



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 9, 2025 – 01:46 am BST

PDB ID : 9H6K / pdb_00009h6k
Title : Human B4GALNT1 in Complex with UDP-GalNac
Authors : Welland, J.W.J.; Deane, J.E.
Deposited on : 2024-10-24
Resolution : 2.75 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

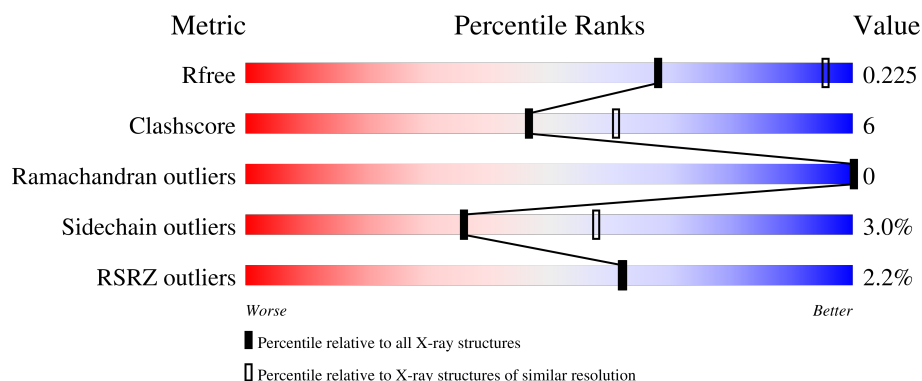
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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	499	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>6%</div> </div> </div>
1	B	499	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>6%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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
6	ACY	A	605	-	-	X	-
6	ACY	B	605	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7590 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 Beta-1,4 N-acetylgalactosaminyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3658	2317	652	680	9			
1	B	468	Total	C	N	O	S	0	0	0
			3658	2317	652	680	9			

There are 24 discrepancies between the modelled and reference sequences:

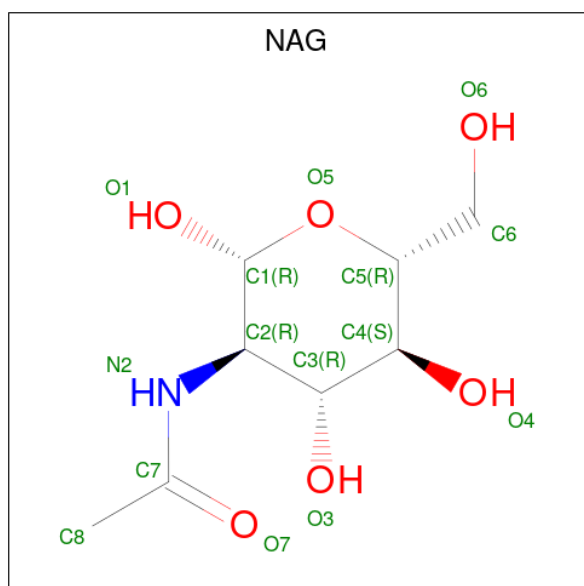
Chain	Residue	Modelled	Actual	Comment	Reference
A	35	HIS	-	expression tag	UNP Q00973
A	36	HIS	-	expression tag	UNP Q00973
A	37	HIS	-	expression tag	UNP Q00973
A	38	HIS	-	expression tag	UNP Q00973
A	39	HIS	-	expression tag	UNP Q00973
A	40	HIS	-	expression tag	UNP Q00973
A	41	HIS	-	expression tag	UNP Q00973
A	42	HIS	-	expression tag	UNP Q00973
A	43	HIS	-	expression tag	UNP Q00973
A	44	HIS	-	expression tag	UNP Q00973
A	45	GLY	-	expression tag	UNP Q00973
A	46	THR	-	expression tag	UNP Q00973
B	35	HIS	-	expression tag	UNP Q00973
B	36	HIS	-	expression tag	UNP Q00973
B	37	HIS	-	expression tag	UNP Q00973
B	38	HIS	-	expression tag	UNP Q00973
B	39	HIS	-	expression tag	UNP Q00973
B	40	HIS	-	expression tag	UNP Q00973
B	41	HIS	-	expression tag	UNP Q00973
B	42	HIS	-	expression tag	UNP Q00973
B	43	HIS	-	expression tag	UNP Q00973
B	44	HIS	-	expression tag	UNP Q00973
B	45	GLY	-	expression tag	UNP Q00973
B	46	THR	-	expression tag	UNP Q00973

- 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
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

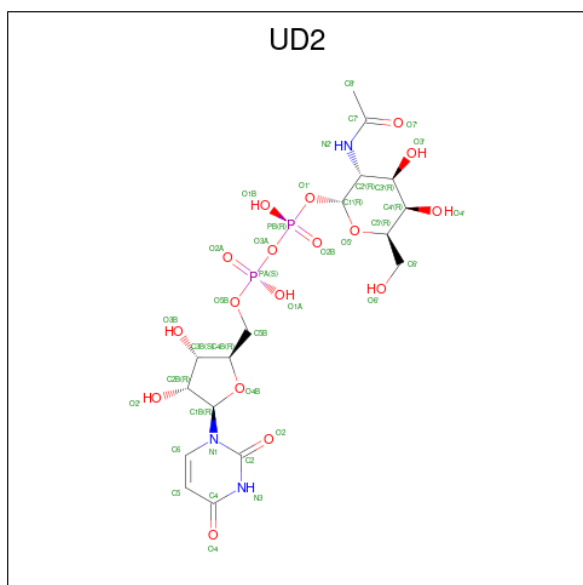


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		

- Molecule 5 is URIDINE-DIPHOSPHATE-N-ACETYLGLACTOSAMINE (CCD ID: UD2) (formula: $C_{17}H_{27}N_3O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
5	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 6 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

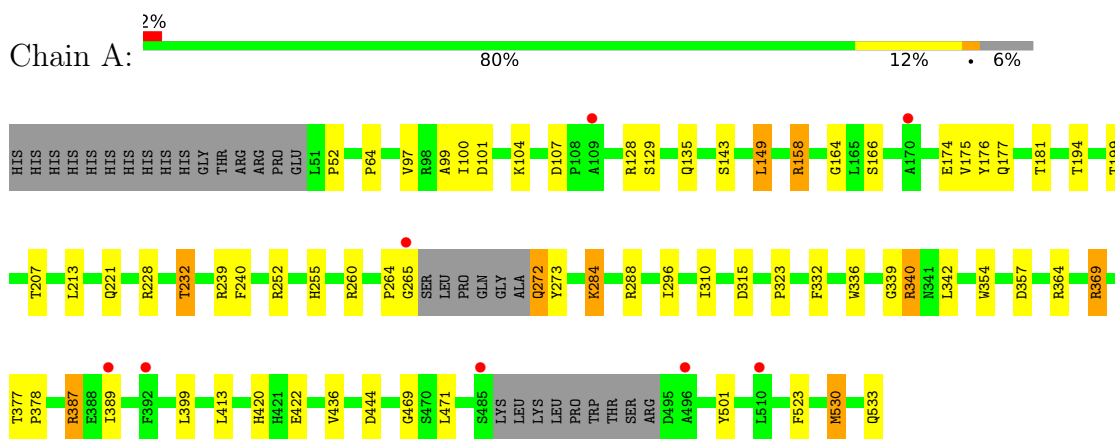
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	36	Total	O	0	0
			36	36		
7	B	38	Total	O	0	0
			38	38		

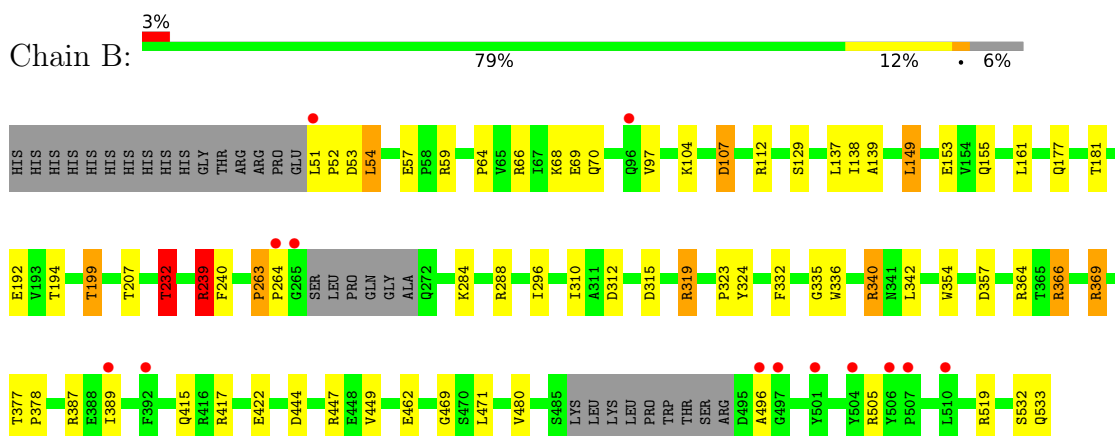
3 Residue-property plots [i](#)

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.

