



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:35 pm BST

PDB ID : 2AG2
Title : Crystal Structure Analysis of GM2-activator protein complexed with Phosphatidylcholine
Authors : Wright, C.S.; Mi, L.Z.; Lee, S.; Rastinejad, F.
Deposited on : 2005-07-26
Resolution : 2.00 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

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

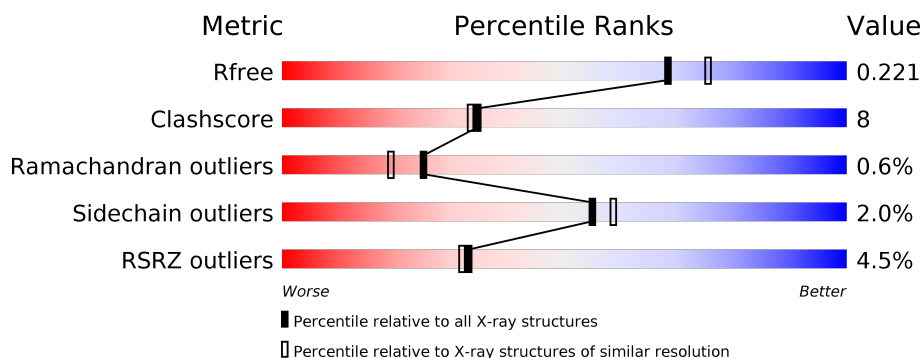
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 ≥ 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	164	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	164	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>
1	C	164	<div> <div>9%</div> <div> <div></div> <div>83%</div> <div>13%</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
6	CH5	B	2341	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4639 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 Ganglioside GM2 activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	9	0	0
			1242	797	195	240	10			
1	B	164	Total	C	N	O	S	8	0	0
			1242	797	195	240	10			
1	C	162	Total	C	N	O	S	0	0	0
			1230	790	193	238	9			

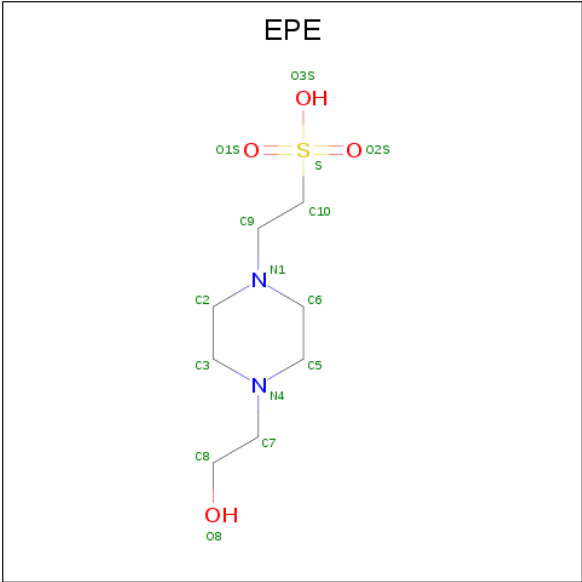
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	CLONING ARTIFACT	UNP P17900
A	2	MET	-	CLONING ARTIFACT	UNP P17900
B	1	HIS	-	CLONING ARTIFACT	UNP P17900
B	2	MET	-	CLONING ARTIFACT	UNP P17900
C	1	HIS	-	CLONING ARTIFACT	UNP P17900
C	2	MET	-	CLONING ARTIFACT	UNP P17900

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

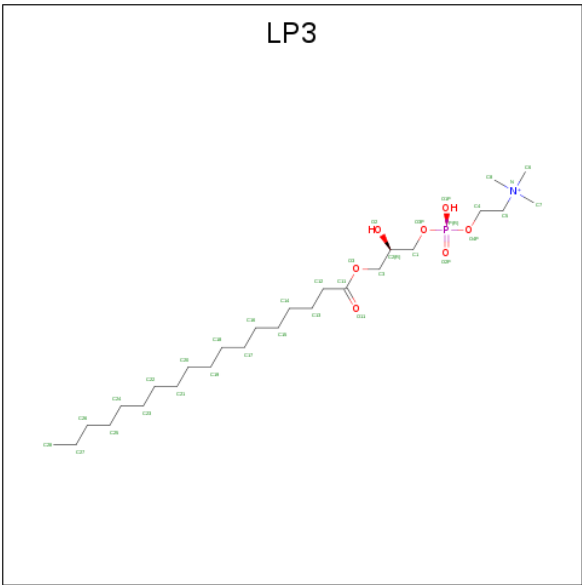
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is (7R)-4,7-DIHYDROXY-N,N,N-TRIMETHYL-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOSAN-1-AMINIUM 4-OXIDE (three-letter code: LP3) (formula: C₂₆H₅₅NO₇P).



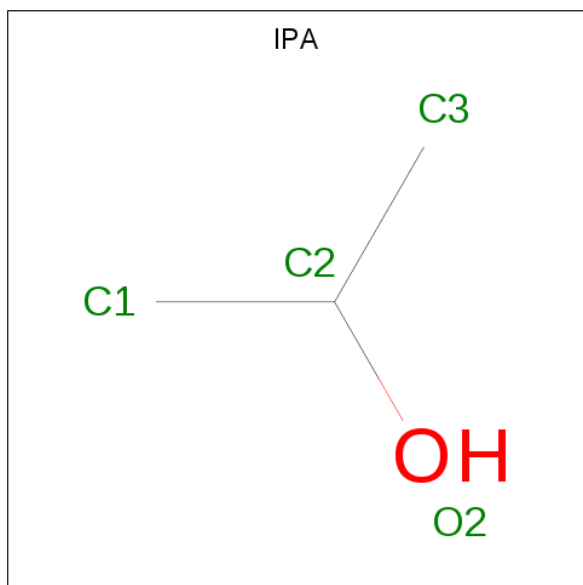
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			35	26	1	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			35	26	1	7	1		
4	B	1	Total	C	N	O	P	0	0
			35	26	1	7	1		
4	C	1	Total	C	N	O	P	0	0
			35	26	1	7	1		

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



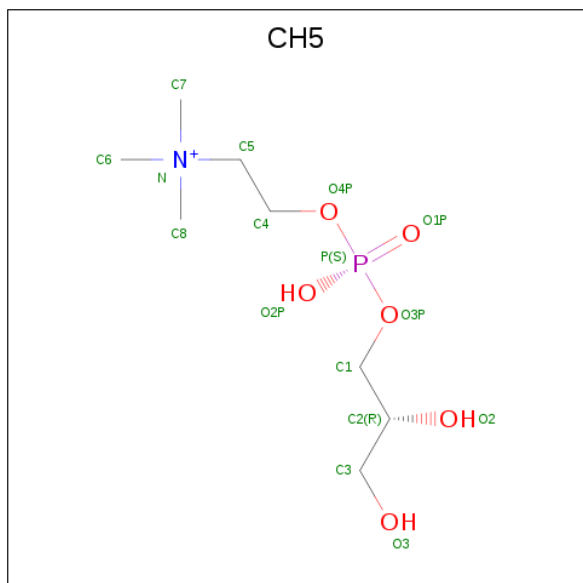
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	3	1		
5	A	1	Total	C	O	0	0
			4	3	1		
5	B	1	Total	C	O	0	0
			4	3	1		
5	B	1	Total	C	O	0	0
			4	3	1		
5	B	1	Total	C	O	0	0
			4	3	1		
5	C	1	Total	C	O	0	0
			4	3	1		
5	C	1	Total	C	O	0	0
			4	3	1		
5	C	1	Total	C	O	0	0
			4	3	1		

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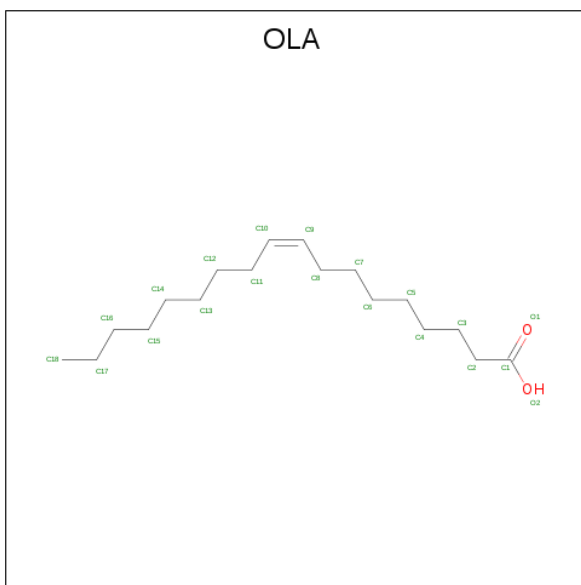
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	3	1		
5	C	1	Total	C	O	0	0
			4	3	1		

- Molecule 6 is 2-(((R)-2,3-DIHYDROXYPROPYL)PHOSPHORYLOXY)-N,N,N-TRIMETHYLETHANAMINIUM (three-letter code: CH5) (formula: C₈H₂₁NO₆P).



