



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:27 AM UTC

PDB ID : 6G6U / pdb_00006g6u
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

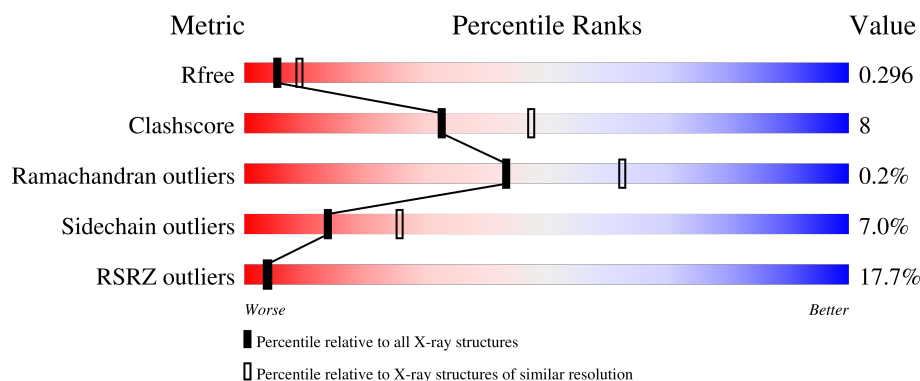
1 Overall quality at a glance

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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	14% 75% 20% ..
1	B	291	20% 78% 17% ..

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.

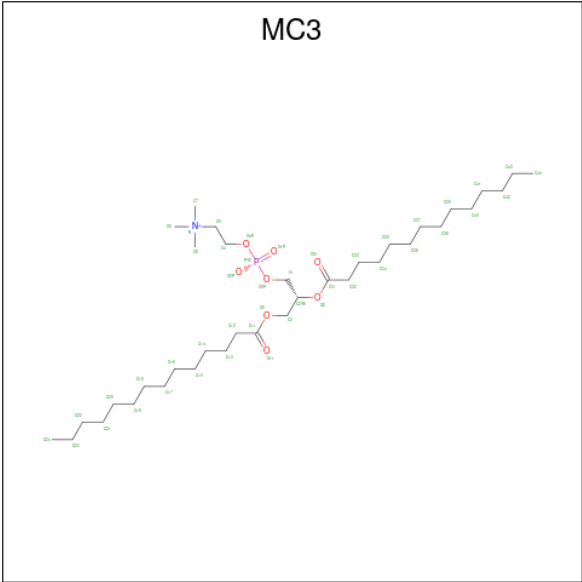
- Molecule 1 is a protein called Voltage-dependent anion-selective channel protein 1.

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:

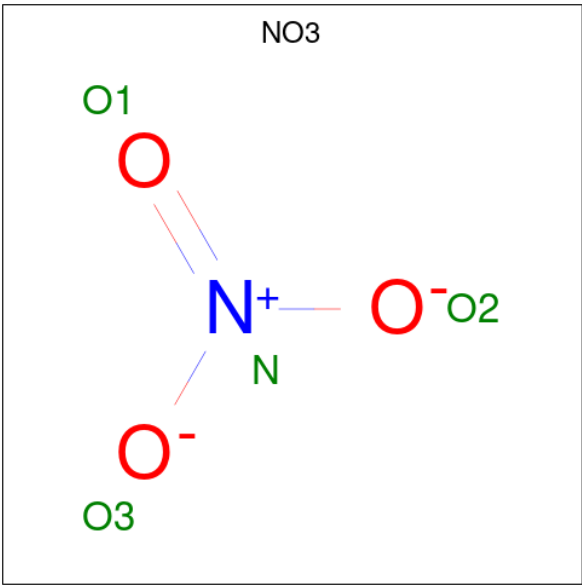
Chain	Residue	Modelled	Actual	Comment	Reference
A	284	LEU	-	expression tag	UNP P21796
A	285	GLU	-	expression tag	UNP P21796
A	286	HIS	-	expression tag	UNP P21796
A	287	HIS	-	expression tag	UNP P21796
A	288	HIS	-	expression tag	UNP P21796
A	289	HIS	-	expression tag	UNP P21796
A	290	HIS	-	expression tag	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 (CCD ID: MC3) (formula: C₃₆H₇₂NO₈P).



