3
1	A	268	VAL	4.2
1	A	264	ASP	3.5
1	A	271	GLY	3.5
1	A	265	GLY	3.4
1	B	162	SER	3.3
1	B	269	ASN	3.2
1	A	37	ASN	3.2
1	A	267	ASN	3.1
1	A	269	ASN	3.0
1	B	135	GLY	2.9
1	B	268	VAL	2.6
1	A	160	ALA	2.6
1	B	281	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	39	LEU	2.3
1	B	41	PHE	2.3
1	A	64	TRP	2.3
1	B	163	ARG	2.3
1	B	283	ALA	2.2
1	B	58	LEU	2.1
1	A	270	ALA	2.1

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

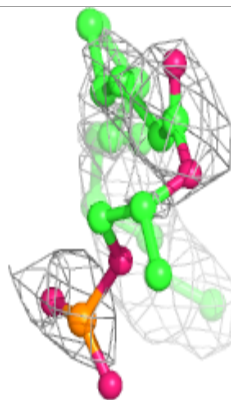
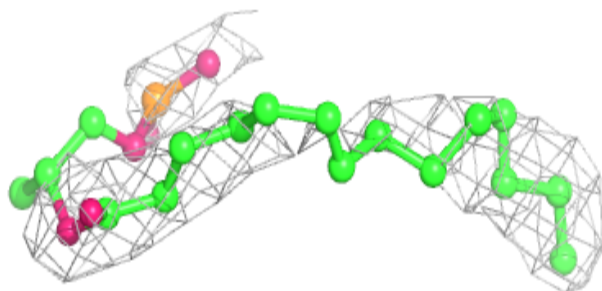
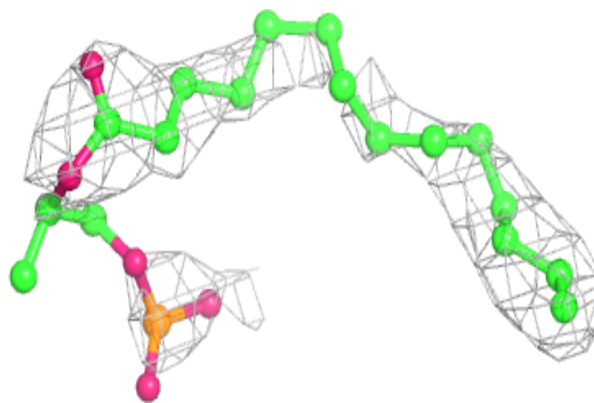
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MC3	B	302	23/46	0.67	0.41	23,46,59,63	23
2	MC3	B	301	23/46	0.83	0.27	29,33,50,52	9
2	MC3	A	301	23/46	0.86	0.21	24,33,52,55	9
3	NO3	A	302	4/4	0.94	0.24	44,47,50,55	0
3	NO3	B	303	4/4	0.94	0.25	47,49,51,53	0

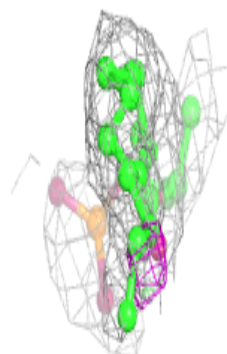
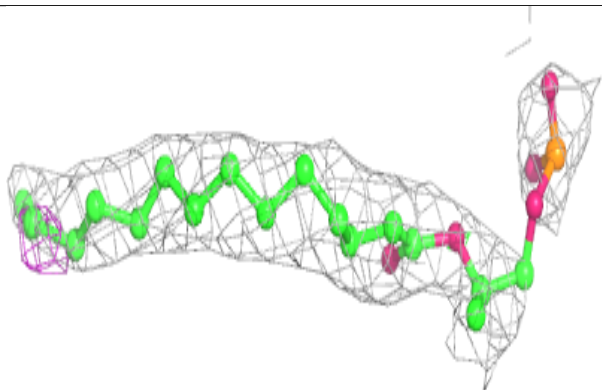
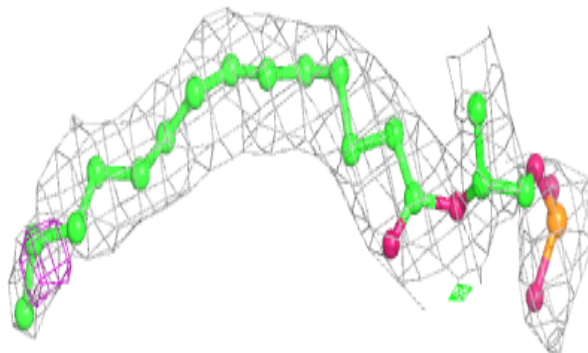
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

