



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:08 AM UTC

PDB ID : 1NN2 / pdb_00001nn2
Title : THREE-DIMENSIONAL STRUCTURE OF THE NEURAMINIDASE OF INFLUENZA VIRUS A(SLASH)TOKYO(SLASH)3(SLASH)67 AT 2.2 ANGSTROMS RESOLUTION
Authors : Varghese, J.N.; Colman, P.M.
Deposited on : 1991-03-28
Resolution : 2.20 Å(reported)

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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

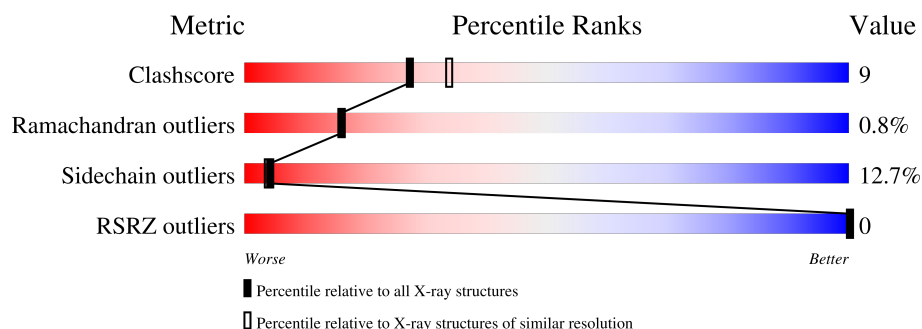
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	388	
2	B	2	
3	C	7	
4	D	6	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4429 atoms, of which 1100 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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	0	0
			3746	1866	724	545	588	23			

There is a discrepancy between the modelled and reference sequences:

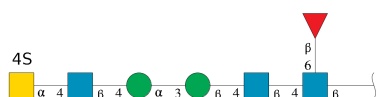
Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	conflict	UNP P06820

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



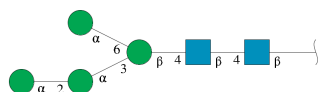
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2	Total	C	H	N	O	28	0	0
			55	16	27	2	10			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-4-O-sulfo-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



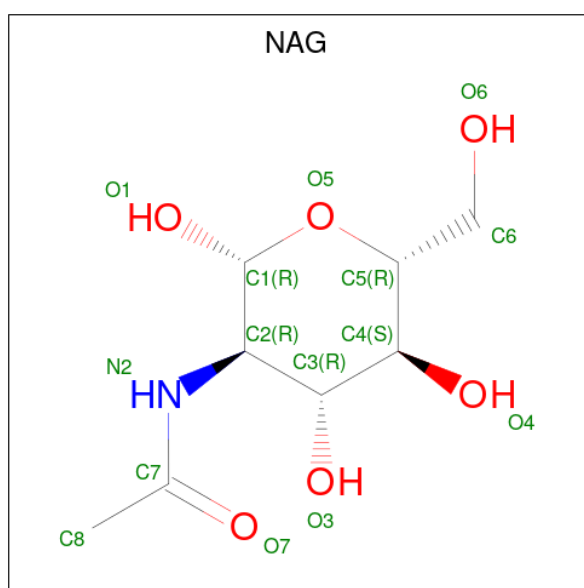
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	7	Total	C	H	N	O	S	69	0	0
			174	50	82	4	37	1			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	6	Total	C	H	N	O	0	0	0
			139	40	67	2	30			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	A	1	Total	C	H	N	O	28	0
			28	8	14	1	5		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	86	Total	H	O	0	0
			258	172	86		

ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  33% 67%

MAG1	MAG2	MAN3	MAN4	MAN5	MAN6
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4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.60Å 139.60Å 191.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20 6.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.20) 59.2 (6.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available) 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.3	EDS
L-test for twinning ¹	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.043 for -1/2*h+1/2*k-1/2*l, 1/2*h-1/2*k-1/2*l, -h-k 0.047 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	0.93	EDS
Total number of atoms	4429	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: BMA, FUL, NGK, NAG, MAN, CA

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	1.27	22/3092 (0.7%)	2.16	139/4194 (3.3%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	VAL	CA-CB	10.68	1.65	1.53
1	A	240	VAL	CA-CB	9.23	1.67	1.54
1	A	418	ILE	CA-CB	9.18	1.65	1.54
1	A	427	ILE	CA-CB	9.10	1.66	1.54
1	A	122	VAL	CA-CB	7.96	1.66	1.54
1	A	424	VAL	CA-CB	7.65	1.64	1.54
1	A	322	VAL	CA-CB	7.31	1.64	1.54
1	A	274	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	184	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	191	HIS	CD2-NE2	-6.48	1.30	1.37
1	A	144	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	155	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	347	GLN	C-O	6.22	1.31	1.24
1	A	150	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	231	VAL	CA-CB	6.08	1.65	1.55
1	A	264	HIS	CD2-NE2	-6.00	1.31	1.37
1	A	297	GLY	C-O	5.82	1.31	1.24
1	A	168	HIS	CD2-NE2	-5.71	1.31	1.37
1	A	293	ASP	C-O	5.53	1.30	1.24
1	A	168	HIS	CG-ND1	-5.18	1.32	1.38
1	A	274	HIS	CG-ND1	-5.11	1.32	1.38
1	A	445	VAL	CA-CB	5.07	1.62	1.54

