



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:49 PM UTC

PDB ID : 6MDS / pdb_00006mds
Title : Crystal structure of Streptococcus pyogenes endo-beta-N-acetylglucosaminidase (EndoS2) with complex biantennary 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

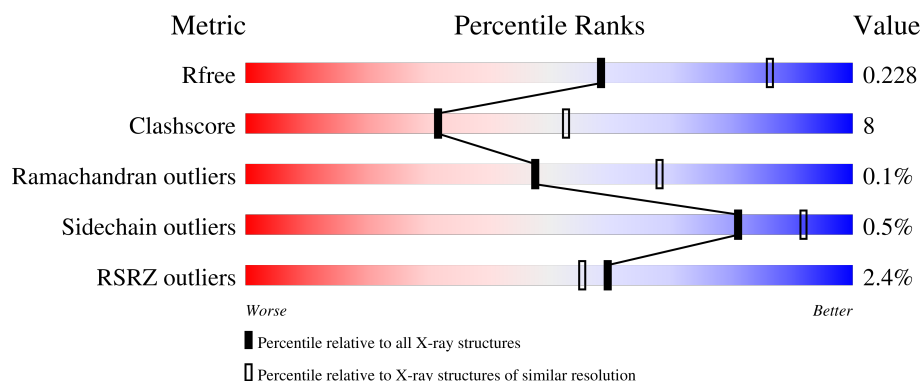
1 Overall quality at a glance

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	% 82% 16% .
1	B	802	3% 78% 20% .
2	C	8	25% 75%
2	D	8	25% 62% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13077 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.

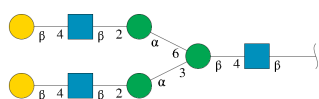
- Molecule 1 is a protein called Endo-beta-N-acetylglucosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	787	Total	C	N	O	S	0	0	0
			6238	3916	1065	1242	15			
1	B	787	Total	C	N	O	S	0	0	0
			6221	3903	1065	1238	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 beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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
			98	54	3	41			
2	D	8	Total	C	N	O	0	0	0
			98	54	3	41			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

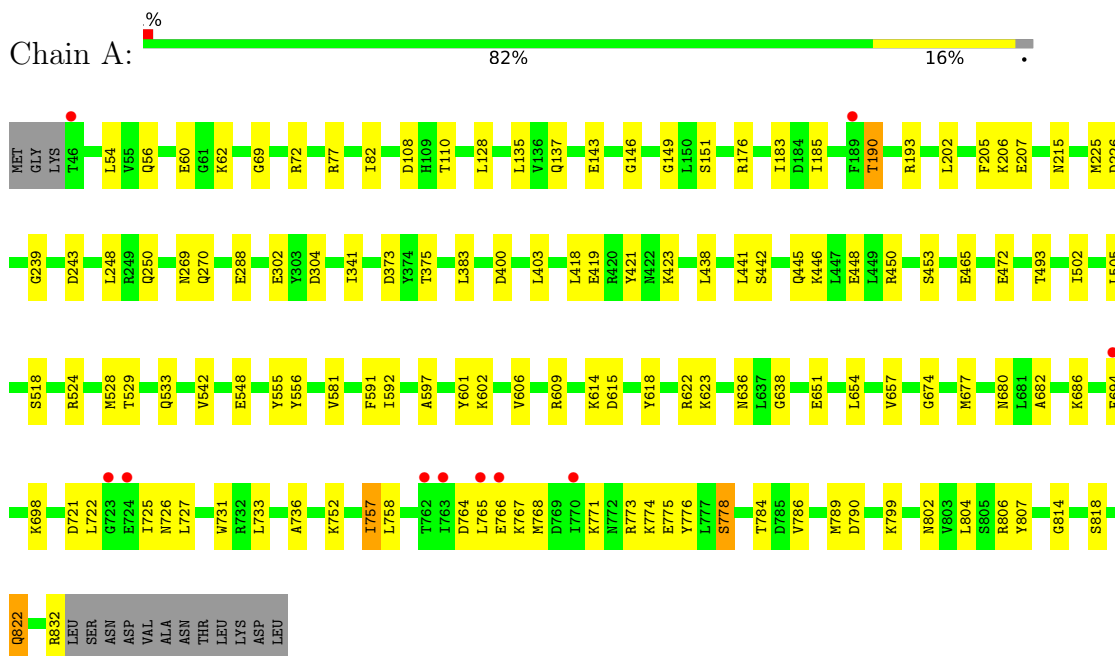
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total 246	O 246	0	0
4	B	174	Total 174	O 174	0	0

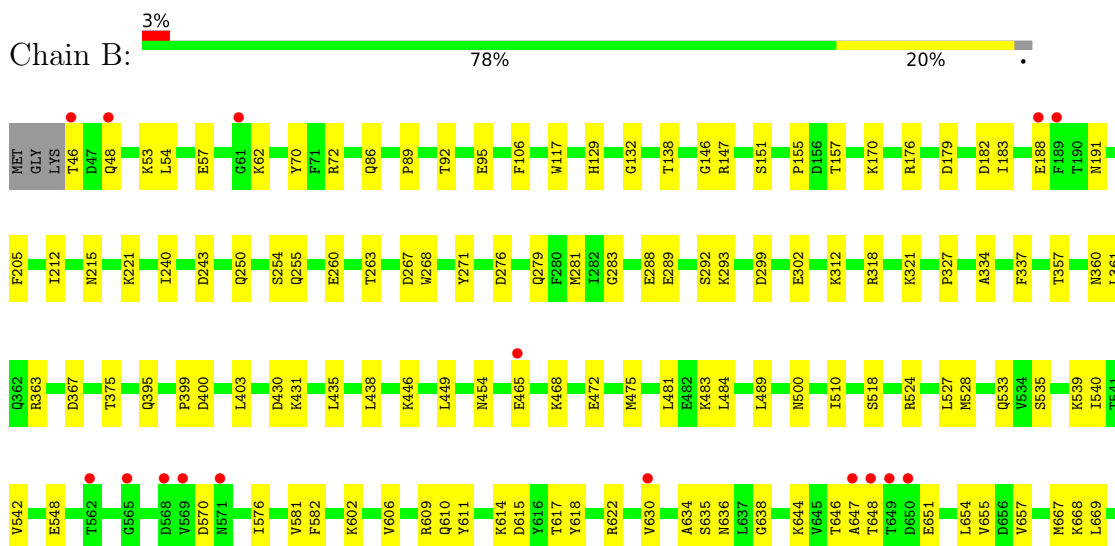
3 Residue-property plots [i](#)

