



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:07 PM UTC

PDB ID : 4AQS / pdb_00004aqs
Title : Laminin beta1 LN-LE1-4 structure
Authors : Carafoli, F.; Hussain, S.; Hohenester, E.
Deposited on : 2012-04-19
Resolution : 3.11 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
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

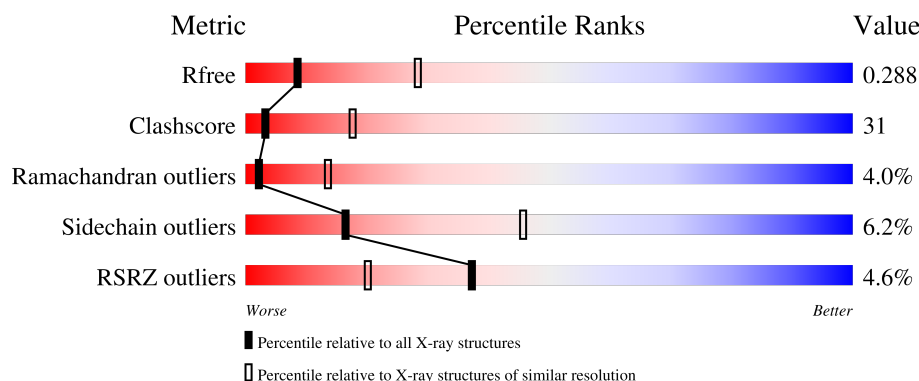
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	525	
2	B	5	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3578 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.

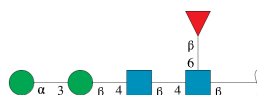
- Molecule 1 is a protein called LAMININ SUBUNIT BETA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	3504	2177	607	673	47	0	0	1

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ALA	-	expression tag	UNP P02469
A	19	PRO	-	expression tag	UNP P02469
A	20	LEU	-	expression tag	UNP P02469
A	21	ALA	-	expression tag	UNP P02469

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	5	60	34	2	24	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	143.99Å 152.95Å 92.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.47 – 3.11 76.47 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.7 (76.47-3.11) 99.8 (76.47-3.11)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.13Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.246 , 0.287 (Not available) , 0.288	Depositor DCC
R_{free} test set	1848 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	90.5	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3578	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: FUL, MAN, BMA, 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	0.53	1/3588 (0.0%)	1.03	14/4857 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	GLN	C-N	-5.53	1.25	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	TYR	N-CA-C	-7.54	104.31	113.97
1	A	146	ALA	N-CA-C	-6.38	104.19	112.23
1	A	154	SER	N-CA-C	-6.35	105.18	113.12
1	A	395	CYS	N-CA-C	6.10	118.68	108.73
1	A	472	CYS	N-CA-C	5.96	117.19	108.14
1	A	476	THR	N-CA-C	5.75	118.33	111.71
1	A	481	CYS	N-CA-C	5.72	118.28	110.55
1	A	60	LYS	CA-C-N	5.67	126.92	119.84
1	A	60	LYS	C-N-CA	5.67	126.92	119.84
1	A	276	HIS	N-CA-C	5.52	120.00	113.16
1	A	133	PHE	N-CA-C	5.49	117.58	108.20
1	A	231	THR	N-CA-C	-5.09	108.10	114.56
1	A	451	ASP	CA-C-N	5.03	125.06	119.32
1	A	451	ASP	C-N-CA	5.03	125.06	119.32

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	3504	0	3237	209	0
2	B	60	0	52	5	0
3	A	14	0	13	5	0
All	All	3578	0	3302	211	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 31.