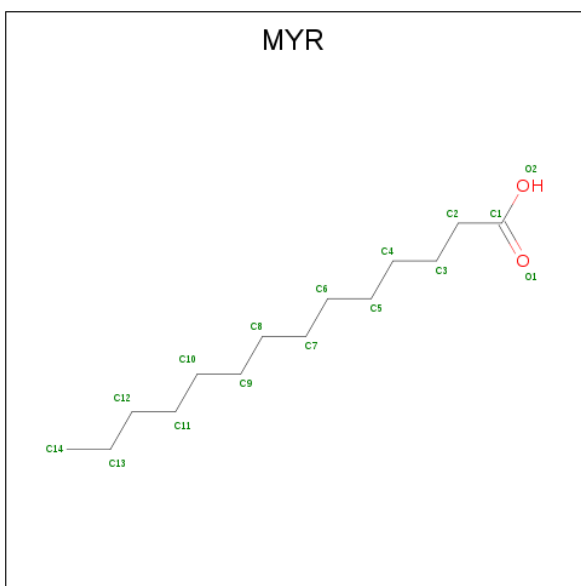
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
6	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 7 is OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).



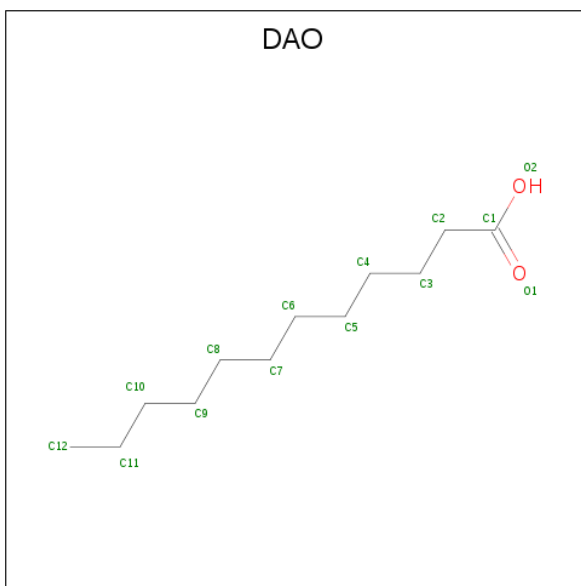
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	2	0
			20	18	2		
7	C	1	Total	C	O	1	0
			20	18	2		

- Molecule 8 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			16	14	2		
8	C	1	Total	C	O	0	0
			16	14	2		

- Molecule 9 is LAURIC ACID (three-letter code: DAO) (formula: C₁₂H₂₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			14	12	2		

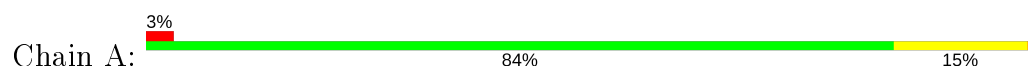
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	211	Total	O	0	0
			211	211		
10	B	192	Total	O	0	0
			192	192		
10	C	191	Total	O	0	0
			191	191		

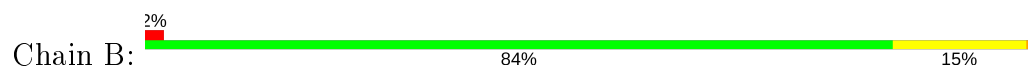
3 Residue-property plots [i](#)

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.

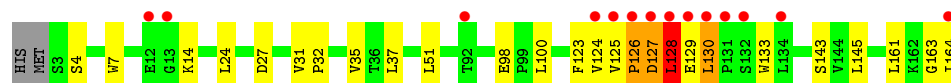
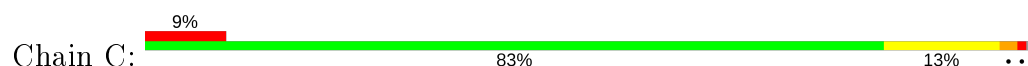
- Molecule 1: Ganglioside GM2 activator



- Molecule 1: Ganglioside GM2 activator



- Molecule 1: Ganglioside GM2 activator



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.53Å 86.19Å 120.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.00 19.76 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.76-2.00) 99.8 (19.76-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.07 (at 2.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.188 , 0.231 0.182 , 0.221	Depositor DCC
R_{free} test set	2289 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4639	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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: OLA, IPA, CL, MYR, LP3, DAO, CH5, EPE

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	0.51	0/1274	0.72	1/1739 (0.1%)
1	B	0.52	0/1274	0.74	0/1739
1	C	0.48	0/1262	0.71	0/1724
All	All	0.50	0/3810	0.73	1/5202 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ARG	NE-CZ-NH2	-6.50	117.05	120.30

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	1242	0	1240	16	0
1	B	1242	0	1240	22	0
1	C	1230	0	1227	22	0
2	A	1	0	0	1	0
2	B	1	0	0	1	0
2	C	1	0	0	0	0
3	A	15	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	15	0	17	2	0
4	A	70	0	108	7	0
4	B	35	0	54	5	0
4	C	35	0	54	2	0
5	A	8	0	16	1	0
5	B	12	0	24	1	0
5	C	20	0	40	1	0
6	B	16	0	20	1	0
6	C	16	0	20	0	0
7	B	20	0	33	4	0
7	C	20	0	33	1	0
8	B	16	0	27	2	0
8	C	16	0	27	0	0
9	B	14	0	23	1	0
10	A	211	0	0	2	0
10	B	192	0	0	2	0
10	C	191	0	0	3	0
All	All	4639	0	4220	68	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 (68) 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:B:51:LEU:HD22	1:B:145:LEU:HD11	1.71	0.71
1:B:132:SER:HB2	1:B:163:GLY:O	1.91	0.70
1:A:128:LEU:O	1:A:130:LEU:HD13	1.96	0.66
4:C:2346:LP3:H63	5:C:1510:IPA:H33	1.78	0.65
1:C:7:TRP:O	3:C:901:EPE:H102	1.96	0.64
1:C:143:SER:OG	4:C:2346:LP3:H42	1.98	0.63
1:B:107:CYS:HA	5:B:1515:IPA:H11	1.83	0.61
1:B:132:SER:HB2	1:B:163:GLY:C	2.22	0.59
1:A:53:VAL:HG21	4:A:2345:LP3:H82	1.85	0.59
1:A:83:CYS:HB2	2:A:801:CL:CL	2.41	0.58
1:C:4:SER:HB2	1:C:27:ASP:OD1	2.03	0.57
1:B:39:VAL:HG13	7:B:3628:OLA:H162	1.87	0.56
1:C:128:LEU:HA	1:C:130:LEU:HD11	1.88	0.55
1:C:125:VAL:O	1:C:127:ASP:N	2.39	0.55
1:A:66:ILE:HD12	1:A:66:ILE:N	2.22	0.54
1:C:35:VAL:HG13	1:C:123:PHE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:GLY:O	1:C:164:ILE:HB	2.08	0.54
1:C:98:GLU:OE1	1:C:98:GLU:HA	2.07	0.54
1:B:31:VAL:HG22	1:B:125:VAL:HG11	1.90	0.53
4:A:2344:LP3:H272	4:A:2345:LP3:H162	1.91	0.53
1:B:112:LYS:HG2	10:B:3723:HOH:O	2.08	0.53
1:B:155:ILE:HG23	4:B:2343:LP3:O2P	2.09	0.52
4:A:2344:LP3:H132	10:A:2516:HOH:O	2.10	0.52
1:B:17:ALA:HB1	4:B:2343:LP3:H32	1.92	0.51
1:B:92:THR:HG22	1:B:93:GLY:N	2.25	0.51
1:C:31:VAL:HG22	1:C:125:VAL:HG11	1.91	0.51
1:B:128:LEU:HD12	1:B:135:THR:HG21	1.94	0.50
1:C:31:VAL:CG2	1:C:125:VAL:HG11	2.42	0.50
1:C:24:LEU:HD11	1:C:35:VAL:HG21	1.94	0.49
1:A:109:CYS:HB3	1:A:110:PRO:HA	1.95	0.48
1:C:14:LYS:HD3	10:C:3656:HOH:O	2.14	0.48
1:B:59:LYS:HD2	6:B:2341:CH5:H83	1.96	0.48
1:B:126:PRO:HB2	9:B:1364:DAO:H122	1.96	0.48
1:C:125:VAL:O	1:C:126:PRO:C	2.52	0.47
1:B:51:LEU:HD22	1:B:145:LEU:CD1	2.43	0.47
1:B:83:CYS:HB2	2:B:802:CL:CL	2.51	0.47
1:A:162:LYS:HD3	10:A:2513:HOH:O	2.14	0.46
1:A:129:GLU:O	1:A:130:LEU:HD12	2.16	0.46
1:C:124:VAL:HG13	1:C:124:VAL:O	2.16	0.46
1:A:57:LEU:HG	1:A:68:ILE:HD12	1.98	0.45
1:C:7:TRP:CZ2	3:C:901:EPE:H22	2.51	0.45
1:C:127:ASP:O	1:C:128:LEU:O	2.34	0.45
1:C:129:GLU:HA	10:C:3811:HOH:O	2.17	0.45
1:A:98:GLU:OE1	1:A:98:GLU:HA	2.17	0.45
4:B:2343:LP3:H121	7:B:3628:OLA:H131	1.99	0.45
1:B:47:LEU:HB2	1:B:111:PHE:HB2	1.99	0.44
1:B:24:LEU:HD21	1:B:29:ILE:HD11	2.00	0.44
1:C:51:LEU:HG	1:C:145:LEU:HD11	2.00	0.44
1:C:100:LEU:N	1:C:100:LEU:HD12	2.33	0.44
1:A:29:ILE:HG23	1:A:35:VAL:CG1	2.48	0.43
1:A:37:LEU:HG	1:A:38:SER:N	2.33	0.43
4:B:2343:LP3:H82	8:B:3046:MYR:H111	2.00	0.43
1:C:31:VAL:HA	1:C:32:PRO:C	2.38	0.43
4:A:2344:LP3:H251	4:A:2345:LP3:H162	2.01	0.43
1:A:143:SER:O	1:A:154:CYS:HA	2.19	0.43
1:A:39:VAL:HG13	4:A:2344:LP3:H262	2.00	0.43
1:B:19:ILE:HG12	1:B:155:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:THR:HG22	1:B:93:GLY:H	1.84	0.43
4:A:2344:LP3:H142	5:A:1504:IPA:H12	2.01	0.43
1:B:41:GLY:HA3	7:B:3628:OLA:H152	2.01	0.43
1:C:24:LEU:HD22	7:C:3629:OLA:H52	2.02	0.42
1:A:29:ILE:HB	1:A:161:LEU:HD23	2.01	0.42
8:B:3046:MYR:H131	10:B:3820:HOH:O	2.19	0.42
1:C:133:TRP:HD1	10:C:3813:HOH:O	2.03	0.42
1:B:19:ILE:HD11	7:B:3628:OLA:H112	2.01	0.41
1:A:100:LEU:HD11	4:A:2345:LP3:H241	2.01	0.41
1:A:52:LYS:HE2	1:A:54:ASP:OD1	2.20	0.41
1:B:143:SER:OG	4:B:2343:LP3:H42	2.20	0.41

