



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:32 AM UTC

PDB ID : 5YDI / pdb_00005ydi
Title : Crystal structure of acetylcholinesterase catalytic subunits of the malaria vector *Anopheles gambiae*, new crystal packing
Authors : Han, Q.; Guan, H.; Ding, H.; Liao, C.; Robinson, H.; Li, J.
Deposited on : 2017-09-13
Resolution : 3.45 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

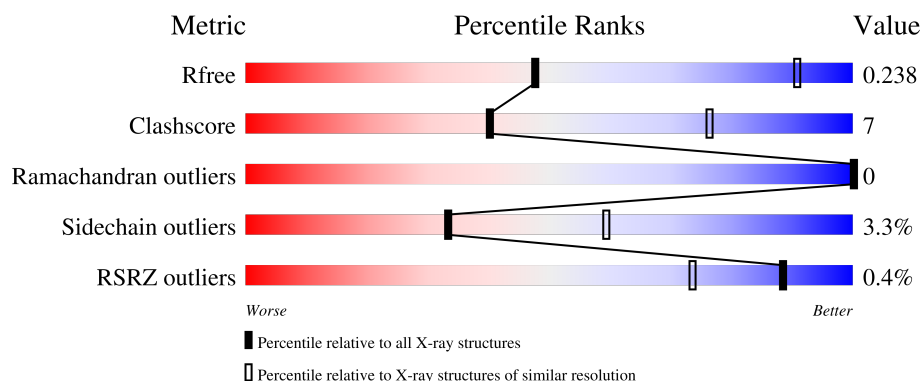
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

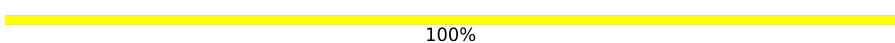
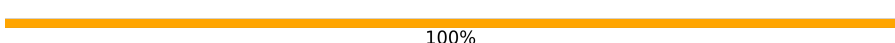
The reported resolution of this entry is 3.45 Å.

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.



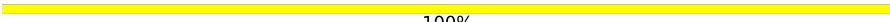
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	553	 80% 16% ..
1	B	553	 80% 17% ..
1	C	553	 81% 15% ..
2	D	3	 100%
2	F	3	 100%

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Mol	Chain	Length	Quality of chain
3	E	6	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	F	1	-	-	X	-
2	NAG	F	2	-	-	X	-

2 Entry composition [i](#)

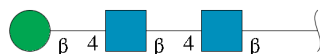
There are 7 unique types of molecules in this entry. The entry contains 12977 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylcholinesterase.

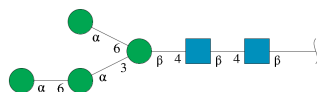
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4249	2707	741	788	13			
1	B	537	Total	C	N	O	S	0	0	0
			4249	2707	741	788	13			
1	C	537	Total	C	N	O	S	0	0	0
			4249	2707	741	788	13			

- Molecule 2 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.



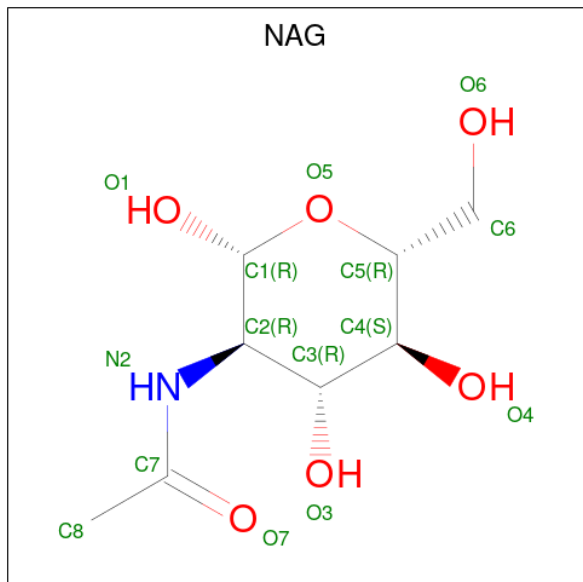
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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.



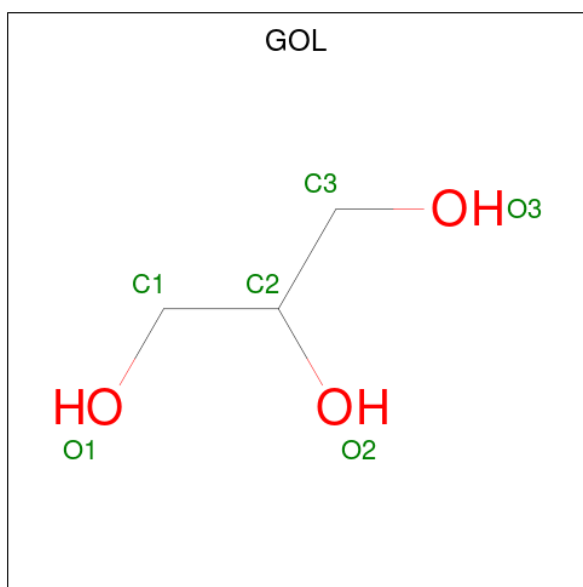
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0
6	B	2	Total Na 2 2	0	0
6	C	1	Total Na 1 1	0	0

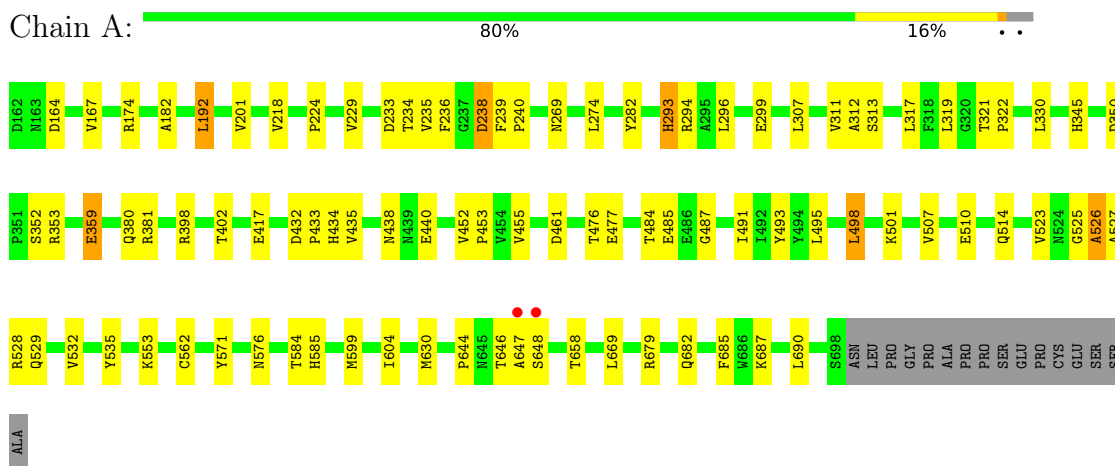
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total O 3 3	0	0
7	B	1	Total O 1 1	0	0
7	C	6	Total O 6 6	0	0