All (211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:MET:HG2	1:A:265:MET:HE3	1.54	0.87
1:A:384:HIS:HB3	1:A:387:ARG:HG3	1.54	0.87
1:A:120:ASN:HB3	3:A:1001:NAG:H83	1.55	0.87
1:A:156:PHE:HA	1:A:232:ASN:HD21	1.43	0.84
1:A:140:PHE:CE2	1:A:145:PRO:HD3	2.13	0.83
1:A:115:GLU:O	1:A:118:VAL:HG22	1.80	0.81
1:A:235:ILE:CD1	1:A:265:MET:HE1	2.12	0.78
1:A:146:ALA:HB3	1:A:239:LYS:HB3	1.64	0.77
1:A:157:GLY:H	1:A:232:ASN:ND2	1.82	0.76
1:A:384:HIS:CB	1:A:387:ARG:HG3	2.15	0.76
1:A:136:LEU:HD11	1:A:265:MET:HE2	1.67	0.75
1:A:109:LYS:HD2	1:A:263:TYR:CE1	2.21	0.75
1:A:142:THR:HG22	1:A:143:PHE:N	2.02	0.74
1:A:290:VAL:HG12	1:A:291:GLU:H	1.53	0.74
1:A:138:MET:CG	1:A:265:MET:HE3	2.17	0.73
1:A:410:ILE:HD12	1:A:410:ILE:O	1.89	0.72
1:A:370:MET:HG2	1:A:371:GLY:N	2.05	0.72
1:A:384:HIS:ND1	1:A:385:PRO:HD2	2.05	0.72
1:A:182:MET:HE3	1:A:187:ASP:O	1.91	0.71
1:A:153:SER:HB3	1:A:232:ASN:HD22	1.57	0.69
1:A:381:TYR:HA	1:A:396:GLU:O	1.93	0.69
1:A:235:ILE:HD11	1:A:265:MET:HE1	1.75	0.68
1:A:59:HIS:C	1:A:60:LYS:HD2	2.19	0.68
1:A:221:SER:HB2	1:A:222:PRO:HD2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:MET:HE1	1:A:148:MET:HE1	1.77	0.66
1:A:120:ASN:CB	3:A:1001:NAG:H83	2.23	0.66
1:A:129:ALA:HB3	1:A:131:PHE:CE1	2.32	0.65
1:A:88:THR:O	1:A:89:LEU:HD23	1.97	0.65
1:A:201:THR:HG22	1:A:202:GLU:N	2.12	0.64
1:A:251:ARG:C	1:A:253:GLU:H	2.05	0.64
1:A:478:TYR:CE1	1:A:488:GLN:HG2	2.33	0.64
1:A:120:ASN:HD22	3:A:1001:NAG:H82	1.62	0.64
1:A:324:ALA:O	1:A:325:GLU:HG3	1.98	0.63
1:A:315:PHE:CE1	1:A:342:SER:HA	2.33	0.63
1:A:201:THR:HG22	1:A:202:GLU:H	1.63	0.62
1:A:142:THR:HG22	1:A:143:PHE:H	1.64	0.62
1:A:404:GLY:O	1:A:429:LYS:HG3	2.00	0.62
1:A:52:VAL:CG2	1:A:96:ILE:HB	2.30	0.61
1:A:128:GLU:HG2	1:A:129:ALA:N	2.16	0.61
1:A:384:HIS:CD2	1:A:387:ARG:HE	2.18	0.61
1:A:412:ASP:HB2	1:A:422:ILE:O	2.00	0.60
1:A:461:ASN:HD21	1:A:463:LEU:HB2	1.67	0.60
1:A:305:LYS:O	1:A:311:LEU:HB2	2.02	0.60
1:A:197:ILE:HG12	1:A:241:HIS:CD2	2.37	0.59
1:A:476:THR:HG22	1:A:478:TYR:CD1	2.38	0.59
1:A:110:ILE:O	1:A:111:TRP:HB3	2.02	0.59
1:A:247:LEU:HD21	1:A:258:TYR:HD2	1.67	0.59
1:A:400:CYS:O	1:A:402:PRO:HD3	2.02	0.59
1:A:52:VAL:HG11	1:A:112:TRP:CZ2	2.38	0.59
1:A:146:ALA:HB3	1:A:239:LYS:CB	2.32	0.59
1:A:417:PHE:O	1:A:419:VAL:N	2.36	0.59
1:A:120:ASN:HD22	3:A:1001:NAG:C8	2.16	0.58
