Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 12:37 PM EDT

PDB ID	:	3A7B
Title	:	Crystal structure of TLR2-Streptococcus Pneumoniae lipoteichoic acid complex
Authors	:	Kang, J.Y.; Jin, M.S.; Lee, J.-O.
Deposited on	:	2009-09-20
Resolution	:	2.53 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:

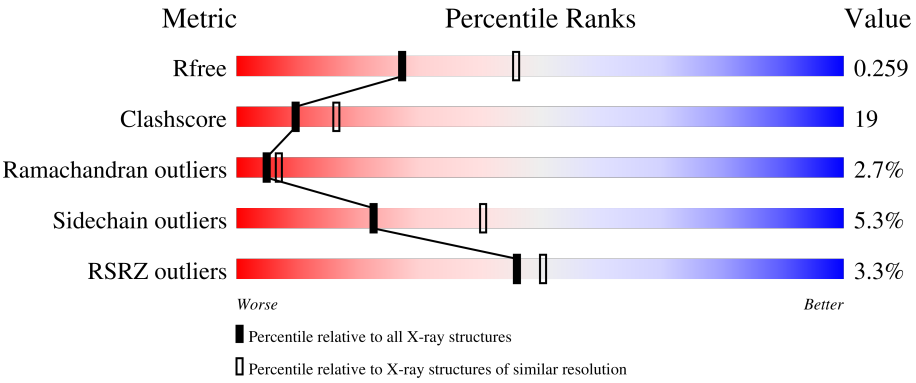
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	580	3%, 61%, 30%, 5%
2	B	2	50%, 50%

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
3	NAG	A	821	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4720 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 Toll-like receptor 2, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	550	4355	2771	736	828	20	0	0	0

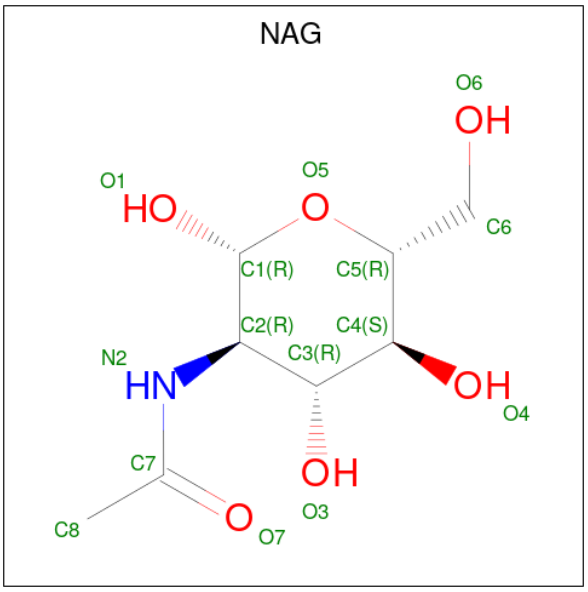
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	507	ALA	-	linker	UNP Q4G1L2
A	508	SER	-	linker	UNP Q4G1L2
A	577	LEU	-	expression tag	UNP Q4G1L2
A	578	VAL	-	expression tag	UNP Q4G1L2
A	579	PRO	-	expression tag	UNP Q4G1L2
A	580	ARG	-	expression tag	UNP Q4G1L2

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

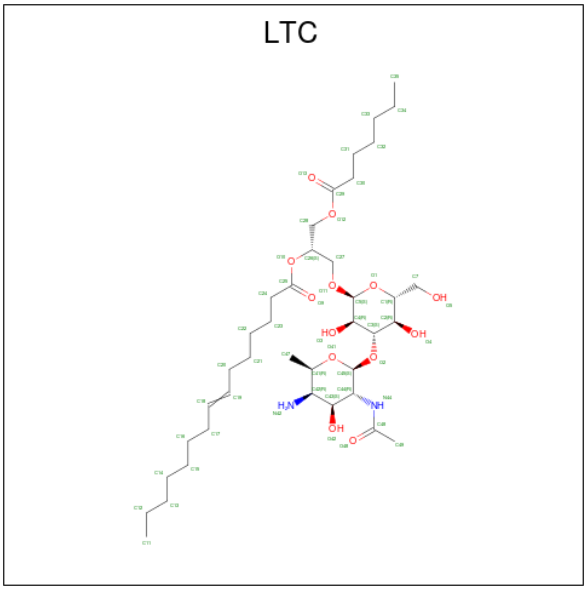
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is (2S)-1-({3-O-[2-(acetylamino)-4-amino-2,4,6-trideoxy-beta-D-galactopyranosyl]-alpha-D-glucopyranosyl}oxy)-3-(heptanoyloxy)propan-2-yl (7Z)-pentadec-7-enoate (three-letter code: LTC) (formula: $C_{39}H_{70}N_2O_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			54	39	2	13		

- Molecule 5 is water.

