Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 11:10 PM JST

PDB ID	:	6AL2
Title	:	Crystal structure of E. coli YidC at 2.8 A resolution
Authors	:	Tanaka, Y.; Tsukazaki, T.; Izumioka, A.; Hamid, A.A.; Fujii, A.
Deposited on	:	2018-09-05
Resolution	:	2.80 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:

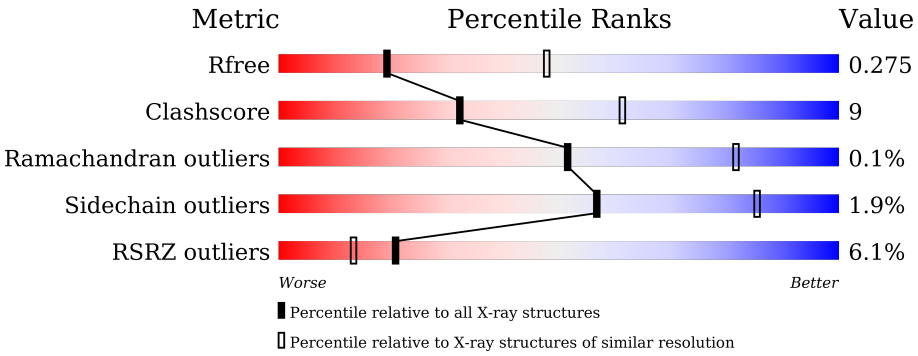
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	551	4% 68% 19% • 12%
1	B	551	6% 66% 21% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7650 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.

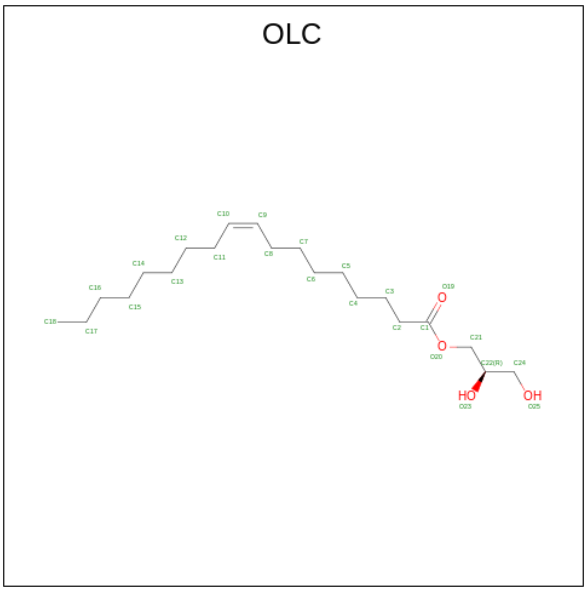
- Molecule 1 is a protein called Membrane protein insertase YidC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3831	2491	620	699	21			
1	B	480	Total	C	N	O	S	0	0	0
			3795	2466	616	692	21			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	541	LEU	-	expression tag	UNP B7MGC7
A	542	GLU	-	expression tag	UNP B7MGC7
A	543	SER	-	expression tag	UNP B7MGC7
A	544	SER	-	expression tag	UNP B7MGC7
A	545	GLY	-	expression tag	UNP B7MGC7
A	546	GLU	-	expression tag	UNP B7MGC7
A	547	ASN	-	expression tag	UNP B7MGC7
A	548	LEU	-	expression tag	UNP B7MGC7
A	549	TYR	-	expression tag	UNP B7MGC7
A	550	PHE	-	expression tag	UNP B7MGC7
A	551	GLN	-	expression tag	UNP B7MGC7
B	541	LEU	-	expression tag	UNP B7MGC7
B	542	GLU	-	expression tag	UNP B7MGC7
B	543	SER	-	expression tag	UNP B7MGC7
B	544	SER	-	expression tag	UNP B7MGC7
B	545	GLY	-	expression tag	UNP B7MGC7
B	546	GLU	-	expression tag	UNP B7MGC7
B	547	ASN	-	expression tag	UNP B7MGC7
B	548	LEU	-	expression tag	UNP B7MGC7
B	549	TYR	-	expression tag	UNP B7MGC7
B	550	PHE	-	expression tag	UNP B7MGC7
B	551	GLN	-	expression tag	UNP B7MGC7

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 19 15 4	0	0

- Molecule 3 is water.

