



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:27 AM UTC

PDB ID : 6MDV / pdb_00006mdv
Title : Crystal structure of Streptococcus pyogenes endo-beta-N-acetylglucosaminidase (EndoS2) with high-mannose glycan
Authors : Klontz, E.H.; Trastoy, B.; Orwenyo, J.; Wang, L.X.; Guerin, M.E.; Sundberg, E.J.
Deposited on : 2018-09-05
Resolution : 2.50 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

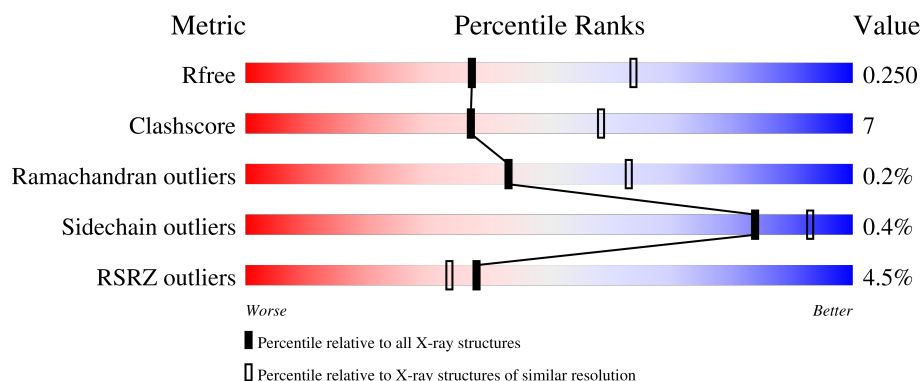
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

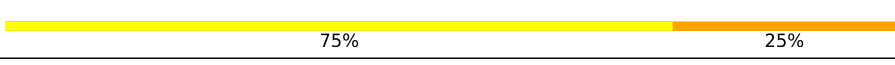
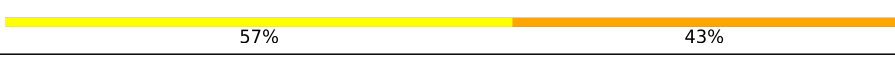
The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	802	
1	B	802	
2	C	8	
3	D	7	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13060 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.

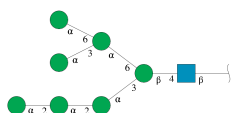
- Molecule 1 is a protein called Endo-beta-N-acetylglucosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	787	Total	C	N	O	S	0	0	0
			6260	3925	1066	1254	15			
1	B	787	Total	C	N	O	S	0	0	0
			6254	3922	1066	1251	15			

There are 4 discrepancies between the modelled and reference sequences:

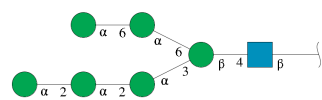
Chain	Residue	Modelled	Actual	Comment	Reference
A	43	MET	-	initiating methionine	UNP T1WGN1
A	844	LEU	-	expression tag	UNP T1WGN1
B	43	MET	-	initiating methionine	UNP T1WGN1
B	844	LEU	-	expression tag	UNP T1WGN1

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			92	50	1	41			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	7	Total	C	N	O	0	0	0
			81	44	1	36			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

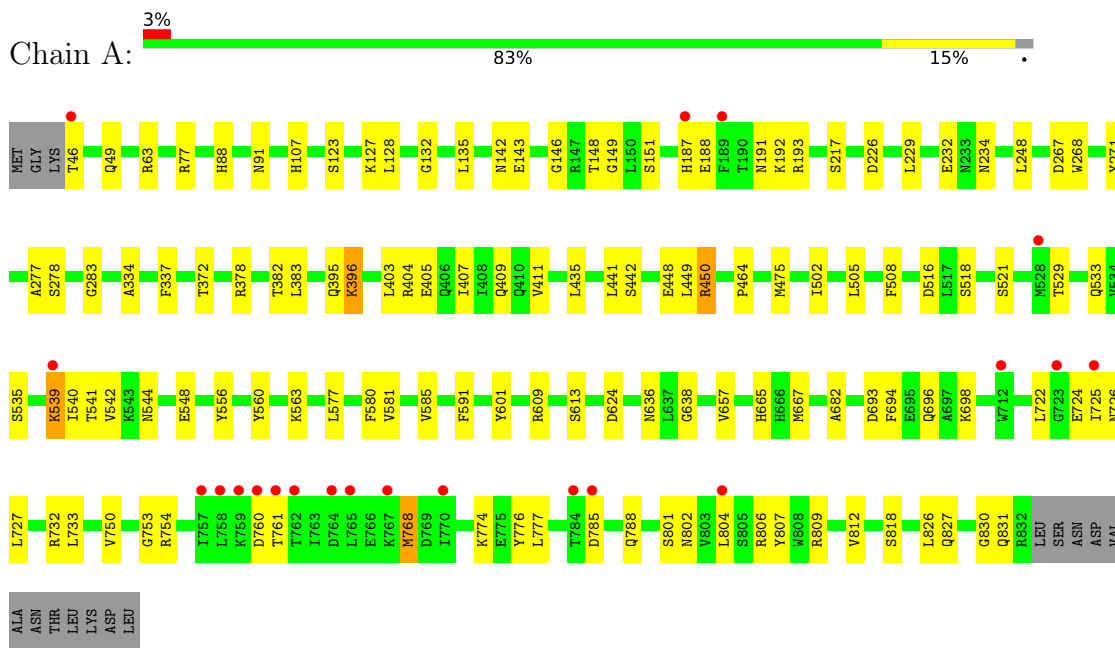
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	207	Total	O	0	0
			207	207		
5	B	164	Total	O	0	0
			164	164		

