



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:32 pm BST

PDB ID : 6G73
Title : The dynamic nature of the VDAC1 channels in bilayers: human VDAC1 at 3.3 Angstrom resolution
Authors : Razeto, A.; Gribbon, P.; Loew, C.
Deposited on : 2018-04-04
Resolution : 3.27 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 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

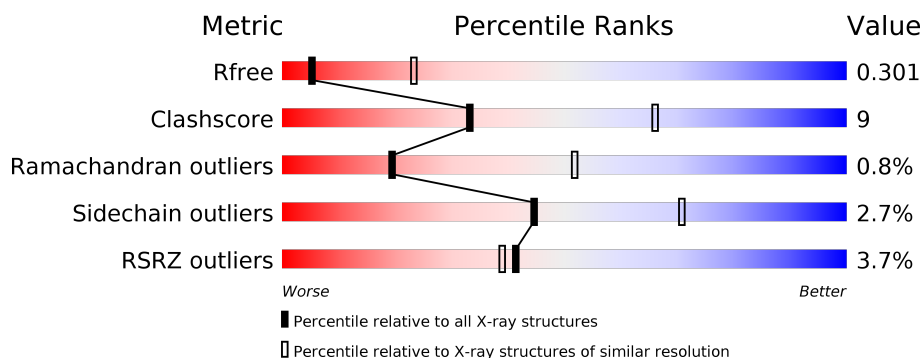
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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 ≥ 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	
1	B	291	
1	C	291	
1	D	291	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MC3	A	301	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8753 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	19	0	0
			2162	1367	365	426	4			
1	B	281	Total	C	N	O	S	20	0	0
			2157	1364	364	425	4			
1	C	281	Total	C	N	O	S	10	0	0
			2157	1364	364	425	4			
1	D	282	Total	C	N	O	S	29	0	0
			2162	1367	365	426	4			

There are 32 discrepancies between the modelled and reference sequences:

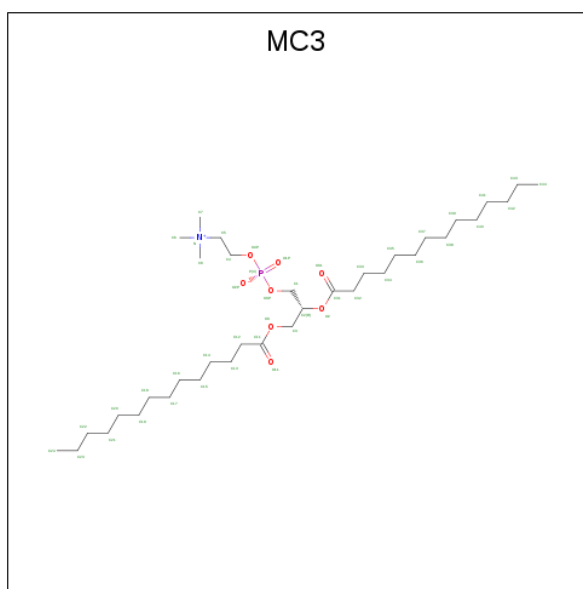
Chain	Residue	Modelled	Actual	Comment	Reference
A	284	LEU	-	expression tag	UNP P21796
A	285	GLU	-	expression tag	UNP P21796
A	286	HIS	-	expression tag	UNP P21796
A	287	HIS	-	expression tag	UNP P21796
A	288	HIS	-	expression tag	UNP P21796
A	289	HIS	-	expression tag	UNP P21796
A	290	HIS	-	expression tag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

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

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: MC3) (formula: $C_{36}H_{72}NO_8P$).

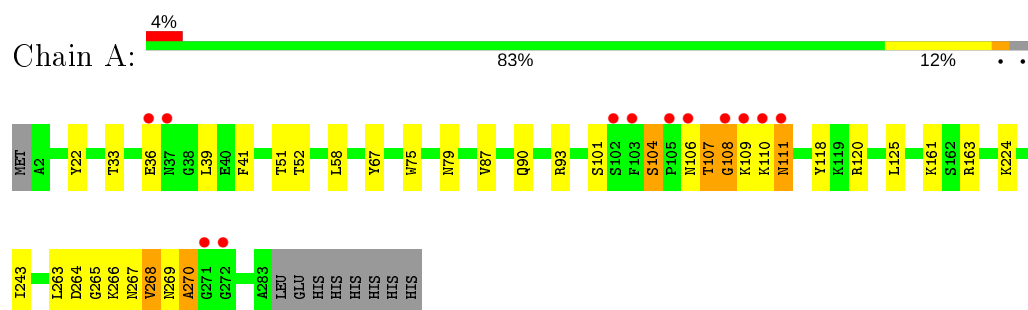


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			23	17	5	1		
2	A	1	Total	C	O	P	0	0
			23	17	5	1		
2	B	1	Total	C	O	P	0	0
			23	17	5	1		
2	B	1	Total	C	O	P	0	0
			23	17	5	1		
2	D	1	Total	C	O	P	0	0
			23	17	5	1		

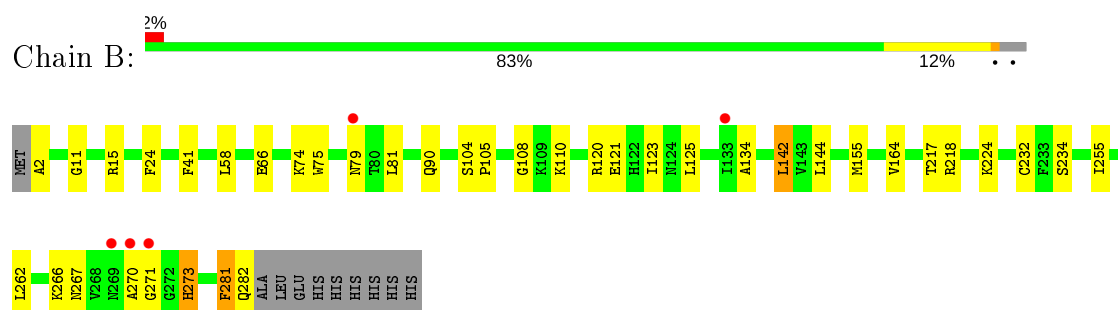
3 Residue-property plots [i](#)

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.