1:A:138:MET:CE	1:A:148:MET:HE1	2.33	0.58
1:A:322:ARG:HD3	2:B:5:FUL:H63	1.86	0.57
1:A:350:VAL:O	1:A:354:THR:HG23	2.05	0.57
1:A:140:PHE:CD1	1:A:140:PHE:N	2.72	0.57
1:A:149:LEU:HD21	1:A:236:LYS:HB2	1.86	0.56
1:A:96:ILE:C	1:A:98:ASN:H	2.13	0.56
1:A:424:GLY:O	1:A:425:GLN:C	2.48	0.56
1:A:185:VAL:HG22	1:A:185:VAL:O	2.04	0.56
1:A:111:TRP:CZ2	1:A:141:LYS:HE2	2.42	0.55
1:A:197:ILE:HG12	1:A:241:HIS:NE2	2.21	0.55
1:A:30:CYS:HB2	1:A:301:ARG:NH1	2.21	0.55
1:A:251:ARG:C	1:A:253:GLU:N	2.64	0.55
1:A:290:VAL:HG12	1:A:291:GLU:N	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LEU:HB3	1:A:453:TYR:HB3	1.89	0.54
1:A:77:PHE:N	1:A:77:PHE:CD1	2.76	0.54
1:A:136:LEU:HD11	1:A:265:MET:CE	2.38	0.54
1:A:99:VAL:HG11	1:A:265:MET:HG2	1.90	0.54
1:A:149:LEU:CD2	1:A:236:LYS:HB2	2.38	0.53
1:A:322:ARG:HD3	2:B:5:FUL:C6	2.38	0.53
1:A:98:ASN:OD1	1:A:110:ILE:HG21	2.09	0.53
1:A:109:LYS:HD2	1:A:263:TYR:HE1	1.74	0.53
1:A:264:ASP:OD1	1:A:264:ASP:C	2.52	0.53
1:A:30:CYS:C	1:A:32:GLU:H	2.15	0.53
1:A:141:LYS:O	1:A:201:THR:HG23	2.09	0.53
1:A:417:PHE:O	1:A:420:GLY:N	2.38	0.53
1:A:64:TYR:HA	1:A:256:GLU:HG3	1.91	0.52
1:A:370:MET:HG2	1:A:371:GLY:H	1.73	0.52
1:A:156:PHE:O	1:A:158:LYS:HG2	2.10	0.52
1:A:338:ASN:O	1:A:339:GLU:HB2	2.09	0.52
1:A:31:ALA:C	1:A:32:GLU:HG3	2.35	0.52
1:A:461:ASN:OD1	1:A:462:PRO:HD2	2.08	0.52
1:A:144:ARG:HD3	1:A:203:GLY:HA3	1.92	0.52
1:A:149:LEU:HD23	1:A:149:LEU:N	2.25	0.52
1:A:144:ARG:HD3	1:A:203:GLY:C	2.35	0.51
1:A:403:ALA:CB	1:A:449:ALA:HB2	2.40	0.51
1:A:52:VAL:HG11	1:A:112:TRP:CE2	2.47	0.50
1:A:110:ILE:HG22	1:A:111:TRP:N	2.26	0.50
1:A:217:GLU:O	1:A:219:PRO:HD3	2.10	0.50
1:A:96:ILE:C	1:A:98:ASN:N	2.68	0.50
1:A:83:ASP:HB2	1:A:90:ASN:ND2	2.27	0.50
1:A:310:GLU:HA	1:A:321:TRP:CZ2	2.47	0.50
1:A:430:LEU:HD23	1:A:453:TYR:CD2	2.47	0.50
1:A:53:THR:HB	1:A:122:THR:H	1.76	0.50
1:A:99:VAL:CG1	1:A:265:MET:HG2	2.41	0.49
1:A:120:ASN:HB3	3:A:1001:NAG:C8	2.35	0.49
1:A:130:GLU:HA	1:A:231:THR:HG22	1.94	0.49
1:A:86:HIS:CD2	1:A:89:LEU:HG	2.47	0.49
1:A:411:CYS:HB2	1:A:424:GLY:O	2.13	0.49
1:A:57:GLY:HA3	1:A:79:CYS:O	2.13	0.49
1:A:149:LEU:HD23	1:A:236:LYS:O	2.13	0.48
1:A:118:VAL:O	1:A:118:VAL:HG23	2.13	0.48
1:A:99:VAL:HG13	1:A:265:MET:N	2.29	0.48
1:A:184:LYS:HD3	1:A:223:ARG:HH12	1.77	0.48
