



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 10:37 PM JST

PDB ID : 7XTJ
Title : Crystal structure of E88A mutant of GH3 beta-xylosidase from *Aspergillus niger* (AnBX)
Authors : Kaenyng, W.; Kongsaree, P.T.; Tagami, T.
Deposited on : 2022-05-17
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

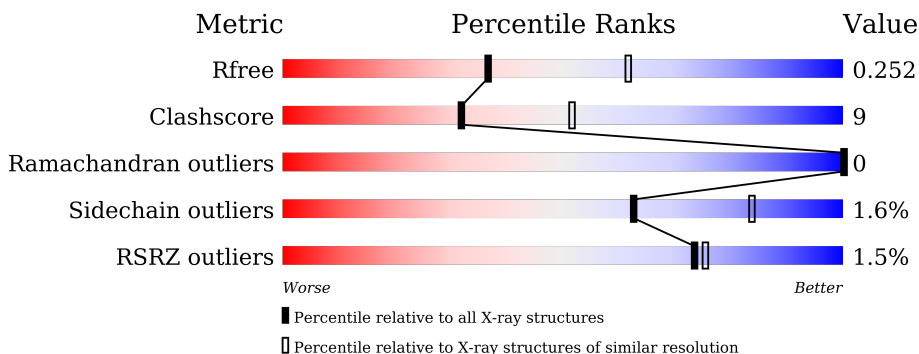
1 Overall quality at a glance

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	788	
1	B	788	
2	C	6	
2	E	6	
3	D	2	
4	F	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	804	-	-	-	X
5	NAG	B	804	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11809 atoms, of which 16 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.

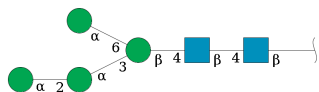
- Molecule 1 is a protein called Xylan 1,4-beta-xylosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	742	Total	C	N	O	S	0	1	0
			5707	3603	968	1124	12			
1	B	743	Total	C	N	O	S	0	0	0
			5704	3599	967	1126	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	ALA	-	expression tag	UNP A0A023J5W7
A	-9	HIS	-	expression tag	UNP A0A023J5W7
A	-8	HIS	-	expression tag	UNP A0A023J5W7
A	-7	HIS	-	expression tag	UNP A0A023J5W7
A	-6	HIS	-	expression tag	UNP A0A023J5W7
A	-5	HIS	-	expression tag	UNP A0A023J5W7
A	-4	HIS	-	expression tag	UNP A0A023J5W7
A	-3	HIS	-	expression tag	UNP A0A023J5W7
A	-2	HIS	-	expression tag	UNP A0A023J5W7
A	-1	ALA	-	expression tag	UNP A0A023J5W7
A	0	ALA	-	expression tag	UNP A0A023J5W7
A	88	ALA	GLU	engineered mutation	UNP A0A023J5W7
B	-10	ALA	-	expression tag	UNP A0A023J5W7
B	-9	HIS	-	expression tag	UNP A0A023J5W7
B	-8	HIS	-	expression tag	UNP A0A023J5W7
B	-7	HIS	-	expression tag	UNP A0A023J5W7
B	-6	HIS	-	expression tag	UNP A0A023J5W7
B	-5	HIS	-	expression tag	UNP A0A023J5W7
B	-4	HIS	-	expression tag	UNP A0A023J5W7
B	-3	HIS	-	expression tag	UNP A0A023J5W7
B	-2	HIS	-	expression tag	UNP A0A023J5W7
B	-1	ALA	-	expression tag	UNP A0A023J5W7
B	0	ALA	-	expression tag	UNP A0A023J5W7
B	88	ALA	GLU	engineered mutation	UNP A0A023J5W7

- Molecule 2 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.



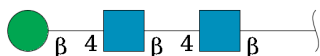
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	6	72	40	2	30	0	0	0
2	E	6	72	40	2	30	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	28	16	2	10	0	0	0

- Molecule 4 is an oligosaccharide called 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
			Total	C	N	O			
4	F	3	39	22	2	15	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		

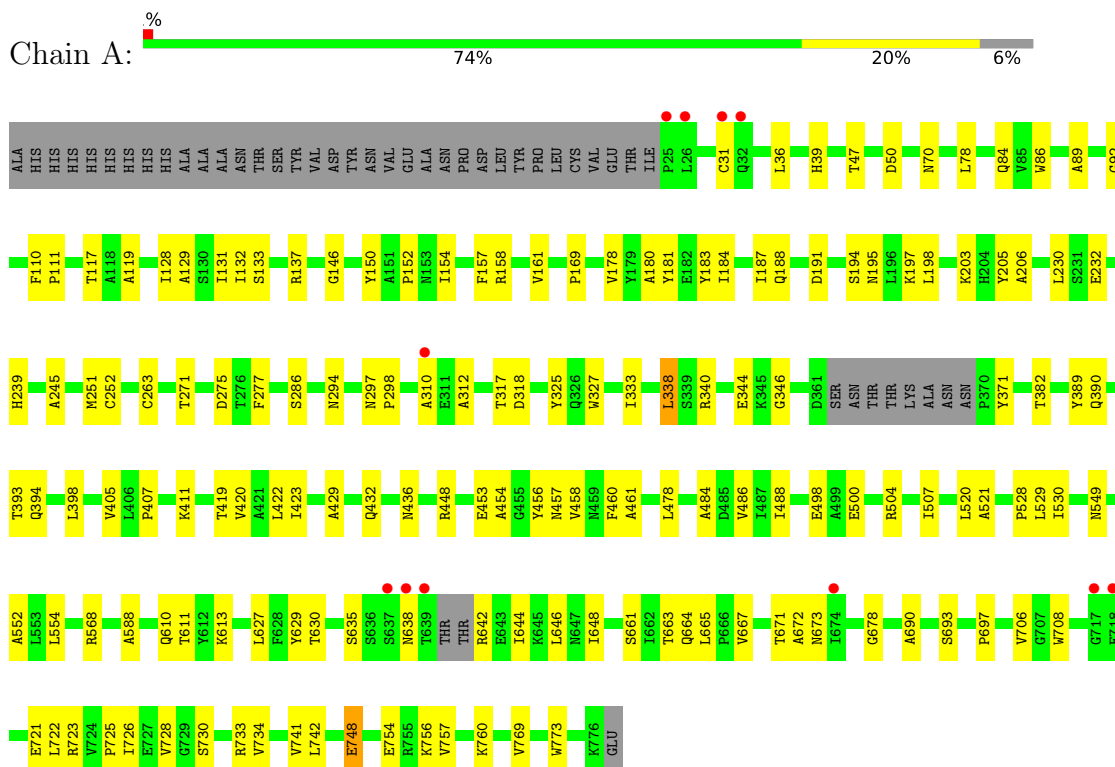
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	23	Total	O	0	0
			23	23		
7	B	10	Total	O	0	0
			10	10		