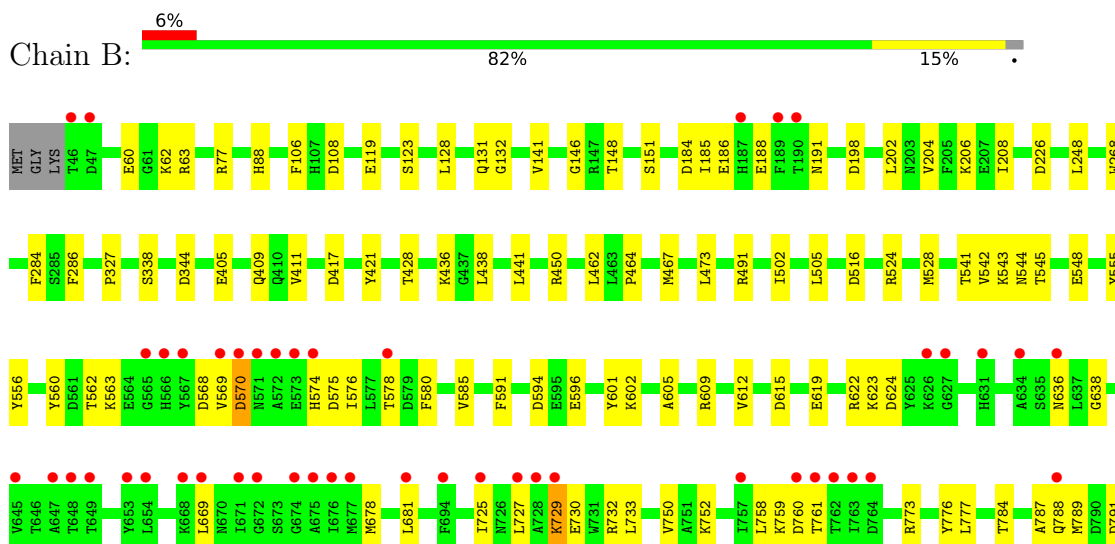
3 Residue-property plots

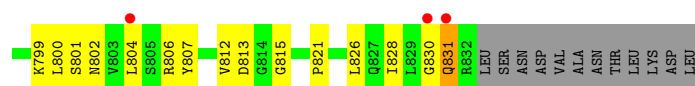
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Endo-beta-N-acetylglucosaminidase



• Molecule 1: Endo-beta-N-acetylglucosaminidase





- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 75% 25%



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 57% 43%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.97Å 105.35Å 257.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.63 – 2.50 29.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.63-2.50) 99.8 (29.63-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.198 , 0.248 0.202 , 0.250	Depositor DCC
R_{free} test set	4299 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13060	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: NAG, MAN, CA, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/6378	0.68	8/8621 (0.1%)
1	B	0.39	2/6371 (0.0%)	0.64	4/8612 (0.0%)
All	All	0.41	2/12749 (0.0%)	0.66	12/17233 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	729	LYS	CD-CE	-5.40	1.36	1.52
1	B	729	LYS	CE-NZ	-5.40	1.33	1.49

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	LYS	CB-CG-CD	9.00	132.01	111.30
1	B	831	GLN	CA-CB-CG	-8.53	97.03	114.10
1	A	396	LYS	CG-CD-CE	-8.15	92.56	111.30
1	A	539	LYS	CA-CB-CG	-7.38	99.35	114.10
1	A	450	ARG	CD-NE-CZ	-6.44	115.38	124.40
1	B	729	LYS	CA-CB-CG	6.27	126.64	114.10
1	B	830	GLY	CA-C-N	-6.05	113.30	122.81
1	B	830	GLY	C-N-CA	-6.05	113.30	122.81
1	A	217	SER	CB-CA-C	5.72	120.29	110.79
1	A	768	MET	CA-C-N	-5.25	113.35	122.64
1	A	768	MET	C-N-CA	-5.25	113.35	122.64
1	A	774	LYS	CB-CG-CD	5.08	122.99	111.30