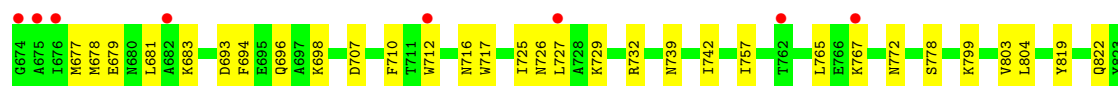
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Endo-beta-N-acetylglucosaminidase



- Molecule 1: Endo-beta-N-acetylglucosaminidase





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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.38Å 105.51Å 259.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.71 – 2.50 39.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.5 (39.71-2.50) 88.5 (39.71-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.193 , 0.242 (Not available) , 0.228	Depositor DCC
R_{free} test set	3800 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.8	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	0.94	EDS
Total number of atoms	13077	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: GAL, MAN, NAG, 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	0.43	0/6356	0.66	1/8595 (0.0%)
1	B	0.42	0/6338	0.71	9/8571 (0.1%)
All	All	0.42	0/12694	0.68	10/17166 (0.1%)

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	B	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	831	GLN	CA-CB-CG	-10.91	92.27	114.10
1	B	767	LYS	CG-CD-CE	10.47	135.37	111.30
1	B	170	LYS	CB-CG-CD	-8.16	92.52	111.30
1	B	644	LYS	CG-CD-CE	7.51	128.57	111.30
1	B	831	GLN	N-CA-C	6.39	119.95	109.85
1	B	170	LYS	CG-CD-CE	5.87	124.81	111.30
1	B	831	GLN	CB-CG-CD	-5.86	102.64	112.60
1	A	757	ILE	CG1-CB-CG2	-5.60	93.89	110.70
1	B	170	LYS	CA-CB-CG	5.55	125.19	114.10
1	B	683	LYS	CA-CB-CG	-5.44	103.22	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	831	GLN	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6238	0	6039	84	1
1	B	6221	0	6012	116	1
2	C	98	0	84	0	0
2	D	98	0	84	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	246	0	0	14	0
4	B	174	0	0	19	1
All	All	13077	0	12219	201	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 8.

