wwPDB X-ray Structure Validation Summary Report (i)

Jan 25, 2024 – 06:08 PM JST

PDB ID	:	8ITT
Title	:	Crystal structure of lysophosphatidylcholine in complex with human serum albumin and myristate
Authors	:	Wang, Y.; Jiang, L.G.; Huang, M.D.
Deposited on	:	2023-03-22
Resolution	:	3.03 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

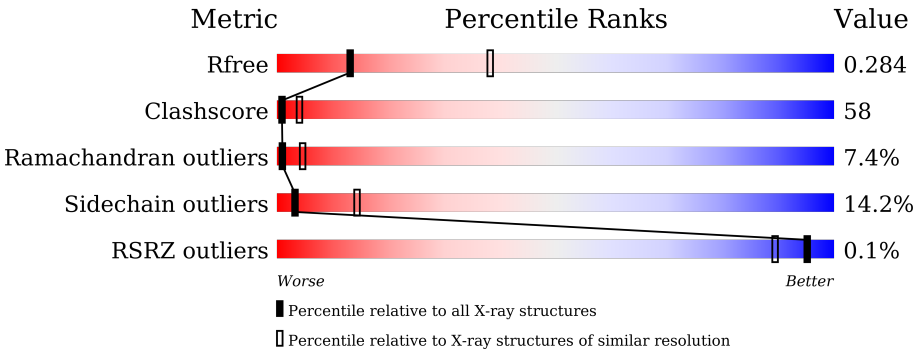
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	580	37% 46% 14% ·
1	B	580	39% 47% 12% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MYR	A	603	-	-	-	X
2	MYR	B	601	-	-	X	-
2	MYR	B	602	-	-	X	-
3	LPC	A	604	-	-	X	X
3	LPC	A	605	-	-	X	-
3	LPC	A	606	-	-	X	X
3	LPC	B	603	-	-	X	X
3	LPC	B	605	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9167 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.

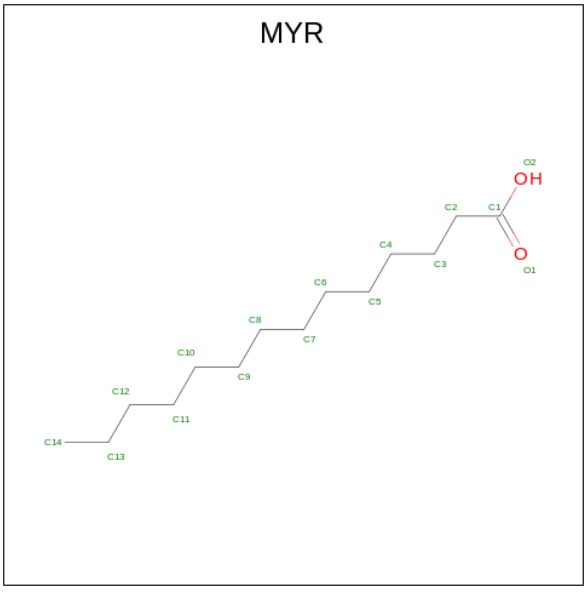
- Molecule 1 is a protein called Albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	0	0
			4443	2808	750	844	41			
1	B	579	Total	C	N	O	S	0	0	0
			4442	2807	752	842	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	580	GLU	GLN	conflict	UNP P02768
B	580	GLU	GLN	conflict	UNP P02768

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$) (labeled as "Ligand of Interest" by depositor).



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

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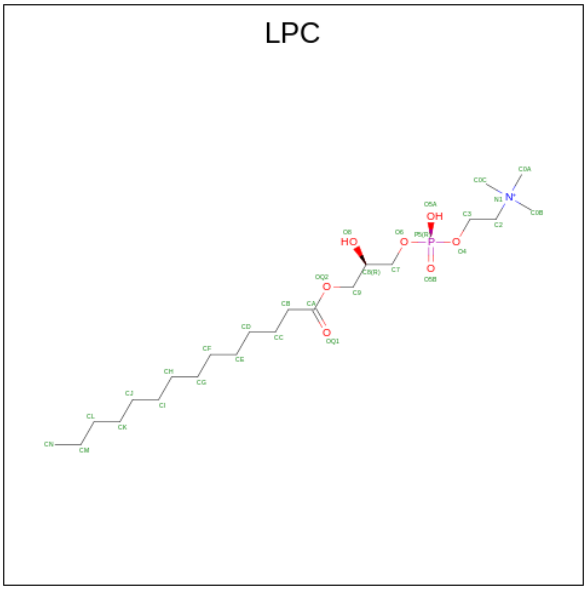
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0

- Molecule 3 is [1-MYRISTOYL-GLYCEROL-3-YL]PHOSPHONYLCHOLINE (three-letter code: LPC) (formula: $C_{22}H_{47}NO_7P$) (labeled as "Ligand of Interest" by depositor).



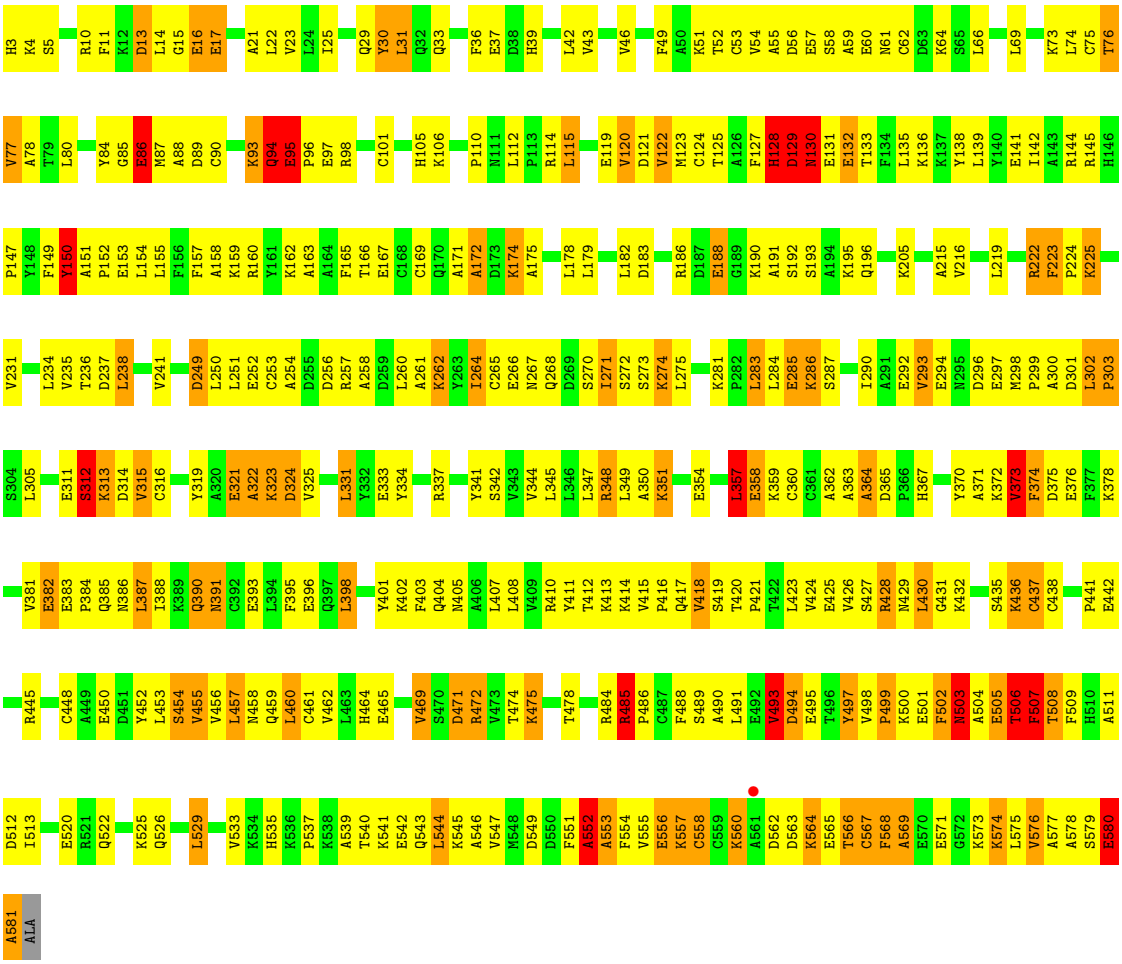
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 22 1 7 1	0	0
3	A	1	Total C N O P 31 22 1 7 1	0	0
3	A	1	Total C N O P 31 22 1 7 1	0	0
3	B	1	Total C N O P 31 22 1 7 1	0	0
3	B	1	Total C N O P 31 22 1 7 1	0	0
3	B	1	Total C N O P 31 22 1 7 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

