



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:48 AM UTC

PDB ID : 1J0I / pdb_00001j0i
Title : Crystal structure of neopullulanase complex with panose
Authors : Hondoh, H.; Kuriki, T.; Matsuura, Y.
Deposited on : 2002-11-14
Resolution : 2.40 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

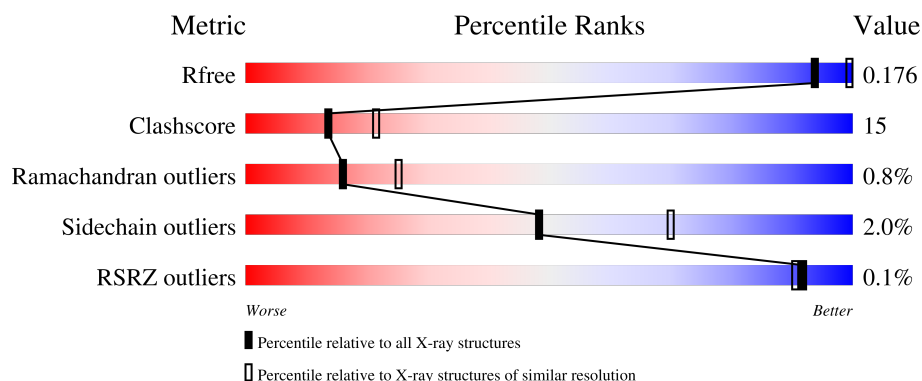
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	588	70% 28% .
1	B	588	69% 28% .
2	C	3	67% 33%
2	D	3	33% 67%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10474 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 neopullulanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4889	3158	816	893	22			
1	B	588	Total	C	N	O	S	0	0	0
			4889	3158	816	893	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ALA	ARG	SEE REMARK 999	UNP P38940
B	290	ALA	ARG	SEE REMARK 999	UNP P38940

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			34	18	16			
2	D	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is water.

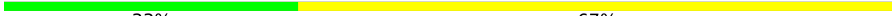
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	346	Total	O	0	0
			346	346		
3	B	282	Total	O	0	0
			282	282		

- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:  67% 33%

GLC1
GLC2
GLC3

- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  33% 67%

GLC1
GLC2
GLC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.45Å 71.44Å 123.69Å 90.00° 91.11° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.40) 94.6 (10.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.177 , 0.238 0.183 , 0.176	Depositor DCC
R_{free} test set	2264 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.792	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.021 for -k,-h,-l 0.020 for k,h,-l 0.030 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10474	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: GLC

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	0.39	0/5047	0.93	20/6857 (0.3%)
1	B	0.38	0/5047	0.90	19/6857 (0.3%)
All	All	0.39	0/10094	0.92	39/13714 (0.3%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ARG	CA-C-N	9.37	131.55	119.84
1	A	9	ARG	C-N-CA	9.37	131.55	119.84
1	B	114	TYR	N-CA-C	9.14	124.04	110.52
1	A	114	TYR	N-CA-C	7.39	121.42	110.48
1	B	281	GLU	N-CA-C	7.05	114.35	108.07
1	A	372	ASP	N-CA-C	-6.58	105.41	113.50
1	A	117	PHE	CA-C-N	6.52	127.99	119.84
1	A	117	PHE	C-N-CA	6.52	127.99	119.84
1	A	584	ALA	N-CA-C	-6.44	99.14	109.96
1	B	117	PHE	CA-C-N	6.23	127.62	119.84
1	B	117	PHE	C-N-CA	6.23	127.62	119.84
1	A	289	PHE	N-CA-C	-6.16	100.72	109.96
1	B	55	GLN	N-CA-C	-6.10	101.49	110.52
1	B	372	ASP	N-CA-C	-6.10	106.00	113.50
1	B	115	PHE	N-CA-C	-6.06	102.53	110.53
1	A	69	ASP	N-CA-C	-6.04	99.55	109.40
1	B	9	ARG	CA-C-N	5.89	127.21	119.84
1	B	9	ARG	C-N-CA	5.89	127.21	119.84
1	A	196	THR	N-CA-C	-5.88	101.49	110.07
1	A	209	THR	N-CA-C	5.86	118.72	110.23
1	A	7	TYR	N-CA-C	5.76	118.59	108.75
1	B	141	PHE	CA-C-N	5.65	126.90	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	PHE	C-N-CA	5.65	126.90	119.84
1	B	289	PHE	N-CA-C	-5.63	101.52	109.96
1	A	82	LEU	N-CA-C	5.60	117.62	108.55
1	A	544	ILE	N-CA-C	5.57	113.38	107.76
1	B	68	PHE	N-CA-C	5.48	118.51	109.85
1	B	69	ASP	N-CA-C	-5.38	101.39	109.95
1	A	130	ASP	N-CA-C	5.31	117.75	111.33
1	B	206	LYS	N-CA-C	5.30	119.05	112.58
1	A	301	ALA	N-CA-C	-5.27	106.90	113.38
1	B	67	LEU	N-CA-C	5.26	120.36	113.88
1	A	478	ASP	CA-C-N	5.25	125.30	119.32
1	A	478	ASP	C-N-CA	5.25	125.30	119.32
1	A	379	PHE	N-CA-C	-5.20	105.53	111.14
1	B	290	ALA	CB-CA-C	-5.12	110.65	116.54
1	B	7	TYR	N-CA-C	5.09	116.79	108.55
1	B	82	LEU	N-CA-C	5.06	117.41	108.75
1	A	290	ALA	CB-CA-C	-5.05	110.73	116.54

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	4889	0	4643	136	0
1	B	4889	0	4643	156	0
2	C	34	0	30	8	0
2	D	34	0	30	2	0
3	A	346	0	0	13	0
3	B	282	0	0	13	0
All	All	10474	0	9346	281	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 15.

