



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:32 AM UTC

PDB ID : 1QBB / pdb_00001qbb
Title : BACTERIAL CHITOBIASE COMPLEXED WITH CHITOBIOSE (DINAG)
Authors : Tews, I.; Perrakis, A.; Oppenheim, A.; Dauter, Z.; Wilson, K.S.; Vorgias, C.E.
Deposited on : 1996-06-07
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

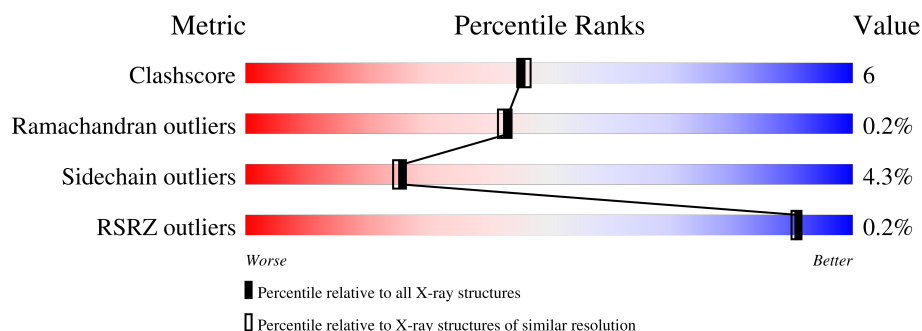
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

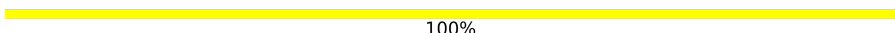
The reported resolution of this entry is 2.00 Å.

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	858	
2	B	2	

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	B	1[A]	X	-	-	-
2	NAG	B	1[B]	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14056 atoms, of which 6501 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 CHITOBIASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	858	Total	C	H	N	O	S	0	13	0
			13306	4306	6501	1189	1286	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	566	GLY	SER	conflict	UNP Q54468
A	828	GLY	ALA	conflict	UNP Q54468

- 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	B	2	Total	C	N	O	0	1	0
			30	16	2	12			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

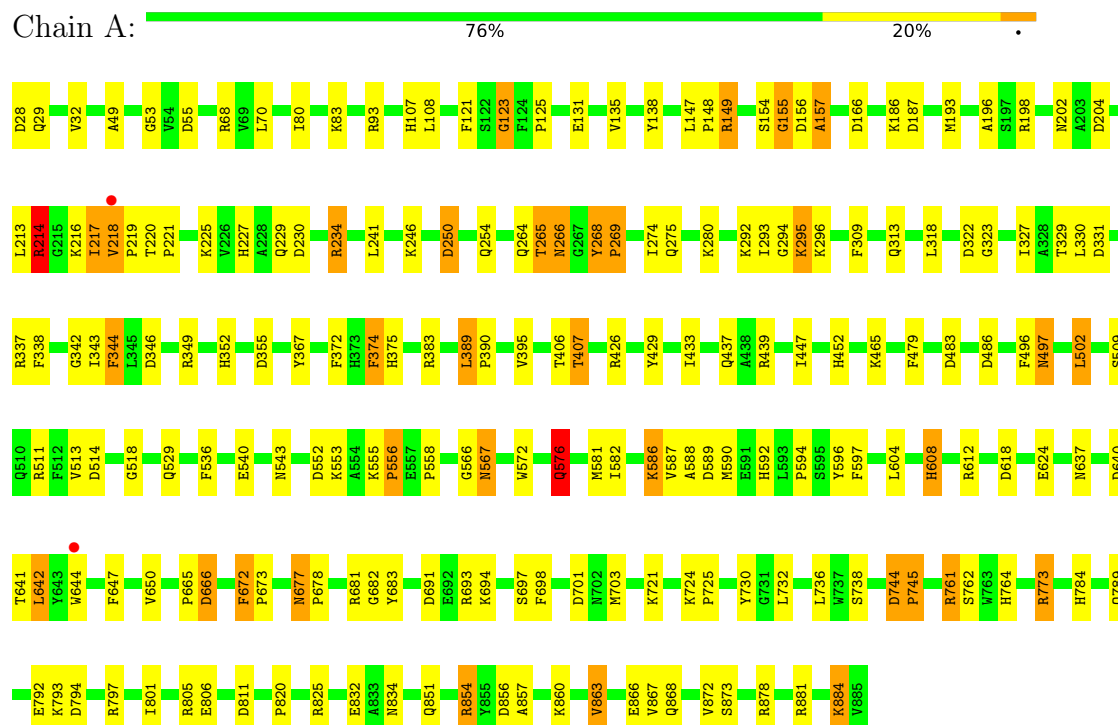
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	700	Total	O	0	0
			700	700		

