



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:25 AM UTC

PDB ID : 8AQ2 / pdb_00008aq2
Title : In meso structure of the membrane integral lipoprotein N-acyltransferase Lnt from *P. aeruginosa* covalently linked with TITC
Authors : Huang, C.-Y.; Weichert, D.; Boland, C.; Smithers, L.; Olieric, V.; Wang, M.; Caffrey, M.
Deposited on : 2022-08-11
Resolution : 2.60 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

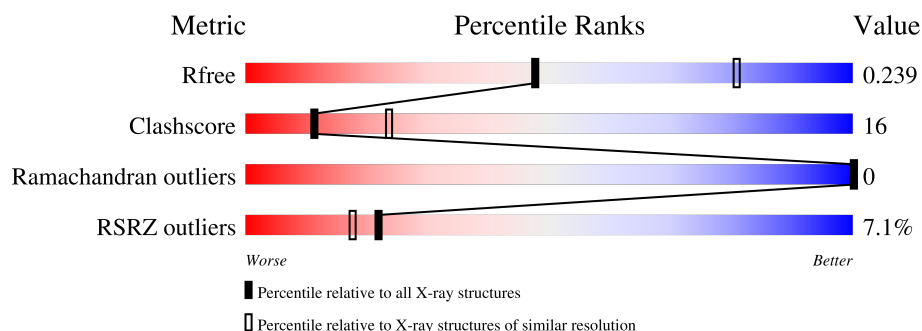
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	531	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4333 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.

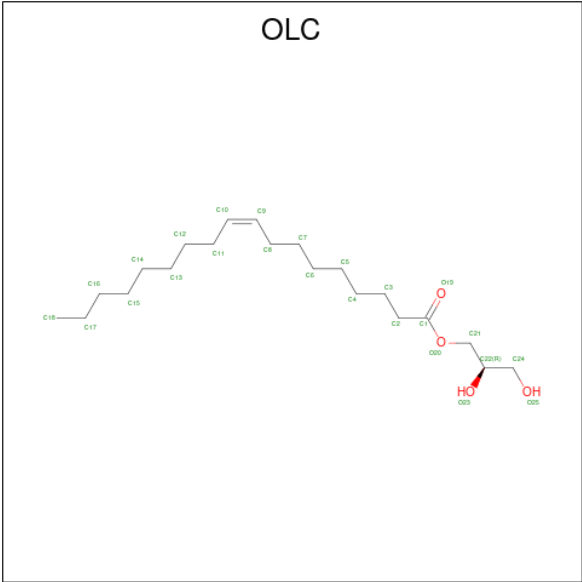
- Molecule 1 is a protein called Apolipoprotein N-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4009	2642	678	678	11			

There are 20 discrepancies between the modelled and reference sequences:

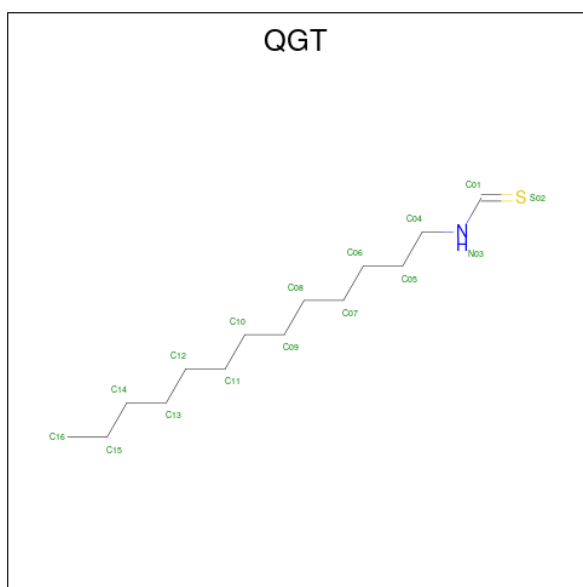
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9ZI86
A	-18	GLY	-	expression tag	UNP Q9ZI86
A	-17	SER	-	expression tag	UNP Q9ZI86
A	-16	SER	-	expression tag	UNP Q9ZI86
A	-15	HIS	-	expression tag	UNP Q9ZI86
A	-14	HIS	-	expression tag	UNP Q9ZI86
A	-13	HIS	-	expression tag	UNP Q9ZI86
A	-12	HIS	-	expression tag	UNP Q9ZI86
A	-11	HIS	-	expression tag	UNP Q9ZI86
A	-10	HIS	-	expression tag	UNP Q9ZI86
A	-9	SER	-	expression tag	UNP Q9ZI86
A	-8	SER	-	expression tag	UNP Q9ZI86
A	-7	GLY	-	expression tag	UNP Q9ZI86
A	-6	LEU	-	expression tag	UNP Q9ZI86
A	-5	VAL	-	expression tag	UNP Q9ZI86
A	-4	PRO	-	expression tag	UNP Q9ZI86
A	-3	ARG	-	expression tag	UNP Q9ZI86
A	-2	GLY	-	expression tag	UNP Q9ZI86
A	-1	SER	-	expression tag	UNP Q9ZI86
A	0	HIS	-	expression tag	UNP Q9ZI86

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



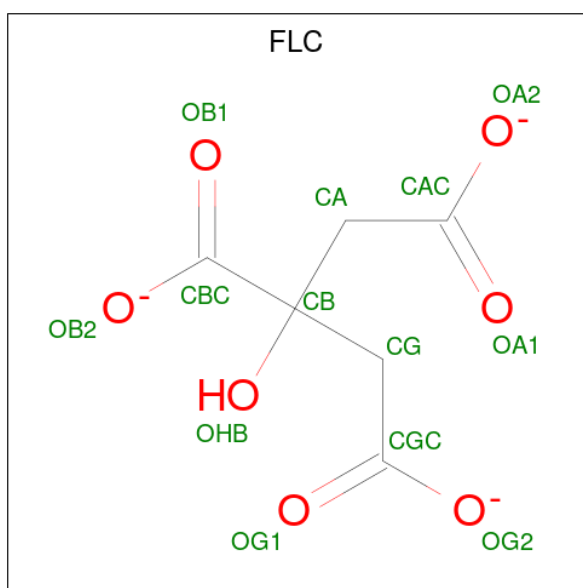
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			22	18	4		
2	A	1	Total	C	O	0	0
			14	10	4		
2	A	1	Total	C	O	0	0
			22	18	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			22	18	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			21	17	4		
2	A	1	Total	C	O	0	0
			14	10	4		

- Molecule 3 is {N}-tridecylmethanethioamide (CCD ID: QGT) (formula: C₁₄H₂₉NS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			16	14	1	1		
3	A	1	Total	C	N	S	0	0
			8	6	1	1		

- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

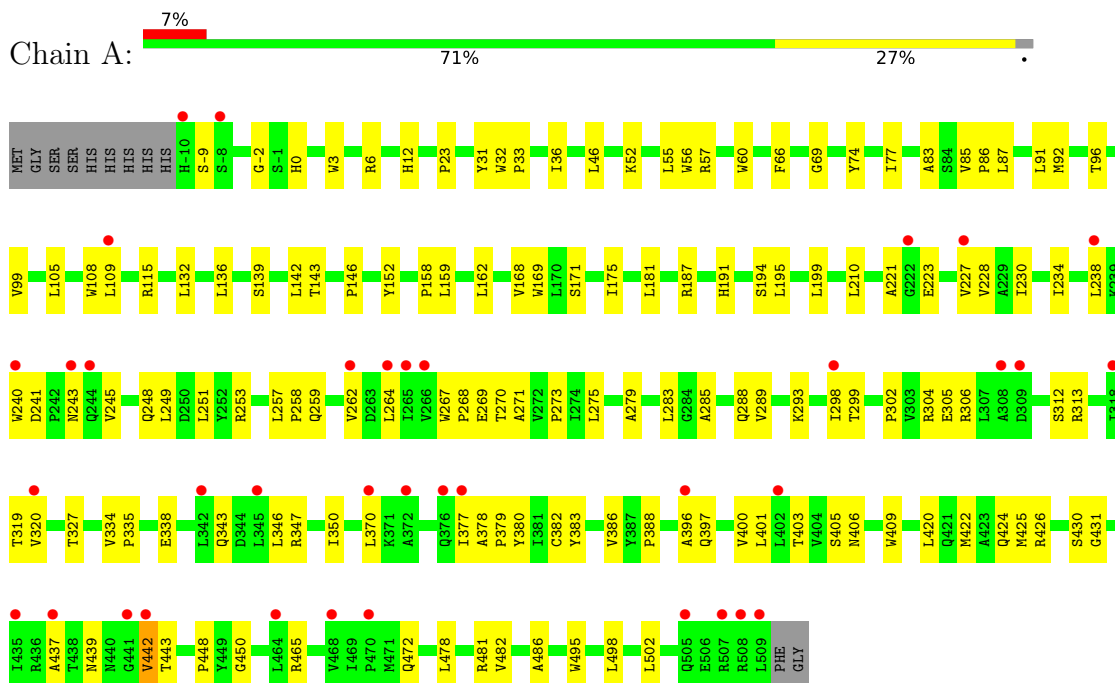
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total	O	0	0
			30	30		

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: Apolipoprotein N-acyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.06Å 116.23Å 73.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.53 – 2.60 48.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.53-2.60) 99.7 (48.53-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.61Å)	Xtriage
Refinement program	PHENIX dev_3494	Depositor
R, R_{free}	0.228 , 0.257 (Not available) , 0.239	Depositor DCC
R_{free} test set	1054 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.7	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	0.91	EDS
Total number of atoms	4333	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: GOL, QGT, FLC, OLC

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	0.34	0/4134	0.53	1/5660 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	442	VAL	N-CA-C	6.90	123.70	109.34

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	4009	0	4024	138	0
2	A	215	0	316	13	0
3	A	24	0	0	0	0
4	A	13	0	5	0	0
5	A	42	0	56	6	0
6	A	30	0	0	3	0
All	All	4333	0	4401	141	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 16.

