Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 06:23 am GMT

PDB ID	:	1E3C
Title	:	Crystal structure of an Arylsulfatase A mutant C69S soaked in synthetic substrate
Authors	:	von Buelow, R.; Schmidt, B.; Dierks, T.; von Figura, K.; Uson, I.
Deposited on	:	2000-06-13
Resolution	:	2.65 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 (i) 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 (i)) were used in the production of this report:

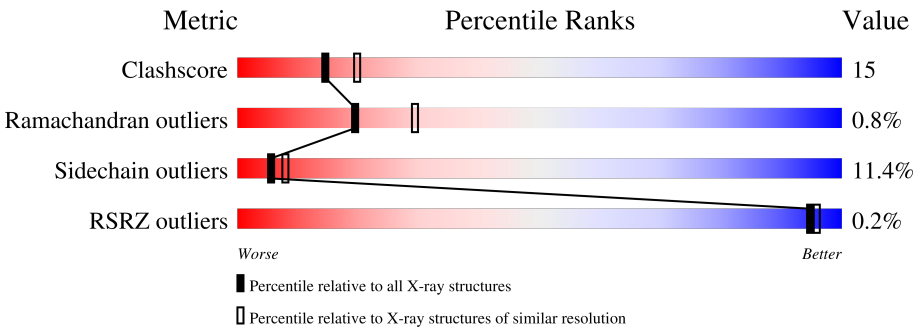
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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))
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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

Mol	Chain	Length	Quality of chain
1	P	489	54% 32% 10% • •
2	A	2	100%

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
2	NAG	A	1	X	-	-	-
2	NAG	A	2	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3784 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 Arylsulfatase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	P	481	3582	2282	610	667	23	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	69	SER	CYS	engineered mutation	UNP P15289
P	215	GLU	GLN	conflict	UNP P15289

- 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	A	2	28	16	2	10	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	P	1	1	1	0	0

- Molecule 4 is water.

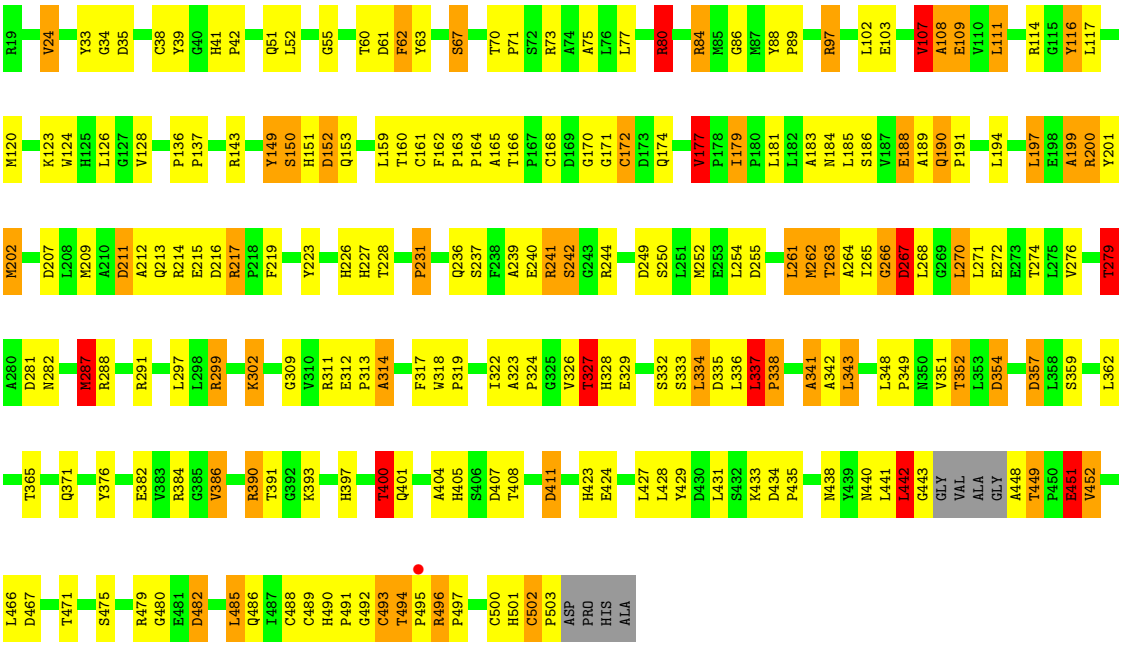
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	P	173	173	173	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Arylsulfatase A