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	6260	0	6056	82	0
1	B	6254	0	6058	95	0
2	C	92	0	78	3	0
3	D	81	0	69	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	207	0	0	2	0
5	B	164	0	0	4	0
All	All	13060	0	12261	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (177) 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:B:576:ILE:HD11	1:B:669:LEU:HD22	1.52	0.90
1:A:192:LYS:HD3	1:A:193:ARG:H	1.42	0.85
1:B:727:LEU:CD1	1:B:729:LYS:HD2	2.08	0.82
1:A:405:GLU:O	1:A:409:GLN:HG3	1.82	0.80
1:A:724:GLU:OE1	1:A:726:ASN:ND2	2.16	0.78
1:A:448:GLU:OE2	1:A:450:ARG:NH2	2.17	0.77
1:A:785:ASP:OD2	1:A:788:GLN:NE2	2.18	0.76
1:B:541:THR:HG23	1:B:544:ASN:H	1.49	0.76
1:B:63:ARG:NH2	1:B:132:GLY:O	2.15	0.76
1:A:636:ASN:HB3	1:A:638:GLY:H	1.50	0.76
1:B:636:ASN:HB3	1:B:638:GLY:H	1.50	0.75
1:B:678:MET:HA	1:B:831:GLN:HE21	1.51	0.75
1:B:800:LEU:O	1:B:802:ASN:N	2.21	0.74
1:A:806:ARG:NH1	1:A:807:TYR:OH	2.21	0.73
1:A:580:PHE:HB3	1:A:667:MET:HE1	1.70	0.73
1:A:560:TYR:O	1:A:563:LYS:NZ	2.19	0.72
1:B:467:MET:HE1	1:B:473:LEU:HB2	1.70	0.71
1:B:560:TYR:O	1:B:563:LYS:NZ	2.23	0.71
1:B:541:THR:CG2	1:B:544:ASN:H	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:MET:HA	1:B:831:GLN:NE2	2.06	0.70
1:B:405:GLU:O	1:B:409:GLN:HG3	1.91	0.70
1:A:192:LYS:HD3	1:A:193:ARG:N	2.06	0.70
1:B:619:GLU:HG2	1:B:622:ARG:NH1	2.07	0.70
1:B:541:THR:HG22	1:B:544:ASN:CG	2.17	0.69
1:A:539:LYS:HG3	1:A:540:ILE:N	2.06	0.69
1:A:768:MET:HE1	1:A:776:TYR:CD2	2.29	0.67
1:B:681:LEU:N	1:B:828:ILE:O	2.27	0.66
1:A:548:GLU:OE2	1:A:609:ARG:HD2	1.98	0.64
1:A:46:THR:HB	1:A:49:GLN:HG3	1.80	0.63
1:B:733:LEU:HD12	1:B:826:LEU:HD13	1.80	0.63
1:A:142:ASN:HB3	1:A:148:THR:HG22	1.81	0.63
1:B:417:ASP:OD2	5:B:1001:HOH:O	2.16	0.63
1:A:146:GLY:N	1:A:151:SER:OG	2.31	0.62
1:A:542:VAL:HG22	1:A:609:ARG:HD3	1.83	0.61
1:A:505:LEU:HD21	1:A:508:PHE:HB3	1.82	0.61
1:B:727:LEU:HD11	1:B:729:LYS:HZ2	1.65	0.60
1:B:619:GLU:HA	1:B:622:ARG:HG2	1.82	0.60
1:B:750:VAL:HG13	1:B:812:VAL:HG13	1.84	0.59
1:B:268:TRP:CD1	1:B:327:PRO:HB3	2.38	0.59
1:A:143:GLU:O	1:A:151:SER:HB2	2.02	0.59
1:B:732:ARG:NH1	5:B:1010:HOH:O	2.34	0.59
1:A:395:GLN:HA	1:A:404:ARG:NH1	2.17	0.58
1:A:777:LEU:O	1:A:809:ARG:NH1	2.36	0.58
1:B:555:TYR:HA	1:B:623:LYS:HE3	1.85	0.58
1:A:187:HIS:HD2	1:A:188:GLU:N	2.02	0.57
1:B:727:LEU:HD12	1:B:729:LYS:HD2	1.87	0.57
1:A:580:PHE:CB	1:A:667:MET:HE1	2.32	0.57
1:A:760:ASP:O	1:A:761:THR:OG1	2.23	0.56
1:A:188:GLU:OE1	2:C:7:MAN:H62	2.05	0.56
1:A:63:ARG:NH2	1:A:132:GLY:O	2.25	0.55
1:A:665:HIS:CD2	1:A:667:MET:HE2	2.41	0.55
1:A:283:GLY:HA3	1:A:337:PHE:CZ	2.42	0.55
1:A:383:LEU:C	1:A:383:LEU:HD23	2.31	0.55
1:B:542:VAL:HG22	1:B:609:ARG:HD3	1.87	0.55
1:B:727:LEU:HA	1:B:804:LEU:HD23	1.88	0.55
1:B:202:LEU:HG	1:B:206:LYS:HE2	1.89	0.55
1:A:142:ASN:ND2	2:C:7:MAN:H61	2.23	0.54
1:B:760:ASP:O	1:B:761:THR:OG1	2.24	0.54
1:B:568:ASP:HB2	1:B:570:ASP:OD1	2.08	0.54
1:A:107:HIS:CE1	2:C:8:MAN:H62	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:ARG:HD3	1:B:807:TYR:CE2	2.43	0.54
1:A:726:ASN:HB3	1:A:831:GLN:O	2.07	0.54
1:B:428:THR:HG22	1:B:450:ARG:HB2	1.90	0.53
1:A:725:ILE:HD11	1:A:804:LEU:HB2	1.91	0.53
1:B:615:ASP:N	1:B:615:ASP:OD1	2.38	0.53
1:A:806:ARG:HD3	1:A:807:TYR:CE2	2.45	0.52
1:A:806:ARG:HD3	1:A:807:TYR:CZ	2.45	0.52
1:B:548:GLU:OE2	1:B:609:ARG:HD2	2.10	0.52
1:B:188:GLU:HG2	1:B:191:ASN:O	2.10	0.52
1:A:556:TYR:OH	1:A:624:ASP:O	2.27	0.51
1:A:724:GLU:HG2	1:A:725:ILE:H	1.73	0.51
1:A:232:GLU:H	1:A:232:GLU:CD	2.18	0.51
1:A:518:SER:OG	1:A:601:TYR:HE1	1.94	0.51
1:B:198:ASP:OD2	5:B:1002:HOH:O	2.19	0.51
1:B:594:ASP:CG	1:B:596:GLU:HG2	2.35	0.51
1:A:581:VAL:HG21	1:A:657:VAL:HG21	1.93	0.51
1:A:665:HIS:NE2	1:A:667:MET:HE2	2.26	0.51
1:B:725:ILE:HG12	1:B:806:ARG:HB2	1.92	0.51
1:B:541:THR:HG23	1:B:543:LYS:N	2.26	0.51
1:A:187:HIS:CD2	1:A:188:GLU:N	2.79	0.50
1:B:60:GLU:OE1	1:B:62:LYS:HE2	2.11	0.50
1:A:694:PHE:CE2	1:A:698:LYS:HE3	2.47	0.50
1:A:187:HIS:HD2	1:A:188:GLU:C	2.20	0.50
1:B:570:ASP:OD2	1:B:574:HIS:NE2	2.38	0.50
1:B:602:LYS:HG2	1:B:612:VAL:HG11	1.94	0.50
1:B:773:ARG:O	1:B:777:LEU:HD12	2.12	0.49
1:B:146:GLY:N	1:B:151:SER:OG	2.42	0.49
1:A:727:LEU:HD11	1:A:802:ASN:HB3	1.92	0.49
1:B:502:ILE:HG22	1:B:505:LEU:HB2	1.95	0.49
1:A:541:THR:HG23	1:A:544:ASN:H	1.77	0.49
1:B:467:MET:HE3	1:B:491:ARG:NH1	2.29	0.48