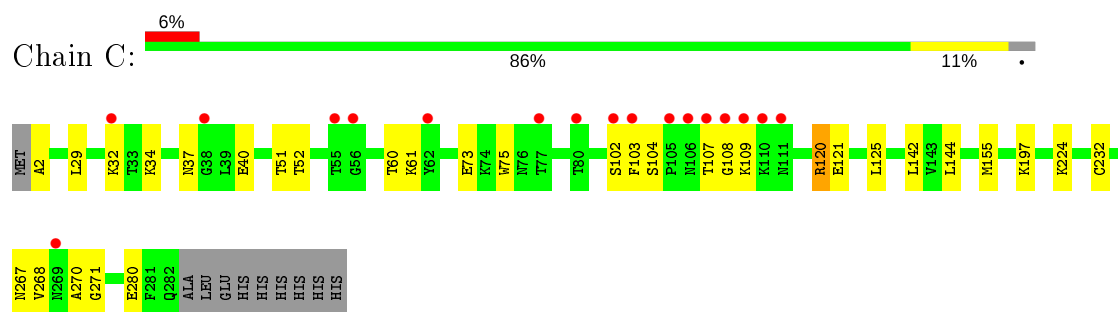
- Molecule 1: Voltage-dependent anion-selective channel protein 1



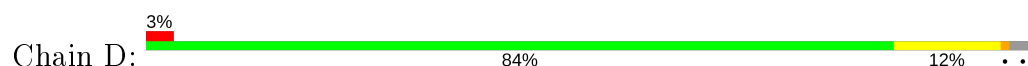
- Molecule 1: Voltage-dependent anion-selective channel protein 1

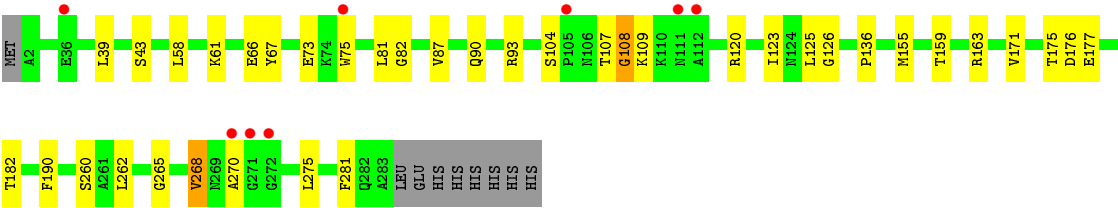


- Molecule 1: Voltage-dependent anion-selective channel protein 1



- 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	60.22Å 83.36Å 156.93Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	19.94 – 3.27 19.94 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.2 (19.94-3.27) 96.7 (19.94-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.298 0.237 , 0.301	Depositor DCC
R_{free} test set	1149 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	96.3	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.208 for h,-k,-l	Xtriage
Reported twinning fraction	0.810 for H, K, L 0.190 for h,-k,-l	Depositor
Outliers	5 of 23411 reflections (0.021%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8753	wwPDB-VP
Average B, all atoms (Å ²)	111.0	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 31.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1272e-03. 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: 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	0.66	0/2203	0.84	0/2976
1	B	0.65	0/2198	0.83	0/2969
1	C	0.64	0/2198	0.80	0/2969
1	D	0.66	0/2203	0.82	0/2976
All	All	0.65	0/8802	0.82	0/11890

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	2162	0	2133	41	0
1	B	2157	0	2128	34	0
1	C	2157	0	2128	39	0
1	D	2162	0	2133	32	0
2	A	46	0	59	3	0
2	B	46	0	60	7	0
2	D	23	0	30	2	0
All	All	8753	0	8671	148	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 9.