All (281) 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:B:571:LEU:HD22	1:B:571:LEU:H	1.35	0.91
1:B:540:GLN:HA	1:B:577:PRO:HG3	1.50	0.91
1:B:436:ILE:HD11	1:B:486:LEU:HD22	1.59	0.85
1:A:559:LEU:HD12	3:A:1498:HOH:O	1.76	0.85
1:B:363:MET:HE1	1:B:409:PRO:HD3	1.58	0.83
1:B:558:LEU:HD21	1:B:584:ALA:HB2	1.60	0.83
1:A:175:LEU:HD13	1:A:219:PHE:HB3	1.60	0.82
1:A:513:ALA:HB2	1:A:521:ILE:HD12	1.64	0.79
1:A:273:ILE:HD13	1:A:278:LEU:HD11	1.65	0.78
1:A:30:LYS:NZ	1:B:2:ARG:HH22	1.82	0.77
1:B:83:ARG:HD3	1:B:114:TYR:HB2	1.68	0.75
1:A:56:MET:HE1	1:A:87:VAL:HG21	1.69	0.74
1:A:402:MET:HA	1:A:402:MET:HE2	1.69	0.74
1:B:1:MET:SD	1:B:95:LEU:HD12	2.26	0.74
1:A:586:GLU:HB3	1:A:588:TRP:HE1	1.52	0.72
1:A:331:ASN:HD22	1:A:331:ASN:N	1.86	0.71
1:B:363:MET:HE1	1:B:408:TYR:HA	1.73	0.71
1:A:36:ARG:HB3	3:A:1593:HOH:O	1.94	0.68
1:B:253:ALA:HB3	1:B:254:PRO:HD3	1.75	0.68
1:B:281:GLU:HA	1:B:282:PRO:C	2.18	0.68
1:A:30:LYS:HZ2	1:B:2:ARG:HH22	1.41	0.68
1:B:331:ASN:N	1:B:331:ASN:HD22	1.90	0.68
1:B:243:ALA:HB2	1:B:325:TRP:CE3	2.30	0.67
1:A:488:GLN:HG2	3:A:1612:HOH:O	1.93	0.66
1:B:536:ASN:O	1:B:578:TYR:HA	1.95	0.66
1:B:556:VAL:HB	1:B:584:ALA:HB3	1.75	0.66
1:B:111:THR:HB	1:B:113:TYR:CE1	2.32	0.65
1:A:586:GLU:HB3	1:A:588:TRP:NE1	2.12	0.65
1:B:389:LYS:HB2	1:B:391:GLU:HG3	1.78	0.64
1:B:288:THR:HG22	1:B:296:PRO:HA	1.80	0.64
1:A:395:ARG:HB2	1:A:516:GLU:HG2	1.80	0.64
1:B:461:ILE:O	1:B:482:GLN:O	2.15	0.64
1:B:402:MET:HE2	1:B:402:MET:HA	1.80	0.63
1:A:226:LYS:HA	1:A:226:LYS:HZ3	1.63	0.63
1:B:140:ILE:O	1:B:142:PRO:HD3	1.98	0.63
1:B:186:VAL:HG21	1:B:235:LYS:HD3	1.80	0.63
1:B:563:ARG:O	1:B:564:PHE:HB3	1.99	0.63
1:A:279:GLN:HG2	1:A:285:ASN:ND2	2.14	0.62
1:B:410:ASN:O	1:B:414:GLU:HG3	1.99	0.62
1:B:546:ILE:HG23	1:B:546:ILE:O	1.98	0.62
1:A:226:LYS:HA	1:A:226:LYS:NZ	2.14	0.62
1:B:279:GLN:H	1:B:285:ASN:ND2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:ILE:HD13	1:B:546:ILE:C	2.24	0.62
1:A:364:PRO:HG2	1:A:365:TRP:CZ3	2.35	0.61
1:B:515:ASP:C	1:B:517:MET:H	2.08	0.61
1:B:523:LYS:HD3	3:B:1624:HOH:O	1.98	0.61
1:A:77:PRO:HB2	1:A:80:ARG:HA	1.83	0.61
1:A:478:ASP:OD2	1:A:481:GLN:HG2	2.00	0.60
1:B:46:ASP:HB3	1:B:51:ALA:HB3	1.83	0.60
1:A:253:ALA:HB3	1:A:254:PRO:HD3	1.82	0.60
1:B:568:ALA:C	1:B:570:THR:H	2.10	0.60
1:B:511:LEU:HD11	3:B:1624:HOH:O	2.00	0.59
1:A:64:SER:HB2	1:A:68:PHE:O	2.02	0.59
1:B:279:GLN:N	1:B:285:ASN:ND2	2.51	0.59
1:A:315:TYR:CE1	1:A:319:GLU:HG3	2.38	0.58
1:B:511:LEU:HD12	1:B:511:LEU:N	2.19	0.58
1:A:108:THR:HB	3:A:1594:HOH:O	2.03	0.58
1:B:191:THR:O	1:B:237:ILE:HA	2.03	0.58
1:A:4:GLU:H	1:A:4:GLU:CD	2.12	0.57
1:A:158:ARG:HG3	1:A:163:GLU:OE1	2.04	0.57
1:A:295:MET:HE1	2:C:2:GLC:H62	1.85	0.57
1:A:383:VAL:HG12	1:A:442:LEU:CD2	2.34	0.57
1:A:233:HIS:HE1	1:A:323:ASP:OD1	1.88	0.57
1:B:84:TYR:O	1:B:114:TYR:HB3	2.05	0.57
1:B:132:VAL:HG11	1:B:353:TYR:CD1	2.40	0.57
1:B:281:GLU:HA	1:B:283:ARG:N	2.20	0.57
1:B:393:SER:HB2	1:B:517:MET:HA	1.86	0.56
1:A:419:LEU:HD23	1:A:419:LEU:H	1.71	0.56
1:A:159:PRO:HB2	1:A:162:SER:HB3	1.86	0.56
1:B:1:MET:HG3	1:B:34:ILE:HD11	1.86	0.56