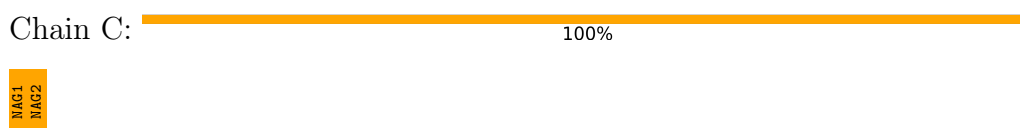
- Molecule 1: Beta-1,4 N-acetylgalactosaminyltransferase 1



- Molecule 1: Beta-1,4 N-acetylgalactosaminyltransferase 1



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



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

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.10Å 134.92Å 86.58Å 90.00° 95.91° 90.00°	Depositor
Resolution (Å)	54.66 – 2.75 54.66 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (54.66-2.75) 99.6 (54.66-2.75)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.189 , 0.225 0.189 , 0.225	Depositor DCC
R_{free} test set	1761 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7590	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: ACY, MN, UD2, 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	0.63	0/3740	1.24	21/5087 (0.4%)
1	B	0.65	0/3740	1.24	22/5087 (0.4%)
All	All	0.64	0/7480	1.24	43/10174 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	7
All	All	0	10

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	NE-CZ-NH2	-7.48	112.47	119.20
1	B	54	LEU	N-CA-CB	7.01	122.33	110.49
1	A	252	ARG	CB-CA-C	6.85	121.00	109.84
1	B	107	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	369	ARG	CB-CA-C	6.75	122.33	110.85
1	A	323	PRO	CB-CA-C	6.75	120.14	111.64
1	B	240	PHE	CA-CB-CG	6.71	120.51	113.80
1	A	471	LEU	N-CA-CB	-6.64	99.52	110.68
1	B	471	LEU	N-CA-CB	-6.50	99.77	110.68
1	B	239	ARG	CB-CG-CD	6.47	126.18	111.30
1	B	369	ARG	CB-CA-C	6.46	121.84	110.85
1	A	284	LYS	CA-CB-CG	-6.43	101.23	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	ARG	CG-CD-NE	-6.42	97.88	112.00
1	A	181	THR	CA-CB-OG1	-6.35	100.07	109.60
1	A	240	PHE	CA-CB-CG	6.09	119.89	113.80
1	A	369	ARG	CA-CB-CG	5.96	126.01	114.10
1	A	523	PHE	CA-CB-CG	-5.86	107.94	113.80
1	B	153	GLU	N-CA-CB	-5.82	100.71	111.13
1	A	369	ARG	N-CA-CB	-5.82	101.55	110.16
1	A	149	LEU	N-CA-CB	-5.70	101.70	110.42
1	B	181	THR	CA-CB-OG1	-5.70	101.05	109.60
1	B	369	ARG	CA-CB-CG	5.69	125.49	114.10
1	B	340	ARG	CD-NE-CZ	5.69	132.37	124.40
1	B	232	THR	CA-CB-OG1	-5.61	101.19	109.60
1	A	340	ARG	CD-NE-CZ	5.58	132.21	124.40
1	A	252	ARG	CB-CG-CD	-5.53	98.58	111.30
1	A	107	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	263	PRO	CB-CA-C	5.51	117.64	110.92
1	B	422	GLU	CB-CG-CD	5.50	121.95	112.60
1	B	340	ARG	NE-CZ-NH2	-5.47	114.28	119.20
1	A	232	THR	CA-CB-OG1	-5.47	101.40	109.60
1	B	462	GLU	N-CA-CB	5.47	118.64	110.22
1	B	149	LEU	N-CA-CB	-5.44	102.09	110.42
1	B	323	PRO	CB-CA-C	5.34	118.37	111.64
1	B	192	GLU	CB-CG-CD	5.30	121.60	112.60
1	A	135	GLN	CB-CA-C	-5.18	100.79	109.65
1	A	199	THR	CA-CB-OG1	-5.16	101.86	109.60
1	B	312	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	496	ALA	CA-C-N	5.09	125.73	120.03
1	B	496	ALA	C-N-CA	5.09	125.73	120.03
1	A	284	LYS	CB-CG-CD	5.05	122.92	111.30
1	B	53	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	272	GLN	CB-CA-C	5.05	119.69	110.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ARG	Sidechain
1	A	158	ARG	Sidechain
1	A	387	ARG	Sidechain
1	B	239	ARG	Sidechain
1	B	366	ARG	Sidechain
1	B	387	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	417	ARG	Sidechain
1	B	505	ARG	Sidechain
1	B	519	ARG	Sidechain
1	B	66	ARG	Sidechain

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	3658	0	3623	44	0
1	B	3658	0	3623	43	0
2	C	28	0	25	2	0
2	D	28	0	25	1	0
3	A	28	0	26	0	0
3	B	28	0	26	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	39	0	25	6	0
5	B	39	0	25	5	0
6	A	4	0	3	2	0
6	B	4	0	3	4	0
7	A	36	0	0	4	0
7	B	38	0	0	2	0
All	All	7590	0	7404	83	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 6.