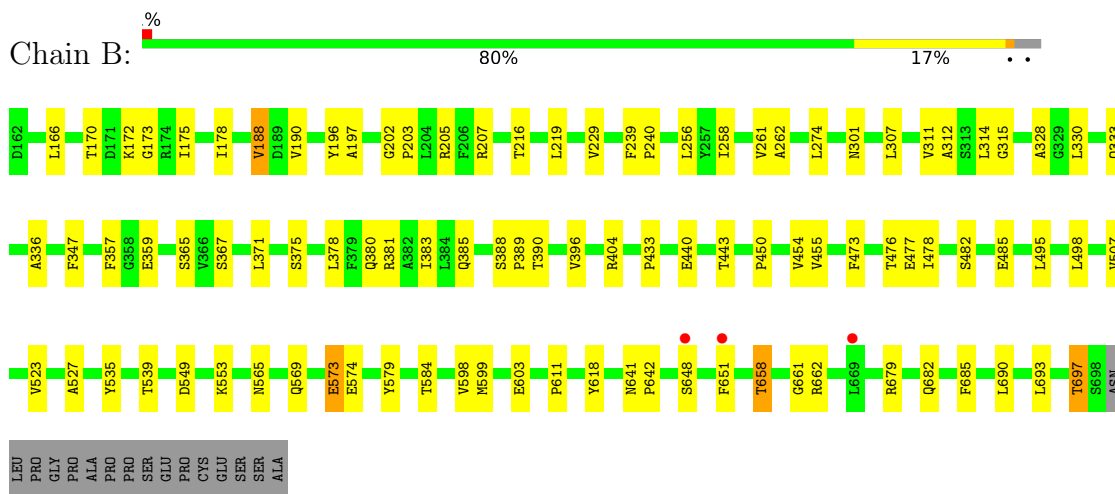
3 Residue-property plots

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.

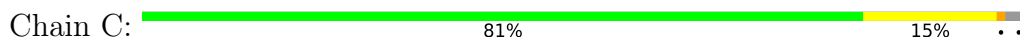
• Molecule 1: Acetylcholinesterase

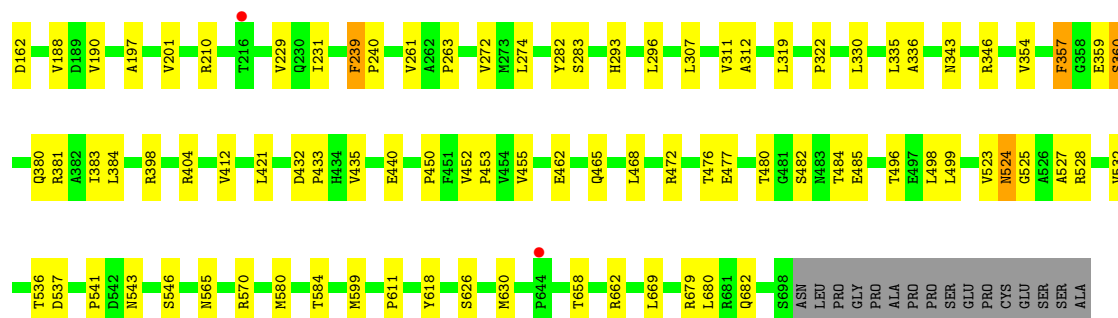


• Molecule 1: Acetylcholinesterase



• Molecule 1: Acetylcholinesterase





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

Chain D: 100%

NAG1
NAG2
BMA3

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

Chain F: 100%

NAG1
NAG2
BMA3

- Molecule 3: alpha-D-mannopyranose-(1-6)-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

Chain E: 100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	127.44Å 235.91Å 167.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.72 – 3.45 63.72 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (63.72-3.45) 99.8 (63.72-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.200 , 0.242 0.197 , 0.238	Depositor DCC
R_{free} test set	1697 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12977	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: MAN, GOL, BMA, NA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/4373	0.81	1/5968 (0.0%)
1	B	0.39	0/4373	0.80	1/5968 (0.0%)
1	C	0.39	0/4373	0.80	3/5968 (0.1%)
All	All	0.39	0/13119	0.80	5/17904 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	648	SER	N-CA-C	-5.85	104.59	110.97
1	C	239	PHE	CA-C-N	5.20	124.87	119.56
1	C	239	PHE	C-N-CA	5.20	124.87	119.56
1	C	283	SER	N-CA-C	5.12	115.00	108.24
1	A	526	ALA	N-CA-C	-5.10	107.05	113.28