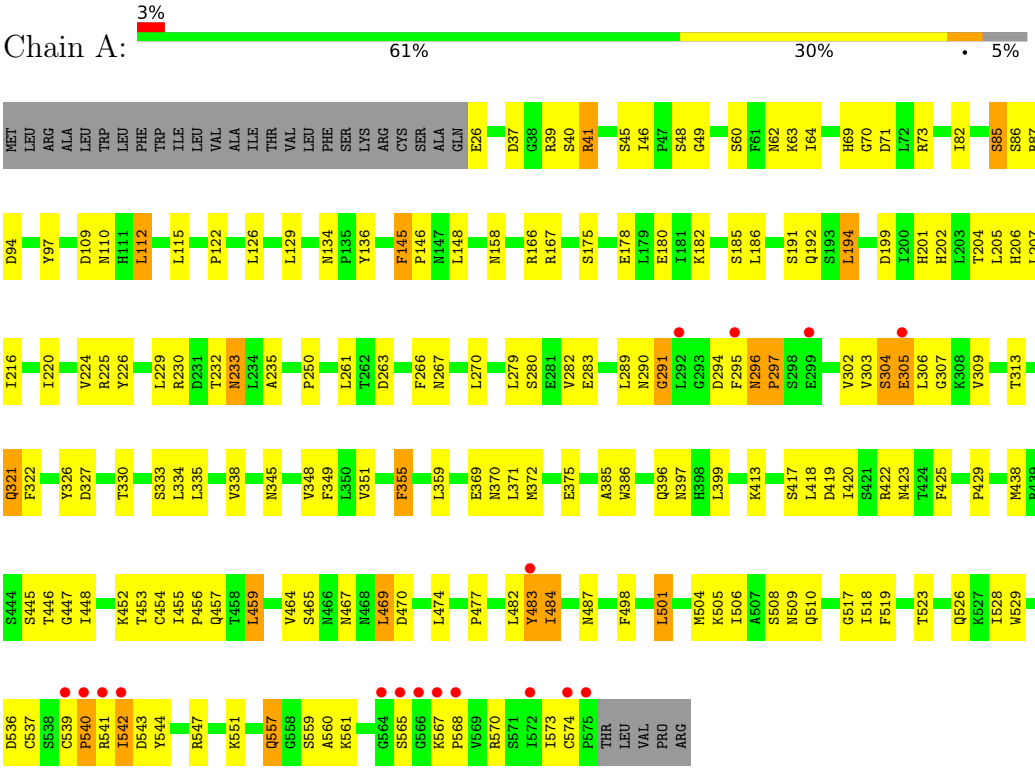
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	269	Total O 269 269	0	0

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: Toll-like receptor 2, Variable lymphocyte receptor B

Chain A:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.58Å 83.19Å 214.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.10 – 2.53 45.10 – 2.53	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.10-2.53) 95.5 (45.10-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	5.42 (at 2.54Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.270 0.225 , 0.259	Depositor DCC
R_{free} test set	4014 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4720	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: LTC, NAG

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	0.66	1/4439 (0.0%)	0.82	3/6013 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	540	PRO	C-N	5.47	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	194	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	351	VAL	N-CA-C	-5.21	96.92	111.00
1	A	86	SER	N-CA-C	-5.17	97.03	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4355	0	4400	171	0
2	B	28	0	25	2	0
3	A	14	0	13	2	0
4	A	54	0	70	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	269	0	0	2	0
All	All	4720	0	4508	173	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 19.