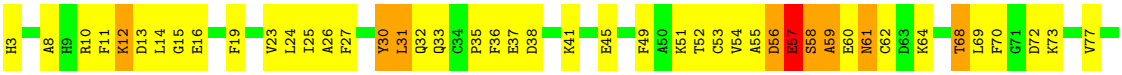
- Molecule 1: Albumin

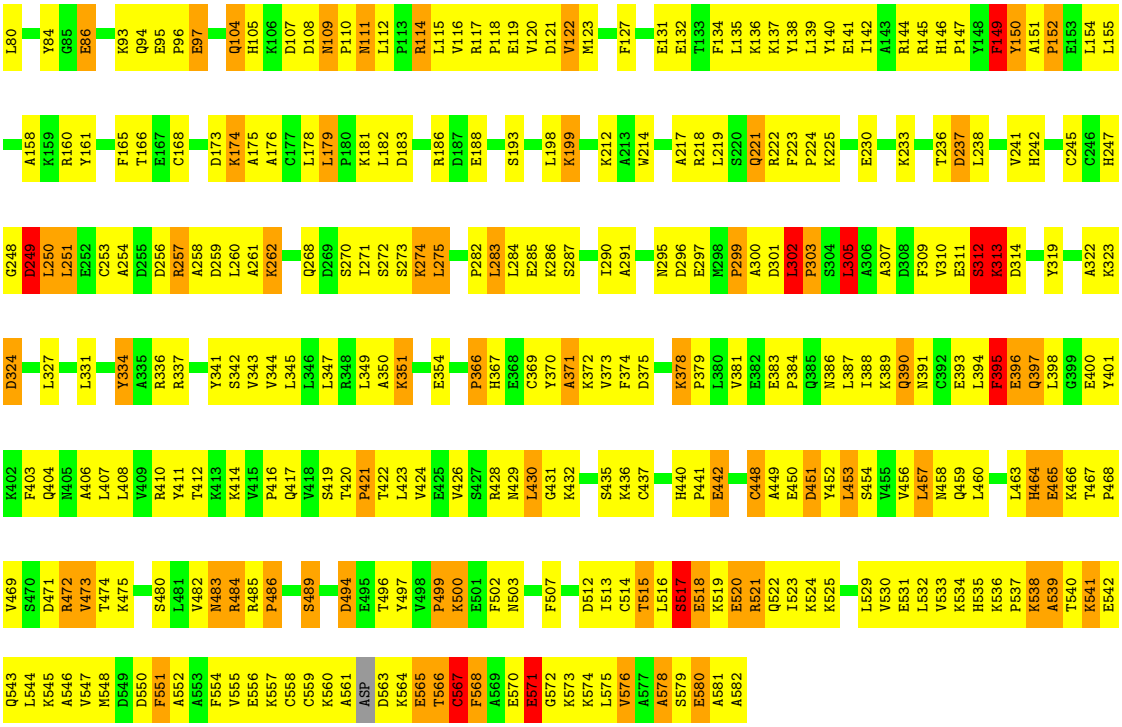
Chain A:



- Molecule 1: Albumin

Chain B:




L80 Y84 G85 E86 K93 Q94 E95 P96 E97 Q104 H105 K106 D107 D108 N109 P110 N111 L112 P113 R114 L115 V116 R117 P118 E119 V120 D121 V122 M123 F127 E131 E132 T133 F134 L135 K136 K137 Y138 L139 Y140 E141 I142 A143 R144 R145 H146 P147 Y148 F149 Y150 A151 P152 E153 L154 L155
A158 K159 R160 Y161 F165 T166 E167 C168 D173 K174 A175 A176 C177 L178 L179 P180 K181 L182 D183 R186 D187 E188 S193 L198 K199 K212 A213 W214 A217 R218 L219 S220 Q221 R222 F223 P224 K225 E230 K233 T236 D237 L238 V241 H242 C245 C246 H247
G248 D249 L250 L251 E252 C253 A254 D255 D256 R257 A258 D259 L260 A261 K262 Q268 D269 S270 I271 S272 S273 K274 L275 P282 L283 L284 E285 K286 S287 I290 A291 N295 D296 E297 M298 P299 A300 D301 L302 P303 S304 L305 A306 A307 D308 F309 V310 E311 S312 K313 D314 Y319 A322 K323
D324 L327 L331 Y334 A335 R336 R337 Y341 S342 V343 V344 L345 L346 L347 R348 L349 A350 K351 E354 P366 H367 E368 C369 Y370 A371 K372 V373 F374 D375 K378 P379 L380 V381 E382 E383 P384 Q385 N386 L387 I388 K389 Q390 N391 C392 E393 L394 F395 E396 Q397 L398 G399 E400 Y401
K402 F403 Q404 N405 A406 L407 L408 V409 R410 Y411 T412 K413 K414 V415 P416 Q417 V418 S419 T420 P421 T422 L423 V424 E425 V426 S427 R428 M429 L430 G431 K432 S435 K436 C437 H440 P441 E442 C448 A449 E450 D451 Y452 L453 S454 V455 V456 L457 N458 Q459 L460 L463 H464 E465 K466 T467 P468
V469 S470 D471 R472 V473 T474 K475 S480 L481 V482 N483 R484 R485 P486 S489 D494 E495 T496 Y497 V498 P499 K500 E501 F502 N503 F507 D512 I513 C514 T515 L516 S517 E518 K519 E520 R521 Q522 I523 K524 K525 L529 V530 E531 L532 V533 K534 H535 K536 P537 K538 A539 T540 K541 E542
Q543 L544 K545 A546 V547 M548 D549 D550 F551 A552 A553 F554 V555 E556 K557 C558 C559 K560 A561 ASP D563 K564 E565 T566 C567 F568 A569 E570 E571 G572 K573 K574 L575 V576 A577 A578 S579 E580 A581 A582

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.26Å 38.47Å 182.46Å 90.00° 104.78° 90.00°	Depositor
Resolution (Å)	47.63 – 3.03 47.63 – 2.74	Depositor EDS
% Data completeness (in resolution range)	86.0 (47.63-3.03) 82.1 (47.63-2.74)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.84 (at 2.73Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.261 , 0.291 0.255 , 0.284	Depositor DCC
R_{free} test set	2383 reflections (7.51%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9167	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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 51.94 % 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 5.2227e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, LPC

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	0.70	4/4530 (0.1%)	1.00	22/6141 (0.4%)
1	B	0.72	5/4528 (0.1%)	0.99	18/6134 (0.3%)
All	All	0.71	9/9058 (0.1%)	0.99	40/12275 (0.3%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	TYR	CB-CG	-8.04	1.39	1.51
1	B	149	PHE	CB-CG	-6.16	1.40	1.51
1	B	150	TYR	CB-CG	-6.15	1.42	1.51
1	A	129	ASP	CB-CG	-5.78	1.39	1.51
1	B	149	PHE	CG-CD2	-5.74	1.30	1.38

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	567	CYS	N-CA-C	-9.41	85.59	111.00
1	A	373	VAL	CB-CA-C	-9.10	94.12	111.40
1	B	567	CYS	CB-CA-C	8.61	127.61	110.40
1	B	571	GLU	N-CA-C	-8.60	87.77	111.00
1	B	567	CYS	CA-CB-SG	8.60	129.48	114.00

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	4443	0	4212	525	1
1	B	4442	0	4216	500	0
2	A	48	0	81	6	0
2	B	48	0	81	29	0
3	A	93	0	138	90	0
3	B	93	0	138	81	0
All	All	9167	0	8866	1042	1

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 58.

The worst 5 of 1042 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:149:PHE:CE2	3:B:603:LPC:H0A1	1.43	1.54
1:A:485:ARG:HH11	3:A:605:LPC:C0B	1.33	1.40
1:B:149:PHE:CE2	3:B:603:LPC:H0C3	1.58	1.37
1:B:158:ALA:HB1	3:B:603:LPC:CK	1.53	1.36
1:B:149:PHE:CZ	3:B:603:LPC:H0C3	1.61	1.34

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:GLU:O	1:A:497:TYR:OH[1_565]	1.93	0.27

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	577/580 (100%)	432 (75%)	97 (17%)	48 (8%)	1 3
1	B	575/580 (99%)	443 (77%)	95 (16%)	37 (6%)	1 6
All	All	1152/1160 (99%)	875 (76%)	192 (17%)	85 (7%)	1 4

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	57	GLU
1	A	95	GLU
1	A	120	VAL
1	A	130	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	462/508 (91%)	391 (85%)	71 (15%)	2 12
1	B	461/508 (91%)	401 (87%)	60 (13%)	4 17
All	All	923/1016 (91%)	792 (86%)	131 (14%)	3 14

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	457	LEU
1	B	486	PRO
1	B	571	GLU
1	A	455	VAL
1	A	454	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	111	ASN

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Mol	Chain	Res	Type
1	B	318	ASN
1	B	440	HIS
1	B	390	GLN
1	B	242	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	MYR	B	602	-	15,15,15	0.91	1 (6%)	15,15,15	1.63	2 (13%)
2	MYR	A	602	-	15,15,15	0.66	0	15,15,15	2.01	5 (33%)
3	LPC	A	605	-	30,30,30	0.98	1 (3%)	35,37,37	0.91	2 (5%)
2	MYR	B	601	-	15,15,15	0.65	0	15,15,15	0.90	0
3	LPC	A	606	-	30,30,30	1.01	1 (3%)	35,37,37	0.95	1 (2%)
3	LPC	B	605	-	30,30,30	1.02	2 (6%)	35,37,37	2.51	13 (37%)
3	LPC	B	604	-	30,30,30	1.11	2 (6%)	35,37,37	0.95	2 (5%)
3	LPC	B	603	-	30,30,30	1.21	1 (3%)	35,37,37	0.93	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	LPC	A	604	-	30,30,30	0.94	4 (13%)	35,37,37	1.23	3 (8%)
2	MYR	A	603	-	15,15,15	0.54	0	15,15,15	0.97	1 (6%)
2	MYR	A	601	-	15,15,15	0.54	0	15,15,15	1.09	1 (6%)
2	MYR	B	606	-	15,15,15	0.52	0	15,15,15	1.22	2 (13%)

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	MYR	B	602	-	-	10/13/13/13	-
2	MYR	A	602	-	-	2/13/13/13	-
3	LPC	A	605	-	-	24/32/32/32	-
2	MYR	B	601	-	-	6/13/13/13	-
3	LPC	A	606	-	-	21/32/32/32	-
3	LPC	B	605	-	-	18/32/32/32	-
3	LPC	B	604	-	-	23/32/32/32	-
3	LPC	B	603	-	-	17/32/32/32	-
3	LPC	A	604	-	-	17/32/32/32	-
2	MYR	A	603	-	-	8/13/13/13	-
2	MYR	A	601	-	-	7/13/13/13	-
2	MYR	B	606	-	-	6/13/13/13	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	LPC	OQ2-CA	5.69	1.50	1.33
3	B	604	LPC	OQ2-CA	4.92	1.47	1.33
3	A	605	LPC	OQ2-CA	4.48	1.46	1.33
3	A	606	LPC	OQ2-CA	4.42	1.46	1.33
2	B	602	MYR	O1-C1	3.09	1.32	1.22

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	605	LPC	C0C-N1-C2	-5.11	89.00	109.92
3	B	605	LPC	C0B-N1-C2	-4.95	89.67	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	605	LPC	C0C-N1-C0B	4.95	121.69	108.97
3	B	605	LPC	C0A-N1-C2	-4.82	90.21	109.92
3	B	605	LPC	CG-CF-CE	-4.80	90.08	114.42

There are no chirality outliers.

