



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:20 PM UTC

PDB ID : 7URU / pdb_00007uru
Title : Crystal structure of the low affinity Fc gamma receptor IIIA variant in complex with the Fc of IgG1.
Authors : Tolbert, W.D.; Pazgier, M.
Deposited on : 2022-04-22
Resolution : 2.40 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

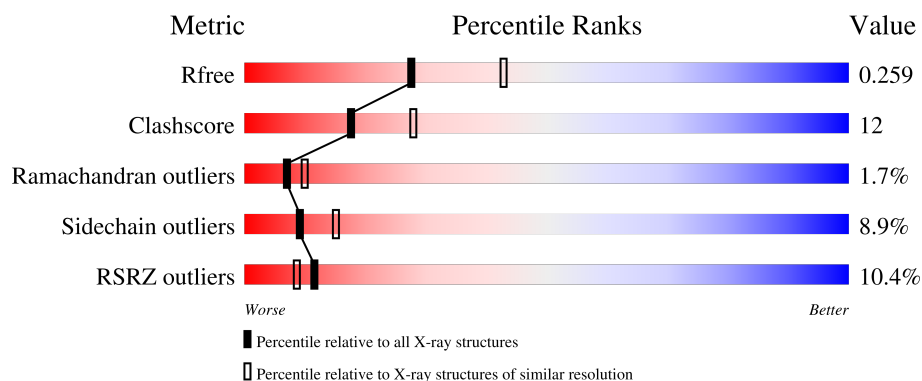
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	223	 13% 65% 28% • 5%
1	B	223	 10% 69% 22% • •
2	C	177	 7% 62% 31% • •
3	D	8	 25% 62% 12%
3	E	8	 38% 50% 12%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5018 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 Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1693	1078	284	325	6			
1	B	213	Total	C	N	O	S	0	0	0
			1700	1083	285	326	6			

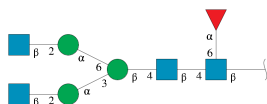
- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	171	Total	C	N	O	S	0	0	0
			1385	884	236	261	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P08637
C	0	SER	-	expression tag	UNP P08637
C	38	GLN	ASN	conflict	UNP P08637
C	74	GLN	ASN	conflict	UNP P08637
C	169	GLN	ASN	conflict	UNP P08637

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



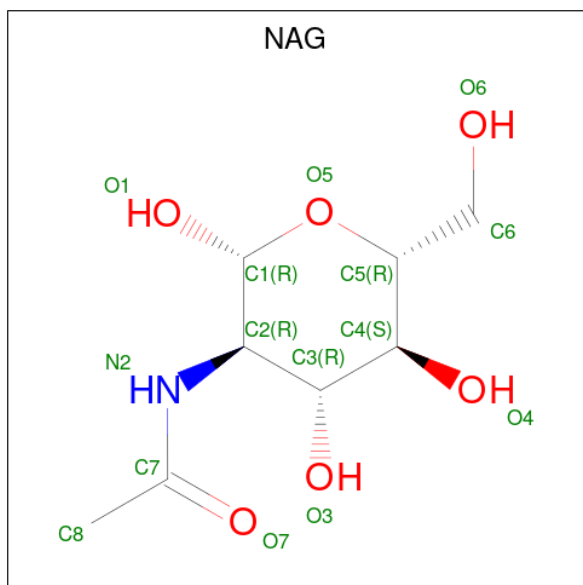
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	8	Total	C	N	O	0	0	0
			99	56	4	39			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	0	0	0
			99	56	4	39			

- 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	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