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	CYS	N-CA-CB	-13.54	88.71	110.77
1	A	329	ASP	CA-CB-CG	12.89	125.49	112.60
1	A	297	GLY	O-C-N	11.15	133.80	123.54
1	A	164	GLY	CA-C-N	-10.21	115.24	122.59
1	A	164	GLY	C-N-CA	-10.21	115.24	122.59
1	A	410	PHE	CA-CB-CG	10.18	123.98	113.80
1	A	455	THR	N-CA-CB	-10.15	95.29	111.43
1	A	397	ILE	N-CA-C	-9.72	103.45	111.81
1	A	293	ASP	CA-C-O	9.70	130.98	120.32
1	A	124	CYS	CB-CA-C	9.69	125.06	110.14
1	A	387	ASN	N-CA-C	9.60	124.62	113.38
1	A	434	THR	N-CA-CB	-9.37	96.58	110.53
1	A	309	ASP	CA-CB-CG	9.29	121.89	112.60
1	A	298	SER	N-CA-C	-9.28	102.47	113.88
1	A	290	ILE	N-CA-C	-8.71	95.03	107.75
1	A	220	GLN	OE1-CD-NE2	-8.54	114.06	122.60
1	A	299	ASN	CA-CB-CG	8.46	121.06	112.60
1	A	277	GLU	N-CA-C	8.37	122.97	111.17
1	A	353	ALA	O-C-N	-8.01	116.20	123.41
1	A	434	THR	N-CA-C	7.93	123.13	113.38
1	A	358	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	A	192	VAL	N-CA-C	-7.55	96.72	107.75
1	A	123	SER	N-CA-C	-7.24	98.30	109.52
1	A	240	VAL	N-CA-C	-7.14	98.19	108.48
1	A	387	ASN	OD1-CG-ND2	-7.14	115.46	122.60
1	A	91	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	A	318	CYS	N-CA-C	7.12	119.66	111.11
1	A	241	MET	CG-SD-CE	-7.11	85.26	100.90
1	A	211	LEU	N-CA-C	-7.00	97.15	108.41
1	A	264	HIS	CB-CG-CD2	-6.99	122.11	131.20
1	A	297	GLY	CA-C-O	6.95	129.06	121.48
1	A	226	GLN	CA-CB-CG	6.88	127.86	114.10
1	A	354	PHE	CA-CB-CG	6.84	120.64	113.80
1	A	195	THR	OG1-CB-CG2	6.82	122.94	109.30
1	A	230	CYS	O-C-N	-6.76	113.81	122.20
1	A	142	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	A	150	HIS	CB-CG-CD2	-6.69	122.51	131.20
1	A	172	ARG	CG-CD-NE	-6.63	97.42	112.00
1	A	147	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	178	TRP	CG-CD2-CE3	6.61	140.51	133.90
1	A	243	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	322	VAL	N-CA-C	6.59	123.06	109.34
1	A	271	SER	CA-CB-OG	6.55	124.19	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	ILE	CB-CG1-CD1	-6.54	100.06	113.80
1	A	185	ASP	N-CA-C	6.54	121.11	113.20
1	A	160	MET	CG-SD-CE	6.51	115.23	100.90
1	A	403	ARG	CB-CG-CD	-6.49	96.38	111.30
1	A	151	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	149	VAL	CB-CA-C	-6.43	102.19	112.16
1	A	178	TRP	CB-CG-CD1	-6.42	117.27	126.90
1	A	153	ILE	O-C-N	-6.41	117.23	121.72
1	A	430	ARG	O-C-N	-6.39	115.32	122.86
1	A	178	TRP	N-CA-C	-6.36	103.97	112.94
1	A	271	SER	N-CA-C	6.34	119.18	111.82
1	A	346	THR	CA-CB-OG1	-6.32	100.12	109.60
1	A	328	ASN	N-CA-C	6.30	118.02	111.03
1	A	384	SER	N-CA-C	6.30	121.12	113.38
1	A	103	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	306	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	A	377	PHE	CA-CB-CG	6.19	119.99	113.80
1	A	324	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	91	GLN	N-CA-C	-6.17	101.34	110.48
1	A	105	SER	N-CA-C	6.16	118.78	111.33
1	A	118	ARG	CA-CB-CG	-6.15	101.79	114.10
1	A	419	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	A	104	ASN	N-CA-C	6.14	120.10	112.24
1	A	296	LYS	N-CA-C	6.14	120.08	112.59
1	A	444	VAL	N-CA-C	-6.14	99.37	108.45
1	A	118	ARG	CB-CG-CD	6.13	125.41	111.30
1	A	366	ILE	N-CA-C	-6.12	104.33	111.00
1	A	449	THR	CA-CB-OG1	-6.11	100.43	109.60
1	A	394	ARG	CG-CD-NE	-6.00	98.80	112.00
1	A	468	PRO	O-C-N	5.96	130.12	122.91
1	A	121	TYR	CA-CB-CG	5.93	124.57	113.90
1	A	142	ASN	O-C-N	-5.83	116.28	123.44
1	A	161	ASN	OD1-CG-ND2	-5.76	116.83	122.60
1	A	299	ASN	N-CA-C	-5.75	102.78	110.55
1	A	104	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	A	169	LEU	N-CA-C	5.73	120.01	113.19
1	A	276	GLU	N-CA-CB	-5.72	100.89	111.53
1	A	97	PHE	CA-CB-CG	-5.70	108.10	113.80
1	A	205	PHE	CA-CB-CG	-5.57	108.23	113.80
1	A	330	ASP	N-CA-C	5.55	119.15	112.38
1	A	181	SER	N-CA-C	-5.54	100.10	108.46
1	A	264	HIS	CB-CG-ND1	5.53	131.00	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	TRP	CG-CD1-NE1	-5.53	103.01	110.20
1	A	276	GLU	CA-CB-CG	5.51	125.13	114.10
1	A	220	GLN	CG-CD-NE2	5.50	124.65	116.40
1	A	322	VAL	N-CA-CB	-5.49	102.17	111.23
1	A	229	GLU	N-CA-C	5.49	117.98	110.24
1	A	320	GLY	N-CA-C	-5.48	108.14	115.32
1	A	309	ASP	CB-CA-C	-5.47	100.13	109.65
1	A	393	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	A	180	SER	N-CA-C	5.46	115.75	108.38
1	A	383	TRP	CG-CD2-CE3	5.43	139.33	133.90
1	A	422	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	468	PRO	CA-C-N	5.40	131.42	121.70
1	A	468	PRO	C-N-CA	5.40	131.42	121.70
1	A	165	VAL	N-CA-C	-5.40	102.31	107.76
1	A	300	ARG	CA-C-N	5.39	125.69	119.92
1	A	300	ARG	C-N-CA	5.39	125.69	119.92
1	A	93	GLN	N-CA-C	-5.38	101.20	109.76
1	A	121	TYR	CA-C-N	-5.37	114.98	122.71
1	A	121	TYR	C-N-CA	-5.37	114.98	122.71
1	A	184	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	A	265	ILE	N-CA-C	-5.35	100.42	108.12
1	A	102	LYS	N-CA-C	-5.33	99.44	110.80
1	A	178	TRP	CA-CB-CG	5.33	123.73	113.60
1	A	442	SER	CA-CB-OG	5.32	121.75	111.10
1	A	441	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	378	LYS	N-CA-C	-5.29	101.66	110.17
1	A	210	ARG	CA-CB-CG	5.26	124.62	114.10
1	A	178	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	A	449	THR	CA-CB-CG2	5.25	119.42	110.50
1	A	173	GLN	CG-CD-NE2	5.24	124.25	116.40
1	A	416	SER	N-CA-C	5.23	119.66	113.12
1	A	361	TRP	CD1-CG-CD2	5.22	114.66	106.30
1	A	275	VAL	CA-C-O	5.22	126.01	120.48
1	A	292	ARG	CA-CB-CG	5.21	124.52	114.10
1	A	221	ASN	O-C-N	5.18	128.27	123.50
1	A	398	VAL	N-CA-C	-5.18	100.61	108.17
1	A	122	VAL	N-CA-C	-5.15	100.83	108.45
1	A	361	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	A	401	ASP	CA-CB-CG	-5.15	107.45	112.60
1	A	297	GLY	N-CA-C	5.14	120.64	111.03
1	A	378	LYS	CB-CG-CD	-5.14	99.48	111.30
1	A	298	SER	CA-CB-OG	-5.13	100.84	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	GLU	N-CA-C	-5.10	102.93	110.48
1	A	287	VAL	N-CA-C	-5.10	100.90	108.45
1	A	383	TRP	CB-CG-CD1	-5.09	119.26	126.90
1	A	168	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	A	276	GLU	O-C-N	-5.09	117.37	123.27
1	A	358	ASN	N-CA-C	-5.08	106.49	113.30
1	A	294	ASN	N-CA-C	5.08	119.47	113.28
1	A	416	SER	N-CA-CB	-5.07	102.66	110.42
1	A	428	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	A	444	VAL	O-C-N	-5.05	117.44	123.05
1	A	438	TRP	CB-CG-CD1	-5.05	119.33	126.90
1	A	226	GLN	CG-CD-NE2	-5.01	108.89	116.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3022	724	2853	52	0
2	B	28	27	25	0	0
3	C	92	82	69	0	0
4	D	72	67	61	0	0
5	A	28	28	26	4	0
6	A	1	0	0	0	0
7	A	86	172	0	1	1
All	All	3329	1100	3034	53	1

