



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:39 PM UTC

PDB ID : 8ITR / pdb_00008itr
Title : Crystal structure of lysophosphatidylcholine in complex with human serum albumin
Authors : Wang, Y.; Jiang, L.G.; Huang, M.D.
Deposited on : 2023-03-22
Resolution : 2.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

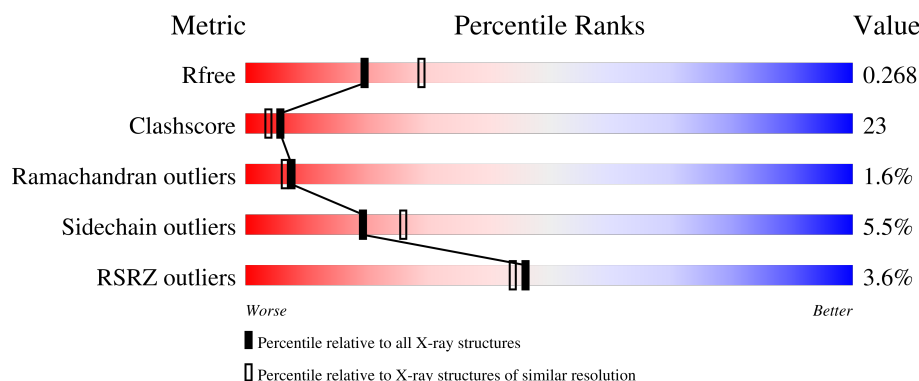
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	582	

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	LPC	A	602	-	-	X	-

2 Entry composition ⓘ

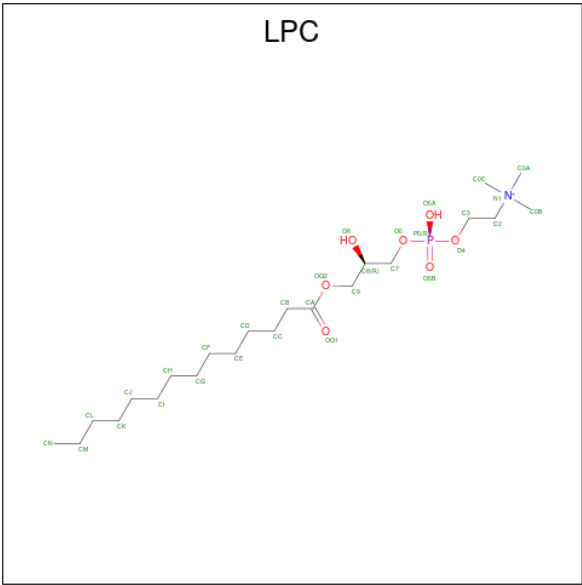
There are 3 unique types of molecules in this entry. The entry contains 4836 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	582	Total	C	N	O	S	0	0	0
			4631	2923	783	884	41			

- Molecule 2 is [1-MYRISTOYL-GLYCEROL-3-YL]PHOSPHONYLCHOLINE (CCD ID: LPC) (formula: C₂₂H₄₇NO₇P) (labeled as "Ligand of Interest" by depositor).



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

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

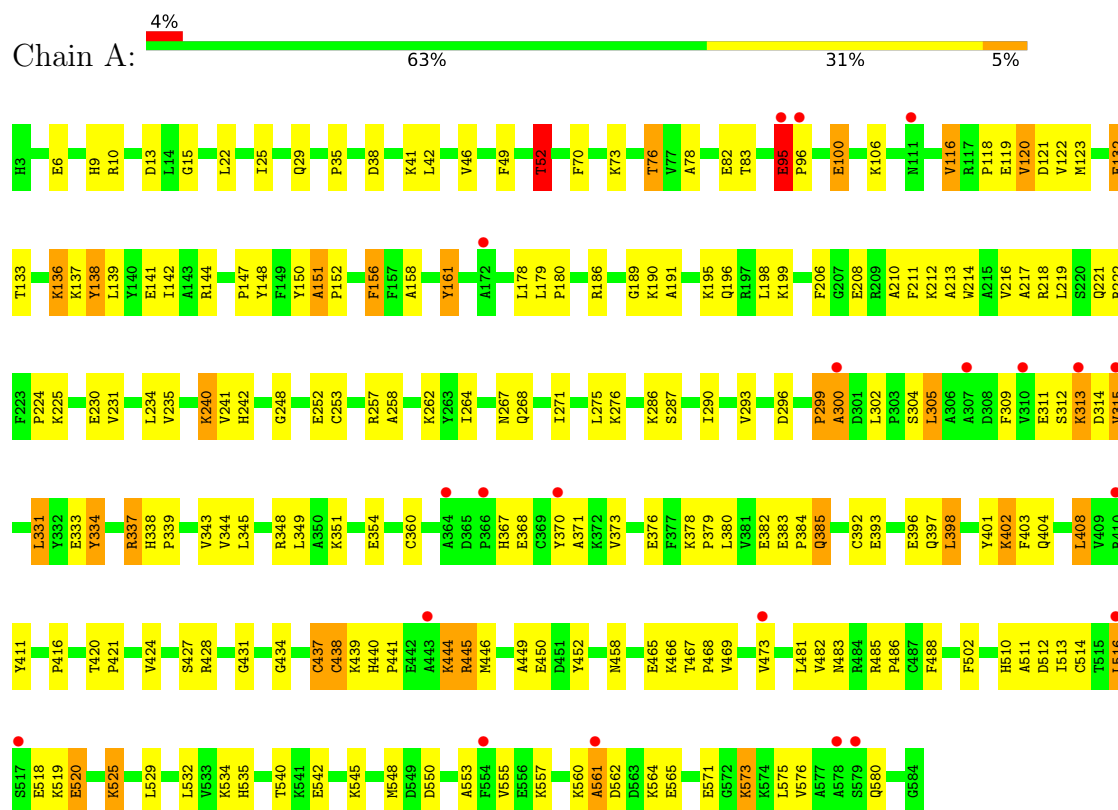
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.73Å 38.84Å 95.19Å 90.00° 105.11° 90.00°	Depositor
Resolution (Å)	46.02 – 2.44 46.02 – 2.44	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.02-2.44) 97.1 (46.02-2.44)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.32Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.255 , 0.267 0.255 , 0.268	Depositor DCC
R_{free} test set	2520 reflections (9.33%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4836	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.73	3/4721 (0.1%)	1.18	43/6366 (0.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	VAL	CA-CB	8.76	1.63	1.53
1	A	293	VAL	CA-CB	5.81	1.59	1.54
1	A	138	TYR	CA-CB	-5.13	1.44	1.53