All (173) 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:372:MET:H	1:A:397:ASN:HD22	1.03	0.93
1:A:63:LYS:HD3	1:A:87:ARG:HD2	1.52	0.91
1:A:283:GLU:HG2	1:A:313:THR:HB	1.53	0.90
1:A:537:CYS:HA	1:A:542:ILE:HG12	1.54	0.89
1:A:303:VAL:HG12	1:A:330:THR:HG23	1.57	0.85
1:A:469:LEU:H	1:A:487:ASN:HD22	1.24	0.84
1:A:539:CYS:SG	1:A:573:ILE:HG13	2.19	0.82
1:A:296:ASN:H	1:A:297:PRO:HD2	1.49	0.78
1:A:348:VAL:H	1:A:370:ASN:ND2	1.82	0.77
1:A:348:VAL:H	1:A:370:ASN:HD22	1.31	0.76
1:A:355:PHE:HE1	1:A:359:LEU:HD21	1.52	0.73
1:A:372:MET:H	1:A:397:ASN:ND2	1.84	0.73
1:A:446:THR:H	1:A:467:ASN:HD21	1.32	0.73
1:A:112:LEU:H	1:A:134:ASN:HD22	1.37	0.72
1:A:561:LYS:HA	1:A:568:PRO:HA	1.72	0.71
2:B:1:NAG:H61	2:B:2:NAG:H82	1.75	0.68
1:A:306:LEU:HD11	4:A:581:LTC:H11	1.75	0.68
1:A:417:SER:HB3	1:A:440:PHE:HB3	1.74	0.67
1:A:372:MET:N	1:A:397:ASN:HD22	1.87	0.67
1:A:279:LEU:HD12	1:A:309:VAL:HG22	1.77	0.67
1:A:446:THR:HG23	1:A:448:ILE:HG23	1.77	0.66
1:A:335:LEU:O	1:A:338:VAL:HG22	1.96	0.66
1:A:456:PRO:HG2	1:A:459:LEU:HD13	1.78	0.66
1:A:304:SER:HB2	1:A:333:SER:OG	1.96	0.65
1:A:63:LYS:NZ	1:A:87:ARG:NE	2.45	0.64
1:A:233:ASN:HD21	1:A:235:ALA:HB3	1.62	0.64
1:A:396:GLN:HG2	1:A:422:ARG:HB3	1.80	0.63
1:A:110:ASN:HB2	1:A:134:ASN:HD21	1.64	0.62
1:A:446:THR:HG22	1:A:467:ASN:HD21	1.63	0.62
1:A:70:GLY:HA2	1:A:73:ARG:HG2	1.82	0.62
1:A:201:HIS:HD2	1:A:225:ARG:HG3	1.64	0.61
1:A:37:ASP:OD1	1:A:39:ARG:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ILE:HG23	1:A:459:LEU:HD22	1.82	0.61
1:A:482:LEU:HD23	1:A:504:MET:CE	2.32	0.59
1:A:467:ASN:HB2	1:A:487:ASN:HD21	1.68	0.58
1:A:509:ASN:O	1:A:510:GLN:HB2	2.04	0.58
1:A:559:SER:HB2	1:A:570:ARG:NH2	2.19	0.58
1:A:396:GLN:HG3	1:A:422:ARG:CZ	2.34	0.58
1:A:220:ILE:HB	1:A:224:VAL:HG23	1.85	0.57
1:A:321:GLN:CD	4:A:581:LTC:H4	2.25	0.57
1:A:447:GLY:H	1:A:467:ASN:ND2	2.02	0.56
1:A:69:HIS:HD2	1:A:94:ASP:OD1	1.87	0.56
1:A:60:SER:OG	1:A:82:ILE:HG22	2.05	0.56
1:A:97:TYR:HA	1:A:122:PRO:HG3	1.87	0.56
1:A:537:CYS:HA	1:A:542:ILE:CG1	2.31	0.56
1:A:306:LEU:HB3	1:A:309:VAL:HB	1.88	0.56
1:A:469:LEU:HD23	1:A:484:ILE:HD11	1.87	0.56
1:A:529:TRP:CZ2	1:A:557:GLN:HG2	2.41	0.56
1:A:205:LEU:HD11	1:A:216:ILE:HG21	1.88	0.55
1:A:498:PHE:HB3	1:A:501:LEU:HG	1.86	0.55
1:A:417:SER:CB	1:A:440:PHE:HB3	2.36	0.55
1:A:349:PHE:CE2	4:A:581:LTC:H28	2.42	0.54
1:A:539:CYS:H	1:A:540:PRO:HD2	1.72	0.54
1:A:469:LEU:H	1:A:487:ASN:ND2	1.99	0.54
1:A:510:GLN:HA	1:A:534:PRO:CD	2.38	0.54
1:A:233:ASN:C	1:A:233:ASN:HD22	2.10	0.54
1:A:542:ILE:HD12	1:A:542:ILE:O	2.08	0.53
2:B:1:NAG:H61	2:B:2:NAG:C8	2.39	0.53
1:A:455:ILE:HB	1:A:474:LEU:HD21	1.90	0.53
1:A:279:LEU:HD12	1:A:309:VAL:CG2	2.39	0.53
1:A:446:THR:HG22	1:A:467:ASN:ND2	2.24	0.53
1:A:532:THR:HG22	1:A:532:THR:O	2.08	0.52
1:A:355:PHE:CE1	1:A:359:LEU:HD21	2.40	0.52
1:A:375:GLU:HB2	5:A:612:HOH:O	2.09	0.52
1:A:464:VAL:HG23	1:A:484:ILE:HG12	1.92	0.52
1:A:175:SER:HA	1:A:199:ASP:O	2.09	0.51
1:A:60:SER:HG	1:A:82:ILE:HG22	1.76	0.51
1:A:518:ILE:HG23	1:A:519:PHE:N	2.25	0.51
1:A:45:SER:HA	1:A:64:ILE:HG23	1.92	0.51
1:A:303:VAL:O	1:A:304:SER:C	2.48	0.51
1:A:317:LEU:CD2	1:A:319:ILE:HD11	2.41	0.51
1:A:399:LEU:H	1:A:423:ASN:ND2	2.07	0.51
1:A:425:PHE:HD1	1:A:446:THR:OG1	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:LEU:H	1:A:423:ASN:HD22	1.59	0.50
1:A:535:TRP:CD1	1:A:560:ALA:HB1	2.47	0.50
1:A:85:SER:HA	1:A:109:ASP:O	2.12	0.50
1:A:26:GLU:CD	5:A:659:HOH:O	2.49	0.50
1:A:220:ILE:HB	1:A:224:VAL:CG2	2.41	0.50
1:A:510:GLN:HA	1:A:534:PRO:HD2	1.94	0.50
1:A:446:THR:H	1:A:467:ASN:ND2	2.06	0.49
1:A:372:MET:HG2	1:A:397:ASN:ND2	2.27	0.49
1:A:280:SER:HA	1:A:309:VAL:HA	1.95	0.49
1:A:385:ALA:O	1:A:386:TRP:C	2.50	0.49
1:A:115:LEU:HD21	1:A:136:TYR:CD2	2.48	0.49
1:A:369:GLU:HA	1:A:396:GLN:O	2.12	0.49
1:A:182:LYS:HA	1:A:206:HIS:HB2	1.94	0.48
1:A:145:PHE:N	1:A:146:PRO:HD2	2.28	0.48