Chain P: 54% 32% 10%



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

Chain A: 100%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	131.80Å 131.80Å 192.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.65 29.47 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.65) 99.4 (29.47-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.15 (at 2.64Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.173 , 0.243 0.150 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 68.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.005 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3784	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MG

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	P	0.97	1/3689 (0.0%)	2.23	165/5042 (3.3%)

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	P	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	503	PRO	N-CD	7.20	1.57	1.47

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	291	ARG	NE-CZ-NH2	-23.56	108.52	120.30
1	P	354	ASP	CB-CG-OD1	17.63	134.17	118.30
1	P	281	ASP	CB-CG-OD1	14.53	131.38	118.30
1	P	217	ARG	NE-CZ-NH2	13.96	127.28	120.30
1	P	384	ARG	NE-CZ-NH2	-13.93	113.33	120.30
1	P	496	ARG	NE-CZ-NH1	13.90	127.25	120.30
1	P	33	TYR	CB-CG-CD2	-12.97	113.22	121.00
1	P	200	ARG	NE-CZ-NH2	12.77	126.69	120.30
1	P	143	ARG	NE-CZ-NH2	-12.01	114.30	120.30
1	P	179	ILE	CA-CB-CG2	11.47	133.85	110.90
1	P	479	ARG	NE-CZ-NH1	11.47	126.03	120.30
1	P	479	ARG	NE-CZ-NH2	-11.32	114.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	120	MET	CG-SD-CE	-10.59	83.25	100.20
1	P	299	ARG	NE-CZ-NH1	-10.07	115.26	120.30
1	P	489	CYS	C-N-CA	9.89	146.43	121.70
1	P	390	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	P	411	ASP	CB-CG-OD2	-9.75	109.53	118.30
1	P	80	ARG	NE-CZ-NH2	9.71	125.15	120.30
1	P	152	ASP	CB-CG-OD2	9.61	126.94	118.30
1	P	33	TYR	CB-CG-CD1	9.31	126.58	121.00
1	P	382	GLU	OE1-CD-OE2	9.24	134.39	123.30
1	P	116	TYR	CB-CG-CD1	9.01	126.40	121.00
1	P	338	PRO	O-C-N	-8.99	108.32	122.70
1	P	80	ARG	NE-CZ-NH1	-8.87	115.86	120.30
1	P	244	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	P	479	ARG	CD-NE-CZ	8.66	135.72	123.60
1	P	291	ARG	NH1-CZ-NH2	8.47	128.72	119.40
1	P	384	ARG	CD-NE-CZ	-8.47	111.75	123.60
1	P	489	CYS	CA-CB-SG	-8.21	99.21	114.00
1	P	223	TYR	CB-CG-CD2	8.05	125.83	121.00
1	P	143	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	P	281	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	P	327	THR	CB-CA-C	-7.92	90.22	111.60
1	P	475	SER	N-CA-CB	-7.82	98.78	110.50
1	P	311	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	P	354	ASP	OD1-CG-OD2	-7.78	108.52	123.30
1	P	357	ASP	CB-CG-OD2	7.76	125.29	118.30
1	P	200	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	P	97	ARG	NE-CZ-NH2	7.73	124.17	120.30
1	P	337	LEU	CA-CB-CG	7.69	132.98	115.30
1	P	242	SER	C-N-CA	-7.64	106.25	122.30