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	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
1	B	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	C	160/164 (98%)	151 (94%)	6 (4%)	3 (2%)	8	3
All	All	484/492 (98%)	468 (97%)	13 (3%)	3 (1%)	25	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	127	ASP
1	C	128	LEU
1	C	126	PRO

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	147/148 (99%)	144 (98%)	3 (2%)	55	58
1	B	147/148 (99%)	145 (99%)	2 (1%)	67	72
1	C	146/148 (99%)	142 (97%)	4 (3%)	44	46
All	All	440/444 (99%)	431 (98%)	9 (2%)	55	58

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

Mol	Chain	Res	Type
1	A	2	MET
1	A	37	LEU
1	A	122	GLU
1	B	37	LEU
1	B	51	LEU
1	C	37	LEU
1	C	128	LEU
1	C	130	LEU
1	C	161	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

Of 26 ligands modelled in this entry, 3 are monoatomic - leaving 23 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
4	LP3	A	2345	-	34,34,34	1.35	3 (8%)	39,41,41	0.83	1 (2%)
6	CH5	C	2342	-	15,15,15	1.27	1 (6%)	19,21,21	0.84	0
5	IPA	A	1502	-	3,3,3	0.51	0	3,3,3	0.92	0
3	EPE	C	901	-	15,15,15	1.25	2 (13%)	18,20,20	0.82	0
7	OLA	C	3629	-	16,19,19	0.23	0	15,19,19	1.24	2 (13%)
5	IPA	C	1513	-	3,3,3	0.54	0	3,3,3	0.92	0
5	IPA	C	1514	-	3,3,3	0.52	0	3,3,3	0.90	0
9	DAO	B	1364	-	10,13,13	0.25	0	9,13,13	0.27	0
5	IPA	A	1504	-	3,3,3	0.44	0	3,3,3	0.91	0
5	IPA	B	1509	-	3,3,3	0.51	0	3,3,3	0.97	0
5	IPA	C	1512	-	3,3,3	0.53	0	3,3,3	0.86	0
4	LP3	C	2346	-	34,34,34	1.33	3 (8%)	39,41,41	0.87	2 (5%)
6	CH5	B	2341	-	15,15,15	1.16	1 (6%)	19,21,21	0.83	0
5	IPA	C	1510	-	3,3,3	0.50	0	3,3,3	0.93	0
8	MYR	B	3046	-	12,15,15	0.18	0	11,15,15	0.50	0
4	LP3	A	2344	-	34,34,34	1.37	2 (5%)	39,41,41	0.85	2 (5%)
5	IPA	C	1511	-	3,3,3	0.49	0	3,3,3	0.88	0
5	IPA	B	1515	-	3,3,3	0.55	0	3,3,3	0.88	0
8	MYR	C	3045	-	12,15,15	0.23	0	11,15,15	0.45	0
4	LP3	B	2343	-	34,34,34	1.30	3 (8%)	39,41,41	0.88	2 (5%)
5	IPA	B	1508	-	3,3,3	0.46	0	3,3,3	0.89	0
7	OLA	B	3628	-	16,19,19	0.26	0	15,19,19	1.28	2 (13%)
3	EPE	A	900	-	15,15,15	1.30	3 (20%)	18,20,20	0.96	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
6	CH5	B	2341	-	-	8/16/16/16	-
8	MYR	B	3046	-	-	5/11/13/13	-
4	LP3	A	2345	-	-	15/36/36/36	-
6	CH5	C	2342	-	-	11/16/16/16	-
9	DAO	B	1364	-	-	4/9/11/11	-
8	MYR	C	3045	-	-	6/11/13/13	-
4	LP3	A	2344	-	-	20/36/36/36	-
4	LP3	B	2343	-	-	15/36/36/36	-
3	EPE	C	901	-	-	1/9/19/19	0/1/1/1
7	OLA	C	3629	-	-	8/15/17/17	-
4	LP3	C	2346	-	-	14/36/36/36	-
7	OLA	B	3628	-	-	9/15/17/17	-
3	EPE	A	900	-	-	0/9/19/19	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2344	LP3	O3-C11	6.08	1.51	1.33
4	A	2345	LP3	O3-C11	6.04	1.51	1.33
4	C	2346	LP3	O3-C11	5.93	1.50	1.33
4	B	2343	LP3	O3-C11	5.71	1.50	1.33
6	C	2342	CH5	O2-C2	2.86	1.51	1.43
4	A	2344	LP3	O2-C2	2.74	1.51	1.43
4	B	2343	LP3	O2-C2	2.57	1.51	1.43
6	B	2341	CH5	O2-C2	2.55	1.51	1.43
4	C	2346	LP3	O2-C2	2.49	1.50	1.43
4	A	2345	LP3	O2-C2	2.42	1.50	1.43
3	C	901	EPE	C6-N1	2.38	1.53	1.46
3	A	900	EPE	C6-N1	2.33	1.53	1.46
3	A	900	EPE	C2-N1	2.24	1.53	1.46
3	A	900	EPE	C10-S	2.23	1.80	1.77
4	B	2343	LP3	C12-C11	2.14	1.57	1.50
4	C	2346	LP3	C12-C11	2.10	1.56	1.50
4	A	2345	LP3	C12-C11	2.04	1.56	1.50
3	C	901	EPE	C10-S	2.03	1.80	1.77

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3628	OLA	C4-C3-C2	-3.59	99.81	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	3629	OLA	C4-C3-C2	-3.42	100.47	113.76
7	B	3628	OLA	C6-C5-C4	-2.83	100.05	114.42
7	C	3629	OLA	C6-C5-C4	-2.81	100.14	114.42
4	A	2344	LP3	O3-C11-C12	2.66	120.27	111.91
4	B	2343	LP3	O3-C11-C12	2.55	119.91	111.91
4	A	2345	LP3	O3-C11-C12	2.48	119.69	111.91
4	C	2346	LP3	O3-C11-C12	2.41	119.46	111.91
4	C	2346	LP3	P-O4P-C4	-2.14	111.06	121.59
4	B	2343	LP3	O3-C11-O11	-2.04	118.45	123.59
4	A	2344	LP3	P-O4P-C4	-2.01	111.71	121.59