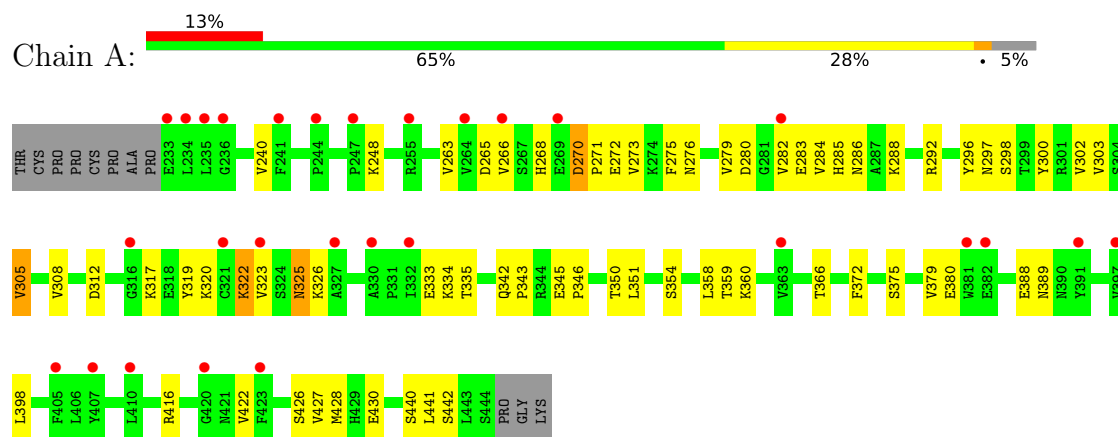
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	5	Total	O	0	0
			5	5		
5	C	4	Total	O	0	0
			4	4		

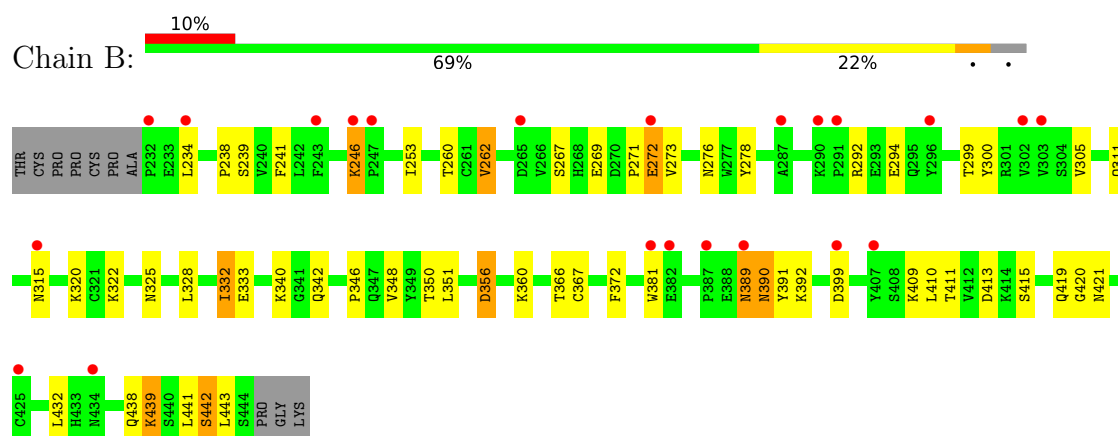
3 Residue-property plots [i](#)

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.

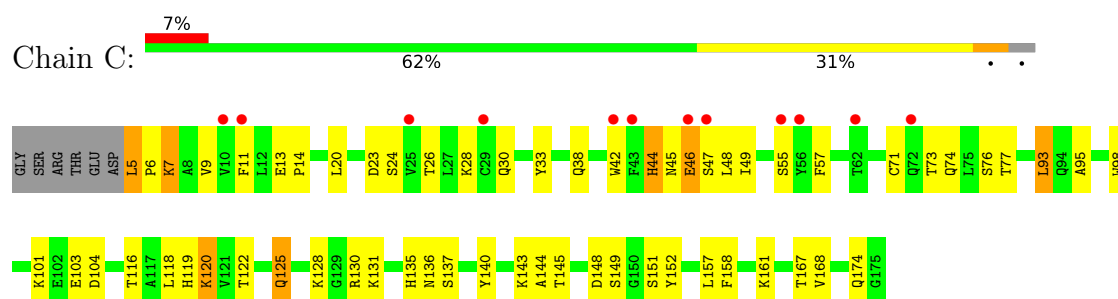
- Molecule 1: Immunoglobulin gamma-1 heavy chain