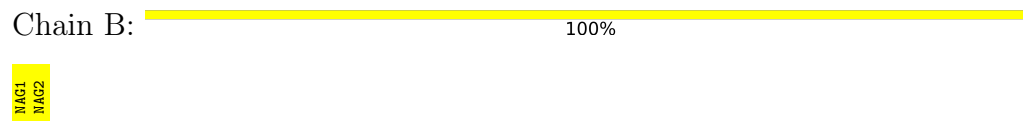
3 Residue-property plots

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: CHITOBIASE



• 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	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.70Å 99.90Å 87.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 15.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.00) 98.6 (15.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.01Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.151 , 0.212 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14056	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: SO4, 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	1.72	23/7040 (0.3%)	1.91	167/9534 (1.8%)

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	1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218[A]	VAL	CA-C	54.48	2.10	1.52
1	A	218[B]	VAL	CA-C	54.48	2.10	1.52
1	A	217	ILE	C-N	27.12	1.64	1.33
1	A	218[A]	VAL	CA-CB	-8.22	1.43	1.54
1	A	218[B]	VAL	CA-CB	-8.22	1.43	1.54
1	A	218[A]	VAL	N-CA	-7.74	1.37	1.46
1	A	218[B]	VAL	N-CA	-7.74	1.37	1.46
1	A	682	GLY	N-CA	-7.62	1.38	1.45
1	A	157	ALA	N-CA	-7.15	1.36	1.46
1	A	452	HIS	CE1-NE2	-6.49	1.26	1.32
1	A	343	ILE	CA-C	6.49	1.61	1.52
1	A	693	ARG	CD-NE	-6.10	1.37	1.46
1	A	773	ARG	CD-NE	-5.91	1.38	1.46
1	A	218[A]	VAL	CB-CG1	-5.67	1.33	1.52
1	A	218[B]	VAL	CB-CG1	-5.67	1.33	1.52
1	A	497	ASN	C-O	-5.46	1.18	1.24
1	A	395	VAL	C-N	-5.22	1.27	1.33
1	A	881	ARG	CB-CG	-5.21	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	GLN	N-CA	-5.19	1.41	1.46
1	A	773	ARG	NE-CZ	-5.18	1.27	1.33
1	A	216	LYS	C-O	-5.15	1.17	1.23
1	A	148	PRO	N-CA	-5.12	1.41	1.47
1	A	294	GLY	N-CA	5.02	1.49	1.44