All (201) 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:95:GLU:OE2	4:B:1001:HOH:O	1.82	0.96
1:B:819:TYR:OH	4:B:1002:HOH:O	1.85	0.92
1:A:445:GLN:NE2	4:A:1001:HOH:O	1.91	0.91
1:B:276:ASP:H	1:B:279:GLN:HE21	1.19	0.87
1:B:830:GLY:C	1:B:831:GLN:HG2	2.01	0.86
1:A:419:GLU:OE2	4:A:1002:HOH:O	1.93	0.84
1:A:207:GLU:OE1	4:A:1005:HOH:O	2.00	0.80
1:A:832:ARG:O	4:A:1003:HOH:O	1.99	0.79
1:A:421:TYR:O	4:A:1004:HOH:O	1.99	0.79
1:A:806:ARG:NH1	1:A:807:TYR:OH	2.16	0.79
1:B:677:MET:O	1:B:831:GLN:NE2	2.16	0.78
1:A:725:ILE:HG13	1:A:804:LEU:HD21	1.65	0.78
1:A:776:TYR:OH	4:A:1006:HOH:O	2.01	0.76
1:A:206:LYS:NZ	1:A:239:GLY:O	2.14	0.76
1:B:46:THR:N	4:B:1014:HOH:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:MET:HE2	1:A:773:ARG:HA	1.66	0.74
1:B:299:ASP:OD1	1:B:318:ARG:NH1	2.20	0.74
1:B:276:ASP:H	1:B:279:GLN:NE2	1.86	0.73
1:A:77:ARG:NH1	4:A:1013:HOH:O	2.22	0.72
1:B:360:ASN:OD1	4:B:1004:HOH:O	2.06	0.71
1:A:448:GLU:OE2	1:A:450:ARG:NH1	2.23	0.71
1:A:383:LEU:O	4:A:1008:HOH:O	2.08	0.71
1:A:56:GLN:O	1:A:60:GLU:HG3	1.91	0.70
1:B:610:GLN:O	4:B:1005:HOH:O	2.09	0.70
1:A:694:PHE:CE1	1:A:698:LYS:HE2	2.28	0.69
1:B:533:GLN:OE1	4:B:1007:HOH:O	2.11	0.68
1:B:729:LYS:O	1:B:799:LYS:HG3	1.93	0.68
1:B:710:PHE:HB3	1:B:822:GLN:HB3	1.76	0.68
1:B:716:ASN:OD1	4:B:1006:HOH:O	2.10	0.68
1:A:636:ASN:HB3	1:A:638:GLY:H	1.59	0.67
1:B:678:MET:HA	1:B:831:GLN:HE21	1.60	0.67
1:B:772:ASN:ND2	4:B:1012:HOH:O	2.17	0.67
1:B:481:LEU:O	4:B:1008:HOH:O	2.12	0.66
1:B:636:ASN:HB3	1:B:638:GLY:H	1.60	0.66
1:B:446:LYS:HG3	1:B:472:GLU:HB2	1.76	0.66
1:B:732:ARG:HD2	1:B:827:GLN:HE21	1.62	0.64
1:B:510:ILE:HD11	1:B:527:LEU:HD13	1.80	0.63
1:A:82:ILE:HD12	1:A:82:ILE:H	1.62	0.63
1:B:739:ASN:O	4:B:1009:HOH:O	2.16	0.63
1:B:732:ARG:HB3	1:B:827:GLN:HG3	1.82	0.61
1:B:727:LEU:HD13	1:B:804:LEU:HG	1.82	0.61
1:B:430:ASP:O	1:B:454:ASN:ND2	2.32	0.60
1:B:732:ARG:HD2	1:B:827:GLN:NE2	2.16	0.60
1:B:321:LYS:NZ	4:B:1021:HOH:O	2.28	0.60
1:A:446:LYS:HG3	1:A:472:GLU:HB2	1.84	0.59
1:B:630:VAL:HG13	1:B:655:VAL:HG23	1.84	0.59
1:B:693:ASP:HB3	1:B:696:GLN:OE1	2.02	0.59
1:B:542:VAL:HG22	1:B:609:ARG:HD3	1.84	0.59
1:B:729:LYS:HB3	1:B:799:LYS:HE3	1.84	0.58
1:A:764:ASP:OD1	1:A:767:LYS:HG3	2.03	0.58
1:B:72:ARG:NH1	1:B:288:GLU:OE1	2.37	0.58
1:B:357:THR:O	1:B:361:LEU:HD23	2.04	0.58
1:A:556:TYR:CD2	1:A:623:LYS:HE3	2.39	0.58
1:B:57:GLU:HG2	1:B:62:LYS:CE	2.34	0.58
1:A:725:ILE:HG13	1:A:804:LEU:CD2	2.34	0.58
1:B:54:LEU:HD21	1:B:132:GLY:HA2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ASP:HB3	1:B:271:TYR:CE2	2.39	0.57
1:B:302:GLU:OE1	4:B:1010:HOH:O	2.17	0.57
1:B:576:ILE:HD11	1:B:669:LEU:HD22	1.84	0.57
1:B:634:ALA:N	4:B:1030:HOH:O	2.37	0.57
1:B:86:GLN:NE2	1:B:89:PRO:HB3	2.19	0.57
1:A:733:LEU:HD22	1:A:789:MET:HE1	1.84	0.57
1:B:292:SER:HB3	1:B:357:THR:HA	1.87	0.57
1:B:281:MET:HG2	1:B:334:ALA:HB3	1.87	0.57
1:A:771:LYS:O	1:A:775:GLU:HG3	2.04	0.56
1:A:654:LEU:HG	1:A:677:MET:HE2	1.86	0.56
1:B:739:ASN:ND2	1:B:742:ILE:HB	2.20	0.56
1:A:597:ALA:O	4:A:1010:HOH:O	2.17	0.56
1:A:373:ASP:OD1	1:A:375:THR:HG23	2.06	0.56
1:A:502:ILE:HG22	1:A:505:LEU:HB2	1.88	0.56
1:B:155:PRO:HB2	1:B:157:THR:HG23	1.88	0.56
1:A:185:ILE:HD12	1:A:225:MET:HE2	1.89	0.55
1:A:721:ASP:OD1	1:A:806:ARG:HG2	2.07	0.55
1:B:655:VAL:CG1	1:B:667:MET:HG3	2.36	0.55
1:A:555:TYR:HA	1:A:623:LYS:HE2	1.87	0.55
1:B:725:ILE:HD11	1:B:804:LEU:HB3	1.90	0.54
1:A:528:MET:HE1	1:A:606:VAL:HG13	1.90	0.53
1:A:548:GLU:OE2	1:A:609:ARG:HD2	2.08	0.53
1:A:250:GLN:NE2	4:A:1031:HOH:O	2.42	0.52
1:A:542:VAL:HG22	1:A:609:ARG:HD3	1.91	0.52
1:A:765:LEU:O	1:A:773:ARG:NH1	2.42	0.52
1:A:694:PHE:CE1	1:A:698:LYS:CE	2.91	0.52
1:B:548:GLU:OE2	1:B:609:ARG:HD2	2.08	0.52
1:B:57:GLU:HG2	1:B:62:LYS:HE2	1.92	0.52
1:A:727:LEU:HD11	1:A:802:ASN:HB3	1.91	0.51
1:B:582:PHE:O	4:B:1013:HOH:O	2.19	0.51
1:B:188:GLU:OE1	4:B:1015:HOH:O	2.19	0.51
1:B:618:TYR:CE2	1:B:622:ARG:HD3	2.45	0.51
1:B:654:LEU:CD2	1:B:668:LYS:HG3	2.40	0.51
1:B:86:GLN:HE22	1:B:89:PRO:HB3	1.74	0.51
1:A:524:ARG:O	1:A:528:MET:HG2	2.11	0.51
1:B:212:ILE:HB	1:B:221:LYS:HB2	1.91	0.51
1:B:830:GLY:O	1:B:831:GLN:HG2	2.11	0.51
1:A:766:GLU:HA	1:A:773:ARG:HH12	1.77	0.50
1:B:500:ASN:ND2	4:B:1034:HOH:O	2.40	0.50
1:B:147:ARG:NH1	1:B:188:GLU:OE2	2.45	0.50
1:B:694:PHE:CE2	1:B:698:LYS:HE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:MET:CE	1:A:773:ARG:HA	2.38	0.50
1:A:682:ALA:HA	1:A:722:LEU:HD22	1.92	0.49
1:B:129:HIS:NE2	1:B:179:ASP:OD1	2.37	0.49
1:B:630:VAL:CG1	1:B:655:VAL:HG23	2.42	0.49