1:A:178:GLU:HG3	1:A:202:HIS:HB3	1.94	0.48
1:A:320:PRO:O	1:A:321:GLN:HG2	2.14	0.48
1:A:506:ILE:HG12	1:A:506:ILE:O	2.13	0.48
1:A:89:ASN:ND2	1:A:90:THR:HG22	2.28	0.48
1:A:505:LYS:HG2	1:A:529:TRP:CE3	2.48	0.48
1:A:225:ARG:HD3	1:A:250:PRO:HB2	1.95	0.48
1:A:483:TYR:HA	1:A:505:LYS:HB2	1.95	0.48
1:A:535:TRP:NE1	1:A:560:ALA:HB1	2.29	0.48
1:A:63:LYS:CD	1:A:87:ARG:HD2	2.33	0.48
1:A:335:LEU:HD21	4:A:581:LTC:H11A	1.96	0.47
1:A:469:LEU:HB2	1:A:487:ASN:ND2	2.29	0.47
1:A:484:ILE:HG23	1:A:484:ILE:O	2.15	0.47
1:A:180:GLU:HG3	1:A:204:THR:HB	1.97	0.47
1:A:191:SER:O	1:A:192:GLN:CB	2.63	0.47
1:A:233:ASN:ND2	1:A:235:ALA:H	2.13	0.47
1:A:447:GLY:H	1:A:467:ASN:HD22	1.61	0.47
1:A:63:LYS:HZ1	1:A:87:ARG:NE	2.11	0.47
1:A:296:ASN:N	1:A:297:PRO:HD2	2.26	0.47
1:A:547:ARG:O	1:A:551:LYS:HG2	2.15	0.47
1:A:71:ASP:OD2	1:A:71:ASP:N	2.48	0.47
1:A:306:LEU:HD11	4:A:581:LTC:C11	2.43	0.47
1:A:191:SER:O	1:A:192:GLN:HB2	2.16	0.46
1:A:452:LYS:C	1:A:454:CYS:H	2.18	0.46
1:A:263:ASP:H	1:A:291:GLY:CA	2.28	0.46
1:A:303:VAL:O	1:A:305:GLU:N	2.48	0.45
1:A:305:GLU:C	1:A:307:GLY:H	2.19	0.45
1:A:420:ILE:HG13	1:A:443:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:GLN:HG2	1:A:477:PRO:HD2	1.97	0.45
1:A:504:MET:O	1:A:528:ILE:HA	2.17	0.45
1:A:541:ARG:O	1:A:542:ILE:HG13	2.16	0.45
1:A:413:LYS:HB2	3:A:821:NAG:H82	1.97	0.45
1:A:206:HIS:CE1	1:A:230:ARG:HD2	2.51	0.45
1:A:263:ASP:HB2	1:A:291:GLY:HA3	1.98	0.45
1:A:536:ASP:O	1:A:542:ILE:HG12	2.17	0.45
1:A:319:ILE:HD12	1:A:319:ILE:N	2.32	0.45
1:A:419:ASP:HA	1:A:442:ASN:HB3	1.99	0.44
1:A:509:ASN:O	1:A:510:GLN:CB	2.65	0.44
1:A:112:LEU:H	1:A:134:ASN:ND2	2.08	0.44
1:A:145:PHE:N	1:A:146:PRO:CD	2.81	0.44
1:A:321:GLN:HE22	4:A:581:LTC:H2	1.83	0.44
1:A:63:LYS:HZ3	1:A:87:ARG:NE	2.14	0.44
1:A:541:ARG:C	1:A:542:ILE:HG13	2.38	0.44
1:A:207:LEU:O	1:A:232:THR:HA	2.18	0.43
1:A:317:LEU:HG	1:A:319:ILE:HD12	2.00	0.43
1:A:348:VAL:HG22	4:A:581:LTC:H24A	2.00	0.43
1:A:447:GLY:N	1:A:467:ASN:ND2	2.65	0.43
1:A:565:SER:C	1:A:567:LYS:H	2.22	0.43
1:A:48:SER:OG	1:A:49:GLY:N	2.52	0.43
1:A:429:PRO:O	1:A:454:CYS:HB2	2.18	0.43
1:A:457:GLN:HG2	1:A:477:PRO:CD	2.48	0.43
1:A:263:ASP:H	1:A:291:GLY:HA2	1.84	0.43
1:A:370:ASN:HB2	1:A:397:ASN:HD21	1.84	0.43
1:A:279:LEU:CD1	1:A:309:VAL:HG22	2.48	0.42
1:A:482:LEU:HD23	1:A:504:MET:HE1	2.01	0.42
1:A:413:LYS:CB	3:A:821:NAG:H82	2.48	0.42
1:A:418:LEU:HB2	1:A:438:MET:HE2	2.01	0.42
1:A:39:ARG:O	1:A:41:ARG:HD2	2.20	0.42
1:A:62:ASN:HB3	1:A:63:LYS:H	1.67	0.42
1:A:270:LEU:HB2	1:A:302:VAL:HG11	2.02	0.42
1:A:63:LYS:HD3	1:A:87:ARG:CD	2.37	0.42
1:A:319:ILE:HG21	1:A:322:PHE:CE1	2.55	0.42
1:A:422:ARG:HA	1:A:445:SER:O	2.20	0.41
1:A:452:LYS:O	1:A:454:CYS:N	2.53	0.41
1:A:505:LYS:HA	1:A:529:TRP:HB2	2.01	0.41
1:A:517:GLY:HA2	1:A:544:TYR:CZ	2.54	0.41
1:A:267:ASN:ND2	1:A:302:VAL:CG1	2.83	0.41
1:A:465:SER:HB3	1:A:483:TYR:CD1	2.55	0.41
1:A:559:SER:HB2	1:A:570:ARG:HH22	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:H	1:A:46:ILE:HG12	1.73	0.41
1:A:498:PHE:HB3	1:A:501:LEU:HB2	2.02	0.41
1:A:508:SER:HA	1:A:532:THR:O	2.21	0.41
1:A:158:ASN:C	1:A:182:LYS:HG2	2.41	0.41
1:A:510:GLN:N	1:A:533:ASN:OD1	2.54	0.41
1:A:185:SER:O	1:A:186:LEU:C	2.58	0.41
1:A:345:ASN:HA	1:A:369:GLU:O	2.20	0.41
1:A:469:LEU:HD23	1:A:484:ILE:CD1	2.51	0.41
1:A:541:ARG:O	1:A:543:ASP:N	2.54	0.41
1:A:518:ILE:CG2	1:A:519:PHE:N	2.84	0.40
1:A:302:VAL:HG23	1:A:305:GLU:CB	2.50	0.40
1:A:539:CYS:N	1:A:540:PRO:HD2	2.35	0.40
1:A:126:LEU:HD21	1:A:129:LEU:HB2	2.03	0.40
1:A:261:LEU:HD13	1:A:266:PHE:HD1	1.87	0.40
1:A:279:LEU:HD11	1:A:282:VAL:HG22	2.02	0.40
1:A:305:GLU:C	1:A:307:GLY:N	2.73	0.40
1:A:567:LYS:HA	1:A:568:PRO:HD3	1.97	0.40
1:A:289:LEU:O	1:A:320:PRO:HD2	2.21	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	548/580 (94%)	483 (88%)	50 (9%)	15 (3%)	5 7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	304	SER
1	A	327	ASP