1:B:727:LEU:C	1:B:727:LEU:HD13	2.38	0.48
1:A:188:GLU:HG2	1:A:191:ASN:O	2.13	0.48
1:B:284:PHE:CZ	1:B:338:SER:HB3	2.47	0.48
1:B:516:ASP:OD1	1:B:601:TYR:OH	2.18	0.48
1:B:108:ASP:OD2	3:D:2:BMA:H62	2.14	0.48
1:B:146:GLY:H	1:B:151:SER:HG	1.62	0.48
1:B:730:GLU:CD	1:B:799:LYS:HG2	2.38	0.48
1:B:148:THR:HG21	3:D:7:MAN:H61	1.96	0.48
1:B:436:LYS:NZ	5:B:1020:HOH:O	2.47	0.47
1:A:518:SER:OG	1:A:601:TYR:CE1	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:VAL:HG12	1:B:591:PHE:HA	1.95	0.47
1:B:815:GLY:HA3	1:B:821:PRO:HG3	1.96	0.47
1:B:752:LYS:HE2	1:B:788:GLN:NE2	2.30	0.47
1:A:123:SER:O	1:A:127:LYS:HG3	2.15	0.47
1:A:585:VAL:HG12	1:A:591:PHE:HA	1.95	0.47
1:A:378:ARG:O	1:A:382:THR:HG23	2.14	0.47
1:B:141:VAL:HB	1:B:185:ILE:HG12	1.97	0.47
1:B:441:LEU:O	1:B:464:PRO:HB3	2.15	0.47
1:B:727:LEU:CD1	1:B:729:LYS:NZ	2.76	0.47
1:A:143:GLU:OE2	1:A:149:GLY:HA3	2.14	0.46
1:B:184:ASP:OD1	1:B:186:GLU:HG3	2.15	0.46
1:B:562:THR:HG21	1:B:580:PHE:CE2	2.50	0.46
1:A:128:LEU:HD12	1:A:135:LEU:HD21	1.98	0.46
1:B:773:ARG:HG3	1:B:777:LEU:CD1	2.46	0.46
1:B:556:TYR:CE2	1:B:623:LYS:HD2	2.51	0.46
1:A:754:ARG:HG2	1:A:788:GLN:OE1	2.16	0.46
1:B:727:LEU:HD11	1:B:729:LYS:NZ	2.31	0.46
1:B:727:LEU:HD13	1:B:729:LYS:HD2	1.93	0.46
1:B:759:LYS:HG3	1:B:784:THR:OG1	2.17	0.45
1:A:226:ASP:HA	1:A:248:LEU:O	2.17	0.45
1:A:541:THR:HG22	1:A:544:ASN:CG	2.41	0.45
1:A:268:TRP:CH2	1:A:277:ALA:HA	2.51	0.45
1:A:502:ILE:HG22	1:A:505:LEU:HB2	1.97	0.45
1:A:727:LEU:O	1:A:830:GLY:HA3	2.17	0.45
1:B:636:ASN:O	1:B:732:ARG:NH2	2.50	0.45
1:B:787:ALA:HB2	1:B:800:LEU:CD2	2.47	0.45
1:A:403:LEU:HD22	1:A:435:LEU:HA	1.98	0.45
1:A:726:ASN:O	1:A:804:LEU:HB2	2.16	0.45
1:A:516:ASP:O	1:A:521:SER:OG	2.27	0.44
1:B:727:LEU:HD21	1:B:802:ASN:HB3	2.00	0.44
1:A:529:THR:O	1:A:533:GLN:HG2	2.18	0.44
1:B:467:MET:CE	1:B:473:LEU:HB2	2.42	0.44
1:B:555:TYR:CA	1:B:623:LYS:HE3	2.47	0.44
1:A:407:ILE:O	1:A:411:VAL:HG22	2.18	0.44
1:A:732:ARG:HB3	1:A:827:GLN:HB2	1.99	0.44
1:B:788:GLN:HG3	1:B:789:MET:N	2.32	0.43
1:B:286:PHE:CE1	1:B:344:ASP:HA	2.54	0.43
1:A:267:ASP:HB3	1:A:271:TYR:CE2	2.54	0.43
1:B:752:LYS:HG3	1:B:813:ASP:HB2	2.00	0.43
1:A:750:VAL:HG13	1:A:812:VAL:HG13	2.00	0.43
1:A:449:LEU:O	1:A:475:MET:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PHE:CE2	3:D:1:NAG:H82	2.54	0.43
1:B:411:VAL:HG13	1:B:421:TYR:HB2	2.01	0.43
1:B:562:THR:HG21	1:B:580:PHE:CD2	2.54	0.43
1:B:727:LEU:CD1	1:B:729:LYS:HZ2	2.28	0.43
1:B:605:ALA:HA	1:B:609:ARG:O	2.19	0.42
1:B:148:THR:O	1:B:151:SER:HB3	2.19	0.42
1:A:278:SER:O	1:A:334:ALA:HB2	2.19	0.42
1:A:724:GLU:HG2	1:A:725:ILE:N	2.34	0.42
1:B:524:ARG:O	1:B:528:MET:HG3	2.20	0.42
1:B:438:LEU:HB3	1:B:462:LEU:O	2.20	0.42
1:B:545:THR:OG1	1:B:609:ARG:NH2	2.48	0.42
1:B:758:LEU:HD12	1:B:758:LEU:O	2.19	0.42
1:B:428:THR:HA	1:B:450:ARG:O	2.20	0.41
1:A:77:ARG:HA	1:A:88:HIS:O	2.20	0.41
1:B:789:MET:HE3	1:B:791:ASP:O	2.20	0.41
1:A:91:ASN:OD1	1:A:372:THR:HG22	2.21	0.41
1:B:128:LEU:O	1:B:131:GLN:HG2	2.20	0.41
1:B:226:ASP:HA	1:B:248:LEU:O	2.20	0.41
1:B:77:ARG:HA	1:B:88:HIS:O	2.21	0.41
1:B:773:ARG:O	1:B:776:TYR:HB3	2.21	0.41
1:A:682:ALA:HA	1:A:722:LEU:HD22	2.02	0.41
1:A:77:ARG:NH1	5:A:1018:HOH:O	2.44	0.41
1:A:753:GLY:C	1:A:754:ARG:HG3	2.46	0.41
1:A:396:LYS:CE	5:A:1001:HOH:O	2.65	0.41
1:B:119:GLU:O	1:B:123:SER:HB3	2.20	0.40
1:B:575:ASP:HB3	1:B:578:THR:HB	2.02	0.40
1:A:229:LEU:HB2	1:A:234:ASN:ND2	2.36	0.40
1:A:441:LEU:O	1:A:464:PRO:HB3	2.20	0.40
1:B:204:VAL:O	1:B:208:ILE:HG13	2.21	0.40
1:B:541:THR:HG23	1:B:543:LYS:H	1.84	0.40
1:B:556:TYR:OH	1:B:624:ASP:O	2.35	0.40
1:A:187:HIS:CD2	1:A:187:HIS:C	2.99	0.40
1:A:577:LEU:HD23	1:A:577:LEU:HA	1.96	0.40
1:A:693:ASP:OD2	1:A:696:GLN:HG2	2.21	0.40
1:A:733:LEU:HD12	1:A:826:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	785/802 (98%)	758 (97%)	26 (3%)	1 (0%)	48	68
1	B	785/802 (98%)	754 (96%)	29 (4%)	2 (0%)	36	55
All	All	1570/1604 (98%)	1512 (96%)	55 (4%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	801	SER
1	A	801	SER
1	B	569	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	679/699 (97%)	675 (99%)	4 (1%)	78	91
1	B	678/699 (97%)	677 (100%)	1 (0%)	88	96
All	All	1357/1398 (97%)	1352 (100%)	5 (0%)	84	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	442	SER
1	A	535	SER
1	A	613	SER