1:B:483:LYS:HG2	1:B:484:LEU:N	2.26	0.49
1:B:138:THR:HG22	1:B:182:ASP:HB3	1.95	0.49
1:B:727:LEU:CD1	1:B:804:LEU:HG	2.43	0.49
1:A:202:LEU:HD11	1:A:206:LYS:HE2	1.95	0.49
1:A:190:THR:N	4:A:1036:HOH:O	2.46	0.49
1:B:528:MET:HE1	1:B:606:VAL:HG11	1.95	0.49
1:B:465:GLU:N	1:B:465:GLU:OE1	2.40	0.48
1:B:732:ARG:HH11	1:B:827:GLN:NE2	2.11	0.48
1:A:529:THR:O	1:A:533:GLN:HG2	2.13	0.48
1:B:630:VAL:HG13	1:B:655:VAL:CG2	2.42	0.48
1:B:717:TRP:CZ2	1:B:778:SER:HB3	2.48	0.48
1:A:680:ASN:HD21	1:A:682:ALA:HB3	1.77	0.48
1:B:535:SER:HB2	1:B:540:ILE:HD11	1.96	0.48
1:A:651:GLU:O	1:A:674:GLY:HA2	2.13	0.48
1:A:686:LYS:HG3	1:A:721:ASP:HB3	1.95	0.48
1:B:215:ASN:ND2	1:B:243:ASP:OD1	2.27	0.48
1:A:302:GLU:O	4:A:1011:HOH:O	2.20	0.48
1:B:602:LYS:NZ	1:B:614:LYS:O	2.37	0.47
1:A:72:ARG:NH1	1:A:288:GLU:OE1	2.46	0.47
1:B:92:THR:HG23	1:B:95:GLU:HG3	1.96	0.47
1:A:618:TYR:CE2	1:A:622:ARG:HD3	2.50	0.47
1:B:524:ARG:O	1:B:528:MET:HG2	2.14	0.47
1:B:188:GLU:HG2	1:B:191:ASN:O	2.14	0.47
1:A:69:GLY:HA3	1:A:341:ILE:HD12	1.97	0.47
1:A:146:GLY:N	1:A:151:SER:OG	2.47	0.47
1:B:255:GLN:O	1:B:263:THR:HG23	2.15	0.47
1:A:193:ARG:HD2	4:A:1059:HOH:O	2.14	0.47
1:A:226:ASP:HA	1:A:248:LEU:O	2.14	0.47
1:B:276:ASP:N	1:B:279:GLN:HE21	2.00	0.46
1:A:758:LEU:HD11	1:A:776:TYR:HE1	1.79	0.46
1:B:435:LEU:HD22	1:B:438:LEU:HD22	1.98	0.46
1:B:70:TYR:CE2	1:B:138:THR:HG21	2.50	0.46
1:B:757:ILE:HG21	1:B:803:VAL:HG11	1.97	0.45
2:D:1:NAG:O7	2:D:1:NAG:H1	2.15	0.45
1:A:215:ASN:ND2	1:A:243:ASP:OD1	2.42	0.45
1:A:438:LEU:HD12	1:A:438:LEU:HA	1.76	0.45
1:A:731:TRP:HH2	1:A:789:MET:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:TRP:CZ3	1:B:176:ARG:NH1	2.84	0.45
1:B:681:LEU:CD2	1:B:726:ASN:HB2	2.46	0.45
1:A:418:LEU:HD22	1:A:441:LEU:HD21	1.99	0.45
1:A:591:PHE:C	1:A:592:ILE:HD12	2.42	0.45
1:B:268:TRP:CD1	1:B:327:PRO:HB3	2.51	0.45
1:B:678:MET:HA	1:B:831:GLN:NE2	2.28	0.45
1:B:70:TYR:HE2	1:B:138:THR:HG21	1.82	0.45
1:B:283:GLY:HA3	1:B:337:PHE:CZ	2.52	0.44
1:A:757:ILE:HG12	1:A:786:VAL:HG13	1.99	0.44
1:B:146:GLY:N	1:B:151:SER:OG	2.49	0.44
1:B:254:SER:OG	1:B:260:GLU:OE1	2.29	0.44
1:B:712:TRP:CD2	1:B:712:TRP:C	2.94	0.44
1:A:202:LEU:O	1:A:206:LYS:HG3	2.17	0.44
1:A:442:SER:HB3	1:A:465:GLU:OE1	2.18	0.44
1:B:679:GLU:O	1:B:829:LEU:HA	2.17	0.44
1:A:774:LYS:O	1:A:778:SER:OG	2.35	0.43
1:B:468:LYS:HG2	1:B:489:LEU:HA	2.01	0.43
1:B:765:LEU:HD23	1:B:765:LEU:HA	1.70	0.43
1:B:106:PHE:HZ	2:D:1:NAG:HO3	1.63	0.43
1:A:143:GLU:OE1	1:A:149:GLY:HA3	2.19	0.43
1:A:137:GLN:CD	1:A:176:ARG:HH11	2.27	0.43
1:B:449:LEU:HD12	1:B:475:MET:HE2	1.99	0.43
1:B:46:THR:HG22	1:B:48:GLN:H	1.84	0.43
1:B:570:ASP:O	1:B:647:ALA:O	2.36	0.43
1:B:712:TRP:O	1:B:712:TRP:CE3	2.71	0.43
1:B:518:SER:HA	1:B:611:TYR:OH	2.18	0.42
1:A:423:LYS:O	1:A:445:GLN:HG3	2.19	0.42
1:A:799:LYS:H	1:A:799:LYS:HG2	1.64	0.42
1:B:400:ASP:HB3	1:B:403:LEU:HB3	2.01	0.42
1:A:269:ASN:HD22	1:A:270:GLN:NE2	2.17	0.42
1:B:581:VAL:HG21	1:B:657:VAL:HG21	2.01	0.42
1:B:646:THR:HG22	1:B:648:THR:HG23	2.00	0.42
1:B:732:ARG:HB3	1:B:827:GLN:HE21	1.83	0.42
1:B:289:GLU:HB2	1:B:367:ASP:O	2.18	0.42
1:B:539:LYS:HD2	1:B:539:LYS:HA	1.65	0.42
1:B:707:ASP:O	1:B:824:THR:HG22	2.20	0.42
1:A:128:LEU:CD1	1:A:135:LEU:HD21	2.50	0.42
1:A:736:ALA:HB2	1:A:822:GLN:O	2.20	0.42
1:B:240:ILE:HG13	1:B:240:ILE:O	2.20	0.42
1:A:108:ASP:C	1:A:110:THR:H	2.27	0.42
1:A:556:TYR:CE2	1:A:623:LYS:HE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:PRO:HD2	4:B:1031:HOH:O	2.19	0.42
1:A:757:ILE:HG13	1:A:784:THR:HB	2.02	0.41
1:B:615:ASP:OD1	1:B:615:ASP:N	2.49	0.41
1:A:614:LYS:NZ	1:A:615:ASP:HB3	2.36	0.41
1:B:617:THR:HG23	4:B:1110:HOH:O	2.19	0.41
1:A:60:GLU:HB2	1:A:62:LYS:HE3	2.03	0.41
1:B:53:LYS:HE3	1:B:57:GLU:OE1	2.21	0.41
1:A:304:ASP:OD1	4:A:1012:HOH:O	2.22	0.41
1:B:176:ARG:HH11	1:B:176:ARG:HD3	1.70	0.41
1:B:312:LYS:HE2	1:B:375:THR:HB	2.03	0.41
1:A:183:ILE:HG13	1:A:205:PHE:CZ	2.56	0.41
1:B:431:LYS:HB3	1:B:431:LYS:HE2	1.77	0.41
1:B:635:SER:OG	1:B:651:GLU:OE1	2.37	0.41
1:A:581:VAL:HG21	1:A:657:VAL:HG21	2.03	0.41
1:A:752:LYS:NZ	1:A:814:GLY:HA3	2.36	0.41
1:A:726:ASN:OD1	1:A:832:ARG:HB2	2.21	0.40
1:B:293:LYS:NZ	4:B:1053:HOH:O	2.53	0.40
1:A:54:LEU:HA	1:A:54:LEU:HD23	1.89	0.40
1:A:400:ASP:HB3	1:A:403:LEU:HB3	2.02	0.40
1:A:518:SER:HB3	1:A:601:TYR:CE1	2.55	0.40
1:B:183:ILE:HG13	1:B:205:PHE:CZ	2.57	0.40
1:B:250:GLN:NE2	2:D:1:NAG:O1	2.49	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:B:1064:HOH:O	4:B:1149:HOH:O[1_565]	1.86	0.34
1:A:602:LYS:O	1:B:363:ARG:NH2[1_655]	2.11	0.09