1:A:546:ILE:HD11	1:A:573:THR:HB	1.87	0.56
1:B:272:HIS:HB2	1:B:287:ASP:HB2	1.87	0.56
1:B:27:LEU:HD21	1:B:88:LEU:HD21	1.87	0.55
1:B:47:TRP:CD1	1:B:48:GLN:N	2.75	0.55
1:A:492:GLN:NE2	1:A:559:LEU:HD22	2.21	0.55
1:B:83:ARG:CD	1:B:114:TYR:HB2	2.35	0.55
1:B:257:ASP:OD2	1:B:265:SER:HB2	2.07	0.55
1:B:571:LEU:H	1:B:571:LEU:CD2	2.13	0.55
1:A:331:ASN:N	1:A:331:ASN:ND2	2.56	0.54
1:B:482:GLN:O	1:B:483:ASN:HB3	2.06	0.54
1:A:436:ILE:O	1:A:440:LYS:HG3	2.08	0.54
1:A:140:ILE:O	1:A:142:PRO:HD3	2.07	0.54
1:B:242:ASP:OD1	1:B:326:ARG:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:GLN:CD	1:A:559:LEU:HD22	2.32	0.54
1:B:419:LEU:HD23	1:B:419:LEU:H	1.73	0.54
1:A:65:ASP:HB2	3:A:1191:HOH:O	2.08	0.54
1:A:360:HIS:HD2	1:A:361:ASP:O	1.90	0.53
1:A:295:MET:CE	2:C:2:GLC:H62	2.38	0.53
1:A:275:GLU:HG2	1:A:285:ASN:HB2	1.89	0.53
1:A:450:THR:HG23	1:A:505:ARG:HA	1.91	0.53
1:B:149:ASN:OD1	1:B:152:ILE:HG12	2.09	0.53
1:B:458:GLY:O	1:B:461:ILE:HG13	2.09	0.53
1:A:364:PRO:HG2	1:A:365:TRP:CE3	2.44	0.53
1:A:385:ARG:HG2	1:A:385:ARG:HH11	1.74	0.53
1:B:143:GLU:HB2	3:B:1033:HOH:O	2.08	0.53
1:B:201:SER:HB3	1:B:206:LYS:HG2	1.91	0.53
1:B:552:GLY:HA3	1:B:588:TRP:OXT	2.09	0.53
1:A:6:ILE:HD13	1:A:88:LEU:HD22	1.91	0.52
1:A:385:ARG:NH2	1:B:111:THR:HG21	2.24	0.52
1:B:279:GLN:N	1:B:285:ASN:HD21	2.07	0.52
1:A:554:TRP:CZ2	1:A:565:ALA:HB2	2.44	0.52
1:B:83:ARG:HD2	3:B:1302:HOH:O	2.09	0.52
1:B:43:ASP:HB3	1:B:46:ASP:OD2	2.09	0.52
1:B:289:PHE:O	1:B:290:ALA:C	2.52	0.52
1:A:291:PHE:HB2	1:B:48:GLN:NE2	2.25	0.52
1:B:160:TRP:CE2	1:B:474:CYS:HB3	2.45	0.52
1:A:26:ARG:NH2	1:A:410:ASN:OD1	2.43	0.51
1:A:41:HIS:HB2	1:A:82:LEU:HD11	1.93	0.51
1:A:30:LYS:HZ1	1:B:2:ARG:HH22	1.58	0.51
1:B:385:ARG:HD2	3:B:1108:HOH:O	2.09	0.51
1:A:357:GLU:OE1	2:C:1:GLC:H1	2.10	0.51
1:B:28:ARG:HD2	1:B:68:PHE:CG	2.45	0.51
1:B:467:ASN:O	1:B:468:ASP:C	2.53	0.51
1:A:218:HIS:HD2	3:A:1471:HOH:O	1.93	0.51
1:A:536:ASN:O	1:A:578:TYR:HA	2.10	0.51
1:B:262:GLY:C	1:B:264:SER:H	2.19	0.51
1:B:389:LYS:CB	1:B:391:GLU:HG3	2.41	0.51
1:B:21:GLU:HG3	3:B:1503:HOH:O	2.09	0.51
1:B:196:THR:HB	1:B:197:PRO:HD2	1.93	0.51
1:B:532:LEU:HD21	1:B:546:ILE:HG13	1.93	0.51
1:A:40:LEU:HG	1:A:54:PHE:CD2	2.46	0.50
1:B:83:ARG:CZ	1:B:116:CYS:HB2	2.41	0.50
1:A:390:GLU:HG2	1:A:537:ARG:HD2	1.93	0.50
1:A:206:LYS:HE3	1:A:216:ASP:CG	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ARG:HG3	3:A:1316:HOH:O	2.11	0.50
1:A:45:TYR:CG	1:B:290:ALA:HA	2.47	0.50
1:B:65:ASP:HB2	3:B:1193:HOH:O	2.12	0.49
1:A:243:ALA:HB2	1:A:325:TRP:CE3	2.47	0.49
1:A:331:ASN:HD22	1:A:331:ASN:H	1.59	0.49
1:A:258:VAL:HG11	1:A:273:ILE:HD11	1.93	0.49
1:A:550:ALA:HB1	1:A:568:ALA:HA	1.95	0.49
1:A:223:GLU:CD	1:A:223:GLU:H	2.21	0.49
1:B:231:ARG:HH21	1:B:234:GLU:CD	2.21	0.49
1:B:327:LEU:HD13	1:B:338:TRP:CZ3	2.47	0.49
1:B:331:ASN:HD22	1:B:331:ASN:H	1.60	0.49
1:B:333:ILE:HD12	1:B:338:TRP:CZ2	2.47	0.49
1:A:88:LEU:HD12	1:A:88:LEU:N	2.28	0.49
1:B:555:LEU:N	1:B:555:LEU:HD12	2.27	0.49
1:B:42:GLY:O	1:B:82:LEU:HD12	2.13	0.49
1:A:291:PHE:C	1:B:48:GLN:HE22	2.21	0.48
1:B:206:LYS:HD2	1:B:219:PHE:CE2	2.48	0.48