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Mol	Chain	Res	Type
1	A	818	SER
1	B	570	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
1	A	234	ASN
1	A	269	ASN
1	A	549	ASN
1	A	566	HIS
1	A	772	ASN
1	A	782	ASN
1	B	269	ASN
1	B	445	GLN
1	B	512	HIS
1	B	549	ASN
1	B	571	ASN
1	B	665	HIS
1	B	726	ASN
1	B	788	GLN
1	B	797	ASN
1	B	802	ASN
1	B	831	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 ⓘ

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	C	1	2	15,15,15	1.22	2 (13%)	21,21,21	1.46	3 (14%)
2	BMA	C	2	2	11,11,12	1.14	1 (9%)	15,15,17	1.15	1 (6%)
2	MAN	C	3	2	11,11,12	1.03	1 (9%)	15,15,17	1.31	2 (13%)
2	MAN	C	4	2	11,11,12	1.38	2 (18%)	15,15,17	1.15	1 (6%)
2	MAN	C	5	2	11,11,12	1.46	2 (18%)	15,15,17	1.23	1 (6%)
2	MAN	C	6	2	11,11,12	1.88	2 (18%)	15,15,17	1.31	2 (13%)
2	MAN	C	7	2	11,11,12	2.02	4 (36%)	15,15,17	1.07	0
2	MAN	C	8	2	11,11,12	2.00	2 (18%)	15,15,17	1.04	1 (6%)
3	NAG	D	1	3	15,15,15	1.00	1 (6%)	21,21,21	0.65	0
3	BMA	D	2	3	11,11,12	1.28	2 (18%)	15,15,17	1.94	2 (13%)
3	MAN	D	3	3	11,11,12	1.27	1 (9%)	15,15,17	1.31	2 (13%)
3	MAN	D	4	3	11,11,12	1.44	2 (18%)	15,15,17	1.16	1 (6%)
3	MAN	D	5	3	11,11,12	1.50	3 (27%)	15,15,17	1.24	1 (6%)
3	MAN	D	6	3	11,11,12	1.46	2 (18%)	15,15,17	1.37	2 (13%)
3	MAN	D	7	3	11,11,12	1.54	3 (27%)	15,15,17	1.15	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2	-	1/6/26/26	0/1/1/1
2	BMA	C	2	2	-	2/2/19/22	0/1/1/1
2	MAN	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	2/2/19/22	0/1/1/1
2	MAN	C	7	2	-	1/2/19/22	0/1/1/1
2	MAN	C	8	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3	-	4/6/26/26	0/1/1/1
3	BMA	D	2	3	-	0/2/19/22	0/1/1/1
3	MAN	D	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	1/2/19/22	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1
3	MAN	D	7	3	-	0/2/19/22	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	MAN	C2-C3	4.54	1.59	1.52
2	C	8	MAN	O5-C5	4.34	1.51	1.43
2	C	7	MAN	C4-C5	4.10	1.61	1.53
2	C	8	MAN	C2-C3	4.08	1.58	1.52
2	C	1	NAG	C1-C2	3.88	1.57	1.52
3	D	1	NAG	O5-C1	3.52	1.51	1.42
2	C	7	MAN	O4-C4	3.28	1.51	1.43
3	D	4	MAN	C2-C3	2.98	1.57	1.52
2	C	5	MAN	C2-C3	2.95	1.57	1.52
2	C	6	MAN	O5-C5	2.84	1.49	1.43
3	D	7	MAN	C2-C3	2.77	1.56	1.52
2	C	7	MAN	C1-C2	2.77	1.58	1.52
3	D	4	MAN	O5-C5	2.64	1.48	1.43
2	C	5	MAN	C4-C3	2.62	1.59	1.52
2	C	4	MAN	C2-C3	2.62	1.56	1.52
3	D	5	MAN	C2-C3	2.61	1.56	1.52
3	D	7	MAN	C1-C2	2.52	1.58	1.52
3	D	6	MAN	C2-C3	2.52	1.56	1.52
3	D	5	MAN	C4-C3	2.50	1.58	1.52
2	C	2	BMA	C4-C3	2.46	1.58	1.52
3	D	2	BMA	O5-C5	2.44	1.48	1.43
3	D	7	MAN	O5-C5	2.37	1.48	1.43
2	C	3	MAN	O5-C5	2.31	1.47	1.43
3	D	6	MAN	C4-C3	2.27	1.58	1.52
2	C	1	NAG	O5-C1	2.22	1.48	1.42
3	D	3	MAN	C4-C5	2.14	1.57	1.53
3	D	2	BMA	C2-C3	2.09	1.55	1.52
3	D	5	MAN	C1-C2	2.05	1.57	1.52
2	C	4	MAN	O5-C5	2.05	1.47	1.43
2	C	7	MAN	O5-C5	2.00	1.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	BMA	C1-O5-C5	6.33	120.67	112.19
2	C	5	MAN	C1-O5-C5	3.81	117.29	112.19
2	C	1	NAG	C1-C2-N2	3.76	115.09	110.73
2	C	6	MAN	O3-C3-C2	3.69	117.58	110.05
2	C	4	MAN	C1-O5-C5	3.62	117.03	112.19
3	D	5	MAN	C1-O5-C5	3.52	116.91	112.19
3	D	3	MAN	O2-C2-C3	-3.46	102.99	110.15
3	D	4	MAN	C1-O5-C5	3.41	116.76	112.19
3	D	6	MAN	C1-O5-C5	3.34	116.66	112.19
2	C	3	MAN	C1-O5-C5	3.17	116.43	112.19
3	D	3	MAN	C1-O5-C5	2.94	116.13	112.19
2	C	3	MAN	O2-C2-C3	-2.92	104.10	110.15
2	C	1	NAG	C1-O5-C5	2.76	118.98	113.65
3	D	7	MAN	C1-O5-C5	2.71	115.81	112.19
2	C	1	NAG	C1-C2-C3	2.64	114.14	110.54
2	C	2	BMA	C1-O5-C5	2.51	115.55	112.19
3	D	2	BMA	C1-C2-C3	2.40	113.13	109.64
2	C	8	MAN	O3-C3-C2	2.19	114.52	110.05
2	C	6	MAN	O6-C6-C5	-2.18	103.90	111.33
3	D	6	MAN	O2-C2-C3	-2.02	105.96	110.15

There are no chirality outliers.