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%)	756 (96%)	28 (4%)	1 (0%)	48	68
1	B	785/802 (98%)	754 (96%)	31 (4%)	0	100	100
All	All	1570/1604 (98%)	1510 (96%)	59 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	THR

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	674/699 (96%)	668 (99%)	6 (1%)	70	87
1	B	669/699 (96%)	668 (100%)	1 (0%)	88	96
All	All	1343/1398 (96%)	1336 (100%)	7 (0%)	81	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	453	SER
1	A	493	THR
1	A	778	SER
1	A	790	ASP
1	A	818	SER
1	A	822	GLN
1	B	395	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	203	ASN
1	A	250	GLN

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Mol	Chain	Res	Type
1	A	270	GLN
1	A	409	GLN
1	A	512	HIS
1	A	680	ASN
1	A	827	GLN
1	B	48	GLN
1	B	75	HIS
1	B	86	GLN
1	B	88	HIS
1	B	107	HIS
1	B	203	ASN
1	B	250	GLN
1	B	255	GLN
1	B	279	GLN
1	B	504	HIS
1	B	512	HIS
1	B	631	HIS
1	B	716	ASN
1	B	739	ASN
1	B	772	ASN
1	B	779	ASN
1	B	827	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 ⓘ

16 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	0.64	0	21,21,21	0.95	1 (4%)
2	BMA	C	2	2	11,11,12	1.02	1 (9%)	15,15,17	0.93	0
2	MAN	C	3	2	11,11,12	1.39	2 (18%)	15,15,17	1.26	3 (20%)
2	NAG	C	4	2	14,14,15	0.21	0	17,19,21	0.52	0
2	GAL	C	5	2	11,11,12	0.84	0	15,15,17	1.12	1 (6%)
2	MAN	C	6	2	11,11,12	1.71	3 (27%)	15,15,17	1.00	1 (6%)
2	NAG	C	7	2	14,14,15	0.59	0	17,19,21	0.69	0
2	GAL	C	8	2	11,11,12	1.27	2 (18%)	15,15,17	0.94	1 (6%)
2	NAG	D	1	2	15,15,15	0.64	1 (6%)	21,21,21	0.79	0
2	BMA	D	2	2	11,11,12	1.30	1 (9%)	15,15,17	0.84	0
2	MAN	D	3	2	11,11,12	1.06	1 (9%)	15,15,17	1.25	2 (13%)
2	NAG	D	4	2	14,14,15	0.29	0	17,19,21	0.52	0
2	GAL	D	5	2	11,11,12	0.89	0	15,15,17	0.99	1 (6%)
2	MAN	D	6	2	11,11,12	1.03	0	15,15,17	1.02	2 (13%)
2	NAG	D	7	2	14,14,15	0.58	0	17,19,21	0.63	0
2	GAL	D	8	2	11,11,12	0.91	1 (9%)	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	C	1	2	-	4/6/26/26	0/1/1/1
2	BMA	C	2	2	-	0/2/19/22	0/1/1/1
2	MAN	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	C	4	2	-	1/6/23/26	0/1/1/1
2	GAL	C	5	2	-	1/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	NAG	C	7	2	-	0/6/23/26	0/1/1/1
2	GAL	C	8	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2	-	4/6/26/26	0/1/1/1
2	BMA	D	2	2	-	0/2/19/22	0/1/1/1
2	MAN	D	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	4	2	-	1/6/23/26	0/1/1/1
2	GAL	D	5	2	-	1/2/19/22	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	0/1/1/1
2	NAG	D	7	2	-	0/6/23/26	0/1/1/1
2	GAL	D	8	2	-	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)
2	C	6	MAN	O5-C5	3.38	1.50	1.43
2	C	6	MAN	C2-C3	3.17	1.57	1.52
2	C	6	MAN	C4-C3	2.54	1.58	1.52
2	C	2	BMA	C2-C3	2.53	1.56	1.52
2	C	8	GAL	C4-C5	2.51	1.58	1.53
2	C	3	MAN	C2-C3	2.48	1.56	1.52
2	C	3	MAN	O3-C3	2.39	1.48	1.43
2	D	2	BMA	C2-C3	2.39	1.56	1.52
2	D	3	MAN	C4-C3	2.25	1.58	1.52
2	C	8	GAL	C1-C2	2.19	1.57	1.52
2	D	1	NAG	O5-C1	-2.14	1.37	1.42
2	D	8	GAL	C1-C2	2.02	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	MAN	C1-O5-C5	3.18	116.45	112.19
2	C	3	MAN	C1-O5-C5	2.91	116.09	112.19
2	D	6	MAN	O2-C2-C3	-2.50	104.97	110.15
2	C	6	MAN	O2-C2-C3	-2.44	105.10	110.15
2	D	3	MAN	O2-C2-C3	-2.42	105.13	110.15
2	C	1	NAG	O1-C1-O5	-2.39	103.30	110.41
2	C	3	MAN	O2-C2-C3	-2.32	105.35	110.15
2	C	3	MAN	O3-C3-C2	2.19	114.53	110.05
2	C	8	GAL	O2-C2-C1	2.15	114.16	109.22
2	D	6	MAN	C1-O5-C5	2.12	115.02	112.19
2	D	5	GAL	C1-O5-C5	2.07	114.96	112.19
2	C	5	GAL	C1-C2-C3	2.06	112.64	109.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C1-C2-N2-C7
2	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	5	GAL	O5-C5-C6-O6
2	C	5	GAL	O5-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7