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	4249	0	4098	55	0
1	B	4249	0	4099	53	0
1	C	4249	0	4099	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	39	0	34	0	0
2	F	39	0	34	13	0
3	E	72	0	61	0	0
4	A	28	0	26	0	0
4	C	14	0	13	1	0
5	A	12	0	16	2	0
5	B	6	0	7	0	0
5	C	6	0	8	2	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	6	0	0	0	0
All	All	12977	0	12495	167	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 (167) 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)
2:F:2:NAG:H83	2:F:2:NAG:H5	1.24	1.09
2:F:1:NAG:H3	2:F:2:NAG:N2	1.71	1.05
2:F:1:NAG:H3	2:F:2:NAG:HN2	1.24	0.99
2:F:2:NAG:H83	2:F:2:NAG:C5	1.97	0.94
1:A:529:GLN:HA	1:A:532:VAL:HG22	1.53	0.90
2:F:2:NAG:H5	2:F:2:NAG:C8	2.02	0.89
1:C:282:TYR:OH	5:C:805:GOL:H32	1.72	0.88
1:A:174:ARG:HD2	1:A:218:VAL:HG22	1.55	0.86
1:A:359:GLU:HG2	1:A:604:ILE:HD11	1.55	0.86
1:C:611:PRO:HA	1:C:618:TYR:HD2	1.41	0.85
1:A:239:PHE:HD1	1:A:240:PRO:HD2	1.45	0.81
1:C:611:PRO:HA	1:C:618:TYR:CD2	2.16	0.81
1:A:282:TYR:OH	5:A:803:GOL:H32	1.80	0.80
1:A:164:ASP:HB3	1:A:167:VAL:HG22	1.64	0.79
2:F:1:NAG:H3	2:F:2:NAG:C2	2.06	0.78
2:F:2:NAG:H62	2:F:3:BMA:O5	1.84	0.77
2:F:1:NAG:C3	2:F:2:NAG:HN2	1.99	0.75
2:F:1:NAG:C3	2:F:2:NAG:C2	2.64	0.71
2:F:2:NAG:H62	2:F:3:BMA:C1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASP:OD1	1:A:235:VAL:HG12	1.90	0.70
1:C:432:ASP:HB3	1:C:435:VAL:HG12	1.76	0.67
1:C:498:LEU:HD23	1:C:499:LEU:HB2	1.76	0.67
1:C:190:VAL:HG12	1:C:261:VAL:HG22	1.77	0.66
2:F:1:NAG:C3	2:F:2:NAG:N2	2.55	0.66
1:B:274:LEU:HD21	1:B:307:LEU:HD23	1.78	0.66
1:B:188:VAL:HG23	1:B:262:ALA:O	1.96	0.65
1:C:282:TYR:HH	5:C:805:GOL:H32	1.61	0.65
1:A:381:ARG:HA	1:A:476:THR:HG21	1.80	0.64
1:C:188:VAL:HG23	1:C:263:PRO:HA	1.82	0.62
1:B:166:LEU:HD21	1:B:178:ILE:HA	1.81	0.62
2:F:2:NAG:H83	2:F:2:NAG:C4	2.29	0.62
1:A:239:PHE:CD1	1:A:240:PRO:HD2	2.33	0.61
1:C:231:ILE:H	1:C:231:ILE:HD12	1.67	0.59
1:B:375:SER:HA	1:B:378:LEU:HD12	1.84	0.59
1:A:498:LEU:HD11	1:A:507:VAL:HG22	1.85	0.59
1:C:485:GLU:O	1:C:599:MET:HA	2.03	0.58
1:B:170:THR:HG22	1:B:172:LYS:H	1.70	0.57
1:A:296:LEU:HA	1:A:630:MET:HE3	1.86	0.56
1:B:203:PRO:O	1:B:207:ARG:NH1	2.38	0.56
1:C:525:GLY:HA2	1:C:528:ARG:HE	1.70	0.56
1:A:239:PHE:HD1	1:A:240:PRO:CD	2.18	0.56
1:B:539:THR:HA	1:C:680:LEU:HD13	1.87	0.56
1:A:644:PRO:O	1:A:648:SER:HB2	2.06	0.55
1:B:611:PRO:HA	1:B:618:TYR:CD2	2.41	0.55
1:B:473:PHE:CZ	1:B:574:GLU:HG3	2.42	0.55
1:B:476:THR:HG22	1:B:477:GLU:N	2.22	0.54
1:A:274:LEU:HD21	1:A:307:LEU:HD23	1.89	0.54
1:C:452:VAL:HB	1:C:453:PRO:HD2	1.90	0.53
1:A:322:PRO:HD3	1:C:398:ARG:NH1	2.23	0.53
1:A:239:PHE:CE2	1:A:501:LYS:HD2	2.43	0.53
1:A:282:TYR:OH	5:A:803:GOL:C3	2.56	0.53
1:C:229:VAL:HG11	1:C:433:PRO:HB2	1.91	0.53
1:A:527:ALA:HB1	1:A:690:LEU:HD11	1.92	0.52
1:B:498:LEU:HD11	1:B:507:VAL:HG22	1.92	0.52
1:C:468:LEU:O	1:C:570:ARG:NH2	2.43	0.51
4:C:804:NAG:H82	4:C:804:NAG:O4	2.10	0.51
1:A:380:GLN:HG2	1:A:381:ARG:HG3	1.92	0.51
1:C:319:LEU:HD23	1:C:421:LEU:HD22	1.92	0.51
1:B:229:VAL:HG11	1:B:433:PRO:HB2	1.93	0.51
1:C:524:ASN:H	1:C:524:ASN:HD22	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:LEU:HD22	1:B:336:ALA:HB3	1.93	0.50
1:A:293:HIS:N	1:A:293:HIS:ND1	2.58	0.50
1:A:350:ASP:HB3	1:A:353:ARG:HB2	1.94	0.50
1:A:525:GLY:HA2	1:A:528:ARG:HB2	1.94	0.50
1:B:312:ALA:HB1	1:B:440:GLU:OE1	2.11	0.50
1:A:571:TYR:O	1:A:576:ASN:HB2	2.12	0.49
1:B:404:ARG:NH1	1:B:450:PRO:O	2.45	0.49
1:C:537:ASP:O	1:C:541:PRO:HA	2.13	0.49
1:B:315:GLY:O	1:B:328:ALA:HB3	2.13	0.49
1:B:205:ARG:HD2	1:B:314:LEU:HD22	1.95	0.49
1:B:381:ARG:HA	1:B:476:THR:HG21	1.95	0.48
1:B:388:SER:OG	1:B:390:THR:HG22	2.13	0.48
1:C:462:GLU:OE2	1:C:472:ARG:HD2	2.12	0.48
1:A:485:GLU:O	1:A:599:MET:HA	2.14	0.48
1:C:274:LEU:HD21	1:C:307:LEU:HD23	1.96	0.48
1:A:526:ALA:HA	1:A:529:GLN:HE22	1.79	0.48
1:C:532:VAL:O	1:C:536:THR:HG22	2.13	0.48
1:C:543:ASN:HB3	1:C:546:SER:HB2	1.95	0.48
1:A:229:VAL:HG11	1:A:433:PRO:HB2	1.96	0.47
1:C:525:GLY:HA2	1:C:528:ARG:NE	2.30	0.47
1:A:312:ALA:HB1	1:A:440:GLU:OE1	2.14	0.47
1:B:175:ILE:HA	1:B:219:LEU:O	2.14	0.47
1:B:569:GLN:O	1:B:573:GLU:HG2	2.15	0.47
1:B:693:LEU:O	1:B:697:THR:HG22	2.15	0.47
1:C:357:PHE:HB3	1:C:383:ILE:HB	1.97	0.47
1:A:238:ASP:OD1	1:A:238:ASP:N	2.48	0.46
1:C:523:VAL:HB	1:C:527:ALA:HB3	1.96	0.46
1:C:307:LEU:HD22	1:C:336:ALA:HB3	1.96	0.46
1:C:343:ASN:HA	1:C:346:ARG:HH11	1.80	0.46
1:B:371:LEU:HD23	1:B:473:PHE:HB3	1.96	0.46
1:C:611:PRO:HG2	1:C:626:SER:HB2	1.97	0.46
1:B:367:SER:HB2	1:B:389:PRO:HD3	1.98	0.46
1:C:296:LEU:HA	1:C:630:MET:HE3	1.97	0.46
1:B:396:VAL:O	1:B:454:VAL:HG23	2.16	0.46
1:C:476:THR:HG22	1:C:477:GLU:N	2.30	0.46
1:A:523:VAL:HB	1:A:527:ALA:HB3	1.98	0.45
1:C:239:PHE:HA	1:C:240:PRO:HD3	1.80	0.45
1:A:321:THR:OG1	1:A:322:PRO:HD2	2.17	0.45
1:A:585:HIS:ND1	1:A:669:LEU:HD11	2.31	0.45
1:B:658:THR:HG23	1:B:661:GLY:HA3	1.97	0.45
1:B:359:GLU:HA	1:B:385:GLN:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:PHE:HZ	1:B:574:GLU:HG3	1.81	0.45
1:B:485:GLU:O	1:B:599:MET:HA	2.17	0.45
1:C:381:ARG:HA	1:C:476:THR:HG21	1.98	0.45
1:C:484:THR:CG2	1:C:584:THR:HG22	2.46	0.45
1:C:662:ARG:HE	1:C:680:LEU:HD21	1.82	0.45
1:A:182:ALA:HA	1:A:294:ARG:HD2	1.99	0.45
1:A:452:VAL:HB	1:A:453:PRO:HD2	1.99	0.45
1:B:523:VAL:HB	1:B:527:ALA:HB3	1.99	0.45
1:A:562:CYS:HB3	1:A:687:LYS:HE2	1.99	0.45
2:F:1:NAG:H4	2:F:2:NAG:H2	1.49	0.45
1:A:269:ASN:OD1	1:A:350:ASP:HB2	2.16	0.44
1:A:535:TYR:HE1	1:A:553:LYS:HB3	1.81	0.44
1:B:175:ILE:HD11	1:B:347:PHE:HZ	1.82	0.44
1:C:462:GLU:OE2	1:C:472:ARG:NH1	2.48	0.44
1:C:380:GLN:O	1:C:476:THR:HG21	2.18	0.44
1:B:196:TYR:CD1	1:B:258:ILE:HG13	2.53	0.44
1:A:234:THR:O	1:A:236:PHE:N	2.51	0.44
1:A:646:THR:O	1:A:647:ALA:HB3	2.18	0.44
1:C:272:VAL:HB	1:C:354:VAL:HA	1.99	0.44
1:C:565:ASN:HB3	1:C:662:ARG:HH22	1.83	0.44
1:A:192:LEU:HD23	1:A:224:PRO:HD3	2.00	0.43
1:B:170:THR:HB	1:B:173:GLY:O	2.18	0.43
1:C:679:ARG:HH21	1:C:682:GLN:HG2	1.84	0.43
1:A:484:THR:CG2	1:A:584:THR:HG22	2.48	0.43
1:B:535:TYR:HE1	1:B:553:LYS:HB3	1.83	0.43
1:B:679:ARG:HH21	1:B:682:GLN:HG2	1.84	0.43
1:A:398:ARG:CZ	1:C:322:PRO:HD3	2.49	0.43
1:B:190:VAL:HG12	1:B:261:VAL:HG22	2.01	0.43
1:A:319:LEU:HA	1:A:402:THR:HG22	2.00	0.43
1:B:579:TYR:OH	1:B:641:ASN:ND2	2.52	0.43
1:C:404:ARG:NH1	1:C:450:PRO:O	2.51	0.43
1:A:235:VAL:CG1	1:A:493:TYR:CE2	3.03	0.42
1:A:235:VAL:HG11	1:A:493:TYR:CE2	2.55	0.42
1:A:679:ARG:HH21	1:A:682:GLN:HG2	1.84	0.42
1:A:476:THR:HG22	1:A:477:GLU:N	2.34	0.42
1:B:380:GLN:O	1:B:476:THR:HG21	2.19	0.42
1:B:333:GLN:OE1	1:B:365:SER:HB3	2.19	0.42
1:C:384:LEU:O	1:C:480:THR:HA	2.19	0.42
1:A:313:SER:O	1:A:317:LEU:HB2	2.20	0.42
1:A:352:SER:O	1:A:380:GLN:HB2	2.19	0.42
1:B:565:ASN:O	1:B:569:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:ASN:HA	1:B:642:PRO:HD3	1.87	0.42
1:B:679:ARG:NH2	1:B:682:GLN:HG2	2.35	0.42
1:C:312:ALA:HB1	1:C:440:GLU:OE1	2.20	0.42
1:B:307:LEU:HD11	1:B:333:GLN:HG2	2.02	0.42
1:B:357:PHE:HA	1:B:383:ILE:O	2.20	0.41
1:C:359:GLU:OE1	1:C:360:SER:HB2	2.20	0.41
1:A:461:ASP:OD2	1:C:210:ARG:NH2	2.53	0.41
1:B:476:THR:CG2	1:B:477:GLU:N	2.82	0.41
1:C:197:ALA:HB2	1:C:335:LEU:HD23	2.03	0.41
1:B:357:PHE:CB	1:B:383:ILE:HB	2.50	0.41
1:C:565:ASN:HA	1:C:580:MET:HE1	2.02	0.41
1:B:569:GLN:CG	1:B:662:ARG:HE	2.33	0.41
1:B:584:THR:C	1:B:598:VAL:HG21	2.46	0.41
1:C:357:PHE:HA	1:C:383:ILE:O	2.20	0.41
1:A:432:ASP:HB3	1:A:435:VAL:HG12	2.01	0.41
1:A:529:GLN:CA	1:A:532:VAL:HG22	2.37	0.41
1:B:682:GLN:O	1:B:685:PHE:HB3	2.20	0.41
1:B:197:ALA:HB3	1:B:256:LEU:HD23	2.03	0.41
1:A:434:HIS:O	1:A:438:ASN:ND2	2.47	0.40
1:A:510:GLU:O	1:A:514:GLN:HG2	2.21	0.40
1:A:682:GLN:O	1:A:685:PHE:HB3	2.21	0.40
1:B:527:ALA:HB1	1:B:690:LEU:HD11	2.03	0.40
1:A:487:GLY:O	1:A:491:ILE:HG13	2.22	0.40
1:B:202:GLY:HA3	1:B:203:PRO:HD3	1.97	0.40
1:B:239:PHE:HA	1:B:240:PRO:HD3	1.90	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	535/553 (97%)	517 (97%)	18 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	535/553 (97%)	518 (97%)	17 (3%)	0	100	100
1	C	535/553 (97%)	519 (97%)	16 (3%)	0	100	100
All	All	1605/1659 (97%)	1554 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	454/467 (97%)	440 (97%)	14 (3%)	35	61
1	B	454/467 (97%)	438 (96%)	16 (4%)	32	58
1	C	454/467 (97%)	439 (97%)	15 (3%)	33	59
All	All	1362/1401 (97%)	1317 (97%)	45 (3%)	33	59