1	P	482	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	P	63	TYR	CB-CG-CD2	-7.48	116.51	121.00
1	P	211	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	P	502	CYS	N-CA-CB	-7.38	97.31	110.60
1	P	448	ALA	O-C-N	-7.35	110.94	122.70
1	P	391	THR	OG1-CB-CG2	-7.34	93.12	110.00
1	P	299	ARG	NH1-CZ-NH2	7.30	127.43	119.40
1	P	109	GLU	OE1-CD-OE2	-7.12	114.76	123.30
1	P	188	GLU	O-C-N	-7.08	111.38	122.70
1	P	255	ASP	CB-CG-OD1	7.07	124.67	118.30
1	P	434	ASP	CB-CG-OD1	7.03	124.62	118.30
1	P	288	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	P	171	GLY	N-CA-C	6.98	130.54	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	207	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	P	482	ASP	CB-CG-OD1	6.85	124.46	118.30
1	P	384	ARG	NH1-CZ-NH2	6.83	126.91	119.40
1	P	267	ASP	CA-C-N	6.79	132.15	117.20
1	P	326	VAL	CA-C-N	6.75	132.04	117.20
1	P	249	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	P	244	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	P	429	TYR	CB-CG-CD1	-6.66	117.00	121.00
1	P	177	VAL	N-CA-CB	-6.64	96.88	111.50
1	P	314	ALA	CB-CA-C	6.64	120.06	110.10
1	P	190	GLN	CB-CG-CD	6.61	128.78	111.60
1	P	279	THR	N-CA-CB	6.59	122.82	110.30
1	P	116	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	P	497	PRO	CA-N-CD	-6.55	102.33	111.50
1	P	67	SER	N-CA-CB	-6.49	100.77	110.50
1	P	186	SER	O-C-N	6.43	132.99	122.70
1	P	199	ALA	N-CA-CB	-6.43	101.10	110.10
1	P	84	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	P	496	ARG	CA-CB-CG	6.38	127.44	113.40
1	P	168	CYS	CA-CB-SG	-6.38	102.52	114.00
1	P	165	ALA	N-CA-CB	-6.35	101.21	110.10
1	P	189	ALA	N-CA-CB	6.31	118.93	110.10
1	P	424	GLU	CA-C-O	-6.30	106.88	120.10
1	P	335	ASP	CB-CG-OD1	6.29	123.96	118.30
1	P	496	ARG	CA-C-O	-6.25	106.97	120.10
1	P	97	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	P	401	GLN	N-CA-CB	-6.22	99.41	110.60
1	P	494	THR	CA-C-O	-6.18	107.13	120.10
1	P	335	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	P	352	THR	CA-C-O	6.10	132.91	120.10
1	P	271	LEU	N-CA-CB	6.06	122.53	110.40
1	P	323	ALA	N-CA-CB	-6.06	101.61	110.10
1	P	400	THR	N-CA-CB	-6.06	98.79	110.30
1	P	496	ARG	NH1-CZ-NH2	-6.05	112.74	119.40
1	P	438	ASN	CB-CA-C	-6.04	98.32	110.40
1	P	291	ARG	CD-NE-CZ	6.03	132.04	123.60
1	P	448	ALA	CA-C-O	6.03	132.75	120.10
1	P	217	ARG	CD-NE-CZ	-6.02	115.17	123.60
1	P	299	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	P	400	THR	CA-CB-CG2	5.97	120.77	112.40
1	P	73	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	P	35	ASP	CB-CG-OD2	-5.95	112.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	449	THR	CA-CB-OG1	-5.89	96.63	109.00
1	P	435	PRO	C-N-CA	5.87	134.62	122.30
1	P	279	THR	CB-CA-C	-5.87	95.76	111.60
1	P	62	PHE	CB-CG-CD2	5.82	124.87	120.80
1	P	267	ASP	CA-C-O	-5.78	107.96	120.10
1	P	299	ARG	N-CA-CB	-5.76	100.22	110.60
1	P	386	VAL	CG1-CB-CG2	-5.76	101.69	110.90