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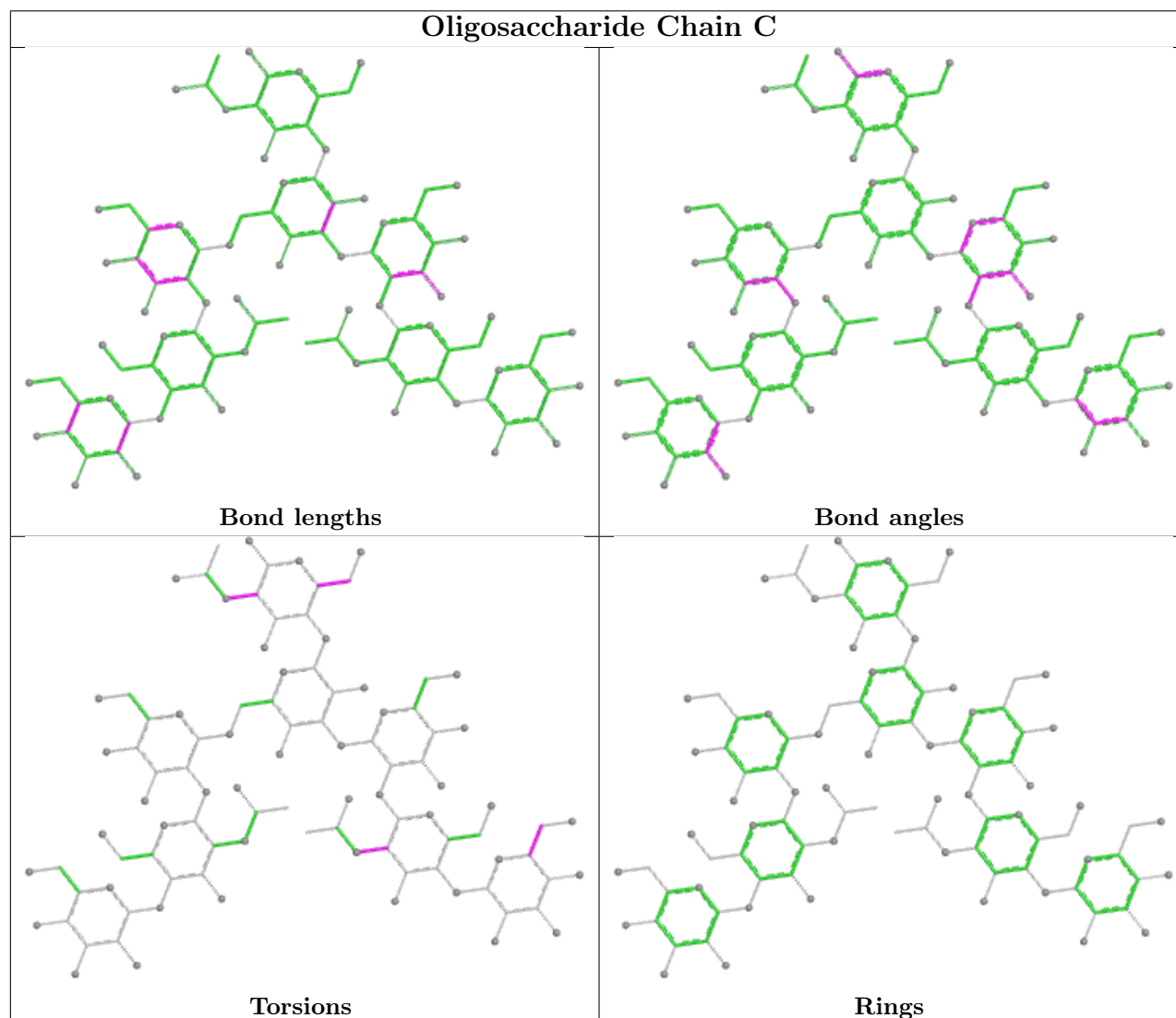
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C3-C2-N2-C7
2	C	4	NAG	C1-C2-N2-C7
2	D	1	NAG	C3-C2-N2-C7
2	D	4	NAG	C4-C5-C6-O6