All (141) 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:442:VAL:HG12	1:A:442:VAL:O	1.56	1.02
1:A:108:TRP:HE1	5:A:618:GOL:H2	1.24	0.99
1:A:437:ALA:HA	1:A:443:THR:HG23	1.43	0.98
1:A:420:LEU:HD22	1:A:442:VAL:HG11	1.43	0.96
1:A:87:LEU:HD22	1:A:91:LEU:HD23	1.51	0.91
1:A:87:LEU:HD22	1:A:91:LEU:CD2	2.05	0.86
1:A:306:ARG:HH21	1:A:306:ARG:HG2	1.42	0.83
1:A:245:VAL:O	1:A:249:LEU:HD13	1.82	0.80
1:A:234:ILE:HG12	1:A:248:GLN:HG3	1.67	0.77
1:A:270:THR:HG23	1:A:302:PRO:HD3	1.65	0.76
1:A:108:TRP:HE3	1:A:109:LEU:HD22	1.49	0.76
1:A:478:LEU:O	1:A:481:ARG:NH1	2.20	0.75
1:A:87:LEU:CD2	1:A:91:LEU:CD2	2.66	0.74
1:A:46:LEU:O	1:A:115:ARG:NH2	2.20	0.73
1:A:99:VAL:HG23	2:A:604:OLC:H9	1.70	0.73
1:A:279:ALA:O	1:A:283:LEU:HD23	1.88	0.72
1:A:83:ALA:HB1	1:A:87:LEU:CD1	2.21	0.70
1:A:334:VAL:HG12	1:A:338:GLU:HG3	1.73	0.70
1:A:268:PRO:HB2	1:A:439:ASN:OD1	1.92	0.70
1:A:96:THR:HG21	2:A:608:OLC:H10	1.73	0.70
1:A:87:LEU:HD22	1:A:87:LEU:O	1.90	0.69
1:A:249:LEU:HD12	1:A:249:LEU:N	2.08	0.67
1:A:238:LEU:HD11	1:A:409:TRP:HZ3	1.60	0.67
1:A:482:VAL:HG12	1:A:486:ALA:HB2	1.74	0.67
1:A:-9:SER:HB3	1:A:187:ARG:HH21	1.60	0.67
1:A:108:TRP:CE3	1:A:109:LEU:HD22	2.31	0.66
1:A:0:HIS:HA	5:A:620:GOL:H2	1.77	0.66
1:A:249:LEU:H	1:A:249:LEU:CD1	2.08	0.66
1:A:87:LEU:HD22	1:A:87:LEU:C	2.21	0.66
1:A:420:LEU:CD2	1:A:442:VAL:HG11	2.24	0.65
1:A:83:ALA:HB1	1:A:87:LEU:HD12	1.78	0.65
1:A:346:LEU:O	1:A:350:ILE:HG12	1.98	0.64
1:A:249:LEU:N	1:A:249:LEU:CD1	2.58	0.64
1:A:304:ARG:HE	1:A:312:SER:HB3	1.61	0.64
1:A:279:ALA:CB	1:A:283:LEU:HD23	2.29	0.62
1:A:257:LEU:HB2	1:A:258:PRO:HD3	1.81	0.62
1:A:343:GLN:O	1:A:347:ARG:HB2	1.98	0.62
1:A:87:LEU:HD21	1:A:91:LEU:HD21	1.82	0.61
1:A:269:GLU:OE2	1:A:406:ASN:N	2.32	0.61
1:A:306:ARG:HG2	1:A:306:ARG:NH2	2.10	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:TRP:CD1	5:A:619:GOL:HO2	2.19	0.60
1:A:74:TYR:HB2	1:A:92:MET:HG3	1.84	0.60
1:A:158:PRO:HB3	1:A:210:LEU:HD11	1.84	0.60
1:A:87:LEU:CD2	1:A:91:LEU:HD21	2.31	0.59
1:A:3:TRP:HD1	5:A:620:GOL:O3	1.86	0.58
1:A:305:GLU:OE1	1:A:313:ARG:NH2	2.28	0.58
1:A:498:LEU:O	1:A:502:LEU:HD23	2.04	0.58
1:A:424:GLN:NE2	1:A:450:GLY:O	2.32	0.58
1:A:87:LEU:O	1:A:91:LEU:HD23	2.04	0.57
1:A:139:SER:HA	1:A:146:PRO:HG3	1.87	0.57
1:A:319:THR:HG1	1:A:327:THR:HG1	1.48	0.56
1:A:241:ASP:N	1:A:241:ASP:OD1	2.38	0.56
1:A:234:ILE:HD11	1:A:251:LEU:HD23	1.88	0.56
1:A:370:LEU:HD13	1:A:379:PRO:HG3	1.88	0.56
1:A:298:ILE:HG12	1:A:320:VAL:HG22	1.88	0.55
1:A:241:ASP:O	1:A:245:VAL:HG23	2.06	0.55
1:A:83:ALA:HB1	1:A:87:LEU:HD13	1.88	0.55
1:A:257:LEU:O	1:A:293:LYS:NZ	2.25	0.55
1:A:396:ALA:O	1:A:397:GLN:HG2	2.07	0.54
1:A:152:TYR:OH	1:A:426:ARG:NH2	2.40	0.54
1:A:230:ILE:HD12	1:A:267:TRP:HE1	1.72	0.54
1:A:99:VAL:CG2	2:A:604:OLC:H9	2.35	0.53
1:A:143:THR:HG21	1:A:335:PRO:CG	2.39	0.53
1:A:285:ALA:O	1:A:289:VAL:HG23	2.09	0.53
1:A:495:TRP:HA	2:A:610:OLC:H5	1.90	0.53
1:A:96:THR:CG2	2:A:608:OLC:H10	2.37	0.52
1:A:152:TYR:CE2	1:A:422:MET:HE3	2.45	0.52
1:A:223:GLU:H	1:A:223:GLU:CD	2.19	0.51
1:A:430:SER:HA	1:A:478:LEU:HD11	1.93	0.51
1:A:259:GLN:OE1	1:A:465:ARG:NH1	2.45	0.50
1:A:108:TRP:NE1	5:A:618:GOL:H2	2.09	0.50
1:A:146:PRO:HB2	6:A:704:HOH:O	2.10	0.50
1:A:279:ALA:HB1	1:A:283:LEU:CD2	2.42	0.50
1:A:87:LEU:CD2	1:A:87:LEU:C	2.85	0.49
1:A:227:VAL:HG22	1:A:264:LEU:HB2	1.93	0.49
2:A:601:OLC:H13	2:A:601:OLC:H18A	1.93	0.49
1:A:56:TRP:CZ3	2:A:609:OLC:H4	2.47	0.49
1:A:92:MET:O	1:A:96:THR:HG22	2.12	0.48
1:A:228:VAL:HG22	1:A:465:ARG:NE	2.28	0.48
1:A:388:PRO:HG3	1:A:426:ARG:NH2	2.28	0.48
1:A:143:THR:HG21	1:A:335:PRO:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ALA:HB2	1:A:472:GLN:HB3	1.95	0.48
1:A:31:TYR:HB3	2:A:605:OLC:H3A	1.95	0.48
1:A:60:TRP:NE1	2:A:609:OLC:O19	2.44	0.48
1:A:66:PHE:CD2	1:A:99:VAL:HG12	2.48	0.48
1:A:85:VAL:CG2	1:A:86:PRO:HD3	2.44	0.48
1:A:257:LEU:CD1	1:A:257:LEU:N	2.76	0.48
1:A:32:TRP:CD2	1:A:33:PRO:HD3	2.49	0.47
1:A:195:LEU:O	1:A:199:LEU:HG	2.14	0.47
1:A:382:CYS:HA	1:A:405:SER:HB3	1.96	0.47
1:A:380:TYR:O	1:A:403:THR:HA	2.14	0.47
1:A:249:LEU:HD11	1:A:273:PRO:HD2	1.95	0.47
1:A:275:LEU:HD12	1:A:304:ARG:HB2	1.96	0.47
1:A:52:LYS:HD3	2:A:607:OLC:H24A	1.97	0.47
1:A:382:CYS:HA	1:A:405:SER:CB	2.44	0.47
1:A:36:ILE:HG13	1:A:175:ILE:HG23	1.97	0.46
1:A:-2:GLY:N	5:A:620:GOL:O1	2.36	0.46
1:A:55:LEU:HB2	1:A:108:TRP:HB2	1.97	0.46
1:A:249:LEU:HD13	1:A:249:LEU:H	1.79	0.46
1:A:279:ALA:CB	1:A:283:LEU:CD2	2.94	0.46
1:A:12:HIS:CE1	1:A:57:ARG:HB2	2.51	0.45
1:A:386:VAL:HG13	1:A:422:MET:HE1	1.97	0.45
1:A:279:ALA:O	1:A:283:LEU:CD2	2.61	0.45
1:A:304:ARG:HG3	1:A:312:SER:HB2	1.98	0.45
1:A:74:TYR:OH	1:A:85:VAL:HG12	2.17	0.45
1:A:23:PRO:HG3	1:A:69:GLY:CA	2.47	0.45
1:A:168:VAL:HG23	1:A:425:MET:HE2	1.99	0.45
1:A:228:VAL:HG23	1:A:262:VAL:HG21	1.98	0.45
1:A:253:ARG:O	1:A:257:LEU:HD13	2.17	0.45
1:A:279:ALA:HB3	1:A:283:LEU:HD23	1.98	0.45
1:A:257:LEU:HA	1:A:293:LYS:HE3	1.99	0.44
1:A:304:ARG:HE	1:A:312:SER:CB	2.28	0.44
1:A:77:ILE:HD11	2:A:602:OLC:H7	1.98	0.44
1:A:6:ARG:HD2	6:A:725:HOH:O	2.18	0.44
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.76	0.44
1:A:159:LEU:HD22	1:A:162:LEU:HD12	1.99	0.44
1:A:431:GLY:C	1:A:448:PRO:HB3	2.43	0.44
1:A:378:ALA:HB3	1:A:401:LEU:HD23	2.00	0.43
2:A:602:OLC:H11	2:A:602:OLC:H8	1.70	0.43
1:A:271:ALA:HB3	1:A:299:THR:OG1	2.19	0.43
1:A:380:TYR:HE2	1:A:401:LEU:HD22	1.84	0.43
1:A:32:TRP:N	1:A:33:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:SER:O	1:A:175:ILE:HG13	2.19	0.42
1:A:85:VAL:HG23	1:A:86:PRO:HD3	2.01	0.42
1:A:383:TYR:O	1:A:386:VAL:HB	2.20	0.42
1:A:288:GLN:NE2	6:A:703:HOH:O	2.30	0.42
1:A:132:LEU:HD11	1:A:169:TRP:HB3	2.00	0.42
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.90	0.41
1:A:228:VAL:CG2	1:A:262:VAL:HG21	2.50	0.41
1:A:279:ALA:HB1	1:A:283:LEU:HD23	1.98	0.41
1:A:228:VAL:HG22	1:A:465:ARG:HE	1.85	0.41
1:A:136:LEU:HD12	1:A:169:TRP:CE3	2.56	0.41
1:A:136:LEU:HD12	1:A:169:TRP:CZ3	2.56	0.41
1:A:105:LEU:O	1:A:109:LEU:HD23	2.21	0.41
1:A:191:HIS:HB2	1:A:194:SER:OG	2.21	0.41
2:A:607:OLC:H16A	2:A:607:OLC:H13A	1.79	0.41
1:A:169:TRP:CD1	1:A:482:VAL:HG22	2.56	0.41
1:A:240:TRP:CH2	1:A:248:GLN:OE1	2.73	0.41
1:A:257:LEU:CB	1:A:258:PRO:HD3	2.50	0.41
1:A:243:ASN:OD1	1:A:243:ASN:N	2.55	0.40
1:A:377:ILE:HG23	1:A:400:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/531 (98%)	503 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 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$
5	GOL	A	617	-	5,5,5	0.36	0	5,5,5	0.20	0
5	GOL	A	614	-	5,5,5	0.34	0	5,5,5	0.35	0
5	GOL	A	620	-	5,5,5	0.45	0	5,5,5	0.63	0
2	OLC	A	601	-	24,24,24	0.68	1 (4%)	25,25,25	0.95	1 (4%)
2	OLC	A	603	-	13,13,24	0.91	1 (7%)	14,14,25	1.11	1 (7%)
3	QGT	A	612	1	6,7,15	1.81	1 (16%)	5,6,14	0.71	0
5	GOL	A	615	-	5,5,5	0.34	0	5,5,5	0.39	0
2	OLC	A	605	-	24,24,24	0.71	1 (4%)	25,25,25	0.94	1 (4%)
2	OLC	A	608	-	24,24,24	0.67	1 (4%)	25,25,25	0.98	1 (4%)
2	OLC	A	609	-	20,20,24	0.77	1 (5%)	21,21,25	0.91	1 (4%)
5	GOL	A	618	-	5,5,5	0.36	0	5,5,5	0.40	0
2	OLC	A	606	-	21,21,24	0.75	1 (4%)	22,22,25	0.98	1 (4%)
2	OLC	A	610	-	13,13,24	0.92	1 (7%)	14,14,25	1.25	1 (7%)
2	OLC	A	604	-	21,21,24	0.74	1 (4%)	22,22,25	0.99	1 (4%)
2	OLC	A	607	-	24,24,24	0.70	1 (4%)	25,25,25	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	QGT	A	611	1	14,15,15	0.94	1 (7%)	13,14,14	2.07	1 (7%)
2	OLC	A	602	-	21,21,24	0.73	1 (4%)	22,22,25	0.95	1 (4%)
5	GOL	A	619	-	5,5,5	0.34	0	5,5,5	0.29	0
5	GOL	A	616	-	5,5,5	0.35	0	5,5,5	0.33	0
4	FLC	A	613	-	12,12,12	1.09	0	17,17,17	1.35	2 (11%)