1:B:567:GLU:H	1:B:571:LEU:HD11	1.78	0.48
1:A:30:LYS:NZ	1:B:2:ARG:NH2	2.57	0.48
1:A:550:ALA:HB2	1:A:569:GLU:OE2	2.13	0.48
1:A:283:ARG:HD2	3:B:1552:HOH:O	2.12	0.48
1:A:29:THR:O	1:A:68:PHE:HB3	2.13	0.48
1:B:10:PRO:O	1:B:11:ALA:HB2	2.13	0.48
1:B:200:ARG:HA	1:B:216:ASP:OD1	2.14	0.48
1:B:196:THR:HB	1:B:197:PRO:CD	2.43	0.48
1:A:246:ASN:N	1:A:333:ILE:HD11	2.29	0.47
1:B:233:HIS:C	1:B:235:LYS:H	2.21	0.47
1:A:304:GLU:HG2	3:A:1215:HOH:O	2.15	0.47
1:B:281:GLU:CA	1:B:282:PRO:C	2.85	0.47
1:A:328:ASP:OD1	2:C:1:GLC:H1	2.13	0.47
1:B:27:LEU:HB3	1:B:71:TRP:HB2	1.96	0.47
1:B:47:TRP:CD1	1:B:47:TRP:C	2.93	0.47
1:B:75:VAL:O	1:B:77:PRO:HD3	2.14	0.47
1:A:194:TYR:CD1	1:A:194:TYR:C	2.93	0.47
1:A:252:PHE:CD2	1:A:254:PRO:HD2	2.50	0.47
1:A:302:ASN:OD1	1:A:304:GLU:HB2	2.14	0.47
1:A:377:TYR:N	1:A:378:PRO:CD	2.78	0.47
1:B:133:LYS:HD2	1:B:505:ARG:HH12	1.80	0.47
1:B:306:LYS:HD3	1:B:340:GLU:OE1	2.15	0.47
1:A:1:MET:HE2	1:A:93:GLU:HB3	1.96	0.47
1:A:270:TRP:CE2	1:A:304:GLU:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ALA:HB1	1:B:48:GLN:OE1	2.14	0.47
1:A:317:ILE:HD13	1:A:352:VAL:HG21	1.96	0.47
1:B:582:LEU:N	1:B:582:LEU:HD12	2.30	0.47
1:A:23:LEU:HD21	1:A:117:PHE:CE2	2.50	0.46
1:A:532:LEU:HB2	1:A:585:ILE:HD11	1.96	0.46
1:B:315:TYR:CE1	1:B:319:GLU:HG3	2.50	0.46
1:A:59:MET:HG2	1:A:73:ALA:HB2	1.98	0.46
1:B:261:ASN:HD22	1:B:265:SER:HB3	1.81	0.46
1:A:502:SER:HB3	1:A:529:GLU:HG3	1.98	0.46
1:B:436:ILE:CD1	1:B:486:LEU:HD22	2.39	0.46
1:B:511:LEU:HD21	3:B:1624:HOH:O	2.14	0.46
1:A:143:GLU:HB2	3:A:1057:HOH:O	2.15	0.46
1:B:28:ARG:HD2	1:B:68:PHE:CD2	2.51	0.45
1:A:75:VAL:O	1:A:77:PRO:HD3	2.16	0.45
1:A:145:PHE:HB3	3:A:1384:HOH:O	2.17	0.45
1:B:400:GLN:HA	1:B:400:GLN:NE2	2.31	0.45
1:B:546:ILE:C	1:B:546:ILE:CD1	2.88	0.45
1:A:154:PRO:HB3	1:A:218:HIS:CE1	2.52	0.45
1:A:385:ARG:HH21	1:B:111:THR:HG21	1.82	0.45
1:A:467:ASN:O	1:A:468:ASP:C	2.58	0.45
1:A:51:ALA:HA	3:A:1594:HOH:O	2.16	0.45
1:B:400:GLN:HA	1:B:400:GLN:HE21	1.82	0.45
1:A:427:ARG:O	1:A:431:VAL:HG23	2.17	0.45
1:B:400:GLN:NE2	3:B:1120:HOH:O	2.50	0.45
1:A:519:TYR:N	1:A:519:TYR:CD2	2.85	0.45
1:B:328:ASP:OD1	2:D:1:GLC:H1	2.17	0.45
1:B:492:GLN:O	1:B:495:ALA:HB3	2.17	0.45
1:A:289:PHE:O	1:A:290:ALA:C	2.58	0.45
1:B:3:LYS:HE2	1:B:95:LEU:HD13	1.99	0.45
1:B:515:ASP:C	1:B:517:MET:N	2.74	0.45
1:A:160:TRP:CE2	1:A:474:CYS:HB3	2.53	0.44
1:B:279:GLN:O	1:B:284:PRO:HA	2.17	0.44
1:A:146:ALA:O	1:A:177:GLY:HA3	2.17	0.44
1:B:23:LEU:O	1:B:74:GLU:HA	2.17	0.44
1:B:462:GLY:HA2	3:B:1086:HOH:O	2.17	0.44
1:B:468:ASP:OD2	1:B:469:PRO:HA	2.17	0.44
1:B:499:GLN:NE2	1:B:500:TYR:CE1	2.85	0.44
1:A:486:LEU:O	1:A:490:VAL:HG23	2.17	0.44
1:B:515:ASP:O	1:B:517:MET:N	2.51	0.44
1:A:9:ARG:HA	1:A:10:PRO:HD2	1.72	0.44
1:B:231:ARG:NH2	1:B:234:GLU:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ALA:HB2	1:A:521:ILE:CD1	2.43	0.44
1:B:41:HIS:HB2	1:B:82:LEU:HD11	1.99	0.44
1:B:306:LYS:HD3	1:B:340:GLU:CD	2.43	0.43
1:B:159:PRO:HB2	1:B:162:SER:HB3	1.99	0.43
1:B:206:LYS:HE2	1:B:216:ASP:CG	2.43	0.43
1:A:582:LEU:N	1:A:582:LEU:HD12	2.33	0.43
1:B:140:ILE:HB	1:B:195:LEU:HD23	1.98	0.43