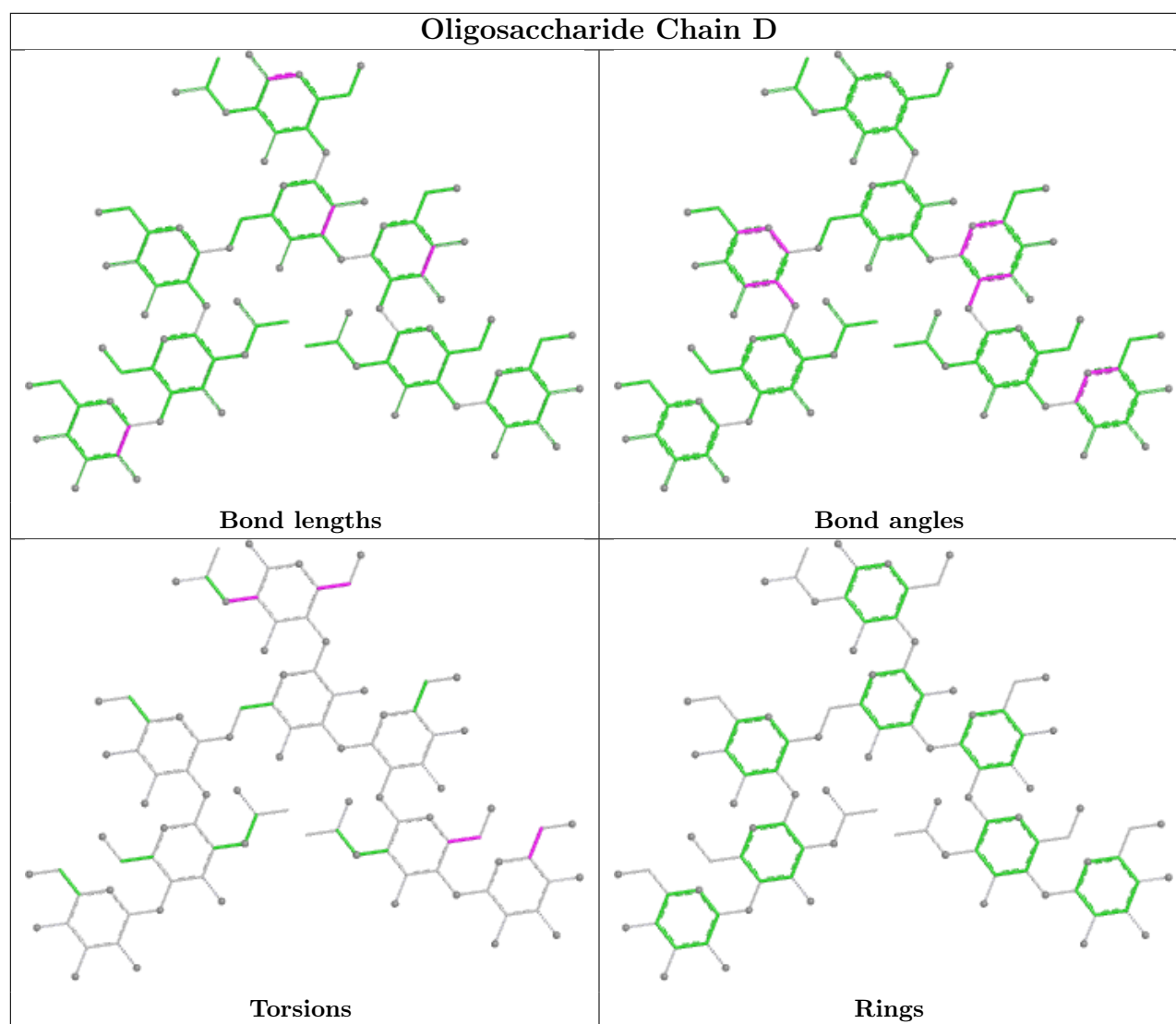
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	3	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%)	0.02	10 (1%) 75 71	28, 43, 62, 97	0
1	B	787/802 (98%)	0.30	27 (3%) 48 43	29, 51, 76, 98	0
All	All	1574/1604 (98%)	0.16	37 (2%) 59 55	28, 46, 72, 98	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	569	VAL	4.3
1	B	568	ASP	4.1
1	A	723	GLY	3.4
1	B	727	LEU	3.3
1	B	676	ILE	2.9
1	B	46	THR	2.9
1	B	48	GLN	2.9
1	B	565	GLY	2.9
1	B	650	ASP	2.8
1	A	765	LEU	2.8
1	B	562	THR	2.7
1	B	648	THR	2.7
1	B	465	GLU	2.6
1	B	682	ALA	2.6
1	A	189	PHE	2.5
1	A	770	ILE	2.4
1	B	630	VAL	2.4
1	B	647	ALA	2.4
1	B	674	GLY	2.4
1	A	694	PHE	2.4
1	B	188	GLU	2.4
1	B	571	ASN	2.3
1	B	649	THR	2.3
1	B	831	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	675	ALA	2.3
1	B	712	TRP	2.3
1	B	61	GLY	2.2
1	B	767	LYS	2.2
1	A	46	THR	2.1
1	A	762	THR	2.1
1	A	724	GLU	2.1
1	B	762	THR	2.1
1	B	828	ILE	2.0
1	B	189	PHE	2.0
1	A	766	GLU	2.0
1	B	826	LEU	2.0
1	A	763	ILE	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	GAL	D	5	11/12	0.53	0.21	77,84,96,99	0
2	GAL	C	8	11/12	0.57	0.17	72,85,94,94	0
2	GAL	C	5	11/12	0.57	0.17	81,84,90,92	0
2	GAL	D	8	11/12	0.57	0.20	79,92,101,101	0
2	NAG	D	7	14/15	0.82	0.13	55,71,83,86	0
2	NAG	D	4	14/15	0.83	0.16	54,65,73,77	0
2	NAG	C	1	15/15	0.83	0.14	43,53,60,65	0
2	MAN	D	6	11/12	0.84	0.12	66,68,71,72	0
2	NAG	D	1	15/15	0.87	0.14	50,58,64,67	0
2	NAG	C	7	14/15	0.87	0.11	51,66,77,83	0
2	MAN	C	6	11/12	0.88	0.12	61,62,65,65	0
2	MAN	D	3	11/12	0.91	0.09	39,47,56,61	0
2	NAG	C	4	14/15	0.91	0.10	49,61,72,74	0
2	BMA	C	2	11/12	0.92	0.10	43,50,54,60	0
2	MAN	C	3	11/12	0.93	0.09	36,45,50,52	0