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
5	GOL	A	617	-	-	0/4/4/4	-
5	GOL	A	614	-	-	2/4/4/4	-
5	GOL	A	620	-	-	0/4/4/4	-
2	OLC	A	601	-	-	11/24/24/24	-
2	OLC	A	603	-	-	5/13/13/24	-
3	QGT	A	612	1	-	2/4/5/13	-
5	GOL	A	615	-	-	1/4/4/4	-
2	OLC	A	605	-	-	16/24/24/24	-
2	OLC	A	608	-	-	9/24/24/24	-
2	OLC	A	609	-	-	7/20/20/24	-
5	GOL	A	618	-	-	0/4/4/4	-
2	OLC	A	606	-	-	6/21/21/24	-
2	OLC	A	610	-	-	5/13/13/24	-
2	OLC	A	604	-	-	10/21/21/24	-
2	OLC	A	607	-	-	7/24/24/24	-
3	QGT	A	611	1	-	3/12/13/13	-
2	OLC	A	602	-	-	7/21/21/24	-
5	GOL	A	619	-	-	0/4/4/4	-
5	GOL	A	616	-	-	0/4/4/4	-
4	FLC	A	613	-	-	7/16/16/16	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	612	QGT	C01-N03	4.37	1.45	1.31
3	A	611	QGT	C01-N03	3.30	1.42	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	OLC	O20-C1	2.86	1.41	1.33
2	A	603	OLC	O20-C1	2.82	1.41	1.33
2	A	604	OLC	O20-C1	2.78	1.41	1.33
2	A	610	OLC	O20-C1	2.75	1.41	1.33
2	A	601	OLC	O20-C1	2.74	1.41	1.33
2	A	607	OLC	O20-C1	2.73	1.41	1.33
2	A	609	OLC	O20-C1	2.70	1.41	1.33
2	A	606	OLC	O20-C1	2.68	1.41	1.33
2	A	602	OLC	O20-C1	2.61	1.41	1.33
2	A	608	OLC	O20-C1	2.59	1.40	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	611	QGT	C04-N03-C01	-7.24	109.83	122.72
4	A	613	FLC	OB2-CBC-CB	3.54	119.93	113.14
2	A	610	OLC	O20-C1-C2	3.24	121.70	111.83
2	A	603	OLC	O20-C1-C2	3.05	121.14	111.83
2	A	606	OLC	O20-C1-C2	2.99	120.94	111.83
2	A	604	OLC	O20-C1-C2	2.98	120.91	111.83
2	A	601	OLC	O20-C1-C2	2.86	120.57	111.83
2	A	605	OLC	O20-C1-C2	2.77	120.28	111.83
2	A	608	OLC	O20-C1-C2	2.64	119.88	111.83
2	A	602	OLC	O20-C1-C2	2.63	119.86	111.83
2	A	609	OLC	O20-C1-C2	2.57	119.68	111.83
4	A	613	FLC	OG2-CGC-CG	2.06	120.88	114.35