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ASN	CA-CB-CG	31.73	144.33	112.60
1	A	773	ARG	CD-NE-CZ	21.97	155.16	124.40
1	A	218[A]	VAL	O-C-N	17.77	141.36	121.10
1	A	218[B]	VAL	O-C-N	17.77	141.36	121.10
1	A	217	ILE	O-C-N	-17.26	99.86	122.47
1	A	218[A]	VAL	N-CA-C	-14.71	77.11	108.88
1	A	218[B]	VAL	N-CA-C	-14.71	77.11	108.88
1	A	693	ARG	CD-NE-CZ	14.49	144.69	124.40
1	A	355	ASP	CA-CB-CG	11.82	124.42	112.60
1	A	266	ASN	OD1-CG-ND2	-11.55	111.05	122.60
1	A	854	ARG	CD-NE-CZ	10.90	139.66	124.40
1	A	218[A]	VAL	CA-CB-CG2	-10.52	92.52	110.40
1	A	218[B]	VAL	CA-CB-CG2	-10.52	92.52	110.40
1	A	214	ARG	CA-CB-CG	10.28	134.66	114.10
1	A	805	ARG	CD-NE-CZ	9.66	137.93	124.40
1	A	640	ASP	CA-CB-CG	9.15	121.75	112.60
1	A	552	ASP	CA-C-N	8.95	135.04	120.63
1	A	552	ASP	C-N-CA	8.95	135.04	120.63
1	A	497	ASN	N-CA-CB	8.62	119.56	108.96
1	A	156	ASP	CA-CB-CG	8.61	121.21	112.60
1	A	218[A]	VAL	N-CA-CB	8.53	123.16	111.21
1	A	218[B]	VAL	N-CA-CB	8.53	123.16	111.21
1	A	374	PHE	CA-CB-CG	8.43	122.23	113.80
1	A	49	ALA	CA-C-N	8.22	130.66	120.22
1	A	49	ALA	C-N-CA	8.22	130.66	120.22
1	A	681	ARG	CD-NE-CZ	8.17	135.83	124.40
1	A	323	GLY	CA-C-N	8.10	133.55	120.60
1	A	323	GLY	C-N-CA	8.10	133.55	120.60
1	A	761	ARG	CD-NE-CZ	8.04	135.66	124.40
1	A	811	ASP	CA-CB-CG	7.90	120.50	112.60
1	A	881	ARG	CA-CB-CG	7.89	129.88	114.10
1	A	567	ASN	CA-CB-CG	7.67	120.27	112.60
1	A	730	TYR	O-C-N	-7.64	111.50	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	ARG	CB-CG-CD	7.63	128.86	111.30
1	A	486	ASP	CA-CB-CG	7.56	120.16	112.60
1	A	155	GLY	CA-C-N	7.52	130.58	120.65
1	A	155	GLY	C-N-CA	7.52	130.58	120.65
1	A	204	ASP	CA-CB-CG	7.49	120.08	112.60
1	A	612	ARG	NE-CZ-NH2	-7.44	112.50	119.20
1	A	738[A]	SER	N-CA-C	7.42	121.64	112.59
1	A	738[B]	SER	N-CA-C	7.42	121.64	112.59
1	A	672	PHE	CA-CB-CG	7.37	121.17	113.80
1	A	346	ASP	CA-CB-CG	7.28	119.88	112.60
1	A	794	ASP	CA-CB-CG	7.23	119.83	112.60
1	A	241	LEU	CA-C-N	7.17	130.61	120.28
1	A	241	LEU	C-N-CA	7.17	130.61	120.28
1	A	268	TYR	CA-C-N	7.04	127.30	119.90
1	A	268	TYR	C-N-CA	7.04	127.30	119.90
1	A	107	HIS	CA-CB-CG	7.03	120.83	113.80
1	A	805	ARG	CG-CD-NE	7.00	127.39	112.00
1	A	677	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	A	536	PHE	CA-CB-CG	6.87	120.67	113.80
1	A	343	ILE	N-CA-CB	6.83	121.10	111.82
1	A	202	ASN	CA-CB-CG	6.79	119.39	112.60
1	A	691	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	156	ASP	CA-C-N	6.65	134.24	121.54
1	A	156	ASP	C-N-CA	6.65	134.24	121.54
1	A	383	ARG	CD-NE-CZ	6.61	133.66	124.40
1	A	338	PHE	CA-CB-CG	6.59	120.39	113.80
1	A	730	TYR	CA-C-O	6.58	127.30	119.60
1	A	250	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	352	HIS	CA-CB-CG	-6.49	107.31	113.80
1	A	437	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	A	784	HIS	CA-CB-CG	6.44	120.24	113.80
1	A	666	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	55	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	594	PRO	CA-C-N	6.32	129.27	120.29
1	A	594	PRO	C-N-CA	6.32	129.27	120.29
1	A	576	GLN	CB-CG-CD	6.26	123.24	112.60
1	A	29	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	A	866	GLU	CA-CB-CG	6.24	126.58	114.10
1	A	483	ASP	CA-C-N	6.18	125.86	119.56
1	A	483	ASP	C-N-CA	6.18	125.86	119.56
1	A	389	LEU	CA-C-N	6.14	126.03	119.28
1	A	389	LEU	C-N-CA	6.14	126.03	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	618	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	390	PRO	N-CA-CB	6.12	110.00	103.39
1	A	265	THR	N-CA-C	6.12	118.75	111.71
1	A	123	GLY	N-CA-C	6.04	119.06	112.29
1	A	597	PHE	CA-C-N	6.04	126.64	119.94
1	A	597	PHE	C-N-CA	6.04	126.64	119.94
1	A	556	PRO	N-CA-CB	6.02	108.53	103.17
1	A	745	PRO	N-CA-CB	6.02	109.89	103.39