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2345	LP3	O3P-C1-C2-C3
4	A	2345	LP3	C1-C2-C3-O3
4	A	2345	LP3	O2-C2-C3-O3
4	A	2345	LP3	C12-C11-O3-C3
4	A	2345	LP3	O11-C11-O3-C3
6	C	2342	CH5	O3P-C1-C2-C3
6	C	2342	CH5	O3P-C1-C2-O2
6	C	2342	CH5	C1-C2-C3-O3
6	C	2342	CH5	O2-C2-C3-O3
6	C	2342	CH5	C4-O4P-P-O1P
4	C	2346	LP3	C1-C2-C3-O3
4	C	2346	LP3	O2-C2-C3-O3
4	C	2346	LP3	C12-C11-O3-C3
4	C	2346	LP3	O11-C11-O3-C3
6	B	2341	CH5	C1-C2-C3-O3
6	B	2341	CH5	O2-C2-C3-O3
4	A	2344	LP3	O3P-C1-C2-C3
4	A	2344	LP3	C1-C2-C3-O3
4	A	2344	LP3	O2-C2-C3-O3
4	A	2344	LP3	C12-C11-O3-C3
4	A	2344	LP3	O11-C11-O3-C3
4	B	2343	LP3	C1-C2-C3-O3
4	B	2343	LP3	O2-C2-C3-O3
4	B	2343	LP3	C12-C11-O3-C3
4	B	2343	LP3	O11-C11-O3-C3
7	B	3628	OLA	C11-C10-C9-C8
4	A	2345	LP3	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	B	2341	CH5	O3P-C1-C2-C3
4	A	2344	LP3	C11-C12-C13-C14
4	C	2346	LP3	O3P-C1-C2-O2
4	B	2343	LP3	O3P-C1-C2-O2
4	C	2346	LP3	O3P-C1-C2-C3
4	B	2343	LP3	O3P-C1-C2-C3
7	B	3628	OLA	C3-C4-C5-C6
4	B	2343	LP3	C22-C23-C24-C25
8	C	3045	MYR	C11-C10-C9-C8
7	C	3629	OLA	C5-C6-C7-C8
4	C	2346	LP3	C16-C17-C18-C19
4	B	2343	LP3	C19-C20-C21-C22
3	C	901	EPE	N4-C7-C8-O8
4	A	2345	LP3	C12-C13-C14-C15
4	B	2343	LP3	C16-C17-C18-C19
4	A	2344	LP3	C23-C24-C25-C26
7	C	3629	OLA	C4-C5-C6-C7
4	C	2346	LP3	C20-C21-C22-C23
8	C	3045	MYR	C5-C6-C7-C8
7	B	3628	OLA	C5-C6-C7-C8
4	A	2344	LP3	C16-C17-C18-C19
4	B	2343	LP3	C21-C22-C23-C24
4	A	2344	LP3	C22-C23-C24-C25
8	B	3046	MYR	C7-C8-C9-C10
8	B	3046	MYR	C9-C10-C11-C12
4	A	2345	LP3	C22-C23-C24-C25
6	B	2341	CH5	O3P-C1-C2-O2
4	B	2343	LP3	C17-C18-C19-C20
9	B	1364	DAO	C5-C6-C7-C8
8	B	3046	MYR	C4-C5-C6-C7
7	C	3629	OLA	C3-C4-C5-C6
9	B	1364	DAO	C3-C4-C5-C6
7	B	3628	OLA	C4-C5-C6-C7
4	A	2344	LP3	C15-C16-C17-C18
8	C	3045	MYR	C4-C5-C6-C7
4	B	2343	LP3	C15-C16-C17-C18
8	B	3046	MYR	C3-C4-C5-C6
4	C	2346	LP3	C22-C23-C24-C25
7	B	3628	OLA	C7-C8-C9-C10
7	B	3628	OLA	C14-C15-C16-C17
4	C	2346	LP3	C18-C19-C20-C21
4	A	2344	LP3	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
7	C	3629	OLA	C13-C14-C15-C16
9	B	1364	DAO	C6-C7-C8-C9
4	B	2343	LP3	C24-C25-C26-C27
4	C	2346	LP3	C17-C18-C19-C20
7	B	3628	OLA	C10-C11-C12-C13
4	A	2345	LP3	C23-C24-C25-C26
4	A	2344	LP3	C12-C13-C14-C15
4	A	2345	LP3	C18-C19-C20-C21
7	C	3629	OLA	C11-C10-C9-C8
4	C	2346	LP3	C21-C22-C23-C24
4	A	2344	LP3	O3P-C1-C2-O2
8	C	3045	MYR	C7-C8-C9-C10
4	B	2343	LP3	C20-C21-C22-C23
4	A	2345	LP3	C21-C22-C23-C24
4	C	2346	LP3	C19-C20-C21-C22
4	A	2344	LP3	C21-C22-C23-C24
9	B	1364	DAO	C11-C10-C9-C8
4	A	2344	LP3	C19-C20-C21-C22
4	A	2344	LP3	C17-C18-C19-C20
6	C	2342	CH5	C4-C5-N-C8
6	C	2342	CH5	C4-O4P-P-O3P
4	A	2344	LP3	C4-O4P-P-O3P
7	C	3629	OLA	C2-C3-C4-C5
4	A	2344	LP3	C2-C1-O3P-P
6	C	2342	CH5	C4-C5-N-C6
8	C	3045	MYR	C9-C10-C11-C12
4	A	2345	LP3	O4P-C4-C5-N
6	C	2342	CH5	O4P-C4-C5-N
4	C	2346	LP3	O4P-C4-C5-N
6	B	2341	CH5	O4P-C4-C5-N
4	A	2344	LP3	O4P-C4-C5-N
4	B	2343	LP3	O4P-C4-C5-N
7	C	3629	OLA	C9-C10-C11-C12
8	C	3045	MYR	C3-C4-C5-C6
6	C	2342	CH5	C4-C5-N-C7
7	B	3628	OLA	C9-C10-C11-C12
4	A	2345	LP3	C4-O4P-P-O3P
6	C	2342	CH5	C1-O3P-P-O4P
6	B	2341	CH5	C1-O3P-P-O4P
7	C	3629	OLA	C6-C7-C8-C9
7	B	3628	OLA	C11-C12-C13-C14
4	A	2344	LP3	C24-C25-C26-C27

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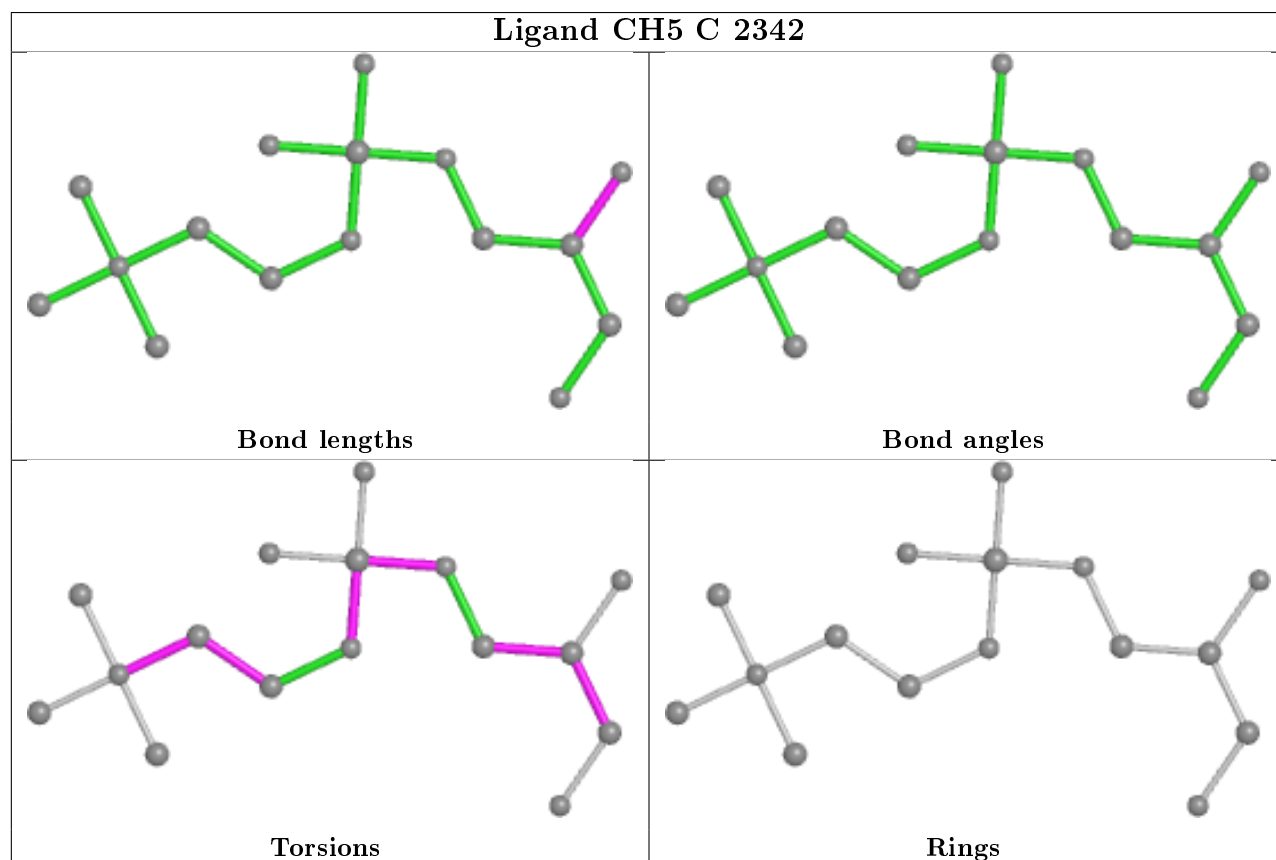
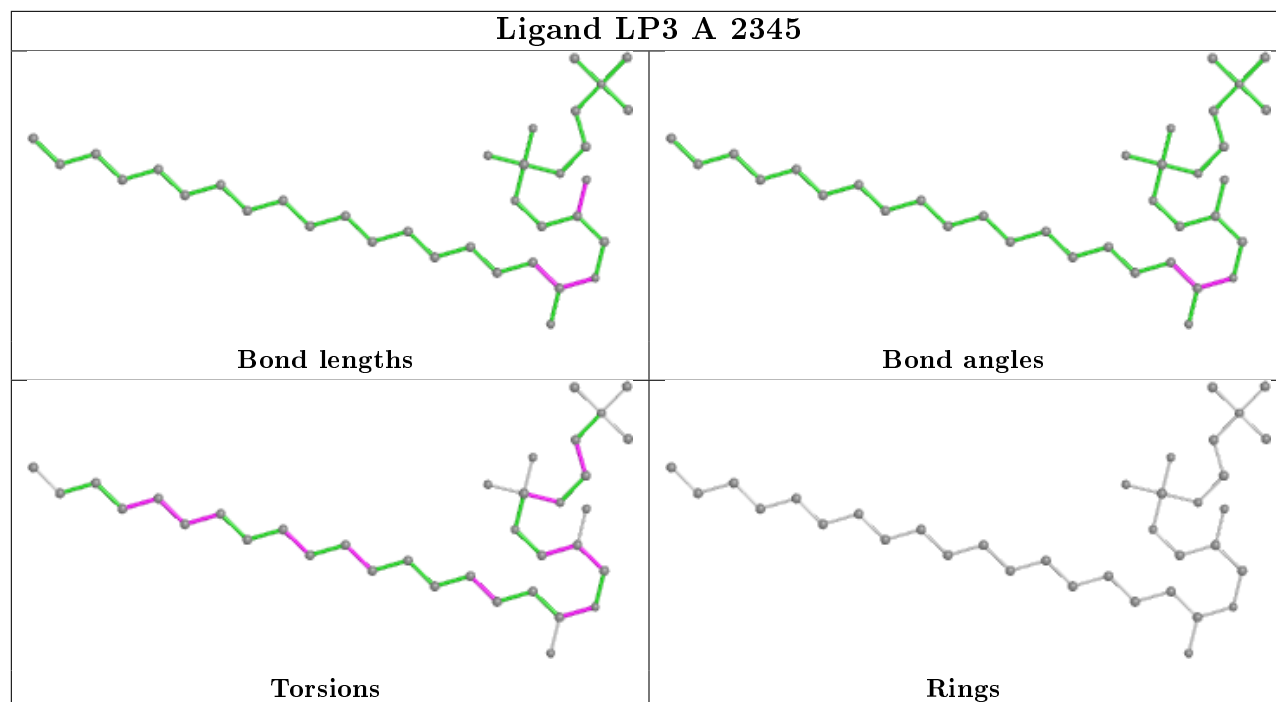
Mol	Chain	Res	Type	Atoms
8	B	3046	MYR	C5-C6-C7-C8
4	A	2345	LP3	C4-O4P-P-O2P
6	B	2341	CH5	C4-O4P-P-O1P
6	B	2341	CH5	C4-C5-N-C6
4	A	2345	LP3	C16-C17-C18-C19