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LEU
1	A	201	VAL
1	A	238	ASP
1	A	293	HIS
1	A	299	GLU
1	A	311	VAL
1	A	330	LEU
1	A	345	HIS
1	A	359	GLU
1	A	417	GLU
1	A	455	VAL
1	A	495	LEU
1	A	498	LEU
1	A	658	THR
1	B	188	VAL
1	B	216	THR

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Mol	Chain	Res	Type
1	B	301	ASN
1	B	311	VAL
1	B	330	LEU
1	B	443	THR
1	B	455	VAL
1	B	478	ILE
1	B	482	SER
1	B	495	LEU
1	B	549	ASP
1	B	573	GLU
1	B	603	GLU
1	B	651	PHE
1	B	658	THR
1	B	697	THR
1	C	162	ASP
1	C	201	VAL
1	C	293	HIS
1	C	311	VAL
1	C	330	LEU
1	C	357	PHE
1	C	360	SER
1	C	412	VAL
1	C	455	VAL
1	C	465	GLN
1	C	482	SER
1	C	496	THR
1	C	524	ASN
1	C	658	THR
1	C	669	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	HIS
1	A	465	GLN
1	A	569	GLN
1	B	576	ASN
1	C	246	ASN
1	C	301	ASN
1	C	524	ASN
1	C	576	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