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 (CCD ID: NO3) (formula: NO₃).



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		

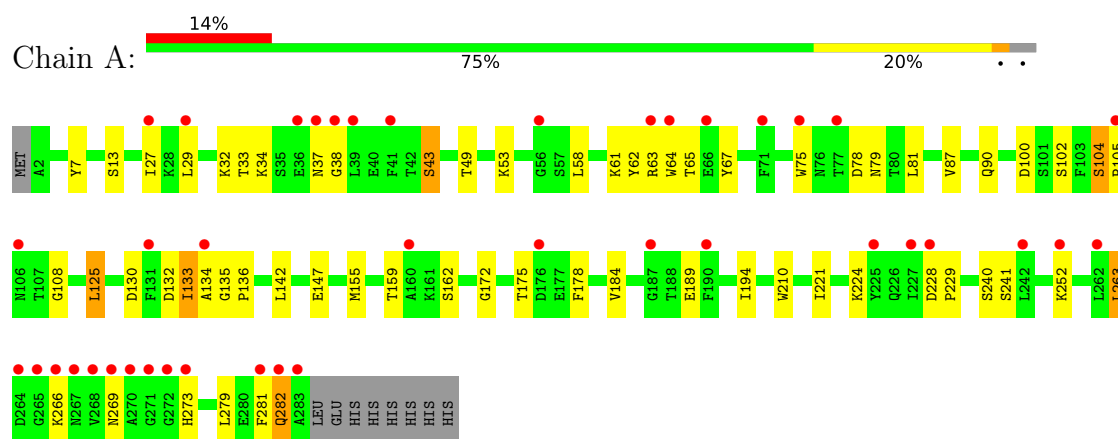
- Molecule 4 is water.

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

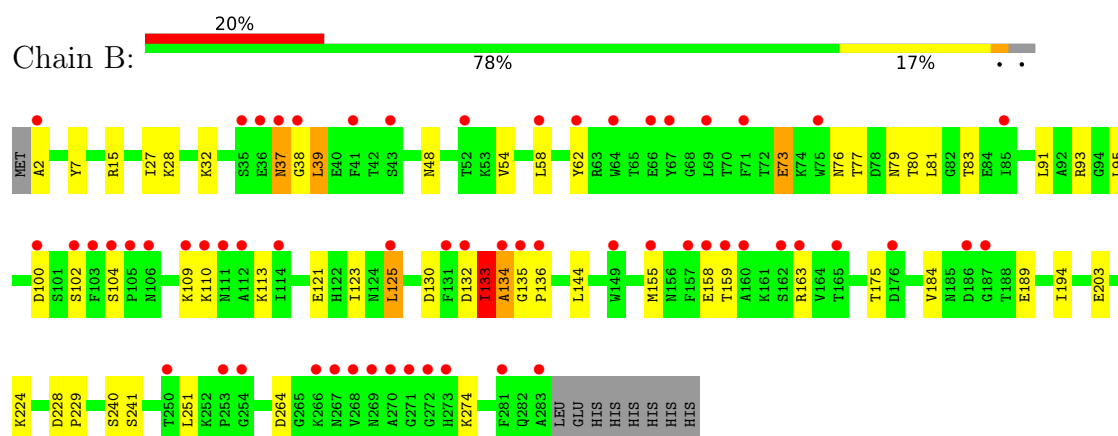
3 Residue-property plots

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: 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, α , β , γ	51.40Å 58.15Å 122.72Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.73Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.256 , 0.287 0.258 , 0.296	Depositor DCC
R_{free} test set	960 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NO3, MC3