5 of 159 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	LPC	C3-O4-P5-O5B
3	A	605	LPC	N1-C2-C3-O4
3	A	605	LPC	C7-O6-P5-O5A
3	A	605	LPC	C7-O6-P5-O5B
3	A	606	LPC	N1-C2-C3-O4

There are no ring outliers.

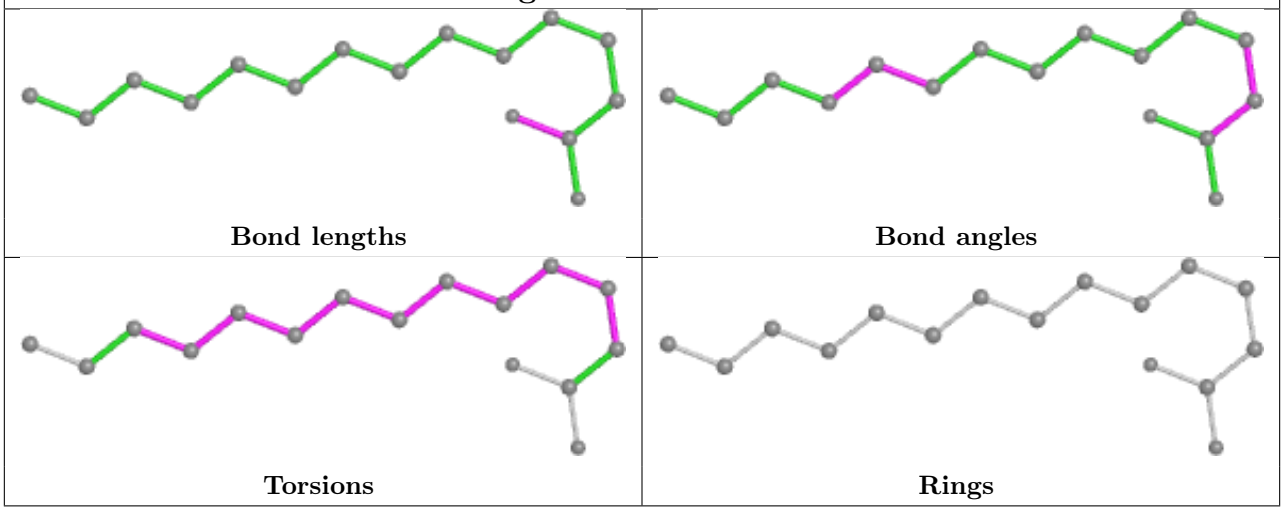
12 monomers are involved in 206 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	MYR	11	0
2	A	602	MYR	4	0
3	A	605	LPC	44	0
2	B	601	MYR	15	0
3	A	606	LPC	21	0
3	B	605	LPC	20	0
3	B	604	LPC	19	0
3	B	603	LPC	42	0
3	A	604	LPC	25	0
2	A	603	MYR	1	0
2	A	601	MYR	1	0
2	B	606	MYR	3	0

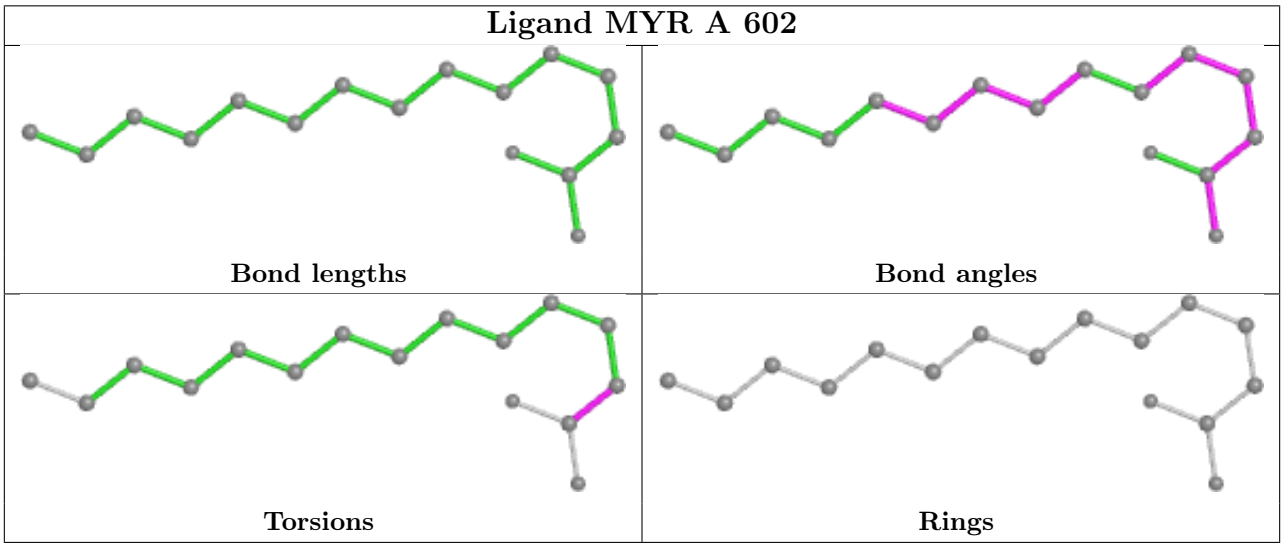
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