12 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	D	1	2,1	14,14,15	0.57	0	17,19,21	1.52	3 (17%)
2	NAG	D	2	2	14,14,15	0.67	0	17,19,21	1.54	2 (11%)
2	BMA	D	3	2	11,11,12	0.62	0	15,15,17	1.62	2 (13%)
3	NAG	E	1	1,3	14,14,15	0.46	0	17,19,21	2.75	6 (35%)
3	NAG	E	2	3	14,14,15	0.73	1 (7%)	17,19,21	2.16	4 (23%)
3	BMA	E	3	3	11,11,12	0.87	0	15,15,17	1.87	5 (33%)
3	MAN	E	4	3	11,11,12	0.51	0	15,15,17	2.96	4 (26%)
3	MAN	E	5	3	11,11,12	0.59	0	15,15,17	1.54	3 (20%)
3	MAN	E	6	3	11,11,12	0.55	0	15,15,17	1.75	3 (20%)
2	NAG	F	1	2,1	14,14,15	0.37	0	17,19,21	0.72	1 (5%)
2	NAG	F	2	2	14,14,15	0.55	0	17,19,21	1.93	3 (17%)
2	BMA	F	3	2	11,11,12	0.26	0	15,15,17	1.05	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	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	1/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
3	MAN	E	6	3	-	2/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	5/6/23/26	0/1/1/1
2	BMA	F	3	2	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	C1-C2	2.08	1.55	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	MAN	C1-O5-C5	9.45	124.85	112.19
3	E	1	NAG	C1-O5-C5	8.52	123.60	112.19
3	E	2	NAG	C1-O5-C5	5.95	120.16	112.19
2	F	2	NAG	C4-C3-C2	5.62	119.26	111.02
3	E	3	BMA	C1-C2-C3	4.92	116.81	109.64
3	E	2	NAG	C4-C3-C2	4.91	118.22	111.02
3	E	1	NAG	O5-C1-C2	4.87	118.83	111.29
3	E	4	MAN	C1-C2-C3	4.87	116.73	109.64
3	E	6	MAN	C1-O5-C5	4.73	118.53	112.19
2	D	2	NAG	C4-C3-C2	4.69	117.89	111.02
2	D	3	BMA	C1-O5-C5	4.52	118.24	112.19
2	F	2	NAG	C1-O5-C5	3.68	117.12	112.19
2	D	1	NAG	C4-C3-C2	3.51	116.16	111.02
3	E	5	MAN	C3-C4-C5	3.46	116.50	110.23
3	E	3	BMA	C2-C3-C4	3.29	116.65	110.86
3	E	6	MAN	C1-C2-C3	3.21	114.32	109.64
3	E	4	MAN	O5-C1-C2	3.12	118.24	110.79
3	E	5	MAN	C1-O5-C5	3.03	116.24	112.19
2	D	3	BMA	C1-C2-C3	2.97	113.97	109.64
2	D	2	NAG	C1-O5-C5	2.89	116.06	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	-2.77	108.47	112.19
3	E	2	NAG	O5-C1-C2	2.70	115.47	111.29
2	D	1	NAG	C3-C4-C5	2.58	114.90	110.23
3	E	1	NAG	C4-C3-C2	2.56	114.77	111.02
2	F	3	BMA	C2-C3-C4	-2.45	106.55	110.86
3	E	1	NAG	C8-C7-N2	2.38	120.07	116.12
3	E	1	NAG	C2-N2-C7	2.28	125.95	122.90
2	F	2	NAG	C1-C2-N2	-2.27	106.86	110.43
3	E	1	NAG	O5-C5-C4	2.26	116.34	110.83
3	E	2	NAG	O5-C5-C6	2.25	112.05	107.66
3	E	3	BMA	C1-O5-C5	-2.18	109.26	112.19
3	E	3	BMA	O5-C5-C6	2.15	111.85	107.66
3	E	5	MAN	O5-C5-C4	2.14	116.02	110.83
3	E	3	BMA	C3-C4-C5	2.11	114.06	110.23
3	E	4	MAN	C3-C4-C5	2.03	113.91	110.23
3	E	6	MAN	C3-C4-C5	2.02	113.89	110.23
2	F	1	NAG	C3-C4-C5	2.01	113.87	110.23

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
3	E	6	MAN	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
3	E	6	MAN	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6

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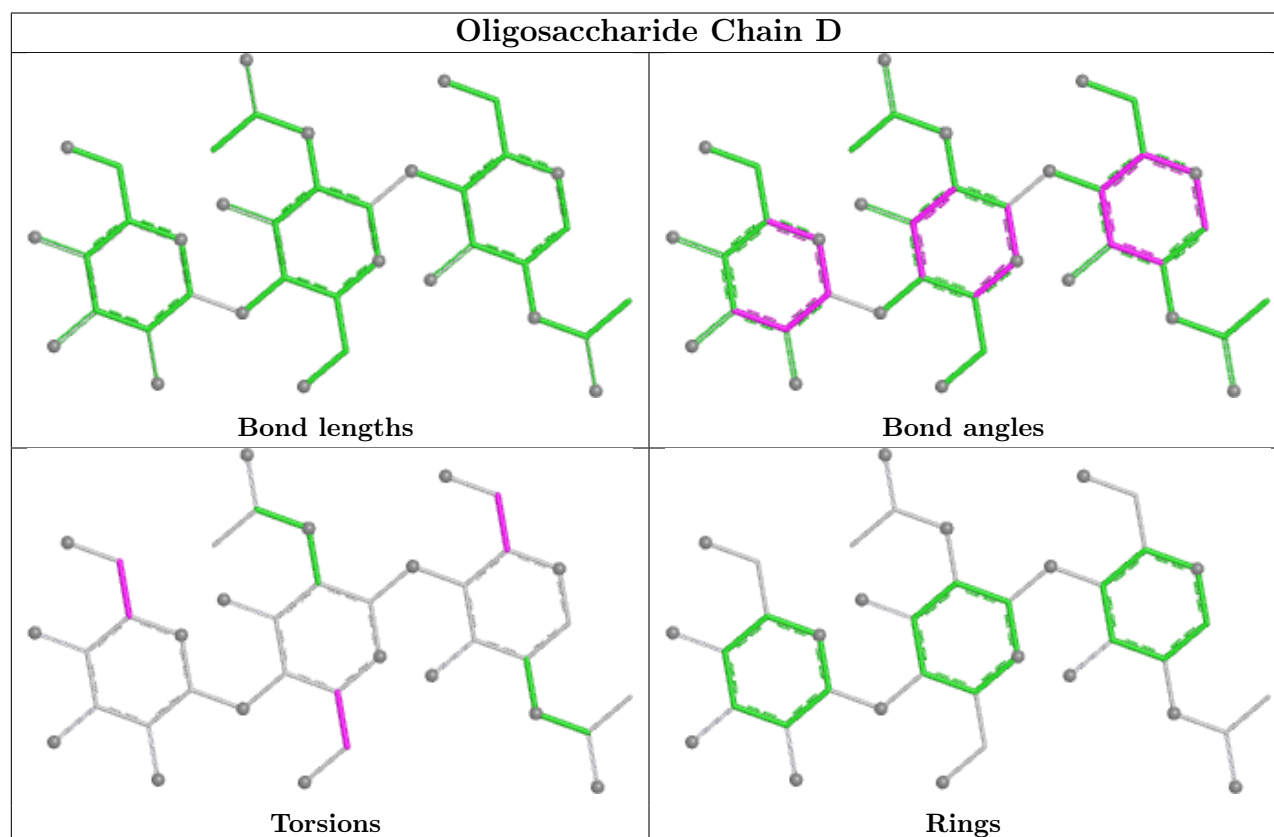
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	D	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6