All (83) 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:284:LYS:HD2	1:A:339:GLY:HA3	1.45	0.96
1:B:177:GLN:HE21	3:B:601:NAG:H82	1.38	0.86
1:A:340:ARG:HD3	1:A:354:TRP:CZ2	2.18	0.79
1:A:64:PRO:HA	7:A:701:HOH:O	1.81	0.79
1:A:444:ASP:OD2	6:A:605:ACY:H3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:HD3	1:B:354:TRP:CZ2	2.18	0.78
5:A:604:UD2:H6'1	7:A:715:HOH:O	1.82	0.77
1:B:447:ARG:HE	6:B:605:ACY:H2	1.49	0.77
1:B:444:ASP:OD1	6:B:605:ACY:H1	1.85	0.76
1:B:199:THR:HG23	1:B:207:THR:HB	1.71	0.73
5:B:604:UD2:O6'	7:B:701:HOH:O	2.06	0.72
1:B:97:VAL:HG22	1:B:533:GLN:HG2	1.74	0.70
1:A:149:LEU:HG	1:B:149:LEU:HG	1.71	0.70
1:A:272:GLN:HG3	1:A:273:TYR:H	1.57	0.68
1:A:239:ARG:HG2	1:A:239:ARG:HH11	1.59	0.67
1:A:444:ASP:OD2	6:A:605:ACY:CH3	2.44	0.66
1:B:444:ASP:OD1	6:B:605:ACY:CH3	2.44	0.65
1:A:97:VAL:HG22	1:A:533:GLN:HG2	1.77	0.65
1:A:501:TYR:OH	5:A:604:UD2:O2A	2.15	0.63
1:A:221:GLN:NE2	1:B:57:GLU:OE1	2.29	0.62
1:A:100:ILE:N	1:A:100:ILE:HD12	2.16	0.61
1:B:340:ARG:CD	1:B:354:TRP:CZ2	2.85	0.59
1:B:336:TRP:CZ2	5:B:604:UD2:H4'	2.37	0.59
1:A:272:GLN:HG3	1:A:273:TYR:N	2.17	0.59
1:A:340:ARG:CD	1:A:354:TRP:CZ2	2.88	0.57
1:A:315:ASP:HB3	1:A:332:PHE:CD2	2.39	0.57
1:A:436:VAL:HG22	5:A:604:UD2:H8'1	1.87	0.56
1:B:288:ARG:NH2	1:B:357:ASP:OD1	2.39	0.55
1:A:101:ASP:HB3	1:A:104:LYS:HE2	1.88	0.55
1:A:288:ARG:NH2	1:A:357:ASP:OD1	2.40	0.55
1:B:315:ASP:HB3	1:B:332:PHE:CD2	2.42	0.55
1:A:336:TRP:CZ2	5:A:604:UD2:H4'	2.42	0.54
1:B:51:LEU:N	1:B:52:PRO:CD	2.72	0.53
1:A:469:GLY:O	1:B:232:THR:HB	2.09	0.53
1:A:52:PRO:HB2	1:B:161:LEU:HD12	1.91	0.52
1:B:335:GLY:HA3	7:B:709:HOH:O	2.10	0.52
1:A:177:GLN:HE21	1:A:207:THR:HG21	1.76	0.51
1:B:415:GLN:NE2	1:B:532:SER:HA	2.26	0.51
1:A:422:GLU:HG2	7:A:736:HOH:O	2.11	0.50
1:A:164:GLY:HA3	1:B:138:ILE:HD12	1.94	0.50
1:A:296:ILE:HD11	1:A:310:ILE:HD11	1.94	0.49
1:B:239:ARG:NH1	1:B:239:ARG:HG2	2.26	0.49
1:A:149:LEU:HD12	1:B:139:ALA:HB2	1.95	0.49
1:A:413:LEU:HD23	1:A:530:MET:HE2	1.93	0.49
1:B:177:GLN:NE2	3:B:601:NAG:H82	2.18	0.48
5:A:604:UD2:H3'	5:A:604:UD2:H5'2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ARG:HE	6:B:605:ACY:CH3	2.20	0.48
1:A:260:ARG:NH2	1:B:449:VAL:O	2.47	0.47
1:B:340:ARG:HD2	1:B:354:TRP:CH2	2.50	0.47
1:B:340:ARG:CD	1:B:354:TRP:CH2	2.97	0.47
1:A:101:ASP:OD1	1:A:104:LYS:HG3	2.14	0.47
1:B:59:ARG:HG3	1:B:59:ARG:HH21	1.79	0.47
1:B:296:ILE:HD11	1:B:310:ILE:HD11	1.96	0.47
1:B:324:TYR:HE1	2:D:2:NAG:H81	1.80	0.46
1:B:342:LEU:C	1:B:342:LEU:HD23	2.40	0.46
1:A:228:ARG:HA	1:A:228:ARG:HD3	1.75	0.46
1:A:264:PRO:O	1:A:265:GLY:C	2.58	0.46
1:A:342:LEU:C	1:A:342:LEU:HD23	2.40	0.45
2:C:2:NAG:H83	2:C:2:NAG:H2	1.87	0.45
1:B:364:ARG:HB3	1:B:480:VAL:HB	1.99	0.45
1:A:194:THR:HB	1:B:64:PRO:HG2	1.98	0.45
5:B:604:UD2:H5'2	5:B:604:UD2:H3'	1.98	0.45
1:A:239:ARG:HH11	1:A:239:ARG:CG	2.28	0.45
1:A:232:THR:HB	1:B:469:GLY:O	2.16	0.45
1:A:364:ARG:HG2	1:A:364:ARG:HH11	1.82	0.45
1:B:319:ARG:HD3	1:B:319:ARG:HA	1.59	0.45
1:B:366:ARG:HA	1:B:366:ARG:HD2	1.85	0.44
1:B:239:ARG:HG2	1:B:239:ARG:HH11	1.82	0.44
1:A:413:LEU:HB3	1:A:530:MET:HB2	2.00	0.43
1:A:340:ARG:CD	1:A:354:TRP:CH2	3.01	0.43
1:A:377:THR:HB	1:A:378:PRO:HD2	2.01	0.43
1:B:284:LYS:NZ	5:B:604:UD2:O2	2.47	0.42
7:A:727:HOH:O	2:C:1:NAG:H81	2.19	0.42
1:A:399:LEU:HD22	1:A:420:HIS:CE1	2.55	0.42
1:B:68:LYS:HG2	1:B:70:GLN:OE1	2.19	0.41
1:B:377:THR:HB	1:B:378:PRO:HD2	2.01	0.41
1:A:176:TYR:CD1	1:A:213:LEU:HD13	2.54	0.41
1:B:263:PRO:HA	1:B:264:PRO:HD3	1.86	0.41
1:A:255:HIS:CD2	1:B:469:GLY:HA2	2.56	0.41
1:B:288:ARG:NH2	5:B:604:UD2:H3B	2.36	0.41
1:A:99:ALA:C	1:A:100:ILE:HD12	2.44	0.40
1:B:51:LEU:HD23	1:B:51:LEU:HA	1.90	0.40
1:A:288:ARG:NH2	5:A:604:UD2:H3B	2.37	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	462/499 (93%)	449 (97%)	13 (3%)	0	100	100
1	B	462/499 (93%)	451 (98%)	11 (2%)	0	100	100
All	All	924/998 (93%)	900 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	395/423 (93%)	386 (98%)	9 (2%)	45	67
1	B	395/423 (93%)	380 (96%)	15 (4%)	28	49
All	All	790/846 (93%)	766 (97%)	24 (3%)	36	58

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

Mol	Chain	Res	Type
1	A	129	SER
1	A	143	SER
1	A	158	ARG
1	A	166	SER
1	A	174	GLU
1	A	175	VAL
1	A	369	ARG
1	A	389	ILE

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Mol	Chain	Res	Type
1	A	530	MET
1	B	54	LEU
1	B	69	GLU
1	B	104	LYS
1	B	107	ASP
1	B	112	ARG
1	B	129	SER
1	B	137	LEU
1	B	155	GLN
1	B	194	THR
1	B	199	THR
1	B	232	THR
1	B	239	ARG
1	B	319	ARG
1	B	369	ARG
1	B	389	ILE

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	94	GLN
1	A	120	GLN
1	A	177	GLN
1	A	245	HIS
1	B	94	GLN
1	B	173	GLN
1	B	177	GLN
1	B	346	GLN
1	B	415	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

4 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	C	1	1,2	14,14,15	0.54	0	17,19,21	2.18	3 (17%)
2	NAG	C	2	2	14,14,15	0.37	0	17,19,21	1.16	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.29	0	17,19,21	0.58	0
2	NAG	D	2	2	14,14,15	0.30	0	17,19,21	0.91	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	C	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	1	NAG	C1-O5-C5	7.34	122.13	112.19
2	C	1	NAG	C2-N2-C7	3.67	128.13	122.90
2	C	2	NAG	C1-C2-N2	3.01	115.62	110.49
2	C	1	NAG	O5-C5-C4	2.60	117.15	110.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