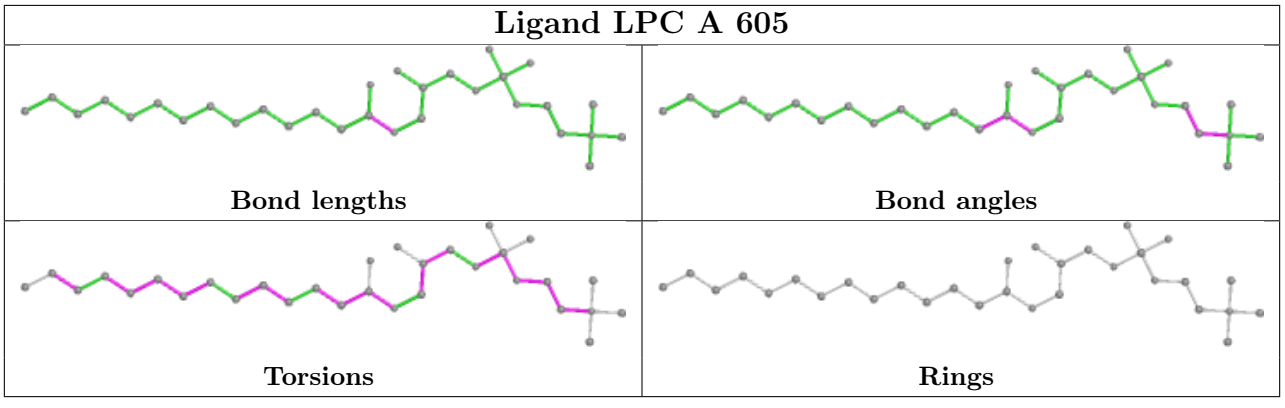
Ligand MYR B 602



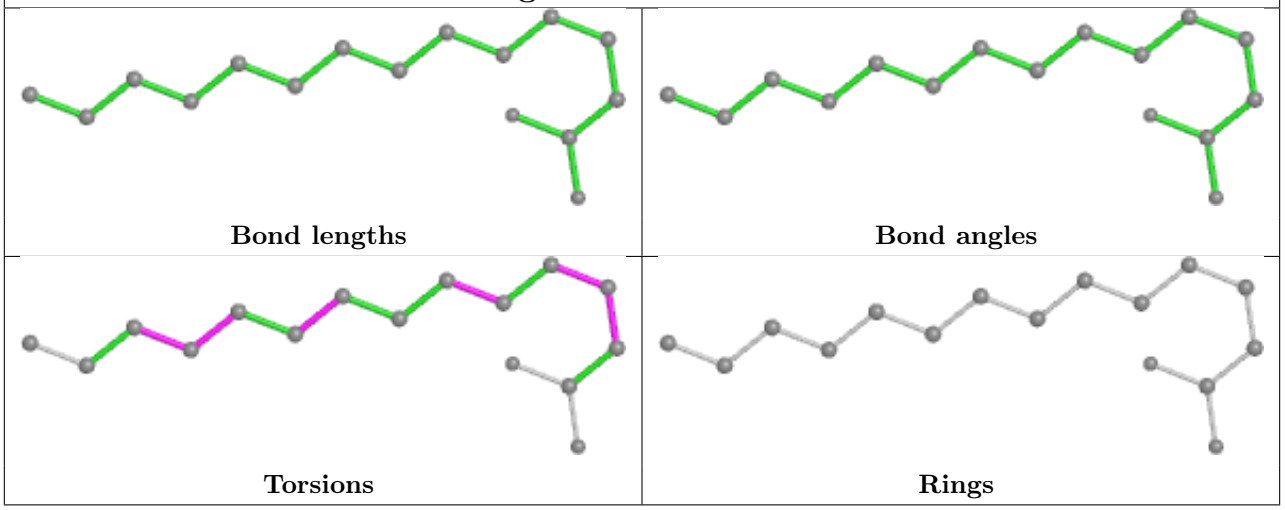
Ligand MYR A 602



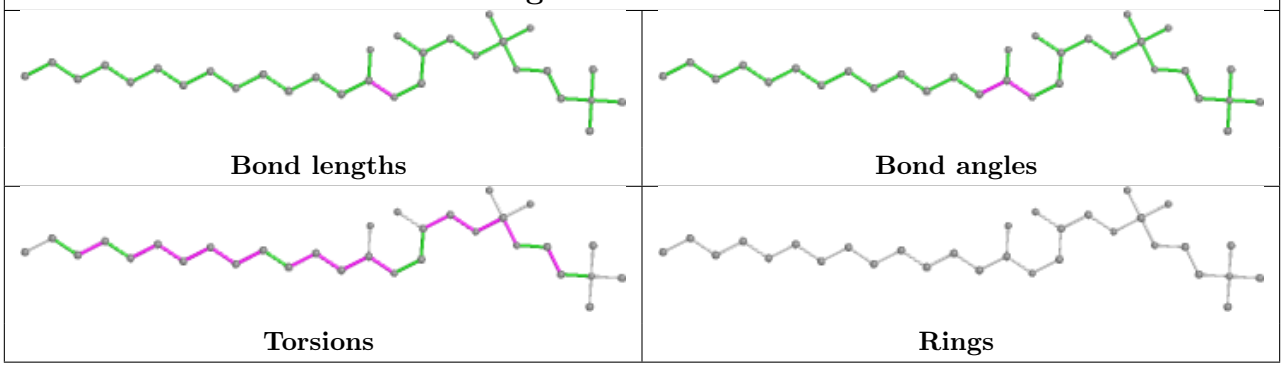
Ligand LPC A 605



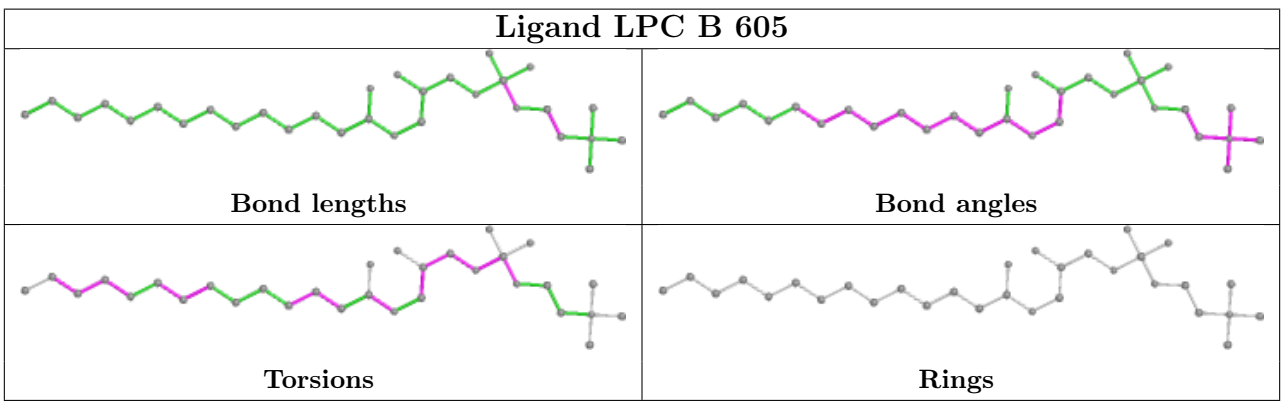
Ligand MYR B 601



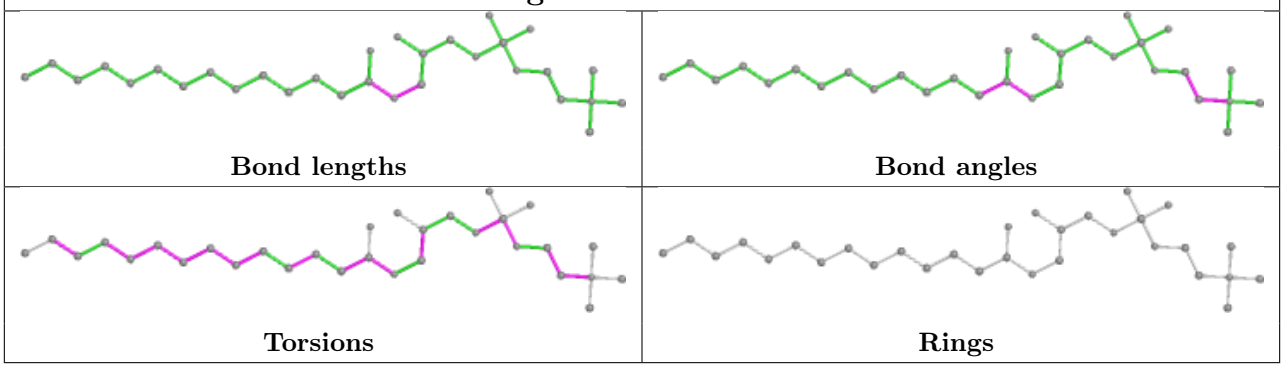
Ligand LPC A 606



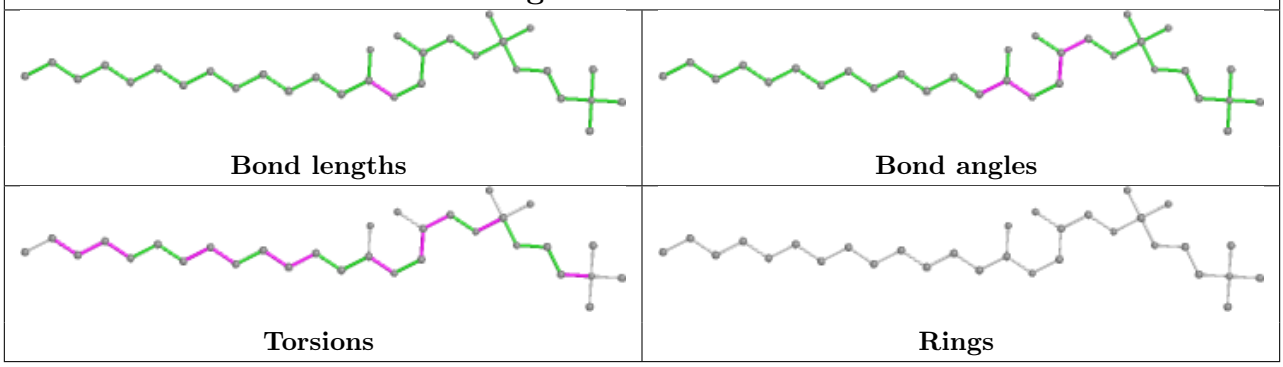
Ligand LPC B 605



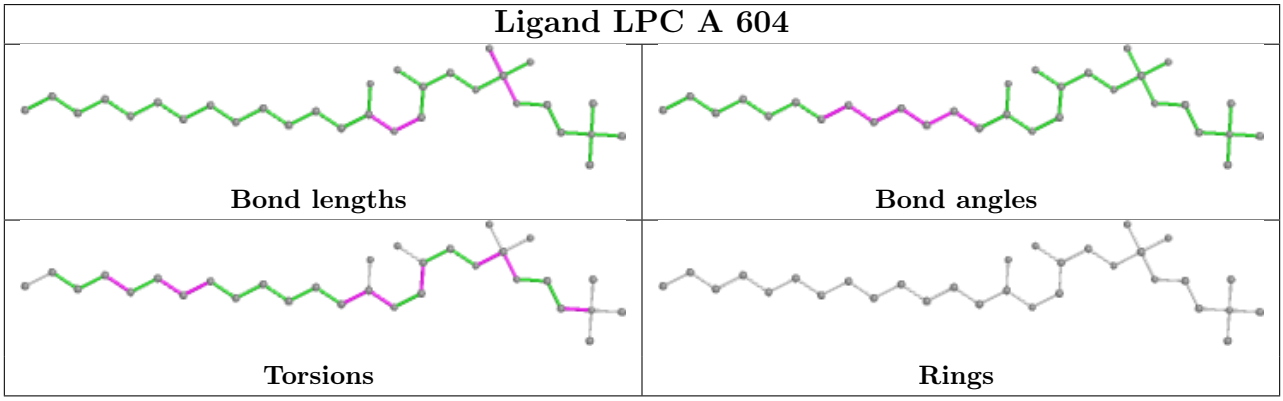
Ligand LPC B 604



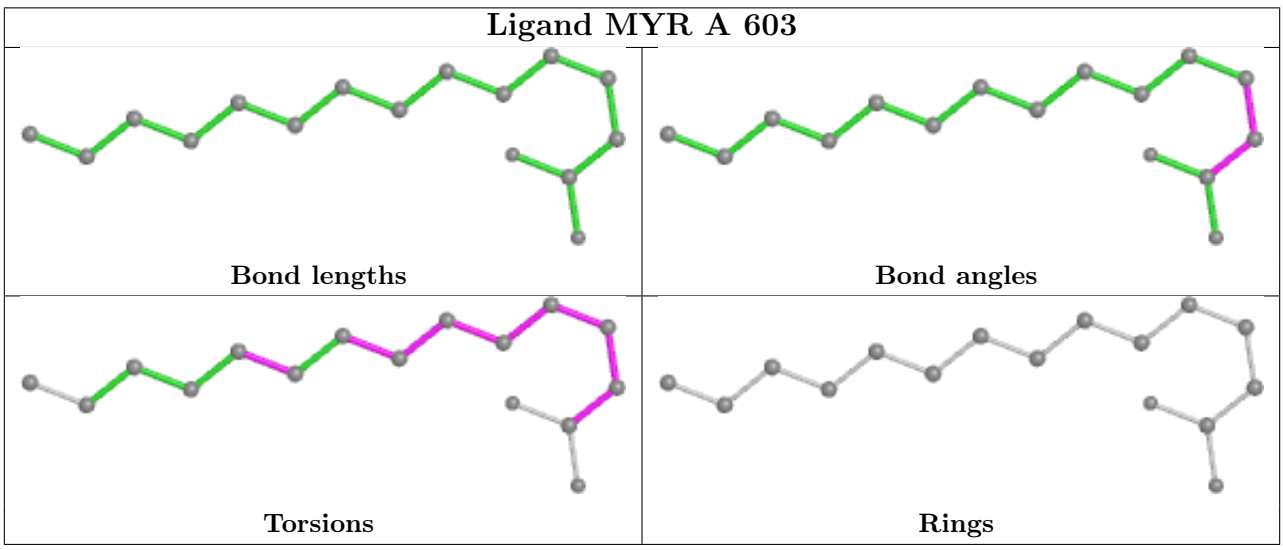
Ligand LPC B 603

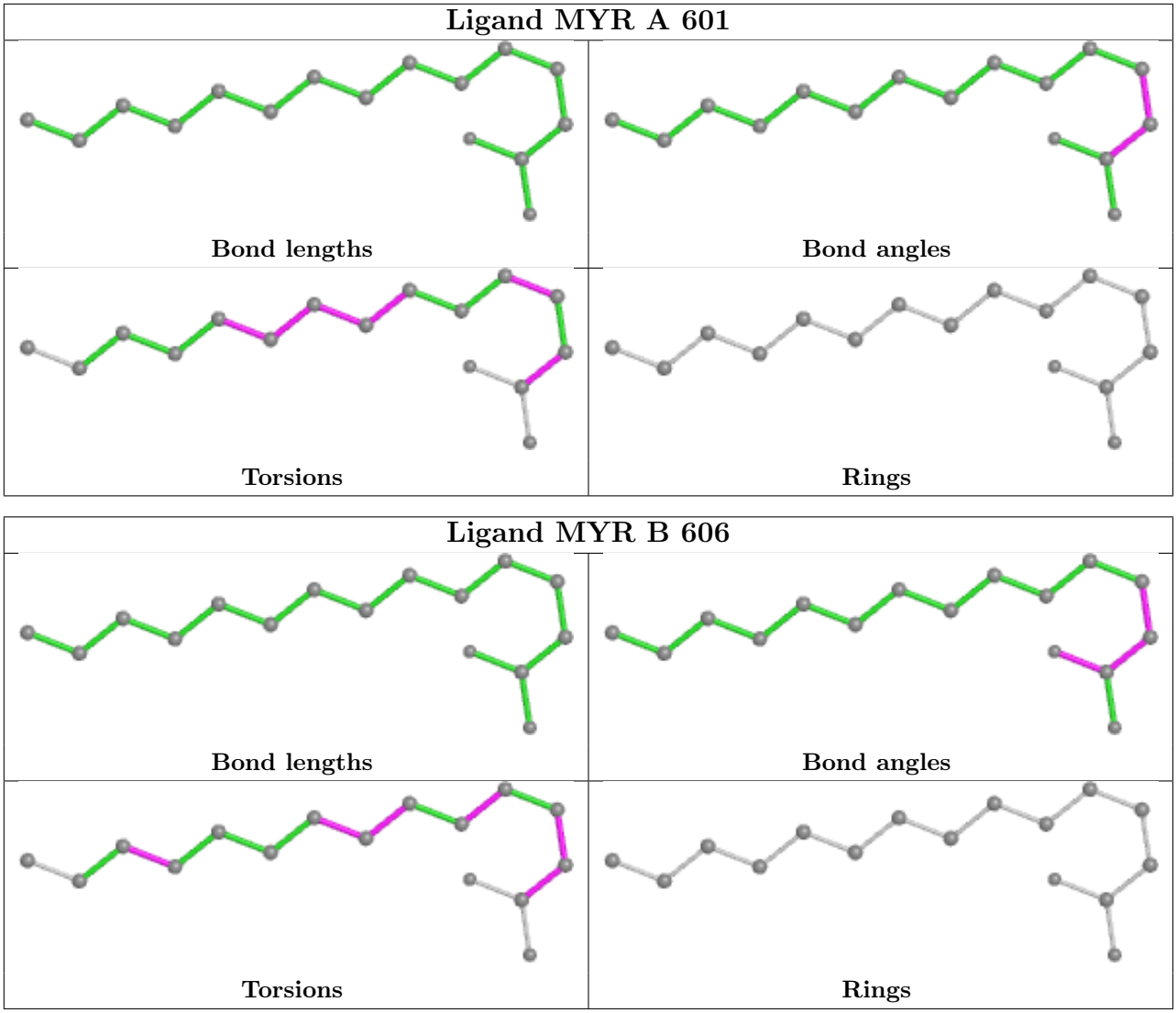


Ligand LPC A 604



Ligand MYR A 603





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	579/580 (99%)	-0.59	1 (0%) 95 87	25, 50, 83, 154	0
1	B	579/580 (99%)	-0.60	0 100 100	21, 49, 83, 124	0
All	All	1158/1160 (99%)	-0.59	1 (0%) 95 89	21, 50, 83, 154	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	561	ALA	3.7