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	OLC	C21-C22-C24-O25
2	A	604	OLC	O20-C21-C22-C24
2	A	607	OLC	C21-C22-C24-O25
4	A	613	FLC	CA-CB-CBC-OB1
4	A	613	FLC	CA-CB-CBC-OB2
4	A	613	FLC	OHB-CB-CBC-OB1
4	A	613	FLC	OHB-CB-CBC-OB2
2	A	609	OLC	C2-C1-O20-C21
3	A	612	QGT	N03-C04-C05-C06
2	A	605	OLC	O20-C21-C22-O23
2	A	609	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
2	A	605	OLC	C11-C12-C13-C14
2	A	606	OLC	O20-C21-C22-O23
2	A	602	OLC	O23-C22-C24-O25
2	A	603	OLC	C1-C2-C3-C4
2	A	605	OLC	C1-C2-C3-C4
2	A	604	OLC	O20-C21-C22-O23
2	A	607	OLC	C11-C12-C13-C14
2	A	606	OLC	O20-C21-C22-C24
5	A	614	GOL	O1-C1-C2-C3
2	A	601	OLC	C1-C2-C3-C4
2	A	605	OLC	C5-C6-C7-C8
2	A	607	OLC	O23-C22-C24-O25
3	A	611	QGT	C06-C07-C08-C09
2	A	604	OLC	C1-C2-C3-C4
2	A	606	OLC	C1-C2-C3-C4
2	A	601	OLC	C14-C15-C16-C17
2	A	605	OLC	C14-C15-C16-C17
2	A	610	OLC	C3-C4-C5-C6
2	A	603	OLC	O20-C21-C22-C24
2	A	602	OLC	C4-C5-C6-C7
2	A	605	OLC	C13-C14-C15-C16
2	A	604	OLC	C2-C3-C4-C5
2	A	609	OLC	C4-C5-C6-C7
2	A	606	OLC	C11-C12-C13-C14
2	A	602	OLC	C5-C6-C7-C8
2	A	604	OLC	C4-C5-C6-C7
2	A	603	OLC	O20-C21-C22-O23
2	A	608	OLC	C10-C11-C12-C13
2	A	603	OLC	C2-C3-C4-C5
3	A	612	QGT	C05-C06-C07-C08
2	A	601	OLC	C15-C16-C17-C18
2	A	608	OLC	C2-C3-C4-C5
2	A	604	OLC	C12-C13-C14-C15
2	A	601	OLC	C4-C5-C6-C7
2	A	601	OLC	O20-C21-C22-C24
2	A	605	OLC	O20-C21-C22-C24
2	A	601	OLC	C6-C7-C8-C9
5	A	614	GOL	O1-C1-C2-O2
2	A	610	OLC	C2-C1-O20-C21
2	A	601	OLC	C2-C1-O20-C21
2	A	609	OLC	C3-C4-C5-C6
2	A	605	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	A	601	OLC	O20-C21-C22-O23
2	A	608	OLC	C12-C13-C14-C15
2	A	608	OLC	C6-C7-C8-C9
2	A	610	OLC	O19-C1-O20-C21
2	A	601	OLC	O19-C1-O20-C21
2	A	601	OLC	C5-C6-C7-C8
2	A	604	OLC	C6-C7-C8-C9
2	A	605	OLC	C10-C11-C12-C13
2	A	605	OLC	C6-C7-C8-C9
2	A	605	OLC	C12-C13-C14-C15
2	A	604	OLC	C7-C8-C9-C10
2	A	608	OLC	C14-C15-C16-C17
2	A	601	OLC	C2-C3-C4-C5
2	A	609	OLC	C11-C12-C13-C14
2	A	610	OLC	C1-C2-C3-C4
2	A	610	OLC	C4-C5-C6-C7
2	A	602	OLC	C1-C2-C3-C4
2	A	602	OLC	C2-C1-O20-C21
2	A	607	OLC	C5-C6-C7-C8
2	A	602	OLC	O19-C1-O20-C21
2	A	605	OLC	C7-C8-C9-C10
2	A	608	OLC	C5-C6-C7-C8
2	A	604	OLC	C5-C6-C7-C8
2	A	605	OLC	C15-C16-C17-C18
3	A	611	QGT	C11-C12-C13-C14
2	A	608	OLC	C7-C8-C9-C10
2	A	603	OLC	C3-C4-C5-C6
3	A	611	QGT	C12-C13-C14-C15
2	A	604	OLC	O23-C22-C24-O25
2	A	607	OLC	C7-C8-C9-C10
4	A	613	FLC	CAC-CA-CB-OHB
2	A	606	OLC	C4-C5-C6-C7
2	A	605	OLC	C9-C10-C11-C12
2	A	608	OLC	C2-C1-O20-C21
2	A	608	OLC	O19-C1-O20-C21
5	A	615	GOL	O1-C1-C2-O2
2	A	606	OLC	C7-C8-C9-C10
2	A	609	OLC	C9-C10-C11-C12
2	A	607	OLC	C9-C10-C11-C12
2	A	609	OLC	O20-C21-C22-O23
4	A	613	FLC	CA-CB-CG-CGC
2	A	605	OLC	O20-C1-C2-C3

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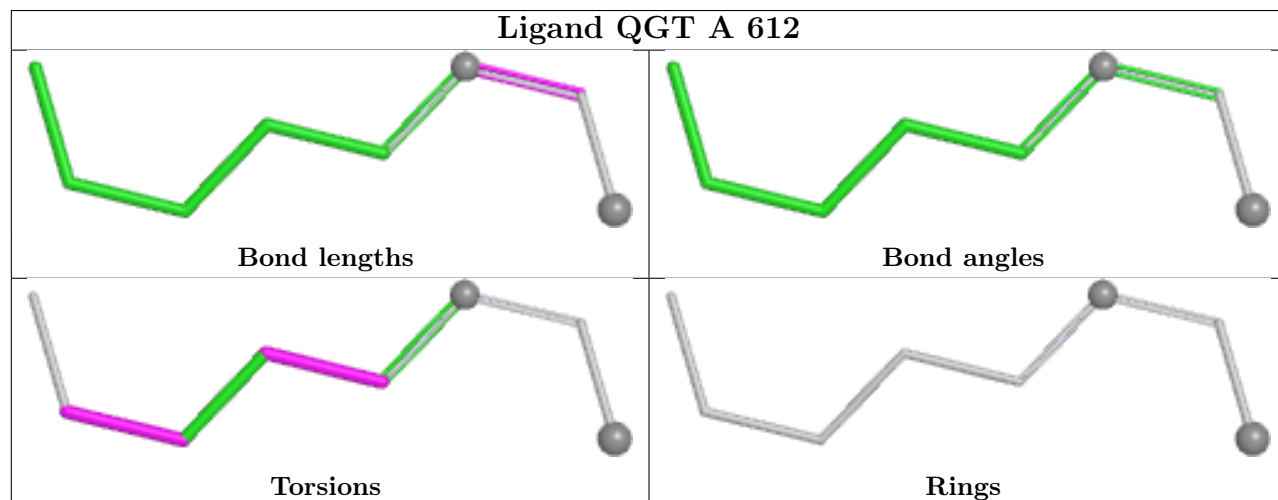
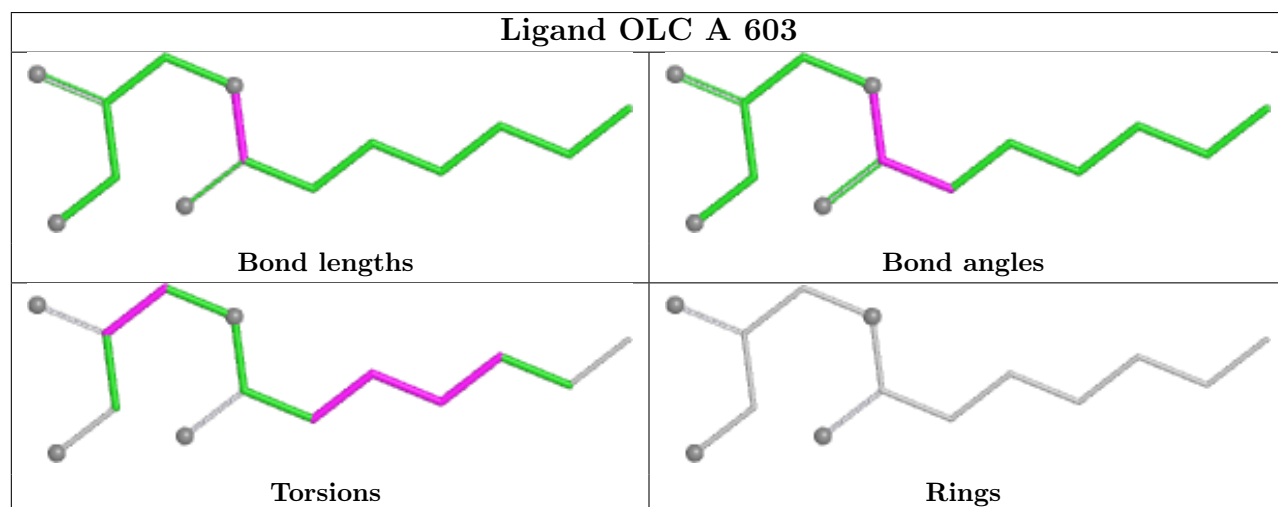
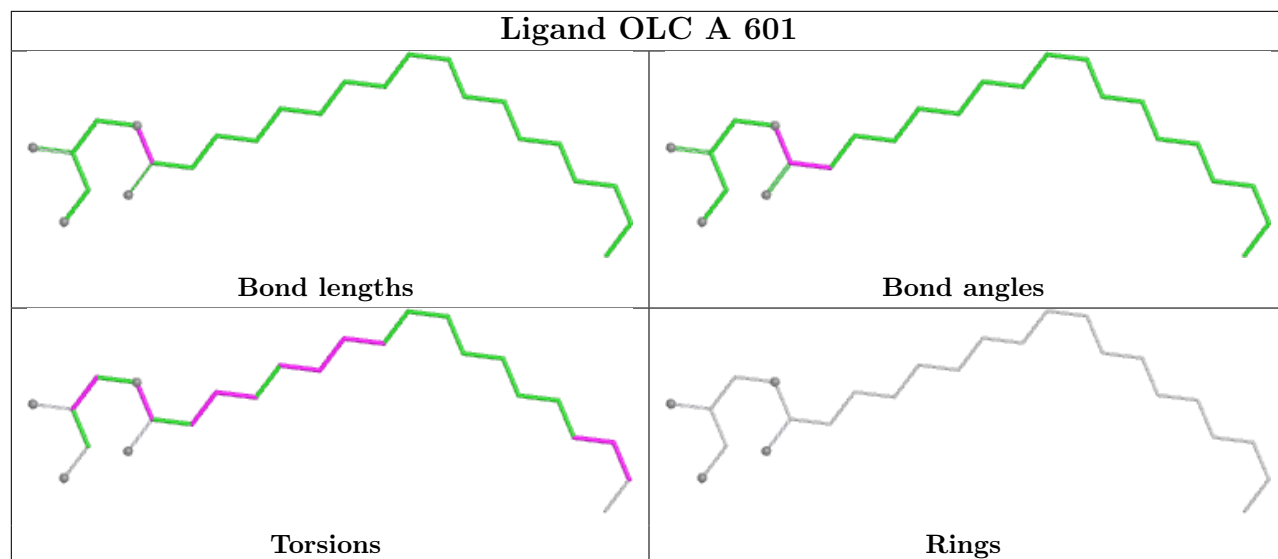
Mol	Chain	Res	Type	Atoms
2	A	607	OLC	C3-C4-C5-C6
4	A	613	FLC	OHB-CB-CG-CGC
2	A	605	OLC	O19-C1-C2-C3