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Mol	Chain	Res	Type
1	A	296	ASN
1	A	320	PRO
1	A	453	THR
1	A	574	CYS
1	A	294	ASP
1	A	297	PRO
1	A	326	TYR
1	A	523	THR
1	A	41	ARG
1	A	542	ILE
1	A	145	PHE
1	A	291	GLY

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	510/537 (95%)	483 (95%)	27 (5%)	22 40

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	SER
1	A	90	THR
1	A	112	LEU
1	A	148	LEU
1	A	166	ARG
1	A	167	ARG
1	A	194	LEU
1	A	209	GLU
1	A	215	GLU
1	A	226	TYR
1	A	229	LEU
1	A	233	ASN
1	A	290	ASN
1	A	295	PHE

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Mol	Chain	Res	Type
1	A	305	GLU
1	A	321	GLN
1	A	334	LEU
1	A	355	PHE
1	A	371	LEU
1	A	459	LEU
1	A	469	LEU
1	A	470	ASP
1	A	483	TYR
1	A	484	ILE
1	A	501	LEU
1	A	526	GLN
1	A	557	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	69	HIS
1	A	89	ASN
1	A	104	HIS
1	A	110	ASN
1	A	134	ASN
1	A	177	ASN
1	A	201	HIS
1	A	233	ASN
1	A	267	ASN
1	A	290	ASN
1	A	321	GLN
1	A	370	ASN
1	A	397	ASN
1	A	423	ASN
1	A	457	GLN
1	A	467	ASN
1	A	487	ASN
1	A	526	GLN
1	A	552	ASN
1	A	554	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

2 monosaccharides 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	NAG	B	1	1,2	14,14,15	0.75	0	17,19,21	0.91	0
2	NAG	B	2	2	14,14,15	0.69	0	17,19,21	0.81	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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C2-N2-C7	-2.06	119.97	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

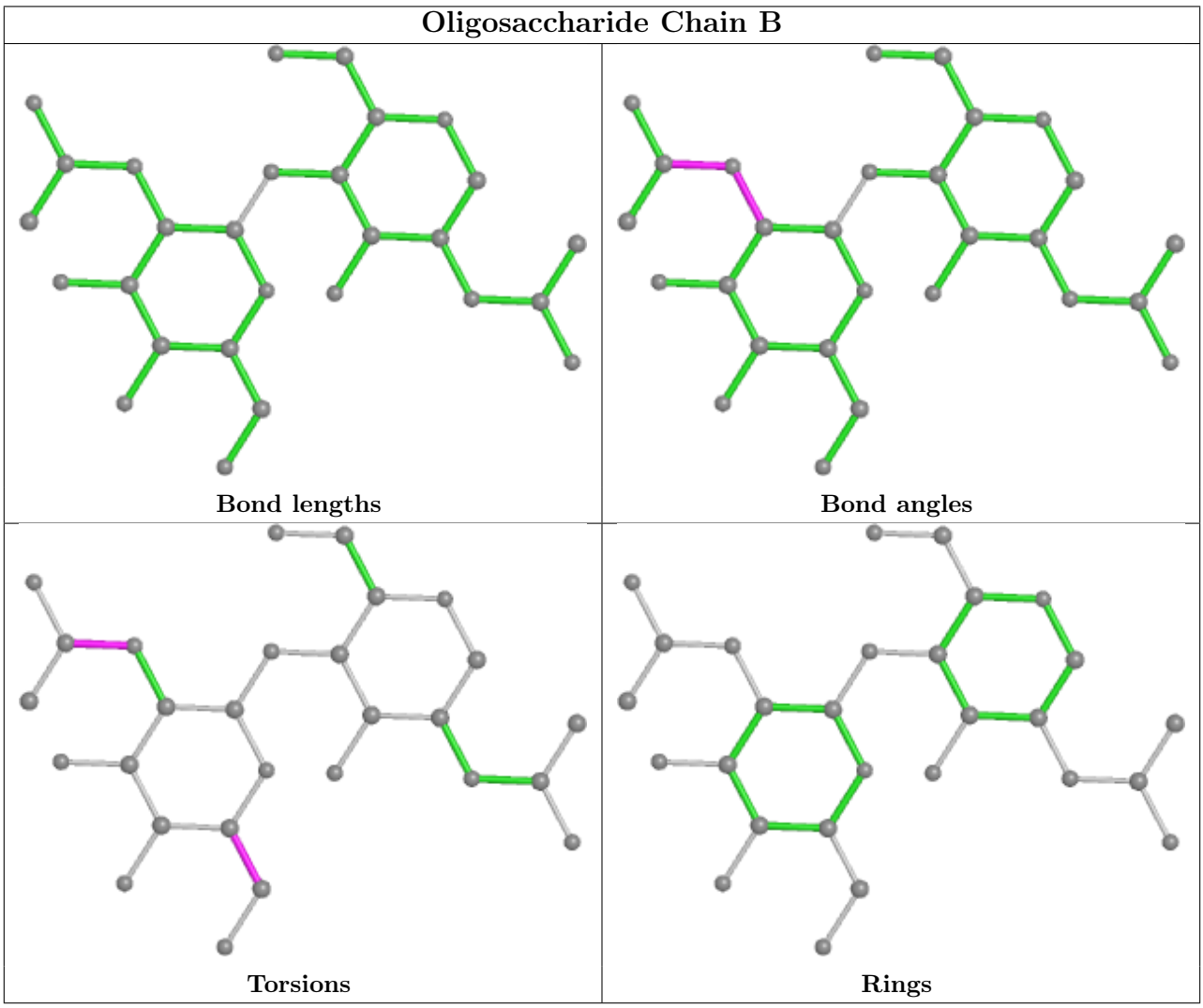
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	2	0
2	B	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	NAG	A	821	1	14,14,15	0.71	0	17,19,21	1.34	3 (17%)
4	LTC	A	581	-	54,55,55	0.81	2 (3%)	69,70,70	1.19	6 (8%)