1	A	407[A]	THR	CA-C-O	6.02	125.45	118.77
1	A	407[B]	THR	CA-C-O	6.02	125.45	118.77
1	A	342	GLY	CA-C-N	6.01	131.52	122.98
1	A	342	GLY	C-N-CA	6.01	131.52	122.98
1	A	496	PHE	CA-C-O	-6.01	114.86	121.89
1	A	383	ARG	NE-CZ-NH2	5.95	124.56	119.20
1	A	576	GLN	OE1-CD-NE2	-5.94	116.66	122.60
1	A	149	ARG	CA-C-O	5.92	129.43	122.03
1	A	724	LYS	CA-C-N	5.92	125.86	119.76
1	A	724	LYS	C-N-CA	5.92	125.86	119.76
1	A	80	ILE	N-CA-CB	5.88	119.06	111.83
1	A	375	HIS	CA-CB-CG	5.85	119.65	113.80
1	A	518	GLY	O-C-N	-5.85	116.34	122.13
1	A	269	PRO	N-CA-CB	5.83	108.49	103.36
1	A	344	PHE	O-C-N	-5.82	116.69	123.27
1	A	797	ARG	CD-NE-CZ	5.80	132.53	124.40
1	A	764	HIS	CA-C-O	5.79	126.70	120.38
1	A	196	ALA	CA-C-O	-5.79	114.28	120.42
1	A	349	ARG	CD-NE-CZ	5.75	132.45	124.40
1	A	266	ASN	CB-CG-ND2	5.75	125.02	116.40
1	A	275	GLN	CA-C-N	5.72	125.85	119.32
1	A	275	GLN	C-N-CA	5.72	125.85	119.32
1	A	558	PRO	N-CA-CB	5.72	108.33	103.35
1	A	642	LEU	CB-CA-C	-5.70	101.90	110.90
1	A	337	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	A	681	ARG	NE-CZ-NH2	-5.66	114.11	119.20
1	A	725	PRO	N-CA-CB	5.66	108.34	103.31
1	A	834	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	A	147	LEU	CA-C-N	5.61	126.07	120.52
1	A	147	LEU	C-N-CA	5.61	126.07	120.52
1	A	274	ILE	CA-C-N	5.61	128.69	122.74
1	A	274	ILE	C-N-CA	5.61	128.69	122.74
1	A	313	GLN	CA-C-N	5.60	128.24	120.29
1	A	313	GLN	C-N-CA	5.60	128.24	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	A	447	ILE	CA-C-N	5.59	128.70	120.82
1	A	447	ILE	C-N-CA	5.59	128.70	120.82
1	A	234	ARG	N-CA-C	5.58	118.13	111.71
1	A	789	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	A	502	LEU	CA-CB-CG	5.58	135.83	116.30
1	A	624	GLU	CB-CG-CD	5.57	122.07	112.60
1	A	806	GLU	N-CA-C	5.57	117.43	111.36
1	A	543	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	A	264	GLN	O-C-N	-5.54	117.06	123.33
1	A	338	PHE	CA-C-N	5.54	125.16	119.56
1	A	338	PHE	C-N-CA	5.54	125.16	119.56
1	A	878	ARG	CD-NE-CZ	5.51	132.11	124.40
1	A	789	GLN	CB-CG-CD	5.50	121.95	112.60
1	A	744	ASP	CA-C-N	5.49	125.32	119.28
1	A	744	ASP	C-N-CA	5.49	125.32	119.28
1	A	53	GLY	N-CA-C	5.47	122.87	115.32
1	A	309	PHE	CA-C-N	5.47	128.06	120.29
1	A	309	PHE	C-N-CA	5.47	128.06	120.29
1	A	540	GLU	N-CA-CB	-5.47	103.70	111.84
1	A	856	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	138	TYR	CA-C-N	5.38	131.06	121.75
1	A	138	TYR	C-N-CA	5.38	131.06	121.75
1	A	514	ASP	O-C-N	-5.37	116.43	122.12
1	A	322	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	637	ASN	CA-CB-CG	5.37	117.97	112.60
1	A	514	ASP	CA-C-O	5.34	126.21	120.55
1	A	229	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	A	221	PRO	N-CA-CB	5.29	108.25	103.33
1	A	439	ARG	O-C-N	-5.29	115.99	122.34
1	A	497	ASN	CB-CA-C	-5.28	107.80	114.40
1	A	187	ASP	CA-CB-CG	-5.26	107.34	112.60
1	A	426	ARG	CD-NE-CZ	-5.23	117.08	124.40
1	A	372	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	367	TYR	CA-C-O	5.16	126.19	119.95
1	A	608	HIS	CA-CB-CG	-5.15	108.65	113.80
1	A	572	TRP	CA-C-N	5.15	127.43	120.38
1	A	572	TRP	C-N-CA	5.15	127.43	120.38
1	A	873	SER	CA-C-N	5.13	124.92	119.28
1	A	873	SER	C-N-CA	5.13	124.92	119.28
1	A	764	HIS	N-CA-C	5.13	117.32	109.07
1	A	213	LEU	CA-C-O	5.11	125.62	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	730	TYR	N-CA-CB	-5.11	102.66	110.33
1	A	529	GLN	CA-C-N	5.09	125.09	119.90
1	A	529	GLN	C-N-CA	5.09	125.09	119.90
1	A	337	ARG	NH1-CZ-NH2	5.08	125.91	119.30
1	A	872	VAL	O-C-N	-5.07	117.67	123.10
1	A	820	PRO	N-CA-CB	5.03	108.01	103.33
1	A	125	PRO	N-CA-CB	5.02	108.00	103.33
1	A	588	ALA	N-CA-C	5.01	117.85	111.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	ILE	Mainchain