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	LEU	N-CA-C	-11.38	95.85	110.53
1	A	271	ILE	N-CA-C	8.79	118.56	111.62
1	A	248	GLY	N-CA-C	8.58	125.18	114.37
1	A	286	LYS	N-CA-C	8.04	120.83	111.02
1	A	275	LEU	N-CA-C	7.75	122.84	113.23
1	A	514	CYS	N-CA-C	-7.29	103.04	112.23
1	A	95	GLU	N-CA-C	7.12	125.55	109.81
1	A	52	THR	N-CA-C	-7.11	103.46	111.07
1	A	339	PRO	N-CA-C	-6.85	105.79	114.35
1	A	437	CYS	N-CA-C	6.64	119.35	111.71
1	A	473	VAL	N-CA-C	-6.53	104.15	110.42
1	A	15	GLY	N-CA-C	-6.44	103.55	112.18
1	A	309	PHE	N-CA-C	6.24	121.83	113.72
1	A	178	LEU	N-CA-C	6.17	117.80	111.14
1	A	446	MET	CA-C-N	-6.15	112.22	119.05
1	A	446	MET	C-N-CA	-6.15	112.22	119.05
1	A	240	LYS	N-CA-C	-6.12	104.53	111.14
1	A	293	VAL	N-CA-C	6.07	119.37	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	ALA	N-CA-C	-6.01	105.78	113.23
1	A	208	GLU	N-CA-C	6.00	118.59	111.33
1	A	304	SER	N-CA-C	-5.96	102.66	110.53
1	A	403	PHE	N-CA-C	-5.92	104.91	111.36
1	A	313	LYS	N-CA-C	-5.91	102.72	110.53
1	A	95	GLU	CA-C-N	-5.87	112.63	119.32
1	A	95	GLU	C-N-CA	-5.87	112.63	119.32
1	A	106	LYS	N-CA-C	-5.80	101.69	110.28
1	A	305	LEU	N-CA-C	-5.80	106.17	113.18
1	A	338	HIS	CA-C-N	-5.62	114.21	120.45
1	A	338	HIS	C-N-CA	-5.62	114.21	120.45
1	A	221	GLN	N-CA-C	-5.55	105.31	111.36
1	A	337	ARG	N-CA-C	-5.49	106.42	113.23
1	A	345	LEU	N-CA-C	-5.48	105.22	111.14
1	A	100	GLU	N-CA-C	-5.45	105.42	111.36
1	A	315	VAL	N-CA-C	-5.44	105.20	110.42
1	A	452	TYR	N-CA-C	5.38	118.31	111.69
1	A	138	TYR	CA-CB-CG	5.38	123.58	113.90
1	A	161	TYR	N-CA-C	-5.32	105.56	111.36
1	A	445	ARG	N-CA-C	5.20	116.75	111.14
1	A	401	TYR	N-CA-C	5.15	116.89	111.28
1	A	151	ALA	N-CA-C	5.08	120.47	113.77
1	A	438	CYS	N-CA-C	5.06	117.69	111.82
1	A	78	ALA	N-CA-C	5.05	116.79	111.28
1	A	360	CYS	N-CA-C	5.02	117.71	111.24

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	4631	0	4552	189	0
2	A	186	0	272	115	0
3	A	19	0	0	0	0
All	All	4836	0	4824	225	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 23.