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	1.27	7/2203 (0.3%)	1.22	8/2976 (0.3%)
1	B	1.23	4/2203 (0.2%)	1.19	11/2976 (0.4%)
All	All	1.25	11/4406 (0.2%)	1.20	19/5952 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	GLU	CA-CB	10.26	1.66	1.53
1	A	279	LEU	CB-CG	-8.44	1.36	1.53
1	A	100	ASP	C-O	-6.91	1.16	1.24
1	B	37	ASN	CA-CB	-6.29	1.44	1.53
1	B	48	ASN	C-O	-5.81	1.16	1.24
1	A	13	SER	N-CA	-5.53	1.39	1.46
1	A	33	THR	C-O	-5.43	1.17	1.23
1	B	109	LYS	CG-CD	-5.38	1.36	1.52
1	A	34	LYS	CA-CB	5.14	1.61	1.53
1	A	147	GLU	C-O	5.09	1.29	1.23
1	A	172	GLY	N-CA	-5.04	1.40	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ILE	N-CA-C	-13.95	98.04	110.74
1	B	133	ILE	N-CA-C	-10.18	100.43	110.30
1	B	264	ASP	CB-CA-C	6.96	123.60	109.76
1	B	109	LYS	CB-CG-CD	6.37	125.95	111.30
1	B	132	ASP	CA-CB-CG	5.95	118.55	112.60
1	B	76	ASN	CA-C-N	5.74	127.97	120.28
1	B	76	ASN	C-N-CA	5.74	127.97	120.28
1	B	39	LEU	N-CA-C	5.44	117.75	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	LEU	CA-C-N	-5.39	118.46	122.18
1	B	144	LEU	C-N-CA	-5.39	118.46	122.18
1	B	104	SER	CA-C-N	5.38	125.45	119.32
1	B	104	SER	C-N-CA	5.38	125.45	119.32
1	A	104	SER	CA-C-N	5.19	125.24	119.32
1	A	104	SER	C-N-CA	5.19	125.24	119.32
1	A	37	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	221	ILE	N-CA-C	-5.12	100.83	108.46
1	A	100	ASP	CA-CB-CG	-5.09	107.51	112.60
1	A	252	LYS	CA-CB-CG	-5.08	103.94	114.10
1	A	64	TRP	CA-CB-CG	5.00	123.11	113.60

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	32	0
2	A	23	0	30	3	0
2	B	46	0	60	1	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	65	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 (65) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:MC3:C3	2:A:301:MC3:C33	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
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: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
1:B:133:ILE:O	1:B:134:ALA:C	2.49	0.54
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:B:7:TYR:CD1	1:B:7:TYR:C	2.89	0.50
1:A:7:TYR:C	1:A:7:TYR:CD1	2.89	0.50
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:HD23	1:B:125:LEU:N	2.31	0.45
1:A:133:ILE:O	1:A:134:ALA:C	2.60	0.45
1:B:77:THR:C	1:B:79:ASN:H	2.25	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:73:GLU:HG2	1:B:83:THR:HG22	2.00	0.43
1:B:155:MET:SD	1:B:155:MET:C	3.02	0.43
1:B:133:ILE:C	1:B:135:GLY:N	2.76	0.43
1:B:240:SER:O	1:B:241:SER:HB2	2.17	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
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
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:155:MET:C	1:A:155:MET:SD	3.03	0.41
1:A:75:TRP:HZ2	1:B:39:LEU:HD13	1.85	0.41
1:A:104:SER:O	1:A:108:GLY:N	2.53	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:224:LYS:HE2	1:A:224:LYS:HB2	1.76	0.41
1:B:38:GLY:HA2	1:B:62:TYR:HE1	1.86	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/291 (96%)	269 (96%)	11 (4%)	0	100	100
1	B	280/291 (96%)	265 (95%)	14 (5%)	1 (0%)	30	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	560/582 (96%)	534 (95%)	25 (4%)	1 (0%)	43 62

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%)	15 28
1	B	229/238 (96%)	212 (93%)	17 (7%)	13 23
All	All	458/476 (96%)	426 (93%)	32 (7%)	14 26

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	78	ASP
1	A	81	LEU
1	A	102	SER
1	A	125	LEU
1	A	162	SER
1	A	194	ILE
1	A	263	LEU
1	A	266	LYS
1	A	269	ASN
1	A	282	GLN
1	B	15	ARG
1	B	27	ILE