1:A:370:MET:O	1:A:374:CYS:HA	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:TYR:HB3	1:A:207:PHE:CZ	2.49	0.48
1:A:152:ARG:HG2	1:A:163:TYR:CZ	2.48	0.48
1:A:132:HIS:CD2	1:A:272:PHE:HB3	2.49	0.47
1:A:255:ARG:C	1:A:257:LYS:H	2.22	0.47
1:A:367:HIS:O	1:A:368:ASN:HB2	2.14	0.47
1:A:414:TYR:CD1	1:A:414:TYR:N	2.82	0.47
1:A:483:ARG:O	1:A:484:LEU:HB2	2.15	0.47
1:A:459:ALA:HB1	1:A:489:ARG:HH21	1.79	0.47
1:A:149:LEU:HD23	1:A:149:LEU:H	1.80	0.47
1:A:458:CYS:HB3	1:A:460:CYS:SG	2.55	0.47
1:A:461:ASN:ND2	1:A:464:GLY:H	2.12	0.47
1:A:144:ARG:HD3	1:A:203:GLY:CA	2.45	0.46
1:A:387:ARG:NH1	1:A:393:ASN:HB2	2.31	0.46
1:A:108:LEU:N	1:A:108:LEU:HD23	2.30	0.46
1:A:144:ARG:HH11	1:A:204:GLU:H	1.62	0.46
1:A:348:MET:O	1:A:352:LEU:HG	2.16	0.46
1:A:322:ARG:HG2	2:B:5:FUL:O4	2.15	0.46
1:A:221:SER:CB	1:A:222:PRO:HD2	2.44	0.46
1:A:368:ASN:O	1:A:378:LYS:HG3	2.15	0.46
1:A:370:MET:CG	1:A:371:GLY:N	2.77	0.46
1:A:167:ALA:O	1:A:195:SER:HB2	2.16	0.46
1:A:197:ILE:C	1:A:199:PRO:HD2	2.41	0.46
1:A:483:ARG:HG2	1:A:484:LEU:HG	1.97	0.46
1:A:52:VAL:HG21	1:A:96:ILE:HB	1.96	0.46
1:A:141:LYS:HG3	1:A:263:TYR:CE2	2.50	0.45
1:A:155:ASP:OD2	1:A:158:LYS:HB2	2.16	0.45
1:A:301:ARG:O	1:A:302:HIS:HB2	2.16	0.45
1:A:96:ILE:O	1:A:98:ASN:N	2.48	0.45
1:A:225:GLN:C	1:A:227:LEU:H	2.24	0.45
1:A:379:PRO:O	1:A:380:PHE:HB2	2.17	0.45
1:A:138:MET:SD	1:A:235:ILE:HD13	2.56	0.45
1:A:345:HIS:CE1	1:A:361:VAL:HG22	2.52	0.45
1:A:444:PHE:CD2	1:A:457:SER:HA	2.52	0.45
1:A:52:VAL:HG22	1:A:96:ILE:HB	1.97	0.45
1:A:171:GLU:OE1	1:A:171:GLU:N	2.50	0.45
1:A:251:ARG:O	1:A:253:GLU:N	2.50	0.45
1:A:451:ASP:OD1	1:A:451:ASP:C	2.59	0.45
1:A:137:ILE:HB	1:A:266:VAL:HG22	1.99	0.45
1:A:201:THR:CG2	1:A:202:GLU:N	2.80	0.45
1:A:110:ILE:HG22	1:A:111:TRP:H	1.80	0.45
1:A:146:ALA:HB3	1:A:239:LYS:C	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:PHE:CD1	1:A:346:PHE:C	2.95	0.45
2:B:4:MAN:H62	2:B:4:MAN:O3	2.17	0.45
1:A:57:GLY:O	1:A:81:SER:N	2.51	0.44
1:A:370:MET:HE2	1:A:370:MET:HB3	1.72	0.44
1:A:43:LEU:HD21	1:A:50:LEU:HD21	1.99	0.44
1:A:246:ASN:C	1:A:248:LEU:N	2.75	0.44
1:A:196:ASP:HB3	1:A:197:ILE:H	1.41	0.44
1:A:64:TYR:O	1:A:76:CYS:HB3	2.18	0.44
1:A:155:ASP:O	1:A:156:PHE:C	2.60	0.43
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.87	0.43
1:A:85:TYR:CD1	1:A:85:TYR:C	2.97	0.43
1:A:136:LEU:HD23	1:A:150:ILE:HD13	2.00	0.43