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

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LPC	B	603	31/31	0.67	0.66	44,53,65,66	0
3	LPC	A	606	31/31	0.68	0.67	49,58,66,70	0
2	MYR	B	601	16/16	0.71	0.37	54,63,72,78	0

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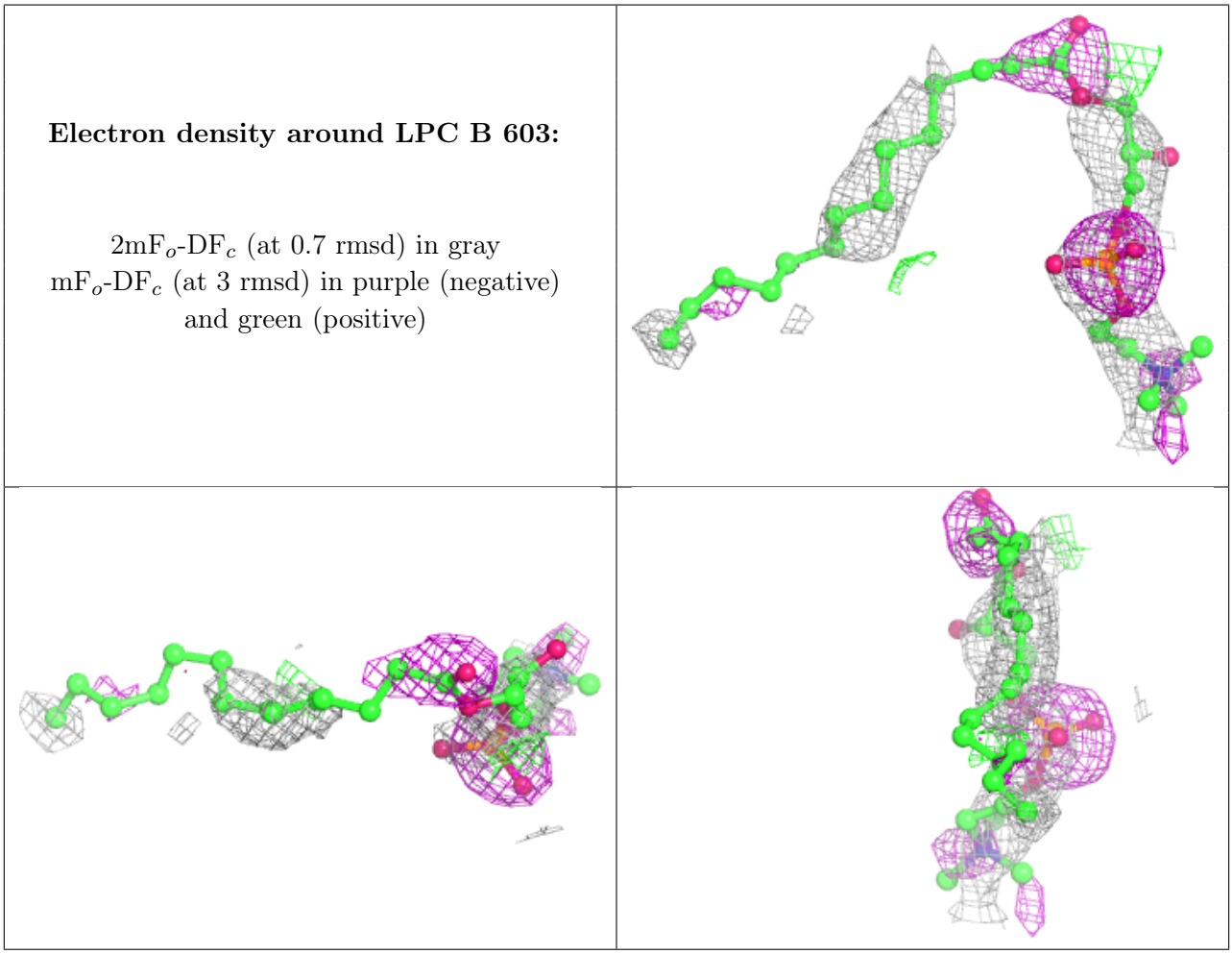
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MYR	B	602	16/16	0.73	0.38	40,48,60,61	0
3	LPC	A	604	31/31	0.73	0.51	43,49,57,59	0
2	MYR	A	603	16/16	0.74	0.44	39,42,61,63	0
3	LPC	B	605	31/31	0.74	0.71	48,56,63,65	0
3	LPC	B	604	31/31	0.80	0.39	42,49,58,60	0
3	LPC	A	605	31/31	0.81	0.41	43,48,55,63	0
2	MYR	A	601	16/16	0.84	0.21	40,48,67,68	0
2	MYR	A	602	16/16	0.85	0.32	47,50,56,56	0
2	MYR	B	606	16/16	0.88	0.30	38,43,50,52	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.