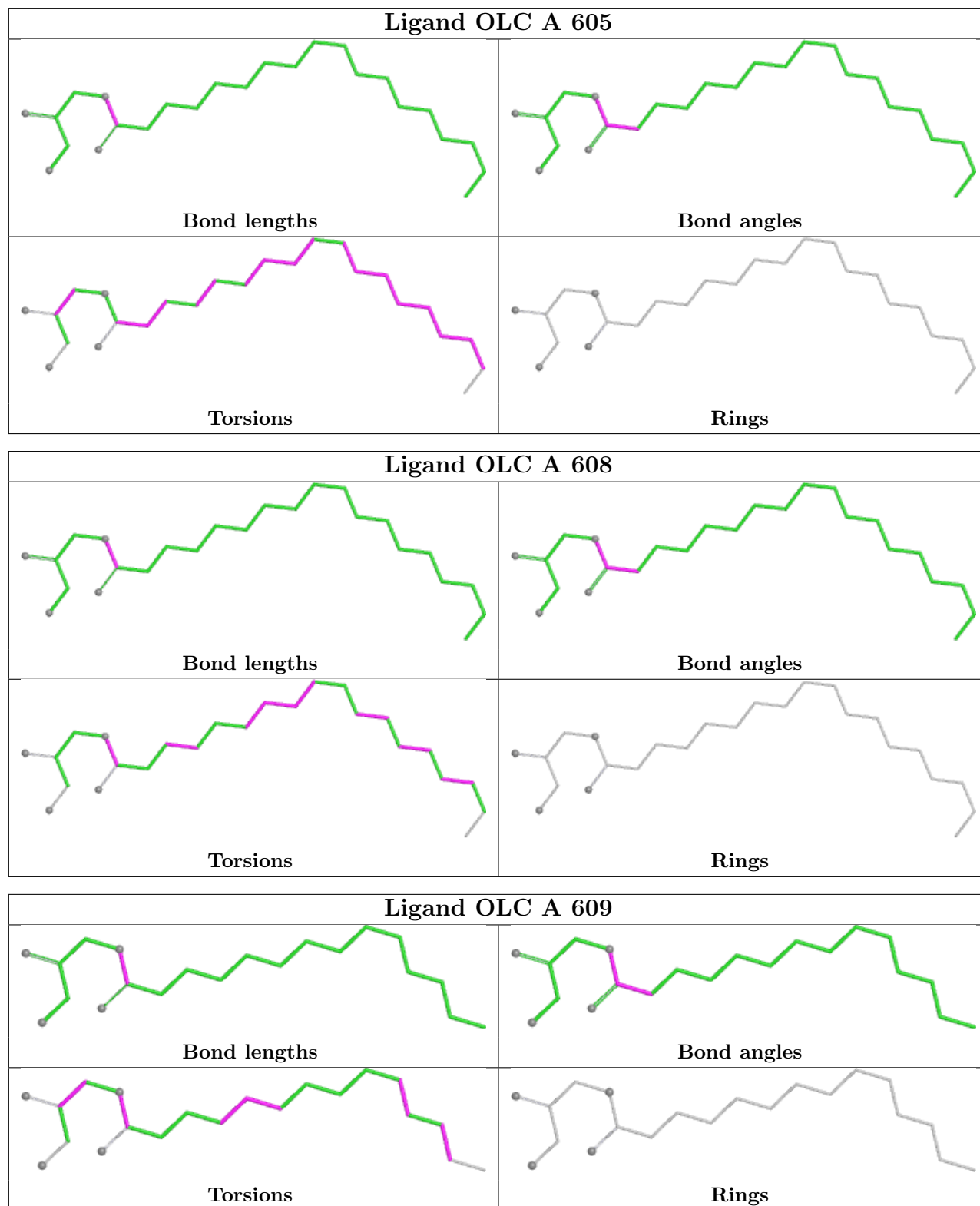
There are no ring outliers.

11 monomers are involved in 19 short contacts:

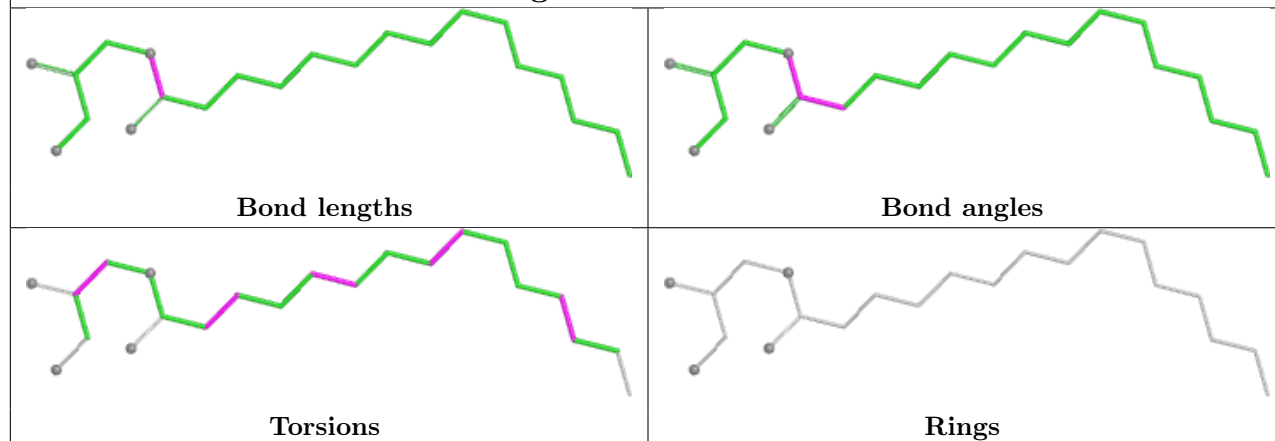
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	620	GOL	3	0
2	A	601	OLC	1	0
2	A	605	OLC	1	0
2	A	608	OLC	2	0
2	A	609	OLC	2	0
5	A	618	GOL	2	0
2	A	610	OLC	1	0
2	A	604	OLC	2	0
2	A	607	OLC	2	0
2	A	602	OLC	2	0
5	A	619	GOL	1	0

