



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:26 AM UTC

PDB ID : 2D7R / pdb_00002d7r
Title : Crystal structure of pp-GalNAc-T10 complexed with GalNAc-Ser on lectin domain
Authors : Kubota, T.; Shiba, T.; Sugioka, S.; Kato, R.; Wakatsuki, S.; Narimatsu, H.
Deposited on : 2005-11-25
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

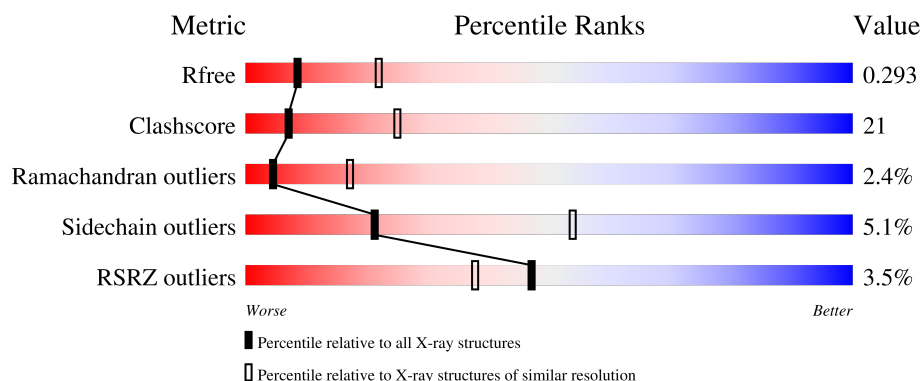
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	570	 3% 56% 33% 6%
2	B	2	 100%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4549 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 Polypeptide N-acetylgalactosaminyltransferase 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4357	2762	778	789	28	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

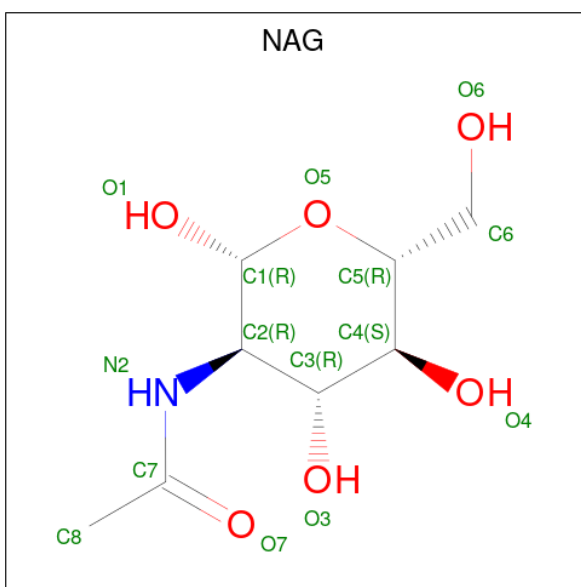
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	HIS	-	expression tag	UNP Q86SR1
A	35	HIS	-	expression tag	UNP Q86SR1
A	36	HIS	-	expression tag	UNP Q86SR1
A	37	HIS	-	expression tag	UNP Q86SR1
A	38	HIS	-	expression tag	UNP Q86SR1
A	39	HIS	-	expression tag	UNP Q86SR1

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



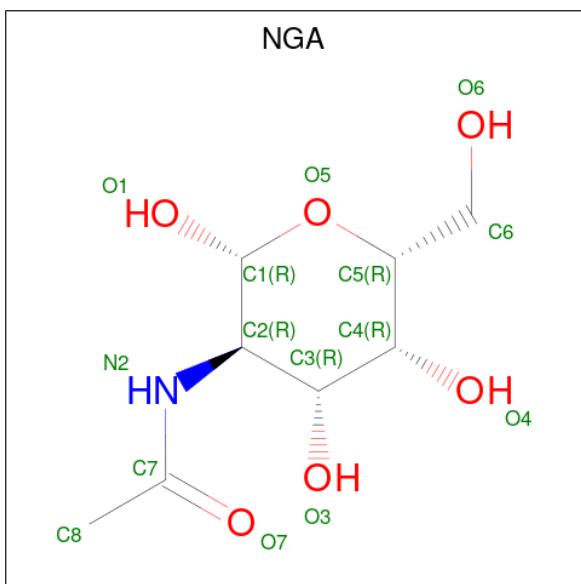
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-galactopyranose (CCD ID: NGA) (formula: $C_8H_{15}NO_6$).

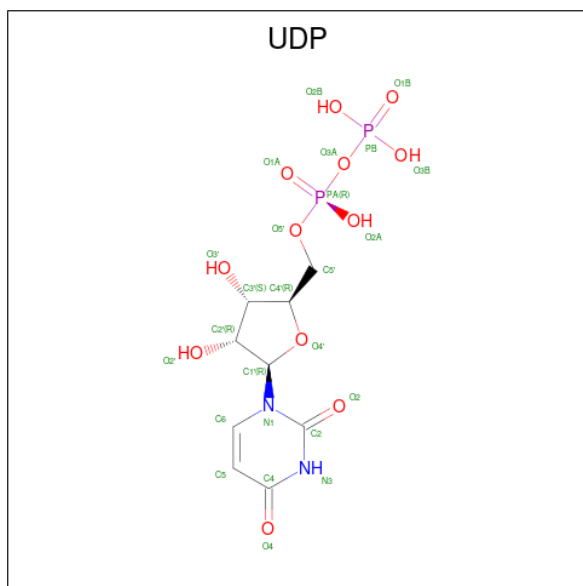


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

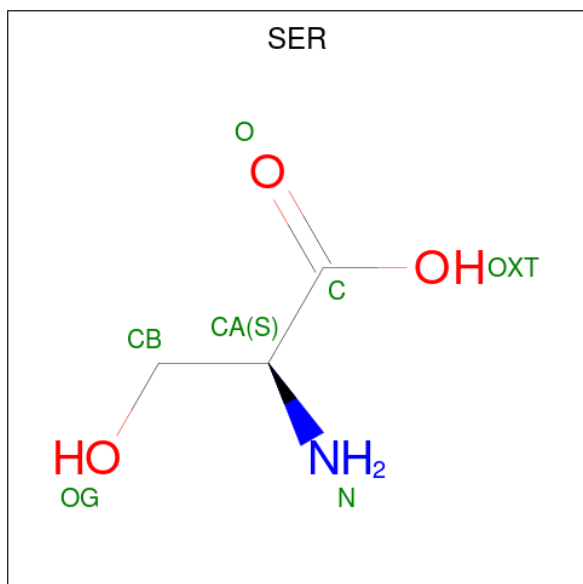
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