1	P	390	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	P	312	GLU	CG-CD-OE1	5.75	129.79	118.30
1	P	471	THR	N-CA-CB	5.74	121.21	110.30
1	P	160	THR	CA-CB-OG1	-5.73	96.97	109.00
1	P	114	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	P	211	ASP	CB-CG-OD1	5.71	123.44	118.30
1	P	441	LEU	CA-C-N	5.70	129.74	117.20
1	P	408	THR	N-CA-CB	5.68	121.10	110.30
1	P	108	ALA	CB-CA-C	5.68	118.62	110.10
1	P	267	ASP	CB-CG-OD1	5.67	123.40	118.30
1	P	219	PHE	O-C-N	-5.67	113.64	122.70
1	P	391	THR	N-CA-CB	5.64	121.02	110.30
1	P	216	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	P	170	GLY	CA-C-N	5.56	127.31	116.20
1	P	250	SER	N-CA-CB	-5.55	102.17	110.50
1	P	263	THR	O-C-N	-5.55	113.81	122.70
1	P	327	THR	OG1-CB-CG2	5.54	122.74	110.00
1	P	63	TYR	CB-CG-CD1	5.52	124.31	121.00
1	P	188	GLU	CA-C-N	5.52	129.34	117.20
1	P	279	THR	CA-CB-OG1	5.48	120.51	109.00
1	P	488	CYS	C-N-CA	5.46	135.36	121.70
1	P	202	MET	CG-SD-CE	5.45	108.92	100.20
1	P	352	THR	O-C-N	-5.44	114.00	122.70
1	P	467	ASP	CA-C-N	5.43	129.15	117.20
1	P	287	MET	O-C-N	-5.41	114.05	122.70
1	P	288	ARG	CG-CD-NE	-5.39	100.49	111.80
1	P	411	ASP	CB-CG-OD1	5.38	123.14	118.30
1	P	451	GLU	OE1-CD-OE2	-5.37	116.85	123.30
1	P	333	SER	O-C-N	-5.36	114.12	122.70
1	P	302	LYS	N-CA-CB	-5.34	101.00	110.60
1	P	357	ASP	OD1-CG-OD2	-5.33	113.18	123.30
1	P	231	PRO	CB-CA-C	-5.32	98.69	112.00
1	P	63	TYR	CB-CA-C	-5.32	99.76	110.40
1	P	38	CYS	CA-CB-SG	5.30	123.54	114.00
1	P	495	PRO	CA-N-CD	-5.29	104.09	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	309	GLY	CA-C-O	-5.28	111.09	120.60
1	P	199	ALA	CB-CA-C	5.25	117.98	110.10
1	P	239	ALA	N-CA-CB	5.25	117.45	110.10
1	P	39	TYR	N-CA-CB	5.25	120.05	110.60
1	P	107	VAL	CA-CB-CG1	-5.25	103.03	110.90
1	P	270	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	P	338	PRO	CA-C-N	5.22	128.68	117.20
1	P	452	VAL	CA-CB-CG2	-5.17	103.15	110.90
1	P	503	PRO	CA-N-CD	-5.16	104.28	111.50
1	P	503	PRO	N-CD-CG	-5.15	95.48	103.20
1	P	150	SER	N-CA-CB	-5.14	102.79	110.50
1	P	67	SER	CA-CB-OG	-5.13	97.34	111.20
1	P	341	ALA	O-C-N	-5.13	114.50	122.70
1	P	404	ALA	CA-C-O	-5.12	109.35	120.10
1	P	332	SER	CB-CA-C	-5.09	100.43	110.10
1	P	188	GLU	OE1-CD-OE2	5.07	129.38	123.30
1	P	209	MET	CG-SD-CE	5.05	108.29	100.20
1	P	442	LEU	CA-C-N	5.05	126.29	116.20
1	P	86	GLY	CA-C-O	-5.04	111.52	120.60
1	P	174	GLN	CG-CD-OE1	-5.04	111.52	121.60
1	P	326	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	P	438	ASN	CB-CG-OD1	-5.04	111.53	121.60
1	P	51	GLN	CA-CB-CG	5.03	124.47	113.40
1	P	312	GLU	OE1-CD-OE2	-5.01	117.29	123.30
1	P	262	MET	CA-CB-CG	5.00	121.81	113.30
1	P	343	LEU	CA-CB-CG	5.00	126.81	115.30
1	P	55	GLY	C-N-CA	-5.00	111.79	122.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	181	LEU	Mainchain
1	P	194	LEU	Mainchain
1	P	241	ARG	Mainchain
1	P	287	MET	Mainchain
1	P	42	PRO	Mainchain
1	P	442	LEU	Mainchain