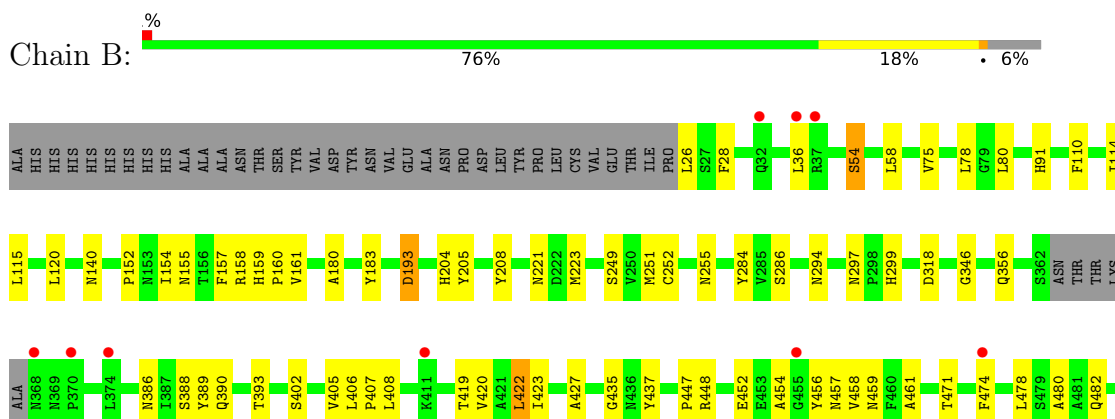
3 Residue-property plots

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: Xylan 1,4-beta-xylosidase



- Molecule 1: Xylan 1,4-beta-xylosidase





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

Chain C: 17% 83%



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

Chain E: 17% 83%



- Molecule 3: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain D: 100%



- Molecule 4: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain F: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.88Å 120.88Å 266.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 2.50 49.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.97-2.50) 99.8 (49.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.214 , 0.256 0.213 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtrriage
Anisotropy	0.488	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11809	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.31	0/5847	0.54	0/7986
1	B	0.31	0/5843	0.53	0/7982
All	All	0.31	0/11690	0.53	0/15968

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5707	0	5438	110	0
1	B	5704	0	5426	90	0
2	C	72	0	61	3	0
2	E	72	0	61	2	0
3	D	28	0	25	0	0
4	F	39	0	34	0	0
5	A	56	0	52	2	0
5	B	70	0	65	3	0
6	A	6	8	8	0	0
6	B	6	8	8	0	0
7	A	23	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	10	0	0	0	0
All	All	11793	16	11178	203	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 9.