All (225) 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:138:TYR:CB	2:A:602:LPC:HI1	1.38	1.51
1:A:138:TYR:CB	2:A:602:LPC:CI	1.94	1.46
1:A:138:TYR:HB3	2:A:602:LPC:CJ	1.60	1.31
1:A:138:TYR:HB3	2:A:602:LPC:CI	1.60	1.26
1:A:138:TYR:CG	2:A:602:LPC:HI1	1.71	1.24
1:A:138:TYR:HB2	2:A:602:LPC:CI	1.59	1.20
1:A:485:ARG:HB2	2:A:604:LPC:C0C	1.72	1.19
1:A:142:ILE:CD1	2:A:602:LPC:HN3	1.74	1.18
1:A:189:GLY:HA3	2:A:602:LPC:H0B1	1.30	1.13
1:A:138:TYR:HB2	2:A:602:LPC:HI2	1.30	1.11
1:A:560:LYS:HG3	1:A:561:ALA:H	0.98	1.09
1:A:22:LEU:HD13	2:A:603:LPC:O8	1.51	1.09
1:A:138:TYR:C	2:A:602:LPC:HJ2	1.80	1.06
1:A:485:ARG:CB	2:A:604:LPC:H0C3	1.85	1.06
1:A:560:LYS:HG3	1:A:561:ALA:N	1.78	0.97
1:A:344:VAL:HG21	2:A:604:LPC:C3	1.94	0.96
1:A:123:MET:HE1	2:A:602:LPC:HC2	1.49	0.93
1:A:46:VAL:HG22	2:A:603:LPC:HJ2	1.52	0.92
1:A:344:VAL:HG21	2:A:604:LPC:H32	1.51	0.92
1:A:485:ARG:HB2	2:A:604:LPC:H0C3	0.92	0.91
1:A:560:LYS:CG	1:A:561:ALA:H	1.83	0.91
1:A:142:ILE:HD13	2:A:602:LPC:HN3	1.53	0.90
2:A:601:LPC:O5A	2:A:601:LPC:HI1	1.71	0.90
2:A:606:LPC:C7	2:A:606:LPC:H0C1	2.03	0.88
1:A:138:TYR:HB3	2:A:602:LPC:HI1	1.24	0.86
1:A:161:TYR:CD1	2:A:602:LPC:HF2	2.11	0.84
2:A:601:LPC:C0B	2:A:601:LPC:HM1	2.07	0.84
1:A:138:TYR:CB	2:A:602:LPC:CJ	2.37	0.84
2:A:606:LPC:H71	2:A:606:LPC:H0B1	1.59	0.84
2:A:601:LPC:HM1	2:A:601:LPC:H0B1	1.58	0.82
1:A:206:PHE:CD1	2:A:606:LPC:O5A	2.32	0.82
1:A:333:GLU:OE1	1:A:337:ARG:NH2	2.13	0.82
1:A:138:TYR:HB3	2:A:602:LPC:HJ2	1.61	0.81
1:A:142:ILE:HD12	2:A:602:LPC:HN3	1.60	0.81
2:A:606:LPC:H0C1	2:A:606:LPC:H72	1.62	0.81
1:A:333:GLU:HB3	1:A:337:ARG:HH21	1.46	0.79
1:A:189:GLY:CA	2:A:602:LPC:H0B1	2.12	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:N	2:A:602:LPC:HJ2	2.00	0.76
1:A:344:VAL:HG21	2:A:604:LPC:H31	1.68	0.76
2:A:606:LPC:H0C1	2:A:606:LPC:H71	1.69	0.75
1:A:138:TYR:HB3	2:A:602:LPC:HJ1	1.65	0.74
1:A:189:GLY:HA3	2:A:602:LPC:C0B	2.16	0.73
1:A:334:TYR:CE2	1:A:349:LEU:HD13	2.24	0.72
1:A:46:VAL:HG22	2:A:603:LPC:HL2	1.71	0.72
1:A:119:GLU:O	1:A:122:VAL:HG22	1.90	0.71
2:A:602:LPC:H92	2:A:602:LPC:O5A	1.90	0.71
1:A:510:HIS:HB2	1:A:512:ASP:OD1	1.89	0.71
2:A:602:LPC:H92	2:A:602:LPC:P5	2.30	0.70
2:A:603:LPC:H92	2:A:603:LPC:HC1	1.72	0.70
1:A:437:CYS:O	1:A:440:HIS:HB2	1.92	0.68
2:A:602:LPC:CL	2:A:602:LPC:CG	2.71	0.68
2:A:602:LPC:HG2	2:A:602:LPC:HL2	1.75	0.68
1:A:142:ILE:CD1	2:A:602:LPC:CN	2.65	0.68
1:A:368:GLU:O	1:A:368:GLU:HG3	1.94	0.67
1:A:485:ARG:H	2:A:604:LPC:H0A1	1.59	0.67
1:A:150:TYR:OH	2:A:603:LPC:H0B2	1.93	0.67
1:A:198:LEU:HD13	1:A:458:ASN:ND2	2.10	0.67
2:A:606:LPC:H71	2:A:606:LPC:C0B	2.24	0.67
1:A:150:TYR:OH	2:A:603:LPC:C0B	2.44	0.66
2:A:602:LPC:CL	2:A:602:LPC:HG1	2.25	0.66
2:A:601:LPC:C0B	2:A:601:LPC:CM	2.73	0.66
1:A:576:VAL:O	1:A:580:GLN:HB2	1.95	0.66
1:A:214:TRP:CH2	2:A:601:LPC:HJ1	2.30	0.65
1:A:138:TYR:CB	2:A:602:LPC:HJ2	2.17	0.65
2:A:605:LPC:H71	2:A:605:LPC:H21	1.77	0.65
1:A:483:ASN:C	1:A:486:PRO:HD2	2.21	0.65
1:A:525:LYS:HG2	2:A:605:LPC:HB1	1.77	0.65
1:A:344:VAL:CG2	2:A:604:LPC:H31	2.26	0.65
1:A:46:VAL:CG2	2:A:603:LPC:HJ2	2.25	0.64
1:A:206:PHE:CG	2:A:606:LPC:O5A	2.51	0.64
1:A:142:ILE:HD12	2:A:602:LPC:CN	2.26	0.64
2:A:601:LPC:HI1	2:A:601:LPC:P5	2.37	0.64
2:A:602:LPC:OQ1	2:A:602:LPC:H8	1.97	0.64
1:A:35:PRO:HG2	1:A:38:ASP:OD1	1.98	0.64
2:A:606:LPC:H0C1	2:A:606:LPC:O4	1.97	0.64
1:A:344:VAL:CG2	2:A:604:LPC:C3	2.72	0.63
1:A:333:GLU:CB	1:A:337:ARG:HH21	2.11	0.63
1:A:424:VAL:O	1:A:428:ARG:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:TRP:HH2	2:A:601:LPC:HJ1	1.64	0.63
1:A:555:VAL:HG11	2:A:605:LPC:O5A	1.99	0.63
2:A:602:LPC:CG	2:A:602:LPC:HL2	2.28	0.62
1:A:82:GLU:OE1	1:A:83:THR:HG23	1.99	0.62
1:A:253:CYS:O	1:A:257:ARG:HG3	1.99	0.61
1:A:373:VAL:HA	1:A:376:GLU:OE2	2.00	0.61
2:A:601:LPC:O5A	2:A:601:LPC:HG2	2.02	0.60
1:A:333:GLU:HB3	1:A:337:ARG:NH2	2.16	0.60
1:A:225:LYS:HG2	1:A:299:PRO:HG3	1.85	0.59
1:A:466:LYS:C	1:A:468:PRO:HD3	2.28	0.59
1:A:73:LYS:O	1:A:76:THR:HB	2.03	0.59
2:A:606:LPC:H71	2:A:606:LPC:C0C	2.31	0.58
2:A:601:LPC:H0B1	2:A:601:LPC:O4	2.03	0.58
1:A:344:VAL:CG2	2:A:604:LPC:H32	2.30	0.58
2:A:602:LPC:HG1	2:A:602:LPC:HL1	1.85	0.58
1:A:466:LYS:O	1:A:468:PRO:HD3	2.03	0.58
1:A:198:LEU:HD13	1:A:458:ASN:HD22	1.69	0.57
1:A:571:GLU:HA	1:A:571:GLU:OE1	2.04	0.57
1:A:367:HIS:O	1:A:371:ALA:HB2	2.04	0.57
1:A:518:GLU:C	1:A:520:GLU:H	2.12	0.57
1:A:351:LYS:NZ	1:A:354:GLU:OE1	2.33	0.56
1:A:218:ARG:HE	1:A:222:ARG:NH2	2.03	0.56
1:A:488:PHE:HB3	2:A:604:LPC:HI2	1.87	0.56
1:A:560:LYS:O	1:A:562:ASP:N	2.38	0.56
1:A:420:THR:HB	1:A:421:PRO:HD3	1.87	0.56
1:A:344:VAL:HG21	2:A:604:LPC:H0B2	1.88	0.55
1:A:434:GLY:O	1:A:438:CYS:HB2	2.07	0.55
1:A:557:LYS:HD3	1:A:571:GLU:HG3	1.87	0.55
1:A:189:GLY:CA	2:A:602:LPC:C0B	2.80	0.55
1:A:219:LEU:HD21	2:A:601:LPC:HD1	1.88	0.55
1:A:138:TYR:CA	2:A:602:LPC:HJ2	2.36	0.54
1:A:485:ARG:CB	2:A:604:LPC:H21	2.36	0.54
1:A:199:LYS:HD2	2:A:601:LPC:H0C1	1.90	0.54
1:A:440:HIS:CE1	1:A:444:LYS:HE3	2.41	0.54
1:A:392:CYS:O	1:A:396:GLU:HG2	2.08	0.53
1:A:555:VAL:CG1	2:A:605:LPC:O5A	2.55	0.53
1:A:210:ALA:HB2	2:A:606:LPC:H72	1.91	0.53
1:A:216:VAL:HG22	1:A:235:VAL:HG21	1.91	0.53
1:A:212:LYS:O	1:A:216:VAL:HG23	2.09	0.53
1:A:550:ASP:HB3	1:A:575:LEU:HD11	1.90	0.53
1:A:408:LEU:HD13	1:A:427:SER:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLU:O	1:A:234:LEU:HG	2.08	0.52
1:A:502:PHE:HB2	1:A:535:HIS:CE1	2.45	0.52
1:A:186:ARG:O	1:A:190:LYS:HG3	2.10	0.52
1:A:73:LYS:HG2	2:A:603:LPC:HL1	1.93	0.51
1:A:398:LEU:HB3	1:A:402:LYS:HB2	1.92	0.51
1:A:344:VAL:HG11	2:A:604:LPC:H0B2	1.93	0.51
1:A:42:LEU:HD22	1:A:73:LYS:HD2	1.92	0.51
1:A:206:PHE:CE2	1:A:481:LEU:HB3	2.46	0.50
1:A:348:ARG:HG3	1:A:482:VAL:CG1	2.42	0.50
1:A:25:ILE:O	1:A:29:GLN:HG3	2.12	0.50
1:A:305:LEU:CD2	1:A:333:GLU:HB3	2.41	0.50
1:A:305:LEU:HD21	1:A:337:ARG:HE	1.76	0.50
1:A:486:PRO:HD3	2:A:604:LPC:H0A1	1.94	0.50
2:A:601:LPC:C0B	2:A:601:LPC:O4	2.60	0.50
1:A:150:TYR:CE2	1:A:152:PRO:HD2	2.47	0.50
1:A:123:MET:HE1	2:A:602:LPC:CC	2.31	0.50
1:A:49:PHE:O	1:A:52:THR:HB	2.12	0.50
1:A:370:TYR:CD1	1:A:370:TYR:C	2.90	0.49
1:A:575:LEU:HD23	2:A:605:LPC:HJ2	1.94	0.49
1:A:305:LEU:HD21	1:A:337:ARG:NE	2.27	0.49
1:A:213:ALA:HB2	2:A:606:LPC:HF1	1.94	0.49
1:A:408:LEU:HD13	1:A:427:SER:CB	2.42	0.49
1:A:411:TYR:HB3	2:A:604:LPC:HM1	1.95	0.49
1:A:141:GLU:HA	1:A:144:ARG:HD3	1.96	0.48
1:A:9:HIS:O	1:A:13:ASP:HB2	2.13	0.48
1:A:70:PHE:HB2	2:A:603:LPC:HG1	1.96	0.48
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.94	0.48
1:A:302:LEU:HB3	1:A:337:ARG:NH1	2.29	0.48
1:A:199:LYS:NZ	2:A:601:LPC:O5B	2.47	0.48
1:A:206:PHE:CD2	1:A:481:LEU:HD23	2.49	0.48
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.48	0.48
1:A:485:ARG:H	2:A:604:LPC:C0A	2.27	0.47
1:A:257:ARG:HH21	1:A:287:SER:HG	1.62	0.47
1:A:118:PRO:HB2	1:A:122:VAL:HG23	1.96	0.47
1:A:382:GLU:HA	1:A:385:GLN:HB2	1.96	0.47
1:A:518:GLU:O	1:A:520:GLU:N	2.47	0.47
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.97	0.47
1:A:485:ARG:CB	2:A:604:LPC:C2	2.93	0.47
2:A:606:LPC:O4	2:A:606:LPC:C0C	2.63	0.47
1:A:302:LEU:HB3	1:A:337:ARG:HH11	1.80	0.46
2:A:603:LPC:H0A3	2:A:603:LPC:O4	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ALA:O	1:A:512:ASP:C	2.58	0.46
1:A:441:PRO:O	1:A:445:ARG:HG3	2.16	0.46
2:A:602:LPC:H32	2:A:602:LPC:H0A3	1.59	0.46
1:A:118:PRO:HD2	1:A:123:MET:HE3	1.98	0.46
1:A:123:MET:CE	2:A:602:LPC:HC2	2.35	0.46
1:A:196:GLN:HG3	2:A:601:LPC:C0A	2.46	0.45
1:A:206:PHE:HB3	2:A:606:LPC:O5A	2.16	0.45
1:A:132:GLU:OE2	1:A:136:LYS:HE3	2.17	0.45
1:A:217:ALA:HB2	1:A:331:LEU:HD22	1.97	0.45
1:A:211:PHE:CD1	1:A:211:PHE:C	2.94	0.45
1:A:6:GLU:O	1:A:10:ARG:HG2	2.16	0.45
1:A:156:PHE:C	1:A:156:PHE:CD1	2.94	0.45
1:A:158:ALA:HA	2:A:602:LPC:HM2	1.98	0.45
1:A:416:PRO:O	1:A:534:LYS:HE2	2.17	0.45
1:A:231:VAL:O	1:A:235:VAL:HG23	2.17	0.45
1:A:142:ILE:HD12	2:A:602:LPC:CM	2.47	0.44
1:A:334:TYR:HE2	1:A:349:LEU:HD13	1.81	0.44
1:A:449:ALA:O	1:A:450:GLU:C	2.58	0.44
2:A:605:LPC:H0B1	2:A:605:LPC:H32	1.52	0.44
1:A:191:ALA:O	1:A:195:LYS:HG3	2.16	0.44
1:A:242:HIS:NE2	2:A:601:LPC:O5B	2.50	0.44
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.48	0.44
1:A:299:PRO:HD2	1:A:302:LEU:HD11	2.00	0.44
1:A:95:GLU:O	1:A:96:PRO:C	2.58	0.44
1:A:469:VAL:HG12	1:A:469:VAL:O	2.18	0.44
2:A:605:LPC:HD1	2:A:605:LPC:HG1	1.33	0.44
1:A:485:ARG:HB3	2:A:604:LPC:C2	2.47	0.43
1:A:264:ILE:HG21	1:A:290:ILE:HD13	1.99	0.43
1:A:404:GLN:HG2	1:A:431:GLY:HA3	2.00	0.43
1:A:513:ILE:HA	1:A:516:LEU:HB2	1.99	0.43
1:A:258:ALA:HB2	2:A:603:LPC:H0A1	1.99	0.43
1:A:199:LYS:HZ1	2:A:601:LPC:HI2	1.83	0.43
1:A:147:PRO:HG2	1:A:148:TYR:CD2	2.54	0.42
1:A:224:PRO:HD2	1:A:296:ASP:HB3	2.00	0.42
1:A:299:PRO:O	1:A:300:ALA:HB3	2.18	0.42
1:A:313:LYS:O	1:A:314:ASP:CB	2.67	0.42
1:A:529:LEU:O	1:A:532:LEU:HB3	2.20	0.42
1:A:349:LEU:HD23	1:A:380:LEU:HD23	2.01	0.42
1:A:378:LYS:HB3	1:A:379:PRO:CD	2.50	0.42
1:A:196:GLN:HG3	2:A:601:LPC:H0A1	2.01	0.42
1:A:305:LEU:HD22	1:A:333:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TYR:HB2	2:A:602:LPC:HI1	1.38	0.42
1:A:518:GLU:C	1:A:520:GLU:N	2.78	0.42
2:A:602:LPC:CG	2:A:602:LPC:CK	2.96	0.42
1:A:138:TYR:C	2:A:602:LPC:CJ	2.71	0.41
1:A:150:TYR:CD2	1:A:152:PRO:HD2	2.55	0.41
1:A:393:GLU:O	1:A:397:GLN:HG3	2.19	0.41
1:A:545:LYS:HA	1:A:548:MET:HE3	2.02	0.41
1:A:73:LYS:CG	2:A:603:LPC:HL1	2.51	0.41
1:A:139:LEU:HD12	1:A:139:LEU:HA	1.85	0.41
1:A:240:LYS:O	1:A:241:VAL:C	2.63	0.41
1:A:118:PRO:HB2	1:A:122:VAL:CG2	2.50	0.41
2:A:606:LPC:H91	2:A:606:LPC:H0B3	2.02	0.41
2:A:604:LPC:H32	2:A:604:LPC:H0B2	1.74	0.41
1:A:469:VAL:O	1:A:469:VAL:CG1	2.69	0.40
1:A:133:THR:O	1:A:137:LYS:HB2	2.21	0.40
1:A:305:LEU:HD21	1:A:333:GLU:HB3	2.03	0.40
1:A:119:GLU:O	1:A:120:VAL:C	2.64	0.40
1:A:481:LEU:HD12	1:A:482:VAL:HG23	2.03	0.40
2:A:602:LPC:P5	2:A:602:LPC:C9	3.06	0.40
2:A:606:LPC:C0B	2:A:606:LPC:H91	2.52	0.40
1:A:252:GLU:H	1:A:252:GLU:HG2	1.69	0.40
1:A:268:GLN:OE1	1:A:276:LYS:HG3	2.20	0.40
1:A:573:LYS:HD2	1:A:573:LYS:HA	1.65	0.40
2:A:602:LPC:HJ1	2:A:602:LPC:HG2	1.92	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	580/582 (100%)	525 (90%)	46 (8%)	9 (2%)	7 6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	519	LYS
1	A	561	ALA
1	A	299	PRO
1	A	312	SER
1	A	565	GLU
1	A	311	GLU
1	A	300	ALA
1	A	564	LYS
1	A	120	VAL