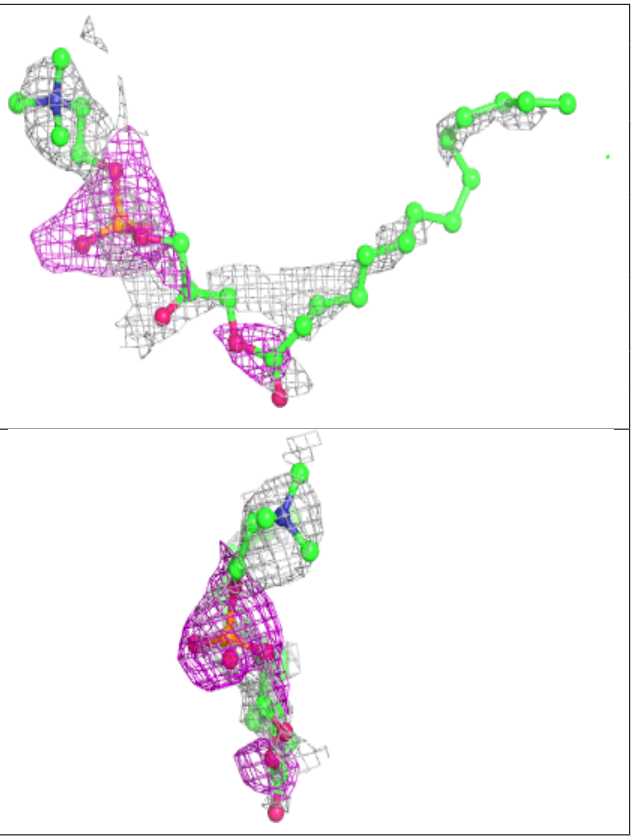
Electron density around LPC B 603:

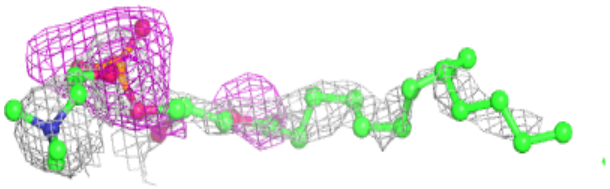
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LPC A 606:

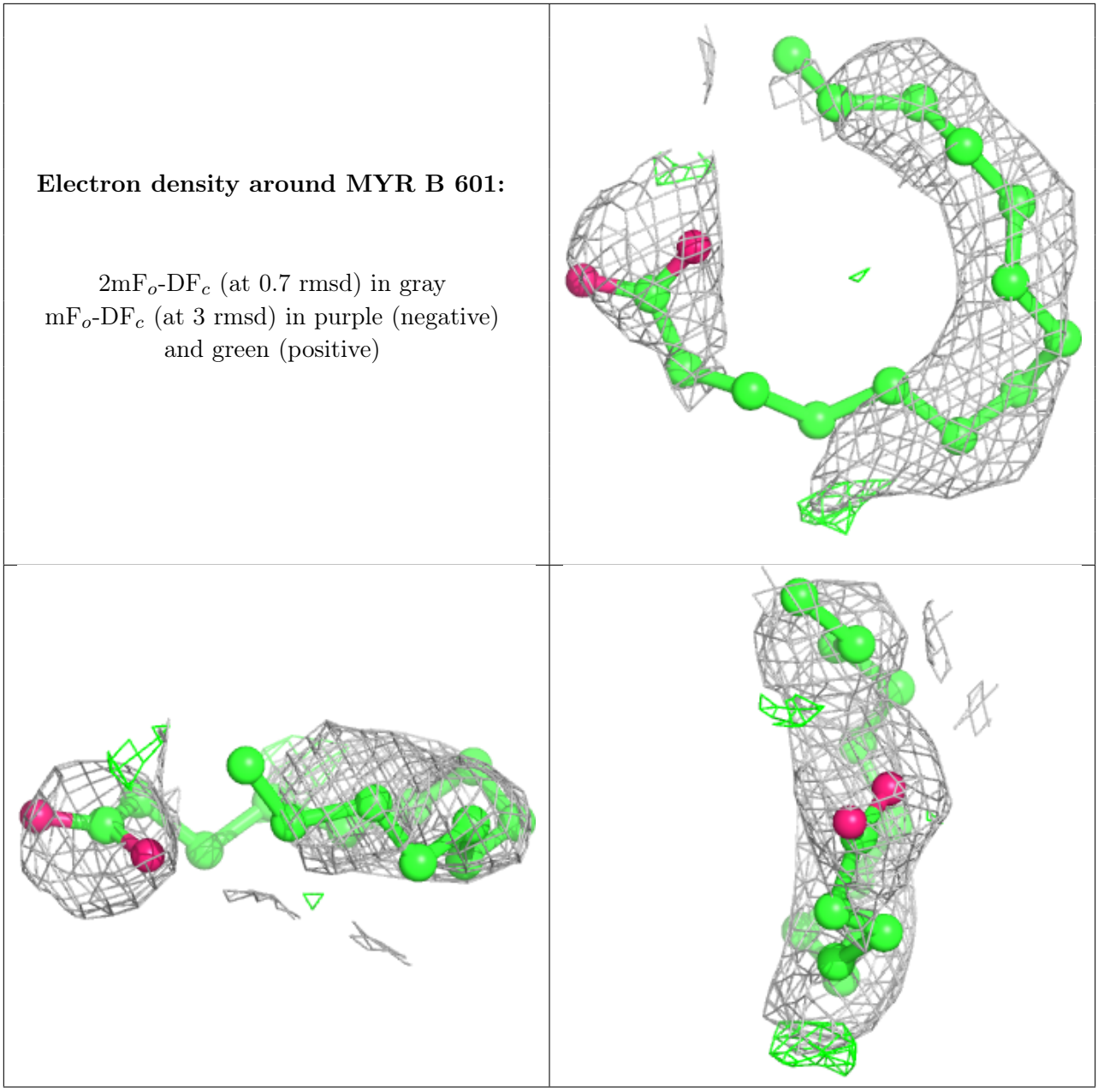
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





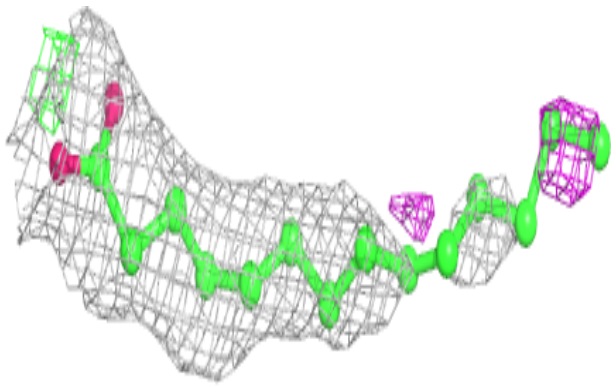
Electron density around MYR B 601:

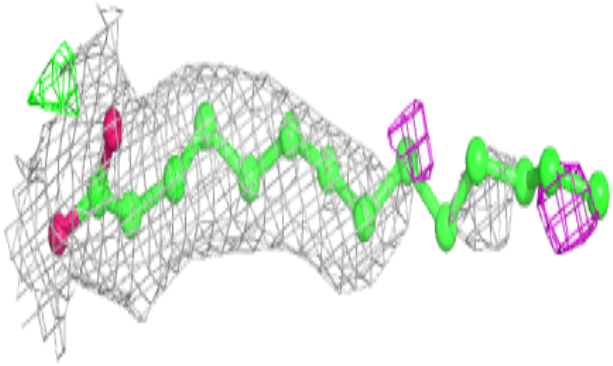
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MYR B 602:

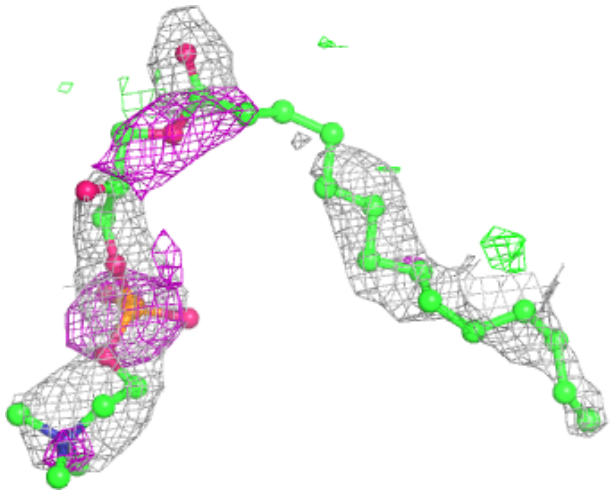
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