All (15) torsion outliers are listed below:

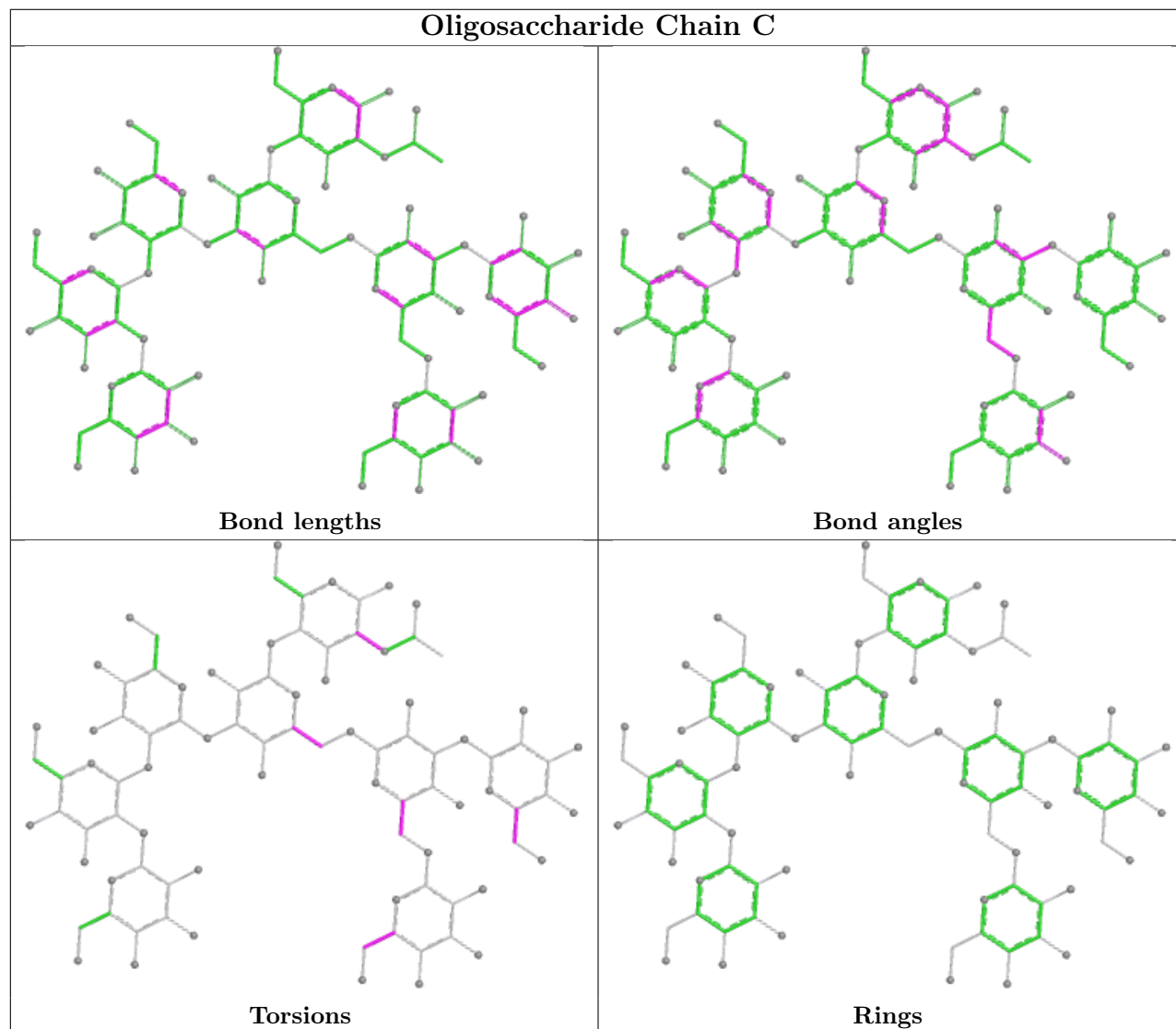
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C1-C2-N2-C7
2	C	8	MAN	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	C	8	MAN	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
2	C	6	MAN	C4-C5-C6-O6
2	C	6	MAN	O5-C5-C6-O6
2	C	2	BMA	C4-C5-C6-O6
2	C	7	MAN	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
3	D	6	MAN	O5-C5-C6-O6
2	C	2	BMA	O5-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6