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	509/509 (100%)	481 (94%)	28 (6%)	19	26

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	52	THR
1	A	76	THR
1	A	95	GLU
1	A	100	GLU
1	A	116	VAL
1	A	121	ASP
1	A	132	GLU
1	A	136	LYS
1	A	156	PHE
1	A	262	LYS
1	A	267	ASN
1	A	315	VAL
1	A	331	LEU
1	A	334	TYR
1	A	385	GLN

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Mol	Chain	Res	Type
1	A	402	LYS
1	A	408	LEU
1	A	439	LYS
1	A	444	LYS
1	A	465	GLU
1	A	467	THR
1	A	516	LEU
1	A	520	GLU
1	A	525	LYS
1	A	540	THR
1	A	542	GLU
1	A	573	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	33	GLN
1	A	39	HIS
1	A	61	ASN
1	A	105	HIS
1	A	109	ASN
1	A	196	GLN
1	A	267	ASN
1	A	318	ASN
1	A	385	GLN
1	A	391	ASN
1	A	440	HIS
1	A	459	GLN
1	A	503	ASN
1	A	580	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	LPC	A	604	-	30,30,30	1.73	6 (20%)	35,37,37	1.40	5 (14%)
2	LPC	A	601	-	30,30,30	2.08	6 (20%)	35,37,37	2.12	9 (25%)
2	LPC	A	603	-	30,30,30	0.94	1 (3%)	35,37,37	0.87	1 (2%)
2	LPC	A	602	-	30,30,30	0.94	1 (3%)	35,37,37	0.86	1 (2%)
2	LPC	A	606	-	30,30,30	2.02	10 (33%)	35,37,37	1.78	7 (20%)
2	LPC	A	605	-	30,30,30	0.94	1 (3%)	35,37,37	0.86	1 (2%)