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 9.

All (53) 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:233:ILE:HG22	1:A:234:ASN:HD22	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HG22	1:A:234:ASN:ND2	2.03	0.74
1:A:334:ASN:HA	1:A:387:ASN:HD21	1.53	0.73
1:A:322:VAL:HG12	1:A:327:ARG:HG3	1.71	0.72
1:A:101:SER:HB3	1:A:445:VAL:HG13	1.77	0.67
1:A:226:GLN:HG3	1:A:278:CYS:O	1.95	0.67
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.76	0.66
1:A:317:VAL:HG23	7:A:551:HOH:O	1.96	0.65
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.79	0.65
1:A:273:GLN:HG3	1:A:340:PRO:HG3	1.79	0.64
1:A:242:THR:HG21	1:A:275:VAL:O	1.99	0.61
1:A:285:PRO:HB2	5:A:485(A):NAG:H82	1.83	0.60
1:A:234:ASN:ND2	5:A:485(A):NAG:C1	2.65	0.60
1:A:309:ASP:HB2	1:A:311:SER:OG	2.02	0.59
1:A:329:ASP:O	1:A:333:SER:HB3	2.01	0.59
1:A:184:HIS:CD2	1:A:186:GLY:H	2.21	0.59
1:A:334:ASN:HA	1:A:387:ASN:ND2	2.19	0.58
1:A:176:ILE:HG22	1:A:195:THR:HG21	1.90	0.53
1:A:245:SER:O	1:A:274:HIS:HE1	1.91	0.53
5:A:485(A):NAG:C1	5:A:485(A):NAG:O7	2.58	0.53
1:A:298:SER:HB2	1:A:341:ASN:HD21	1.74	0.52
1:A:326:PRO:HA	1:A:368:LYS:O	2.09	0.51
1:A:365:THR:HG21	1:A:371:ARG:HA	1.92	0.51
1:A:349:VAL:CG2	1:A:371:ARG:HE	2.25	0.50
1:A:349:VAL:HG23	1:A:371:ARG:NE	2.27	0.50
1:A:131:GLN:NE2	1:A:164:GLY:H	2.11	0.48
1:A:428:ARG:NH2	1:A:462:ALA:O	2.47	0.48
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.76	0.47
1:A:437:TRP:HD1	1:A:469:ILE:HG22	1.79	0.47
1:A:403:ARG:NH2	1:A:429:GLY:O	2.48	0.47
1:A:241:MET:HE3	1:A:255:LEU:HG	1.97	0.46
1:A:204:SER:HB3	1:A:211:LEU:HD11	1.97	0.46
1:A:242:THR:HG22	1:A:252:THR:HG23	1.98	0.46
1:A:183:CYS:SG	1:A:232:CYS:SG	3.14	0.45
1:A:240:VAL:HG21	1:A:278:CYS:SG	2.57	0.45
1:A:425:GLU:HG2	1:A:427:ILE:HG22	1.99	0.45
1:A:184:HIS:HD2	1:A:186:GLY:H	1.63	0.45
1:A:349:VAL:HG23	1:A:371:ARG:HE	1.82	0.45
1:A:131:GLN:HE21	1:A:163:LEU:HD12	1.82	0.44
1:A:298:SER:O	1:A:322:VAL:HG13	2.19	0.43
1:A:418:ILE:HD11	1:A:420:ARG:NH1	2.34	0.43
1:A:100:PHE:HB3	1:A:445:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:SER:HB3	1:A:350:LYS:CE	2.47	0.42
1:A:278:CYS:HB3	1:A:289:CYS:HB3	2.01	0.42
1:A:246:ALA:O	1:A:274:HIS:NE2	2.53	0.42
1:A:205:PHE:CE1	1:A:262:ILE:HD11	2.55	0.42
1:A:352:TRP:NE1	1:A:374:TYR:OH	2.53	0.42
1:A:290:ILE:HG12	1:A:353:ALA:HB3	2.02	0.41
1:A:411:SER:HB3	1:A:418:ILE:CD1	2.50	0.41
1:A:366:ILE:HG21	1:A:400:SER:HB3	2.03	0.41
1:A:285:PRO:CB	5:A:485(A):NAG:H82	2.50	0.40
1:A:297:GLY:O	1:A:345:GLY:O	2.39	0.40
1:A:452:THR:HG22	1:A:453:TYR:H	1.86	0.40