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
3	NAG	A	821	1	1/1/5/7	0/6/23/26	0/1/1/1
4	LTC	A	581	-	-	13/44/84/84	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	581	LTC	C19-C18	3.79	1.53	1.31
4	A	581	LTC	O11-C5	2.04	1.43	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	581	LTC	O10-C25-C24	3.95	120.02	111.50
3	A	821	NAG	C2-N2-C7	-3.39	118.08	122.90
4	A	581	LTC	C26-O10-C25	-3.27	109.73	117.79
4	A	581	LTC	C45-O2-C3	-2.66	111.39	117.96
4	A	581	LTC	C5-O1-C1	-2.47	108.83	113.69
4	A	581	LTC	O12-C29-C30	2.39	119.40	111.91
3	A	821	NAG	O5-C1-C2	2.27	114.88	111.29
4	A	581	LTC	C47-C41-C42	-2.23	109.41	114.10
3	A	821	NAG	C3-C4-C5	-2.08	106.53	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	821	NAG	C1

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	581	LTC	O1-C5-O11-C27
4	A	581	LTC	C4-C5-O11-C27
4	A	581	LTC	O48-C48-N44-C44
4	A	581	LTC	C49-C48-N44-C44
4	A	581	LTC	C27-C26-C28-O12
4	A	581	LTC	C17-C18-C19-C20
4	A	581	LTC	O10-C26-C28-O12
4	A	581	LTC	C16-C17-C18-C19
4	A	581	LTC	C20-C21-C22-C23
4	A	581	LTC	C18-C19-C20-C21
4	A	581	LTC	O12-C29-C30-C31
4	A	581	LTC	O41-C45-O2-C3
4	A	581	LTC	O13-C29-C30-C31

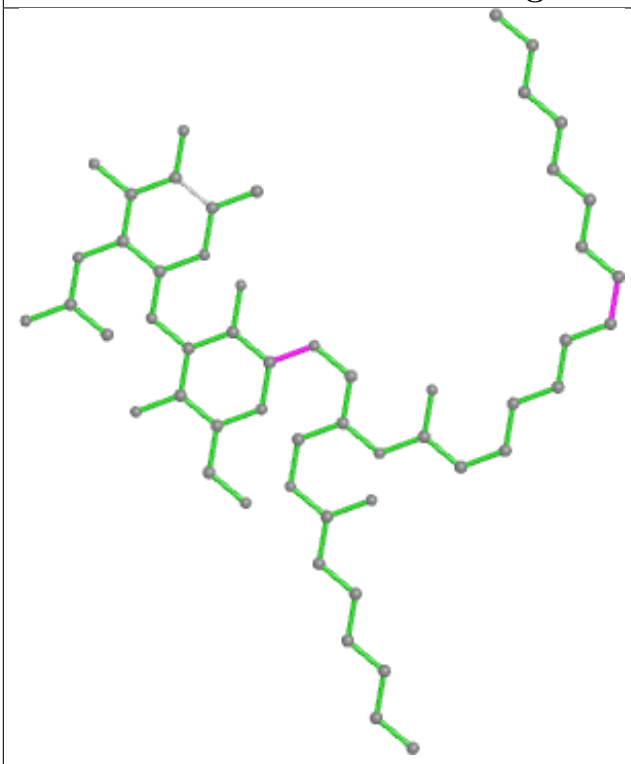
There are no ring outliers.