1:A:507:GLU:O	1:A:524:LYS:HA	2.18	0.43
1:A:515:ASP:C	1:A:517:MET:H	2.25	0.43
1:B:19:ASP:OD2	1:B:19:ASP:C	2.61	0.43
1:B:131:TRP:CZ3	1:B:238:ARG:HG3	2.53	0.43
1:B:566:ALA:HB1	1:B:571:LEU:HD21	2.00	0.43
1:A:336:GLU:HG3	3:A:1450:HOH:O	2.17	0.43
1:A:545:PRO:O	1:A:547:PRO:HD3	2.19	0.43
1:B:229:ILE:HD12	1:B:320:PHE:HB3	2.01	0.43
1:A:401:MET:HE2	1:A:401:MET:HA	2.00	0.43
1:B:293:PRO:HB2	1:B:294:GLN:NE2	2.33	0.43
1:B:328:ASP:OD1	2:D:1:GLC:C1	2.66	0.43
1:B:383:VAL:HG12	1:B:442:LEU:CD2	2.49	0.43
1:B:263:GLU:HB2	1:B:276:PHE:CG	2.53	0.43
1:B:194:TYR:CD1	1:B:194:TYR:C	2.96	0.42
1:B:327:LEU:HB2	1:B:356:GLY:HA2	2.01	0.42
1:B:515:ASP:HB3	1:B:519:TYR:CD1	2.54	0.42
1:A:25:LEU:HD12	1:A:39:LEU:HD21	2.02	0.42
1:A:385:ARG:HG2	1:A:385:ARG:NH1	2.33	0.42
1:B:317:ILE:HA	1:B:322:ILE:HG12	2.01	0.42
1:B:568:ALA:C	1:B:570:THR:N	2.76	0.42
1:A:468:ASP:OD1	2:C:2:GLC:O3	2.29	0.42
1:A:295:MET:HE1	2:C:2:GLC:O5	2.20	0.42
1:A:196:THR:HB	1:A:197:PRO:HD2	2.02	0.42
1:A:295:MET:HE1	2:C:2:GLC:C6	2.49	0.42
1:B:12:ASP:O	1:B:409:PRO:HG3	2.19	0.42
1:B:343:GLN:HA	3:B:1622:HOH:O	2.20	0.42
1:B:482:GLN:O	1:B:483:ASN:CB	2.66	0.42
1:A:18:TYR:HB2	1:A:24:HIS:CD2	2.54	0.41
1:B:275:GLU:HG2	1:B:285:ASN:HB2	2.02	0.41
1:B:546:ILE:O	1:B:546:ILE:CG2	2.66	0.41
1:A:10:PRO:HD3	1:A:115:PHE:CD1	2.56	0.41
1:A:365:TRP:HB3	1:A:371:PHE:CD2	2.55	0.41
1:A:534:ILE:HD13	1:A:573:THR:HG21	2.02	0.41
1:B:133:LYS:HD2	1:B:505:ARG:NH1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLN:H	1:B:294:GLN:CD	2.28	0.41
1:A:44:PRO:HB3	1:A:83:ARG:CG	2.50	0.41
1:A:331:ASN:ND2	1:A:331:ASN:H	2.16	0.41
1:B:6:ILE:HA	1:B:28:ARG:O	2.20	0.41
1:B:377:TYR:N	1:B:378:PRO:CD	2.83	0.41
1:B:419:LEU:H	1:B:419:LEU:CD2	2.33	0.41
1:A:216:ASP:OD2	1:A:218:HIS:HB2	2.21	0.41
1:A:279:GLN:HG2	1:A:285:ASN:HD21	1.83	0.41
1:A:7:TYR:O	1:A:27:LEU:HD12	2.20	0.41
1:A:28:ARG:HB3	1:A:70:TYR:CD1	2.56	0.41
1:A:30:LYS:HZ2	1:B:2:ARG:NH2	2.11	0.41
1:A:544:ILE:O	1:A:573:THR:HG22	2.21	0.41
1:B:129:PRO:O	1:B:132:VAL:HG22	2.21	0.41
1:A:44:PRO:HG2	1:A:45:TYR:CD1	2.56	0.41
1:A:315:TYR:CD1	1:A:319:GLU:HG3	2.56	0.41
1:B:83:ARG:CG	1:B:83:ARG:HH11	2.34	0.41
1:B:151:SER:HB3	3:B:1618:HOH:O	2.19	0.41
1:B:363:MET:HE2	1:B:407:SER:O	2.20	0.41
1:B:511:LEU:N	1:B:511:LEU:CD1	2.83	0.41
1:B:567:GLU:HG2	1:B:568:ALA:N	2.36	0.41
1:A:328:ASP:OD1	2:C:1:GLC:C1	2.69	0.41
1:A:376:ASN:O	1:A:379:PHE:HB3	2.22	0.40
1:A:428:ILE:HD12	1:A:439:VAL:HG13	2.03	0.40
1:A:581:VAL:HG23	3:A:1164:HOH:O	2.21	0.40
1:A:20:SER:CB	1:A:122:ARG:NH1	2.84	0.40
1:A:40:LEU:HD11	1:A:106:VAL:HG11	2.03	0.40
1:A:43:ASP:HB3	1:A:46:ASP:HB2	2.04	0.40
1:A:263:GLU:HB2	1:A:276:PHE:CD2	2.56	0.40
1:B:57:MET:HE1	1:B:75:VAL:HG22	2.04	0.40
1:B:363:MET:CE	1:B:407:SER:O	2.69	0.40
1:A:196:THR:HB	1:A:197:PRO:CD	2.52	0.40
1:B:444:LEU:HA	1:B:493:LEU:HD13	2.03	0.40
1:A:223:GLU:CD	1:A:223:GLU:N	2.80	0.40
1:B:233:HIS:C	1:B:235:LYS:N	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	586/588 (100%)	557 (95%)	26 (4%)	3 (0%)	24	37
1	B	586/588 (100%)	535 (91%)	45 (8%)	6 (1%)	12	20
All	All	1172/1176 (100%)	1092 (93%)	71 (6%)	9 (1%)	16	25