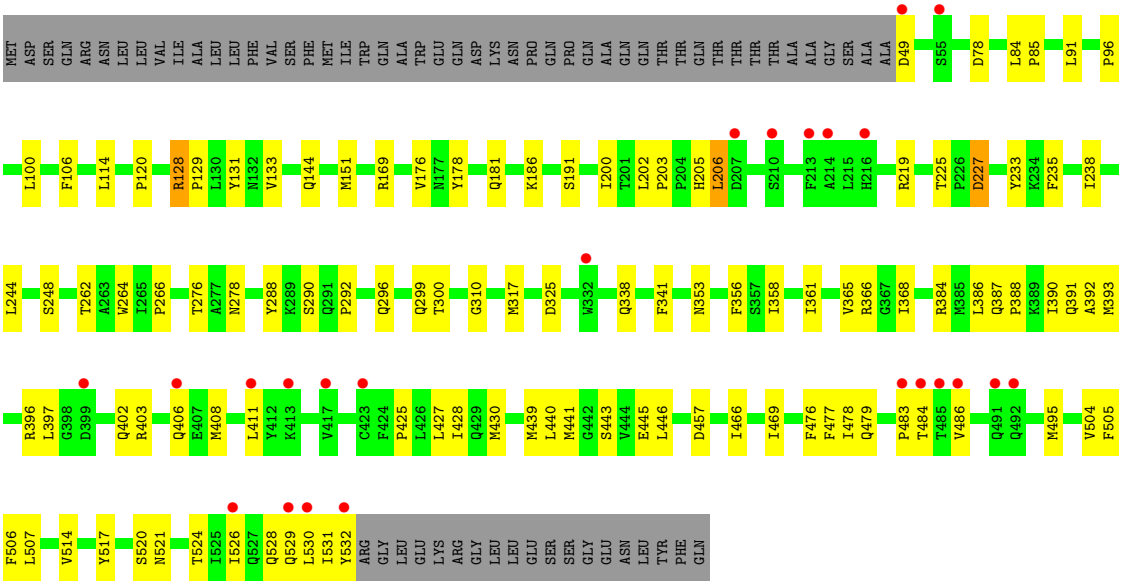
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0
3	B	2	Total O 2 2	0	0

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.

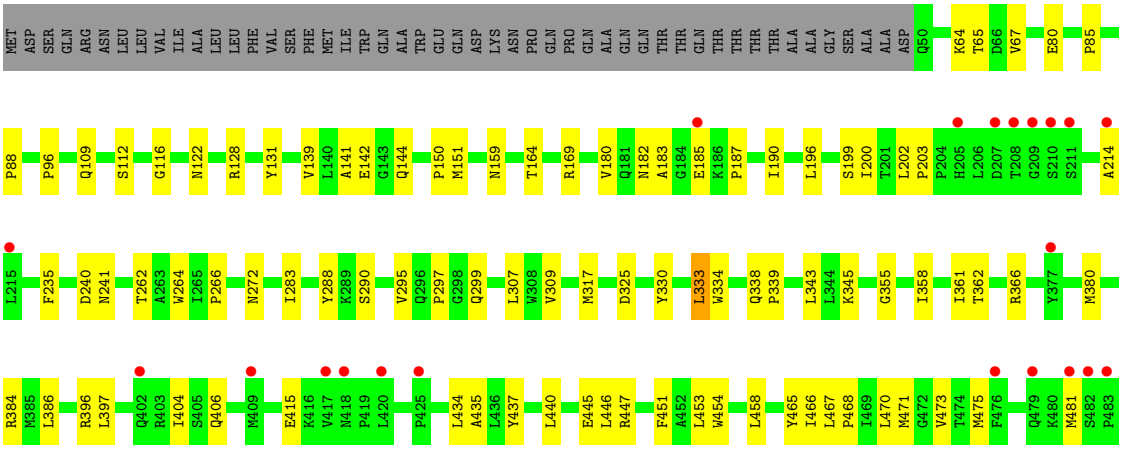
• Molecule 1: Membrane protein insertase YidC