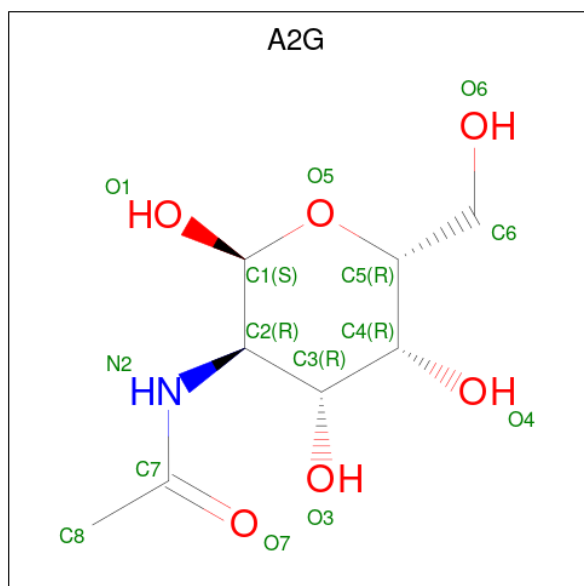
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	25	9	2	12	2	0	0

- Molecule 7 is SERINE (CCD ID: SER) (formula: C₃H₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 8 is 2-acetamido-2-deoxy- α -D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



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

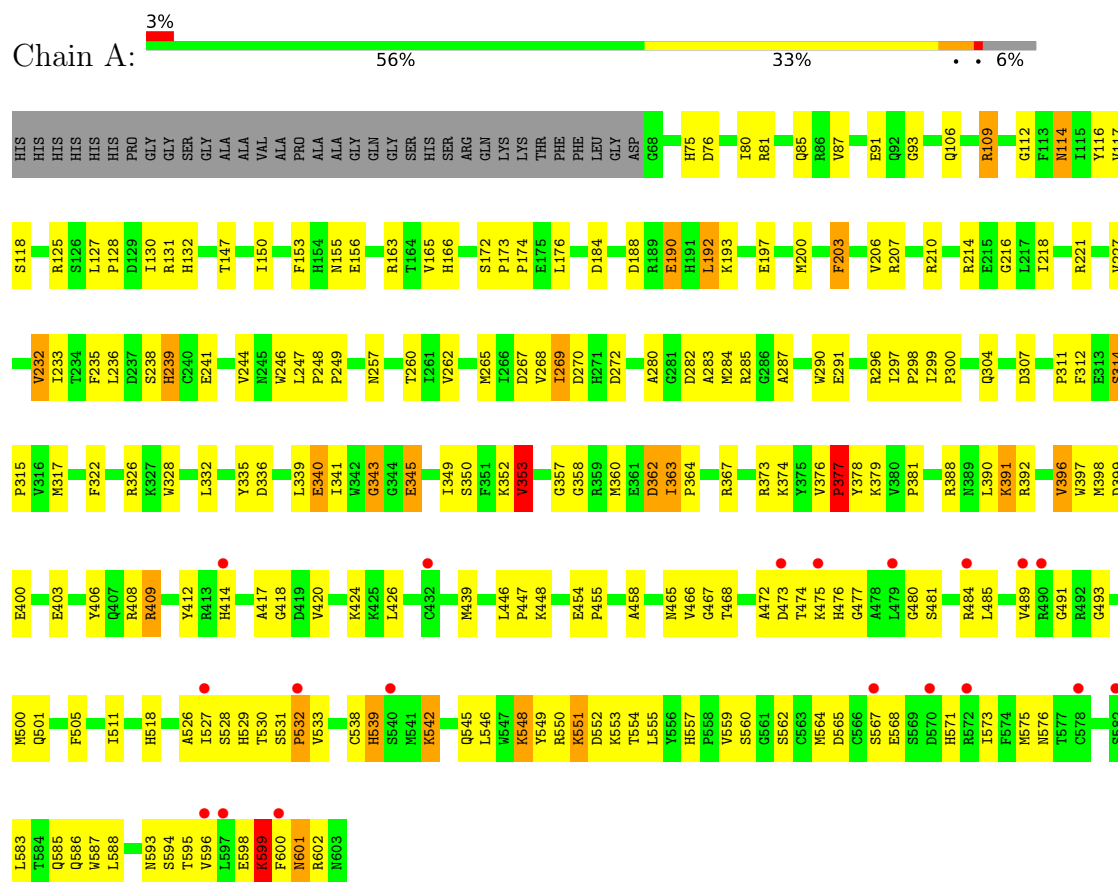
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	74	Total	O	0	0
			74	74		

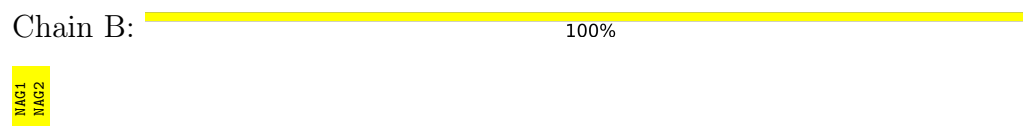
3 Residue-property plots

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: Polypeptide N-acetylgalactosaminyltransferase 10



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	80.19Å 132.81Å 138.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 40.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.80) 98.8 (40.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.298 0.229 , 0.293	Depositor DCC
R_{free} test set	1840 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.028 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4549	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: MN, NGA, NAG, A2G, UDP