- Molecule 1: Immunoglobulin gamma-1 heavy chain



- Molecule 2: Low affinity immunoglobulin gamma Fc region receptor III-A



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

Chain D:  25% 62% 12%



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

Chain E:  38% 50% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.98Å 100.75Å 124.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.43 – 2.40 32.43 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (32.43-2.40) 95.8 (32.43-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.215 , 0.262 0.215 , 0.259	Depositor DCC
R_{free} test set	1734 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5018	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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, NAG, FUC, 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	0.51	0/1739	0.69	0/2369
1	B	0.54	0/1747	0.72	0/2380
2	C	0.55	0/1424	0.80	1/1934 (0.1%)
All	All	0.53	0/4910	0.73	1/6683 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	47	SER	N-CA-C	-5.15	108.26	114.75

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	1693	0	1661	38	0
1	B	1700	0	1669	34	0
2	C	1385	0	1328	51	0
3	D	99	0	85	1	0
3	E	99	0	85	1	0
4	C	28	0	26	2	0
5	A	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	0	0
5	C	4	0	0	0	0
All	All	5018	0	4854	122	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 12.

All (122) 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:C:26:THR:HG22	2:C:57:PHE:CD1	1.55	1.39
2:C:26:THR:HG22	2:C:57:PHE:CE1	1.74	1.21
2:C:26:THR:CG2	2:C:57:PHE:CE1	2.27	1.18
2:C:26:THR:CG2	2:C:57:PHE:HE1	1.65	1.04
2:C:26:THR:HG21	2:C:57:PHE:HE1	1.23	1.00
2:C:5:LEU:HD23	2:C:6:PRO:HD2	1.43	0.99
2:C:26:THR:CG2	2:C:57:PHE:CD1	2.47	0.97
2:C:26:THR:HG22	2:C:57:PHE:HD1	1.15	0.93
1:A:273:VAL:HG11	1:A:302:VAL:HG11	1.52	0.92
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.61	0.82
1:A:276:ASN:HB2	1:A:322:LYS:HG2	1.61	0.81
2:C:45:ASN:O	2:C:46:GLU:C	2.22	0.81
1:A:320:LYS:HG3	1:A:335:THR:HG22	1.62	0.81
2:C:13:GLU:HB2	2:C:26:THR:OG1	1.81	0.81
2:C:26:THR:HG21	2:C:57:PHE:CE1	2.06	0.77
1:B:292:ARG:HD3	1:B:300:TYR:CE2	2.20	0.77
1:A:272:GLU:O	1:A:325:ASN:ND2	2.20	0.74
2:C:9:VAL:HG22	2:C:30:GLN:HB3	1.69	0.74
2:C:103:GLU:HG2	2:C:143:LYS:HD3	1.70	0.73
1:B:294:GLU:HG2	1:B:300:TYR:CE1	2.24	0.72
1:B:238:PRO:O	2:C:161:LYS:NZ	2.24	0.71