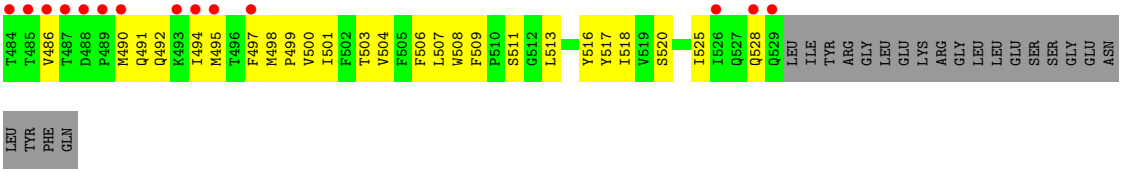
Chain A:



• Molecule 1: Membrane protein insertase YidC

Chain B:




T484 T485 V486 T487 D488 P489 M490 Q491 Q492 K493 I494 M495 T496 F497 M498 P499 V500 I501 F502 T503 V504 F505 F506 L507 W508 F509 P510 S511 G512 L513 Y516 Y517 I518 V519 S520 I525 I526 Q527 Q528 Q529 LEU ILE TYR ARG GLY LEU GLU LYS ARG GLY LEU LEU GLU SER SER GLY GLU ASN
LEU TYR PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	42.91Å 76.19Å 91.95Å 78.03° 82.61° 78.05°	Depositor
Resolution (Å)	41.84 – 2.80 41.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.84-2.80) 99.7 (41.84-2.80)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.218 , 0.275 0.218 , 0.275	Depositor DCC
R_{free} test set	1995 reflections (7.32%)	wwPDB-VP
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7650	wwPDB-VP
Average B, all atoms (Å^2)	59.0	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 40.09 % 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 2.8797e-04. 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: 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	0.26	0/3935	0.45	0/5359
1	B	0.26	0/3898	0.45	0/5308
All	All	0.26	0/7833	0.45	0/10667