All (148) 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:267:ASN:O	1:A:269:ASN:N	1.61	1.32
2:B:302:MC3:P	2:B:302:MC3:C3	2.24	1.24
1:D:87:VAL:HG11	1:D:90:GLN:OE1	1.44	1.15
2:B:302:MC3:O31	2:B:302:MC3:H11	1.32	1.07
1:C:267:ASN:OD1	1:C:271:GLY:HA3	1.53	1.07
2:B:302:MC3:C1	2:B:302:MC3:O31	2.06	1.04
1:B:41:PHE:HE1	1:B:58:LEU:HD11	1.18	1.03
1:A:39:LEU:HD21	1:B:75:TRP:HZ2	1.24	1.02
1:A:264:ASP:OD1	1:A:265:GLY:N	1.97	0.97
1:A:110:LYS:O	1:A:111:ASN:HB2	1.61	0.96
1:A:267:ASN:C	1:A:269:ASN:H	1.69	0.95
1:D:125:LEU:HD23	1:D:126:GLY:N	1.88	0.89
1:A:106:ASN:O	1:A:107:THR:O	1.91	0.88
1:B:266:LYS:HG2	1:B:266:LYS:O	1.73	0.86
1:B:41:PHE:CE1	1:B:58:LEU:HD11	2.09	0.85
1:B:41:PHE:HE1	1:B:58:LEU:CD1	1.91	0.83
1:C:267:ASN:OD1	1:C:271:GLY:CA	2.27	0.83
2:B:302:MC3:O2P	2:B:302:MC3:C3	2.27	0.83
2:A:301:MC3:H382	2:A:301:MC3:C42	2.08	0.83
1:A:41:PHE:HE1	1:A:58:LEU:CD1	1.93	0.81
1:A:39:LEU:HD21	1:B:75:TRP:CZ2	2.15	0.81
1:A:106:ASN:O	1:A:107:THR:C	2.20	0.80
1:B:79:ASN:O	1:B:105:PRO:HD2	1.81	0.80
1:C:267:ASN:HB2	1:C:270:ALA:HB3	1.63	0.78
2:A:301:MC3:H422	2:A:301:MC3:H382	1.66	0.77
1:A:39:LEU:CD2	1:B:75:TRP:HZ2	1.99	0.75
1:A:41:PHE:CE1	1:A:58:LEU:CD1	2.69	0.74
1:A:268:VAL:O	1:A:268:VAL:CG1	2.35	0.74
1:C:107:THR:OG1	1:C:109:LYS:HE3	1.88	0.74
1:C:75:TRP:CZ2	1:D:39:LEU:HD21	2.23	0.73
1:A:118:TYR:HB3	1:A:125:LEU:HD11	1.69	0.72
1:A:269:ASN:O	1:A:270:ALA:O	2.08	0.71
1:A:22:TYR:CZ	1:A:234:SER:HB3	2.25	0.71
1:A:268:VAL:O	1:A:268:VAL:HG12	1.91	0.69
1:C:60:THR:HG22	1:C:73:GLU:HB3	1.72	0.69
1:B:142:LEU:O	1:B:142:LEU:HD23	1.93	0.69
1:C:104:SER:HB3	1:C:109:LYS:HG2	1.72	0.69
1:D:260:SER:O	1:D:275:LEU:HD12	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LEU:C	1:B:142:LEU:HD23	2.15	0.67
2:B:301:MC3:H431	2:B:301:MC3:H382	1.76	0.67
1:A:41:PHE:CE1	1:A:58:LEU:HD11	2.31	0.66
1:B:255:ILE:HD11	1:B:281:PHE:CZ	2.31	0.66
1:B:267:ASN:O	1:B:270:ALA:HB3	1.97	0.65
1:A:161:LYS:HB2	1:A:163:ARG:HG2	1.79	0.64
1:A:110:LYS:O	1:A:111:ASN:CB	2.39	0.63
1:B:255:ILE:HD11	1:B:281:PHE:CE1	2.34	0.63
1:D:136:PRO:HG2	1:D:159:THR:HB	1.81	0.63
1:D:58:LEU:HD23	1:D:58:LEU:O	1.99	0.63
1:D:75:TRP:CD1	1:D:81:LEU:HD11	2.35	0.62
1:B:267:ASN:HB3	1:B:270:ALA:HB2	1.82	0.62
1:B:41:PHE:CE1	1:B:58:LEU:CD1	2.76	0.62
1:C:102:SER:O	1:C:103:PHE:CD1	2.53	0.61
1:C:102:SER:C	1:C:103:PHE:CD1	2.73	0.61
1:D:39:LEU:HB2	1:D:61:LYS:O	2.00	0.61
1:B:266:LYS:CG	1:B:266:LYS:O	2.45	0.61
1:C:107:THR:CB	1:C:109:LYS:HE3	2.30	0.61
1:C:102:SER:C	1:C:103:PHE:HD1	2.04	0.60
1:B:224:LYS:HE3	1:B:234:SER:OG	2.02	0.60
1:A:39:LEU:CD2	1:B:75:TRP:CZ2	2.79	0.60
1:C:267:ASN:HB2	1:C:271:GLY:H	1.67	0.59
1:C:268:VAL:O	1:C:268:VAL:HG12	2.02	0.59
1:C:267:ASN:OD1	1:C:271:GLY:N	2.36	0.58
1:C:51:THR:O	1:C:52:THR:OG1	2.19	0.58
1:A:33:THR:HG22	1:A:41:PHE:HD2	1.68	0.58
1:A:75:TRP:CD1	1:B:41:PHE:CE2	2.92	0.57
1:B:217:THR:OG1	1:C:120:ARG:HD3	2.04	0.57
1:A:41:PHE:HE1	1:A:58:LEU:HD13	1.69	0.56
1:A:51:THR:O	1:A:52:THR:OG1	2.20	0.56
1:D:190:PHE:CE2	2:D:700:MC3:H361	2.41	0.56
1:D:73:GLU:OE1	1:D:82:GLY:O	2.24	0.56
1:B:267:ASN:HB3	1:B:270:ALA:CB	2.37	0.55
1:D:171:VAL:HG12	1:D:182:THR:OG1	2.07	0.54
1:A:79:ASN:OD1	1:A:106:ASN:ND2	2.40	0.54
1:D:87:VAL:CG1	1:D:90:GLN:OE1	2.37	0.53
1:B:142:LEU:HD21	1:B:144:LEU:HG	1.89	0.53
1:C:29:LEU:HD23	1:D:43:SER:OG	2.09	0.53
1:A:104:SER:OG	1:A:104:SER:O	2.24	0.52
1:C:155:MET:SD	1:C:155:MET:C	2.88	0.52
1:C:104:SER:CB	1:C:109:LYS:HG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:HD2	1:A:266:LYS:O	2.10	0.52
1:C:144:LEU:N	1:C:144:LEU:HD12	2.24	0.52
1:A:224:LYS:HE3	1:A:232:CYS:SG	2.50	0.52
1:C:2:ALA:N	1:C:121:GLU:OE1	2.43	0.52
1:C:107:THR:OG1	1:C:109:LYS:HG2	2.10	0.51
1:D:104:SER:O	1:D:108:GLY:CA	2.58	0.51
1:C:107:THR:HG21	1:C:109:LYS:HE3	1.93	0.51
1:C:32:LYS:NZ	1:C:280:GLU:OE2	2.44	0.51
1:C:142:LEU:HG	1:C:144:LEU:CD1	2.41	0.51
1:B:155:MET:HG3	1:B:164:VAL:HG13	1.93	0.50
1:D:66:GLU:C	1:D:67:TYR:HD1	2.15	0.50
1:D:66:GLU:C	1:D:67:TYR:CD1	2.85	0.50
1:B:2:ALA:N	1:B:121:GLU:OE1	2.45	0.50
1:C:267:ASN:CB	1:C:271:GLY:H	2.25	0.50
1:A:67:TYR:O	1:A:90:GLN:OE1	2.30	0.49
1:D:66:GLU:O	1:D:67:TYR:HD1	1.95	0.49
1:D:104:SER:O	1:D:108:GLY:N	2.45	0.49
1:A:161:LYS:CB	1:A:163:ARG:HG2	2.42	0.48
1:A:267:ASN:C	1:A:269:ASN:N	2.38	0.48
1:A:41:PHE:CD1	1:A:58:LEU:HD11	2.48	0.48
1:A:22:TYR:OH	1:A:235:ALA:N	2.46	0.48
1:C:40:GLU:OE1	1:C:61:LYS:HD2	2.14	0.48
1:A:264:ASP:OD1	1:A:264:ASP:C	2.50	0.48
1:D:75:TRP:CD1	1:D:81:LEU:CD1	2.97	0.47
1:D:107:THR:C	1:D:109:LYS:H	2.18	0.47
1:D:123:ILE:O	1:D:123:ILE:HG13	2.15	0.47
1:A:22:TYR:OH	1:A:234:SER:HB3	2.13	0.47
1:B:123:ILE:CG2	1:B:125:LEU:CD1	2.93	0.46
2:B:302:MC3:H351	2:B:302:MC3:H322	1.52	0.46
1:B:74:LYS:O	1:B:81:LEU:HD12	2.16	0.46
1:C:104:SER:O	1:C:108:GLY:N	2.46	0.46
1:D:104:SER:O	1:D:108:GLY:HA2	2.14	0.46
1:D:75:TRP:HD1	1:D:81:LEU:CD1	2.30	0.45
1:C:142:LEU:HG	1:C:144:LEU:HD11	1.99	0.45
1:C:267:ASN:CG	1:C:271:GLY:H	2.20	0.45
1:C:142:LEU:CG	1:C:144:LEU:HD11	2.46	0.45
1:B:104:SER:O	1:B:108:GLY:N	2.46	0.45
1:C:224:LYS:HE3	1:C:232:CYS:SG	2.57	0.45
2:A:301:MC3:C38	2:A:301:MC3:C42	2.90	0.45
1:C:34:LYS:HB2	1:C:40:GLU:HG2	1.98	0.44
2:B:302:MC3:H443	2:B:302:MC3:H411	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:GLY:O	1:D:268:VAL:HG23	2.18	0.44
1:C:107:THR:CG2	1:C:109:LYS:HE3	2.46	0.44
1:B:58:LEU:HB3	1:B:75:TRP:HB3	2.00	0.44
1:B:224:LYS:HE2	1:B:232:CYS:SG	2.57	0.44
1:D:171:VAL:HG13	1:D:171:VAL:O	2.17	0.44
1:C:125:LEU:CD2	1:C:142:LEU:HD13	2.48	0.43
1:D:75:TRP:HD1	1:D:81:LEU:HD11	1.79	0.43
1:C:267:ASN:CB	1:C:270:ALA:HB3	2.41	0.43
1:D:73:GLU:CD	1:D:82:GLY:O	2.58	0.42
1:B:11:GLY:O	1:B:15:ARG:HG3	2.19	0.42
1:D:171:VAL:CG1	1:D:182:THR:OG1	2.67	0.42
1:A:118:TYR:O	1:A:125:LEU:HG	2.19	0.42
1:B:281:PHE:HD1	1:B:282:GLN:N	2.18	0.42
1:D:67:TYR:N	1:D:67:TYR:CD1	2.85	0.42
1:A:118:TYR:HB3	1:A:125:LEU:CD1	2.44	0.42
1:C:109:LYS:HE2	1:C:109:LYS:HB3	1.70	0.42
1:D:190:PHE:CZ	2:D:700:MC3:H332	2.55	0.42
1:A:243:ILE:HB	1:A:263:LEU:HB2	2.02	0.41
1:A:107:THR:HB	1:A:108:GLY:H	1.77	0.41
1:B:123:ILE:HG23	1:B:125:LEU:CD1	2.50	0.41
1:C:125:LEU:HD21	1:C:142:LEU:HD13	2.02	0.41
1:C:107:THR:OG1	1:C:109:LYS:CE	2.62	0.41
1:D:107:THR:C	1:D:109:LYS:N	2.74	0.41
1:A:22:TYR:OH	1:A:234:SER:C	2.59	0.40
1:B:262:LEU:O	1:B:273:HIS:HB2	2.20	0.40
1:B:24:PHE:CD2	1:B:262:LEU:HD12	2.55	0.40
1:D:175:THR:HG23	1:D:177:GLU:H	1.85	0.40
1:A:87:VAL:HG12	1:A:90:GLN:HB2	2.03	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%)	263 (94%)	12 (4%)	5 (2%)	8	36
1	B	279/291 (96%)	267 (96%)	10 (4%)	2 (1%)	22	56
1	C	279/291 (96%)	261 (94%)	18 (6%)	0	100	100
1	D	280/291 (96%)	264 (94%)	14 (5%)	2 (1%)	22	56
All	All	1118/1164 (96%)	1055 (94%)	54 (5%)	9 (1%)	19	52