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Mol	Chain	Res	Type
1	B	28	LYS
1	B	32	LYS
1	B	37	ASN
1	B	73	GLU
1	B	80	THR
1	B	81	LEU
1	B	93	ARG
1	B	102	SER
1	B	110	LYS
1	B	125	LEU
1	B	133	ILE
1	B	163	ARG
1	B	175	THR
1	B	251	LEU
1	B	274	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	179	GLN
1	A	181	HIS
1	A	183	ASN
1	A	267	ASN
1	A	282	GLN
1	B	79	ASN
1	B	90	GLN
1	B	111	ASN
1	B	156	ASN
1	B	181	HIS
1	B	183	ASN
1	B	226	GLN
1	B	267	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	MC3	B	302	-	19,22,45	1.12	1 (5%)	19,24,53	1.73	3 (15%)
2	MC3	A	301	-	19,22,45	1.30	2 (10%)	19,24,53	1.54	3 (15%)
3	NO3	A	302	-	1,3,3	0.44	0	0,3,3	-	-
2	MC3	B	301	-	19,22,45	1.57	3 (15%)	19,24,53	2.46	7 (36%)
3	NO3	B	303	-	1,3,3	0.44	0	0,3,3	-	-

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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	C34-C33	2.41	1.63	1.51
2	B	301	MC3	O3P-C1	2.16	1.50	1.44
2	A	301	MC3	O2-C2	-2.12	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	-6.52	89.18	113.13
2	B	302	MC3	O2-C31-C32	4.68	121.61	111.48
2	B	301	MC3	O2-C31-C32	4.68	121.61	111.48
2	A	301	MC3	O2-C31-C32	4.33	120.85	111.48
2	B	301	MC3	O2-C2-C3	4.23	117.44	107.96
2	B	302	MC3	C2-O2-C31	-3.52	112.71	117.78
2	B	301	MC3	C33-C32-C31	-3.08	102.41	113.69
2	A	301	MC3	C3-C2-C1	-2.53	105.58	112.69
2	B	301	MC3	O31-C31-C32	-2.51	113.98	123.78
2	B	301	MC3	C3-C2-C1	-2.42	105.90	112.69
2	A	301	MC3	C2-O2-C31	-2.35	114.40	117.78
2	B	301	MC3	O2-C2-C1	2.06	110.95	106.21
2	B	302	MC3	C33-C32-C31	-2.05	106.19	113.69

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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	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	B	302	MC3	C38-C39-C40-C41