All (1) 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)
7:A:490:HOH:H1	7:A:490:HOH:H1[16_665]	0.83	0.77

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	378/388 (97%)	345 (91%)	30 (8%)	3 (1%)	16 16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ASP
1	A	222	ILE
1	A	322	VAL

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	338/338 (100%)	295 (87%)	43 (13%)	4 4

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

Mol	Chain	Res	Type
1	A	82	VAL
1	A	118	ARG
1	A	122	VAL
1	A	134	LEU
1	A	149	VAL
1	A	161	ASN
1	A	165	VAL
1	A	178	TRP
1	A	192	VAL
1	A	195	THR
1	A	202	THR
1	A	204	SER
1	A	224	ARG
1	A	226	GLN
1	A	231	VAL
1	A	240	VAL
1	A	242	THR
1	A	253	ARG
1	A	255	LEU
1	A	257	ILE
1	A	271	SER
1	A	288	ARG
1	A	311	SER
1	A	315	SER
1	A	324	ASP
1	A	332	SER
1	A	346	THR
1	A	364	ARG
1	A	387	ASN
1	A	388	SER

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Mol	Chain	Res	Type
1	A	390	SER
1	A	394	ARG
1	A	401	ASP
1	A	412	VAL
1	A	413	GLU
1	A	418	ILE
1	A	424	VAL
1	A	427	ILE
1	A	434	THR
1	A	445	VAL
1	A	452	THR
1	A	455	THR
1	A	464	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	136	GLN
1	A	161	ASN
1	A	173	GLN
1	A	191	HIS
1	A	220	GLN
1	A	226	GLN
1	A	234	ASN
1	A	334	ASN
1	A	358	ASN
1	A	387	ASN
1	A	393	ASN
1	A	419	ASN
1	A	432	GLN
1	A	441	ASN

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 ⓘ

15 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1	2,1	14,14,15	0.66	0	17,19,21	0.88	0
2	NAG	B	2	2	14,14,15	0.69	0	17,19,21	1.63	3 (17%)
3	NAG	C	1	3,1	14,14,15	1.07	1 (7%)	17,19,21	2.89	6 (35%)
3	NAG	C	2	3	14,14,15	1.04	1 (7%)	17,19,21	1.33	2 (11%)
3	BMA	C	3	3	11,11,12	1.00	0	15,15,17	1.38	3 (20%)
3	MAN	C	4	3	11,11,12	0.89	0	15,15,17	1.37	2 (13%)
3	NAG	C	5	3	14,14,15	1.60	3 (21%)	17,19,21	2.76	5 (29%)
3	NGK	C	6	3	18,18,19	1.66	2 (11%)	21,26,28	2.40	5 (23%)
3	FUL	C	7	3	10,10,11	3.23	4 (40%)	14,14,16	5.11	9 (64%)
4	NAG	D	1	4,1	14,14,15	0.88	0	17,19,21	1.28	3 (17%)
4	NAG	D	2	4	14,14,15	1.12	1 (7%)	17,19,21	1.49	5 (29%)
4	BMA	D	3	4	11,11,12	0.83	0	15,15,17	1.05	0
4	MAN	D	4	4	11,11,12	0.57	0	15,15,17	1.27	2 (13%)
4	MAN	D	5	4	11,11,12	0.84	0	15,15,17	1.16	1 (6%)
4	MAN	D	6	4	11,11,12	0.68	0	15,15,17	0.87	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	5	3	-	2/6/23/26	0/1/1/1
3	NGK	C	6	3	-	4/11/28/31	0/1/1/1
3	FUL	C	7	3	-	-	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	2/2/19/22	0/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	7	FUL	C4-C5	7.84	1.70	1.52
3	C	7	FUL	C4-C3	4.88	1.65	1.52
3	C	6	NGK	O4-S	-4.80	1.42	1.57
3	C	5	NAG	C1-C2	4.01	1.57	1.52
3	C	6	NGK	C1-C2	3.75	1.57	1.52
4	D	2	NAG	C1-C2	-3.27	1.47	1.52
3	C	7	FUL	C1-C2	2.66	1.58	1.52
3	C	1	NAG	C1-C2	2.61	1.55	1.52
3	C	7	FUL	C6-C5	2.51	1.57	1.51
3	C	5	NAG	C4-C5	2.46	1.58	1.53
3	C	5	NAG	O4-C4	2.22	1.48	1.43
3	C	2	NAG	C4-C5	2.19	1.57	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	7	FUL	C6-C5-C4	10.36	132.03	113.08
3	C	7	FUL	O3-C3-C2	10.10	130.67	110.05
3	C	5	NAG	C1-O5-C5	8.84	124.04	112.19
3	C	1	NAG	C1-C2-N2	8.84	124.36	110.43
3	C	6	NGK	C8-C7-N2	6.66	127.16	116.12
3	C	7	FUL	O2-C2-C1	6.61	124.36	109.22
3	C	7	FUL	C1-C2-C3	6.39	118.95	109.64
3	C	6	NGK	C1-O5-C5	5.98	120.20	112.19
3	C	7	FUL	C3-C4-C5	4.87	117.21	109.81
3	C	7	FUL	O2-C2-C3	-4.36	101.12	110.15
3	C	6	NGK	O7-C7-N2	-4.32	114.34	121.98
3	C	1	NAG	C8-C7-N2	3.93	122.64	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	NAG	O5-C1-C2	3.73	117.06	111.29
3	C	4	MAN	C1-O5-C5	3.71	117.16	112.19
3	C	7	FUL	O4-C4-C3	3.64	118.95	110.38
2	B	2	NAG	C1-O5-C5	3.62	117.03	112.19
3	C	1	NAG	C1-O5-C5	3.50	116.88	112.19
4	D	5	MAN	C1-O5-C5	3.50	116.88	112.19
3	C	5	NAG	C3-C4-C5	-3.45	103.98	110.23
2	B	2	NAG	C1-C2-N2	-3.43	105.02	110.43
3	C	5	NAG	O4-C4-C5	3.37	117.63	109.32
3	C	1	NAG	C4-C3-C2	-3.34	106.13	111.02
3	C	3	BMA	C1-O5-C5	2.76	115.89	112.19
3	C	7	FUL	C2-C3-C4	-2.75	106.02	110.86
2	B	2	NAG	C6-C5-C4	2.75	119.77	113.02
3	C	5	NAG	C4-C3-C2	-2.72	107.03	111.02
3	C	1	NAG	O7-C7-N2	-2.59	117.40	121.98
4	D	1	NAG	C8-C7-N2	2.59	120.42	116.12
4	D	1	NAG	C1-O5-C5	2.54	115.58	112.19
4	D	4	MAN	C1-O5-C5	2.53	115.58	112.19
3	C	2	NAG	C1-O5-C5	2.47	115.50	112.19
3	C	2	NAG	C8-C7-N2	2.44	120.16	116.12
4	D	2	NAG	C8-C7-N2	2.40	120.10	116.12
4	D	1	NAG	O7-C7-C8	-2.40	117.78	122.05
3	C	3	BMA	C3-C4-C5	2.35	114.50	110.23
3	C	6	NGK	C2-N2-C7	2.31	125.99	122.90
4	D	4	MAN	C3-C4-C5	-2.20	106.25	110.23
3	C	7	FUL	C1-O5-C5	2.20	118.14	112.97
4	D	2	NAG	O5-C5-C4	-2.19	105.50	110.83
3	C	3	BMA	C2-C3-C4	-2.09	107.18	110.86
4	D	2	NAG	C1-O5-C5	2.07	114.96	112.19
3	C	1	NAG	O4-C4-C3	-2.06	105.51	110.38
4	D	2	NAG	C1-C2-N2	2.05	113.66	110.43
4	D	2	NAG	O4-C4-C3	-2.05	105.55	110.38
3	C	4	MAN	C3-C4-C5	2.03	113.92	110.23
3	C	6	NGK	O7-C7-C8	-2.02	118.46	122.05