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3831	0	3816	59	0
1	B	3795	0	3781	76	0
2	A	19	0	25	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
All	All	7650	0	7622	135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (135) 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:504:VAL:HA	1:A:507:LEU:HD13	1.49	0.91
1:A:49:ASP:HB3	1:A:292:PRO:HG3	1.69	0.75
1:A:440:LEU:HD23	1:A:446:LEU:HD13	1.70	0.74
1:B:185:GLU:HA	1:B:297:PRO:HB3	1.68	0.74
1:B:486:VAL:HG21	1:B:492:GLN:HB2	1.69	0.74
1:B:88:PRO:O	1:B:447:ARG:NH2	2.22	0.72
1:B:465:TYR:HE1	1:B:508:TRP:HE1	1.35	0.72
1:B:440:LEU:HD13	1:B:446:LEU:HD13	1.71	0.71
1:A:144:GLN:O	1:A:169:ARG:NH1	2.25	0.69
1:A:353:ASN:HD22	1:A:356:PHE:H	1.42	0.68
1:A:528:GLN:HA	1:A:531:ILE:HG22	1.77	0.67
1:B:486:VAL:HB	1:B:491:GLN:HG3	1.77	0.67
1:B:504:VAL:HA	1:B:507:LEU:HD11	1.76	0.66
1:A:477:PHE:HZ	1:A:529:GLN:HE21	1.41	0.66
1:A:78:ASP:OD2	1:A:128:ARG:NH1	2.29	0.66
1:B:468:PRO:HG2	1:B:507:LEU:HA	1.80	0.64
1:A:366:ARG:NH2	1:A:524:THR:OG1	2.30	0.64
1:A:296:GLN:N	1:A:299:GLN:OE1	2.24	0.63
1:B:150:PRO:HA	1:B:164:THR:HG22	1.80	0.63
1:A:484:THR:HG23	1:A:486:VAL:HG13	1.80	0.63
1:B:358:ILE:O	1:B:361:ILE:HG22	1.98	0.63
1:A:120:PRO:HB2	1:A:129:PRO:HG3	1.81	0.63
1:A:106:PHE:HB2	1:A:203:PRO:HG3	1.79	0.62
1:A:84:LEU:HD21	1:A:310:GLY:HA2	1.84	0.60
1:A:225:THR:HG22	1:A:227:ASP:H	1.66	0.59
1:B:486:VAL:HG12	1:B:491:GLN:HE21	1.67	0.59
1:A:386:LEU:HD22	1:A:411:LEU:HD11	1.85	0.59
1:B:196:LEU:HD13	1:B:262:THR:HG23	1.83	0.59
1:A:427:LEU:O	1:A:430:MET:HG2	2.03	0.58
1:B:202:LEU:HD12	1:B:203:PRO:HD2	1.84	0.58
1:B:470:LEU:HA	1:B:473:VAL:HB	1.85	0.57
1:B:498:MET:HA	1:B:501:ILE:HD12	1.85	0.57
1:A:317:MET:HE3	1:A:325:ASP:HA	1.88	0.56
1:B:466:ILE:O	1:B:470:LEU:HD12	2.06	0.55
1:B:131:TYR:HB3	1:B:151:MET:HB3	1.87	0.55
1:B:333:LEU:HD21	1:B:434:LEU:HB3	1.88	0.55
1:B:525:ILE:O	1:B:528:GLN:HG2	2.06	0.54
1:A:244:LEU:HB3	1:A:276:THR:HG23	1.89	0.54
1:B:141:ALA:HB3	1:B:144:GLN:HG3	1.90	0.54
1:B:317:MET:HE3	1:B:325:ASP:HA	1.88	0.54
1:A:526:ILE:O	1:A:530:LEU:HD13	2.08	0.54
1:A:445:GLU:OE1	1:A:445:GLU:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:VAL:HG11	1:B:492:GLN:HA	1.90	0.54
1:A:85:PRO:HA	1:A:96:PRO:HB3	1.90	0.53
1:B:517:TYR:HA	1:B:520:SER:HB3	1.89	0.53
1:B:343:LEU:HD12	1:B:361:ILE:HD12	1.90	0.53
1:B:159:ASN:ND2	1:B:183:ALA:H	2.06	0.52
1:B:454:TRP:CZ2	1:B:466:ILE:HD11	2.44	0.52
1:B:437:TYR:HD1	1:B:513:LEU:HD22	1.74	0.52
1:B:491:GLN:HA	1:B:494:ILE:HG12	1.92	0.52
1:A:388:PRO:HA	1:A:391:GLN:HG2	1.92	0.52
1:B:506:PHE:HA	1:B:509:PHE:HD2	1.74	0.52
1:A:466:ILE:O	1:A:469:ILE:HG13	2.10	0.51
1:B:386:LEU:HD21	1:B:415:GLU:HG2	1.93	0.51
1:A:479:GLN:NE2	1:A:495:MET:O	2.44	0.51
1:B:144:GLN:O	1:B:169:ARG:NH2	2.45	0.50
1:B:445:GLU:OE2	1:B:445:GLU:N	2.37	0.50
1:B:397:LEU:HD23	1:B:404:ILE:HG13	1.93	0.50
1:A:203:PRO:HB2	1:A:205:HIS:CE1	2.45	0.50
1:B:458:LEU:HA	1:B:511:SER:HB2	1.94	0.50
1:A:366:ARG:HH22	1:A:524:THR:HG1	1.58	0.50
1:A:365:VAL:HA	1:A:368:ILE:HG22	1.94	0.49
1:A:91:LEU:HD22	1:A:457:ASP:HB2	1.94	0.49
1:A:266:PRO:HB3	1:A:288:TYR:CE1	2.47	0.49
1:B:475:MET:HE3	1:B:499:PRO:HA	1.95	0.48
1:A:506:PHE:HD2	1:A:514:VAL:HG22	1.77	0.48
1:B:343:LEU:HD12	1:B:361:ILE:CD1	2.43	0.48