All (203) 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:221:ASN:HB3	1:B:223:MET:HE3	1.44	1.00
1:B:667:VAL:HG13	1:B:728:VAL:HG22	1.51	0.93
1:A:706:VAL:HG12	1:A:730:SER:HB3	1.59	0.85
1:A:84:GLN:HE21	1:A:86:TRP:H	1.25	0.81
1:A:158:ARG:HH11	1:A:610:GLN:HE22	1.27	0.81
1:A:70:ASN:HD22	1:A:84:GLN:HE22	1.28	0.78
1:B:514:LEU:O	1:B:518:GLN:HG3	1.83	0.77
1:A:436:ASN:HD21	1:A:500:GLU:H	1.34	0.74
1:B:740:TRP:HB2	1:B:771:LEU:HB3	1.68	0.74
1:A:263:CYS:HB3	1:A:317:THR:HG21	1.69	0.73
1:B:158:ARG:HH11	1:B:610:GLN:HE22	1.35	0.73
1:A:422:LEU:HD13	1:A:448:ARG:HA	1.70	0.73
1:B:665:LEU:O	1:B:728:VAL:HG23	1.89	0.73
1:B:452:GLU:HG3	1:B:458:VAL:HG21	1.71	0.71
1:B:667:VAL:CG1	1:B:728:VAL:HG22	2.21	0.70
1:A:610:GLN:O	1:A:611:THR:HB	1.92	0.69
1:A:197:LYS:HD3	1:A:371:TYR:CE1	2.27	0.69
1:B:386:ASN:O	1:B:390:GLN:HG3	1.93	0.68
1:B:155:ASN:ND2	1:B:204:HIS:H	1.90	0.68
1:A:436:ASN:ND2	1:A:500:GLU:H	1.92	0.67
1:A:646:LEU:HD13	1:A:667:VAL:CG2	2.25	0.66
1:B:155:ASN:HD21	1:B:204:HIS:H	1.41	0.66
2:E:1:NAG:H62	2:E:2:NAG:C1	2.26	0.66
1:B:221:ASN:HB3	1:B:223:MET:CE	2.23	0.66
1:B:452:GLU:HG3	1:B:458:VAL:CG2	2.26	0.66
1:A:191:ASP:OD2	1:A:194:SER:HB2	1.95	0.66
1:B:671:THR:HA	1:B:722:LEU:O	1.96	0.66
1:A:398:LEU:HD23	1:A:627:LEU:HB2	1.78	0.65
1:A:671:THR:HA	1:A:722:LEU:O	1.97	0.65
1:B:538:GLN:HB3	1:B:585:GLN:HG3	1.79	0.65
1:B:251:MET:HA	1:B:286:SER:O	1.96	0.65
1:B:389:TYR:O	1:B:393:THR:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:VAL:HG22	1:B:769:VAL:HG22	1.80	0.63
1:A:530:ILE:HD12	1:A:552:ALA:HB3	1.81	0.63
1:A:294:ASN:HA	1:A:297:ASN:O	1.99	0.63
1:A:398:LEU:HA	1:A:554:LEU:HD23	1.79	0.62
1:B:489:TYR:OH	1:B:513:GLN:HB3	2.00	0.62
1:B:402:SER:O	1:B:405:VAL:HG23	1.99	0.62
1:A:611:THR:HG22	1:A:613:LYS:H	1.66	0.61
1:B:420:VAL:CG2	1:B:458:VAL:HG12	2.31	0.61
1:A:47:THR:HG22	1:A:50:ASP:HB2	1.81	0.60
1:B:459:ASN:HB3	1:B:480:ALA:HB1	1.84	0.59
1:B:294:ASN:HA	1:B:297:ASN:O	2.03	0.58
1:A:47:THR:HG23	1:A:50:ASP:H	1.67	0.58
1:B:160:PRO:HG3	1:B:586:TYR:CD2	2.38	0.58
1:A:661:SER:H	1:A:664:GLN:HE21	1.52	0.58
1:A:419:THR:OG1	1:A:484:ALA:HA	2.05	0.57
1:A:667:VAL:HB	1:A:728:VAL:HG12	1.87	0.57
1:A:84:GLN:NE2	1:A:86:TRP:H	1.99	0.57
1:A:488:ILE:HD13	1:A:530:ILE:HB	1.87	0.57
1:B:427:ALA:O	1:B:447:PRO:HD2	2.05	0.57
1:A:706:VAL:CG1	1:A:730:SER:HB3	2.33	0.56
1:A:420:VAL:CG2	1:A:458:VAL:HG22	2.36	0.56
1:B:750:GLY:HA3	1:B:755:ARG:HG2	1.86	0.56
1:B:630:THR:HB	1:B:680:VAL:HG12	1.85	0.56
1:B:158:ARG:NH1	1:B:610:GLN:HE22	2.03	0.56
1:B:435:GLY:HA2	1:B:558:TYR:CD2	2.41	0.56
1:A:638:ASN:HB3	1:A:642:ARG:NH2	2.21	0.56
5:B:804:NAG:O3	5:B:804:NAG:H82	2.06	0.56
1:B:422:LEU:HD12	1:B:448:ARG:HA	1.89	0.55
1:B:407:PRO:HB2	1:B:572:THR:O	2.07	0.55
1:B:159:HIS:ND1	1:B:161:VAL:HG22	2.21	0.55
1:B:406:LEU:HD23	1:B:408:LEU:HG	1.88	0.55
1:A:741:VAL:HG22	1:A:769:VAL:HG22	1.90	0.54
1:A:754:GLU:HB2	1:A:756:LYS:HE3	1.88	0.54
1:B:208:TYR:HB2	1:B:255:ASN:OD1	2.08	0.54
1:B:408:LEU:HD11	1:B:530:ILE:HD11	1.90	0.54
1:A:423:ILE:HA	1:A:461:ALA:O	2.09	0.53
1:A:665:LEU:O	1:A:728:VAL:HG13	2.08	0.53
1:B:471:THR:O	1:B:474:PHE:HB2	2.07	0.53
2:C:1:NAG:H62	2:C:2:NAG:C1	2.38	0.53
1:A:205:TYR:CD1	1:A:206:ALA:HB2	2.44	0.53
1:B:645:LYS:O	1:B:646:LEU:HD23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:THR:OG1	1:A:325:TYR:OH	2.27	0.52
1:A:398:LEU:HD13	1:A:554:LEU:HD21	1.91	0.52
1:B:28:PHE:HZ	1:B:140:ASN:HD21	1.58	0.52
1:A:697:PRO:O	1:A:733:ARG:NH2	2.43	0.52
1:A:672:ALA:HB2	1:A:757:VAL:HG11	1.90	0.52
1:A:84:GLN:HE21	1:A:86:TRP:N	2.02	0.52
1:A:271:THR:O	1:A:275:ASP:HB2	2.11	0.51
1:B:454:ALA:HB3	1:B:456:TYR:HD1	1.75	0.51
1:B:478:LEU:HD21	1:B:519:LYS:HB3	1.93	0.51
1:A:158:ARG:NH1	1:A:610:GLN:HE22	2.04	0.51
1:A:630:THR:OG1	1:A:678:GLY:HA3	2.10	0.51
1:A:419:THR:HA	1:A:457:ASN:O	2.11	0.51
1:B:423:ILE:HA	1:B:461:ALA:O	2.11	0.51
1:A:131:ILE:HG23	1:A:382:THR:HB	1.92	0.51
1:A:644:ILE:O	1:A:644:ILE:HG22	2.11	0.51
1:A:36:LEU:HD21	1:A:78:LEU:HB3	1.93	0.51
1:A:47:THR:CG2	1:A:50:ASP:H	2.23	0.51
1:A:498:GLU:O	1:A:498:GLU:HG3	2.10	0.51
1:A:429:ALA:HB1	1:A:432:GLN:HB2	1.94	0.50
1:A:251:MET:HA	1:A:286:SER:O	2.10	0.50
1:B:54:SER:O	1:B:58:LEU:HG	2.12	0.50
1:A:232:GLU:HB2	1:A:734:VAL:HG21	1.93	0.50
1:B:423:ILE:O	1:B:489:TYR:HA	2.12	0.50
1:B:706:VAL:HG12	1:B:730:SER:HB3	1.93	0.49
1:A:184:ILE:O	1:A:188:GLN:HG3	2.12	0.49
1:A:663:THR:HA	1:A:728:VAL:CG2	2.43	0.49
1:B:454:ALA:HB3	1:B:456:TYR:CD1	2.48	0.49
1:A:420:VAL:HG22	1:A:458:VAL:HG22	1.94	0.49
1:B:746:THR:HG23	1:B:762:VAL:HG22	1.93	0.49
1:B:75:VAL:HG23	1:B:80:LEU:HD23	1.94	0.48
1:B:161:VAL:HB	1:B:504:ARG:O	2.13	0.48
1:B:510:PRO:HG2	1:B:513:GLN:NE2	2.28	0.48
1:A:411:LYS:HD2	1:A:411:LYS:N	2.28	0.48
1:A:389:TYR:O	1:A:393:THR:HG23	2.13	0.48
1:A:394:GLN:OE1	2:C:1:NAG:H83	2.14	0.48
1:A:152:PRO:HB3	1:A:183:TYR:CD1	2.49	0.48
1:A:178:VAL:HG21	1:A:708:TRP:CZ2	2.49	0.48
1:A:721:GLU:OE1	1:A:723:ARG:NH2	2.46	0.48
1:B:406:LEU:CD2	1:B:408:LEU:HG	2.44	0.47
1:B:775:GLY:O	1:B:776:LYS:HB3	2.15	0.47
1:A:638:ASN:HB3	1:A:642:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ASN:ND2	1:B:204:HIS:HD2	2.12	0.47
1:A:312:ALA:HB1	1:A:317:THR:OG1	2.15	0.47
1:A:327:TRP:HA	5:A:804:NAG:H62	1.97	0.47
1:A:390:GLN:OE1	2:C:2:NAG:H5	2.15	0.47
1:A:420:VAL:HG12	1:A:486:VAL:HG22	1.95	0.47
1:A:460:PHE:HE2	5:A:802:NAG:H82	1.80	0.47
1:A:507:ILE:HG13	1:A:588:ALA:HA	1.97	0.47
1:B:154:ILE:HG21	1:B:180:ALA:HB2	1.96	0.46
1:B:422:LEU:HD12	1:B:448:ARG:CA	2.45	0.46
1:B:580:ARG:HA	1:B:625:HIS:O	2.14	0.46
1:B:615:TYR:CZ	1:B:617:GLY:HA3	2.50	0.46
1:B:693:SER:OG	5:B:804:NAG:H83	2.15	0.46
1:A:129:ALA:HB1	1:A:187:ILE:HG12	1.97	0.46
1:A:340:ARG:O	1:A:344:GLU:HG3	2.15	0.46
1:A:390:GLN:O	1:A:394:GLN:HG3	2.15	0.46
1:A:754:GLU:CB	1:A:756:LYS:HE3	2.46	0.46
1:B:604:GLU:O	1:B:607:ASN:HB3	2.16	0.46
1:A:419:THR:HG22	1:A:457:ASN:HB3	1.98	0.46
1:B:193:ASP:HA	1:B:356:GLN:HE21	1.81	0.46
1:A:646:LEU:HD13	1:A:667:VAL:HG22	1.96	0.45
1:A:310:ALA:HA	1:A:338:LEU:HD23	1.98	0.45
1:B:26:LEU:HG	1:B:26:LEU:O	2.16	0.45
1:B:407:PRO:HB3	1:B:629:TYR:CE2	2.51	0.45
1:B:510:PRO:HG2	1:B:513:GLN:HE21	1.81	0.45
1:A:110:PHE:HB3	1:A:111:PRO:HD2	1.98	0.45
1:A:333:ILE:HD13	1:A:338:LEU:HD12	1.98	0.45
1:B:205:TYR:O	1:B:252:CYS:HA	2.16	0.45
1:A:239:HIS:CD2	1:A:277:PHE:HA	2.52	0.45
1:A:648:ILE:HG23	1:A:742:LEU:HD23	1.98	0.45
1:B:223:MET:HB3	1:B:599:MET:HG3	1.99	0.45
1:A:398:LEU:HD12	1:A:554:LEU:HD23	1.99	0.45
1:A:150:TYR:O	1:A:203:LYS:HE2	2.17	0.44
1:A:117:THR:HG21	1:A:169:PRO:O	2.16	0.44
1:A:205:TYR:O	1:A:252:CYS:HA	2.16	0.44
1:B:630:THR:OG1	1:B:678:GLY:HA3	2.17	0.44
1:A:420:VAL:HG12	1:A:486:VAL:CG2	2.48	0.44
1:A:529:LEU:C	1:A:530:ILE:HD13	2.38	0.44
1:B:695:ALA:O	1:B:733:ARG:HD3	2.18	0.44
1:A:137:ARG:NH1	1:A:197:LYS:O	2.44	0.44
1:A:405:VAL:CG1	1:A:528:PRO:HB3	2.47	0.44
1:B:559:PRO:HG2	1:B:563:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HD3	1:A:197:LYS:O	2.17	0.44
1:A:89:ALA:HA	1:A:92:GLY:O	2.18	0.43
1:A:407:PRO:HB3	1:A:629:TYR:CE2	2.54	0.43
1:B:114:ILE:HG23	1:B:115:LEU:N	2.33	0.43
1:B:91:HIS:NE2	1:B:437:TYR:O	2.51	0.43
1:A:478:LEU:HD23	1:A:520:LEU:HD23	2.00	0.43
1:B:419:THR:HA	1:B:457:ASN:O	2.19	0.43
1:B:710:ARG:HE	2:E:1:NAG:H81	1.84	0.43
1:B:152:PRO:HB3	1:B:183:TYR:CD1	2.54	0.43
1:B:408:LEU:CD1	1:B:486:VAL:HG11	2.48	0.43
1:A:725:PRO:O	1:A:726:ILE:HD13	2.19	0.43
1:A:661:SER:H	1:A:664:GLN:NE2	2.16	0.43
1:B:498:GLU:HG3	1:B:498:GLU:O	2.18	0.43
1:B:673:ASN:C	1:B:674:ILE:HD13	2.39	0.43
1:A:263:CYS:CB	1:A:317:THR:HG21	2.45	0.42
1:B:490:ALA:HA	1:B:532:LEU:HB2	1.99	0.42
1:B:26:LEU:N	1:B:26:LEU:HD23	2.35	0.42
1:A:146:GLY:HA3	7:A:909:HOH:O	2.19	0.42
1:A:181:TYR:HA	1:A:245:ALA:HB2	2.01	0.42
1:A:521:ALA:HB1	1:A:549:ASN:HB2	2.01	0.42
1:B:513:GLN:O	1:B:517:ILE:HG13	2.20	0.42
1:B:249:SER:HA	1:B:284:TYR:O	2.19	0.42
1:B:748:GLU:HB3	5:B:804:NAG:HN2	1.84	0.42
1:A:635:SER:OG	1:A:673:ASN:HB2	2.20	0.41
1:B:507:ILE:HG13	1:B:588:ALA:HA	2.02	0.41
1:A:297:ASN:HA	1:A:298:PRO:HA	1.90	0.41
1:A:133:SER:HB2	1:A:197:LYS:HE3	2.02	0.41
1:B:36:LEU:HD21	1:B:78:LEU:HB3	2.02	0.41
1:A:690:ALA:HA	1:A:748:GLU:O	2.21	0.41
1:B:294:ASN:O	1:B:299:HIS:HB2	2.19	0.41
1:B:521:ALA:HB1	1:B:549:ASN:HB3	2.01	0.41
1:B:721:GLU:HG3	1:B:722:LEU:N	2.35	0.41
1:A:128:ILE:O	1:A:132:ILE:HG13	2.21	0.41
1:A:154:ILE:HG21	1:A:180:ALA:HB2	2.02	0.41
1:A:119:ALA:HB1	1:A:394:GLN:HB3	2.02	0.41
1:A:188:GLN:HA	1:A:198:LEU:O	2.21	0.41
1:B:120:LEU:HD12	1:B:685:THR:HB	2.02	0.41
1:A:454:ALA:HB3	1:A:456:TYR:HD1	1.86	0.40
1:B:755:ARG:O	1:B:758:ARG:NH1	2.53	0.40
1:A:36:LEU:HA	1:A:39:HIS:HD2	1.86	0.40
1:A:183:TYR:CE1	1:A:187:ILE:HG13	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:GLU:OE1	1:A:568:ARG:NH1	2.39	0.40
1:A:318:ASP:HB3	1:A:346:GLY:CA	2.52	0.40
1:B:110:PHE:HA	1:B:388:SER:OG	2.22	0.40
1:B:756:LYS:HA	1:B:756:LYS:HD3	1.93	0.40
1:A:161:VAL:HB	1:A:504:ARG:O	2.21	0.40
1:A:230:LEU:HD23	1:A:773:TRP:HZ2	1.86	0.40
1:B:318:ASP:HB3	1:B:346:GLY:CA	2.52	0.40