1:B:356:ASP:OD1	1:B:356:ASP:N	2.24	0.70
1:A:240:VAL:HG11	1:A:323:VAL:HG11	1.75	0.68
1:B:294:GLU:HG2	1:B:300:TYR:HE1	1.60	0.67
1:A:271:PRO:O	1:A:292:ARG:NH1	2.28	0.67
1:A:265:ASP:OD2	2:C:120:LYS:NZ	2.27	0.67
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.77	0.65
2:C:103:GLU:OE1	2:C:143:LYS:NZ	2.30	0.64
1:A:296:TYR:CE1	2:C:128:LYS:HD2	2.33	0.64
1:B:238:PRO:HD2	1:B:328:LEU:HD13	1.80	0.63
2:C:130:ARG:NH2	2:C:148:ASP:OD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:TYR:HB2	1:B:320:LYS:HB3	1.79	0.63
2:C:46:GLU:O	2:C:46:GLU:HG3	1.99	0.62
1:B:328:LEU:HD21	1:B:332:ILE:HG13	1.80	0.62
2:C:145:THR:HG22	2:C:148:ASP:OD2	2.01	0.61
1:A:279:VAL:HG23	1:A:284:VAL:HG21	1.83	0.61
1:B:246:LYS:HD2	1:B:246:LYS:H	1.67	0.60
2:C:5:LEU:CD2	2:C:6:PRO:HD2	2.26	0.60
1:A:263:VAL:HB	1:A:302:VAL:HG12	1.83	0.59
1:A:270:ASP:N	1:A:270:ASP:OD1	2.36	0.59
1:B:292:ARG:HD3	1:B:300:TYR:HE2	1.67	0.58
1:B:238:PRO:HD2	1:B:328:LEU:CD1	2.34	0.58
1:A:268:HIS:NE2	1:A:298:SER:O	2.23	0.58
1:B:390:ASN:OD1	1:B:411:THR:HB	2.02	0.58
2:C:101:LYS:HG3	2:C:174:GLN:HB2	1.86	0.58
3:D:5:NAG:H3	3:D:5:NAG:H83	1.87	0.57
2:C:120:LYS:O	4:C:1001:NAG:H81	2.05	0.56
1:A:388:GLU:OE1	1:A:416:ARG:NH2	2.30	0.56
2:C:11:PHE:HB2	2:C:28:LYS:HD2	1.85	0.56
2:C:116:THR:HB	2:C:158:PHE:CZ	2.41	0.56
1:A:271:PRO:HB2	1:A:292:ARG:NH1	2.21	0.55
1:B:421:ASN:O	1:B:442:SER:OG	2.24	0.55
2:C:145:THR:CG2	2:C:148:ASP:OD2	2.54	0.55
1:A:325:ASN:ND2	1:A:326:LYS:H	2.06	0.54
3:E:5:NAG:H3	3:E:5:NAG:H83	1.88	0.54
2:C:33:TYR:HB3	2:C:38:GLN:HA	1.89	0.54
1:A:351:LEU:HB2	1:A:366:THR:HB	1.89	0.53
1:A:248:LYS:NZ	1:A:380:GLU:OE2	2.24	0.53
1:B:311:GLN:O	1:B:315:ASN:HB2	2.09	0.53
1:B:269:GLU:OE1	1:B:269:GLU:N	2.36	0.53
1:A:275:PHE:HZ	1:A:302:VAL:HG13	1.73	0.52
1:B:348:VAL:HG13	1:B:439:LYS:HG2	1.92	0.52
1:B:390:ASN:O	1:B:410:LEU:HD12	2.10	0.52
1:B:438:GLN:O	1:B:439:LYS:HD3	2.10	0.51
2:C:13:GLU:HB2	2:C:26:THR:HG1	1.71	0.51
2:C:101:LYS:N	2:C:104:ASP:OD1	2.37	0.51
2:C:118:LEU:HB3	2:C:136:ASN:HB2	1.91	0.51
1:A:322:LYS:HB2	1:A:333:GLU:HG2	1.93	0.51
2:C:120:LYS:HD3	2:C:157:LEU:HD22	1.92	0.51
1:A:312:ASP:HB3	1:A:319:TYR:OH	2.10	0.50
1:A:430:GLU:HG2	5:A:503:HOH:O	2.10	0.50
1:B:241:PHE:HB2	1:B:262:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:THR:HB	1:B:441:LEU:HB2	1.93	0.50
1:B:320:LYS:HE3	1:B:333:GLU:OE1	2.12	0.49
1:A:297:ASN:O	1:A:298:SER:HB3	2.13	0.49
1:B:389:ASN:O	1:B:391:TYR:N	2.47	0.48