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	PRO
1	A	567	GLU
1	B	10	PRO
1	B	571	LEU
1	A	550	ALA
1	B	516	GLU
1	B	564	PHE
1	B	263	GLU
1	B	282	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	521/521 (100%)	514 (99%)	7 (1%)	61	80
1	B	521/521 (100%)	507 (97%)	14 (3%)	39	62
All	All	1042/1042 (100%)	1021 (98%)	21 (2%)	48	70

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	120	LEU
1	A	226	LYS
1	A	268	LYS
1	A	304	GLU
1	A	331	ASN
1	A	572	CYS
1	B	4	GLU
1	B	21	GLU
1	B	28	ARG
1	B	40	LEU
1	B	83	ARG
1	B	106	VAL
1	B	259	TRP
1	B	281	GLU
1	B	331	ASN
1	B	419	LEU
1	B	529	GLU
1	B	546	ILE
1	B	567	GLU
1	B	571	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	49	ASN
1	A	121	HIS
1	A	139	GLN
1	A	218	HIS
1	A	233	HIS
1	A	279	GLN
1	A	294	GLN
1	A	331	ASN
1	A	360	HIS
1	A	446	GLN
1	A	492	GLN
1	B	49	ASN
1	B	121	HIS
1	B	176	GLN
1	B	261	ASN