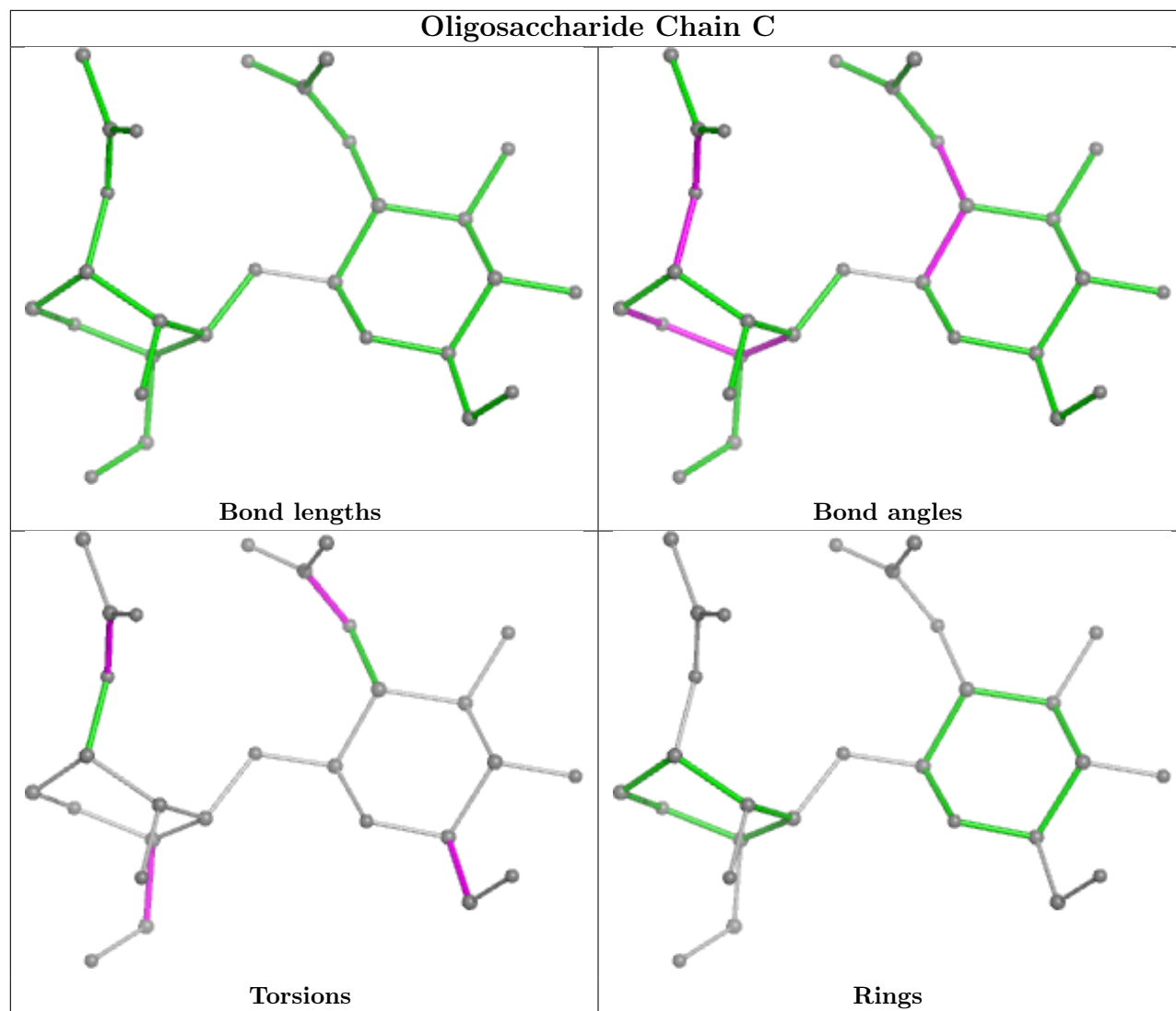
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6

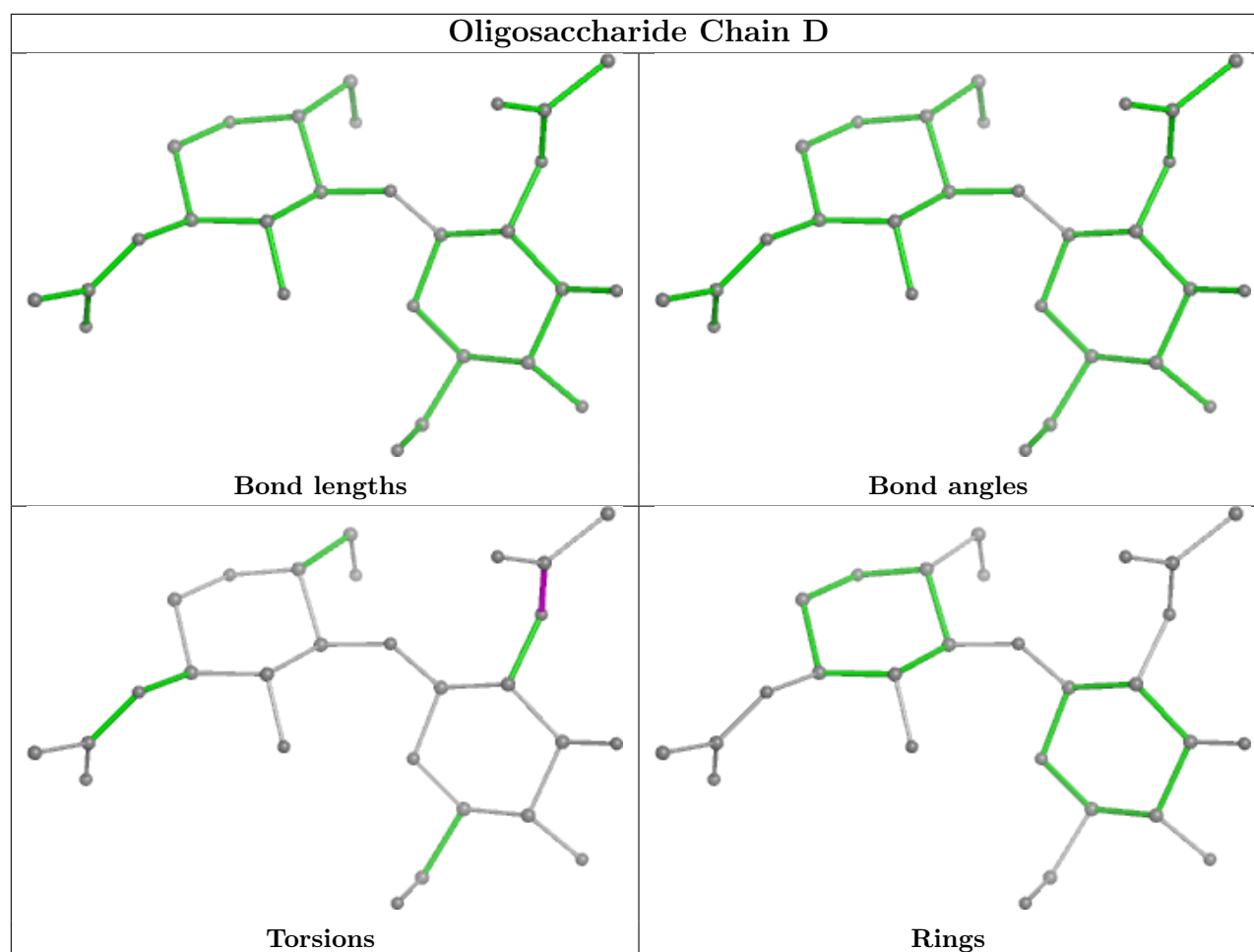
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
2	C	2	NAG	1	0
2	C	1	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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	ACY	B	605	-	3,3,3	0.92	0	3,3,3	0.97	0
3	NAG	A	601	1	14,14,15	0.34	0	17,19,21	1.38	3 (17%)
6	ACY	A	605	-	3,3,3	0.91	0	3,3,3	1.00	0
3	NAG	B	602	1	14,14,15	0.42	0	17,19,21	1.12	2 (11%)
3	NAG	B	601	1	14,14,15	0.44	0	17,19,21	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	602	1	14,14,15	0.48	0	17,19,21	1.37	2 (11%)
5	UD2	B	604	4	38,41,41	0.49	0	57,62,62	1.15	5 (8%)
5	UD2	A	604	4	38,41,41	0.49	0	57,62,62	1.14	5 (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	601	1	-	3/6/23/26	0/1/1/1
3	NAG	B	602	1	-	2/6/23/26	0/1/1/1
3	NAG	B	601	1	-	3/6/23/26	0/1/1/1
3	NAG	A	602	1	-	2/6/23/26	0/1/1/1
5	UD2	B	604	4	-	5/26/63/63	0/3/3/3
5	UD2	A	604	4	-	10/26/63/63	0/3/3/3