1:B:351:LEU:HB2	1:B:366:THR:HB	1.95	0.47
2:C:93:LEU:HA	2:C:93:LEU:HD12	1.69	0.47
1:A:345:GLU:OE2	5:A:501:HOH:O	2.20	0.47
2:C:119:HIS:CE1	2:C:135:HIS:ND1	2.83	0.47
1:B:272:GLU:O	1:B:325:ASN:ND2	2.46	0.46
1:A:379:VAL:HG22	1:A:427:VAL:HG22	1.97	0.46
2:C:7:LYS:HA	2:C:77:THR:OG1	2.15	0.46
1:A:240:VAL:O	1:A:334:LYS:NZ	2.49	0.45
1:A:283:GLU:OE2	1:A:285:HIS:NE2	2.49	0.45
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.99	0.45
2:C:125:GLN:NE2	2:C:130:ARG:HH12	2.15	0.44
2:C:33:TYR:HB2	2:C:38:GLN:HG3	1.99	0.44
2:C:101:LYS:CG	2:C:174:GLN:HB2	2.47	0.44
1:A:422:VAL:HG22	1:A:442:SER:HB3	1.99	0.44
2:C:140:TYR:C	2:C:140:TYR:CD1	2.95	0.44
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.52	0.44
1:A:350:THR:HB	1:A:441:LEU:HD13	1.98	0.43
2:C:13:GLU:O	2:C:26:THR:OG1	2.34	0.43
1:A:288:LYS:O	1:A:305:VAL:HG13	2.19	0.43
1:A:273:VAL:CG1	1:A:302:VAL:HG11	2.37	0.43
2:C:98:TRP:HZ3	2:C:168:VAL:HG21	1.83	0.43
1:B:234:LEU:HD23	1:B:234:LEU:O	2.19	0.42
2:C:44:HIS:NE2	4:C:1002:NAG:H82	2.35	0.42
2:C:95:ALA:HB3	2:C:98:TRP:CE2	2.55	0.42
1:B:267:SER:OG	1:B:269:GLU:HG2	2.19	0.42
2:C:98:TRP:CZ3	2:C:168:VAL:HG21	2.55	0.42
1:B:328:LEU:CD2	1:B:332:ILE:HG13	2.50	0.42
2:C:11:PHE:CB	2:C:28:LYS:HD2	2.49	0.42
2:C:28:LYS:HB3	2:C:55:SER:OG	2.20	0.42
2:C:42:TRP:CZ3	2:C:71:CYS:HB3	2.55	0.42
2:C:45:ASN:O	2:C:46:GLU:O	2.38	0.42
1:A:296:TYR:C	1:A:298:SER:H	2.28	0.41
1:B:413:ASP:OD1	1:B:413:ASP:N	2.53	0.41
2:C:73:THR:OG1	2:C:76:SER:OG	2.24	0.41
2:C:13:GLU:HA	2:C:14:PRO:HA	1.93	0.41
2:C:125:GLN:HB2	2:C:152:TYR:CE2	2.56	0.41
1:A:248:LYS:HE3	1:A:428:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PHE:CZ	1:A:302:VAL:HG13	2.54	0.41
1:A:280:ASP:O	1:A:282:VAL:HG23	2.20	0.41
1:B:342:GLN:HE21	1:B:342:GLN:HB2	1.70	0.41
1:A:308:VAL:HG23	1:A:319:TYR:CE2	2.56	0.41
1:A:342:GLN:OE1	1:A:343:PRO:HD2	2.21	0.40
1:A:266:VAL:HG12	1:A:300:TYR:HB2	2.03	0.40
1:B:432:LEU:HA	1:B:432:LEU:HD23	1.81	0.40
1:B:292:ARG:CD	1:B:300:TYR:CE2	2.99	0.40
2:C:20:LEU:O	2:C:23:ASP:HB2	2.21	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	210/223 (94%)	198 (94%)	10 (5%)	2 (1%)	12	20
1	B	211/223 (95%)	206 (98%)	2 (1%)	3 (1%)	9	13
2	C	169/177 (96%)	150 (89%)	14 (8%)	5 (3%)	3	3
All	All	590/623 (95%)	554 (94%)	26 (4%)	10 (2%)	7	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	49	ILE
1	A	359	THR
1	B	390	ASN
2	C	46	GLU
1	A	358	LEU
1	B	271	PRO
2	C	44	HIS
2	C	48	LEU