There are no symmetry-related clashes.

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	737/788 (94%)	716 (97%)	21 (3%)	0	100	100
1	B	737/788 (94%)	716 (97%)	21 (3%)	0	100	100
All	All	1474/1576 (94%)	1432 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	599/638 (94%)	592 (99%)	7 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	599/638 (94%)	587 (98%)	12 (2%)	55 79
All	All	1198/1276 (94%)	1179 (98%)	19 (2%)	62 84

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	CYS
1	A	157	PHE
1	A	195	ASN
1	A	338	LEU
1	A	693	SER
1	A	748	GLU
1	A	760	LYS
1	B	54	SER
1	B	157	PHE
1	B	193	ASP
1	B	422	LEU
1	B	482	GLN
1	B	527	LYS
1	B	542	SER
1	B	574	ARG
1	B	637	SER
1	B	680	VAL
1	B	713	ASP
1	B	748	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	195	ASN
1	A	216	HIS
1	A	239	HIS
1	A	436	ASN
1	A	610	GLN
1	A	638	ASN
1	A	664	GLN
1	B	39	HIS
1	B	112	GLN
1	B	155	ASN
1	B	204	HIS

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Mol	Chain	Res	Type
1	B	282	HIS
1	B	294	ASN
1	B	356	GLN
1	B	432	GLN
1	B	482	GLN
1	B	546	ASN
1	B	610	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

17 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	1,2	14,14,15	0.34	0	17,19,21	0.58	0
2	NAG	C	2	2	14,14,15	0.33	0	17,19,21	0.59	0
2	BMA	C	3	2	11,11,12	1.02	1 (9%)	15,15,17	1.10	1 (6%)
2	MAN	C	4	2	11,11,12	0.97	1 (9%)	15,15,17	1.13	2 (13%)
2	MAN	C	5	2	11,11,12	1.10	1 (9%)	15,15,17	0.81	0
2	MAN	C	6	2	11,11,12	0.99	0	15,15,17	1.02	0
3	NAG	D	1	1,3	14,14,15	0.72	1 (7%)	17,19,21	0.48	0
3	NAG	D	2	3	14,14,15	0.48	0	17,19,21	0.70	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.28	0	17,19,21	0.56	0
2	NAG	E	2	2	14,14,15	0.57	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	E	3	2	11,11,12	0.64	0	15,15,17	1.02	1 (6%)
2	MAN	E	4	2	11,11,12	0.80	0	15,15,17	1.17	1 (6%)
2	MAN	E	5	2	11,11,12	0.84	0	15,15,17	0.85	0
2	MAN	E	6	2	11,11,12	1.15	1 (9%)	15,15,17	1.09	1 (6%)
4	NAG	F	1	4,1	14,14,15	0.23	0	17,19,21	0.38	0
4	NAG	F	2	4	14,14,15	0.30	0	17,19,21	0.40	0
4	BMA	F	3	4	11,11,12	1.02	0	15,15,17	0.93	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	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	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	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	O5-C1	-2.40	1.39	1.43
2	C	5	MAN	C2-C3	2.39	1.56	1.52
2	C	3	BMA	C1-C2	2.19	1.57	1.52
2	E	6	MAN	O5-C5	2.14	1.47	1.43
2	C	4	MAN	C1-C2	2.14	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	MAN	C1-O5-C5	2.94	116.18	112.19
2	C	4	MAN	C1-O5-C5	2.72	115.88	112.19
2	E	6	MAN	C1-O5-C5	2.64	115.77	112.19
2	E	3	BMA	C1-C2-C3	2.23	112.41	109.67
2	C	3	BMA	O2-C2-C3	-2.18	105.76	110.14
3	D	2	NAG	C1-O5-C5	2.10	115.04	112.19
2	C	4	MAN	O2-C2-C3	-2.02	106.08	110.14

There are no chirality outliers.