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

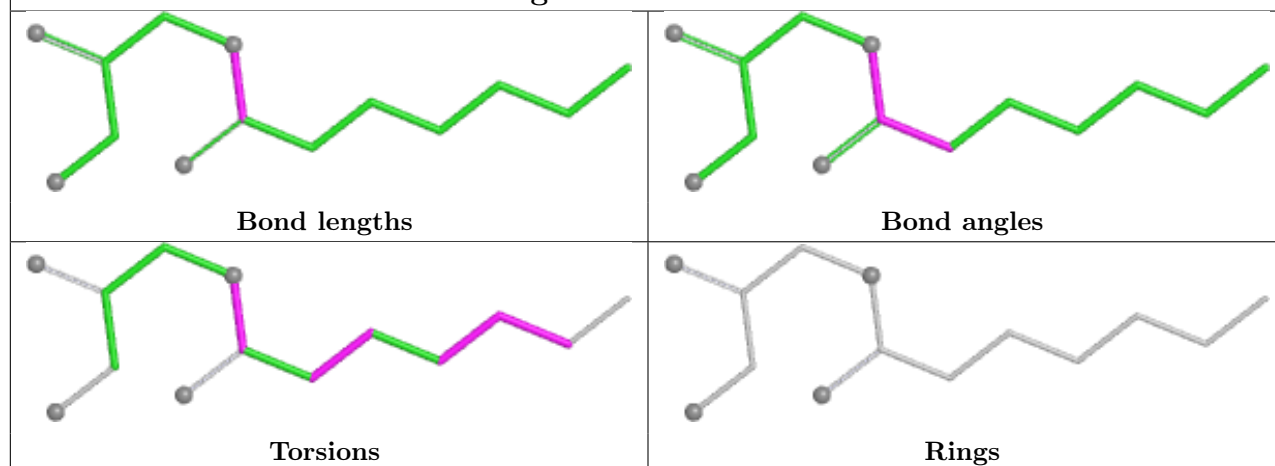




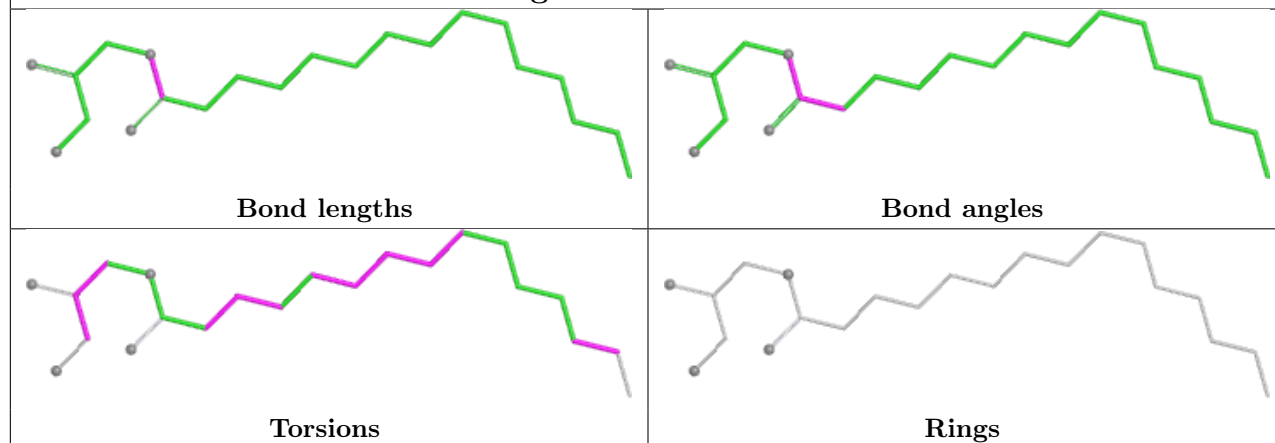
Ligand OLC A 606

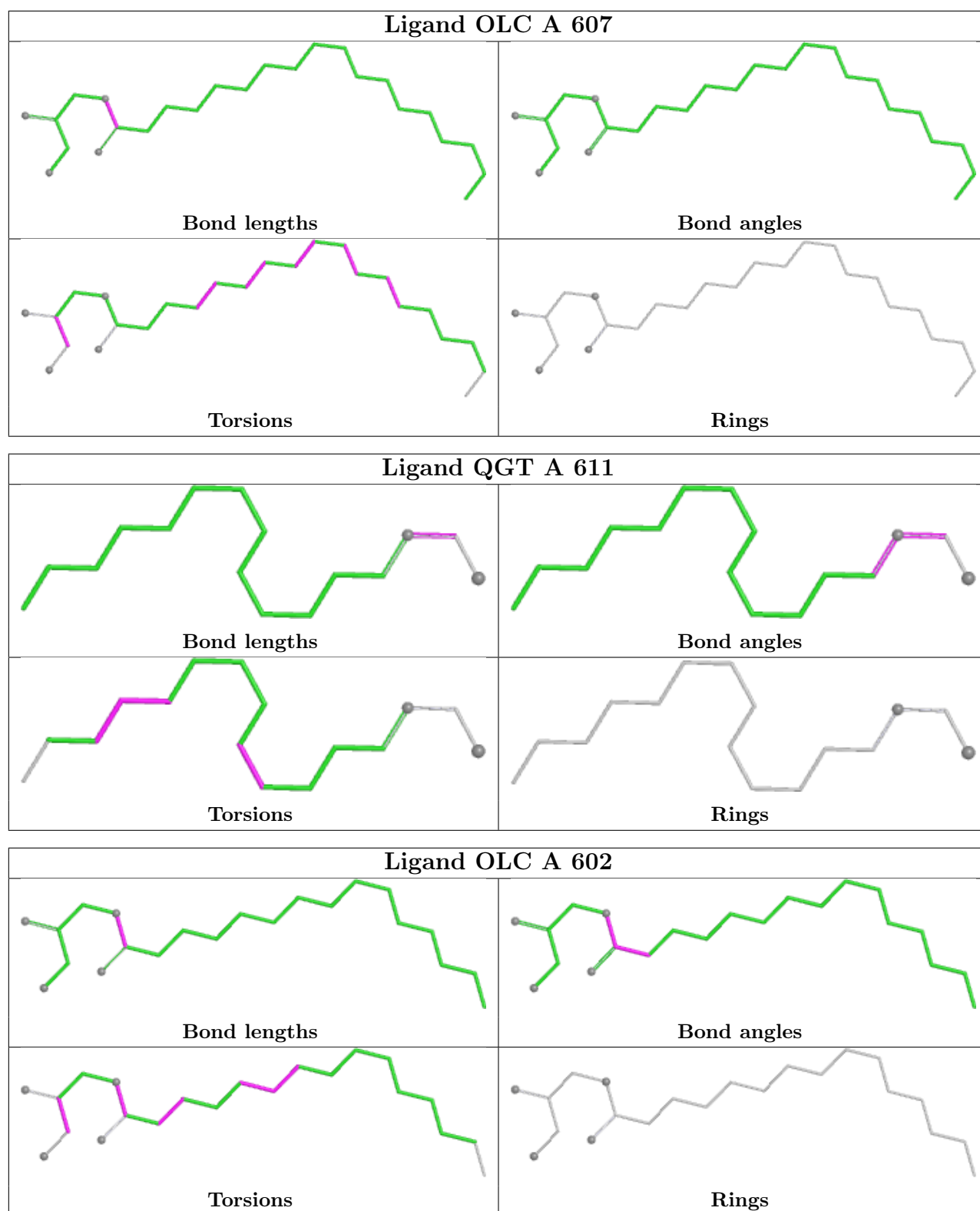


Ligand OLC A 610



Ligand OLC A 604





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, 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	520/531 (97%)	0.41	37 (7%) 22 17	40, 68, 115, 173	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	VAL	6.1
1	A	441	GLY	5.0
1	A	464	LEU	4.8
1	A	377	ILE	4.4
1	A	468	VAL	4.4
1	A	435	ILE	4.3
1	A	370	LEU	4.1
1	A	318	ILE	3.7
1	A	402	LEU	3.7
1	A	372	ALA	3.6
1	A	-8	SER	3.6
1	A	238	LEU	3.6
1	A	222	GLY	3.4
1	A	309	ASP	3.3
1	A	376	GLN	3.2
1	A	266	VAL	3.1
1	A	509	LEU	3.0
1	A	507	ARG	3.0
1	A	264	LEU	3.0
1	A	-10	HIS	2.9
1	A	244	GLN	2.8
1	A	265	ILE	2.7
1	A	262	VAL	2.7
1	A	437	ALA	2.7
1	A	320	VAL	2.5
1	A	308	ALA	2.5
1	A	298	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	342	LEU	2.3
1	A	109	LEU	2.3
1	A	396	ALA	2.2
1	A	470	PRO	2.2
1	A	505	GLN	2.2
1	A	442	VAL	2.2
1	A	508	ARG	2.2
1	A	243	ASN	2.2
1	A	240	TRP	2.1
1	A	345	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