5.2 Too-close contacts (i)

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	P	3582	0	3453	109	1
2	A	28	0	25	0	0
3	P	1	0	0	0	0
4	P	173	0	0	18	1
All	All	3784	0	3478	109	2

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 (109) 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:P:102:LEU:O	4:P:2030:HOH:O	1.65	1.12
1:P:109:GLU:OE1	4:P:2034:HOH:O	1.90	0.88
1:P:423:HIS:HD2	4:P:2150:HOH:O	1.61	0.84
1:P:449:THR:HG22	1:P:451:GLU:H	1.53	0.74
1:P:24:VAL:HG13	1:P:276:VAL:HG22	1.71	0.73
1:P:279:THR:HG23	1:P:314:ALA:HB2	1.72	0.70
1:P:357:ASP:OD2	4:P:2121:HOH:O	2.09	0.70
1:P:261:LEU:O	1:P:265:ILE:HG13	1.92	0.69
1:P:442:LEU:O	1:P:443:GLY:C	2.30	0.68
1:P:449:THR:HG22	1:P:451:GLU:N	2.06	0.68
1:P:163:PRO:HG2	1:P:236:GLN:HG3	1.77	0.66
1:P:150:SER:H	1:P:153:GLN:NE2	1.95	0.64
1:P:150:SER:H	1:P:153:GLN:HE21	1.43	0.64
1:P:482:ASP:HB3	1:P:485:LEU:HD22	1.79	0.64
1:P:211:ASP:O	1:P:215:GLU:HG3	1.99	0.63
1:P:34:GLY:O	1:P:41:HIS:HB2	1.99	0.62
1:P:242:SER:HB3	1:P:252:MET:HE2	1.82	0.61
1:P:449:THR:CG2	1:P:451:GLU:H	2.12	0.61
1:P:84:ARG:HH11	1:P:84:ARG:HG2	1.66	0.61
1:P:357:ASP:OD1	1:P:359:SER:OG	2.17	0.59
1:P:199:ALA:O	1:P:200:ARG:C	2.40	0.59
1:P:500:CYS:O	1:P:501:HIS:HB3	2.02	0.59
1:P:60:THR:OG1	1:P:328:HIS:HD2	1.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:124:TRP:CE2	1:P:126:LEU:HB2	2.37	0.58
1:P:177:VAL:HB	1:P:486:GLN:OE1	2.03	0.58
1:P:407:ASP:CB	4:P:2141:HOH:O	2.51	0.57
1:P:327:THR:HG23	4:P:2113:HOH:O	2.03	0.57
1:P:179:ILE:O	1:P:191:PRO:HA	2.05	0.57
1:P:318:TRP:HB2	1:P:322:ILE:HD12	1.87	0.56
1:P:75:ALA:HB1	1:P:334:LEU:HD13	1.87	0.56
1:P:400:THR:HG23	4:P:2147:HOH:O	2.06	0.55
1:P:241:ARG:CB	1:P:252:MET:HE1	2.37	0.55
1:P:151:HIS:CD2	1:P:231:PRO:HD2	2.42	0.55
1:P:263:THR:O	1:P:264:ALA:C	2.43	0.54
1:P:341:ALA:O	1:P:342:ALA:C	2.46	0.54
1:P:136:PRO:HB2	1:P:137:PRO:HD3	1.89	0.54
1:P:149:TYR:HE1	1:P:179:ILE:HD11	1.73	0.54
1:P:400:THR:HB	1:P:423:HIS:HE1	1.73	0.54
1:P:213:GLN:NE2	1:P:268:LEU:HB3	2.23	0.54
1:P:449:THR:HG22	1:P:452:VAL:H	1.72	0.53
1:P:390:ARG:HD2	1:P:431:LEU:HD12	1.90	0.53
1:P:150:SER:HB3	1:P:153:GLN:NE2	2.24	0.52
1:P:265:ILE:HD13	1:P:274:THR:HG21	1.91	0.52
1:P:201:TYR:OH	1:P:226:HIS:HE1	1.92	0.52
1:P:109:GLU:OE2	4:P:2034:HOH:O	2.19	0.51
1:P:70:THR:N	1:P:71:PRO:HD2	2.26	0.50
1:P:159:LEU:HD21	1:P:191:PRO:HG3	1.94	0.50
1:P:337:LEU:HD12	1:P:338:PRO:N	2.27	0.49
1:P:400:THR:CG2	4:P:2147:HOH:O	2.59	0.49
1:P:407:ASP:CG	4:P:2141:HOH:O	2.50	0.49
1:P:151:HIS:NE2	1:P:231:PRO:HD2	2.28	0.48
1:P:440:ASN:ND2	1:P:442:LEU:H	2.10	0.48
1:P:501:HIS:O	1:P:501:HIS:CG	2.67	0.48