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	NAG	C2-N2-C7	4.03	128.65	122.90
5	B	604	UD2	O3B-C3B-C2B	3.47	123.05	111.82
5	A	604	UD2	C6'-C5'-C4'	3.28	120.68	113.00
5	B	604	UD2	C2'-N2'-C7'	3.22	131.02	123.18
3	A	601	NAG	C4-C3-C2	3.09	115.54	111.02
3	A	602	NAG	C1-C2-N2	2.97	115.56	110.49
5	A	604	UD2	C3'-C4'-C5'	-2.93	105.01	110.24
3	A	601	NAG	C1-C2-N2	-2.93	105.49	110.49
5	A	604	UD2	PB-O1'-C1'	2.73	130.30	119.74
3	B	602	NAG	C1-O5-C5	2.49	115.57	112.19
5	B	604	UD2	PB-O1'-C1'	2.43	129.14	119.74
5	A	604	UD2	O6'-C6'-C5'	2.32	119.25	111.29
5	B	604	UD2	O5'-C1'-O1'	2.25	114.31	111.36
3	B	602	NAG	C2-N2-C7	2.21	126.06	122.90
3	A	602	NAG	C2-N2-C7	2.18	126.00	122.90
5	B	604	UD2	O2'-C2B-C1B	2.16	117.25	110.02
3	A	601	NAG	O5-C5-C6	-2.14	103.84	107.20
5	A	604	UD2	O3B-C3B-C2B	2.11	118.64	111.82
3	B	601	NAG	C4-C3-C2	2.01	113.97	111.02

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	NAG	C1-C2-N2-C7
3	B	601	NAG	C8-C7-N2-C2
3	B	601	NAG	O7-C7-N2-C2
5	A	604	UD2	C5B-O5B-PA-O1A
3	B	602	NAG	C4-C5-C6-O6
5	B	604	UD2	O5'-C5'-C6'-O6'
3	B	602	NAG	O5-C5-C6-O6
5	A	604	UD2	C4'-C5'-C6'-O6'
3	A	601	NAG	C8-C7-N2-C2
3	A	602	NAG	O5-C5-C6-O6
5	A	604	UD2	O5'-C5'-C6'-O6'
3	A	602	NAG	C4-C5-C6-O6
5	B	604	UD2	C4'-C5'-C6'-O6'
3	A	601	NAG	O7-C7-N2-C2
5	A	604	UD2	C1'-O1'-PB-O3A
5	B	604	UD2	C1'-O1'-PB-O3A
3	A	601	NAG	O5-C5-C6-O6
5	A	604	UD2	C3B-C4B-C5B-O5B
5	A	604	UD2	O4B-C4B-C5B-O5B
5	A	604	UD2	C5B-O5B-PA-O3A
5	B	604	UD2	PB-O3A-PA-O1A
5	A	604	UD2	C5B-O5B-PA-O2A
5	A	604	UD2	PB-O3A-PA-O1A
5	A	604	UD2	PB-O3A-PA-O2A
5	B	604	UD2	PB-O3A-PA-O2A

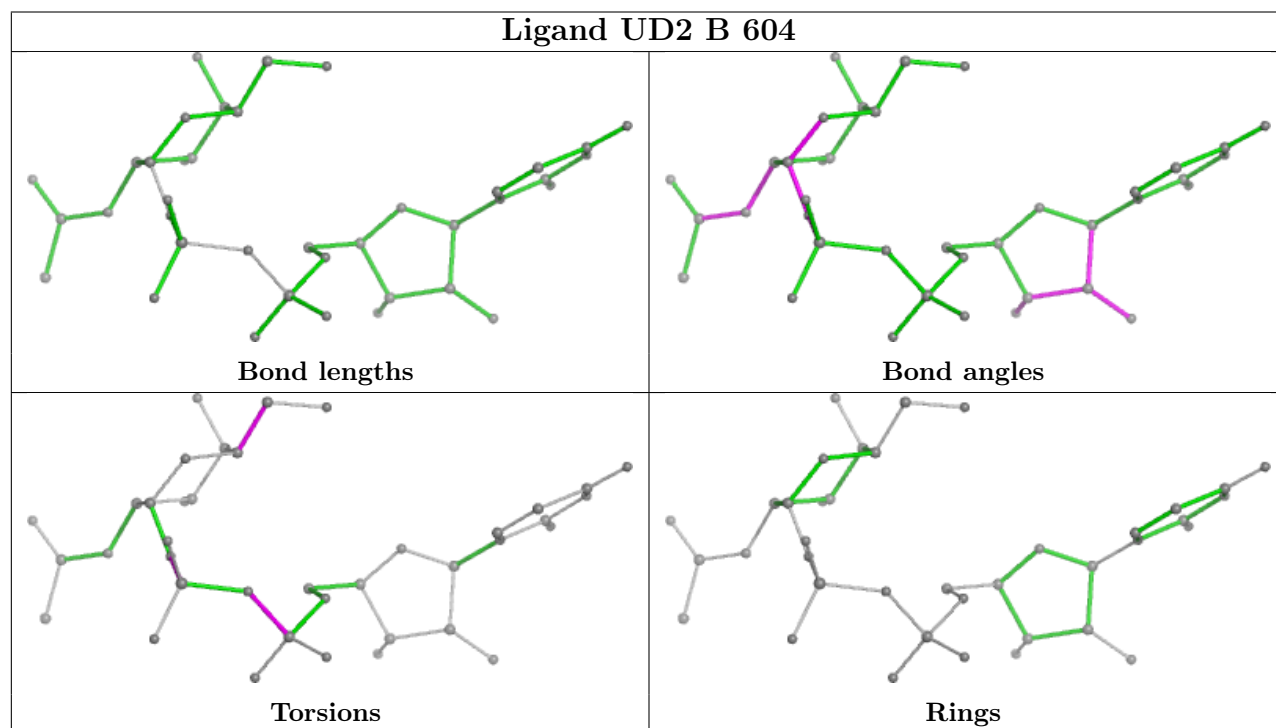
There are no ring outliers.