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C1-C2-N2-C7
3	C	6	NGK	C3-C4-O4-S
3	C	3	BMA	O5-C5-C6-O6

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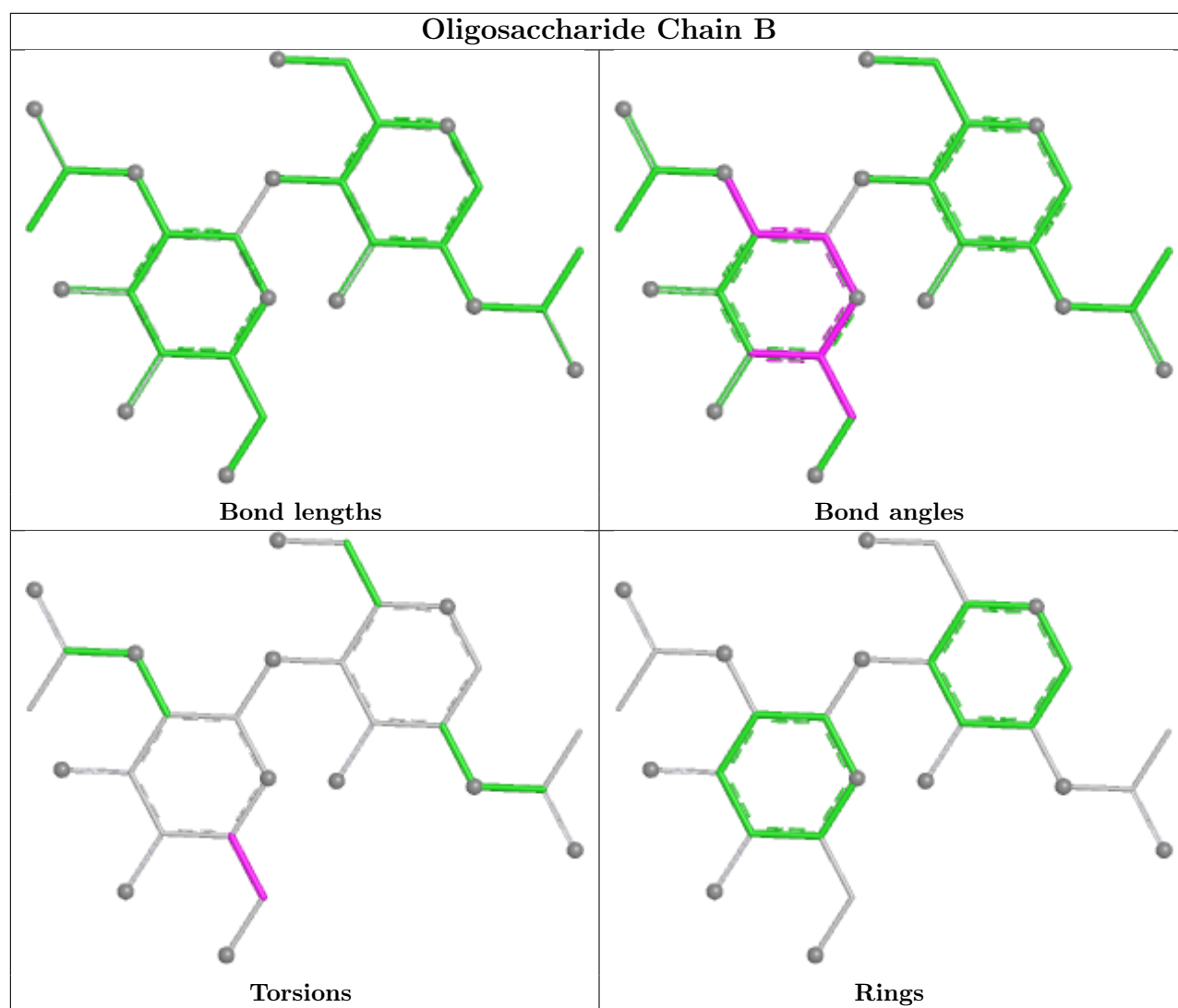
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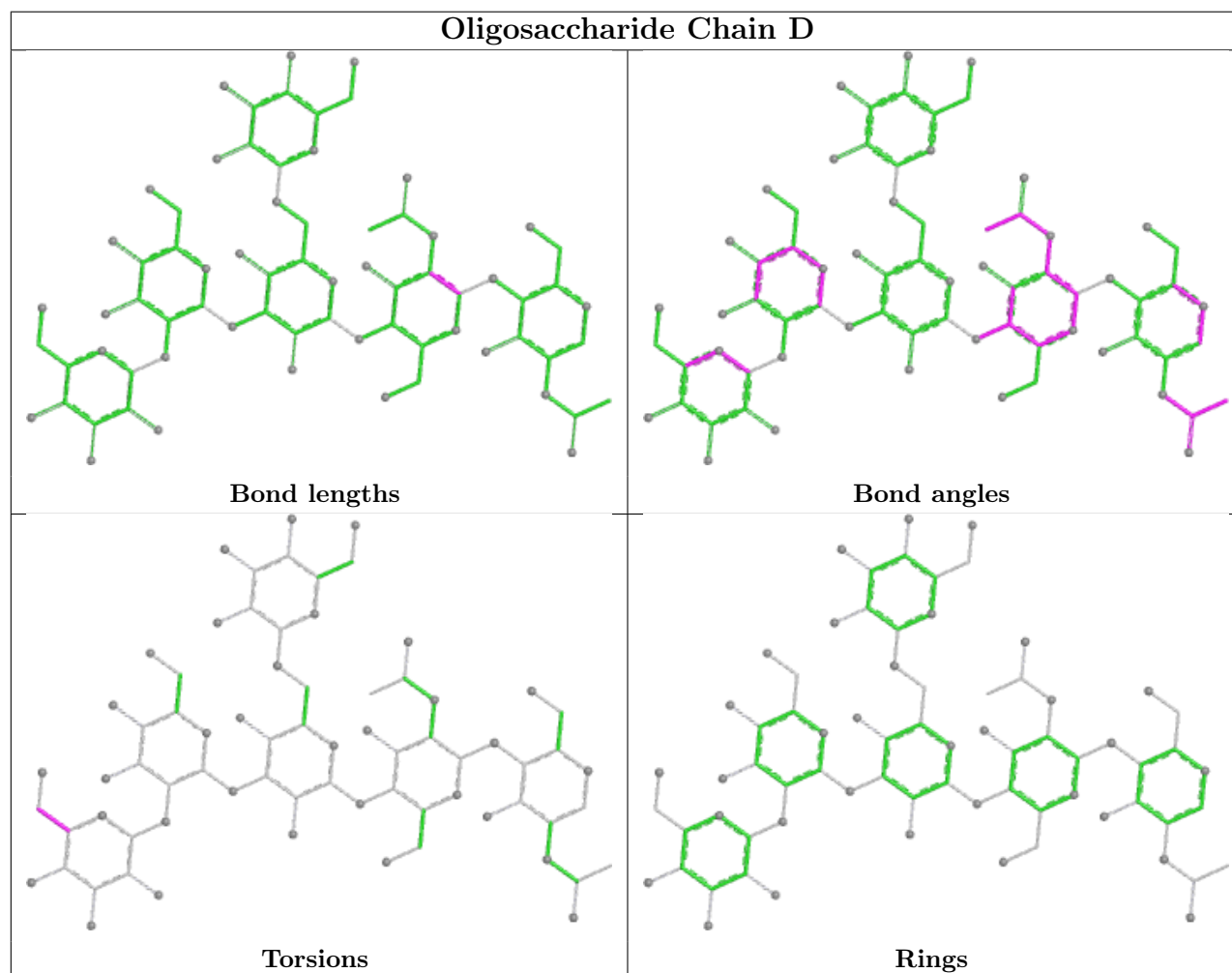
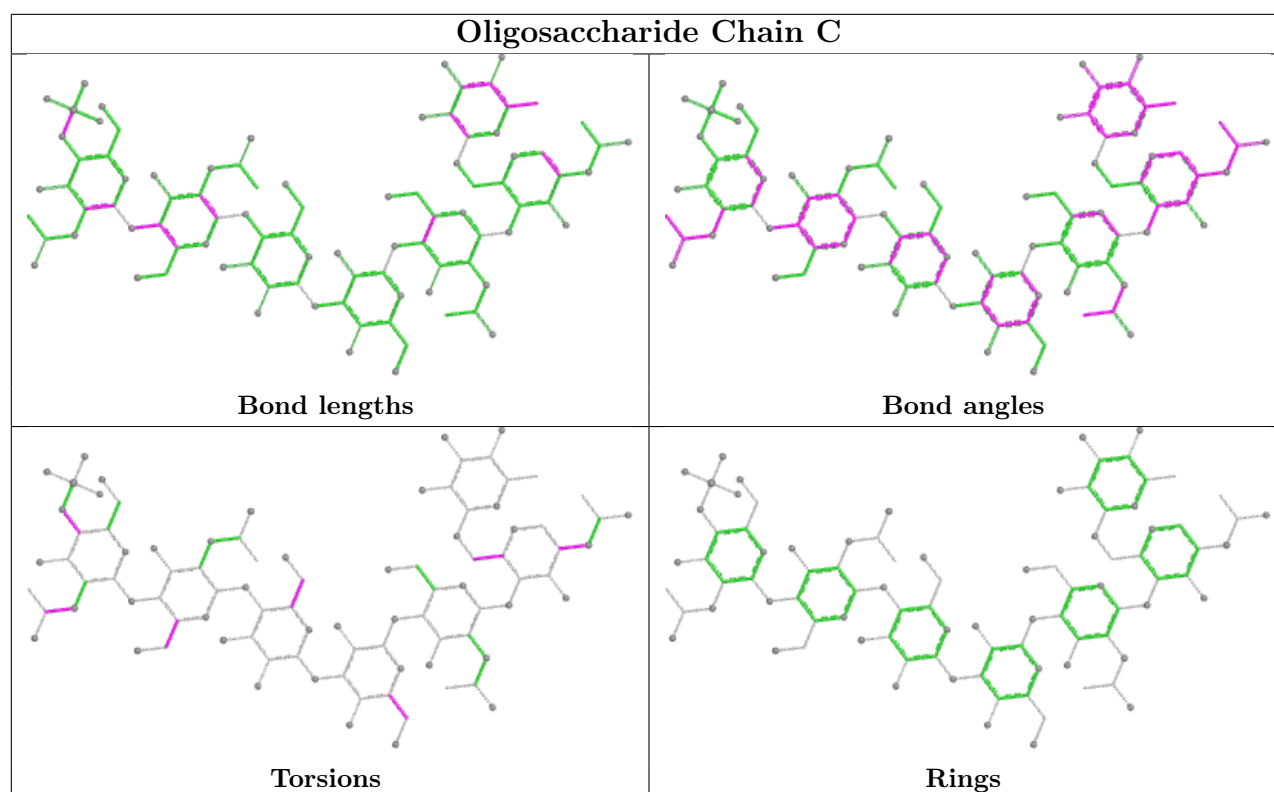
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	5	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	C	6	NGK	C8-C7-N2-C2
3	C	6	NGK	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	C	5	NAG	C4-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6
3	C	6	NGK	C5-C4-O4-S
4	D	5	MAN	C4-C5-C6-O6
3	C	4	MAN	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.