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	6805	6501	6597	77	0
2	B	30	0	16	0	0
3	A	20	0	0	1	0
4	A	700	0	0	11	2
All	All	7555	6501	6613	77	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 6.

All (77) 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:218[A]:VAL:CB	1:A:218[A]:VAL:CG2	2.31	1.08
1:A:218[A]:VAL:CG1	1:A:801:ILE:HD13	1.98	0.92
1:A:566:GLY:HA3	4:A:1256:HOH:O	1.70	0.90
1:A:218[A]:VAL:HG11	1:A:801:ILE:HG21	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LYS:HG3	1:A:331:ASP:OD1	1.85	0.77
1:A:218[A]:VAL:HG11	1:A:801:ILE:HD13	1.70	0.72
1:A:218[A]:VAL:HG12	1:A:801:ILE:HD13	1.72	0.71
1:A:832:GLU:OE1	4:A:1366:HOH:O	2.11	0.68
1:A:218[A]:VAL:CG1	1:A:801:ILE:HG21	2.25	0.67
1:A:465:LYS:HD2	4:A:1228:HOH:O	1.93	0.67
1:A:825:ARG:NH2	4:A:1366:HOH:O	2.30	0.65
1:A:697[B]:SER:OG	4:A:1270:HOH:O	2.14	0.64
1:A:250:ASP:O	1:A:254[B]:GLN:HG3	1.98	0.64
1:A:642:LEU:HD21	1:A:703[B]:MET:HE3	1.80	0.64
1:A:193[A]:MET:HE1	1:A:198:ARG:HA	1.79	0.63
1:A:581:MET:HE3	4:A:1395:HOH:O	1.98	0.63
1:A:28:ASP:N	1:A:154:SER:HG	1.98	0.61
1:A:732:LEU:HD23	1:A:762:SER:HB3	1.85	0.58
1:A:497:ASN:HB3	3:A:1:SO4:O1	2.05	0.55
1:A:641:THR:HG22	1:A:665:PRO:HG2	1.88	0.55
1:A:218[A]:VAL:CB	1:A:218[A]:VAL:CG1	2.87	0.53
1:A:295:LYS:O	1:A:295:LYS:HD2	2.11	0.50
1:A:673:PRO:HD3	1:A:683:TYR:O	2.12	0.50
1:A:642:LEU:HD21	1:A:703[B]:MET:HB3	1.94	0.49
1:A:193[A]:MET:CE	1:A:198:ARG:HA	2.43	0.48
1:A:857:ALA:O	1:A:860:LYS:NZ	2.41	0.48
1:A:642:LEU:HD22	1:A:647:PHE:HB3	1.96	0.48
1:A:68:ARG:HG2	1:A:135:VAL:HG22	1.96	0.47
1:A:576:GLN:HG3	4:A:1315:HOH:O	2.13	0.47
1:A:296:LYS:HA	1:A:296:LYS:HD2	1.69	0.47
1:A:318:LEU:HD11	1:A:330:LEU:HD21	1.96	0.47
1:A:744:ASP:N	1:A:745:PRO:CD	2.77	0.47
1:A:698:PHE:O	1:A:761:ARG:HD2	2.15	0.46
1:A:429:TYR:CE2	1:A:433:ILE:HD11	2.50	0.46
1:A:604:LEU:O	1:A:608:HIS:HD2	1.99	0.45
1:A:589:ASP:OD1	1:A:592:HIS:ND1	2.44	0.45
1:A:295:LYS:HD2	4:A:1267:HOH:O	2.16	0.45
1:A:650:VAL:HG21	1:A:703[A]:MET:HE1	1.98	0.45
1:A:70:LEU:HD11	1:A:131:GLU:HB3	1.99	0.44
1:A:214:ARG:NH2	1:A:230:ASP:OD1	2.44	0.43
1:A:863:VAL:HG11	1:A:867:VAL:HG21	1.99	0.43
1:A:389:LEU:HD21	1:A:479:PHE:CD2	2.53	0.43
1:A:227:HIS:HB2	1:A:329:THR:OG1	2.19	0.43
1:A:268:TYR:HA	1:A:269:PRO:HD3	1.75	0.42
1:A:509:SER:O	1:A:513:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:HG2	1:A:166:ASP:HA	2.02	0.42
1:A:218[A]:VAL:CG2	1:A:218[A]:VAL:CG1	2.98	0.42
1:A:344:PHE:CD1	1:A:344:PHE:C	2.97	0.42
1:A:121:PHE:CZ	1:A:123:GLY:HA2	2.54	0.41
1:A:293:ILE:HD13	1:A:327:ILE:HD12	2.01	0.41
1:A:32:VAL:HG23	1:A:154:SER:HB3	2.02	0.41
1:A:582:ILE:HD12	1:A:590:MET:HE2	2.03	0.41
1:A:269:PRO:HD2	1:A:296:LYS:O	2.21	0.41
1:A:672:PHE:HA	1:A:683:TYR:O	2.21	0.41
1:A:406:THR:HG23	1:A:407[A]:THR:HG23	2.02	0.41
1:A:566:GLY:CA	4:A:1256:HOH:O	2.48	0.41
1:A:576:GLN:CG	4:A:1315:HOH:O	2.68	0.41
1:A:677:ASN:HA	1:A:678:PRO:HD3	1.94	0.41
1:A:68:ARG:HD3	4:A:1151:HOH:O	2.22	0.40
1:A:555:LYS:N	1:A:556:PRO:HD3	2.36	0.40
1:A:586:LYS:NZ	1:A:596[A]:TYR:OH	2.45	0.40
1:A:868:GLN:HG2	1:A:884:LYS:HG3	2.04	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:A:1388:HOH:O	4:A:1388:HOH:O[2_565]	1.63	0.57
4:A:1338:HOH:O	4:A:1441:HOH:O[3_556]	2.15	0.05