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	0.50	0/4481	0.96	22/6073 (0.4%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	ASP	CB-CA-C	-8.17	107.14	116.54
1	A	132	HIS	N-CA-C	-7.55	100.57	110.39
1	A	601	ASN	N-CA-C	-6.92	105.78	114.56
1	A	374	LYS	N-CA-C	-6.59	103.93	112.23
1	A	409	ARG	CA-C-N	6.46	126.68	119.32
1	A	409	ARG	C-N-CA	6.46	126.68	119.32
1	A	203	PHE	CA-C-N	6.45	127.91	119.84
1	A	203	PHE	C-N-CA	6.45	127.91	119.84
1	A	357	GLY	N-CA-C	6.10	121.94	114.69
1	A	112	GLY	N-CA-C	-6.06	107.33	115.21
1	A	396	VAL	N-CA-C	5.94	118.51	111.09
1	A	216	GLY	N-CA-C	-5.90	106.02	112.04
1	A	340	GLU	N-CA-C	5.74	123.02	110.80
1	A	398	MET	N-CA-C	5.67	120.04	113.18
1	A	291	GLU	N-CA-C	-5.56	106.08	112.92
1	A	353	VAL	CB-CA-C	-5.40	104.97	111.88
1	A	244	VAL	N-CA-C	5.31	116.10	108.93
1	A	314	SER	CA-C-N	5.25	124.43	118.97
1	A	314	SER	C-N-CA	5.25	124.43	118.97
1	A	341	ILE	N-CA-C	5.15	116.61	111.00
1	A	190	GLU	N-CA-C	5.14	117.55	111.33
1	A	269	ILE	N-CA-C	-5.07	98.73	107.24

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	4357	0	4229	183	0
2	B	28	0	25	1	0
3	A	28	0	26	1	0
4	A	15	0	15	2	0
5	A	1	0	0	0	0
6	A	25	0	11	0	0
7	A	7	0	3	0	0
8	A	14	0	12	0	0
9	A	74	0	0	3	0
All	All	4549	0	4321	184	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 21.