1:B:486:VAL:HB	1:B:491:GLN:CG	2.44	0.48
1:B:380:MET:O	1:B:384:ARG:HG3	2.13	0.48
1:B:481:MET:HE1	1:B:528:GLN:OE1	2.13	0.48
1:B:85:PRO:HA	1:B:96:PRO:HB3	1.94	0.48
1:A:387:GLN:HA	1:A:390:ILE:HG12	1.95	0.48
1:A:391:GLN:HG3	1:A:392:ALA:N	2.29	0.48
1:A:517:TYR:HA	1:A:520:SER:HB3	1.96	0.48
1:B:495:MET:HA	1:B:498:MET:HG2	1.96	0.48
1:B:345:LYS:HB3	1:B:345:LYS:HE3	1.58	0.47
1:A:341:PHE:HB2	1:A:439:MET:HG3	1.96	0.47
1:B:80:GLU:HA	1:B:109:GLN:HG2	1.96	0.47
1:A:425:PRO:HA	1:A:428:ILE:HD11	1.97	0.47
1:A:358:ILE:O	1:A:361:ILE:HG22	2.16	0.46
1:B:64:LYS:HB2	1:B:139:VAL:HG12	1.98	0.46
1:B:214:ALA:HB3	1:B:437:TYR:OH	2.15	0.46
1:A:191:SER:OG	1:A:290:SER:O	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASP:OD1	1:A:325:ASP:N	2.42	0.46
1:A:531:ILE:HG23	1:A:532:TYR:CD2	2.51	0.46
1:A:477:PHE:HZ	1:A:529:GLN:NE2	2.11	0.45
1:A:402:GLN:O	1:A:406:GLN:HG3	2.17	0.45
1:B:65:THR:HG22	1:B:67:VAL:H	1.81	0.45
1:B:468:PRO:CG	1:B:507:LEU:HA	2.47	0.45
1:B:497:PHE:O	1:B:500:VAL:HG12	2.17	0.45
1:A:202:LEU:HD13	1:A:219:ARG:NE	2.33	0.44
1:A:202:LEU:HD23	1:A:206:LEU:HG	1.99	0.44
1:A:181:GLN:HG3	1:A:300:THR:HG23	1.99	0.44
1:B:159:ASN:HD22	1:B:183:ALA:H	1.65	0.44
1:B:507:LEU:HD12	1:B:507:LEU:H	1.83	0.44
1:A:114:LEU:HD21	1:A:178:TYR:CG	2.52	0.44
1:B:467:LEU:O	1:B:518:ILE:HD11	2.18	0.44
1:B:180:VAL:HG11	1:B:295:VAL:HG21	1.98	0.44
1:A:133:VAL:HG22	1:A:151:MET:HG2	1.99	0.44
1:B:199:SER:HA	1:B:283:ILE:HA	2.00	0.44
1:B:180:VAL:HG21	1:B:190:ILE:HD13	1.99	0.44
1:B:325:ASP:OD1	1:B:325:ASP:N	2.44	0.43
1:B:471:MET:O	1:B:475:MET:HE2	2.18	0.43
1:B:343:LEU:CD1	1:B:361:ILE:HD12	2.48	0.43
1:A:397:LEU:HD13	1:A:403:ARG:HG3	2.00	0.43
1:B:355:GLY:HA3	1:B:451:PHE:CD1	2.54	0.43
1:A:131:TYR:HB3	1:A:151:MET:HB3	2.00	0.43
1:A:176:VAL:HG21	1:A:264:TRP:HH2	1.84	0.43
1:B:240:ASP:O	1:B:241:ASN:HB2	2.19	0.42
1:B:266:PRO:HB3	1:B:288:TYR:CE2	2.53	0.42
1:A:524:THR:O	1:A:528:GLN:HG2	2.20	0.42
1:B:116:GLY:O	1:B:122:ASN:ND2	2.48	0.42
1:A:200:ILE:HG23	1:A:235:PHE:HB3	2.01	0.42
1:A:393:MET:HE3	1:A:408:MET:HB2	2.01	0.42
1:B:187:PRO:HG3	1:B:297:PRO:HD3	2.01	0.42
1:B:272:ASN:HD22	1:B:290:SER:HA	1.84	0.42
1:B:490:MET:O	1:B:494:ILE:HG23	2.19	0.42
1:A:443:SER:HB2	1:A:446:LEU:HD12	2.02	0.42
1:B:112:SER:O	1:B:128:ARG:NH2	2.53	0.41
1:B:338:GLN:HB3	1:B:339:PRO:HD3	2.01	0.41
1:A:100:LEU:HD21	1:A:262:THR:HG21	2.03	0.41
1:A:106:PHE:CD1	1:A:203:PRO:HD3	2.55	0.41
1:A:478:ILE:HD11	1:A:521:ASN:HB3	2.01	0.41
1:B:330:TYR:HB2	1:B:334:TRP:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:LEU:HD13	1:B:435:ALA:HA	2.03	0.41
1:B:453:LEU:HB3	1:B:454:TRP:CE3	2.54	0.41
1:B:264:TRP:CZ3	1:B:307:LEU:HB2	2.55	0.41
1:B:362:THR:HG22	1:B:516:TYR:CD2	2.56	0.41
1:B:500:VAL:HA	1:B:503:THR:HB	2.02	0.41
1:A:238:ILE:O	1:A:278:ASN:HB2	2.20	0.40
1:B:200:ILE:HG23	1:B:235:PHE:HB3	2.04	0.40
1:A:384:ARG:HD3	1:A:483:PRO:HB2	2.04	0.40
1:B:159:ASN:ND2	1:B:182:ASN:HD22	2.19	0.40
1:B:202:LEU:HD12	1:B:203:PRO:CD	2.50	0.40
1:B:366:ARG:NH2	1:B:520:SER:O	2.53	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	482/551 (88%)	463 (96%)	18 (4%)	1 (0%)	47 78
1	B	478/551 (87%)	462 (97%)	16 (3%)	0	100 100
All	All	960/1102 (87%)	925 (96%)	34 (4%)	1 (0%)	51 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	LEU