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	869/858 (101%)	847 (98%)	20 (2%)	2 (0%)	43 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
1	A	155	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	A	718/705 (102%)	688 (96%)	30 (4%)	26	25

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	108	LEU
1	A	186	LYS
1	A	214	ARG
1	A	225	LYS
1	A	234	ARG
1	A	246	LYS
1	A	265	THR
1	A	266	ASN
1	A	280	LYS
1	A	295	LYS
1	A	374	PHE
1	A	502	LEU
1	A	553	LYS
1	A	567	ASN
1	A	576	GLN
1	A	586	LYS
1	A	587	VAL
1	A	644	TRP
1	A	666	ASP
1	A	701	ASP
1	A	721	LYS
1	A	736	LEU
1	A	773	ARG
1	A	792	GLU

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Mol	Chain	Res	Type
1	A	793	LYS
1	A	851	GLN
1	A	854	ARG
1	A	863	VAL
1	A	884	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	140	GLN
1	A	172	GLN
1	A	567	ASN
1	A	599	GLN
1	A	851	GLN
1	A	853	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 ⓘ

3 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[A]	-	15,15,15	1.18	1 (6%)	21,21,21	2.07	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1[B]	-	15,15,15	1.36	2 (13%)	21,21,21	2.23	8 (38%)
2	NAG	B	2	2	14,14,15	1.45	3 (21%)	17,19,21	3.02	5 (29%)

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[A]	-	1/1/6/7	0/6/26/26	0/1/1/1
2	NAG	B	1[B]	-	1/1/6/7	0/6/26/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-2.80	1.39	1.43
2	B	2	NAG	C3-C2	-2.64	1.47	1.52
2	B	1[B]	NAG	O1-C1	-2.58	1.31	1.39
2	B	2	NAG	O5-C5	-2.51	1.38	1.43
2	B	1[A]	NAG	C3-C2	2.22	1.57	1.53
2	B	1[B]	NAG	C3-C2	2.22	1.57	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	9.78	125.29	112.19
2	B	2	NAG	O3-C3-C2	5.31	120.44	109.40
2	B	1[A]	NAG	O5-C5-C4	5.02	118.75	109.70
2	B	1[B]	NAG	O5-C5-C4	5.02	118.75	109.70
2	B	1[A]	NAG	O5-C1-C2	4.20	113.74	109.52
2	B	1[B]	NAG	O5-C1-C2	4.20	113.74	109.52
2	B	1[B]	NAG	O1-C1-C2	3.48	116.44	109.22
2	B	1[A]	NAG	O3-C3-C2	-3.30	103.01	109.58
2	B	1[B]	NAG	O3-C3-C2	-3.30	103.01	109.58
2	B	1[A]	NAG	C1-O5-C5	3.19	119.82	113.65
2	B	1[B]	NAG	C1-O5-C5	3.19	119.82	113.65
2	B	2	NAG	O5-C5-C6	2.48	112.49	107.66
2	B	2	NAG	C1-C2-N2	2.44	114.27	110.43
2	B	2	NAG	O4-C4-C3	2.30	115.81	110.38
2	B	1[B]	NAG	O1-C1-O5	2.25	117.11	110.41
2	B	1[A]	NAG	C6-C5-C4	2.23	118.49	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1[B]	NAG	C6-C5-C4	2.23	118.49	113.02
2	B	1[A]	NAG	O4-C4-C5	2.21	114.77	109.32
2	B	1[B]	NAG	O4-C4-C5	2.21	114.77	109.32