1:A:386:GLU:O	1:A:387:ARG:O	2.36	0.43
1:A:478:TYR:CE1	1:A:488:GLN:CG	3.00	0.43
1:A:101:THR:HG23	1:A:264:ASP:HB2	2.01	0.43
1:A:59:HIS:O	1:A:60:LYS:HD2	2.18	0.43
1:A:429:LYS:HD3	1:A:452:PRO:O	2.17	0.43
1:A:432:VAL:HG12	1:A:433:GLU:N	2.33	0.43
1:A:131:PHE:CD1	1:A:131:PHE:N	2.87	0.43
1:A:143:PHE:O	1:A:144:ARG:C	2.60	0.43
1:A:320:PRO:HB3	1:A:346:PHE:CZ	2.53	0.43
1:A:366:GLN:HB3	1:A:367:HIS:CD2	2.53	0.43
1:A:98:ASN:HB3	1:A:110:ILE:HG22	2.00	0.43
1:A:112:TRP:CH2	1:A:121:VAL:HG11	2.54	0.43
1:A:140:PHE:N	1:A:140:PHE:HD1	2.15	0.42
1:A:459:ALA:HB1	1:A:489:ARG:NH2	2.35	0.42
1:A:319:LEU:HD12	1:A:333:LYS:HB2	2.01	0.42
1:A:407:ASN:C	1:A:409:GLY:H	2.27	0.42
1:A:367:HIS:CD2	1:A:367:HIS:N	2.88	0.42
1:A:393:ASN:O	1:A:394:LEU:C	2.62	0.42
1:A:30:CYS:HB2	1:A:301:ARG:CZ	2.50	0.42
1:A:375:GLU:H	1:A:375:GLU:CD	2.27	0.42
1:A:301:ARG:O	1:A:304:THR:OG1	2.33	0.42
1:A:169:ASP:C	1:A:171:GLU:H	2.28	0.41
1:A:179:THR:O	1:A:180:GLY:O	2.38	0.41
1:A:212:PRO:C	1:A:214:PHE:H	2.28	0.41
1:A:407:ASN:HB2	1:A:410:ILE:HG13	2.02	0.41
1:A:64:TYR:HA	1:A:256:GLU:CG	2.50	0.41
1:A:56:CYS:C	1:A:79:CYS:SG	3.03	0.41
1:A:362:CYS:SG	1:A:373:ASN:HA	2.60	0.41
1:A:58:LEU:O	1:A:82:ARG:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASP:HB3	1:A:44:ILE:HG13	2.03	0.41
1:A:439:VAL:HG12	1:A:440:CYS:N	2.36	0.41
1:A:483:ARG:O	1:A:484:LEU:CB	2.69	0.41
1:A:30:CYS:SG	1:A:278:SER:HB3	2.60	0.41
1:A:80:ASP:OD1	1:A:82:ARG:HG2	2.21	0.41
1:A:86:HIS:CD2	1:A:88:THR:H	2.38	0.41
1:A:111:TRP:CE2	1:A:141:LYS:HE2	2.56	0.41
1:A:169:ASP:C	1:A:171:GLU:N	2.79	0.41
1:A:312:CYS:C	1:A:313:MET:O	2.64	0.41
1:A:400:CYS:HB3	1:A:405:SER:OG	2.21	0.41
1:A:403:ALA:HB2	1:A:449:ALA:HB2	2.02	0.41
1:A:303:ASN:O	1:A:313:MET:HB2	2.20	0.41
1:A:380:PHE:HA	1:A:398:CYS:SG	2.61	0.40
1:A:403:ALA:HA	1:A:449:ALA:CB	2.51	0.40
2:B:1:NAG:H61	2:B:2:NAG:H82	2.02	0.40
1:A:86:HIS:HD2	1:A:88:THR:H	1.68	0.40
1:A:169:ASP:O	1:A:171:GLU:N	2.54	0.40
1:A:375:GLU:HB2	1:A:389:ILE:HD11	2.03	0.40
1:A:452:PRO:HG2	1:A:453:TYR:CE1	2.55	0.40
1:A:453:TYR:CD1	1:A:453:TYR:N	2.88	0.40
1:A:76:CYS:C	1:A:77:PHE:CD1	3.00	0.40
1:A:210:LEU:O	1:A:211:ASP:C	2.64	0.40
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.83	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	448/525 (85%)	364 (81%)	66 (15%)	18 (4%)	2 13