2 monomers are involved in 9 short contacts:

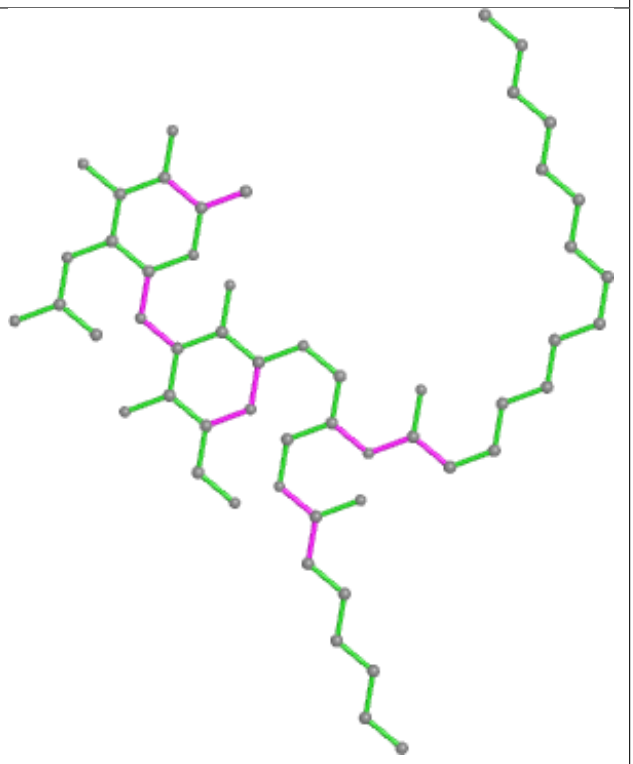
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	821	NAG	2	0
4	A	581	LTC	7	0

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 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.

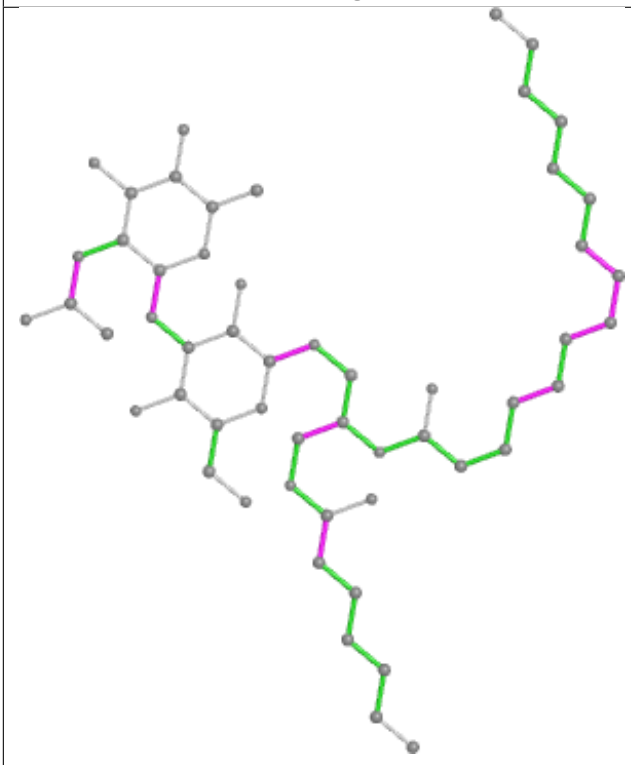
Ligand LTC A 581



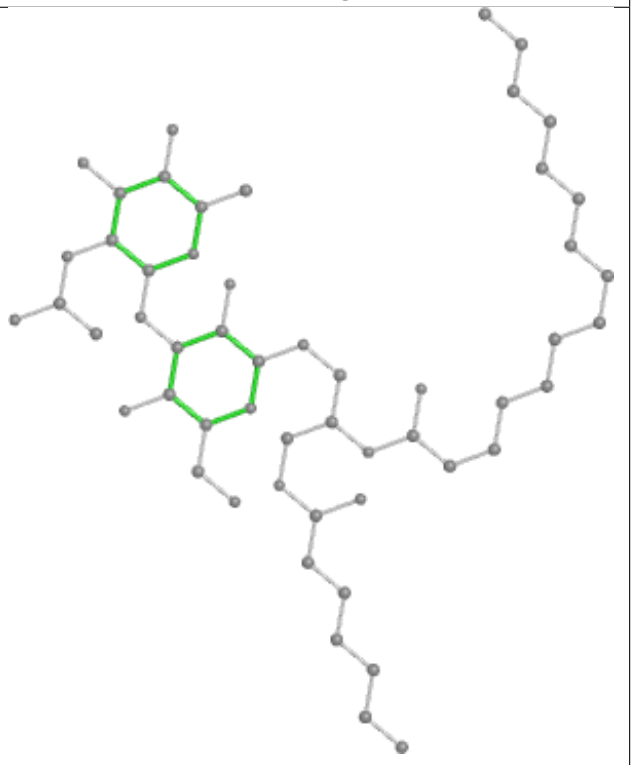
Bond lengths



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	550/580 (94%)	-0.03	18 (3%) 46 50	34, 53, 100, 123	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	PHE	6.2
1	A	539	CYS	5.9
1	A	483	TYR	5.7
1	A	566	GLY	4.8
1	A	564	GLY	4.5
1	A	541	ARG	4.4
1	A	540	PRO	4.0
1	A	542	ILE	3.4
1	A	572	ILE	3.2
1	A	299	GLU	3.1
1	A	575	PRO	3.0
1	A	567	LYS	3.0
1	A	535	TRP	2.8
1	A	292	LEU	2.8
1	A	305	GLU	2.7
1	A	565	SER	2.7
1	A	574	CYS	2.6
1	A	568	PRO	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