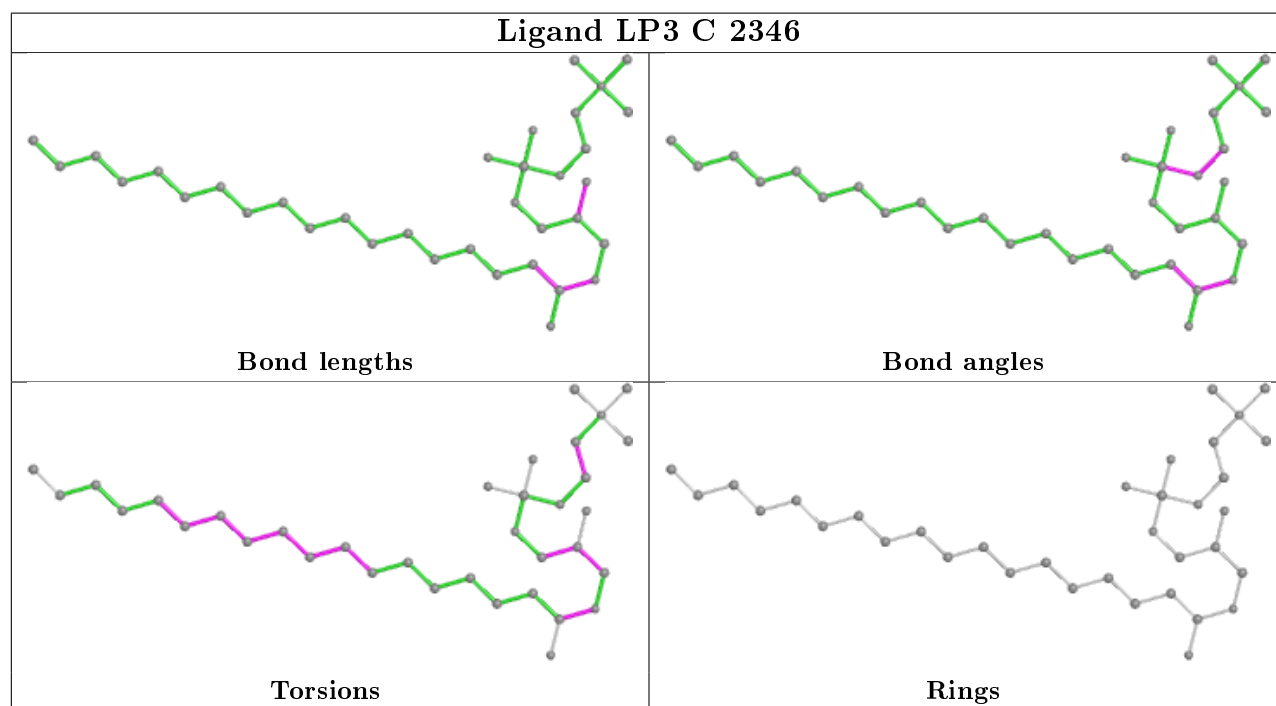
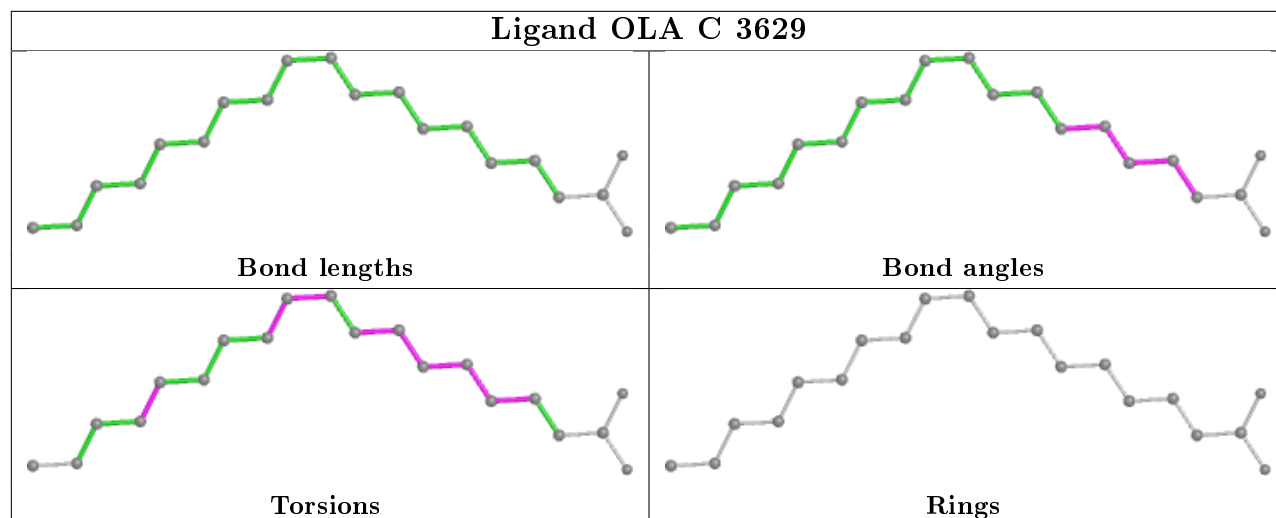
There are no ring outliers.