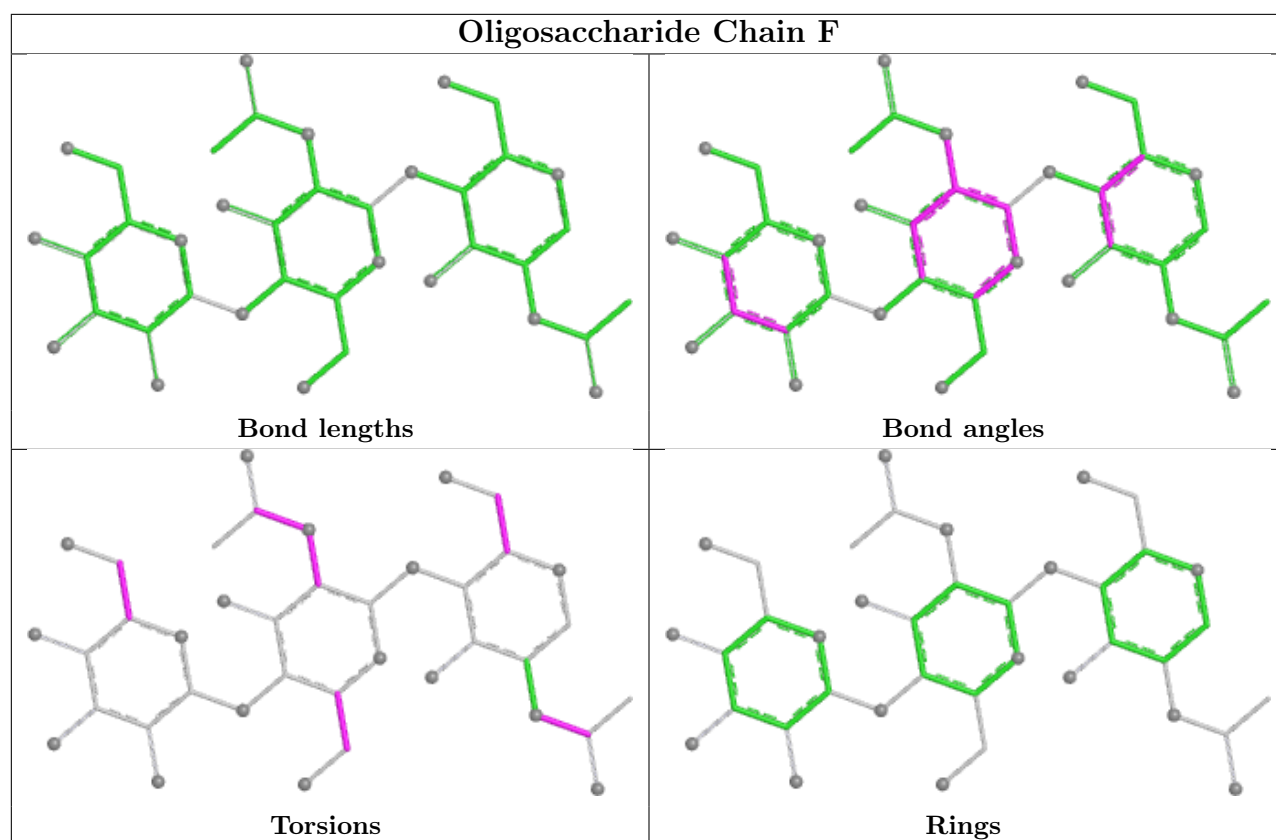
There are no ring outliers.

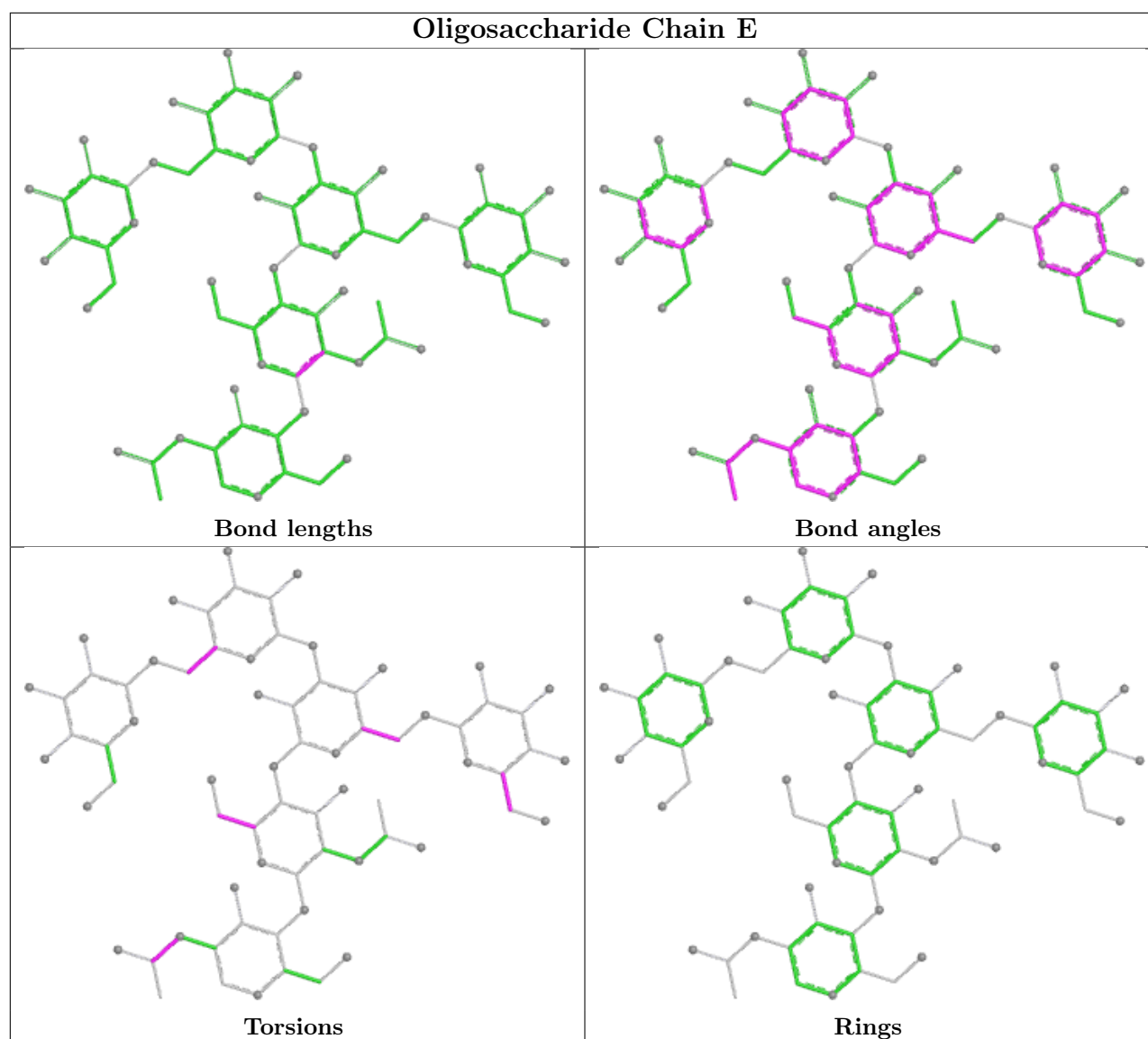
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	BMA	2	0
2	F	2	NAG	13	0
2	F	1	NAG	7	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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	C	805	-	5,5,5	0.32	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	802	1	14,14,15	0.58	0	17,19,21	3.18	6 (35%)
5	GOL	B	810	6	5,5,5	1.06	0	5,5,5	0.65	0
5	GOL	A	803	-	5,5,5	0.31	0	5,5,5	0.35	0
5	GOL	A	804	6	5,5,5	0.41	0	5,5,5	0.24	0
4	NAG	A	801	1	14,14,15	0.29	0	17,19,21	0.55	0
4	NAG	C	804	1	14,14,15	0.38	0	17,19,21	0.72	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	GOL	C	805	-	-	0/4/4/4	-
4	NAG	A	802	1	-	5/6/23/26	0/1/1/1
5	GOL	B	810	6	-	0/4/4/4	-
5	GOL	A	803	-	-	2/4/4/4	-
5	GOL	A	804	6	-	2/4/4/4	-
4	NAG	A	801	1	-	2/6/23/26	0/1/1/1
4	NAG	C	804	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	NAG	C2-N2-C7	9.12	135.12	122.90
4	A	802	NAG	C1-O5-C5	6.01	120.24	112.19
4	A	802	NAG	C1-C2-N2	4.17	117.01	110.43
4	A	802	NAG	C8-C7-N2	3.76	122.35	116.12
4	A	802	NAG	O7-C7-C8	-2.56	117.50	122.05
4	A	802	NAG	C3-C4-C5	2.21	114.23	110.23