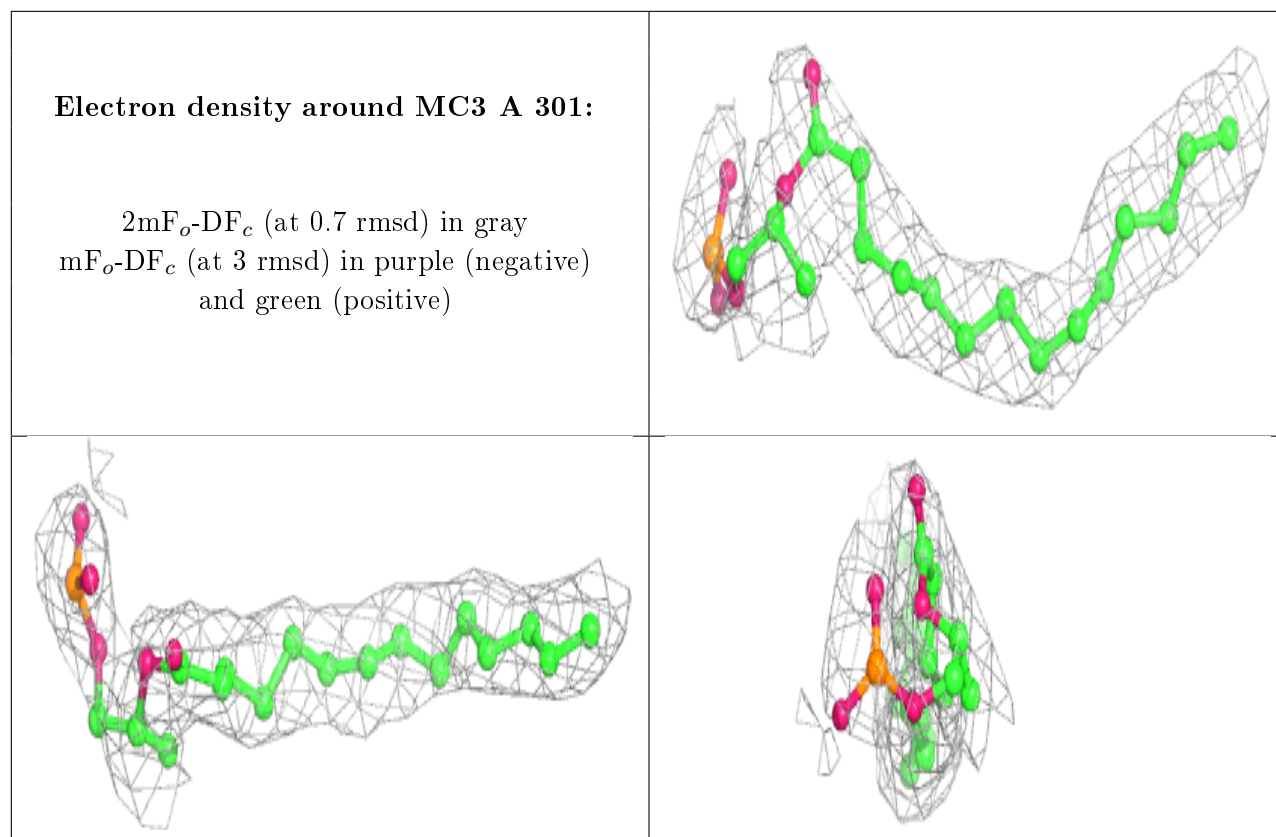
**Electron density around MC3 B 302:**

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

**Electron density around MC3 B 301:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.