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	415/471 (88%)	405 (98%)	10 (2%)	49 81
1	B	411/471 (87%)	405 (98%)	6 (2%)	65 89
All	All	826/942 (88%)	810 (98%)	16 (2%)	57 85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ARG
1	A	186	LYS
1	A	227	ASP
1	A	233	TYR
1	A	248	SER
1	A	338	GLN
1	A	396	ARG
1	A	441	MET
1	A	476	PHE
1	A	505	PHE
1	B	142	GLU
1	B	299	GLN
1	B	309	VAL
1	B	333	LEU
1	B	396	ARG
1	B	406	GLN

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	175	ASN
1	A	296	GLN
1	A	353	ASN
1	A	448	GLN
1	A	529	GLN
1	B	159	ASN
1	B	182	ASN
1	B	195	GLN
1	B	272	ASN
1	B	281	ASN
1	B	299	GLN

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Mol	Chain	Res	Type
1	B	461	GLN
1	B	479	GLN
1	B	491	GLN
1	B	492	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	OLC	A	601	-	18,18,24	1.06	1 (5%)	18,19,25	0.97	1 (5%)

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	OLC	A	601	-	-	6/18/18/24	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	OLC	O20-C1	4.27	1.45	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	OLC	O20-C1-C2	2.61	120.11	111.91

There are no chirality outliers.