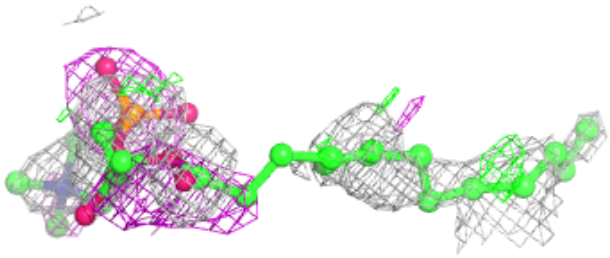


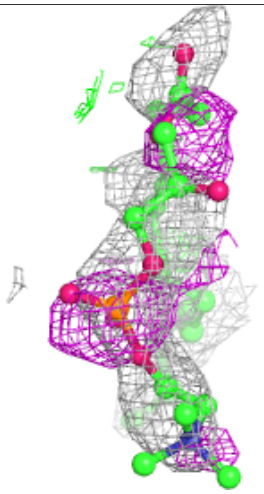


Electron density around LPC A 604:

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

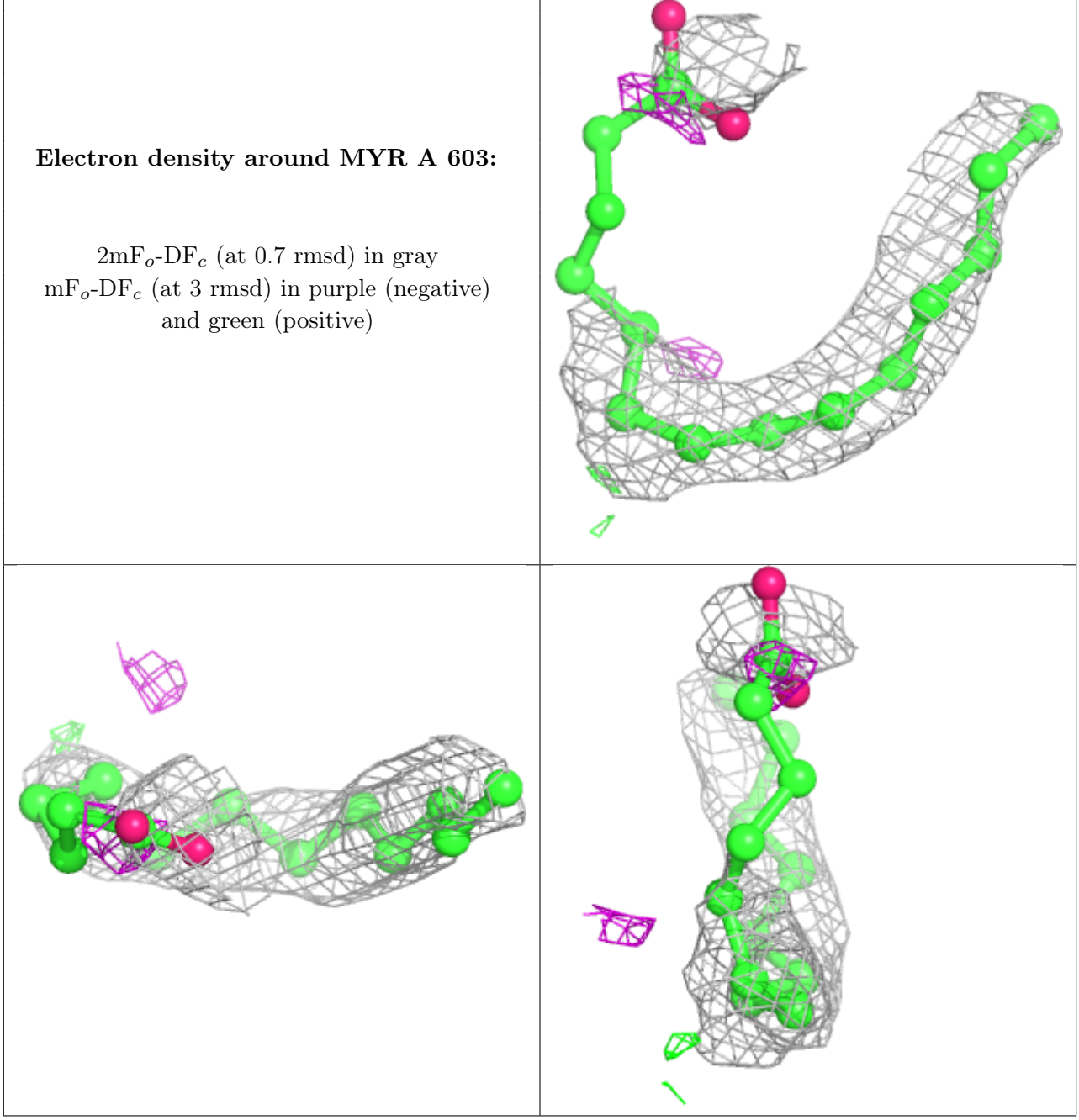






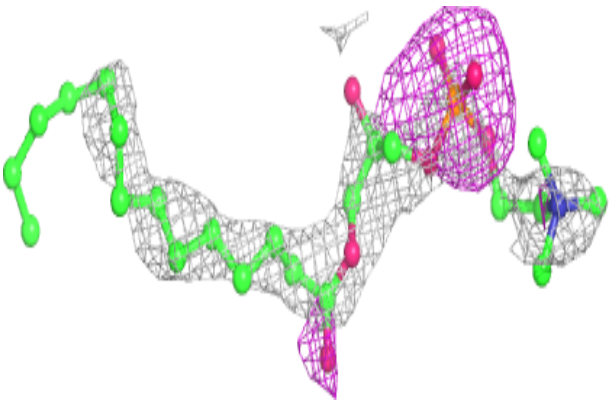
Electron density around MYR A 603:

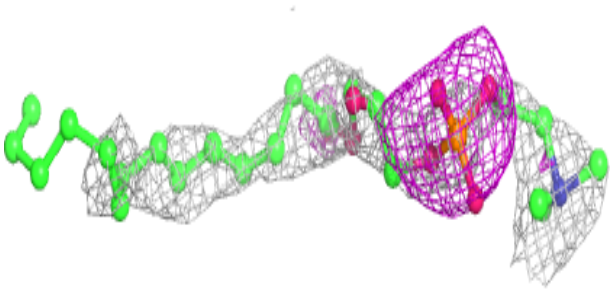
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

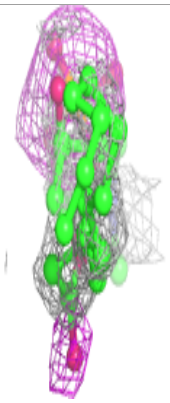


Electron density around LPC B 605:

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

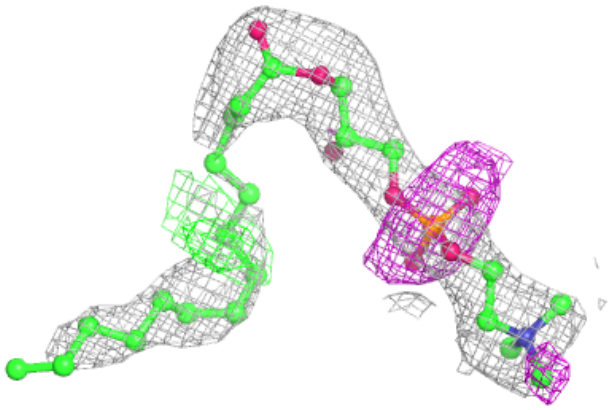


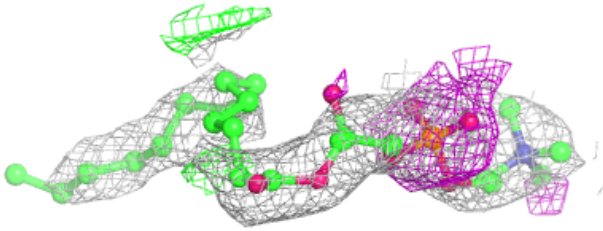


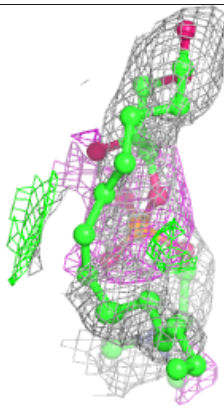


Electron density around LPC B 604:

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

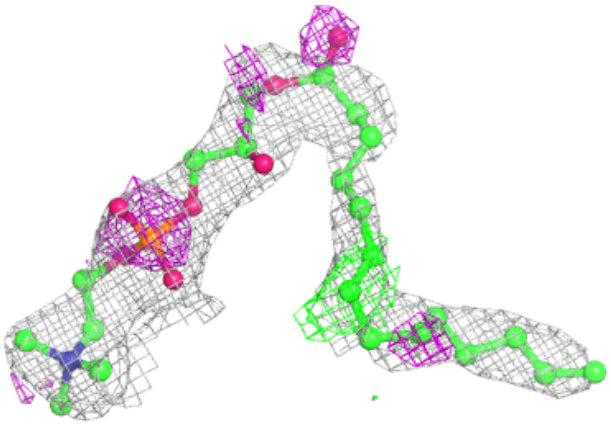


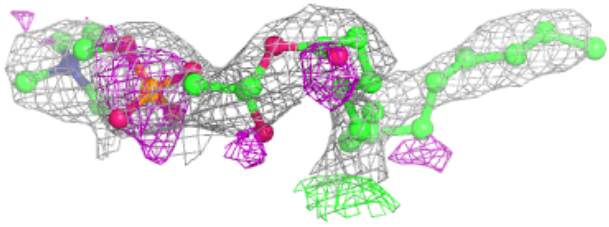


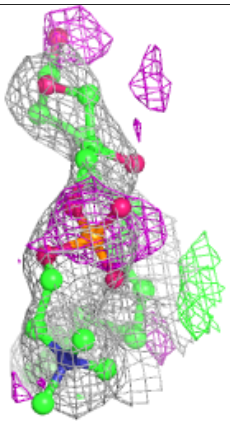


Electron density around LPC A 605:

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

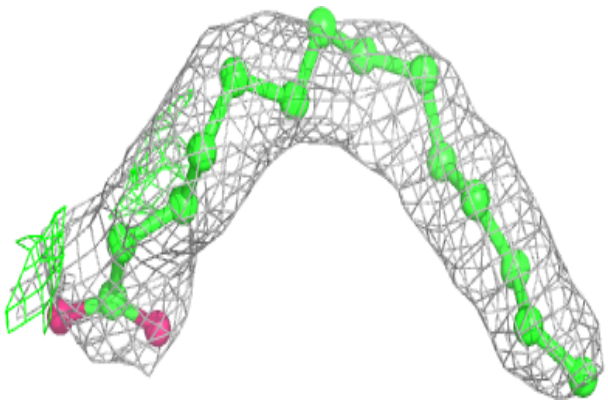


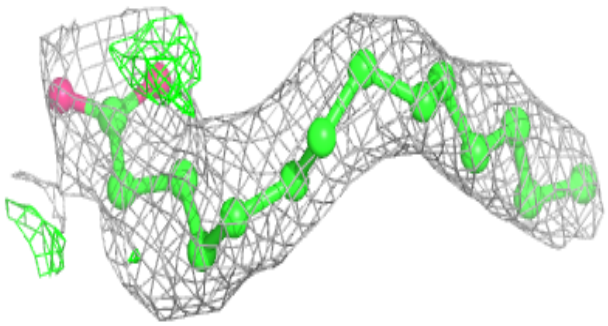


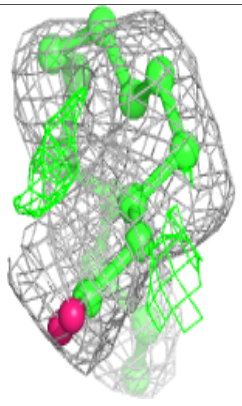


Electron density around MYR A 601:

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

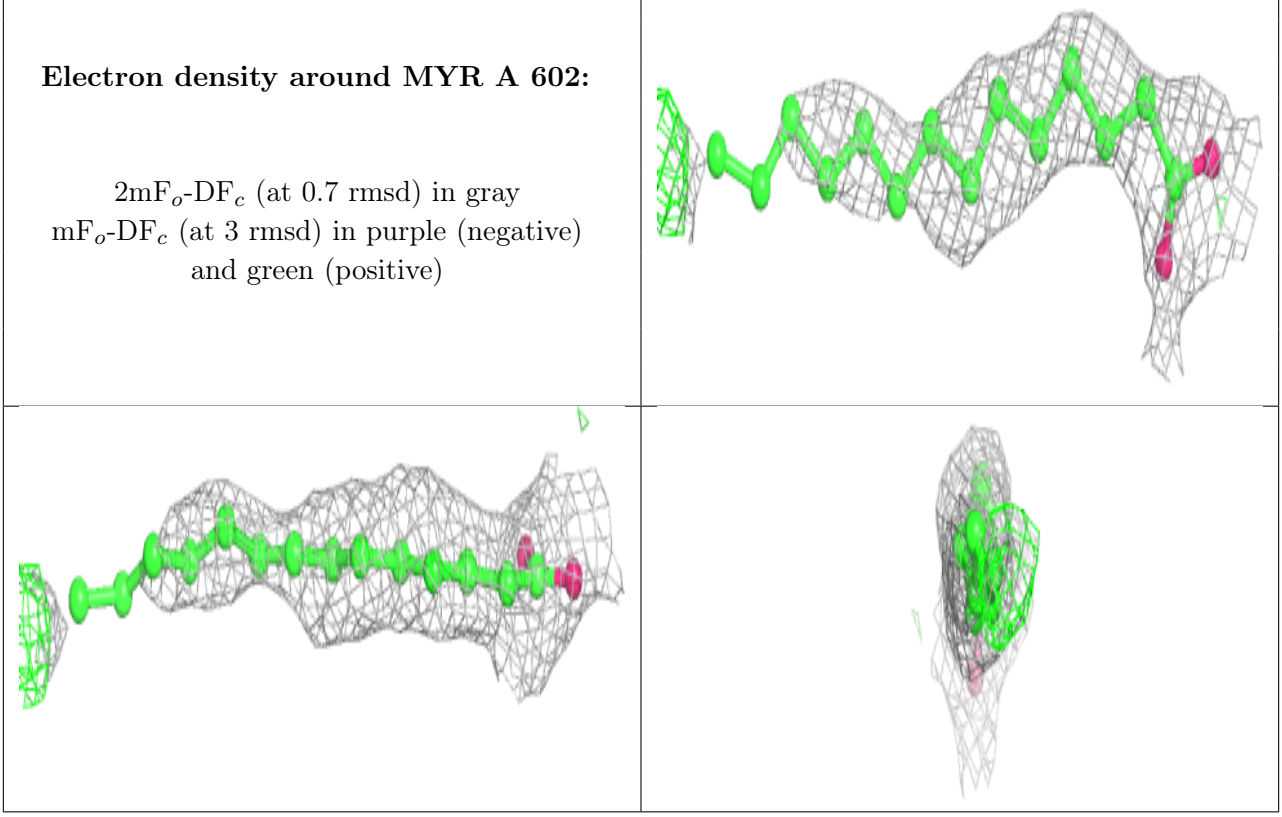






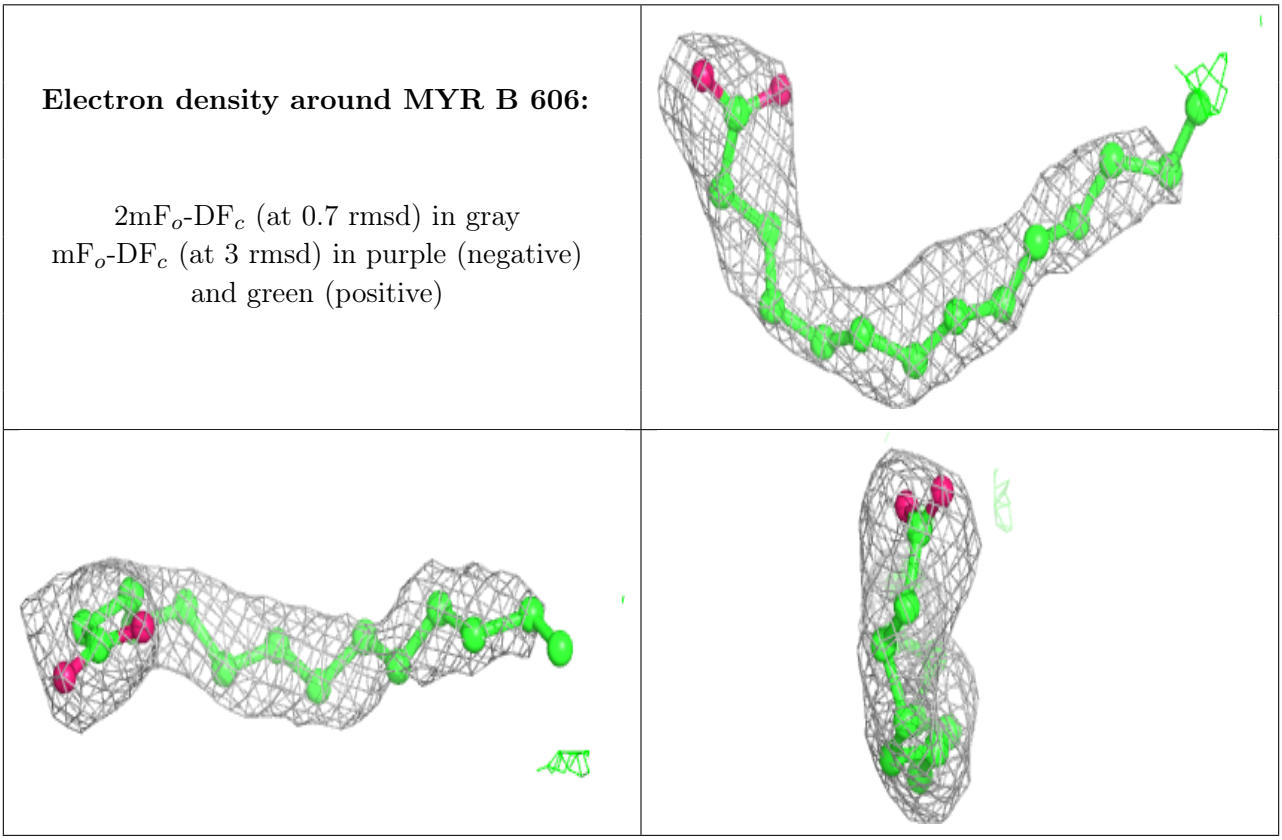
Electron density around MYR A 602:

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



Electron density around MYR B 606:

$2mF_o$-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.