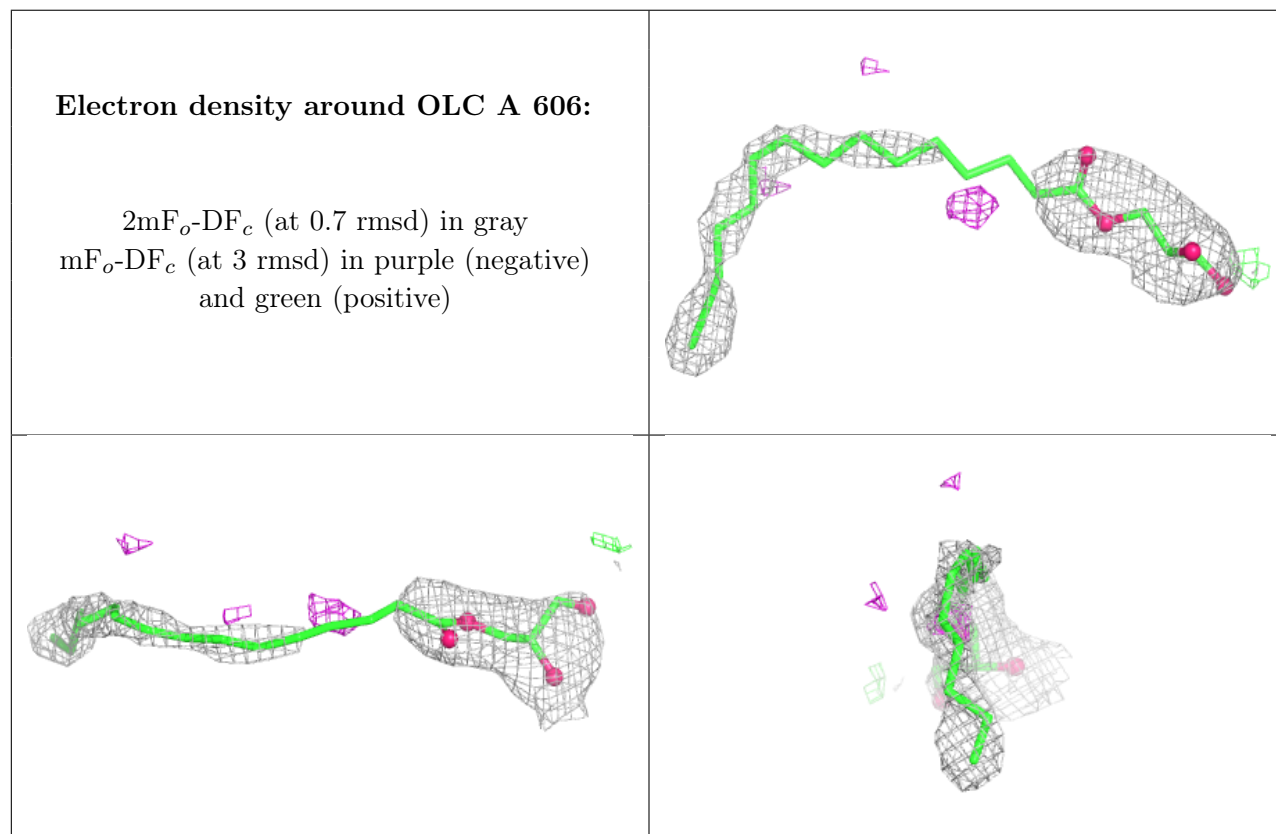
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FLC	A	613	13/13	0.63	0.13	126,132,135,137	0
5	GOL	A	616	6/6	0.69	0.18	108,110,113,113	0
5	GOL	A	620	6/6	0.69	0.16	105,107,109,110	0
5	GOL	A	619	6/6	0.75	0.16	104,106,106,107	0
5	GOL	A	614	6/6	0.75	0.12	104,111,112,113	0
5	GOL	A	617	6/6	0.76	0.18	75,89,89,99	0
5	GOL	A	618	6/6	0.77	0.17	110,113,114,119	0
2	OLC	A	606	22/25	0.79	0.20	63,81,92,95	0
2	OLC	A	607	25/25	0.80	0.17	73,103,112,115	0
2	OLC	A	605	25/25	0.82	0.22	78,97,108,111	0
5	GOL	A	615	6/6	0.84	0.14	95,98,101,104	0
3	QGT	A	612	8/16	0.84	0.17	84,95,107,111	0
2	OLC	A	610	14/25	0.85	0.12	81,95,110,114	0

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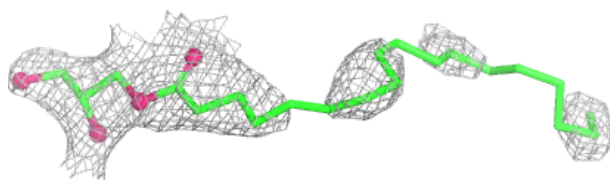
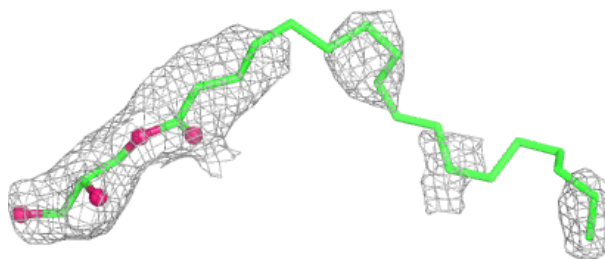
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OLC	A	608	25/25	0.85	0.17	73,80,102,105	0
2	OLC	A	601	25/25	0.87	0.18	76,88,102,110	0
2	OLC	A	609	21/25	0.87	0.15	75,86,93,96	0
3	QGT	A	611	16/16	0.88	0.16	56,66,91,97	0
2	OLC	A	604	22/25	0.88	0.13	48,76,86,89	0
2	OLC	A	603	14/25	0.90	0.14	64,92,103,111	0
2	OLC	A	602	22/25	0.90	0.16	67,84,99,106	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.

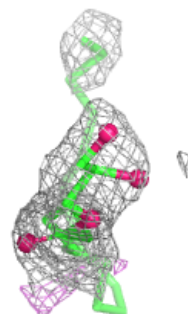
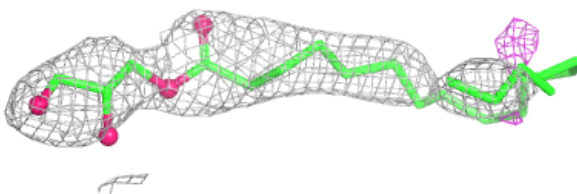
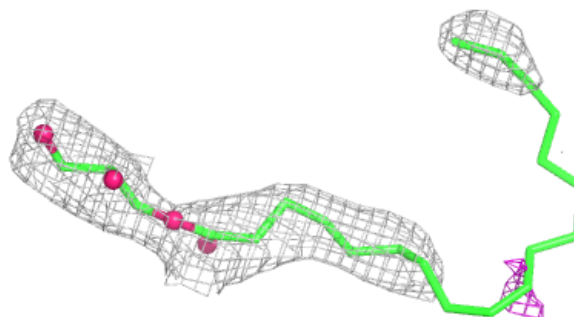


Electron density around OLC A 607:

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

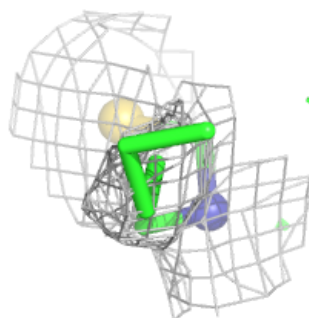
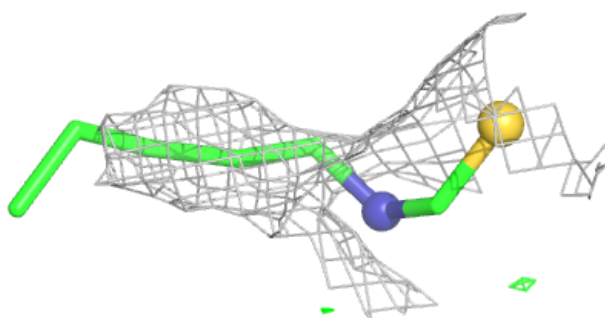
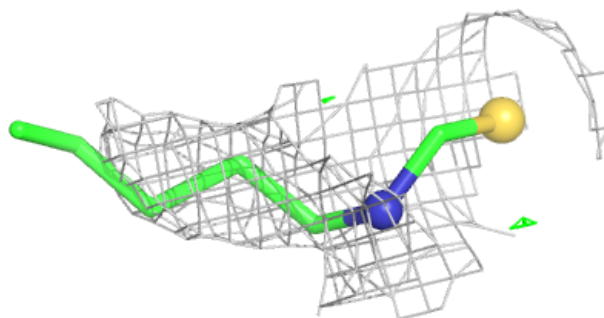
**Electron density around OLC A 605:**

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

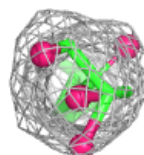
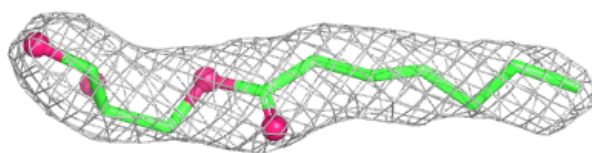
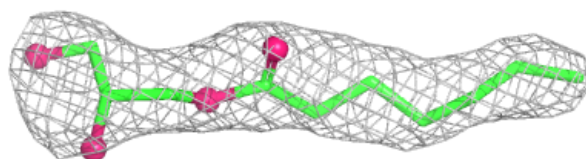


Electron density around QGT A 612:

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

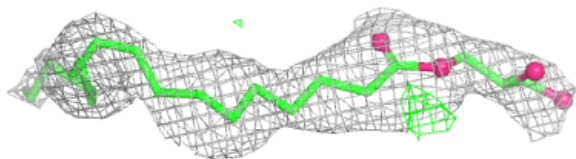
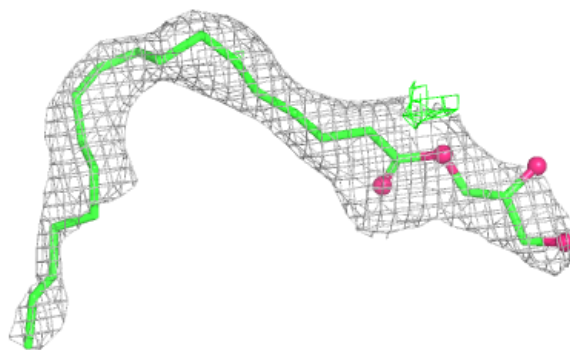
**Electron density around OLC A 610:**

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

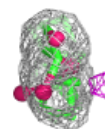
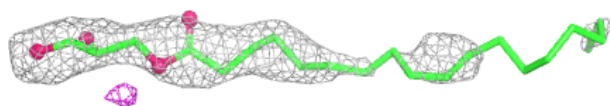
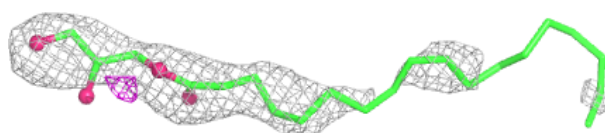


Electron density around OLC A 608:

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

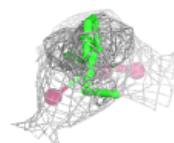
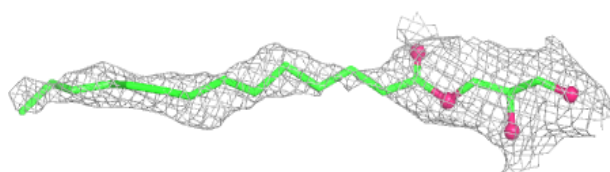
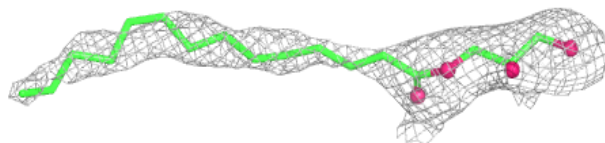
**Electron density around OLC A 601:**

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

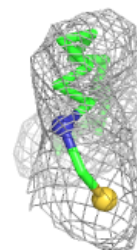
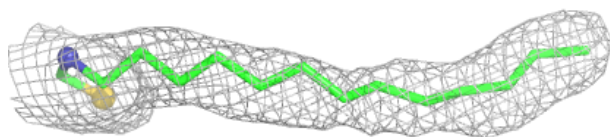
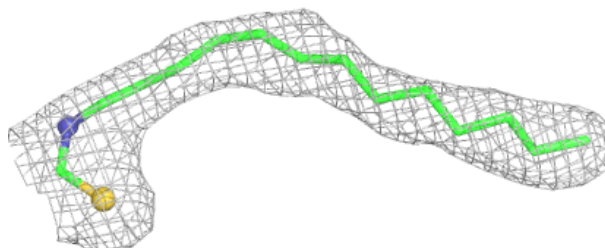


Electron density around OLC A 609:

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

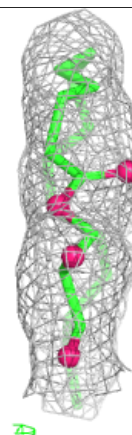
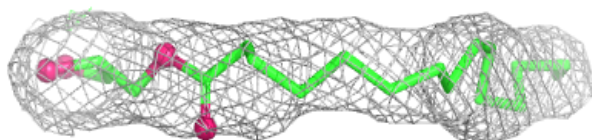
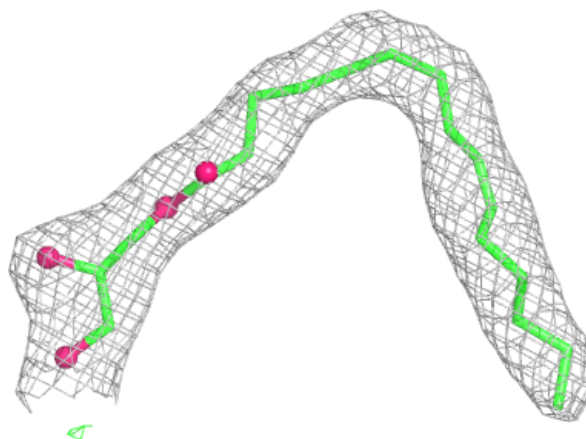
**Electron density around QGT A 611:**

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

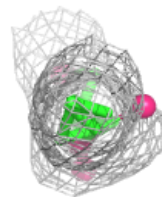
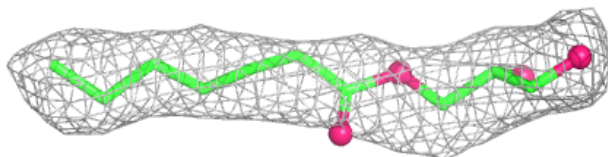
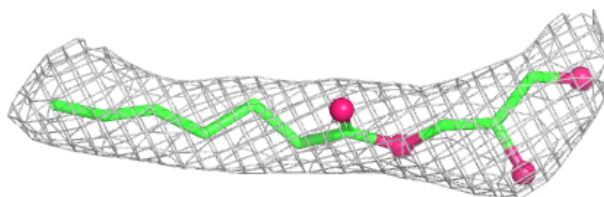


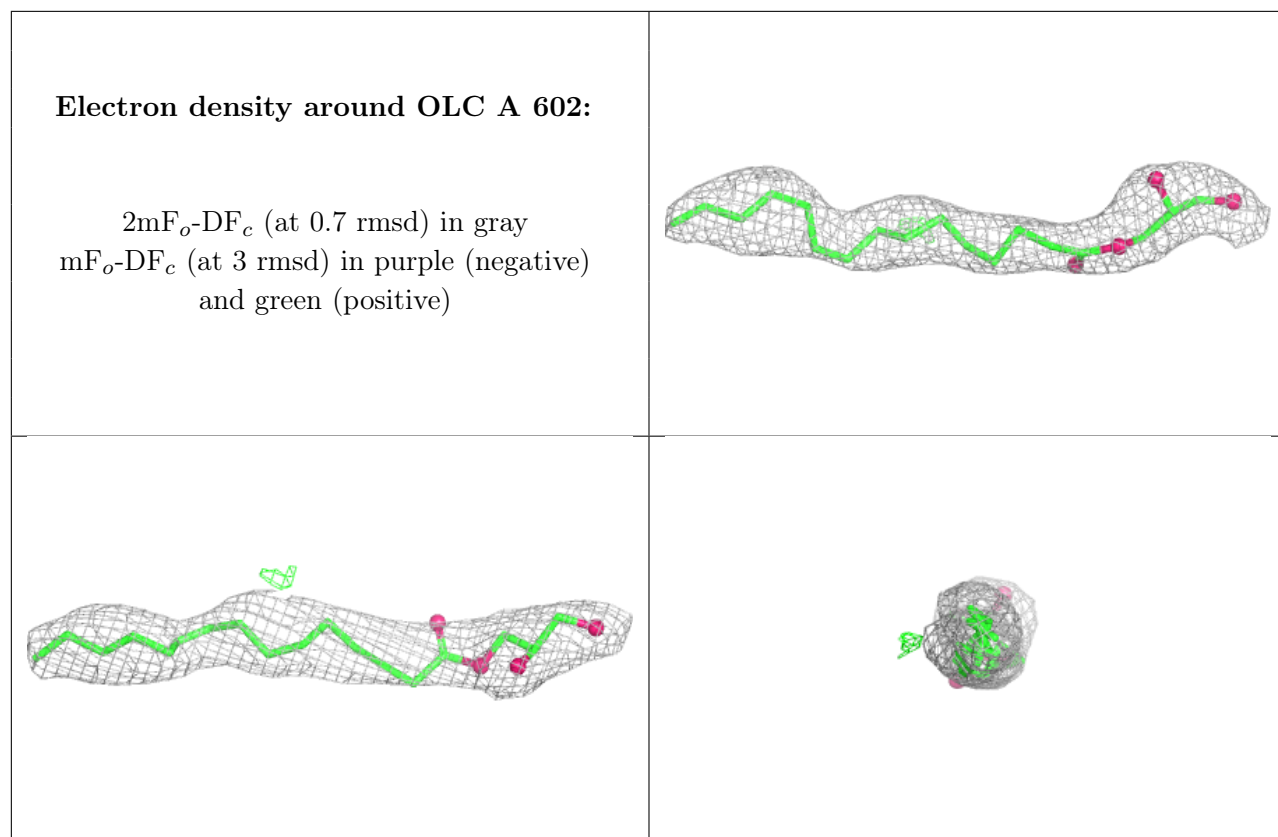
Electron density around OLC A 604:

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

**Electron density around OLC 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.