All (184) 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:75:HIS:HE1	1:A:131:ARG:HH12	0.99	0.94
1:A:75:HIS:CE1	1:A:131:ARG:HH12	1.87	0.92
1:A:284:MET:HE3	1:A:296:ARG:NH1	1.86	0.90
1:A:155:ASN:HD21	1:A:188:ASP:H	1.16	0.89
1:A:287:ALA:HB1	1:A:446:LEU:HD12	1.59	0.84
1:A:548:LYS:HD2	1:A:601:ASN:HA	1.59	0.83
1:A:598:GLU:HG3	1:A:599:LYS:NZ	1.99	0.78
1:A:551:LYS:HZ3	1:A:551:LYS:HA	1.48	0.78
1:A:594:SER:O	1:A:598:GLU:HG2	1.85	0.77
1:A:75:HIS:HE1	1:A:131:ARG:NH1	1.81	0.75
1:A:218:ILE:HG13	1:A:345:GLU:CG	2.16	0.75
1:A:218:ILE:HG13	1:A:345:GLU:HG2	1.70	0.74
1:A:363:ILE:HD12	1:A:363:ILE:N	2.04	0.72
1:A:467:GLY:HA2	1:A:583:LEU:HD12	1.71	0.72
1:A:335:TYR:CE2	1:A:345:GLU:HB2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LYS:HD2	1:A:417:ALA:HB2	1.73	0.69
1:A:565:ASP:HB2	1:A:585:GLN:HE21	1.56	0.69
1:A:81:ARG:O	1:A:85:GLN:HG3	1.92	0.69
1:A:551:LYS:HA	1:A:551:LYS:NZ	2.08	0.69
1:A:598:GLU:HG3	1:A:599:LYS:HZ3	1.58	0.69
1:A:533:VAL:HG22	1:A:575:MET:HE3	1.74	0.68
1:A:155:ASN:HD21	1:A:188:ASP:N	1.90	0.68
1:A:184:ASP:HB3	1:A:210:ARG:HG2	1.76	0.66
1:A:221:ARG:HD2	1:A:235:PHE:CD2	2.31	0.66
1:A:114:ASN:C	1:A:114:ASN:HD22	2.03	0.66
1:A:150:ILE:HD12	1:A:233:ILE:HG23	1.78	0.66
1:A:114:ASN:HD21	1:A:116:TYR:HB2	1.61	0.66
1:A:265:MET:HE1	1:A:362:ASP:HB3	1.78	0.66
1:A:538:CYS:HA	1:A:545:GLN:HE22	1.61	0.66
1:A:297:ILE:HB	1:A:298:PRO:HD2	1.79	0.65
1:A:529:HIS:HB2	1:A:562:SER:HB3	1.79	0.64
1:A:448:LYS:HD3	9:A:840:HOH:O	1.97	0.63
1:A:184:ASP:OD1	1:A:210:ARG:NH1	2.32	0.63
1:A:362:ASP:O	1:A:364:PRO:HD3	1.98	0.63
1:A:599:LYS:HZ2	1:A:599:LYS:CB	2.13	0.62
1:A:489:VAL:HG12	1:A:491:GLY:H	1.64	0.62
1:A:485:LEU:HD13	1:A:573:ILE:HD11	1.82	0.61
1:A:218:ILE:HD12	1:A:218:ILE:H	1.65	0.61
1:A:328:TRP:CH2	1:A:332:LEU:HD21	2.36	0.61
1:A:562:SER:HB2	1:A:576:ASN:O	2.02	0.60
1:A:599:LYS:HZ2	1:A:599:LYS:HB2	1.66	0.60
1:A:285:ARG:HD3	1:A:299:ILE:HA	1.86	0.58
1:A:595:THR:HA	1:A:598:GLU:OE2	2.05	0.57
1:A:262:VAL:HB	1:A:363:ILE:CD1	2.35	0.57
1:A:468:THR:HG22	1:A:568:GLU:OE2	2.05	0.57
1:A:518:HIS:CE1	9:A:834:HOH:O	2.59	0.56
1:A:564:MET:HE3	1:A:573:ILE:HG21	1.88	0.56
1:A:557:HIS:NE2	1:A:559:VAL:HG12	2.21	0.56
1:A:109:ARG:HH11	1:A:109:ARG:HB3	1.72	0.55
1:A:420:VAL:HG23	1:A:424:LYS:HE3	1.88	0.55
1:A:476:HIS:CE1	1:A:500:MET:HB2	2.42	0.55
1:A:377:PRO:HG2	1:A:378:TYR:H	1.72	0.55
1:A:218:ILE:HG13	1:A:345:GLU:HG3	1.87	0.54
1:A:262:VAL:HB	1:A:363:ILE:HD11	1.87	0.54
1:A:439:MET:HE1	1:A:446:LEU:HD22	1.89	0.54
1:A:466:VAL:HG23	1:A:586:GLN:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ARG:HH11	1:A:214:ARG:HG2	1.73	0.54
1:A:282:ASP:CG	1:A:283:ALA:H	2.15	0.54
1:A:284:MET:HE3	1:A:296:ARG:HH12	1.69	0.53
1:A:363:ILE:N	1:A:363:ILE:CD1	2.71	0.53
1:A:349:ILE:O	1:A:353:VAL:HG22	2.08	0.53
1:A:474:THR:C	1:A:476:HIS:H	2.17	0.53
1:A:118:SER:OG	1:A:163:ARG:NH1	2.41	0.53
1:A:583:LEU:N	1:A:583:LEU:HD23	2.24	0.53
1:A:218:ILE:HD12	1:A:218:ILE:N	2.24	0.52
1:A:473:ASP:OD1	1:A:501:GLN:HG2	2.09	0.52
1:A:489:VAL:HG13	1:A:493:GLY:H	1.74	0.52
1:A:147:THR:HB	1:A:232:VAL:HG22	1.92	0.51
1:A:420:VAL:O	1:A:424:LYS:HG3	2.10	0.51
1:A:468:THR:HG22	1:A:568:GLU:CD	2.34	0.51
3:A:705:NAG:H3	3:A:705:NAG:H82	1.92	0.51
1:A:114:ASN:ND2	1:A:117:VAL:H	2.08	0.51
1:A:76:ASP:O	1:A:80:ILE:HD13	2.11	0.51
1:A:127:LEU:HD11	1:A:241:GLU:HB3	1.91	0.51
1:A:150:ILE:HD12	1:A:233:ILE:CG2	2.41	0.51
1:A:595:THR:O	1:A:599:LYS:NZ	2.41	0.51
1:A:345:GLU:OE1	4:A:704:NGA:H62	2.11	0.51
1:A:109:ARG:HB3	1:A:109:ARG:NH1	2.26	0.51
1:A:350:SER:O	1:A:353:VAL:HG23	2.10	0.51
1:A:599:LYS:HZ2	1:A:599:LYS:N	2.08	0.51
1:A:550:ARG:HH11	1:A:551:LYS:HG2	1.76	0.51
1:A:350:SER:HA	1:A:360:MET:CE	2.41	0.50
1:A:553:LYS:O	1:A:586:GLN:HA	2.11	0.50
1:A:114:ASN:CG	1:A:117:VAL:HG23	2.36	0.50
1:A:531:SER:HB2	1:A:532:PRO:HD2	1.92	0.50
1:A:538:CYS:HA	1:A:545:GLN:NE2	2.27	0.50
1:A:599:LYS:NZ	1:A:599:LYS:N	2.59	0.50
1:A:599:LYS:HZ2	1:A:599:LYS:CA	2.24	0.50
1:A:270:ASP:OD2	1:A:272:ASP:HB2	2.12	0.50
1:A:350:SER:HA	1:A:360:MET:HE1	1.93	0.50
1:A:446:LEU:N	1:A:447:PRO:HD2	2.27	0.50
1:A:153:PHE:CE1	1:A:192:LEU:HG	2.47	0.49
1:A:542:LYS:HB3	1:A:546:LEU:HD22	1.93	0.49
1:A:593:ASN:ND2	1:A:596:VAL:HG23	2.27	0.49
1:A:599:LYS:NZ	1:A:599:LYS:CA	2.75	0.49
1:A:353:VAL:O	1:A:358:GLY:N	2.45	0.49
1:A:528:SER:C	1:A:530:THR:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:VAL:HG13	1:A:493:GLY:HA3	1.94	0.49
1:A:114:ASN:OD1	1:A:117:VAL:HG23	2.13	0.48
1:A:87:VAL:C	1:A:91:GLU:HG3	2.37	0.48
1:A:554:THR:HG22	1:A:555:LEU:H	1.79	0.48
1:A:362:ASP:C	1:A:363:ILE:HD12	2.37	0.48
1:A:336:ASP:HB3	1:A:339:LEU:HG	1.96	0.48
1:A:248:PRO:HD2	1:A:249:PRO:HD2	1.95	0.48
1:A:207:ARG:HH12	1:A:227:VAL:CG1	2.27	0.47
1:A:270:ASP:C	1:A:272:ASP:H	2.22	0.47
1:A:550:ARG:HH11	1:A:551:LYS:CG	2.27	0.47
1:A:466:VAL:HG21	1:A:586:GLN:NE2	2.29	0.47
1:A:526:ALA:O	1:A:557:HIS:HE1	1.96	0.47
1:A:147:THR:HG21	1:A:247:LEU:HD11	1.97	0.47
1:A:465:ASN:HD22	1:A:468:THR:H	1.63	0.47
1:A:221:ARG:HB3	1:A:235:PHE:CE2	2.50	0.47
1:A:392:ARG:O	1:A:396:VAL:HG23	2.14	0.47
1:A:567:SER:OG	1:A:571:HIS:HB2	2.15	0.47
1:A:280:ALA:O	1:A:284:MET:HE2	2.15	0.46
1:A:554:THR:HG22	1:A:555:LEU:N	2.31	0.46
1:A:388:ARG:NH1	1:A:418:GLY:HA3	2.30	0.46
1:A:530:THR:HA	1:A:575:MET:O	2.15	0.46
1:A:114:ASN:C	1:A:114:ASN:ND2	2.73	0.46
1:A:550:ARG:HB3	1:A:552:ASP:OD2	2.15	0.46
1:A:203:PHE:CZ	2:B:2:NAG:H82	2.50	0.46
1:A:233:ILE:HD11	1:A:326:ARG:HG3	1.97	0.46
1:A:156:GLU:HG2	1:A:238:SER:OG	2.16	0.46
1:A:248:PRO:N	1:A:249:PRO:HD2	2.31	0.46
1:A:282:ASP:CG	1:A:283:ALA:N	2.74	0.46
1:A:332:LEU:O	1:A:426:LEU:HD21	2.15	0.46
1:A:518:HIS:HE1	9:A:834:HOH:O	1.98	0.46
1:A:218:ILE:CG1	1:A:345:GLU:HG3	2.46	0.45
1:A:420:VAL:CG2	1:A:424:LYS:HE3	2.46	0.45
1:A:221:ARG:NH2	1:A:345:GLU:OE2	2.49	0.45
1:A:257:ASN:HB2	1:A:260:THR:OG1	2.17	0.45
1:A:557:HIS:CD2	1:A:559:VAL:HG12	2.52	0.45
1:A:214:ARG:HG2	1:A:214:ARG:NH1	2.32	0.45
1:A:377:PRO:HG2	1:A:378:TYR:N	2.30	0.44
1:A:299:ILE:HD11	1:A:312:PHE:CE1	2.52	0.44
1:A:352:LYS:HG2	1:A:397:TRP:CH2	2.53	0.44
1:A:548:LYS:HE2	1:A:549:TYR:N	2.32	0.44
1:A:268:VAL:HG12	1:A:269:ILE:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:PHE:HE2	1:A:364:PRO:HG3	1.82	0.44
1:A:314:SER:HA	1:A:315:PRO:HD3	1.85	0.44
1:A:193:LYS:O	1:A:197:GLU:HG3	2.17	0.44
1:A:93:GLY:HA3	1:A:128:PRO:HD3	2.00	0.43
1:A:599:LYS:HB3	1:A:600:PHE:H	1.62	0.43
1:A:290:TRP:HB2	1:A:408:ARG:NE	2.34	0.43
1:A:249:PRO:HB2	1:A:363:ILE:HG21	2.00	0.43
1:A:317:MET:HE2	1:A:360:MET:SD	2.59	0.43
1:A:467:GLY:HA2	1:A:583:LEU:HB2	2.00	0.43
1:A:284:MET:CE	1:A:296:ARG:HH12	2.32	0.43
1:A:409:ARG:HD3	1:A:412:TYR:CE1	2.54	0.43
1:A:173:PRO:HB2	1:A:176:LEU:HD12	2.01	0.43
1:A:564:MET:HG3	1:A:575:MET:HE1	2.00	0.42
1:A:472:ALA:HA	1:A:485:LEU:HD12	2.01	0.42
1:A:248:PRO:CD	1:A:249:PRO:HD2	2.49	0.42
1:A:300:PRO:O	1:A:304:GLN:HG3	2.20	0.42
1:A:477:GLY:HA3	1:A:481:SER:OG	2.20	0.42
1:A:505:PHE:CD2	1:A:511:ILE:HG12	2.55	0.42
1:A:549:TYR:OH	1:A:588:LEU:HA	2.19	0.42
1:A:106:GLN:HA	1:A:109:ARG:HG2	2.02	0.42
1:A:239:HIS:HE1	1:A:373:ARG:NH2	2.17	0.42
1:A:403:GLU:HA	1:A:406:TYR:CD2	2.54	0.42
1:A:173:PRO:HA	1:A:174:PRO:HD2	1.84	0.42
1:A:454:GLU:HA	1:A:455:PRO:HD3	1.94	0.42
1:A:529:HIS:HB3	1:A:560:SER:O	2.20	0.42
1:A:505:PHE:HD2	1:A:511:ILE:HG12	1.85	0.42
1:A:172:SER:HA	1:A:173:PRO:HD3	1.94	0.42
1:A:465:ASN:HB2	1:A:587:TRP:CZ3	2.55	0.42
1:A:267:ASP:OD1	1:A:367:ARG:HB3	2.20	0.41
1:A:489:VAL:HG12	1:A:491:GLY:N	2.34	0.41
1:A:539:HIS:O	1:A:539:HIS:ND1	2.53	0.41
1:A:489:VAL:HG13	1:A:493:GLY:CA	2.50	0.41
1:A:265:MET:HB2	1:A:367:ARG:HG2	2.02	0.41
1:A:343:GLY:HA2	4:A:704:NGA:H61	2.02	0.41
1:A:284:MET:CE	1:A:296:ARG:NH1	2.70	0.41
1:A:489:VAL:HG13	1:A:493:GLY:N	2.35	0.41
1:A:564:MET:CE	1:A:573:ILE:HG21	2.50	0.41
1:A:322:PHE:CD1	1:A:322:PHE:C	2.97	0.41
1:A:246:TRP:O	1:A:249:PRO:HG2	2.20	0.41
1:A:307:ASP:OD2	1:A:307:ASP:C	2.63	0.41
1:A:153:PHE:HE1	1:A:192:LEU:HG	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ALA:HB3	1:A:505:PHE:HD1	1.86	0.41
1:A:218:ILE:H	1:A:218:ILE:CD1	2.32	0.40
1:A:474:THR:C	1:A:476:HIS:N	2.79	0.40
1:A:165:VAL:O	1:A:166:HIS:C	2.61	0.40
1:A:200:MET:SD	1:A:206:VAL:HG11	2.61	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	534/570 (94%)	460 (86%)	61 (11%)	13 (2%)	4 17