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	LPC	A	604	-	-	19/32/32/32	-
2	LPC	A	601	-	-	22/32/32/32	-
2	LPC	A	603	-	-	17/32/32/32	-
2	LPC	A	602	-	-	21/32/32/32	-
2	LPC	A	606	-	-	17/32/32/32	-
2	LPC	A	605	-	-	25/32/32/32	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	LPC	OQ2-CA	-6.03	1.15	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	LPC	OQ1-CA	5.91	1.40	1.22
2	A	601	LPC	CB-CA	-4.55	1.37	1.50
2	A	606	LPC	OQ2-CA	-4.37	1.20	1.33
2	A	605	LPC	OQ2-CA	4.29	1.45	1.33
2	A	603	LPC	OQ2-CA	4.29	1.45	1.33
2	A	602	LPC	OQ2-CA	4.28	1.45	1.33
2	A	604	LPC	OQ1-CA	4.22	1.35	1.22
2	A	606	LPC	OQ2-C9	4.02	1.54	1.45
2	A	604	LPC	OQ2-CA	-3.92	1.21	1.33
2	A	606	LPC	O8-C8	-3.44	1.33	1.43
2	A	604	LPC	OQ2-C9	3.28	1.52	1.45
2	A	604	LPC	O8-C8	-3.05	1.34	1.43
2	A	606	LPC	O6-C7	2.96	1.55	1.44
2	A	606	LPC	CB-CA	-2.90	1.42	1.50
2	A	601	LPC	O8-C8	-2.89	1.35	1.43
2	A	606	LPC	CD-CC	-2.88	1.37	1.51
2	A	604	LPC	CB-CA	-2.75	1.42	1.50
2	A	606	LPC	CG-CF	-2.69	1.38	1.51
2	A	606	LPC	CE-CD	-2.63	1.38	1.51
2	A	606	LPC	P5-O5A	-2.58	1.43	1.55
2	A	604	LPC	C7-C8	-2.50	1.43	1.51
2	A	601	LPC	C0B-N1	-2.27	1.43	1.50
2	A	601	LPC	CC-CB	2.16	1.60	1.52
2	A	606	LPC	OQ1-CA	2.16	1.28	1.22

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	LPC	CF-CE-CD	-5.94	84.32	114.37
2	A	601	LPC	OQ2-CA-OQ1	5.66	137.78	123.63
2	A	606	LPC	OQ2-CA-CB	5.59	128.89	111.83
2	A	604	LPC	CG-CF-CE	-4.43	91.97	114.37
2	A	601	LPC	CE-CD-CC	-4.29	92.66	114.37
2	A	606	LPC	CD-CC-CB	-3.53	100.15	113.13
2	A	606	LPC	OQ1-CA-CB	-3.52	110.00	123.78
2	A	601	LPC	O8-C8-C9	3.48	121.72	109.70
2	A	601	LPC	CJ-CI-CH	-3.45	96.92	114.37
2	A	606	LPC	CF-CE-CD	-2.88	99.82	114.37
2	A	604	LPC	O8-C8-C7	2.77	119.26	109.70
2	A	606	LPC	OQ2-C9-C8	2.74	118.76	105.85
2	A	603	LPC	OQ2-CA-CB	2.74	120.19	111.83
2	A	602	LPC	OQ2-CA-CB	2.72	120.12	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	LPC	OQ2-CA-CB	2.72	120.12	111.83
2	A	601	LPC	OQ1-CA-CB	-2.70	113.21	123.78
2	A	606	LPC	CJ-CI-CH	-2.68	100.82	114.37
2	A	604	LPC	OQ1-CA-CB	-2.65	113.44	123.78
2	A	601	LPC	CH-CG-CF	2.58	127.41	114.37
2	A	604	LPC	OQ2-CA-OQ1	2.52	129.93	123.63
2	A	606	LPC	O8-C8-C7	2.42	118.07	109.70
2	A	601	LPC	O8-C8-C7	2.29	117.61	109.70
2	A	604	LPC	CJ-CI-CH	-2.26	102.92	114.37
2	A	601	LPC	CC-CB-CA	-2.22	105.56	113.69

There are no chirality outliers.

All (121) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	LPC	C3-O4-P5-O5A
2	A	601	LPC	C3-O4-P5-O5B
2	A	601	LPC	C7-O6-P5-O4
2	A	601	LPC	O6-C7-C8-O8
2	A	601	LPC	C7-C8-C9-OQ2
2	A	602	LPC	C3-O4-P5-O5B
2	A	602	LPC	C7-O6-P5-O4
2	A	602	LPC	C7-O6-P5-O5A
2	A	602	LPC	C7-C8-C9-OQ2
2	A	603	LPC	C3-O4-P5-O5B
2	A	603	LPC	C7-O6-P5-O4
2	A	603	LPC	O8-C8-C9-OQ2
2	A	604	LPC	N1-C2-C3-O4
2	A	604	LPC	C3-O4-P5-O6
2	A	604	LPC	O8-C8-C9-OQ2
2	A	605	LPC	N1-C2-C3-O4
2	A	605	LPC	C3-O4-P5-O5A
2	A	605	LPC	C3-O4-P5-O5B
2	A	605	LPC	C3-O4-P5-O6
2	A	605	LPC	C7-O6-P5-O5B
2	A	606	LPC	C3-O4-P5-O5A
2	A	606	LPC	C3-O4-P5-O6
2	A	606	LPC	C7-O6-P5-O4
2	A	606	LPC	C7-O6-P5-O5A
2	A	606	LPC	C7-O6-P5-O5B
2	A	606	LPC	O6-C7-C8-C9
2	A	603	LPC	OQ1-CA-OQ2-C9

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Mol	Chain	Res	Type	Atoms
2	A	603	LPC	CB-CA-OQ2-C9
2	A	601	LPC	CB-CA-OQ2-C9
2	A	601	LPC	OQ1-CA-OQ2-C9
2	A	606	LPC	O6-C7-C8-O8
2	A	602	LPC	O8-C8-C9-OQ2
2	A	605	LPC	CB-CA-OQ2-C9
2	A	605	LPC	OQ1-CA-OQ2-C9
2	A	604	LPC	O6-C7-C8-C9
2	A	604	LPC	CB-CA-OQ2-C9
2	A	605	LPC	CD-CE-CF-CG
2	A	602	LPC	C8-C9-OQ2-CA
2	A	604	LPC	O6-C7-C8-O8
2	A	604	LPC	OQ1-CA-OQ2-C9
2	A	601	LPC	C3-C2-N1-C0B
2	A	601	LPC	C3-C2-N1-C0C
2	A	604	LPC	C3-C2-N1-C0B
2	A	604	LPC	C3-C2-N1-C0C
2	A	605	LPC	C3-C2-N1-C0A
2	A	605	LPC	C3-C2-N1-C0B
2	A	606	LPC	C3-C2-N1-C0B
2	A	606	LPC	C3-C2-N1-C0C
2	A	603	LPC	C7-C8-C9-OQ2
2	A	601	LPC	C3-C2-N1-C0A
2	A	604	LPC	C3-C2-N1-C0A
2	A	605	LPC	C3-C2-N1-C0C
2	A	606	LPC	C3-C2-N1-C0A
2	A	605	LPC	CF-CG-CH-CI
2	A	601	LPC	CG-CH-CI-CJ
2	A	602	LPC	CJ-CK-CL-CM
2	A	604	LPC	CJ-CK-CL-CM
2	A	602	LPC	CI-CJ-CK-CL
2	A	603	LPC	CF-CG-CH-CI
2	A	603	LPC	CH-CI-CJ-CK
2	A	602	LPC	CB-CA-OQ2-C9
2	A	602	LPC	CE-CF-CG-CH
2	A	605	LPC	CI-CJ-CK-CL
2	A	602	LPC	CC-CD-CE-CF
2	A	602	LPC	CF-CG-CH-CI
2	A	605	LPC	CH-CI-CJ-CK
2	A	602	LPC	OQ1-CA-OQ2-C9
2	A	606	LPC	CG-CH-CI-CJ
2	A	606	LPC	CF-CG-CH-CI