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	THR
1	A	268	VAL
1	A	270	ALA
1	B	271	GLY
1	D	108	GLY
1	A	108	GLY
1	A	111	ASN
1	D	270	ALA
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%)	223 (97%)	6 (3%)	46	71
1	B	229/238 (96%)	221 (96%)	8 (4%)	36	64
1	C	229/238 (96%)	226 (99%)	3 (1%)	69	82
1	D	229/238 (96%)	221 (96%)	8 (4%)	36	64
All	All	916/952 (96%)	891 (97%)	25 (3%)	44	71

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	93	ARG

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Mol	Chain	Res	Type
1	A	101	SER
1	A	104	SER
1	A	109	LYS
1	A	120	ARG
1	B	66	GLU
1	B	90	GLN
1	B	110	LYS
1	B	120	ARG
1	B	142	LEU
1	B	218	ARG
1	B	273	HIS
1	B	281	PHE
1	C	37	ASN
1	C	120	ARG
1	C	197	LYS
1	D	93	ARG
1	D	120	ARG
1	D	155	MET
1	D	163	ARG
1	D	176	ASP
1	D	262	LEU
1	D	268	VAL
1	D	281	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	106	ASN
1	A	156	ASN
1	C	106	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	D	700	-	19,22,45	1.42	1 (5%)	19,24,53	2.35	4 (21%)
2	MC3	A	302	-	19,22,45	1.18	1 (5%)	19,24,53	1.37	4 (21%)
2	MC3	B	302	-	19,22,45	1.16	2 (10%)	19,24,53	1.50	3 (15%)
2	MC3	A	301	-	19,22,45	1.23	1 (5%)	19,24,53	1.74	3 (15%)
2	MC3	B	301	-	19,22,45	1.29	1 (5%)	19,24,53	1.21	2 (10%)

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	D	700	-	-	13/20/22/49	-
2	MC3	A	302	-	-	11/20/22/49	-
2	MC3	B	302	-	-	13/20/22/49	-
2	MC3	A	301	-	-	14/20/22/49	-
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	D	700	MC3	O2-C31	5.45	1.49	1.34
2	B	301	MC3	O2-C31	4.92	1.48	1.34
2	A	301	MC3	O2-C31	4.35	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	MC3	O2-C31	4.34	1.46	1.34
2	B	302	MC3	O2-C31	4.09	1.45	1.34
2	B	302	MC3	O2-C2	-2.11	1.43	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	700	MC3	C2-O2-C31	7.44	127.45	117.88
2	A	301	MC3	C2-O2-C31	-5.34	111.01	117.88
2	D	700	MC3	O2-C2-C3	4.95	119.24	107.93
2	B	302	MC3	C2-O2-C31	-4.17	112.51	117.88
2	A	301	MC3	O2-C31-C32	3.92	119.95	111.50
2	A	302	MC3	O2-C2-C3	3.71	116.40	107.93
2	D	700	MC3	O2-C31-C32	3.65	119.36	111.50
2	B	302	MC3	O2-C31-C32	3.42	118.88	111.50
2	B	301	MC3	O2-C31-C32	3.20	118.40	111.50
2	A	302	MC3	O2-C31-C32	2.89	117.73	111.50
2	D	700	MC3	O2-C2-C1	2.47	111.86	106.13
2	A	302	MC3	C2-O2-C31	2.22	120.73	117.88
2	B	302	MC3	O2-C2-C1	2.19	111.21	106.13
2	A	301	MC3	O2-C2-C1	2.16	111.14	106.13
2	B	301	MC3	O2-C2-C1	2.05	110.88	106.13
2	A	302	MC3	C3-C2-C1	-2.03	106.81	112.63