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	LYS
1	A	114	ASN
1	A	340	GLU
1	A	539	HIS
1	A	527	ILE
1	A	599	LYS
1	A	475	LYS
1	A	484	ARG
1	A	377	PRO
1	A	532	PRO
1	A	130	ILE
1	A	343	GLY
1	A	480	GLY

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	471/494 (95%)	447 (95%)	24 (5%)	21 54

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

Mol	Chain	Res	Type
1	A	109	ARG
1	A	125	ARG
1	A	190	GLU
1	A	192	LEU
1	A	232	VAL
1	A	236	LEU
1	A	239	HIS
1	A	311	PRO
1	A	345	GLU
1	A	353	VAL
1	A	362	ASP
1	A	363	ILE
1	A	376	VAL
1	A	377	PRO
1	A	379	LYS
1	A	381	PRO
1	A	390	LEU
1	A	391	LYS
1	A	400	GLU
1	A	414	HIS
1	A	548	LYS
1	A	551	LYS
1	A	599	LYS
1	A	602	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS

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Mol	Chain	Res	Type
1	A	92	GLN
1	A	114	ASN
1	A	134	ASN
1	A	155	ASN
1	A	170	ASN
1	A	191	HIS
1	A	304	GLN
1	A	423	GLN
1	A	465	ASN
1	A	476	HIS
1	A	499	ASN
1	A	517	GLN
1	A	518	HIS
1	A	545	GLN
1	A	557	HIS
1	A	579	ASN
1	A	585	GLN
1	A	586	GLN
1	A	591	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 ⓘ