5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
5	NAG	A	486(B)	-	14,14,15	0.56	0	17,19,21	1.02	1 (5%)
5	NAG	A	485(A)	-	14,14,15	0.86	0	17,19,21	1.33	3 (17%)

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
5	NAG	A	486(B)	-	-	0/6/23/26	0/1/1/1
5	NAG	A	485(A)	-	-	3/6/23/26	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(°)	Ideal(°)
5	A	485(A)	NAG	C8-C7-N2	2.86	120.87	116.12
5	A	485(A)	NAG	C6-C5-C4	2.57	119.32	113.02
5	A	486(B)	NAG	O3-C3-C2	2.29	114.16	109.40
5	A	485(A)	NAG	O7-C7-C8	-2.28	118.00	122.05

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	485(A)	NAG	C1-C2-N2-C7
5	A	485(A)	NAG	C4-C5-C6-O6
5	A	485(A)	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	485(A)	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/388 (100%)	-0.64	0 100 100	8, 20, 35, 53	0

There are no RSRZ outliers to report.

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

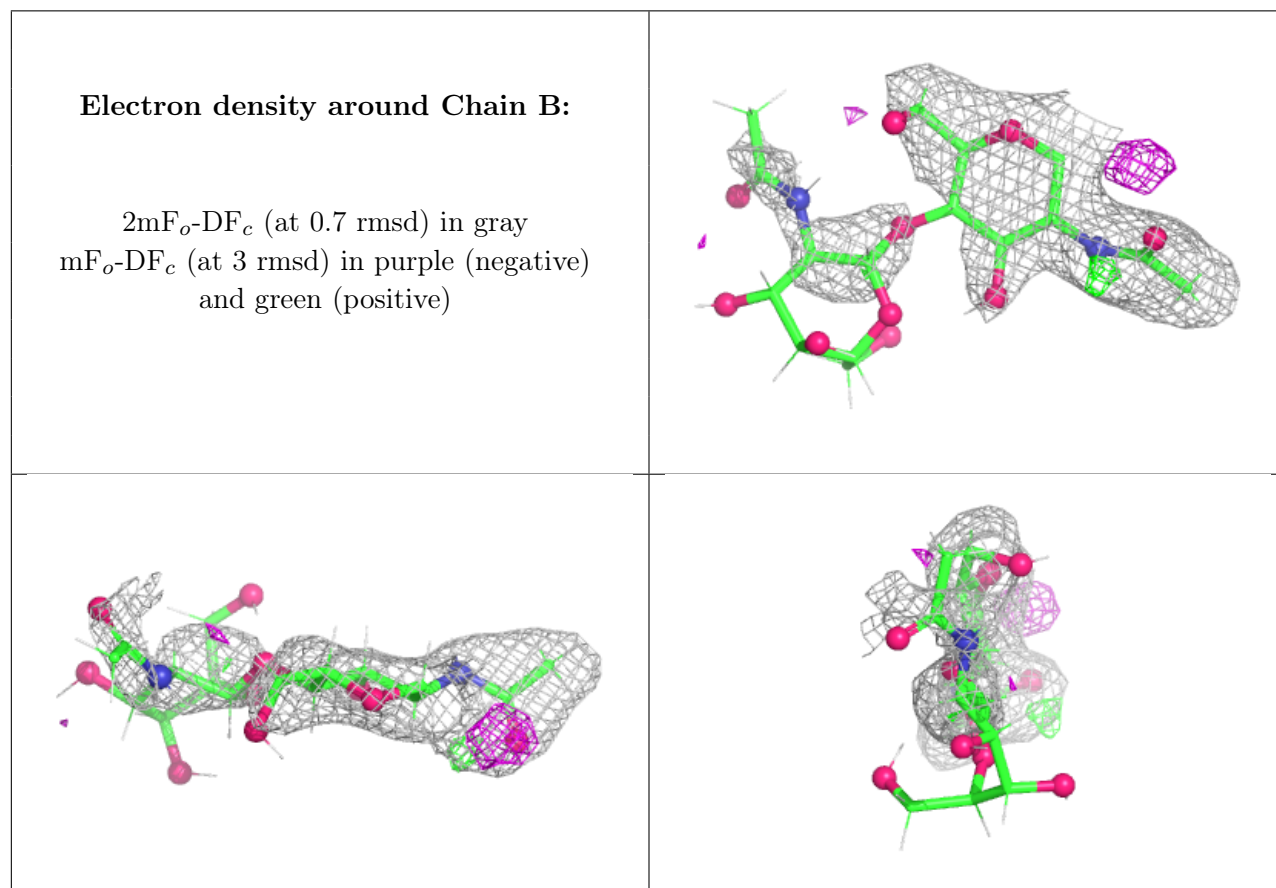
There are no non-standard protein/DNA/RNA residues in this entry.

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.