All (15) torsion outliers are listed below:

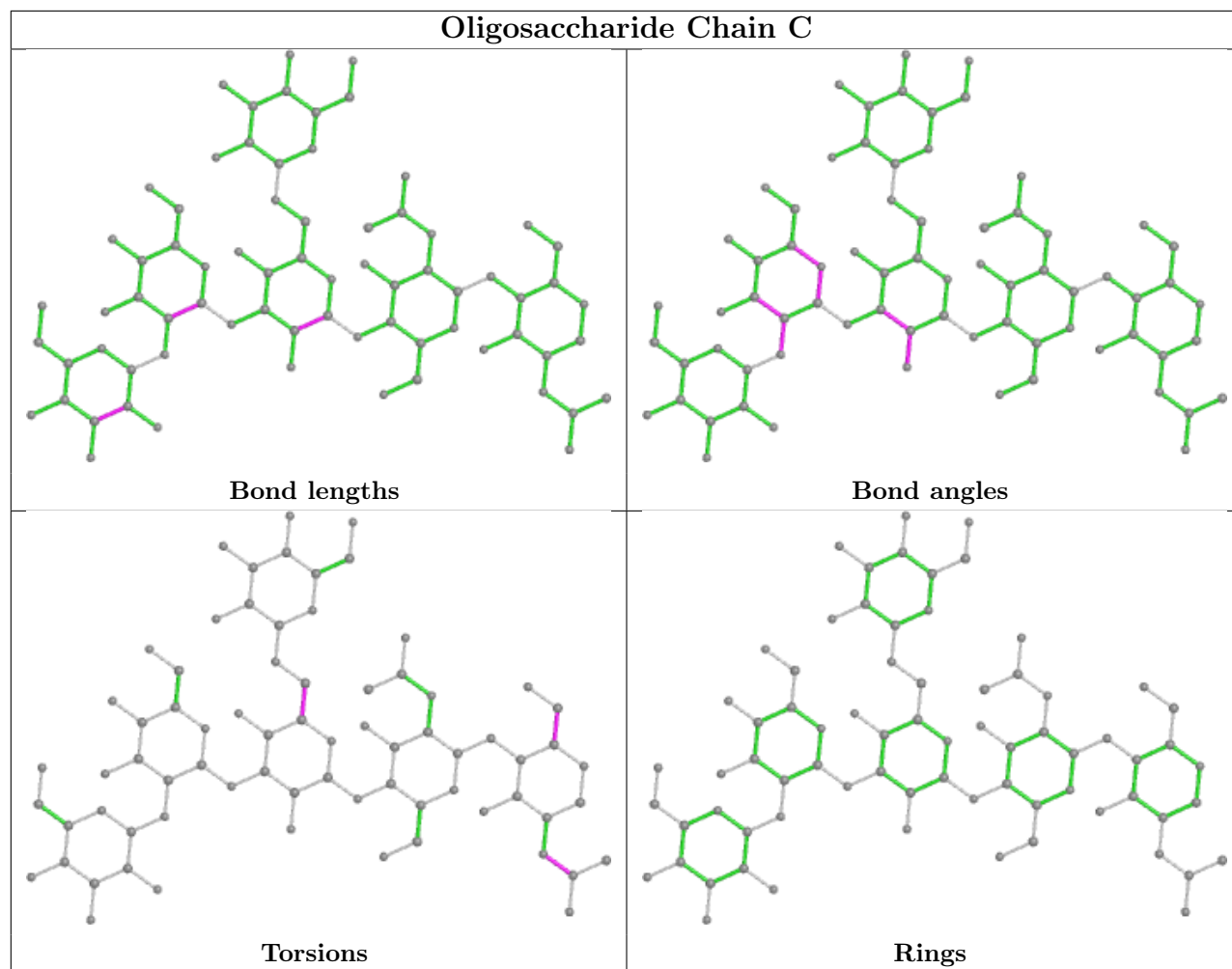
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6

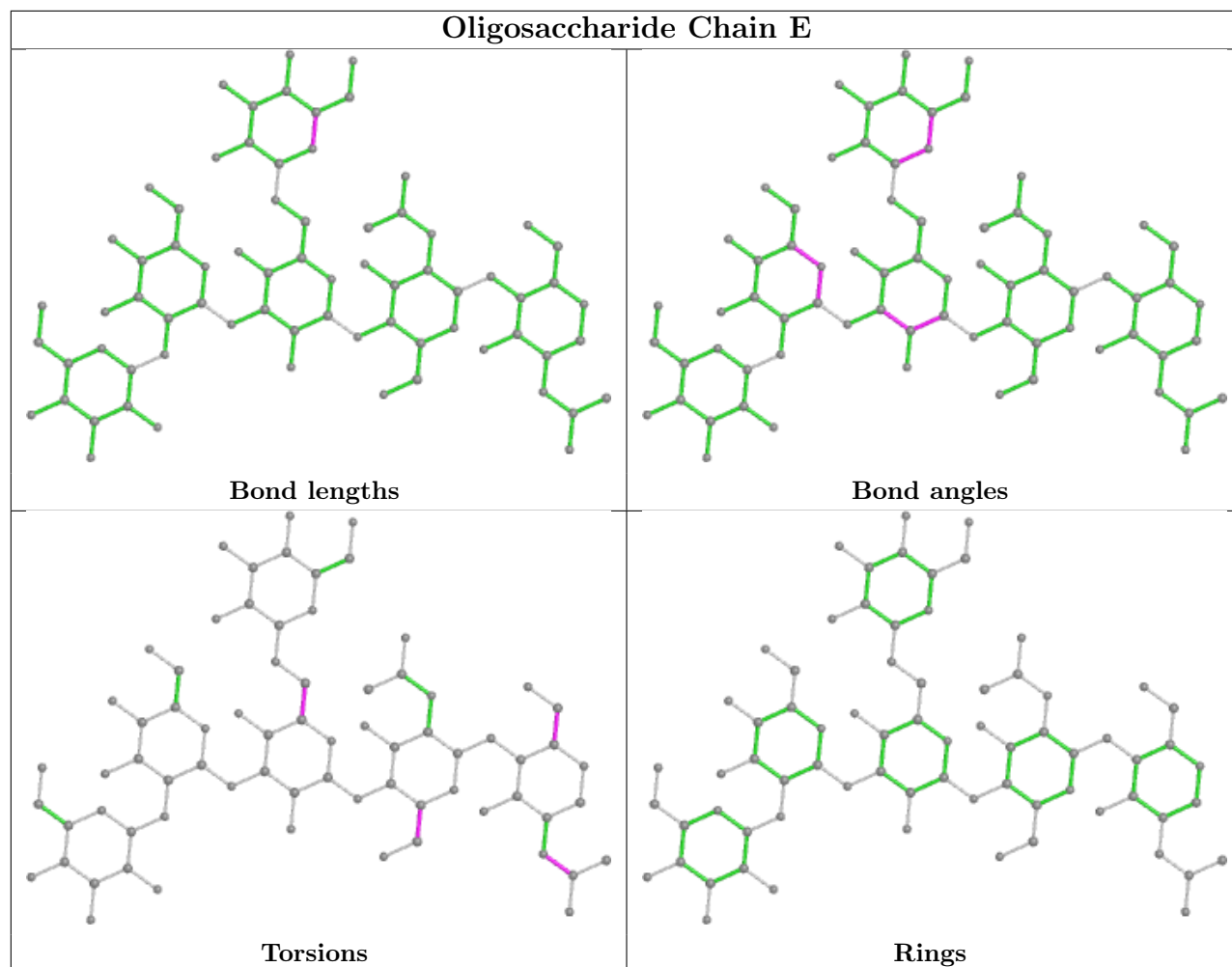
There are no ring outliers.