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Mol	Chain	Res	Type
1	B	294	GLN
1	B	331	ASN
1	B	343	GLN
1	B	400	GLN
1	B	446	GLN
1	B	492	GLN
1	B	499	GLN
1	B	512	HIS
1	B	587	HIS

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 ⓘ

6 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	GLC	C	1	2	12,12,12	0.43	0	17,17,17	0.51	0
2	GLC	C	2	2	11,11,12	0.51	0	15,15,17	0.81	1 (6%)
2	GLC	C	3	2	11,11,12	0.57	0	15,15,17	0.77	1 (6%)
2	GLC	D	1	2	12,12,12	0.46	0	17,17,17	0.47	0
2	GLC	D	2	2	11,11,12	0.59	0	15,15,17	0.74	1 (6%)
2	GLC	D	3	2	11,11,12	0.55	0	15,15,17	0.57	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	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	2/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	2/2/19/22	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	C	3	GLC	C1-O5-C5	2.50	115.54	112.19
2	C	2	GLC	C1-O5-C5	2.35	115.33	112.19
2	D	2	GLC	C1-O5-C5	2.10	115.00	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

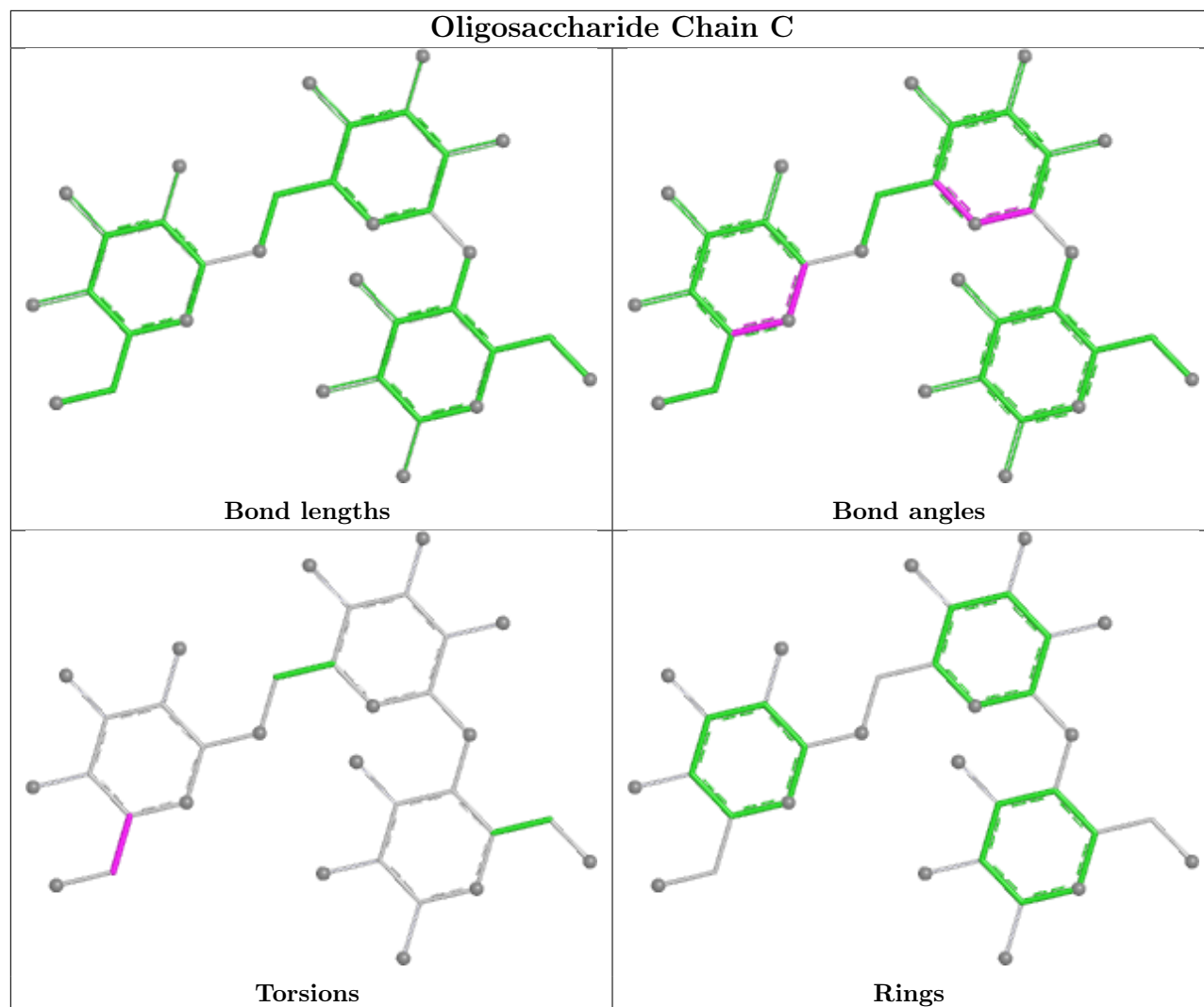
Mol	Chain	Res	Type	Atoms
2	D	3	GLC	O5-C5-C6-O6
2	D	3	GLC	C4-C5-C6-O6
2	C	3	GLC	C4-C5-C6-O6
2	C	3	GLC	O5-C5-C6-O6

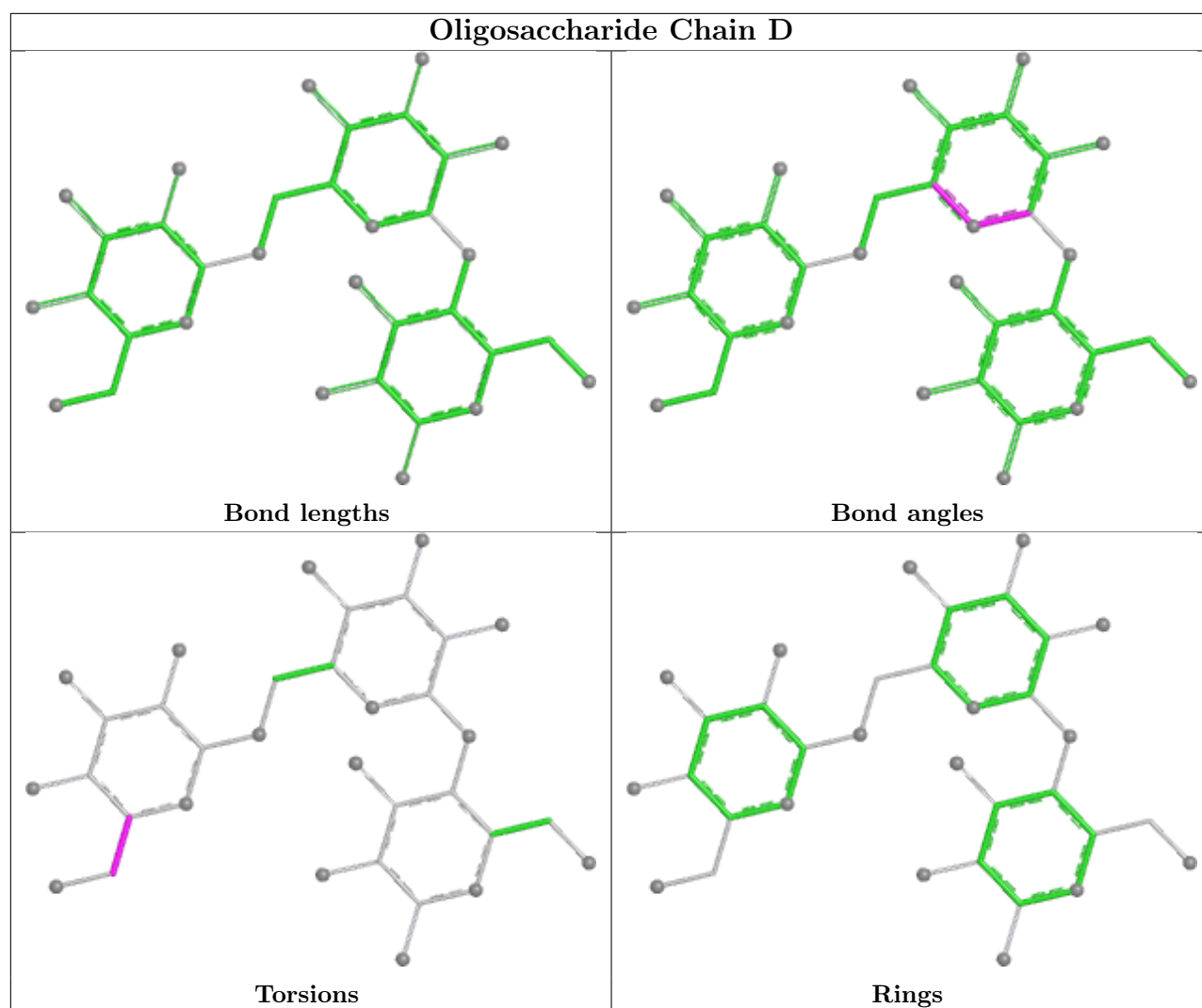
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	3	0
2	D	1	GLC	2	0
2	C	2	GLC	5	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](#)