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	700	MC3	O3P-C1-C2-C3
2	D	700	MC3	C3-C2-O2-C31
2	A	302	MC3	C3-C2-O2-C31
2	B	302	MC3	C2-C1-O3P-P
2	B	302	MC3	C1-C2-O2-C31
2	A	301	MC3	C2-C1-O3P-P
2	A	301	MC3	C3-C2-O2-C31
2	A	301	MC3	C32-C31-O2-C2
2	A	301	MC3	O31-C31-O2-C2
2	B	301	MC3	O3P-C1-C2-C3
2	B	301	MC3	O3P-C1-C2-O2
2	B	301	MC3	C3-C2-O2-C31
2	B	301	MC3	C32-C31-O2-C2
2	B	301	MC3	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
2	A	301	MC3	C38-C39-C40-C41
2	B	302	MC3	C32-C33-C34-C35
2	A	302	MC3	C34-C35-C36-C37
2	D	700	MC3	C32-C33-C34-C35
2	A	301	MC3	C37-C38-C39-C40
2	A	302	MC3	C32-C33-C34-C35
2	D	700	MC3	C31-C32-C33-C34
2	A	301	MC3	C36-C37-C38-C39
2	B	302	MC3	C36-C37-C38-C39
2	A	302	MC3	C32-C31-O2-C2
2	B	302	MC3	C37-C38-C39-C40
2	B	302	MC3	C34-C35-C36-C37
2	A	302	MC3	O31-C31-O2-C2
2	D	700	MC3	C40-C41-C42-C43
2	A	301	MC3	C40-C41-C42-C43
2	A	302	MC3	C33-C34-C35-C36
2	A	302	MC3	C39-C40-C41-C42
2	B	301	MC3	C34-C35-C36-C37
2	A	302	MC3	C37-C38-C39-C40
2	B	301	MC3	C38-C39-C40-C41
2	A	302	MC3	C36-C37-C38-C39
2	A	301	MC3	C34-C35-C36-C37
2	D	700	MC3	O3P-C1-C2-O2
2	D	700	MC3	C41-C42-C43-C44
2	D	700	MC3	C34-C35-C36-C37
2	B	302	MC3	C33-C34-C35-C36
2	A	301	MC3	C33-C34-C35-C36
2	B	302	MC3	C38-C39-C40-C41
2	A	301	MC3	C41-C42-C43-C44
2	A	302	MC3	C38-C39-C40-C41
2	D	700	MC3	C37-C38-C39-C40
2	B	301	MC3	C2-C1-O3P-P
2	B	301	MC3	C33-C34-C35-C36
2	B	302	MC3	C41-C42-C43-C44
2	B	302	MC3	C40-C41-C42-C43
2	B	302	MC3	C35-C36-C37-C38
2	A	302	MC3	C35-C36-C37-C38
2	B	301	MC3	C40-C41-C42-C43
2	A	301	MC3	O3P-C1-C2-O2
2	A	301	MC3	C35-C36-C37-C38
2	B	302	MC3	O2-C31-C32-C33
2	D	700	MC3	O31-C31-O2-C2

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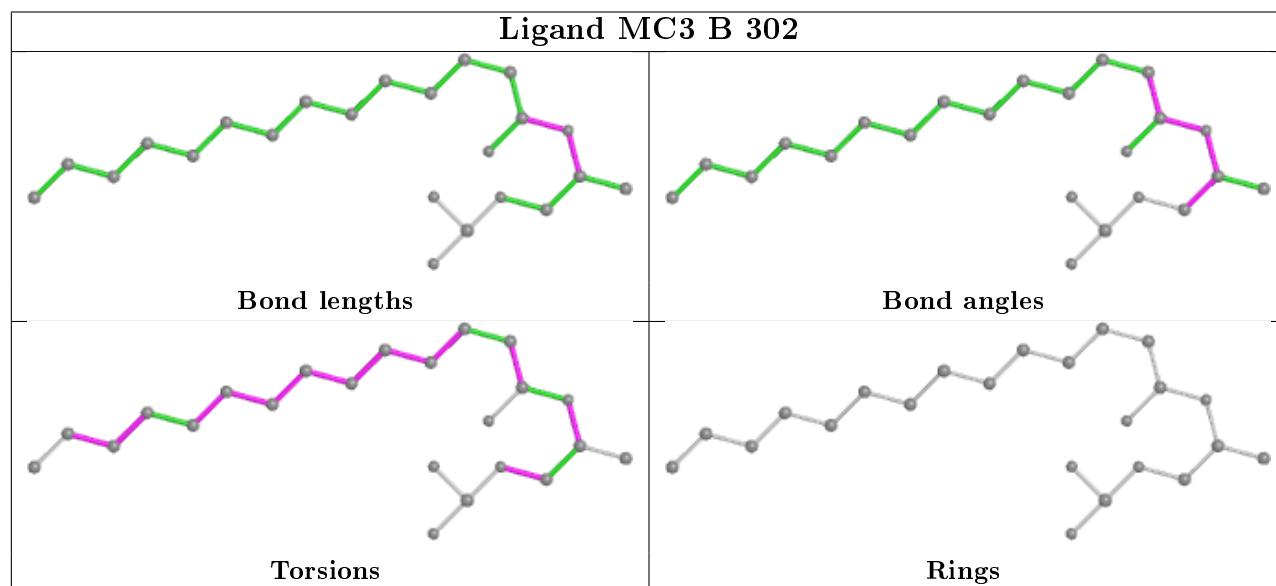
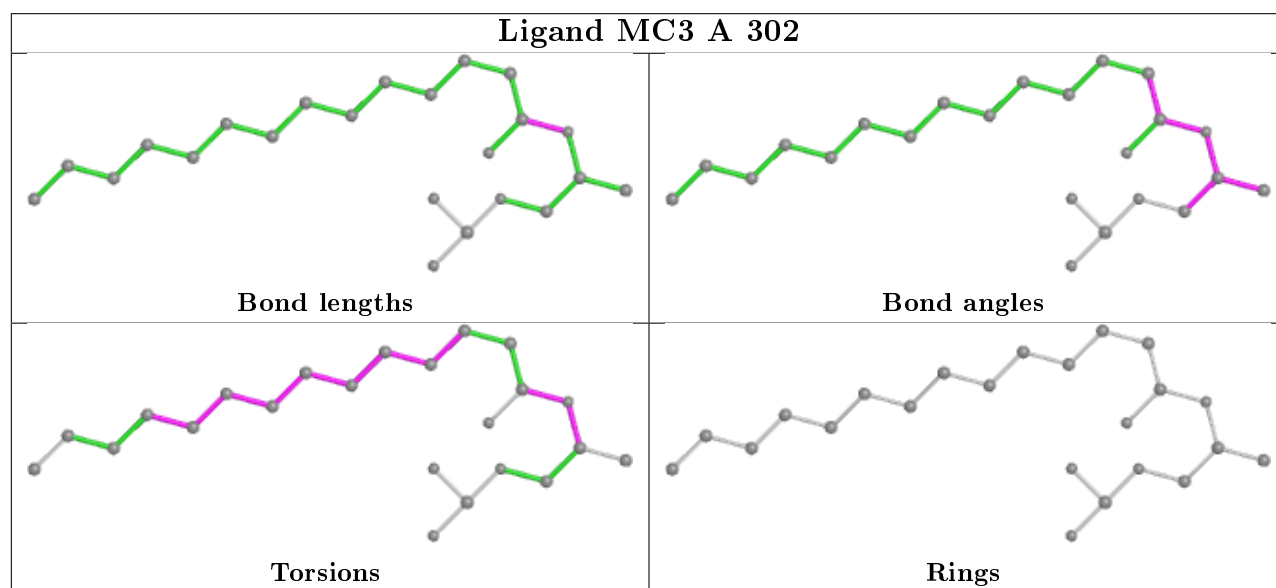
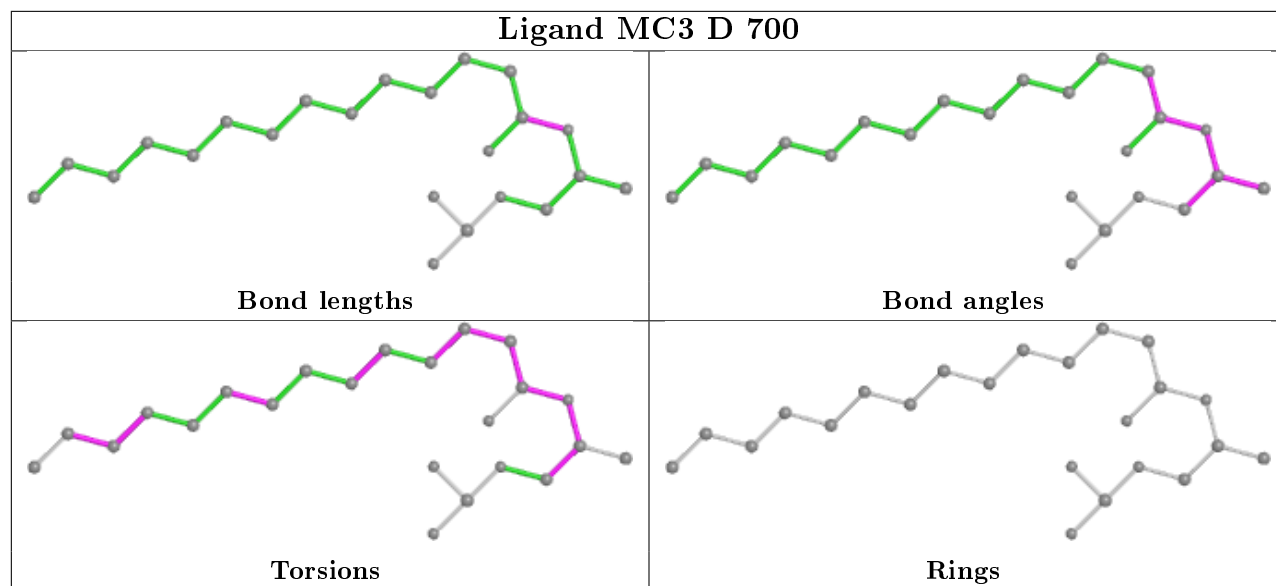
Mol	Chain	Res	Type	Atoms
2	B	301	MC3	C39-C40-C41-C42
2	D	700	MC3	C32-C31-O2-C2
2	B	302	MC3	O31-C31-C32-C33
2	A	301	MC3	C32-C33-C34-C35
2	D	700	MC3	O2-C31-C32-C33
2	D	700	MC3	O31-C31-C32-C33