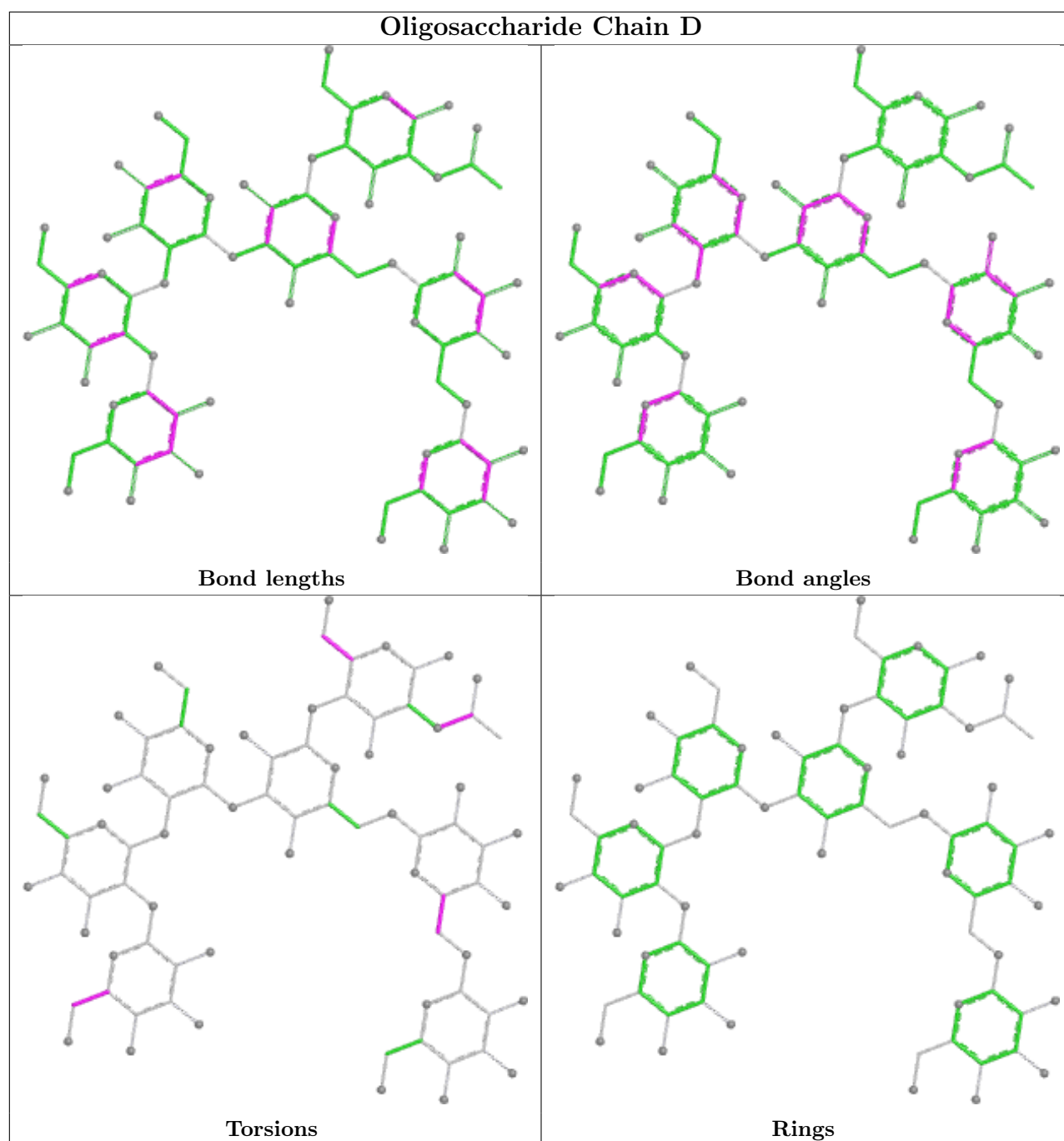
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7	MAN	2	0
3	D	2	BMA	1	0
2	C	8	MAN	1	0
3	D	7	MAN	1	0
3	D	1	NAG	1	0

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





5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	787/802 (98%)	0.03	21 (2%) 56 51	30, 48, 72, 99	0
1	B	787/802 (98%)	0.23	50 (6%) 25 22	34, 53, 81, 92	0
All	All	1574/1604 (98%)	0.13	71 (4%) 38 33	30, 51, 78, 99	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	647	ALA	5.2
1	B	569	VAL	4.5
1	B	668	LYS	4.4
1	B	676	ILE	4.2
1	B	572	ALA	4.2
1	A	758	LEU	4.1
1	B	830	GLY	4.0
1	B	46	THR	3.6
1	B	648	THR	3.6
1	B	728	ALA	3.6
1	A	761	THR	3.5
1	A	189	PHE	3.4
1	B	669	LEU	3.3
1	B	189	PHE	3.3
1	A	759	LYS	3.3
1	A	46	THR	3.2
1	A	723	GLY	3.2
1	B	761	THR	3.1
1	A	770	ILE	3.1
1	B	831	GLN	3.0
1	B	654	LEU	3.0
1	A	804	LEU	3.0
1	B	672	GLY	3.0
1	B	674	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	725	ILE	3.0
1	B	574	HIS	2.9
1	B	764	ASP	2.9
1	B	627	GLY	2.8
1	B	725	ILE	2.7
1	A	762	THR	2.7
1	B	631	HIS	2.7
1	B	762	THR	2.7
1	B	567	TYR	2.6
1	A	757	ILE	2.6
1	B	187	HIS	2.6
1	A	712	TRP	2.5
1	A	785	ASP	2.5
1	B	645	VAL	2.5
1	A	539	LYS	2.5
1	B	729	LYS	2.5
1	B	190	THR	2.5
1	B	804	LEU	2.5
1	B	626	LYS	2.5
1	A	760	ASP	2.5
1	B	636	ASN	2.4
1	A	767	LYS	2.4
1	B	763	ILE	2.4
1	B	565	GLY	2.4
1	B	653	TYR	2.4
1	B	571	ASN	2.3
1	B	634	ALA	2.3
1	B	675	ALA	2.3
1	A	765	LEU	2.3
1	A	528	MET	2.3
1	A	187	HIS	2.2
1	B	694	PHE	2.2
1	B	788	GLN	2.2
1	B	671	ILE	2.2
1	A	764	ASP	2.2
1	B	727	LEU	2.1
1	B	760	ASP	2.1
1	B	681	LEU	2.1
1	B	573	GLU	2.1
1	B	566	HIS	2.1
1	A	784	THR	2.1
1	B	570	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	677	MET	2.0
1	B	578	THR	2.0
1	B	649	THR	2.0
1	B	757	ILE	2.0
1	B	47	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

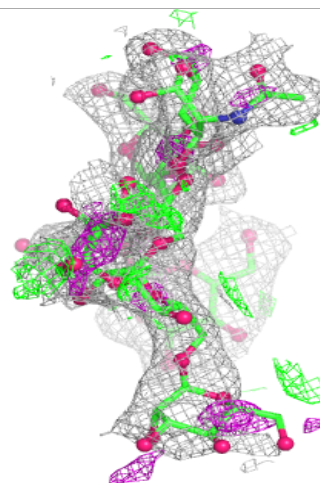
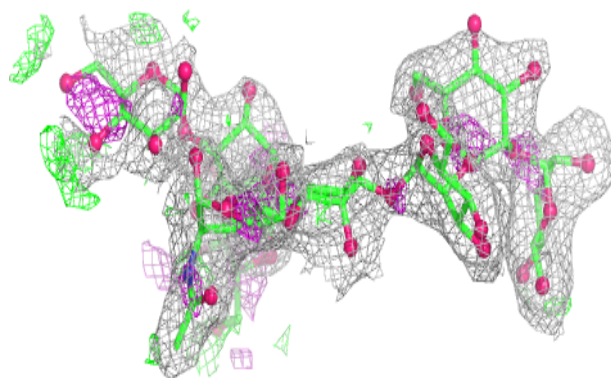
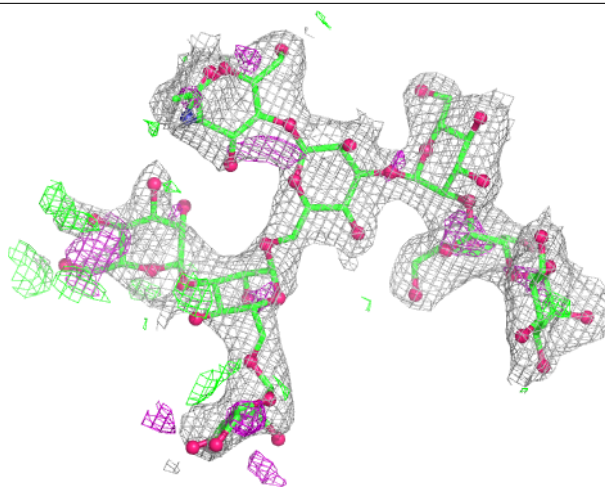
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