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PHE
1	A	200	SER
1	A	387	ARG
1	A	418	SER
1	A	488	GLN
1	A	180	GLY
1	A	197	ILE
1	A	145	PRO
1	A	192	SER
1	A	196	ASP
1	A	217	GLU
1	A	256	GLU
1	A	416	ASP
1	A	170	CYS
1	A	198	GLU
1	A	252	MET
1	A	425	GLN
1	A	61	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/457 (84%)	362 (94%)	24 (6%)	16	46

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	53	THR
1	A	61	PRO
1	A	77	PHE
1	A	78	ILE
1	A	88	THR
1	A	97	GLU
1	A	108	LEU
1	A	132	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	139	THR
1	A	140	PHE
1	A	152	ARG
1	A	195	SER
1	A	200	SER
1	A	216	ILE
1	A	257	LYS
1	A	291	GLU
1	A	299	MET
1	A	361	VAL
1	A	402	PRO
1	A	406	GLU
1	A	451	ASP
1	A	453	TYR
1	A	475	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	90	ASN
1	A	132	HIS
1	A	232	ASN
1	A	308	ASN
1	A	345	HIS
1	A	407	ASN
1	A	431	HIS
1	A	461	ASN

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 ⓘ

5 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	0.64	0	17,19,21	1.11	2 (11%)
2	NAG	B	2	2	14,14,15	0.73	0	17,19,21	0.58	0
2	BMA	B	3	2	11,11,12	0.79	0	15,15,17	0.51	0
2	MAN	B	4	2	11,11,12	0.65	0	15,15,17	0.60	1 (6%)
2	FUL	B	5	2	10,10,11	0.58	0	14,14,16	0.35	0

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	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
2	FUL	B	5	2	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C2-N2-C7	-2.69	119.29	122.90
2	B	1	NAG	C6-C5-C4	2.48	119.10	113.02
2	B	4	MAN	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