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1[A]	NAG	C1
2	B	1[B]	NAG	C1

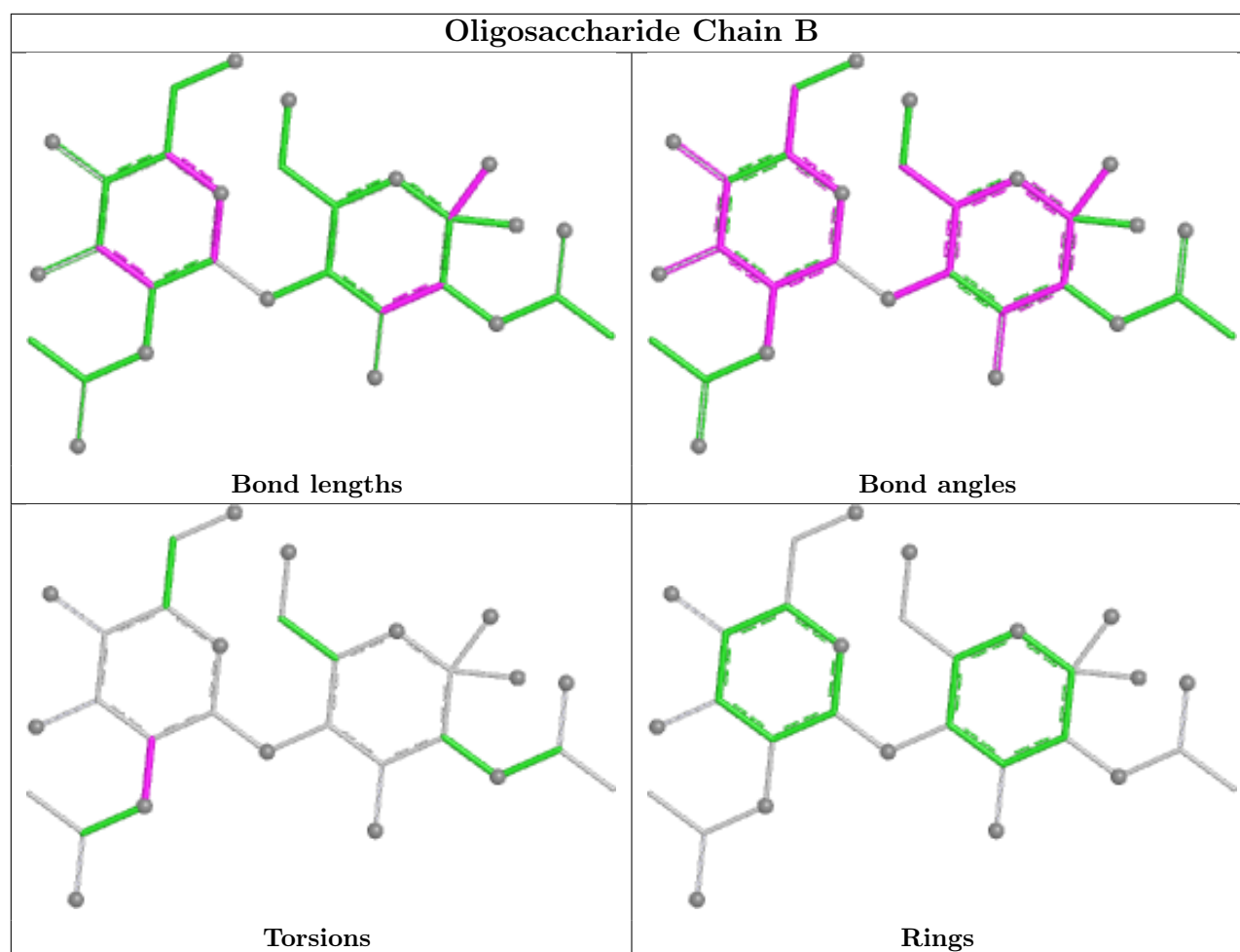
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C1-C2-N2-C7

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.