1:P:327:THR:CG2	4:P:2113:HOH:O	2.61	0.48
1:P:400:THR:CG2	1:P:423:HIS:HE1	2.26	0.48
1:P:268:LEU:O	1:P:270:LEU:HG	2.14	0.48
1:P:400:THR:HB	1:P:423:HIS:CE1	2.48	0.48
1:P:111:LEU:O	1:P:116:TYR:HB2	2.13	0.47
1:P:84:ARG:NH2	1:P:354:ASP:OD1	2.44	0.47
1:P:407:ASP:OD1	4:P:2141:HOH:O	2.20	0.47
1:P:197:LEU:HA	1:P:197:LEU:HD23	1.69	0.47
1:P:348:LEU:O	1:P:349:PRO:C	2.52	0.46
1:P:123:LYS:HD2	1:P:150:SER:HA	1.97	0.46
1:P:128:VAL:HB	4:P:2040:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:162:PHE:HB2	1:P:166:THR:HB	1.96	0.46
1:P:279:THR:CG2	1:P:313:PRO:O	2.64	0.46
1:P:428:LEU:H	1:P:440:ASN:ND2	2.14	0.46
1:P:190:GLN:HA	1:P:191:PRO:HA	1.73	0.45
1:P:327:THR:HG22	1:P:329:GLU:H	1.82	0.45
1:P:188:GLU:HG3	1:P:188:GLU:O	2.16	0.45
1:P:302:LYS:HD3	1:P:405:HIS:HB3	1.97	0.45
1:P:492:GLY:O	1:P:493:CYS:O	2.34	0.45
1:P:152:ASP:HB3	1:P:231:PRO:HD3	1.98	0.45
1:P:329:GLU:OE2	4:P:2113:HOH:O	2.21	0.45
1:P:400:THR:CB	1:P:423:HIS:HE1	2.30	0.45
1:P:77:LEU:HD12	1:P:126:LEU:CD1	2.47	0.45
1:P:24:VAL:CG1	1:P:276:VAL:HG22	2.45	0.44
1:P:393:LYS:NZ	4:P:2134:HOH:O	2.30	0.44
1:P:88:TYR:HB2	1:P:89:PRO:HA	1.99	0.44
1:P:299:ARG:HH21	1:P:411:ASP:CG	2.20	0.44
1:P:62:PHE:CE1	1:P:279:THR:HG21	2.52	0.44
1:P:318:TRP:CB	1:P:322:ILE:HD12	2.47	0.43
1:P:152:ASP:O	1:P:172:CYS:HB3	2.18	0.43
1:P:279:THR:HG22	1:P:313:PRO:O	2.19	0.43
1:P:149:TYR:HE1	1:P:179:ILE:CD1	2.31	0.43
1:P:123:LYS:NZ	1:P:150:SER:HB2	2.34	0.42
1:P:266:GLY:O	1:P:267:ASP:C	2.57	0.42
1:P:97:ARG:NH1	1:P:480:GLY:HA3	2.35	0.42
1:P:80:ARG:HG2	1:P:80:ARG:NH1	2.34	0.42
1:P:397:HIS:HB2	1:P:427:LEU:HB2	2.01	0.42
1:P:297:LEU:H	1:P:297:LEU:HD23	1.84	0.42
1:P:327:THR:CG2	1:P:329:GLU:H	2.33	0.42
1:P:108:ALA:O	1:P:109:GLU:C	2.58	0.42
1:P:423:HIS:CD2	4:P:2150:HOH:O	2.50	0.42
1:P:490:HIS:O	1:P:491:PRO:C	2.58	0.42
1:P:317:PHE:CE1	1:P:319:PRO:HD3	2.55	0.42
1:P:376:TYR:CZ	1:P:386:VAL:HG12	2.55	0.41
1:P:227:HIS:HA	1:P:228:THR:HA	1.79	0.41
1:P:502:CYS:O	1:P:502:CYS:SG	2.77	0.41
1:P:407:ASP:HB3	4:P:2141:HOH:O	2.19	0.41
1:P:202:MET:SD	1:P:261:LEU:CD1	3.09	0.41
1:P:329:GLU:OE1	4:P:2114:HOH:O	2.22	0.40
1:P:107:VAL:HG13	1:P:337:LEU:HB2	2.03	0.40
1:P:183:ALA:O	1:P:184:ASN:C	2.58	0.40
1:P:117:LEU:HD23	1:P:212:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:149:TYR:HB2	1:P:153:GLN:NE2	2.36	0.40
1:P:337:LEU:HD12	1:P:337:LEU:C	2.41	0.40
1:P:163:PRO:HA	1:P:164:PRO:C	2.42	0.40
1:P:492:GLY:O	1:P:493:CYS:C	2.59	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:2148:HOH:O	4:P:2148:HOH:O[5_555]	1.84	0.36
1:P:490:HIS:NE2	1:P:490:HIS:NE2[16_554]	2.17	0.03