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	2,1	14,14,15	0.81	1 (7%)	17,19,21	1.06	1 (5%)
2	NAG	B	2	2	14,14,15	0.71	0	17,19,21	0.69	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	2,1	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	2.42	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C2-N2-C7	-2.51	119.53	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

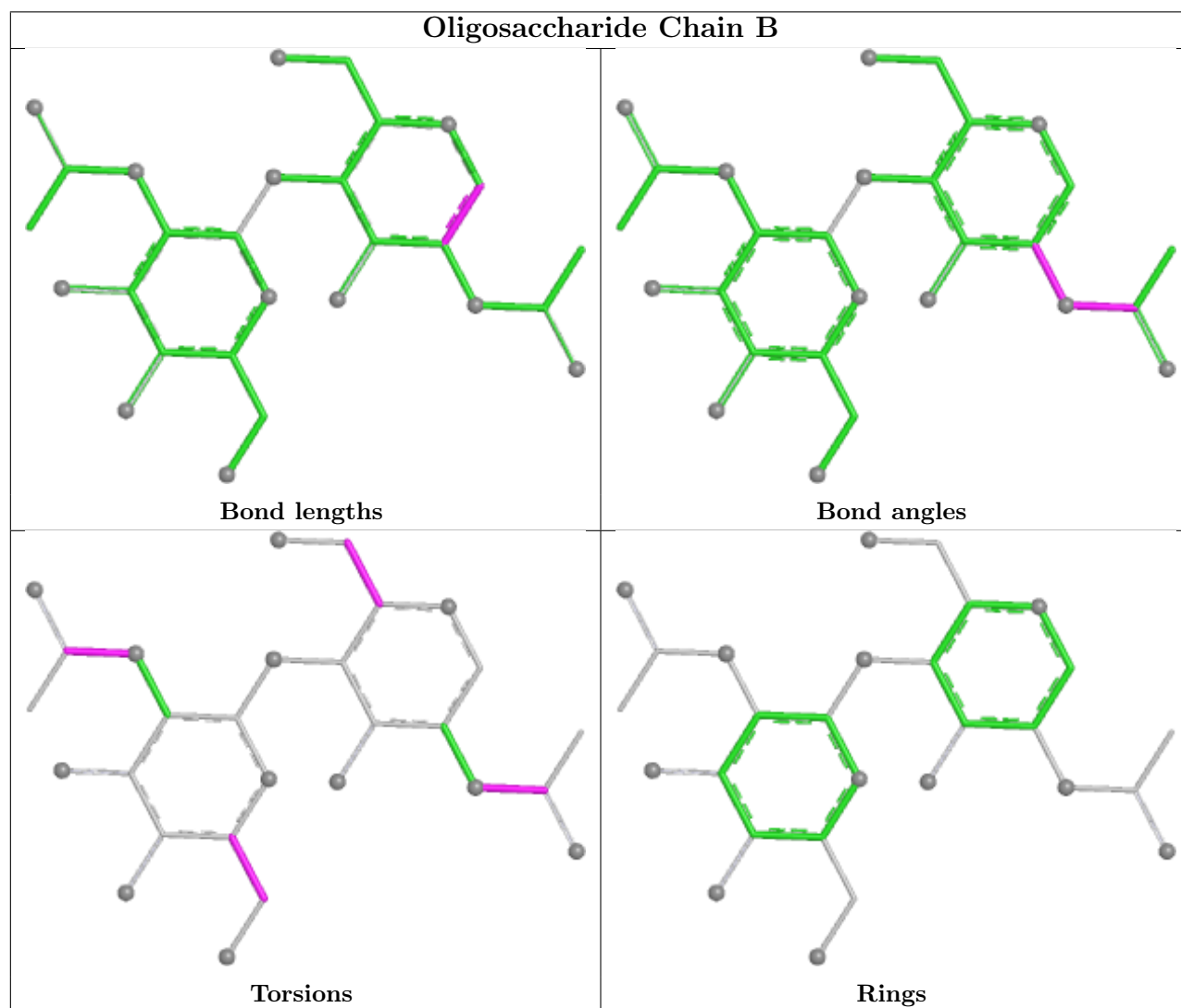
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
6	UDP	A	707	5	25,26,26	0.95	1 (4%)	38,40,40	1.53	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	A2G	A	709	7	14,14,15	1.07	1 (7%)	17,19,21	0.82	0
3	NAG	A	703	1	14,14,15	0.63	0	17,19,21	0.79	0
3	NAG	A	705	1	14,14,15	0.77	1 (7%)	17,19,21	0.65	0
4	NGA	A	704	-	15,15,15	0.59	0	21,21,21	0.75	0
7	SER	A	708	8	4,6,6	1.13	1 (25%)	2,7,7	1.72	1 (50%)

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
6	UDP	A	707	5	-	1/16/32/32	0/2/2/2
8	A2G	A	709	7	-	2/6/23/26	0/1/1/1
3	NAG	A	703	1	-	5/6/23/26	0/1/1/1
3	NAG	A	705	1	-	3/6/23/26	0/1/1/1
4	NGA	A	704	-	-	1/6/26/26	0/1/1/1
7	SER	A	708	8	-	2/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	709	A2G	C1-C2	2.84	1.56	1.52
6	A	707	UDP	C6-C5	2.32	1.40	1.35
3	A	705	NAG	C1-C2	2.19	1.55	1.52
7	A	708	SER	OXT-C	-2.13	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	707	UDP	C4-N3-C2	-4.84	120.61	126.61
6	A	707	UDP	C5-C4-N3	3.98	120.38	114.80
6	A	707	UDP	N3-C2-N1	3.69	119.70	114.89
6	A	707	UDP	O4-C4-C5	-2.43	120.97	125.16
7	A	708	SER	OXT-C-O	-2.36	118.72	124.08
6	A	707	UDP	O3B-PB-O3A	2.28	112.28	104.64
6	A	707	UDP	O2B-PB-O3A	2.12	111.75	104.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