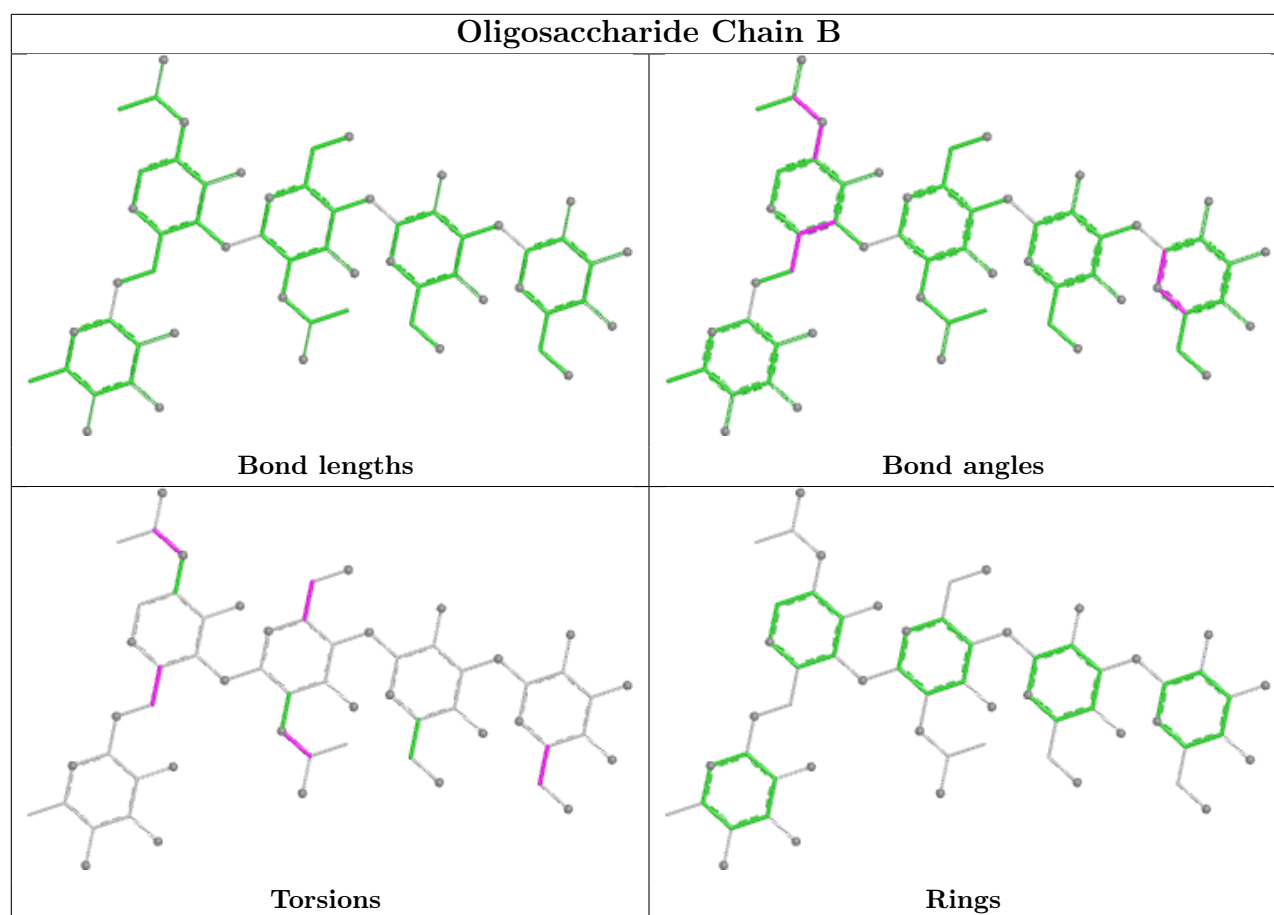
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	4	MAN	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	MAN	1	0
2	B	1	NAG	1	0
2	B	5	FUL	3	0
2	B	2	NAG	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 oligosaccharide.



5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	NAG	A	1001	1	14,14,15	1.10	1 (7%)	17,19,21	0.60	0

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	1001	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	NAG	C1-C2	2.48	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	NAG	C8-C7-N2-C2
3	A	1001	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	NAG	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	454/525 (86%)	0.42	21 (4%) 37 20	58, 87, 119, 134	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	LEU	5.1
1	A	69	HIS	4.7
1	A	242	THR	3.8
1	A	102	THR	3.4
1	A	290	VAL	2.7
1	A	252	MET	2.6
1	A	163	TYR	2.6
1	A	493	CYS	2.5
1	A	253	GLU	2.5
1	A	198	GLU	2.4
1	A	249	ASP	2.4
1	A	196	ASP	2.4
1	A	258	TYR	2.3
1	A	72	GLU	2.3
1	A	138	MET	2.3
1	A	251	ARG	2.3
1	A	76	CYS	2.2
1	A	29	GLY	2.2
1	A	248	LEU	2.2
1	A	133	PHE	2.1
1	A	246	ASN	2.0