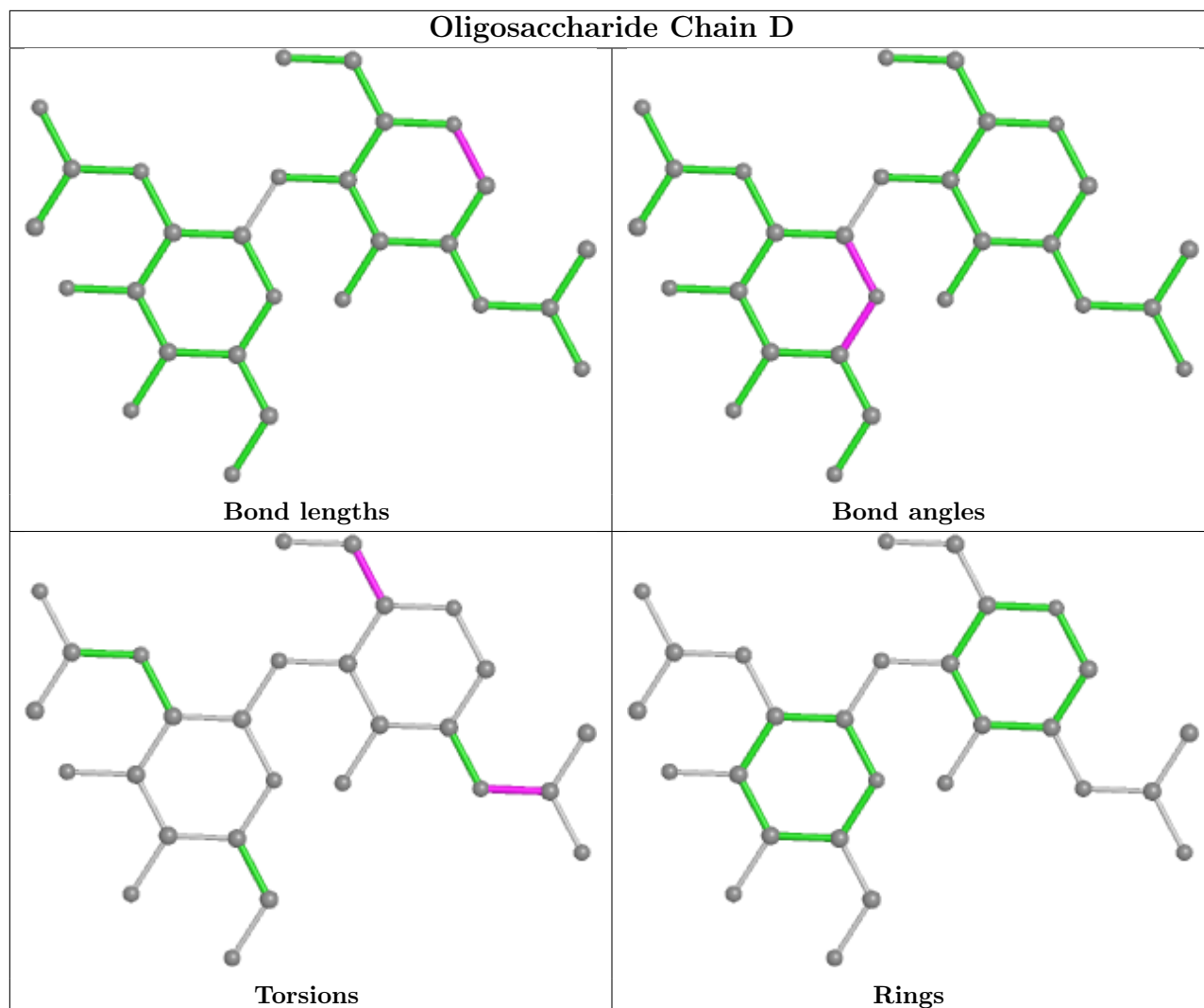
4 monomers are involved in 5 short contacts:

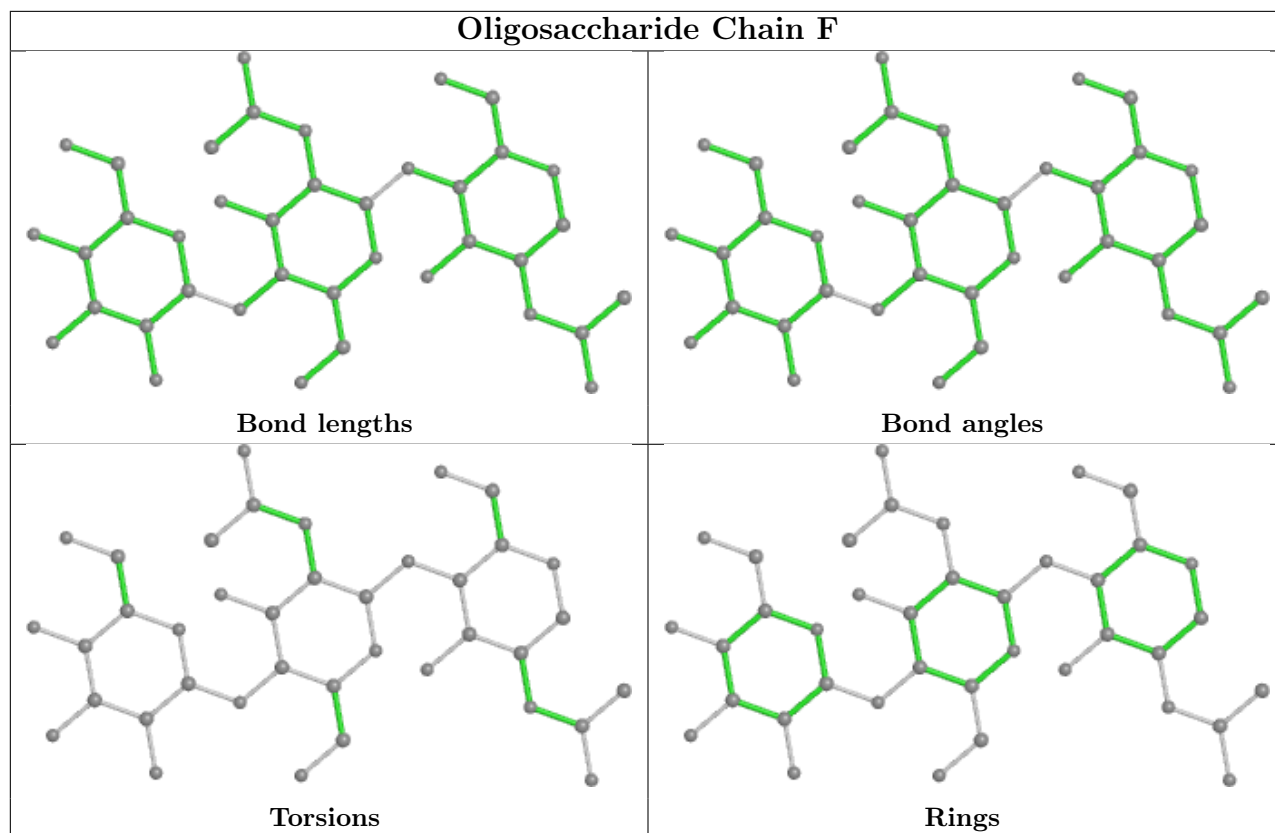
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	2	0
2	C	2	NAG	2	0
2	C	1	NAG	2	0
2	E	2	NAG	1	0