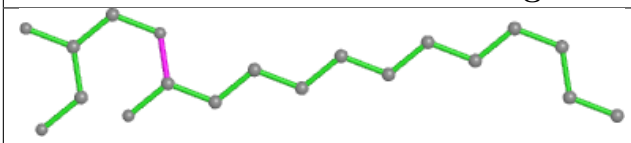
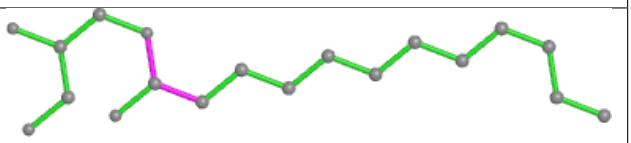
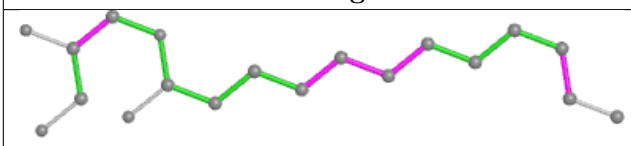
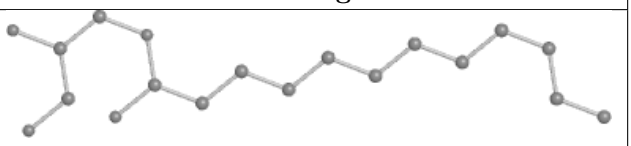
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	OLC	O20-C21-C22-O23
2	A	601	OLC	O20-C21-C22-C24
2	A	601	OLC	C4-C5-C6-C7
2	A	601	OLC	C9-C10-C11-C12
2	A	601	OLC	C5-C6-C7-C8
2	A	601	OLC	C3-C4-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

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 OLC A 601	
 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

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	484/551 (87%)	0.04	24 (4%) 28 19	22, 50, 110, 162	0
1	B	480/551 (87%)	0.13	35 (7%) 15 8	25, 53, 128, 185	0
All	All	964/1102 (87%)	0.08	59 (6%) 21 13	22, 51, 118, 185	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	485	THR	10.4
1	A	486	VAL	8.7
1	A	532	TYR	8.0
1	B	493	LYS	7.2
1	B	486	VAL	7.0
1	B	214	ALA	6.9
1	B	208	THR	5.8
1	A	55	SER	5.6
1	B	484	THR	5.3
1	B	482	SER	4.7
1	B	417	VAL	4.3
1	A	484	THR	4.2
1	B	487	THR	4.1
1	B	490	MET	4.0
1	A	213	PHE	3.9
1	A	49	ASP	3.9
1	A	485	THR	3.8
1	B	483	PRO	3.7
1	B	185	GLU	3.6
1	B	481	MET	3.5
1	B	205	HIS	3.5
1	A	406	GLN	3.4
1	B	495	MET	3.4
1	A	207	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	214	ALA	3.3
1	B	377	TYR	3.2
1	A	529	GLN	3.2
1	B	528	GLN	3.1
1	B	489	PRO	3.1
1	B	402	GLN	3.0
1	A	417	VAL	3.0
1	B	418	ASN	3.0
1	A	210	SER	2.8
1	A	413	LYS	2.7
1	B	207	ASP	2.7
1	B	211	SER	2.6
1	B	420	LEU	2.6
1	B	526	ILE	2.5
1	A	526	ILE	2.5
1	A	530	LEU	2.4
1	A	411	LEU	2.4
1	B	209	GLY	2.3
1	B	529	GLN	2.3
1	A	216	HIS	2.3
1	B	479	GLN	2.3
1	B	476	PHE	2.3
1	B	210	SER	2.3
1	A	399	ASP	2.2
1	B	494	ILE	2.2
1	B	409	MET	2.1
1	B	497	PHE	2.1
1	A	491	GLN	2.1
1	A	483	PRO	2.1
1	B	215	LEU	2.1
1	A	492	GLN	2.1
1	A	423	CYS	2.1
1	A	332	TRP	2.0
1	B	488	ASP	2.0
1	B	425	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