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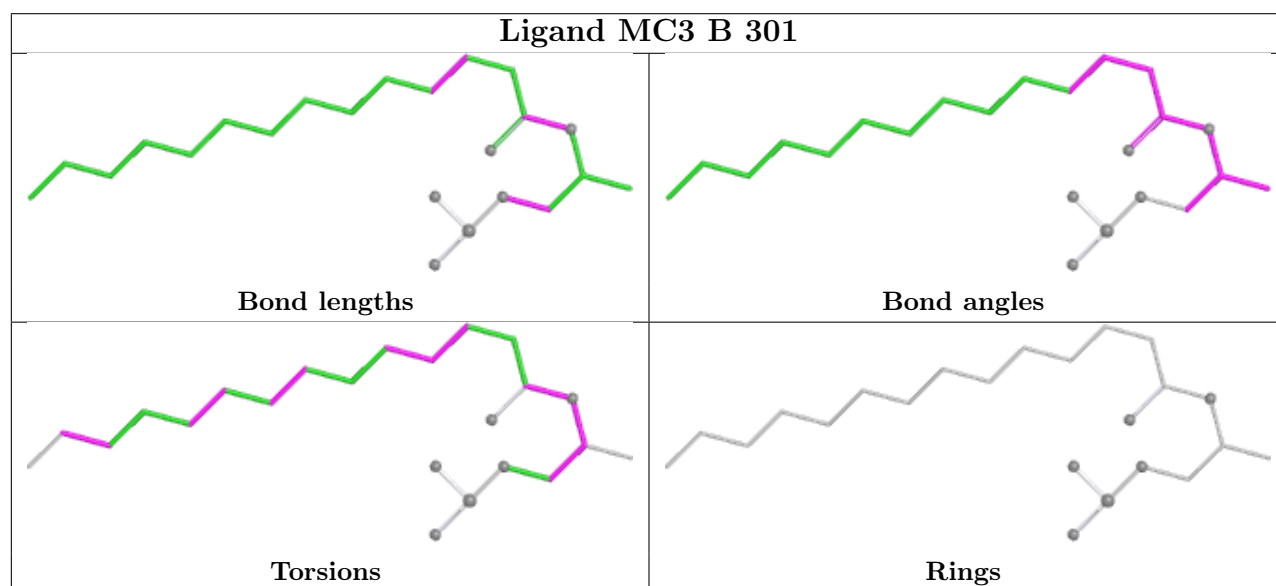
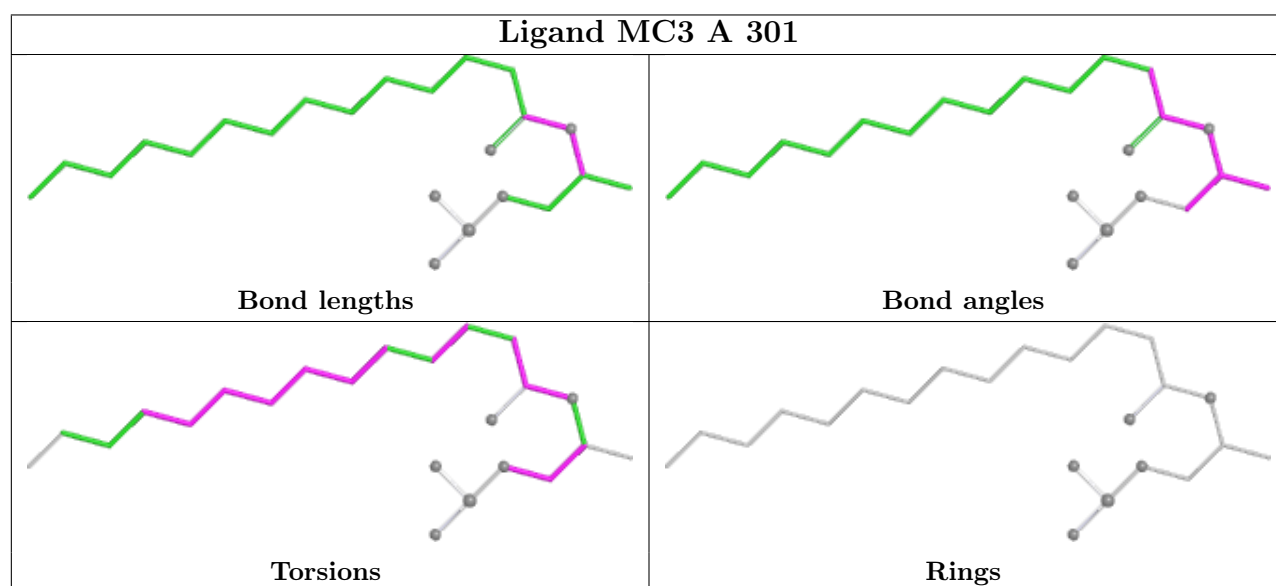
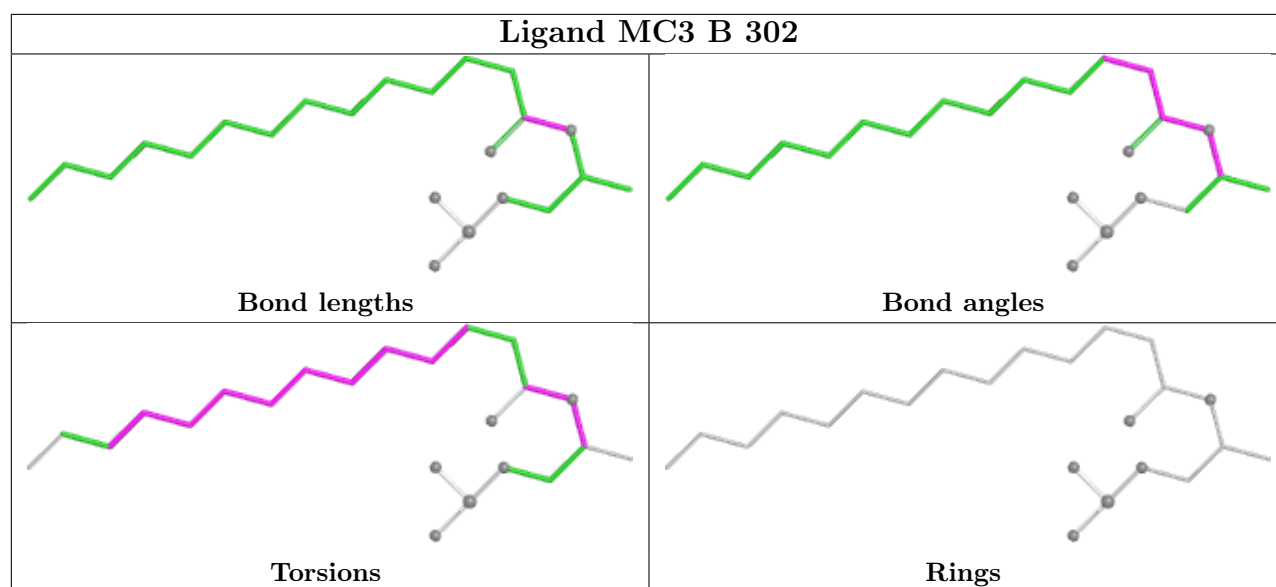
Mol	Chain	Res	Type	Atoms
2	A	301	MC3	C34-C35-C36-C37
2	B	302	MC3	C35-C36-C37-C38
2	A	301	MC3	C32-C33-C34-C35
2	A	301	MC3	C37-C38-C39-C40
2	B	302	MC3	C37-C38-C39-C40
2	B	301	MC3	C32-C33-C34-C35
2	B	301	MC3	C38-C39-C40-C41
2	A	301	MC3	C39-C40-C41-C42
2	B	301	MC3	C36-C37-C38-C39
2	B	302	MC3	C40-C41-C42-C43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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