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Mol	Chain	Res	Type	Atoms
2	A	602	LPC	CG-CH-CI-CJ
2	A	603	LPC	CC-CD-CE-CF
2	A	601	LPC	CK-CL-CM-CN
2	A	606	LPC	CI-CJ-CK-CL
2	A	604	LPC	CG-CH-CI-CJ
2	A	602	LPC	CH-CI-CJ-CK
2	A	601	LPC	CJ-CK-CL-CM
2	A	605	LPC	CA-CB-CC-CD
2	A	605	LPC	CE-CF-CG-CH
2	A	601	LPC	CH-CI-CJ-CK
2	A	606	LPC	CH-CI-CJ-CK
2	A	604	LPC	CK-CL-CM-CN
2	A	606	LPC	CA-CB-CC-CD
2	A	604	LPC	CF-CG-CH-CI
2	A	603	LPC	CI-CJ-CK-CL
2	A	603	LPC	CB-CC-CD-CE
2	A	601	LPC	CC-CD-CE-CF
2	A	601	LPC	CF-CG-CH-CI
2	A	602	LPC	CD-CE-CF-CG
2	A	606	LPC	CJ-CK-CL-CM
2	A	605	LPC	O6-C7-C8-O8
2	A	606	LPC	CK-CL-CM-CN
2	A	601	LPC	CB-CC-CD-CE
2	A	601	LPC	C3-O4-P5-O6
2	A	601	LPC	C7-O6-P5-O5B
2	A	602	LPC	C3-O4-P5-O5A
2	A	602	LPC	C3-O4-P5-O6
2	A	603	LPC	C3-O4-P5-O5A
2	A	603	LPC	C3-O4-P5-O6
2	A	603	LPC	C7-O6-P5-O5B
2	A	604	LPC	C3-O4-P5-O5B
2	A	604	LPC	C7-O6-P5-O5B
2	A	605	LPC	C7-O6-P5-O4
2	A	605	LPC	C7-O6-P5-O5A
2	A	602	LPC	C8-C7-O6-P5
2	A	604	LPC	CD-CE-CF-CG
2	A	605	LPC	CG-CH-CI-CJ
2	A	605	LPC	CK-CL-CM-CN
2	A	602	LPC	CB-CC-CD-CE
2	A	604	LPC	CA-CB-CC-CD
2	A	601	LPC	C8-C7-O6-P5
2	A	605	LPC	O6-C7-C8-C9

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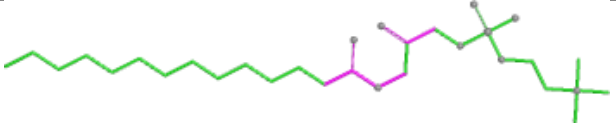
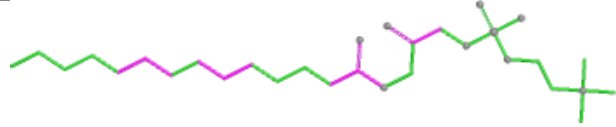
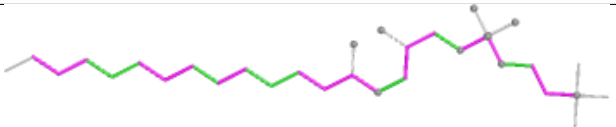
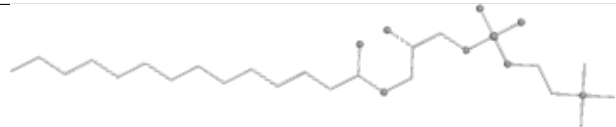
Mol	Chain	Res	Type	Atoms
2	A	602	LPC	CK-CL-CM-CN
2	A	601	LPC	CE-CF-CG-CH
2	A	605	LPC	CC-CD-CE-CF
2	A	603	LPC	C3-C2-N1-C0B
2	A	605	LPC	OQ2-CA-CB-CC
2	A	601	LPC	CA-CB-CC-CD
2	A	603	LPC	C3-C2-N1-C0C
2	A	604	LPC	OQ2-CA-CB-CC
2	A	605	LPC	OQ1-CA-CB-CC
2	A	603	LPC	OQ2-CA-CB-CC

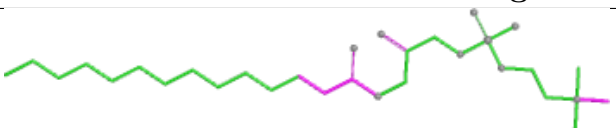
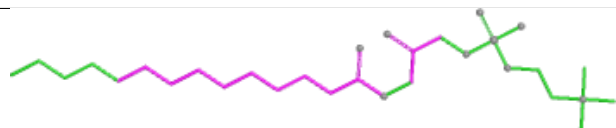
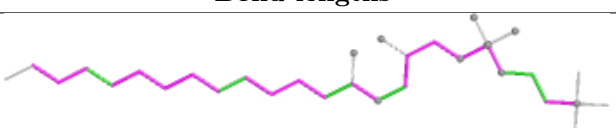
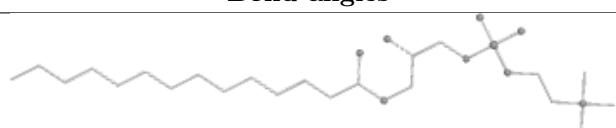
There are no ring outliers.

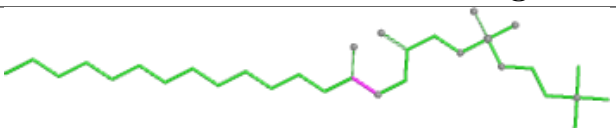
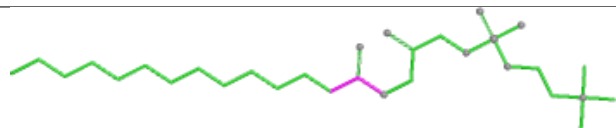
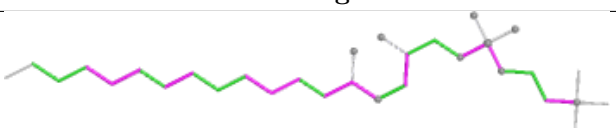
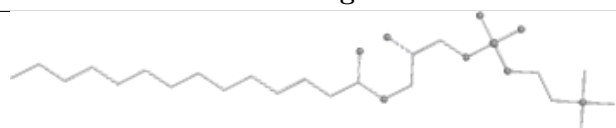
6 monomers are involved in 115 short contacts:

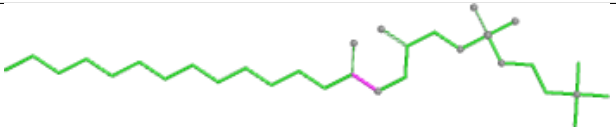
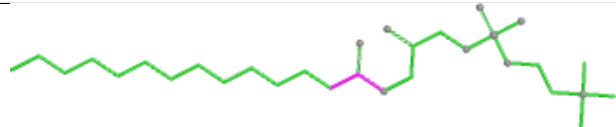
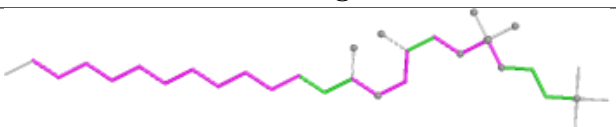
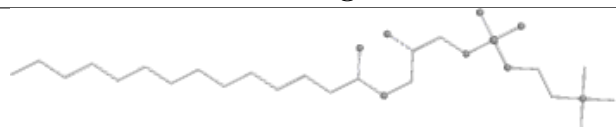
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	LPC	20	0
2	A	601	LPC	17	0
2	A	603	LPC	12	0
2	A	602	LPC	44	0
2	A	606	LPC	15	0
2	A	605	LPC	7	0

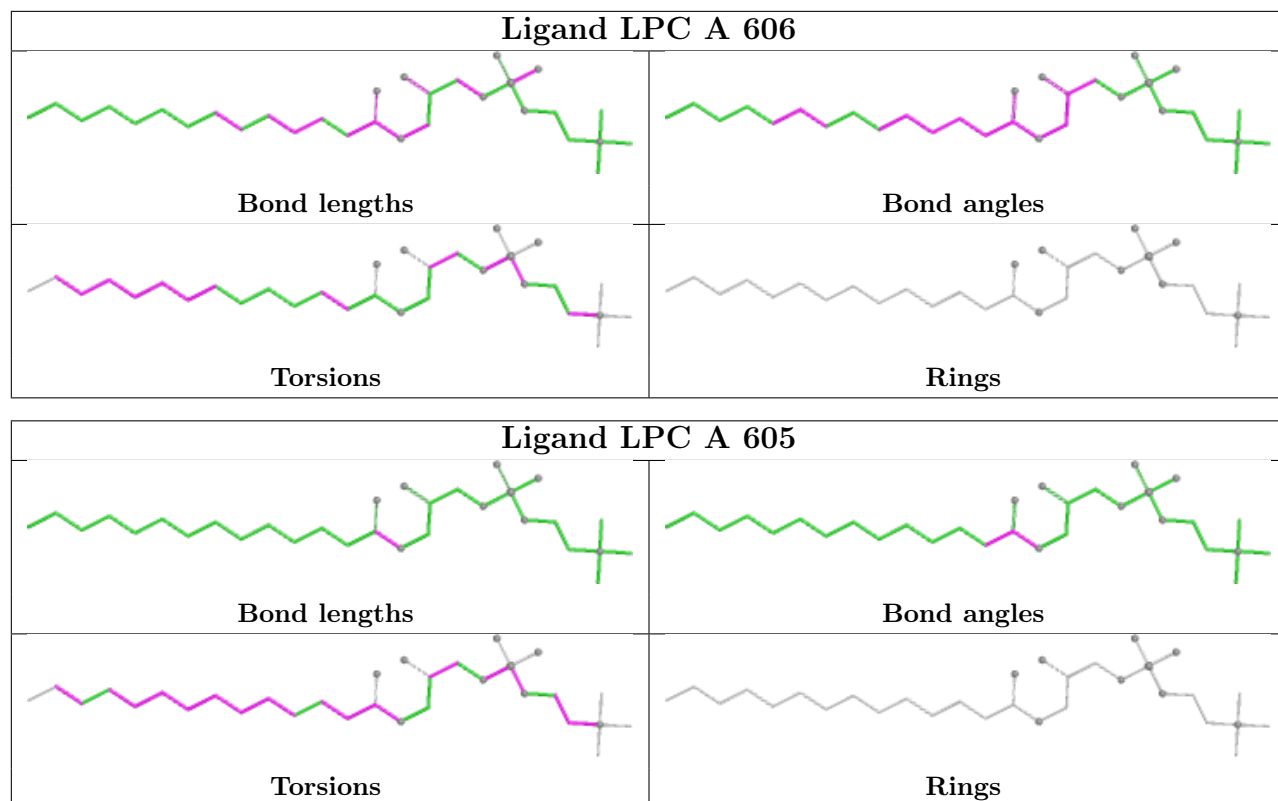
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand LPC A 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LPC A 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LPC A 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LPC A 602	
 Bond lengths	 Bond angles
 Torsions	 Rings



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	582/582 (100%)	0.40	21 (3%)	46 44	42, 66, 99, 162	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	VAL	5.3
1	A	443	ALA	3.6
1	A	517	SER	3.2
1	A	554	PHE	3.1
1	A	364	ALA	2.9
1	A	366	PRO	2.8
1	A	307	ALA	2.7
1	A	561	ALA	2.7
1	A	172	ALA	2.6
1	A	111	ASN	2.6
1	A	315	VAL	2.5
1	A	300	ALA	2.4
1	A	95	GLU	2.4
1	A	516	LEU	2.4
1	A	313	LYS	2.3
1	A	96	PRO	2.3
1	A	370	TYR	2.2
1	A	578	ALA	2.2
1	A	473	VAL	2.1
1	A	579	SER	2.1
1	A	410	ARG	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

There are no oligosaccharides in this entry.

6.4 Ligands

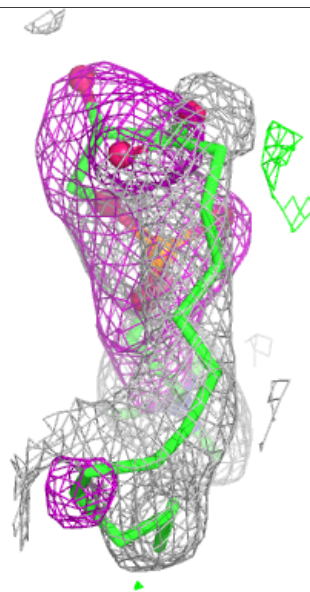
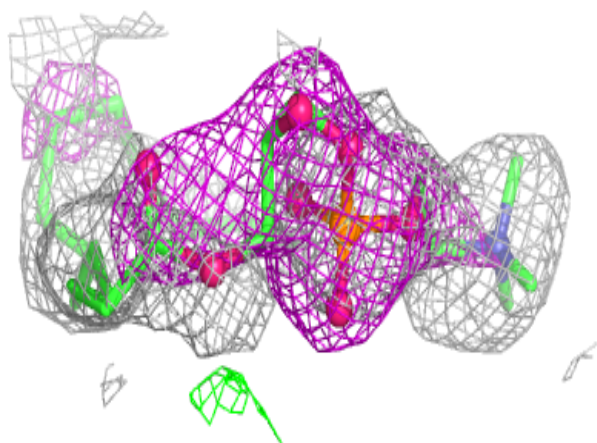
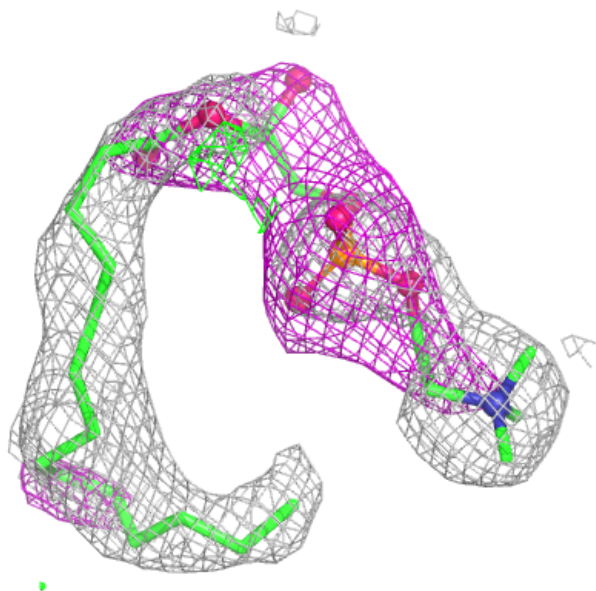
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LPC	A	602	31/31	0.56	0.18	52,61,67,68	0
2	LPC	A	601	31/31	0.59	0.19	51,58,62,64	0
2	LPC	A	606	31/31	0.60	0.20	46,58,67,72	0
2	LPC	A	604	31/31	0.66	0.19	51,57,64,70	0
2	LPC	A	605	31/31	0.72	0.16	62,90,115,115	0
2	LPC	A	603	31/31	0.78	0.15	47,56,63,70	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.