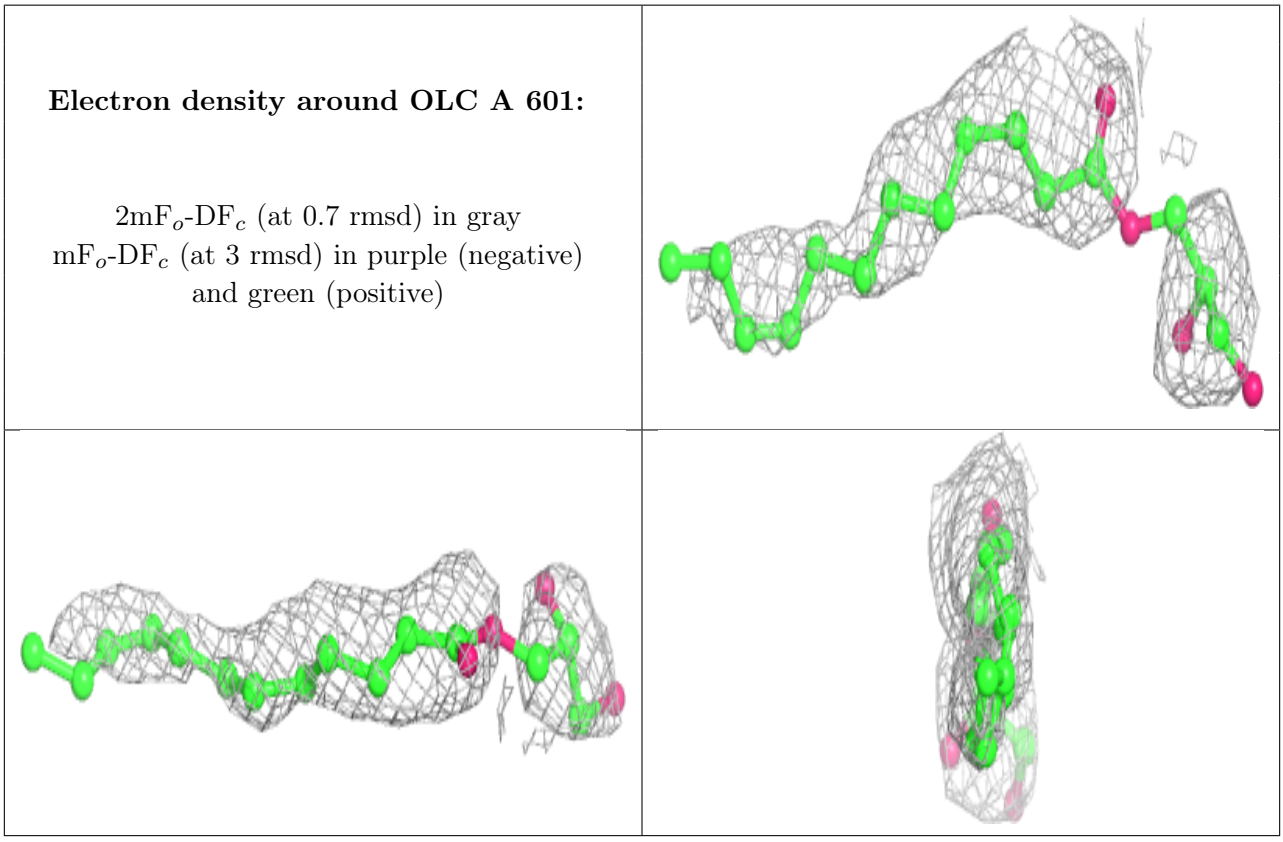
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	OLC	A	601	19/25	0.73	0.31	69,77,101,103	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 601:

$2mF_o$-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.