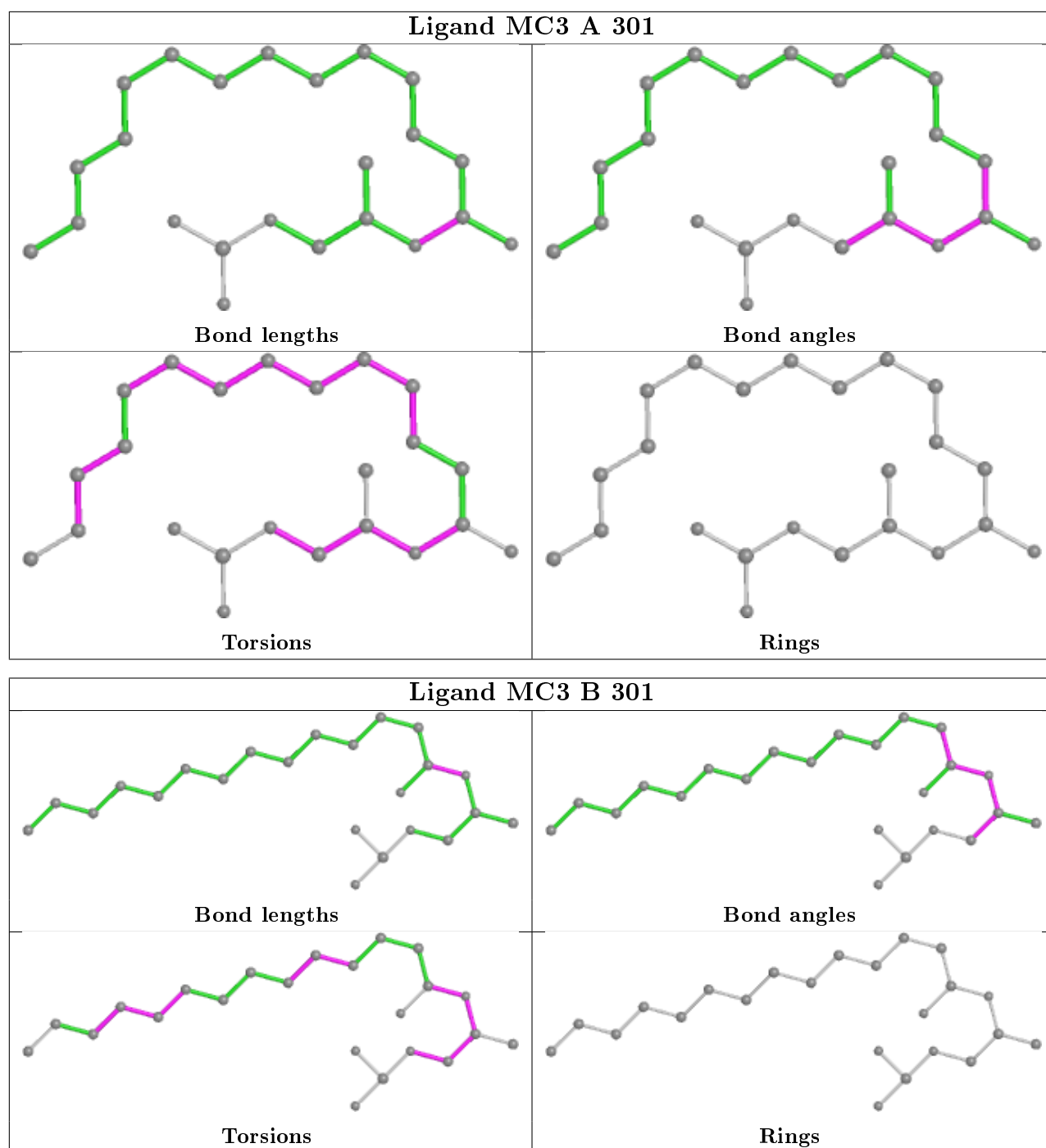
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	700	MC3	2	0
2	B	302	MC3	6	0
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%)	-0.26	12 (4%) 35 33	61, 103, 149, 176	57 (20%)
1	B	281/291 (96%)	-0.40	5 (1%) 68 66	59, 108, 165, 217	46 (16%)
1	C	281/291 (96%)	0.00	17 (6%) 21 21	58, 109, 161, 201	70 (24%)
1	D	282/291 (96%)	-0.33	8 (2%) 53 51	53, 111, 169, 241	47 (16%)
All	All	1126/1164 (96%)	-0.25	42 (3%) 41 39	53, 108, 164, 241	220 (19%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	LYS	9.0
1	C	106	ASN	7.3
1	C	77	THR	7.2
1	C	103	PHE	6.8
1	C	111	ASN	6.6
1	D	271	GLY	6.2
1	C	38	GLY	6.1
1	C	107	THR	5.9
1	A	36	GLU	5.9
1	C	105	PRO	4.9
1	A	103	PHE	4.5
1	C	269	ASN	4.4
1	D	111	ASN	4.4
1	A	37	ASN	4.4
1	D	36	GLU	4.4
1	C	102	SER	4.2
1	A	271	GLY	4.2
1	B	270	ALA	4.1
1	C	109	LYS	4.0
1	A	102	SER	4.0
1	D	270	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	79	ASN	3.8
1	B	271	GLY	3.7
1	C	108	GLY	3.4
1	C	56	GLY	3.4
1	D	105	PRO	3.0
1	B	133	ILE	2.8
1	A	105	PRO	2.5
1	C	55	THR	2.5
1	D	75	TRP	2.5
1	A	110	LYS	2.4
1	A	111	ASN	2.4
1	C	80	THR	2.4
1	D	112	ALA	2.3
1	A	272	GLY	2.2
1	A	106	ASN	2.2
1	C	62	TYR	2.2
1	B	269	ASN	2.2
1	A	109	LYS	2.2
1	A	108	GLY	2.2
1	C	32	LYS	2.1
1	D	272	GLY	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, 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.