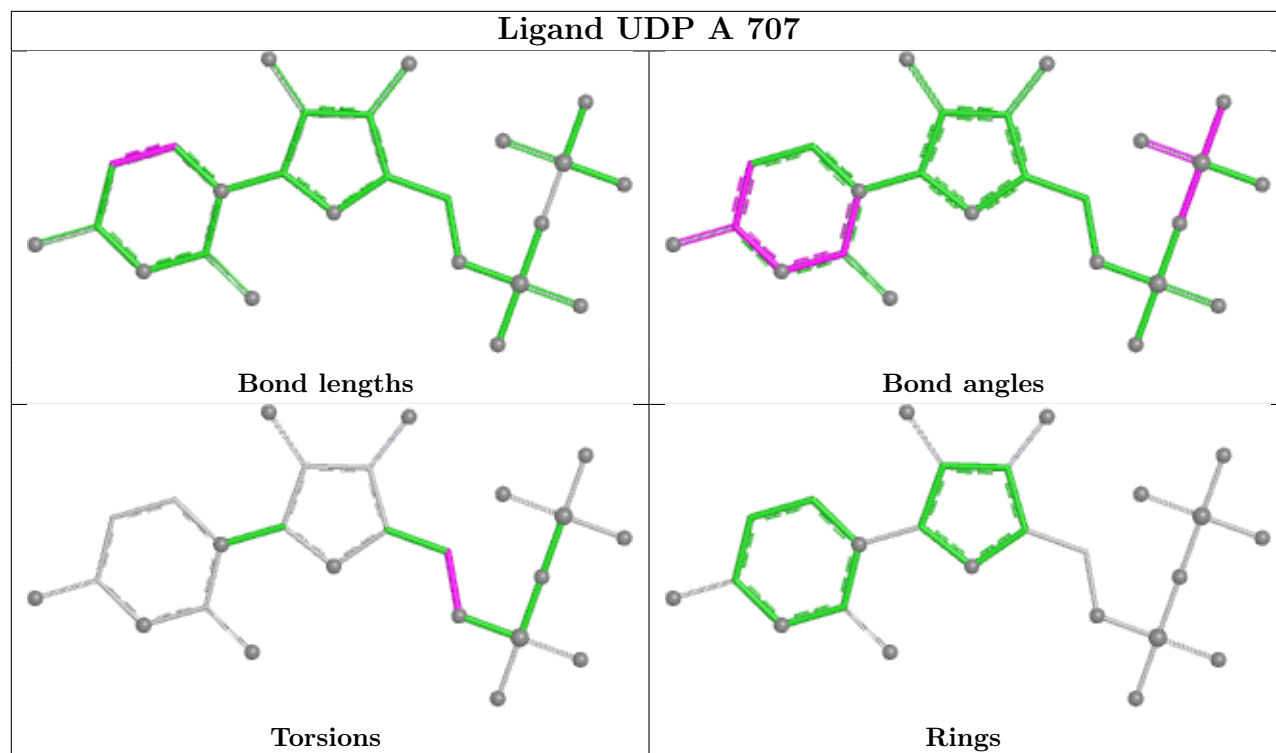
Mol	Chain	Res	Type	Atoms
3	A	703	NAG	C8-C7-N2-C2
3	A	703	NAG	O7-C7-N2-C2
3	A	705	NAG	C1-C2-N2-C7
3	A	705	NAG	C8-C7-N2-C2
3	A	705	NAG	O7-C7-N2-C2
3	A	703	NAG	C4-C5-C6-O6
8	A	709	A2G	O5-C5-C6-O6
3	A	703	NAG	O5-C5-C6-O6
4	A	704	NGA	O5-C5-C6-O6
3	A	703	NAG	C3-C2-N2-C7
6	A	707	UDP	C4'-C5'-O5'-PA
8	A	709	A2G	C4-C5-C6-O6
7	A	708	SER	OXT-C-CA-N
7	A	708	SER	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	NAG	1	0
4	A	704	NGA	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	536/570 (94%)	0.14	19 (3%) 47 38	22, 47, 98, 108	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	SER	4.1
1	A	600	PHE	3.3
1	A	414	HIS	3.0
1	A	582	SER	2.9
1	A	527	ILE	2.7
1	A	484	ARG	2.6
1	A	532	PRO	2.6
1	A	570	ASP	2.6
1	A	489	VAL	2.3
1	A	432	CYS	2.3
1	A	572	ARG	2.3
1	A	479	LEU	2.2
1	A	578	CYS	2.2
1	A	567	SER	2.2
1	A	475	LYS	2.1
1	A	490	ARG	2.1
1	A	597	LEU	2.0
1	A	596	VAL	2.0
1	A	473	ASP	2.0

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

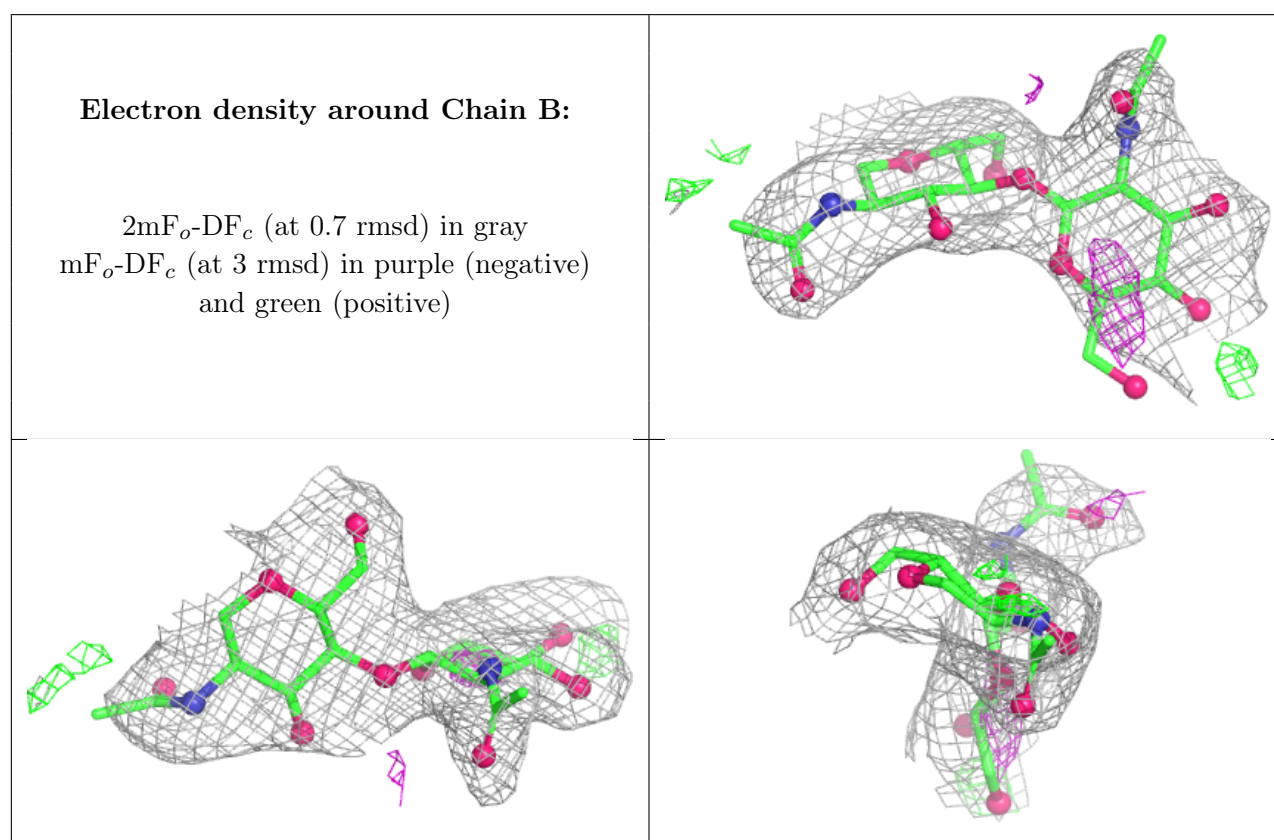
There are no non-standard protein/DNA/RNA residues in this entry.