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

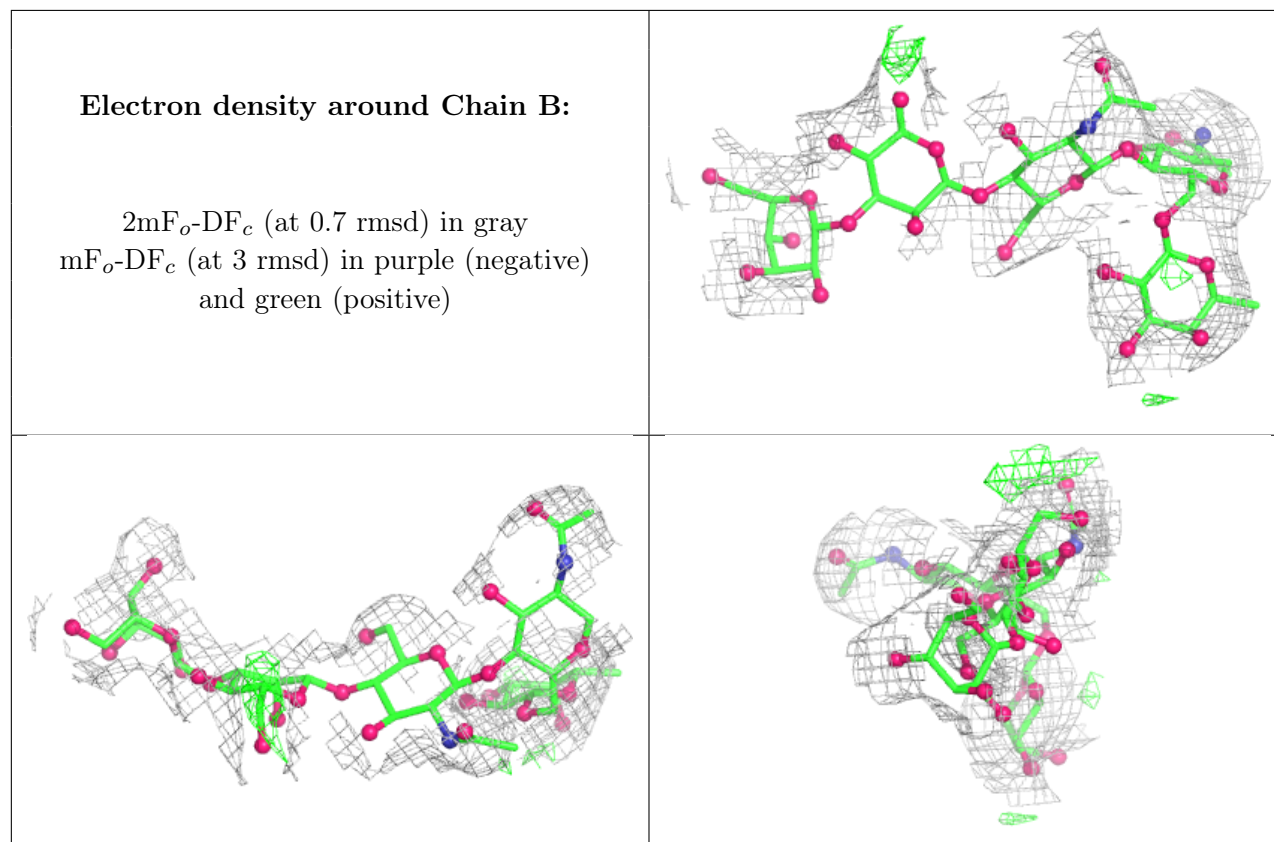
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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
2	MAN	B	4	11/12	0.39	0.15	154,156,156,156	0
2	BMA	B	3	11/12	0.46	0.13	148,149,151,154	0
2	FUL	B	5	10/11	0.83	0.19	117,119,120,120	0
2	NAG	B	2	14/15	0.87	0.14	128,132,138,144	0
2	NAG	B	1	14/15	0.90	0.13	100,104,115,120	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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	1001	14/15	0.20	0.19	122,124,129,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.