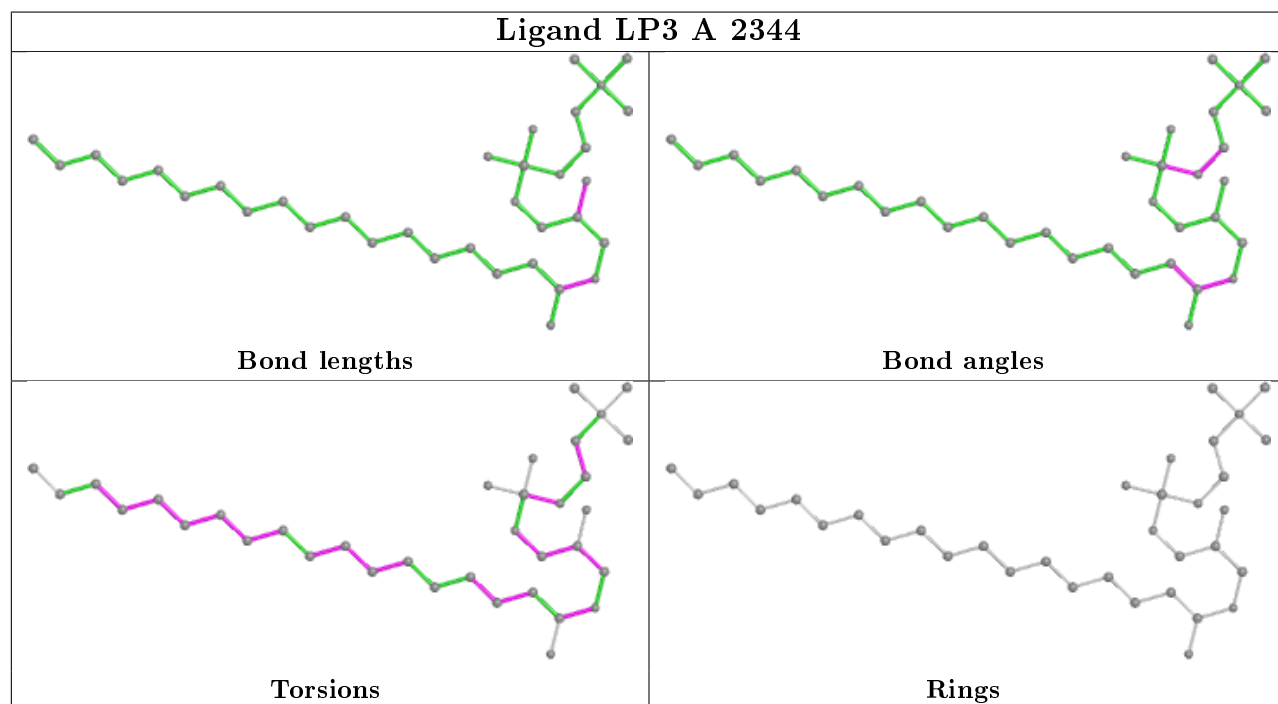
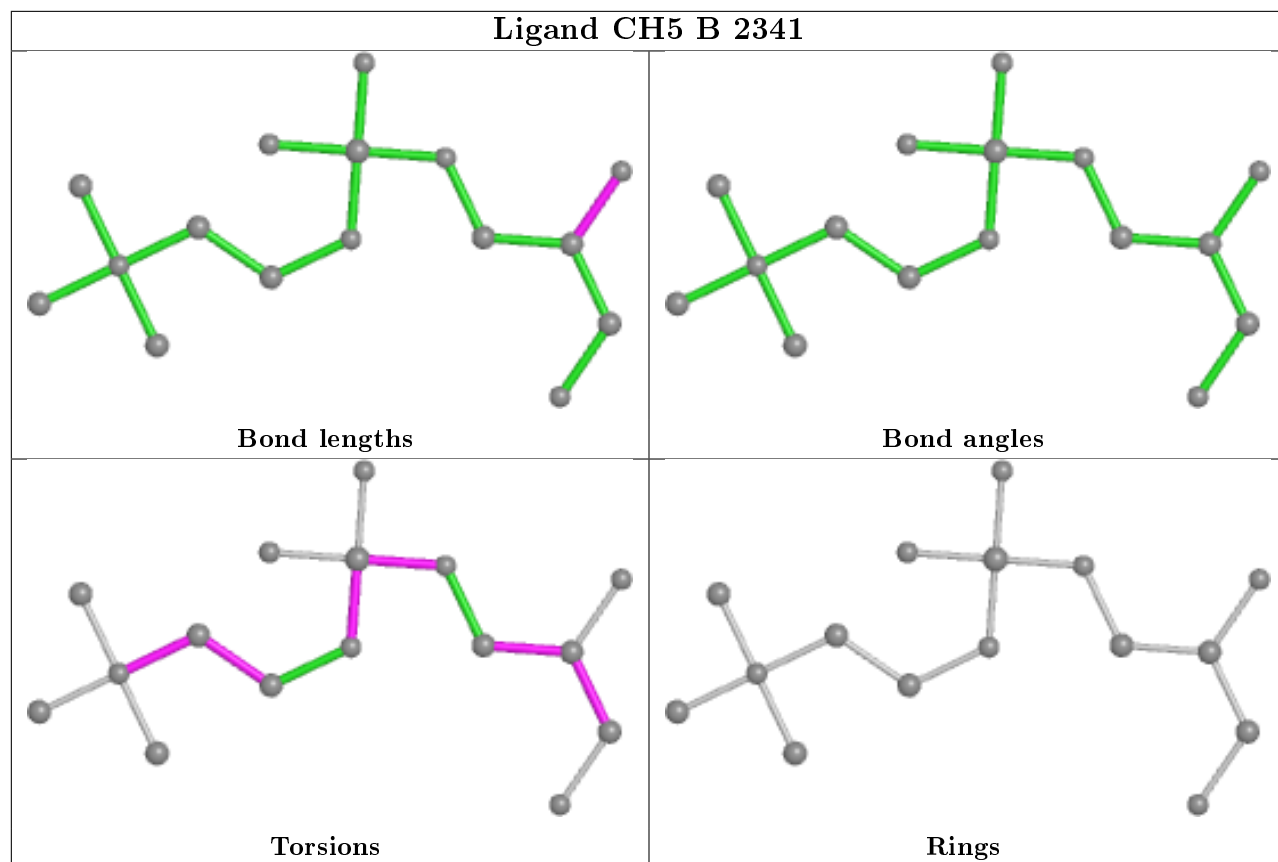
13 monomers are involved in 24 short contacts:

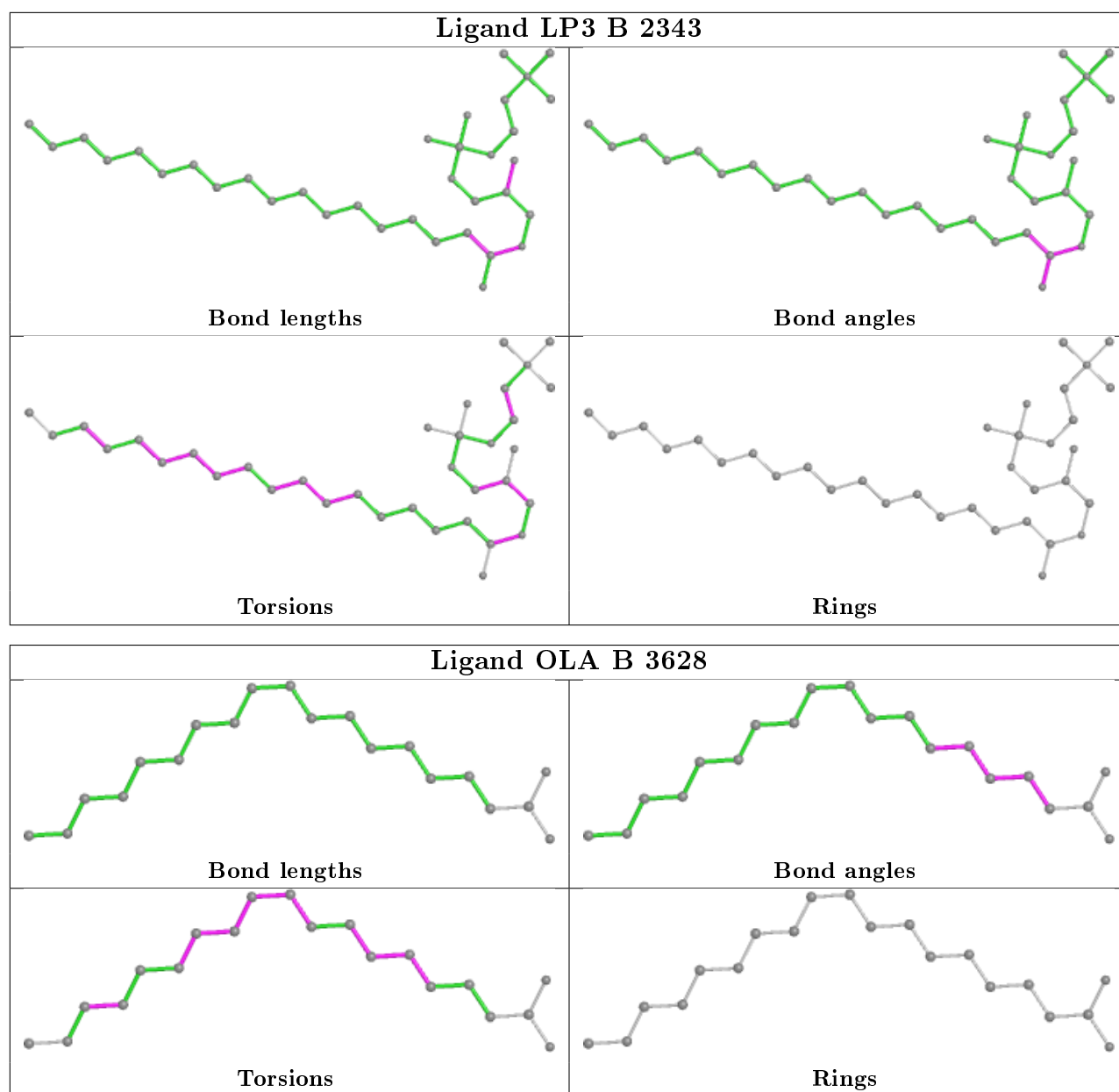
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2345	LP3	4	0
3	C	901	EPE	2	0
7	C	3629	OLA	1	0
9	B	1364	DAO	1	0
5	A	1504	IPA	1	0
4	C	2346	LP3	2	0
6	B	2341	CH5	1	0
5	C	1510	IPA	1	0
8	B	3046	MYR	2	0
4	A	2344	LP3	5	0
5	B	1515	IPA	1	0
4	B	2343	LP3	5	0
7	B	3628	OLA	4	0