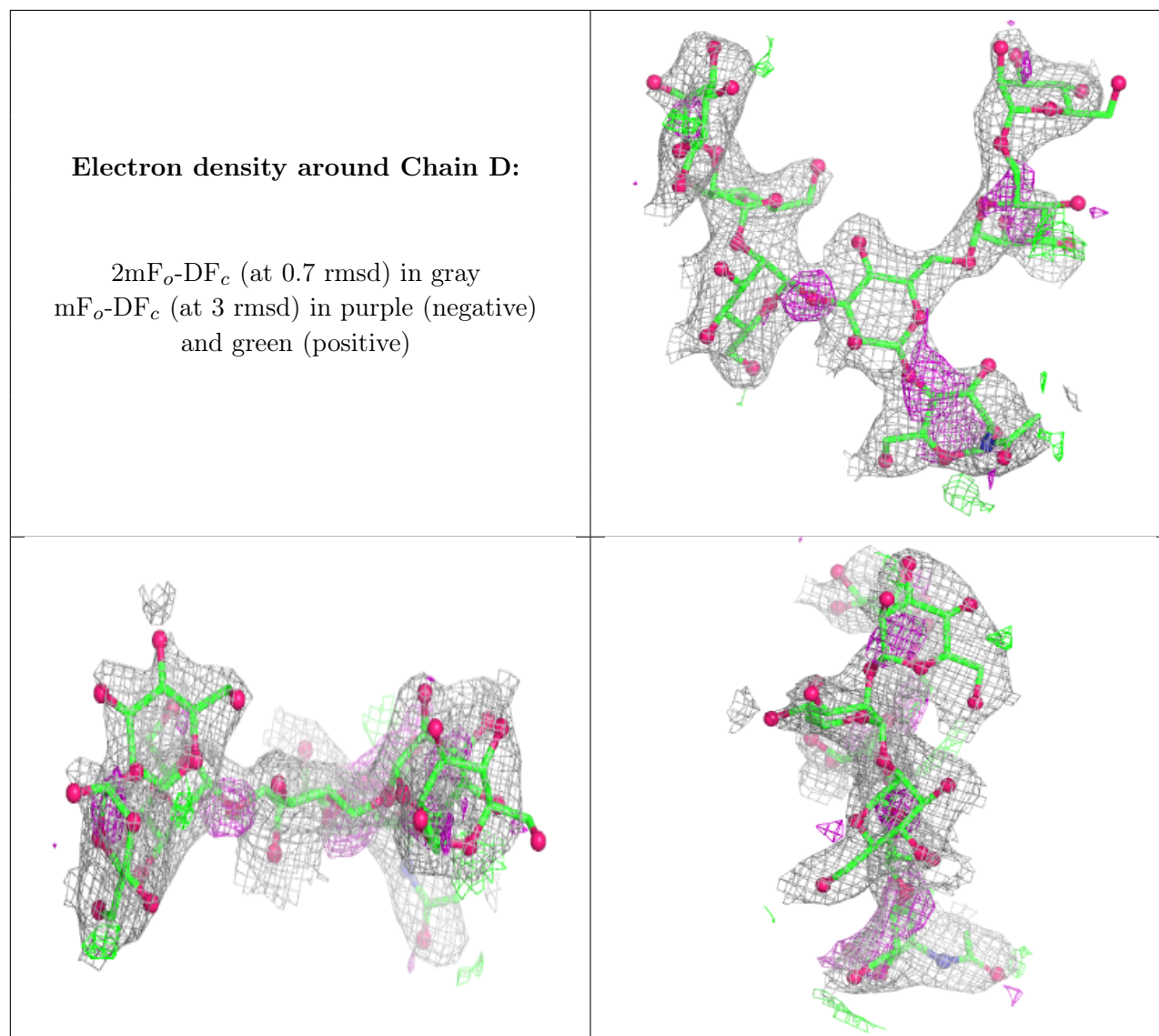
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	C	7	11/12	0.42	0.24	75,83,90,93	0
2	MAN	C	8	11/12	0.51	0.21	86,90,96,97	0
3	MAN	D	6	11/12	0.57	0.18	80,84,92,94	0
3	MAN	D	7	11/12	0.66	0.16	84,88,91,94	0
3	MAN	D	5	11/12	0.75	0.16	56,70,77,77	0
2	MAN	C	6	11/12	0.78	0.12	76,80,88,88	0
3	NAG	D	1	15/15	0.82	0.16	50,59,68,70	0
2	MAN	C	5	11/12	0.83	0.13	46,61,67,70	0
2	MAN	C	4	11/12	0.83	0.13	60,65,71,72	0
3	BMA	D	2	11/12	0.85	0.12	48,62,70,75	0
3	MAN	D	4	11/12	0.86	0.11	67,71,75,76	0
2	NAG	C	1	15/15	0.87	0.12	43,53,57,65	0
2	BMA	C	2	11/12	0.89	0.11	44,58,67,76	0
3	MAN	D	3	11/12	0.90	0.10	47,52,61,64	0
2	MAN	C	3	11/12	0.93	0.08	38,44,57,64	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(Å ²)	Q<0.9
4	CA	B	901	1/1	0.96	0.09	75,75,75,75	0
4	CA	A	901	1/1	0.98	0.10	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.