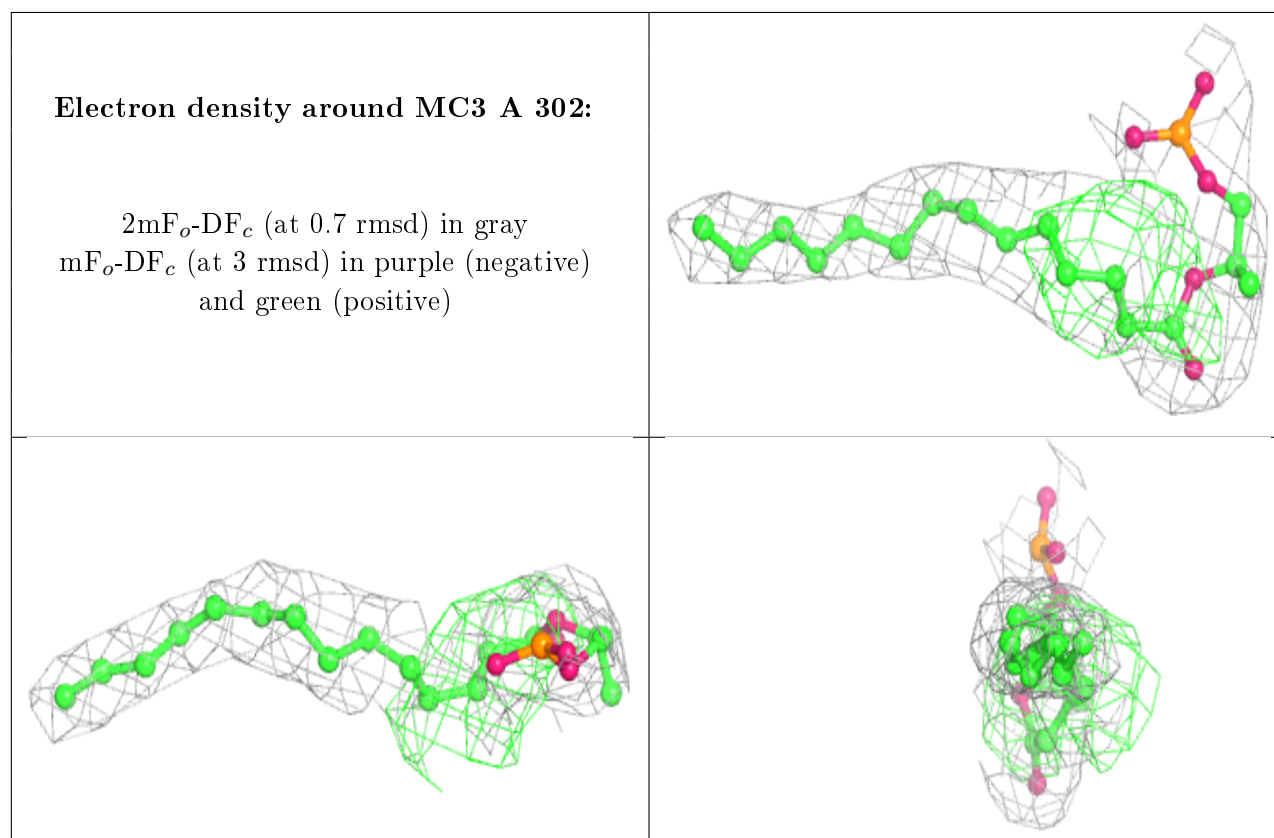
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MC3	A	302	23/46	0.68	0.36	44,85,123,131	11
2	MC3	B	301	23/46	0.71	0.39	50,71,88,101	10