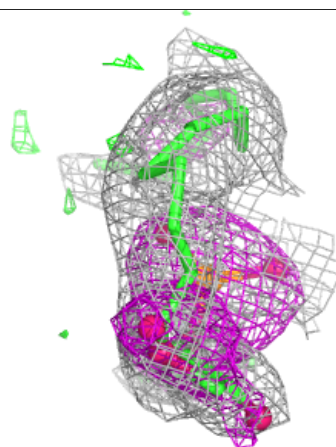
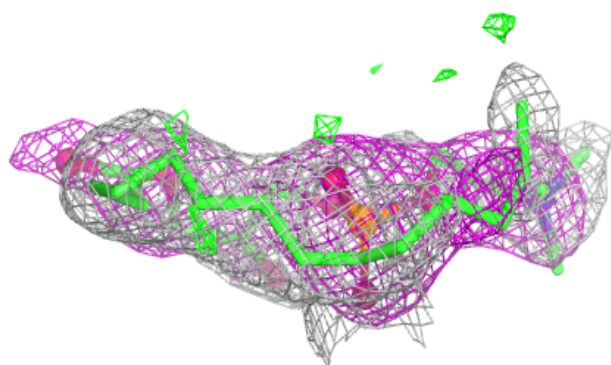
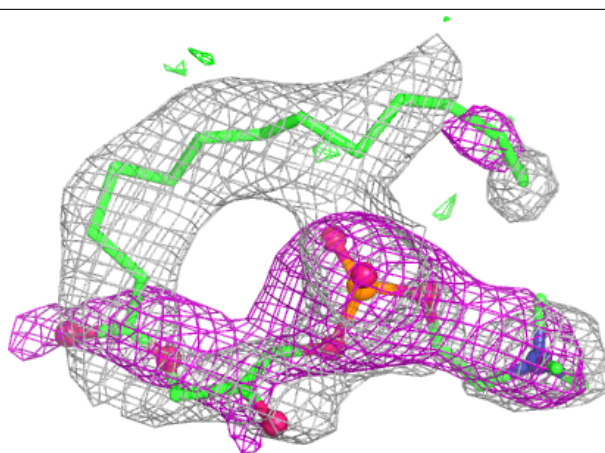
Electron density around LPC A 602:

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



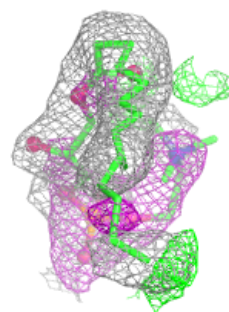
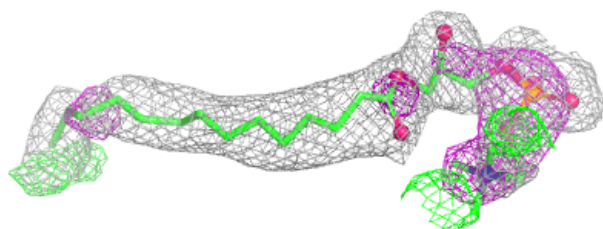
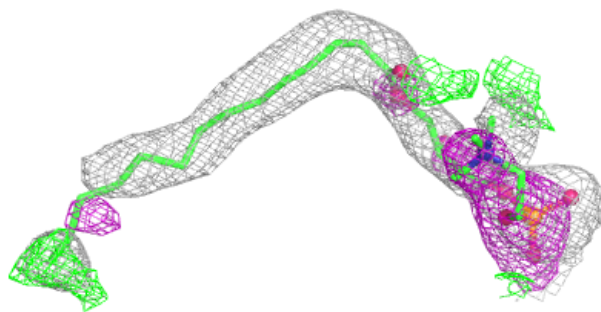
Electron density around LPC A 601:

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

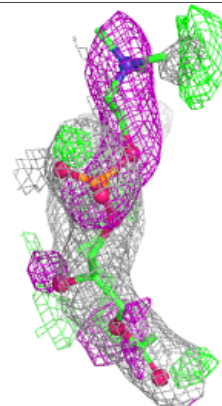
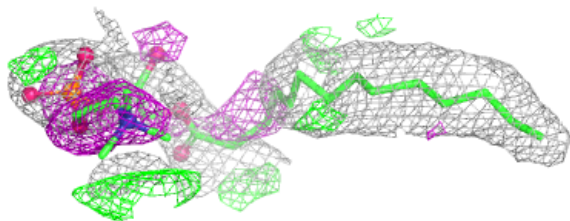
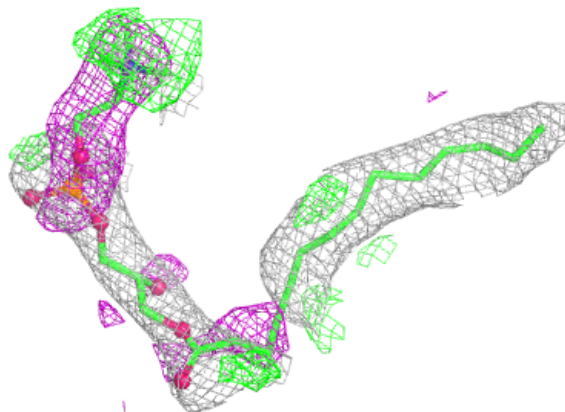


Electron density around LPC A 606:

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

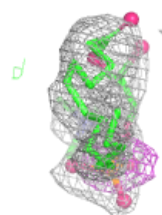
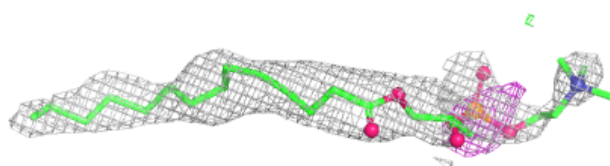
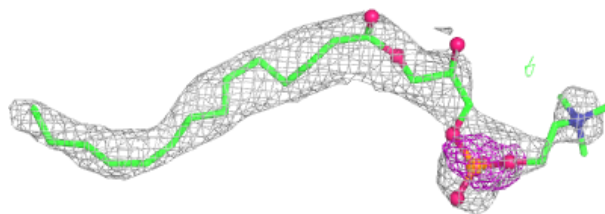
**Electron density around LPC A 604:**

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

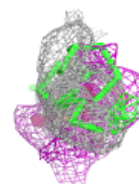
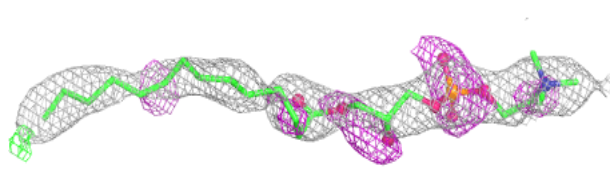
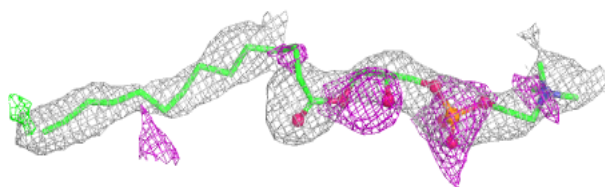


Electron density around LPC A 605:

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

**Electron density around LPC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.