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	164/164 (100%)	-0.23	5 (3%)	50	49	10, 20, 46, 61	2 (1%)
1	B	164/164 (100%)	-0.32	3 (1%)	68	66	11, 20, 50, 70	2 (1%)
1	C	162/164 (98%)	-0.06	14 (8%)	10	9	14, 24, 59, 80	0
All	All	490/492 (99%)	-0.21	22 (4%)	33	32	10, 22, 54, 80	4 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	128	LEU	7.0
1	C	131	PRO	4.7
1	C	127	ASP	4.6
1	C	134	LEU	4.3
1	A	127	ASP	3.9
1	C	126	PRO	3.8
1	C	164	ILE	3.7
1	B	93	GLY	3.7
1	C	129	GLU	3.6
1	A	1	HIS	3.5
1	C	132	SER	3.1
1	C	124	VAL	3.0
1	C	130	LEU	3.0
1	A	164	ILE	2.9
1	C	125	VAL	2.7
1	C	12	GLU	2.5
1	B	92	THR	2.4
1	C	13	GLY	2.3
1	A	126	PRO	2.1
1	C	92	THR	2.1
1	A	2	MET	2.1
1	B	127	ASP	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](#)

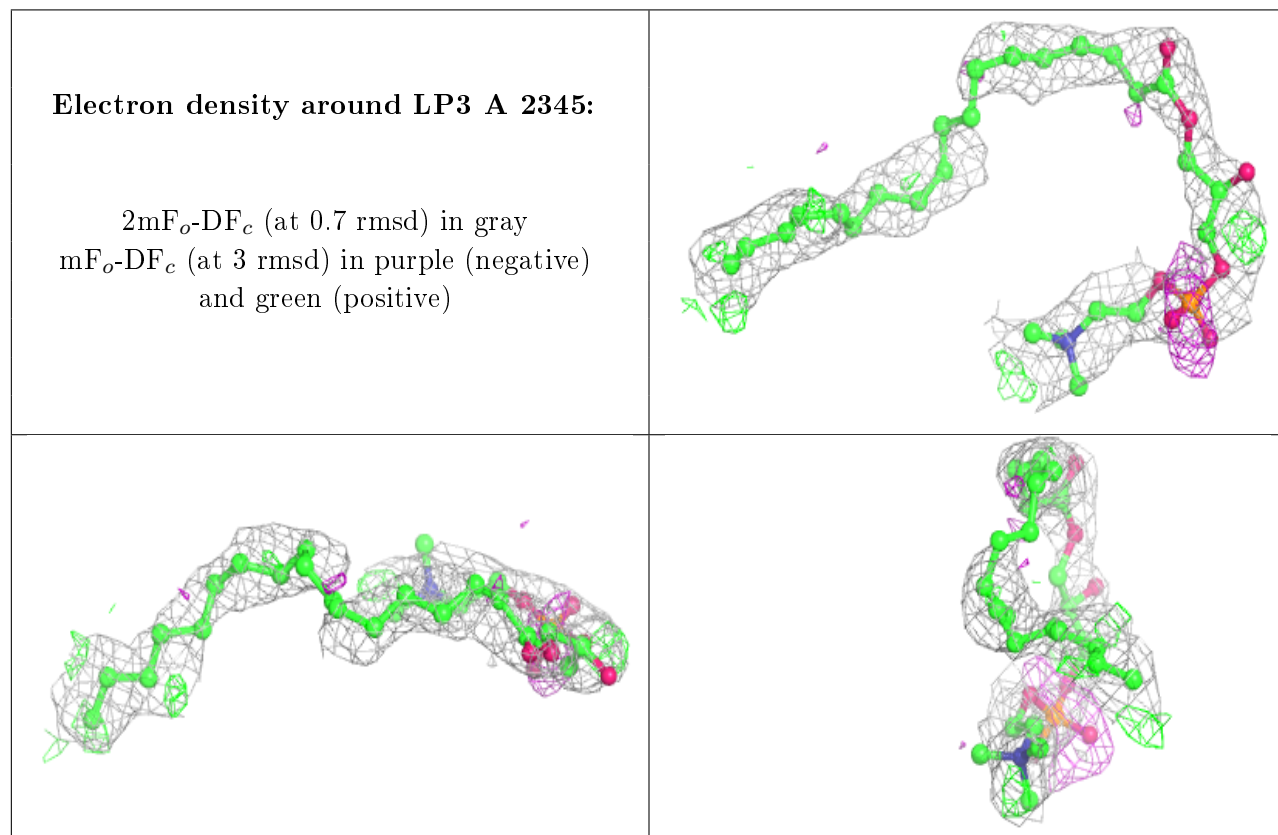
There are no carbohydrates in this entry.

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.

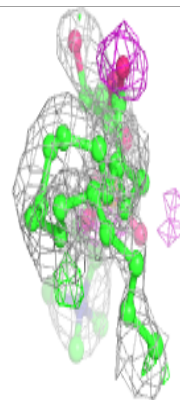
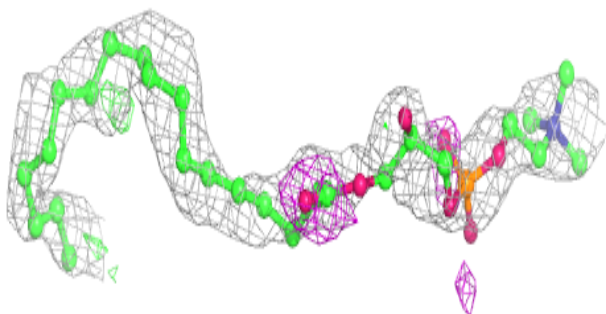
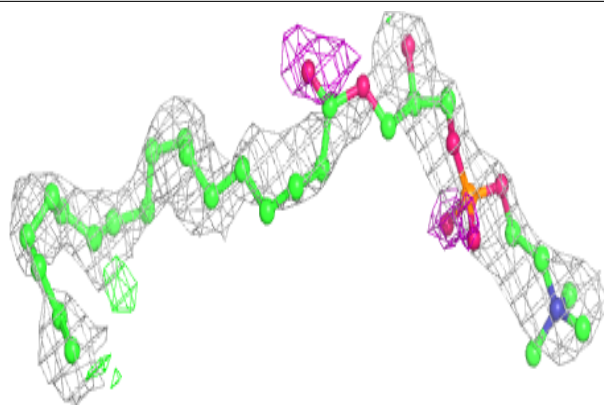
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MYR	B	3046	16/16	0.57	0.24	59,62,67,67	0
4	LP3	A	2345	35/35	0.66	0.28	58,66,80,80	0
4	LP3	A	2344	35/35	0.66	0.32	55,74,80,80	0
8	MYR	C	3045	16/16	0.66	0.21	58,66,68,69	0
6	CH5	B	2341	16/16	0.67	0.40	73,76,80,80	0
4	LP3	C	2346	35/35	0.68	0.30	50,69,80,80	0
9	DAO	B	1364	14/14	0.69	0.28	64,67,70,71	0
5	IPA	C	1512	4/4	0.75	0.25	59,61,62,62	0
7	OLA	C	3629	20/20	0.76	0.23	63,66,71,71	1
4	LP3	B	2343	35/35	0.77	0.29	58,70,80,80	0
5	IPA	B	1515	4/4	0.79	0.37	59,60,61,61	0
3	EPE	C	901	15/15	0.79	0.31	75,78,80,80	0
6	CH5	C	2342	16/16	0.80	0.28	69,76,80,80	0
7	OLA	B	3628	20/20	0.80	0.22	52,56,61,62	2
5	IPA	A	1504	4/4	0.86	0.18	56,56,57,61	0
5	IPA	B	1509	4/4	0.88	0.24	36,41,43,43	0
3	EPE	A	900	15/15	0.88	0.23	29,36,43,46	0
5	IPA	B	1508	4/4	0.90	0.44	59,60,60,61	0
5	IPA	C	1510	4/4	0.90	0.37	57,59,60,62	0
5	IPA	C	1514	4/4	0.91	0.18	64,65,66,67	0
5	IPA	A	1502	4/4	0.92	0.29	47,48,50,51	0
5	IPA	C	1513	4/4	0.92	0.16	51,52,52,54	0
5	IPA	C	1511	4/4	0.94	0.15	40,41,41,43	0
2	CL	C	803	1/1	0.98	0.06	23,23,23,23	0
2	CL	B	802	1/1	0.99	0.06	19,19,19,19	0
2	CL	A	801	1/1	1.00	0.04	16,16,16,16	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.