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, 95th 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 ²)	Q < 0.9
1	A	282/291 (96%)	1.32	41 (14%)	6 6	12, 52, 80, 104	38 (13%)
1	B	282/291 (96%)	1.58	59 (20%)	2 2	4, 55, 90, 115	39 (13%)
All	All	564/582 (96%)	1.45	100 (17%)	4 4	4, 53, 88, 115	77 (13%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	GLU	39.9
1	A	272	GLY	23.6
1	A	271	GLY	20.3
1	A	270	ALA	20.3
1	A	268	VAL	19.6
1	B	272	GLY	18.9
1	B	268	VAL	18.6
1	B	269	ASN	18.0
1	B	270	ALA	17.6
1	A	269	ASN	17.4
1	A	266	LYS	15.8
1	B	271	GLY	15.7
1	B	267	ASN	14.1
1	B	266	LYS	13.1
1	A	267	ASN	12.7
1	A	273	HIS	10.3
1	A	37	ASN	9.5
1	B	37	ASN	6.4
1	B	41	PHE	6.3
1	B	58	LEU	5.8
1	A	281	PHE	5.7
1	B	105	PRO	5.6
1	B	134	ALA	5.1
1	B	71	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	69	LEU	4.6
1	B	273	HIS	4.4
1	A	38	GLY	4.3
1	B	176	ASP	4.2
1	B	283	ALA	4.2
1	B	160	ALA	4.1
1	B	35	SER	4.1
1	B	103	PHE	3.9
1	B	157	PHE	3.6
1	A	264	ASP	3.2
1	A	252	LYS	3.2
1	B	67	TYR	3.2
1	A	106	ASN	3.1
1	A	66	GLU	3.1
1	A	71	PHE	3.1
1	B	136	PRO	3.1
1	B	162	SER	3.1
1	B	2	ALA	3.0
1	A	36	GLU	3.0
1	A	105	PRO	3.0
1	A	134	ALA	3.0
1	B	102	SER	2.9
1	B	165	THR	2.9
1	A	39	LEU	2.8
1	A	225	TYR	2.8
1	B	104	SER	2.8
1	B	111	ASN	2.8
1	A	283	ALA	2.8
1	B	131	PHE	2.8
1	A	160	ALA	2.7
1	B	155	MET	2.7
1	B	52	THR	2.7
1	B	186	ASP	2.7
1	B	158	GLU	2.6
1	B	100	ASP	2.6
1	B	253	PRO	2.6
1	A	187	GLY	2.6
1	B	75	TRP	2.5
1	A	41	PHE	2.5
1	B	159	THR	2.5
1	B	132	ASP	2.5
1	B	85	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	176	ASP	2.5
1	A	265	GLY	2.5
1	B	62	TYR	2.5
1	B	187	GLY	2.5
1	B	110	LYS	2.4
1	B	125	LEU	2.4
1	B	135	GLY	2.4
1	A	64	TRP	2.4
1	A	227	ILE	2.3
1	A	75	TRP	2.3
1	B	149	TRP	2.3
1	B	250	THR	2.2
1	A	56	GLY	2.2
1	A	190	PHE	2.2
1	B	281	PHE	2.2
1	A	77	THR	2.2
1	A	228	ASP	2.2
1	A	131	PHE	2.2
1	B	106	ASN	2.2
1	B	66	GLU	2.2
1	B	109	LYS	2.2
1	A	242	LEU	2.2
1	B	43	SER	2.2
1	B	64	TRP	2.1
1	B	163	ARG	2.1
1	A	282	GLN	2.1
1	A	63	ARG	2.1
1	A	29	LEU	2.0
1	A	27	ILE	2.0
1	B	38	GLY	2.0
1	B	114	ILE	2.0
1	B	254	GLY	2.0
1	B	112	ALA	2.0
1	A	262	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