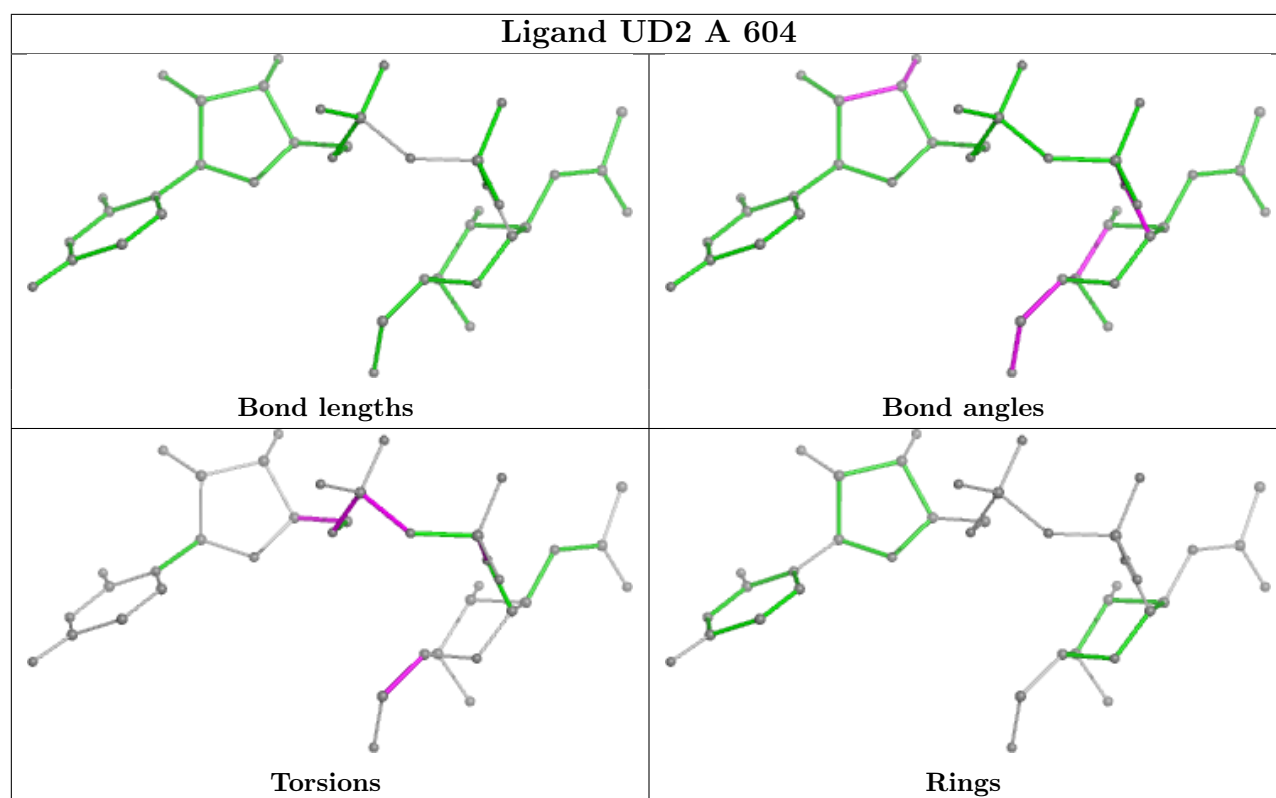
5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	605	ACY	4	0
6	A	605	ACY	2	0
3	B	601	NAG	2	0
5	B	604	UD2	5	0
5	A	604	UD2	6	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

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, 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	468/499 (93%)	-0.20	8 (1%) 69 70	33, 71, 130, 164	0
1	B	468/499 (93%)	-0.18	13 (2%) 55 56	34, 68, 132, 182	0
All	All	936/998 (93%)	-0.19	21 (2%) 62 62	33, 69, 131, 182	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	265	GLY	4.6
1	A	389	ILE	4.5
1	B	96	GLN	3.6
1	A	496	ALA	3.2
1	B	51	LEU	3.2
1	B	497	GLY	3.0
1	B	264	PRO	2.9
1	B	496	ALA	2.9
1	B	510	LEU	2.9
1	B	504	TYR	2.8
1	A	170	ALA	2.8
1	B	389	ILE	2.6
1	A	392	PHE	2.5
1	A	485	SER	2.4
1	B	392	PHE	2.4
1	B	507	PRO	2.4
1	A	109	ALA	2.4
1	A	510	LEU	2.3
1	B	501	TYR	2.3
1	A	265	GLY	2.1
1	B	506	TYR	2.0

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

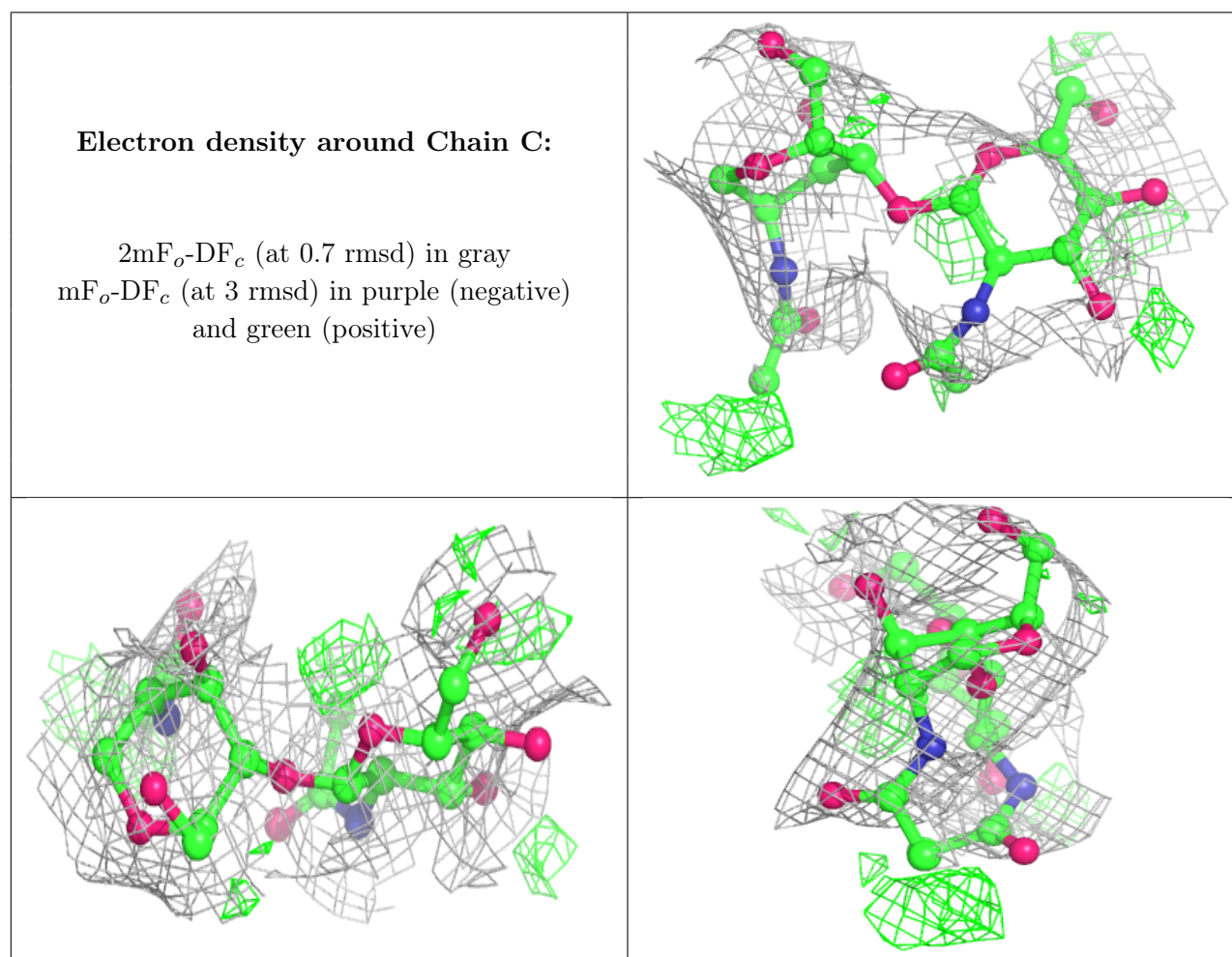
There are no non-standard protein/DNA/RNA residues in this entry.