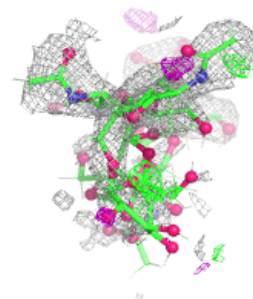
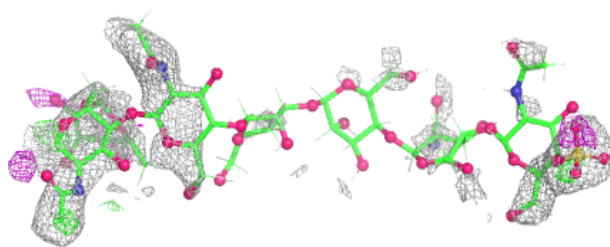
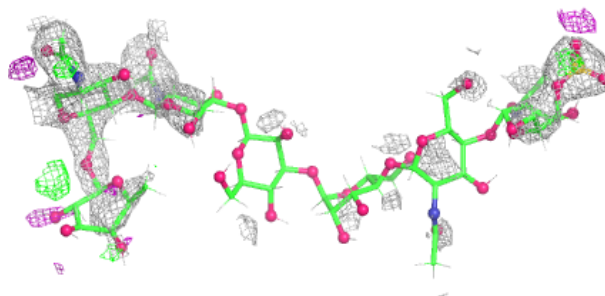
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	D	6	11/12	0.60	0.15	0,0,61,63	0
2	NAG	B	2	14/15	-	-	0,0,55,55	28
3	FUL	C	7	10/11	0.63	0.21	0,0,87,89	0
3	NAG	C	2	14/15	0.68	0.15	0,0,79,79	0
3	BMA	C	3	11/12	-	-	0,0,80,81	21
3	MAN	C	4	11/12	-	-	0,0,84,87	21
3	NAG	C	5	14/15	-	-	0,0,92,94	27
4	MAN	D	5	11/12	0.75	0.11	0,0,61,65	0
2	NAG	B	1	14/15	0.81	0.10	0,0,54,55	0
3	NAG	C	1	14/15	0.83	0.12	0,66,74,82	0
4	MAN	D	4	11/12	0.83	0.10	0,0,51,53	0
3	NGK	C	6	18/19	0.84	0.15	0,93,99,100	0
4	BMA	D	3	11/12	0.88	0.09	0,41,49,54	0
4	NAG	D	1	14/15	0.88	0.09	0,0,38,40	0
4	NAG	D	2	14/15	0.89	0.08	0,0,36,38	0

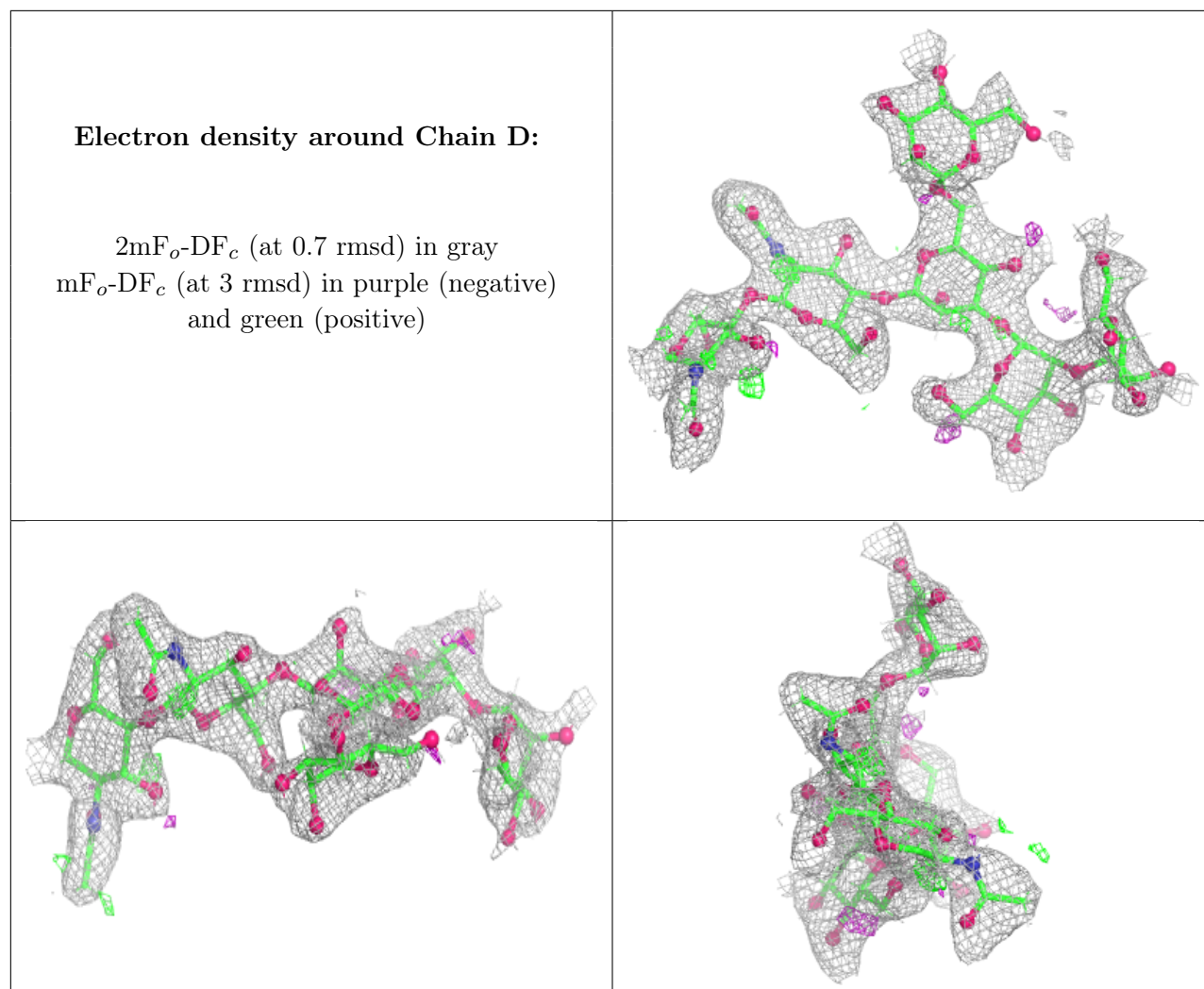
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain C:

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





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
5	NAG	A	485(A)	14/15	0.66	0.15	0,0,78,79	0
5	NAG	A	486(B)	14/15	-	-	0,0,92,92	28
6	CA	A	1	1/1	0.89	0.04	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.