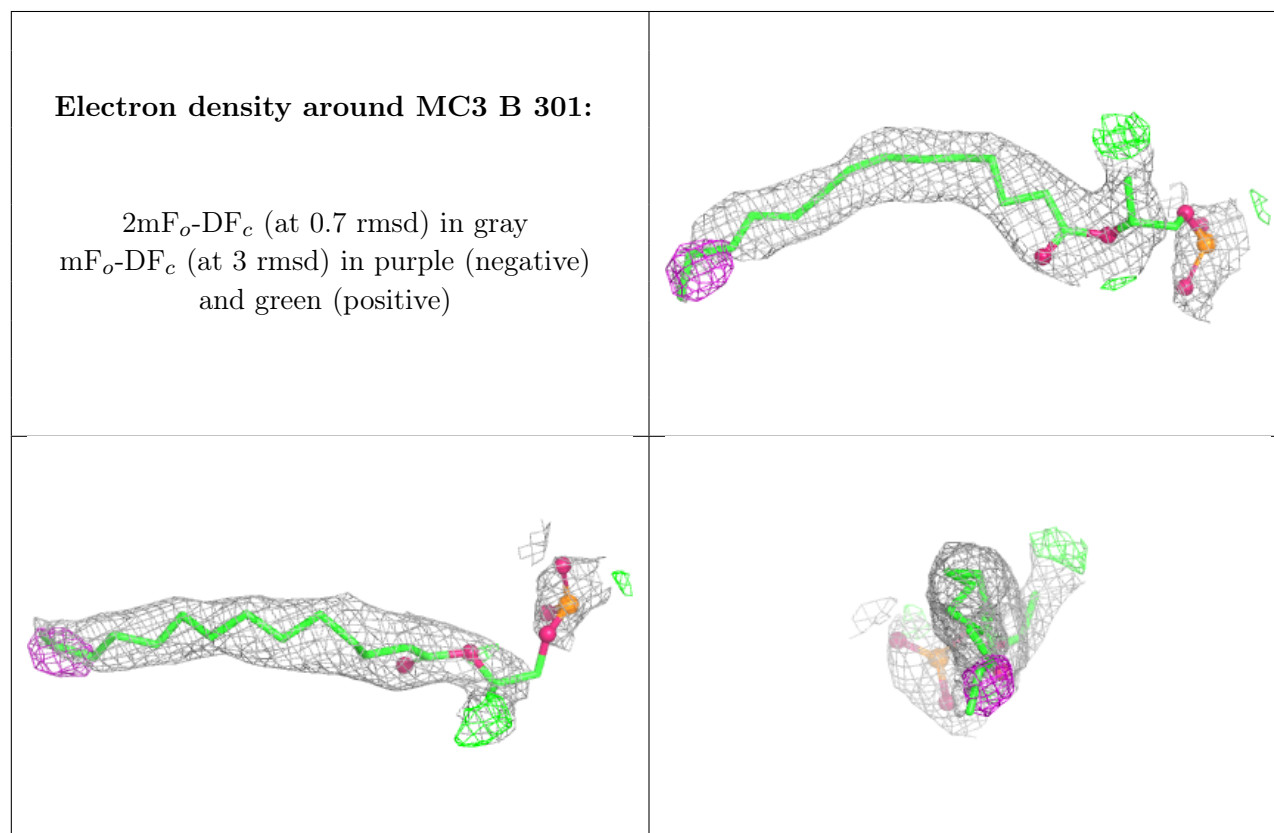
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