5.6 Ligand geometry [i](#)

4 ligands 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	$\# Z > 2$
3	SO4	A	4	-	4,4,4	0.83	0	6,6,6	0.58	0
3	SO4	A	3	-	4,4,4	0.95	0	6,6,6	0.91	0
3	SO4	A	1	-	4,4,4	1.02	0	6,6,6	0.88	0
3	SO4	A	2	-	4,4,4	0.89	0	6,6,6	0.54	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	217:ILE	C	218:VAL	N	1.64

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	858/858 (100%)	-1.11	2 (0%) 91 90	3, 11, 37, 77	13 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	644	TRP	4.3
1	A	218[A]	VAL	2.9

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

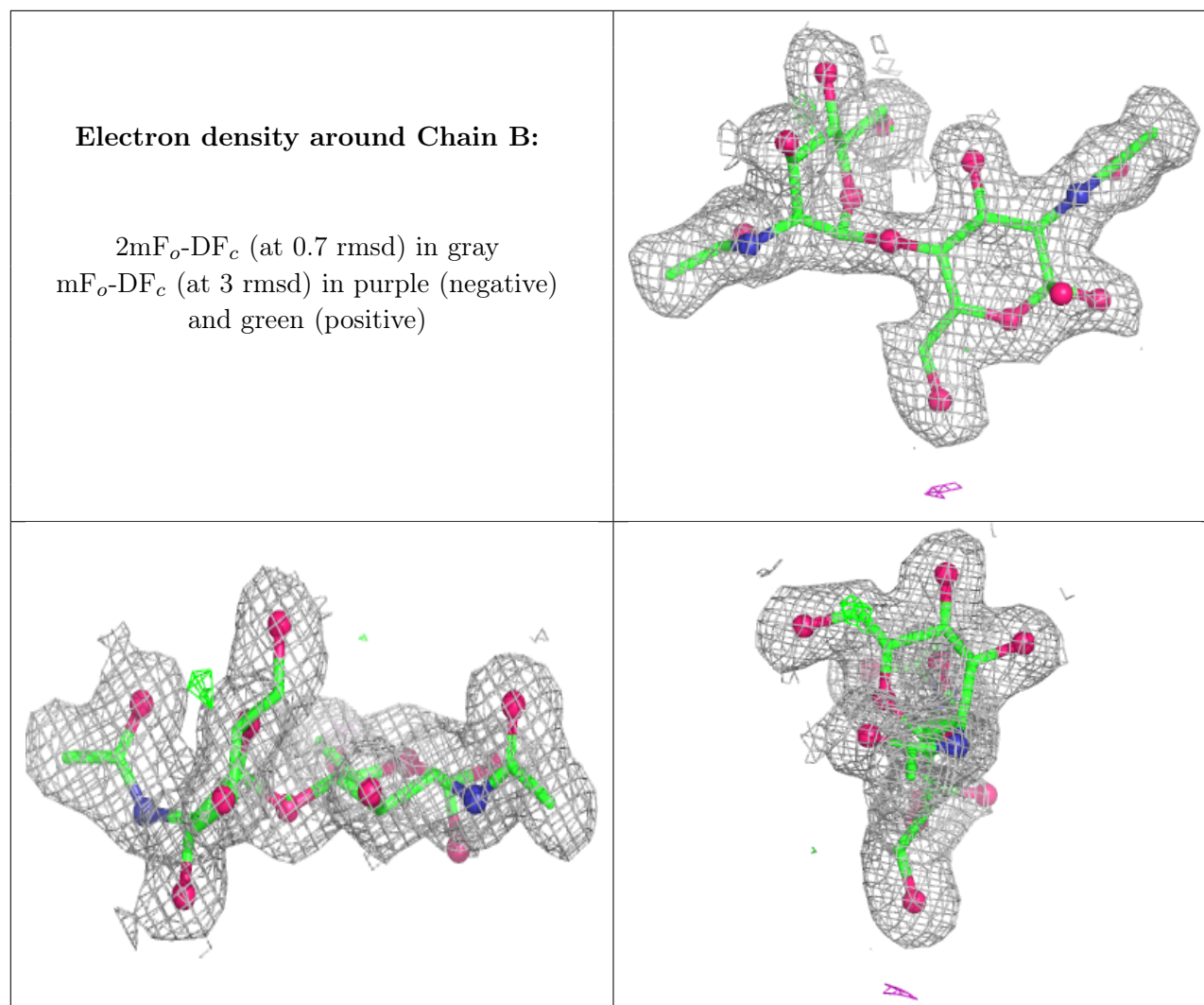
There are no non-standard protein/DNA/RNA residues in this entry.

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	B	1[A]	15/15	0.98	0.04	3,7,10,10	1
2	NAG	B	1[B]	15/15	0.98	0.04	3,6,8,10	1
2	NAG	B	2	14/15	0.98	0.04	2,4,7,7	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 [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($\text{\AA}^2$)	Q<0.9
3	SO4	A	2	5/5	0.77	0.16	70,71,72,75	0
3	SO4	A	4	5/5	0.87	0.14	15,29,30,32	5
3	SO4	A	1	5/5	0.95	0.08	13,14,26,29	0
3	SO4	A	3	5/5	0.96	0.07	28,28,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.