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](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	803	1	14,14,15	0.44	0	17,19,21	0.48	0
5	NAG	A	801	1	14,14,15	0.19	0	17,19,21	0.49	0
5	NAG	B	805	1	14,14,15	0.45	0	17,19,21	0.41	0
6	GOL	B	806	-	5,5,5	1.06	0	5,5,5	1.40	1 (20%)
5	NAG	A	802	1	14,14,15	0.32	0	17,19,21	0.55	0
5	NAG	B	801	1	14,14,15	0.24	0	17,19,21	0.33	0
5	NAG	B	802	1	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	A	804	1	14,14,15	0.35	0	17,19,21	0.48	0
5	NAG	B	804	1	14,14,15	0.67	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	A	805	-	5,5,5	0.75	0	5,5,5	0.65	0
5	NAG	A	803	1	14,14,15	0.63	0	17,19,21	0.60	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
5	NAG	B	803	1	-	2/6/23/26	0/1/1/1
5	NAG	A	801	1	-	2/6/23/26	0/1/1/1
5	NAG	B	805	1	-	0/6/23/26	0/1/1/1
6	GOL	B	806	-	-	0/4/4/4	-
5	NAG	A	802	1	-	0/6/23/26	0/1/1/1
5	NAG	B	801	1	-	0/6/23/26	0/1/1/1
5	NAG	B	802	1	-	2/6/23/26	0/1/1/1
5	NAG	A	804	1	-	0/6/23/26	0/1/1/1
5	NAG	B	804	1	-	3/6/23/26	0/1/1/1
6	GOL	A	805	-	-	2/4/4/4	-
5	NAG	A	803	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	806	GOL	C3-C2-C1	-2.81	100.78	111.70

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	801	NAG	C8-C7-N2-C2
5	A	801	NAG	O7-C7-N2-C2
5	A	803	NAG	C8-C7-N2-C2
5	A	803	NAG	O7-C7-N2-C2
5	B	802	NAG	C8-C7-N2-C2
5	B	802	NAG	O7-C7-N2-C2
5	B	803	NAG	C8-C7-N2-C2
5	B	803	NAG	O7-C7-N2-C2
5	B	804	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	B	804	NAG	O7-C7-N2-C2
5	B	804	NAG	O5-C5-C6-O6
6	A	805	GOL	O1-C1-C2-C3
6	A	805	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	802	NAG	1	0
5	A	804	NAG	1	0
5	B	804	NAG	3	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

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	742/788 (94%)	0.04	11 (1%) 73 75	45, 56, 74, 103	0
1	B	743/788 (94%)	0.09	11 (1%) 73 75	46, 60, 80, 99	0
All	All	1485/1576 (94%)	0.07	22 (1%) 73 75	45, 58, 78, 103	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	637	SER	3.2
1	B	32	GLN	3.1
1	A	717	GLY	3.0
1	B	368	ASN	2.9
1	A	25	PRO	2.8
1	B	36	LEU	2.7
1	B	474	PHE	2.6
1	B	374	LEU	2.6
1	A	26	LEU	2.5
1	B	629	TYR	2.4
1	A	638	ASN	2.3
1	A	32	GLN	2.3
1	B	370	PRO	2.2
1	A	31	CYS	2.2
1	A	639	THR	2.2
1	A	674	ILE	2.2
1	B	455	GLY	2.2
1	A	310	ALA	2.1
1	A	718	GLU	2.1
1	B	411	LYS	2.1
1	B	37	ARG	2.1
1	B	578	ALA	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](#)

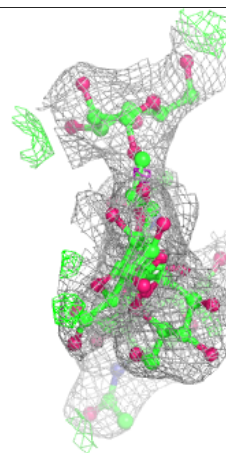
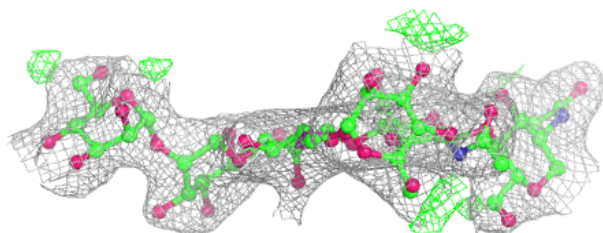
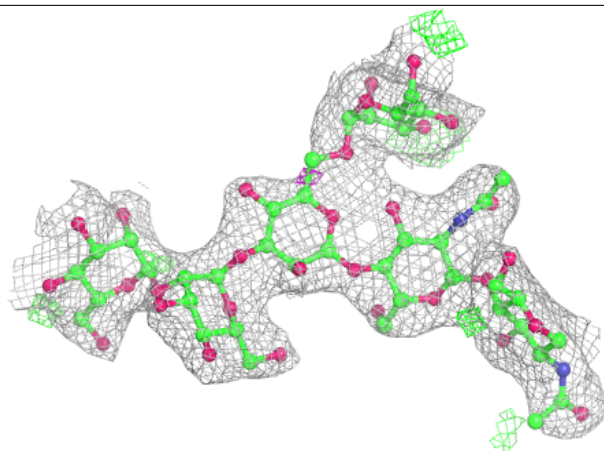
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	E	6	11/12	0.70	0.23	74,77,82,82	0
4	BMA	F	3	11/12	0.79	0.17	76,80,84,86	0
2	MAN	C	5	11/12	0.81	0.21	80,85,90,92	0
2	MAN	E	5	11/12	0.85	0.29	91,97,101,101	0
3	NAG	D	2	14/15	0.86	0.21	57,62,66,67	0
2	MAN	C	6	11/12	0.87	0.12	70,72,74,76	0
2	MAN	E	4	11/12	0.92	0.15	70,79,81,90	0
2	NAG	E	1	14/15	0.94	0.15	58,62,65,66	0
2	BMA	C	3	11/12	0.94	0.20	65,71,75,77	0
4	NAG	F	2	14/15	0.94	0.09	59,68,73,79	0
2	MAN	C	4	11/12	0.94	0.18	68,73,76,79	0
3	NAG	D	1	14/15	0.95	0.15	56,62,65,72	0
4	NAG	F	1	14/15	0.95	0.11	60,64,67,67	0
2	NAG	C	2	14/15	0.96	0.12	60,65,68,74	0
2	BMA	E	3	11/12	0.96	0.18	72,75,78,79	0
2	NAG	E	2	14/15	0.97	0.13	63,66,71,72	0
2	NAG	C	1	14/15	0.97	0.13	52,58,64,66	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.