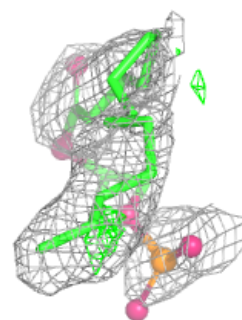
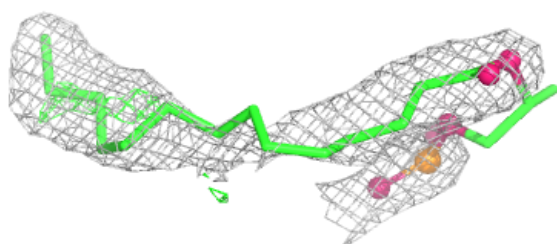
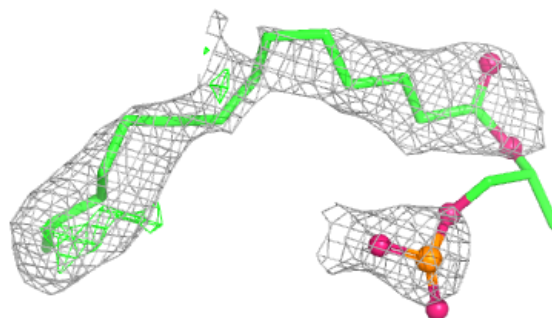
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MC3	B	301	23/46	0.75	0.20	29,33,50,52	9
2	MC3	B	302	23/46	0.75	0.29	23,46,59,63	23
2	MC3	A	301	23/46	0.80	0.18	24,33,52,55	9
3	NO3	A	302	4/4	0.97	0.09	44,47,50,55	0
3	NO3	B	303	4/4	0.97	0.06	47,49,51,53	0

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.

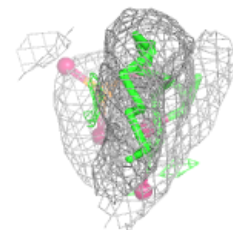
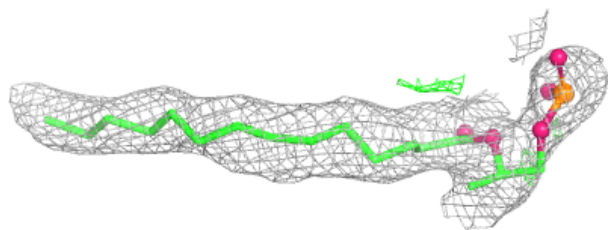
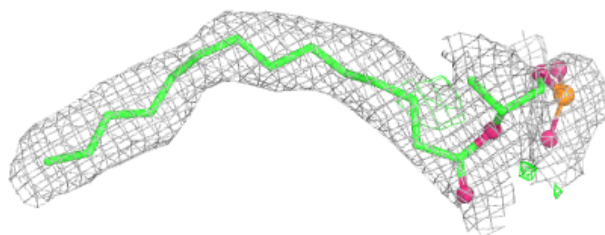


Electron density around MC3 B 302:

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

**Electron density around MC3 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 [i](#)

There are no such residues in this entry.