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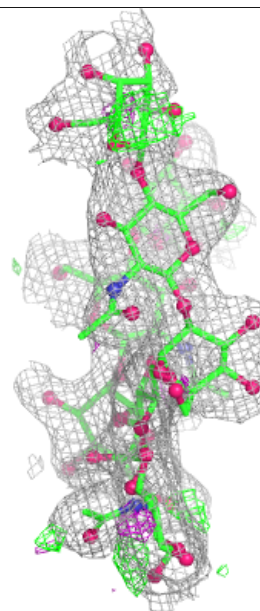
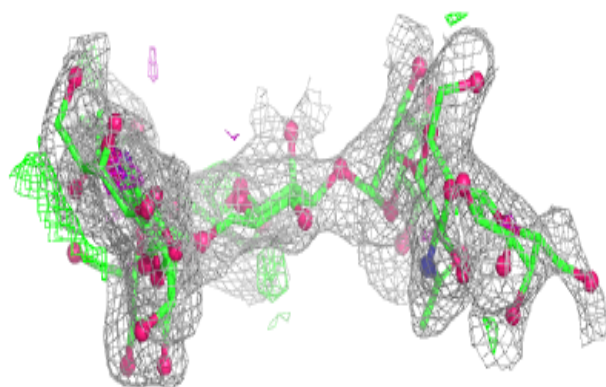
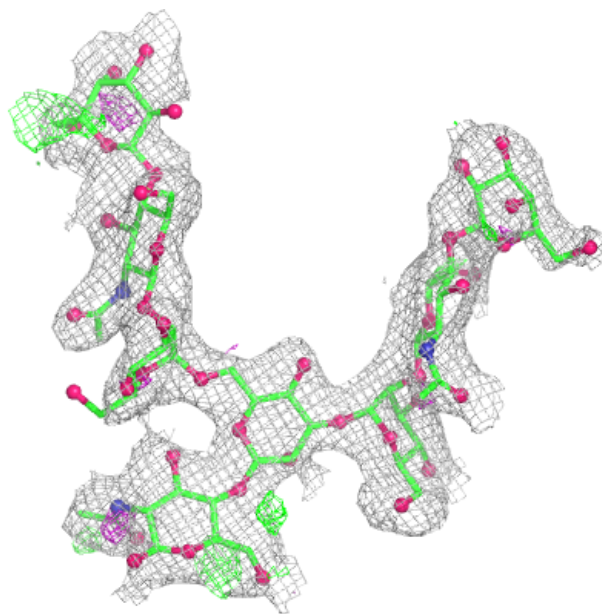
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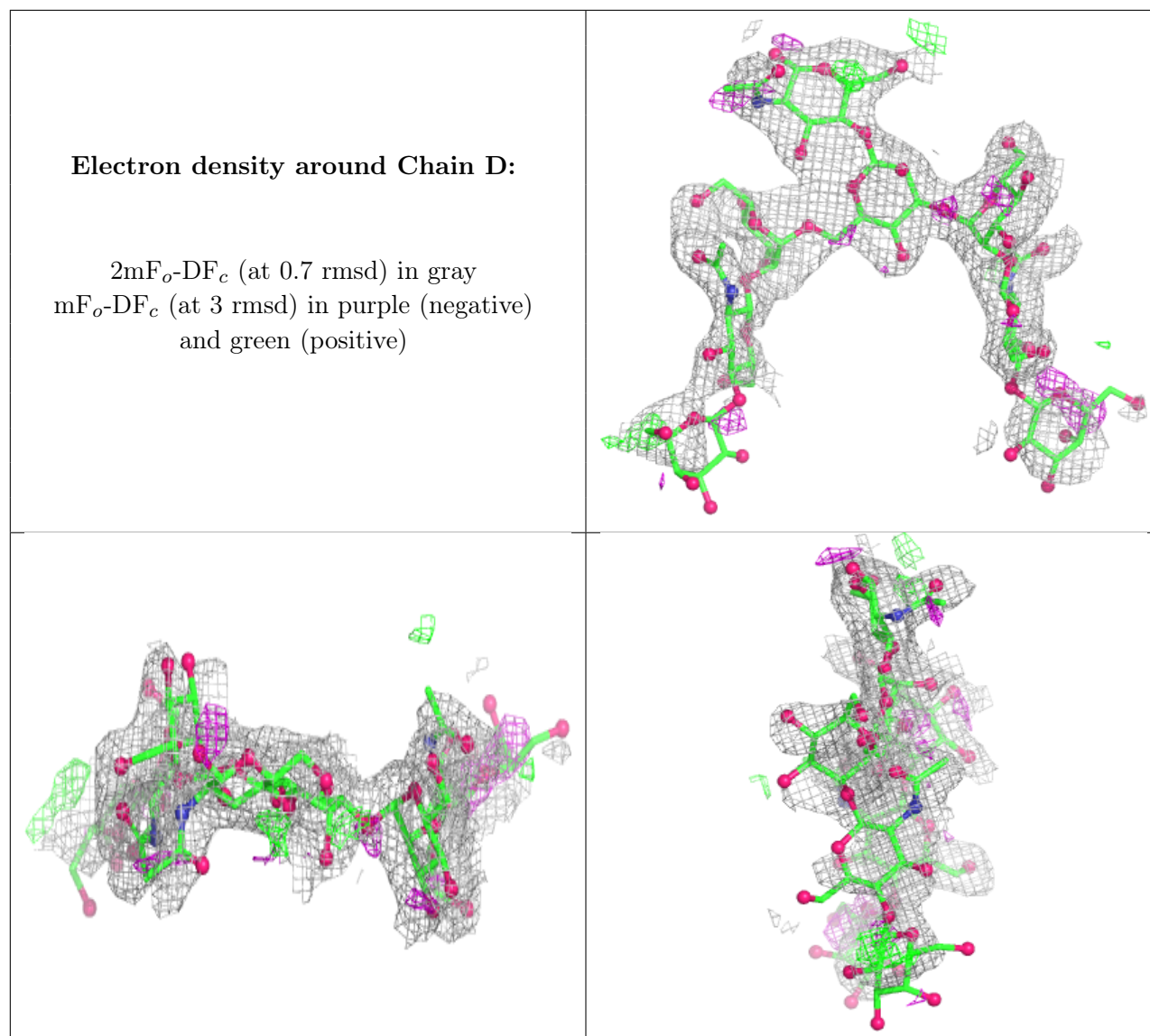
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	D	2	11/12	0.93	0.07	47,52,57,67	0

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
3	CA	B	901	1/1	0.90	0.12	74,74,74,74	0
3	CA	A	909	1/1	0.96	0.07	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.