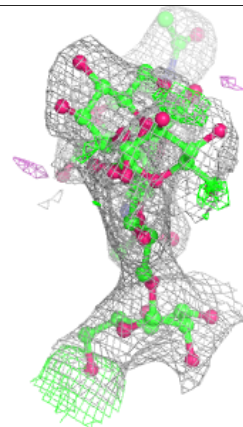
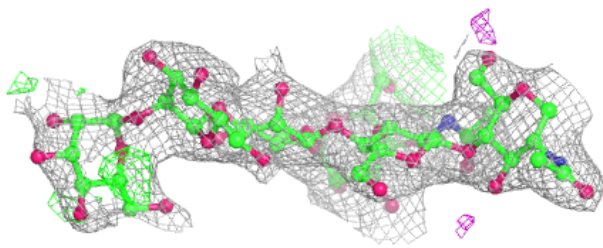
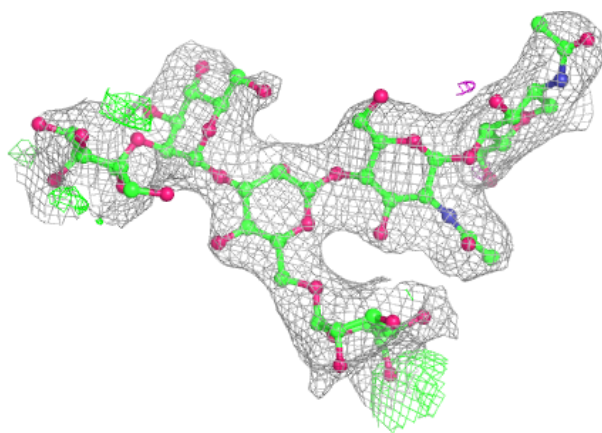
Electron density around Chain C:

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

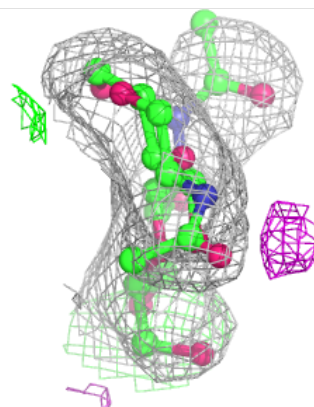
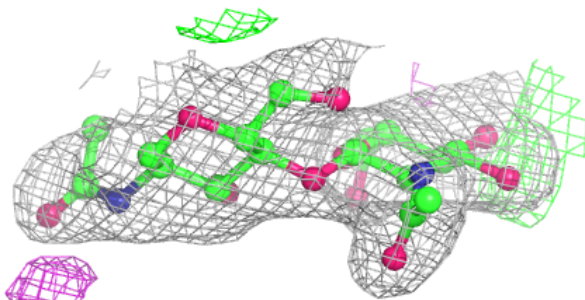
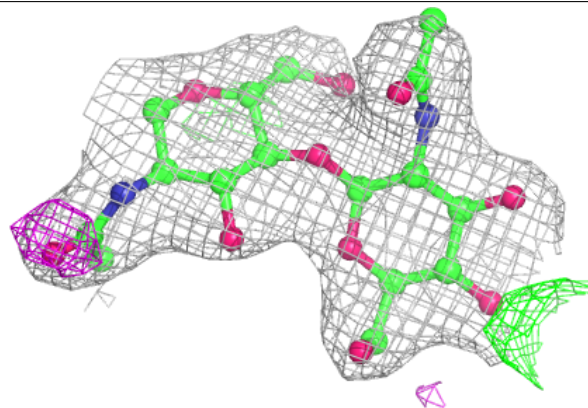


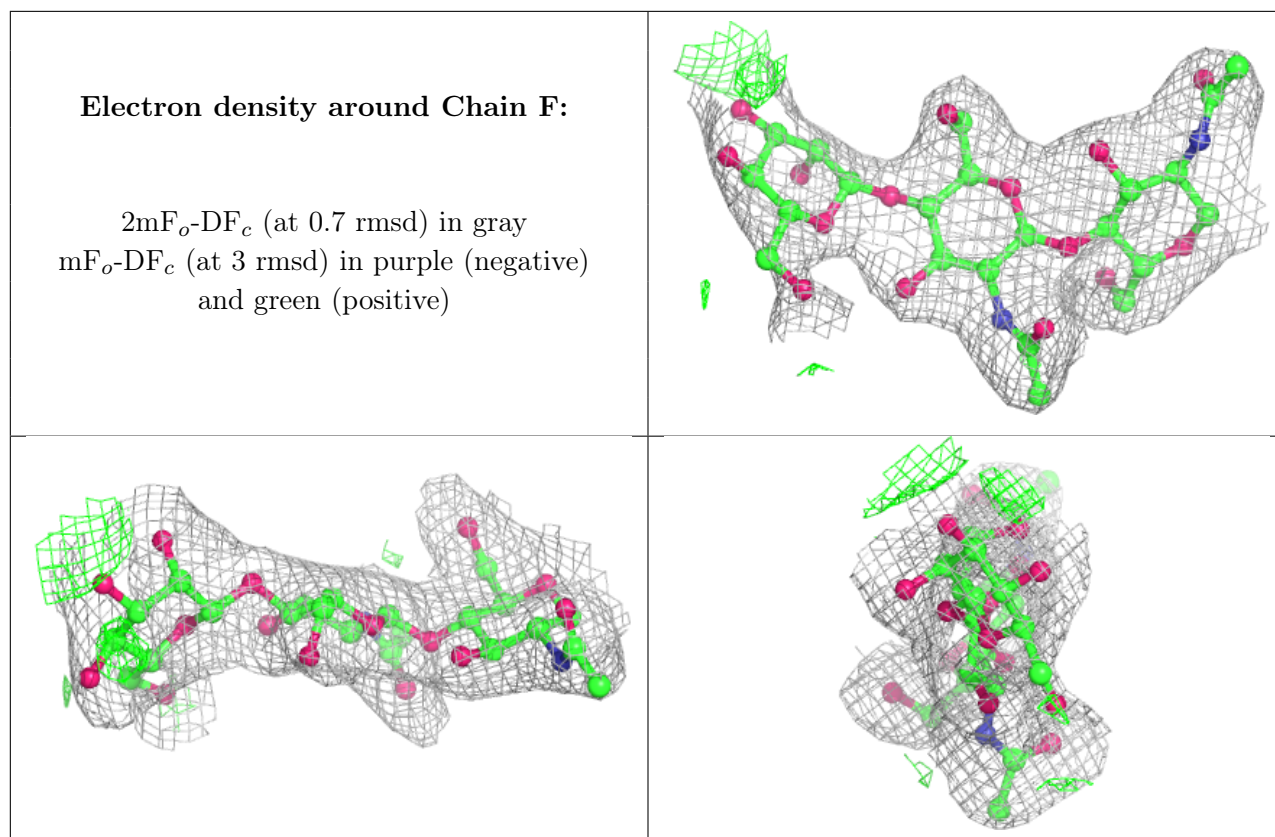
Electron density around Chain E:

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

**Electron density around Chain D:**

$2mF_o-DF_c$ (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
5	NAG	A	804	14/15	0.67	0.45	75,85,91,92	0
6	GOL	A	805	6/6	0.74	0.32	47,60,69,73	0
5	NAG	B	804	14/15	0.78	0.49	79,89,94,103	0
5	NAG	A	803	14/15	0.79	0.19	75,84,89,89	0
6	GOL	B	806	6/6	0.79	0.22	73,88,99,99	0
5	NAG	B	802	14/15	0.85	0.22	77,82,83,84	0
5	NAG	B	805	14/15	0.85	0.23	66,77,83,87	0
5	NAG	B	801	14/15	0.86	0.19	80,86,90,92	0
5	NAG	A	802	14/15	0.88	0.33	64,71,75,76	0
5	NAG	B	803	14/15	0.89	0.14	71,88,92,93	0
5	NAG	A	801	14/15	0.93	0.40	74,82,85,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.