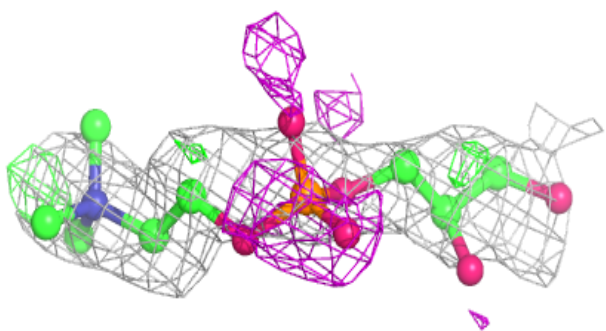
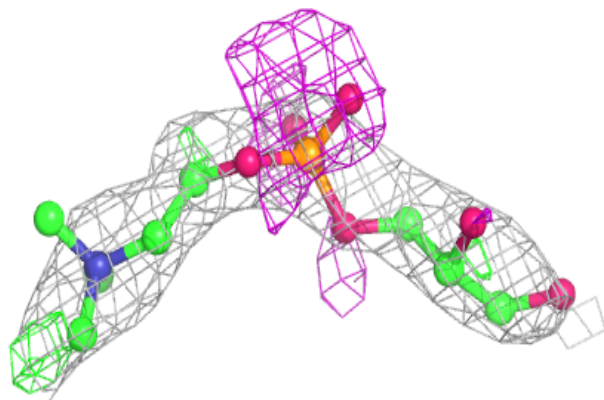


Electron density around LP3 A 2344:

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

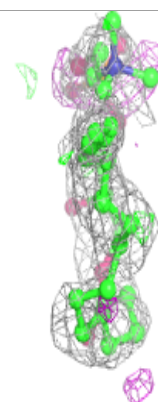
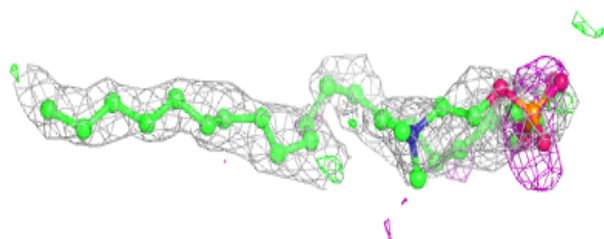
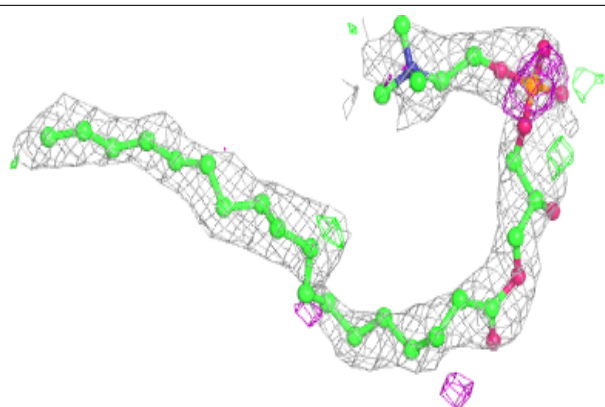
**Electron density around CH5 B 2341:**

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

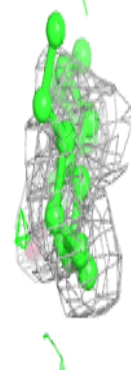
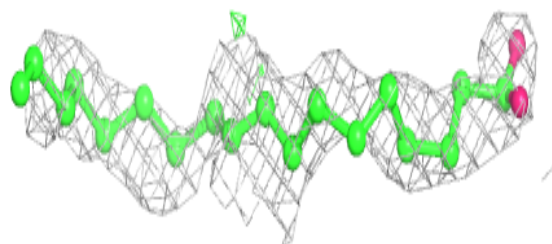
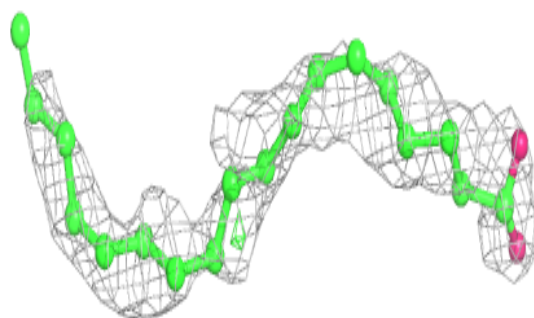


Electron density around LP3 C 2346:

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

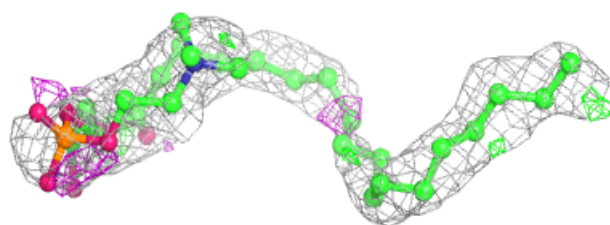
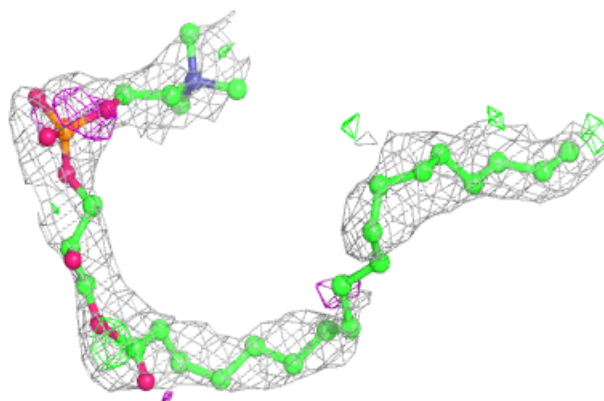
**Electron density around OLA C 3629:**

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

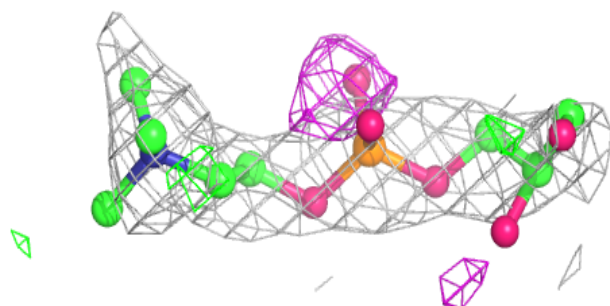
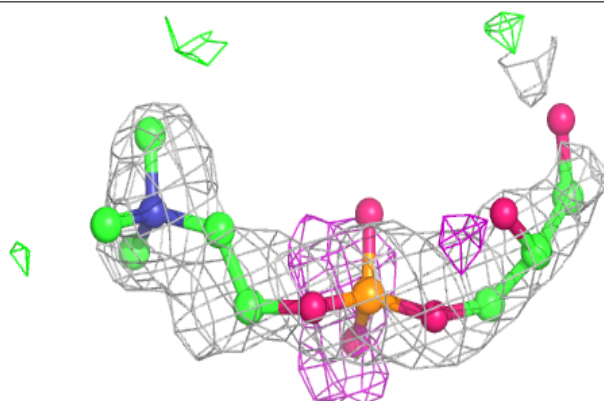


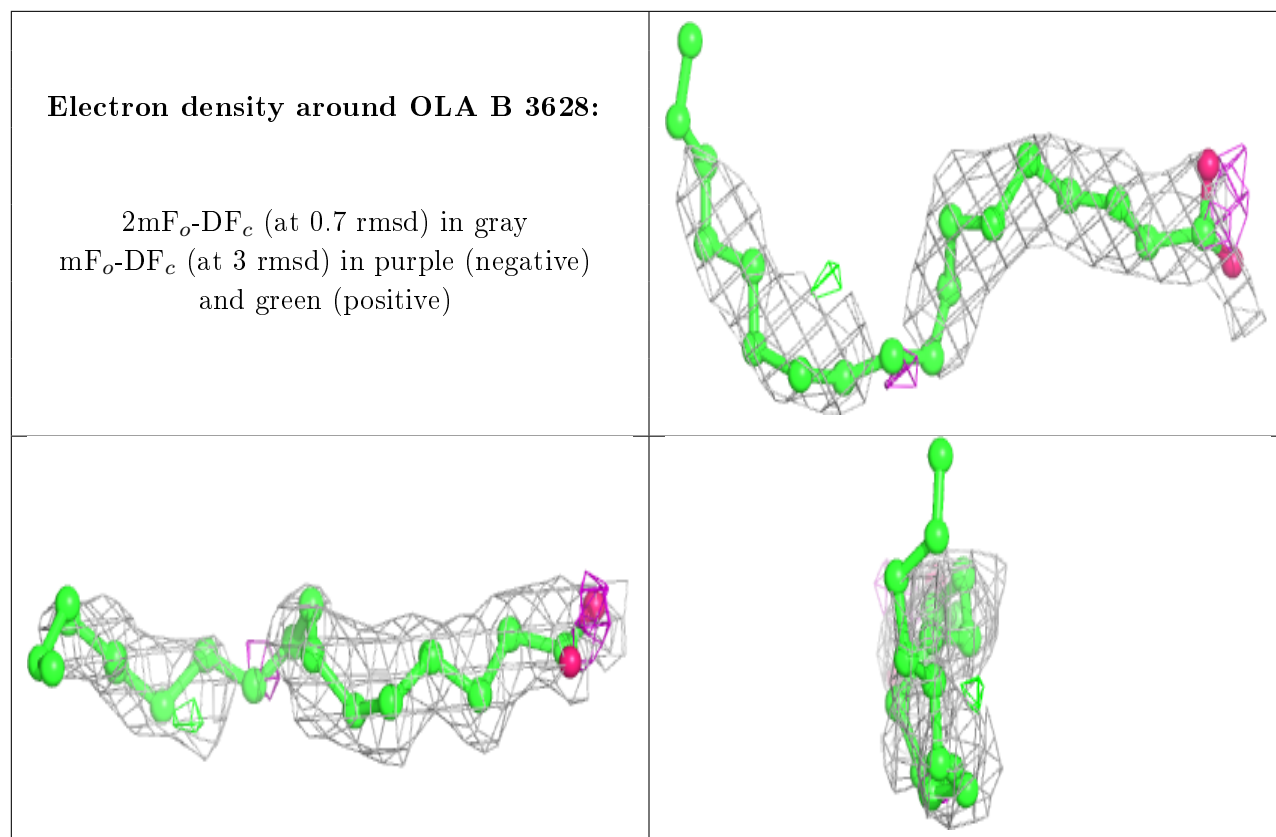
Electron density around LP3 B 2343:

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

**Electron density around CH5 C 2342:**

$2mF_o-DF_c$ (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.