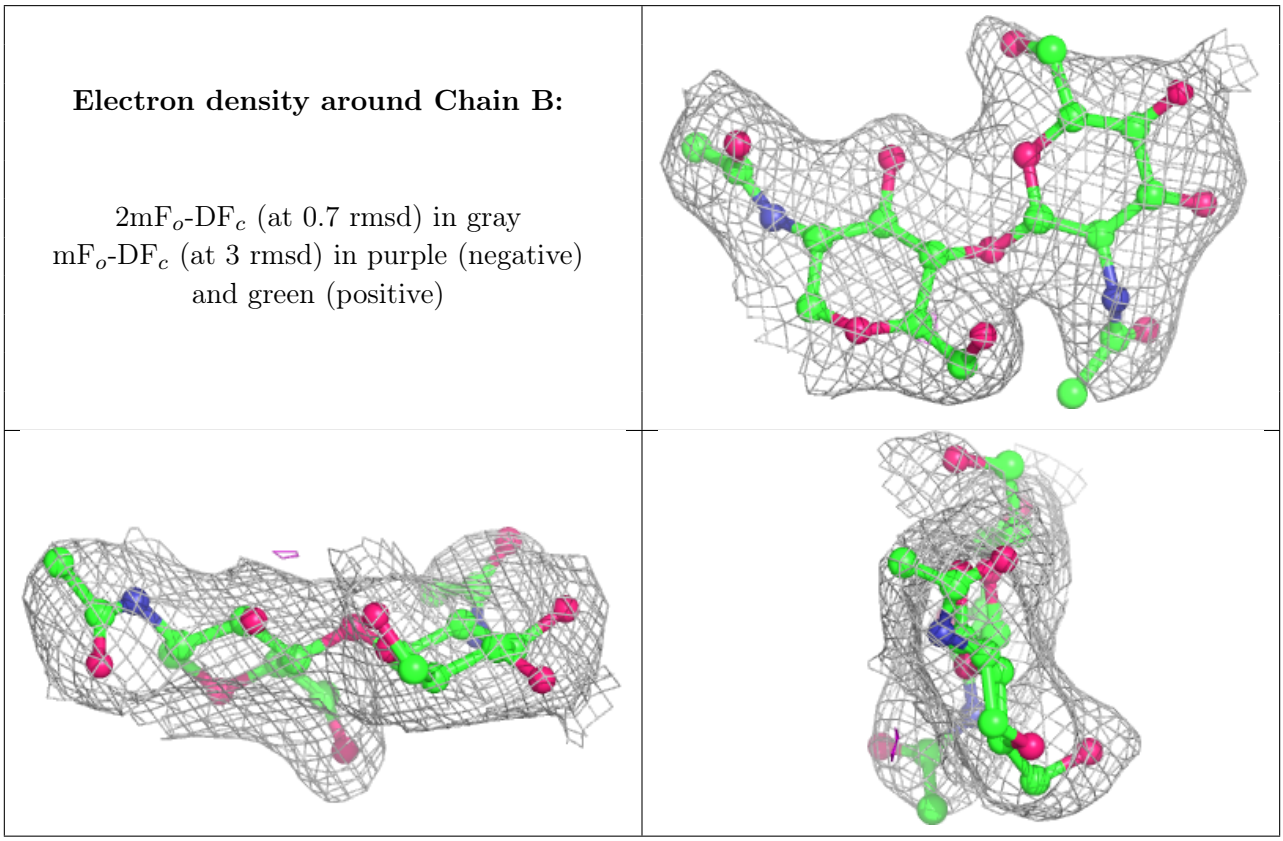
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (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	NAG	B	2	14/15	0.91	0.17	69,75,78,80	0
2	NAG	B	1	14/15	0.98	0.13	50,54,56,63	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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
4	LTC	A	581	54/54	0.64	0.37	81,91,97,101	0

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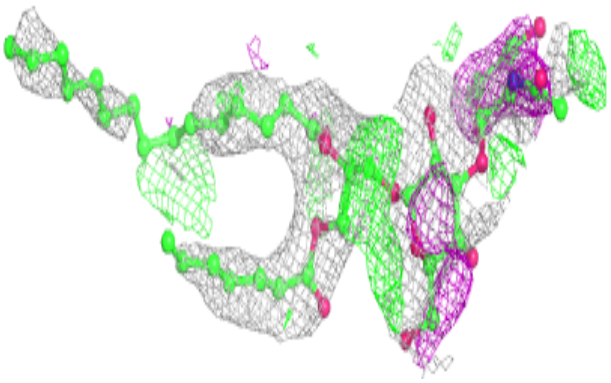
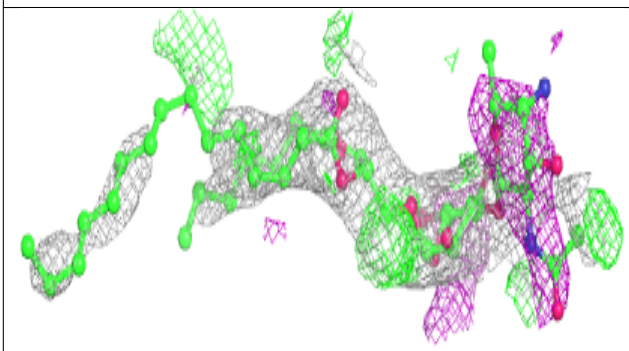
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	A	821	14/15	0.91	0.20	65,67,69,69	0

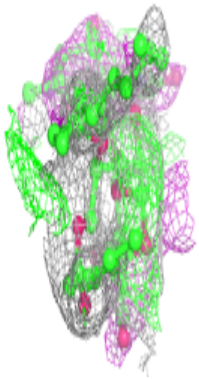
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LTC A 581:

$2mF_o$-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.