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	NAG	C8-C7-N2-C2
4	A	801	NAG	O7-C7-N2-C2
4	A	802	NAG	C1-C2-N2-C7
4	C	804	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	C	804	NAG	C8-C7-N2-C2
4	C	804	NAG	O7-C7-N2-C2
5	A	803	GOL	O1-C1-C2-C3
5	A	804	GOL	O2-C2-C3-O3
4	A	802	NAG	O5-C5-C6-O6
4	A	802	NAG	C8-C7-N2-C2
4	A	802	NAG	O7-C7-N2-C2
5	A	804	GOL	C1-C2-C3-O3
5	A	803	GOL	O1-C1-C2-O2
4	A	802	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	805	GOL	2	0
5	A	803	GOL	2	0
4	C	804	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	537/553 (97%)	-0.22	2 (0%) 88 73	34, 54, 83, 139	0
1	B	537/553 (97%)	-0.10	3 (0%) 85 66	33, 61, 90, 125	0
1	C	537/553 (97%)	-0.02	2 (0%) 88 73	39, 63, 99, 136	0
All	All	1611/1659 (97%)	-0.11	7 (0%) 88 73	33, 58, 91, 139	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	647	ALA	2.5
1	A	648	SER	2.4
1	B	648	SER	2.4
1	B	669	LEU	2.3
1	B	651	PHE	2.3
1	C	644	PRO	2.1
1	C	216	THR	2.1

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

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

6.3 Carbohydrates [i](#)

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

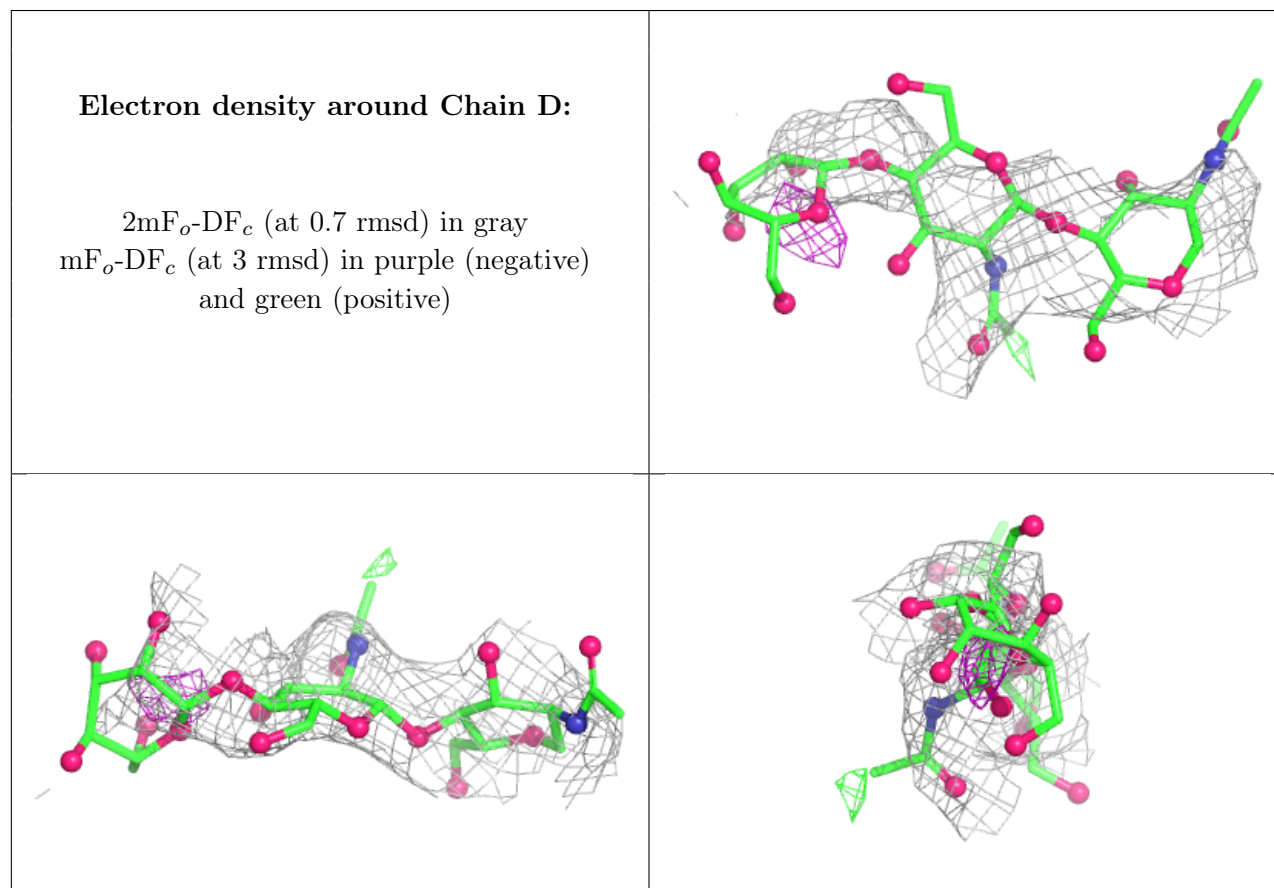
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	2	14/15	0.17	0.15	145,154,157,158	0