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	NAG	B	2	14/15	0.80	0.14	65,69,72,74	0
2	NAG	B	1	14/15	0.87	0.11	53,56,61,66	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.

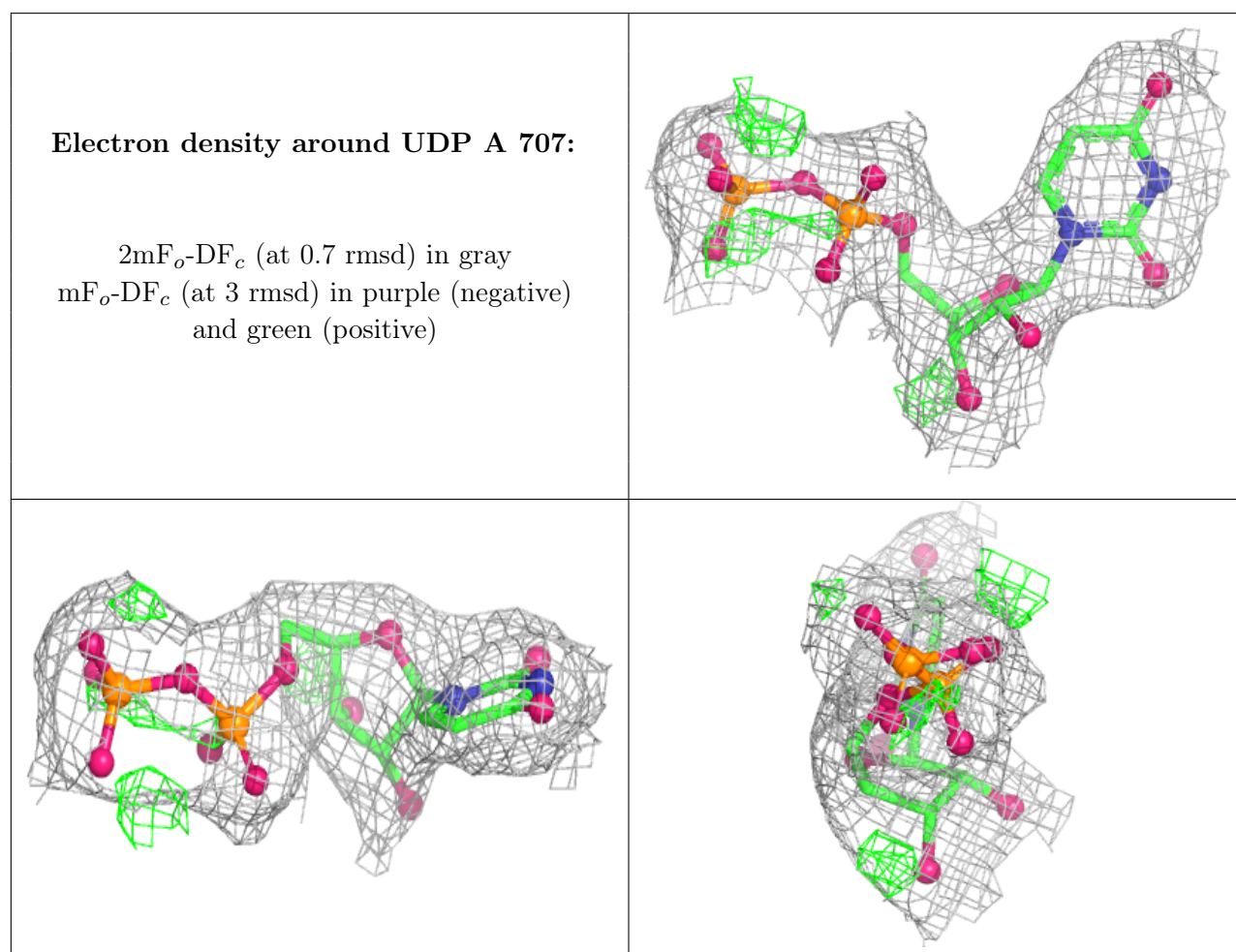
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SER	A	708	7/7	0.60	0.13	103,103,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	705	14/15	0.61	0.15	76,79,80,80	0
8	A2G	A	709	14/15	0.77	0.14	102,104,105,105	0
3	NAG	A	703	14/15	0.78	0.14	74,77,78,79	0
4	NGA	A	704	15/15	0.95	0.08	43,45,47,50	0
6	UDP	A	707	25/25	0.96	0.10	49,53,57,59	0
5	MN	A	706	1/1	0.99	0.02	24,24,24,24	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.