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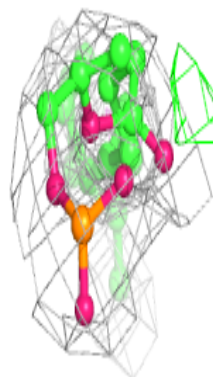
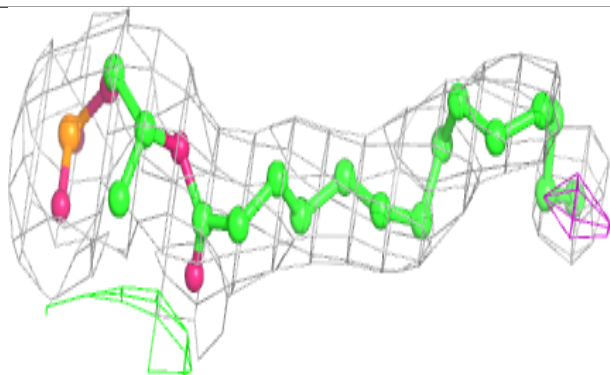
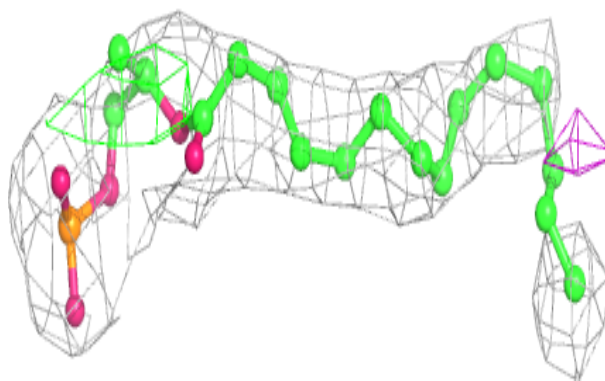
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MC3	A	301	23/46	0.76	0.41	26,46,82,87	23
2	MC3	D	700	23/46	0.80	0.22	75,91,108,114	6
2	MC3	B	302	23/46	0.83	0.33	38,56,118,127	23

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.

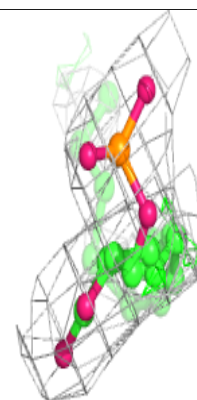
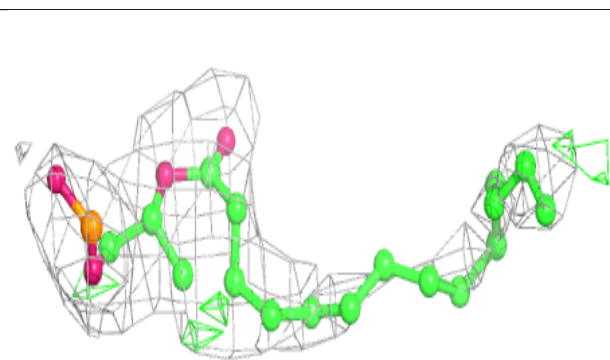
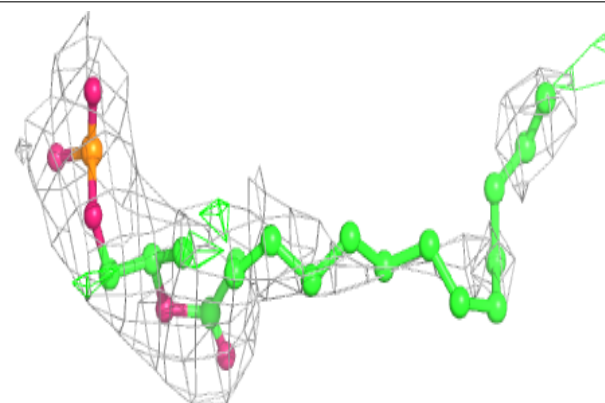


Electron density around MC3 B 301:

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

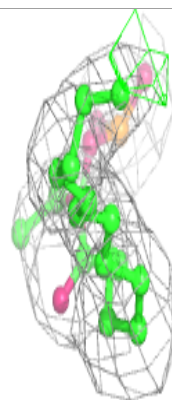
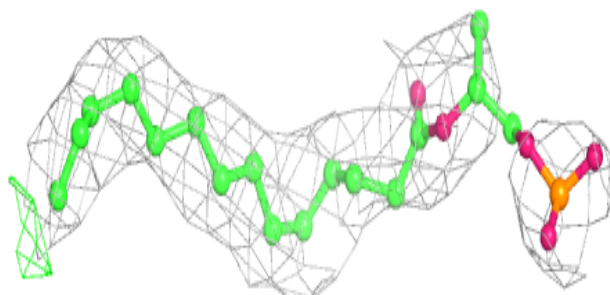
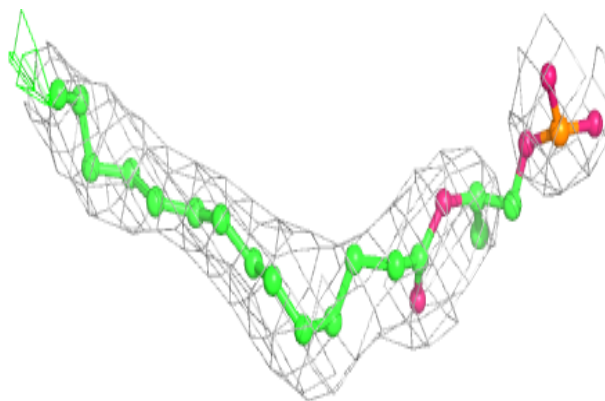
**Electron density around MC3 A 301:**

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

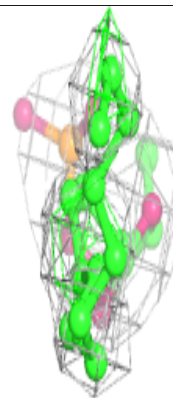
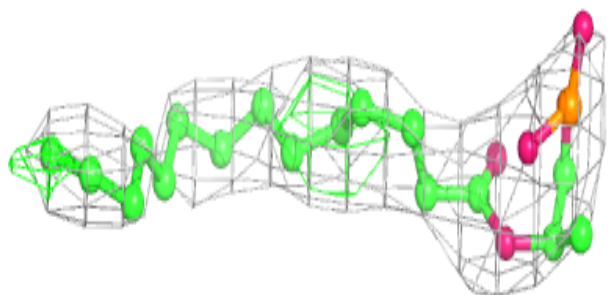
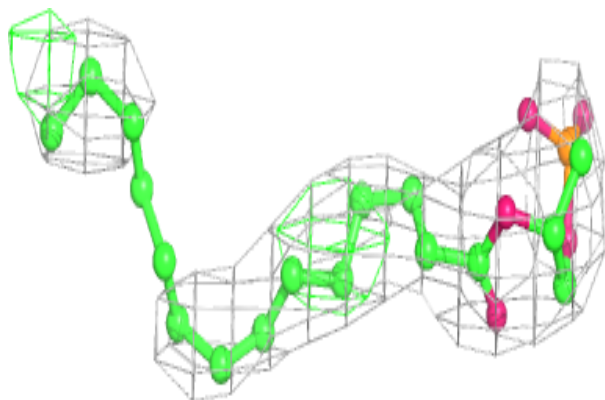


Electron density around MC3 D 700:

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

**Electron density around MC3 B 302:**

$2mF_o-DF_c$ (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.