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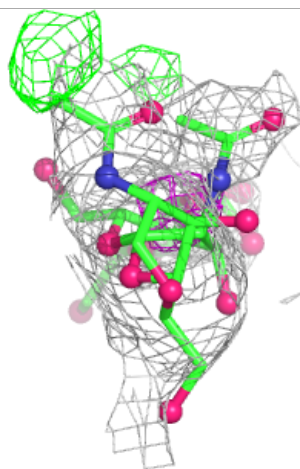
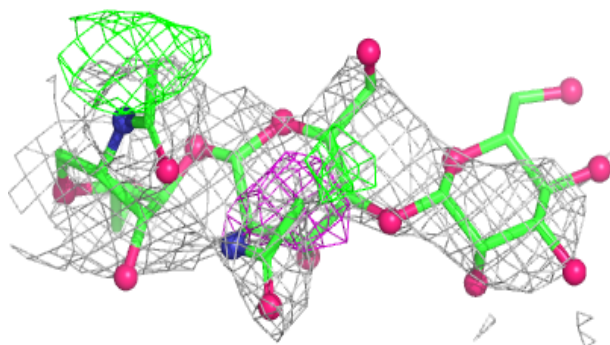
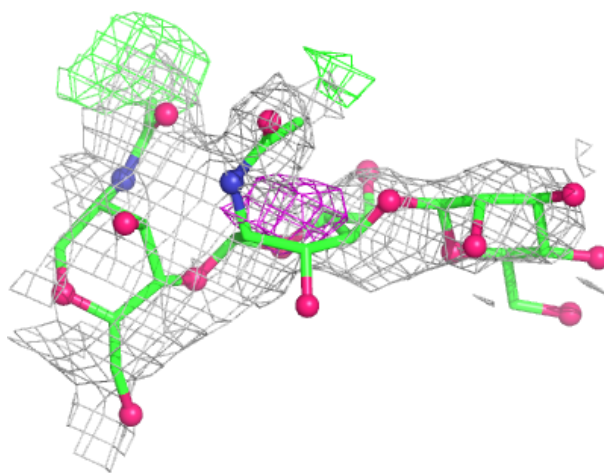
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	E	5	11/12	0.25	0.14	198,200,204,206	0
3	MAN	E	4	11/12	0.30	0.13	188,191,195,201	0
2	NAG	F	1	14/15	0.31	0.18	114,127,135,139	0
3	MAN	E	6	11/12	0.36	0.15	148,165,167,168	0
3	BMA	E	3	11/12	0.38	0.11	166,169,175,182	0
2	BMA	D	3	11/12	0.39	0.16	171,174,177,180	0
2	BMA	F	3	11/12	0.50	0.12	143,156,159,160	0
3	NAG	E	2	14/15	0.55	0.15	138,152,161,166	0
2	NAG	D	1	14/15	0.56	0.14	135,143,147,147	0
3	NAG	E	1	14/15	0.57	0.13	119,127,134,143	0
2	NAG	D	2	14/15	0.57	0.13	135,152,160,167	0

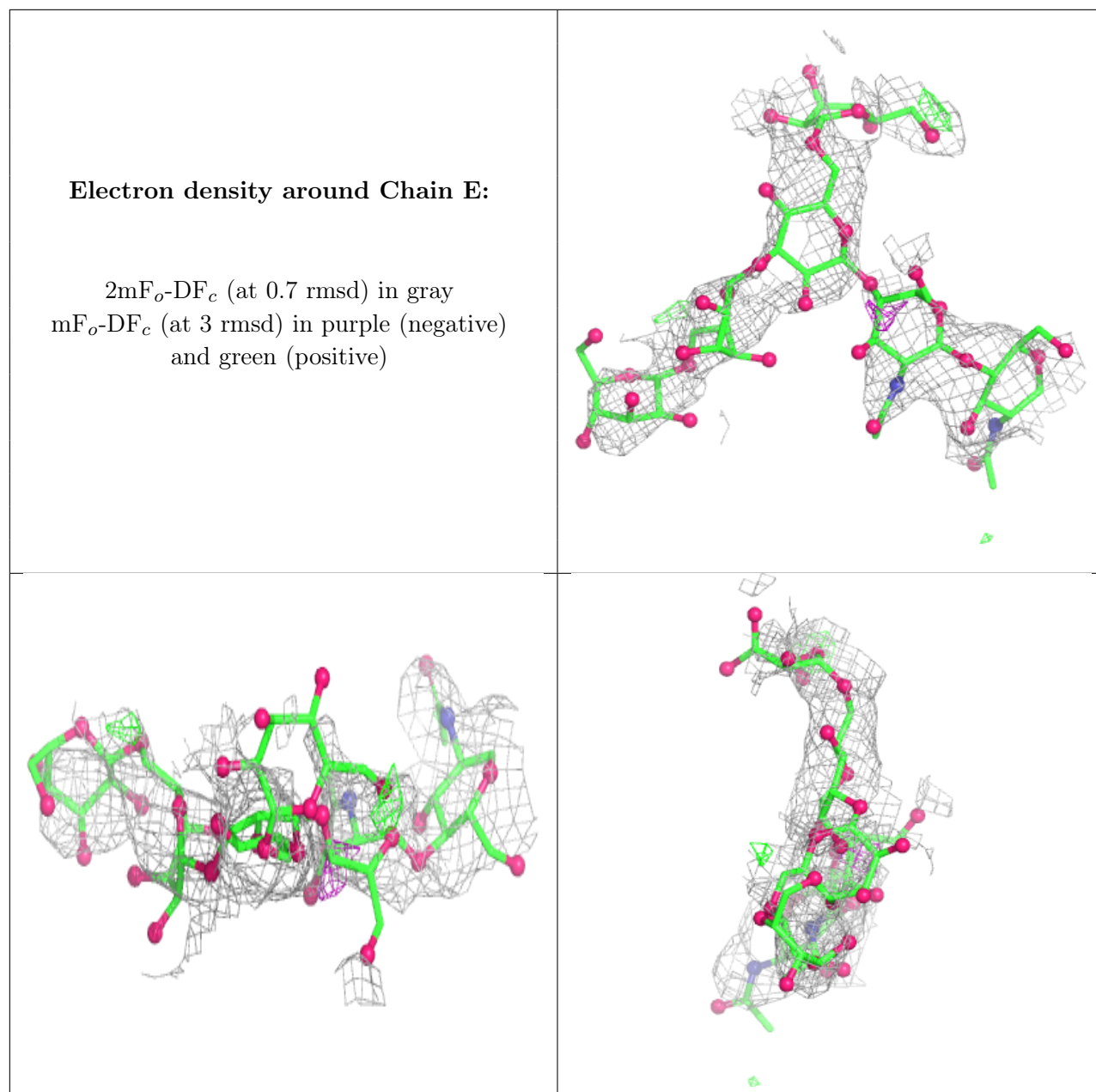
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain F:

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





6.4 Ligands ⓘ

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	NAG	C	804	14/15	0.19	0.18	118,127,130,130	0
4	NAG	A	802	14/15	0.44	0.16	112,119,121,122	0
4	NAG	A	801	14/15	0.62	0.14	109,115,117,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	C	805	6/6	0.79	0.18	43,46,46,46	0
5	GOL	A	803	6/6	0.80	0.18	49,51,53,55	0
6	NA	B	812	1/1	0.82	0.24	50,50,50,50	0
5	GOL	A	804	6/6	0.85	0.20	48,53,53,53	0
5	GOL	B	810	6/6	0.86	0.14	31,31,32,32	0
6	NA	A	805	1/1	0.90	0.25	22,22,22,22	0
6	NA	B	811	1/1	0.98	0.08	30,30,30,30	0
6	NA	C	806	1/1	0.98	0.12	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.