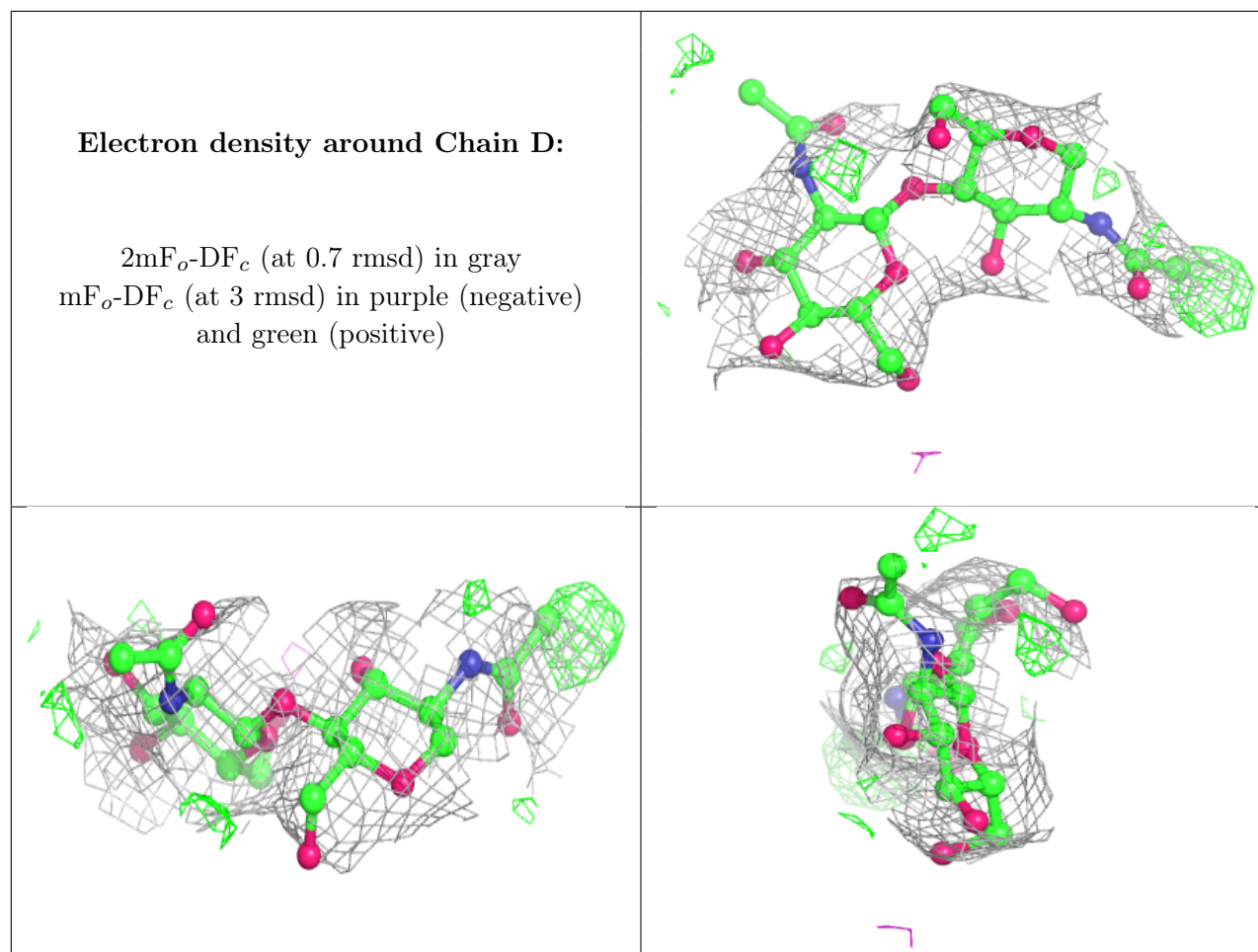
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
2	NAG	C	2	14/15	0.62	0.15	125,153,182,195	0
2	NAG	D	2	14/15	0.71	0.14	109,142,153,156	0
2	NAG	D	1	14/15	0.84	0.12	100,118,129,132	0
2	NAG	C	1	14/15	0.84	0.13	108,134,146,154	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 ⓘ

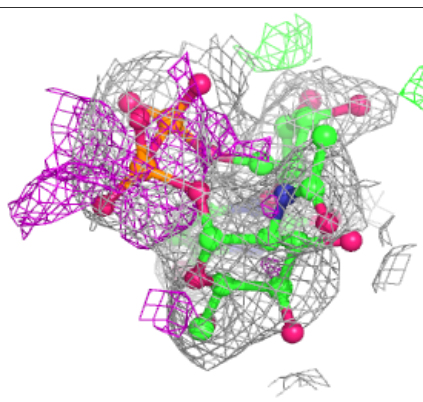
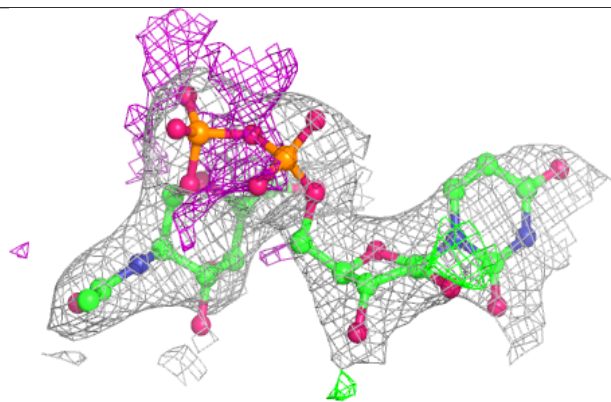
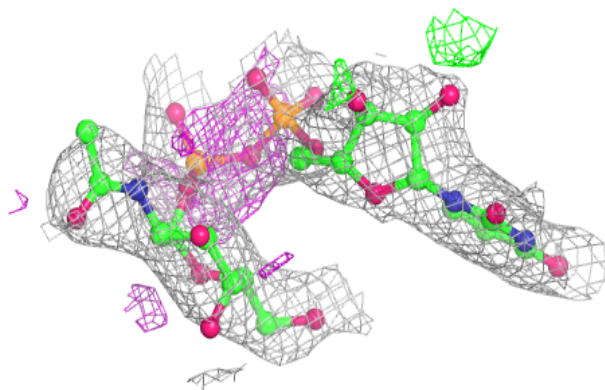
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	601	14/15	0.59	0.17	121,151,170,173	0
3	NAG	A	602	14/15	0.67	0.14	83,119,128,131	0
3	NAG	B	602	14/15	0.73	0.14	89,132,142,145	0
3	NAG	B	601	14/15	0.79	0.11	99,109,117,136	0
5	UD2	B	604	39/39	0.91	0.11	60,93,107,109	0
6	ACY	A	605	4/4	0.92	0.14	40,53,56,59	0
6	ACY	B	605	4/4	0.93	0.15	42,55,57,66	0
5	UD2	A	604	39/39	0.97	0.06	48,61,71,78	0
4	MN	A	603	1/1	0.98	0.04	74,74,74,74	0
4	MN	B	603	1/1	0.99	0.06	88,88,88,88	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.

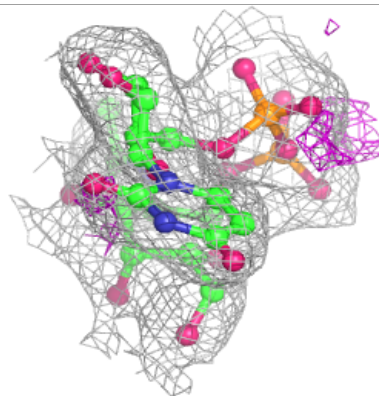
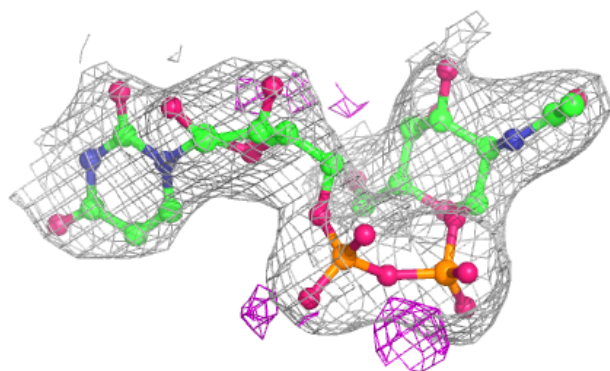
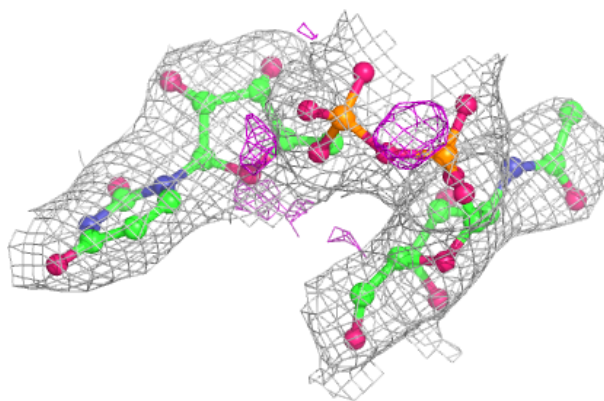
Electron density around UD2 B 604:

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



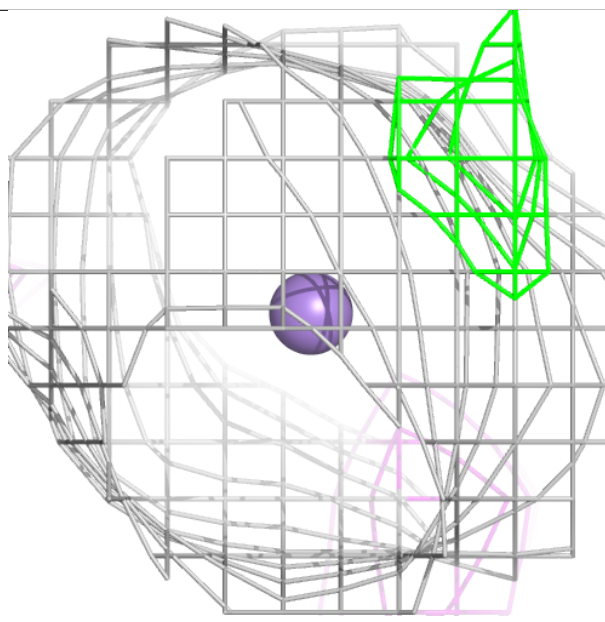
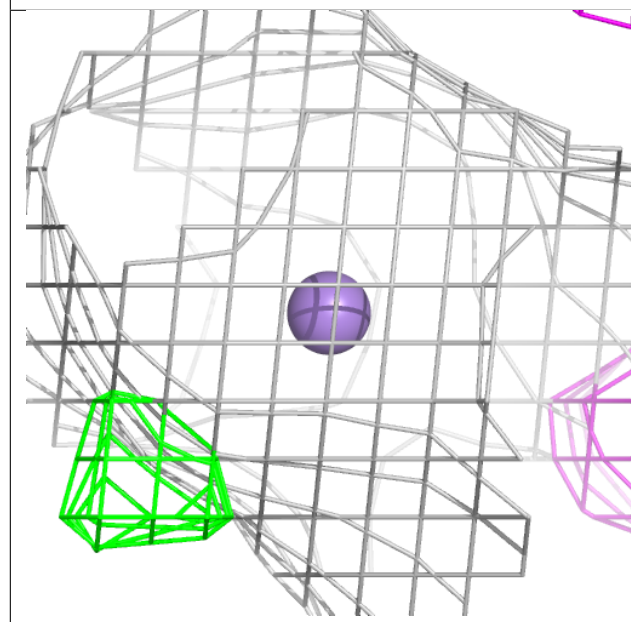
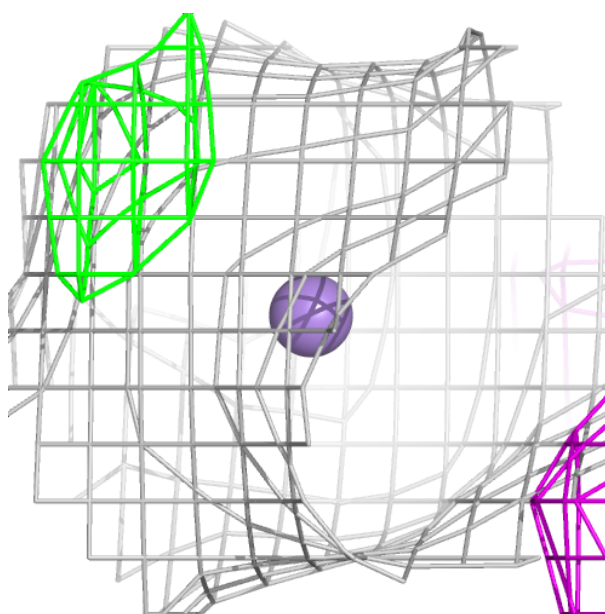
Electron density around UD2 A 604:

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



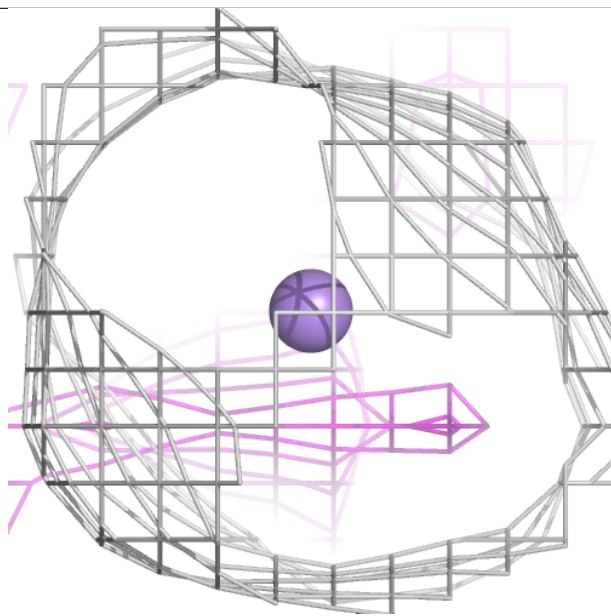
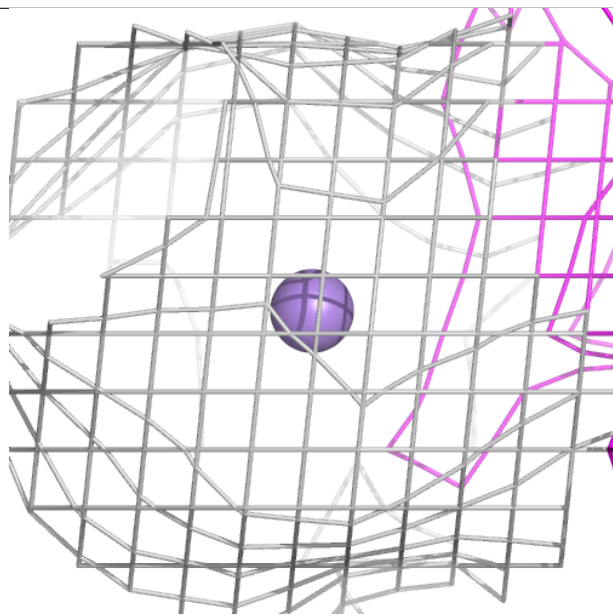
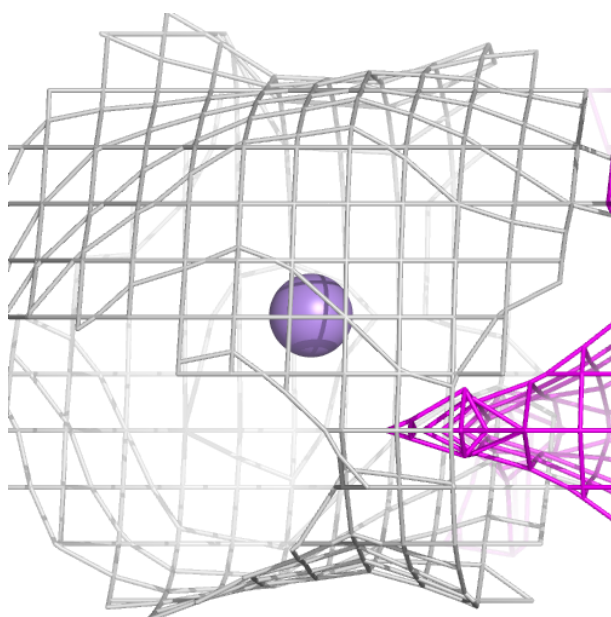
Electron density around MN A 603:

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



Electron density around MN B 603:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.