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	P	477/489 (98%)	438 (92%)	35 (7%)	4 (1%)	19 29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	493	CYS
1	P	267	ASP
1	P	172	CYS
1	P	266	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	377/385 (98%)	334 (89%)	43 (11%)	5 8

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	24	VAL
1	P	52	LEU
1	P	61	ASP
1	P	67	SER
1	P	80	ARG
1	P	103	GLU
1	P	107	VAL
1	P	111	LEU
1	P	149	TYR
1	P	161	CYS
1	P	177	VAL
1	P	185	LEU
1	P	197	LEU
1	P	214	ARG
1	P	217	ARG
1	P	237	SER
1	P	240	GLU
1	P	254	LEU
1	P	261	LEU
1	P	262	MET
1	P	272	GLU
1	P	279	THR
1	P	282	ASN
1	P	287	MET
1	P	324	PRO
1	P	327	THR
1	P	334	LEU
1	P	336	LEU
1	P	337	LEU
1	P	343	LEU
1	P	351	VAL
1	P	352	THR
1	P	362	LEU
1	P	365	THR
1	P	371	GLN

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Mol	Chain	Res	Type
1	P	400	THR
1	P	433	LYS
1	P	442	LEU
1	P	451	GLU
1	P	466	LEU
1	P	485	LEU
1	P	494	THR
1	P	496	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	153	GLN
1	P	226	HIS
1	P	328	HIS
1	P	423	HIS
1	P	440	ASN
1	P	465	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

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	A	1	2,1	14,14,15	2.00	4 (28%)	17,19,21	3.55	11 (64%)
2	NAG	A	2	2	14,14,15	1.30	2 (14%)	17,19,21	2.51	6 (35%)

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	A	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	2	2	1/1/5/7	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAG	O7-C7	-4.23	1.13	1.23
2	A	1	NAG	C2-N2	4.06	1.53	1.46
2	A	2	NAG	O7-C7	-2.95	1.16	1.23
2	A	1	NAG	O4-C4	-2.84	1.36	1.43
2	A	1	NAG	O5-C5	-2.63	1.38	1.43
2	A	2	NAG	C2-N2	2.21	1.50	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	NAG	C8-C7-N2	6.98	127.92	116.10
2	A	1	NAG	O7-C7-N2	-6.47	110.06	121.95
2	A	1	NAG	O4-C4-C3	5.36	122.75	110.35
2	A	2	NAG	C1-O5-C5	5.16	119.19	112.19
2	A	2	NAG	O3-C3-C2	-5.13	98.84	109.47
2	A	2	NAG	C2-N2-C7	-4.80	116.08	122.90
2	A	1	NAG	O5-C1-C2	4.36	118.18	111.29
2	A	1	NAG	O4-C4-C5	-4.16	98.96	109.30
2	A	1	NAG	C2-N2-C7	-3.46	117.98	122.90
2	A	1	NAG	C1-O5-C5	3.27	116.62	112.19
2	A	1	NAG	C3-C4-C5	-3.18	104.56	110.24
2	A	2	NAG	C1-C2-N2	3.08	115.75	110.49
2	A	1	NAG	C6-C5-C4	-3.02	105.93	113.00
2	A	1	NAG	O3-C3-C2	2.96	115.58	109.47
2	A	1	NAG	O5-C5-C6	2.32	110.84	107.20
2	A	2	NAG	C3-C4-C5	2.18	114.13	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2	NAG	C4-C3-C2	2.06	114.03	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1	NAG	C1
2	A	2	NAG	C1

All (4) torsion outliers are listed below:

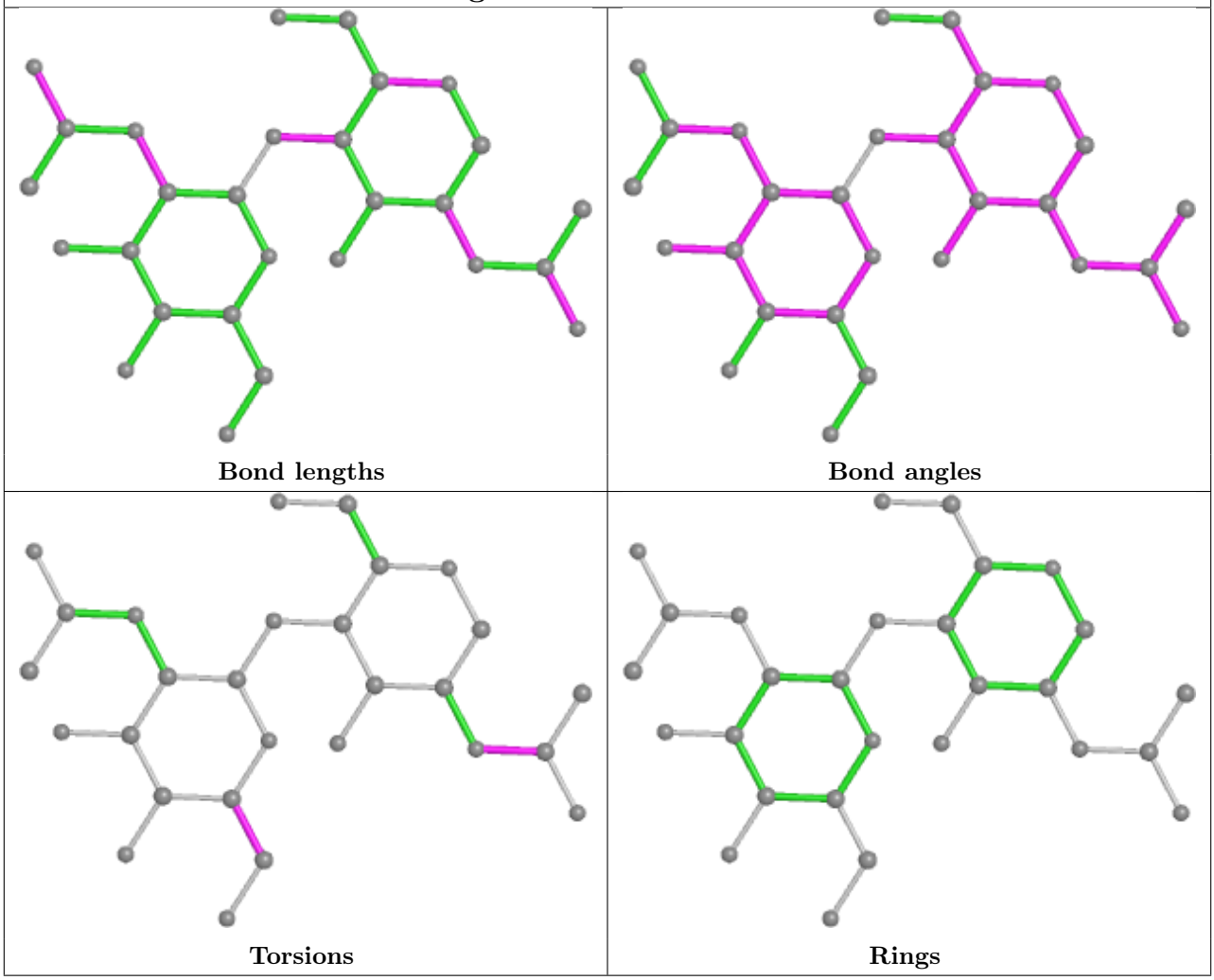
Mol	Chain	Res	Type	Atoms
2	A	1	NAG	C8-C7-N2-C2
2	A	1	NAG	O7-C7-N2-C2
2	A	2	NAG	O5-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain A



5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	P	481/489 (98%)	-0.79	1 (0%) 95 96	15, 34, 61, 95	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	495	PRO	2.5

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)

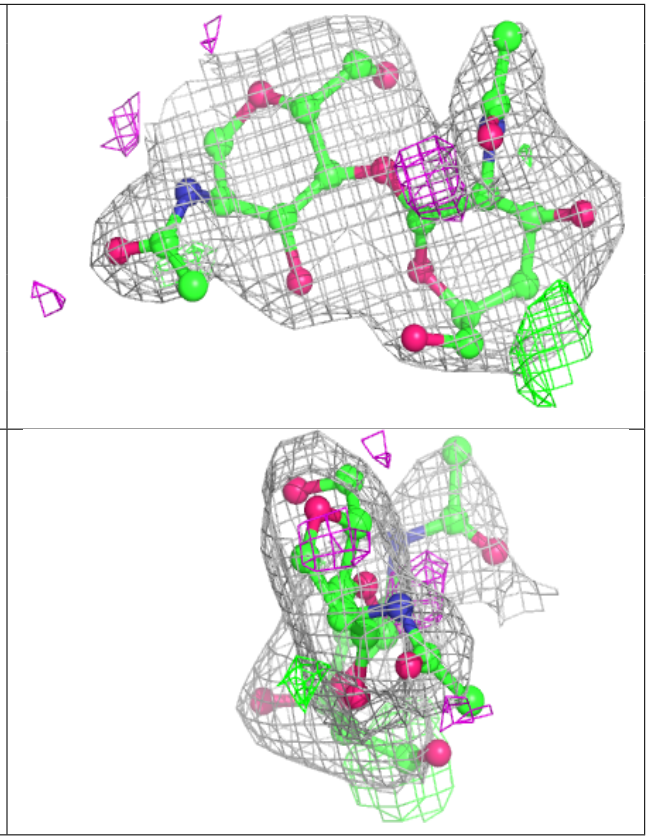
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	A	2	14/15	0.90	0.25	70,84,97,98	0
2	NAG	A	1	14/15	0.96	0.17	43,54,65,70	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 A:

$2mF_o$-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)

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
3	MG	P	603	1/1	0.98	0.27	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.