There are no ligands in this entry.

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	588/588 (100%)	-0.74	0 100 100	18, 31, 55, 86	0
1	B	588/588 (100%)	-0.57	1 (0%) 91 89	18, 35, 69, 96	0
All	All	1176/1176 (100%)	-0.66	1 (0%) 92 90	18, 33, 64, 96	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	571	LEU	2.8

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](#)

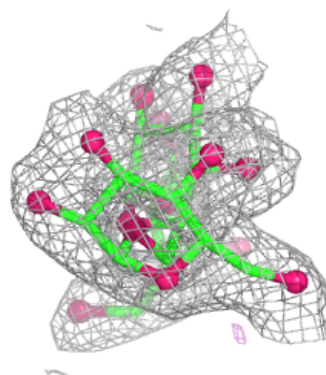
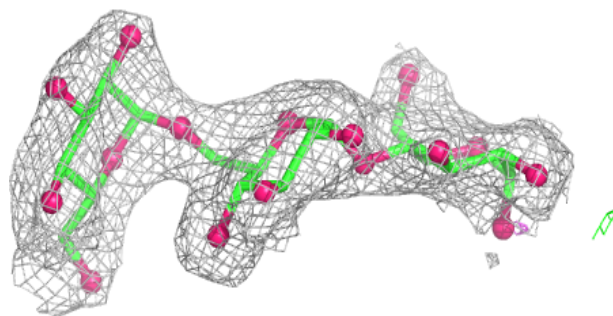
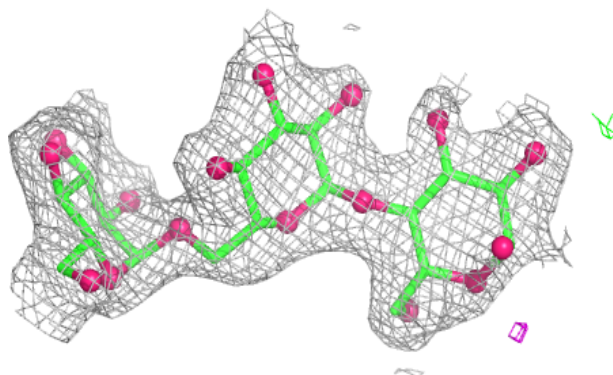
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	GLC	D	1	12/12	0.78	0.11	42,45,49,49	0
2	GLC	D	3	11/12	0.82	0.09	52,54,55,55	0
2	GLC	C	3	11/12	0.83	0.08	45,48,49,50	0
2	GLC	C	1	12/12	0.90	0.08	38,40,43,46	0
2	GLC	D	2	11/12	0.93	0.06	40,44,48,48	0
2	GLC	C	2	11/12	0.93	0.07	36,38,41,45	0

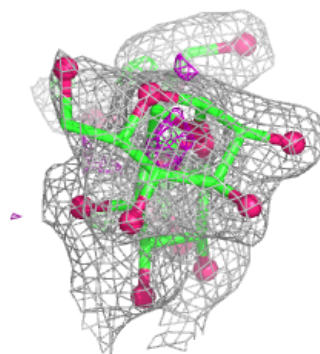
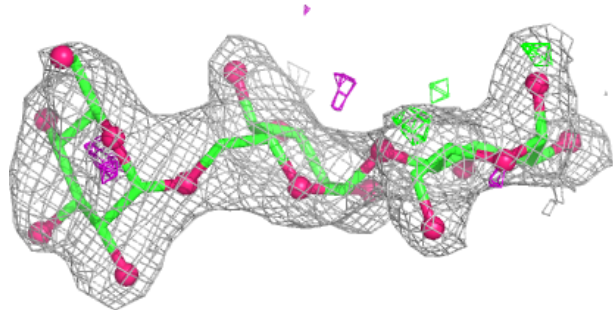
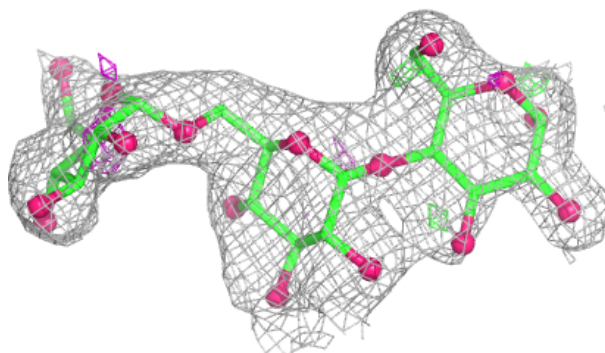
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

**Electron density around Chain D:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.