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Mol	Chain	Res	Type
2	C	144	ALA
1	B	420	GLY

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	197/206 (96%)	183 (93%)	14 (7%)	13	23
1	B	198/206 (96%)	176 (89%)	22 (11%)	6	9
2	C	154/159 (97%)	141 (92%)	13 (8%)	10	17
All	All	549/571 (96%)	500 (91%)	49 (9%)	9	15

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	ASP
1	A	286	ASN
1	A	303	VAL
1	A	305	VAL
1	A	317	LYS
1	A	322	LYS
1	A	325	ASN
1	A	354	SER
1	A	360	LYS
1	A	375	SER
1	A	389	ASN
1	A	398	LEU
1	A	426	SER
1	A	440	SER
1	B	239	SER
1	B	246	LYS
1	B	253	ILE
1	B	260	THR
1	B	262	VAL
1	B	272	GLU

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Mol	Chain	Res	Type
1	B	273	VAL
1	B	299	THR
1	B	305	VAL
1	B	332	ILE
1	B	340	LYS
1	B	356	ASP
1	B	360	LYS
1	B	389	ASN
1	B	392	LYS
1	B	399	ASP
1	B	409	LYS
1	B	415	SER
1	B	419	GLN
1	B	439	LYS
1	B	442	SER
1	B	443	LEU
2	C	5	LEU
2	C	7	LYS
2	C	24	SER
2	C	74	GLN
2	C	93	LEU
2	C	120	LYS
2	C	122	THR
2	C	125	GLN
2	C	131	LYS
2	C	137	SER
2	C	149	SER
2	C	151	SER
2	C	167	THR

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	325	ASN
1	A	362	GLN
1	A	389	ASN
1	A	390	ASN
1	B	276	ASN
1	B	325	ASN
1	B	342	GLN
2	C	119	HIS

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
3	NAG	D	1	1,3	14,14,15	0.23	0	17,19,21	1.05	1 (5%)
3	NAG	D	2	3	14,14,15	0.47	0	17,19,21	0.67	0
3	BMA	D	3	3	11,11,12	0.90	0	15,15,17	0.98	1 (6%)
3	MAN	D	4	3	11,11,12	1.27	1 (9%)	15,15,17	1.26	1 (6%)
3	NAG	D	5	3	14,14,15	0.64	0	17,19,21	1.31	1 (5%)
3	MAN	D	6	3	11,11,12	0.82	1 (9%)	15,15,17	1.92	5 (33%)
3	NAG	D	7	3	14,14,15	0.34	0	17,19,21	0.43	0
3	FUC	D	8	3	10,10,11	1.06	0	14,14,16	1.65	4 (28%)
3	NAG	E	1	1,3	14,14,15	0.64	1 (7%)	17,19,21	0.74	1 (5%)
3	NAG	E	2	3	14,14,15	0.58	0	17,19,21	0.67	0
3	BMA	E	3	3	11,11,12	0.92	1 (9%)	15,15,17	0.89	0
3	MAN	E	4	3	11,11,12	1.09	2 (18%)	15,15,17	0.99	1 (6%)
3	NAG	E	5	3	14,14,15	0.44	0	17,19,21	1.44	2 (11%)
3	MAN	E	6	3	11,11,12	1.35	1 (9%)	15,15,17	1.49	1 (6%)
3	NAG	E	7	3	14,14,15	0.68	0	17,19,21	0.49	0
3	FUC	E	8	3	10,10,11	0.81	0	14,14,16	0.96	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
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	NAG	D	5	3	-	6/6/23/26	0/1/1/1
3	MAN	D	6	3	-	1/2/19/22	0/1/1/1
3	NAG	D	7	3	-	4/6/23/26	0/1/1/1
3	FUC	D	8	3	-	-	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	NAG	E	5	3	-	4/6/23/26	0/1/1/1
3	MAN	E	6	3	-	1/2/19/22	0/1/1/1
3	NAG	E	7	3	-	4/6/23/26	0/1/1/1
3	FUC	E	8	3	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	6	MAN	C2-C3	-2.84	1.48	1.52
3	D	4	MAN	O5-C1	-2.81	1.39	1.43
3	E	1	NAG	O5-C1	-2.27	1.39	1.43
3	E	4	MAN	C4-C3	2.17	1.58	1.52
3	D	6	MAN	C1-C2	2.12	1.57	1.52
3	E	4	MAN	O5-C1	-2.06	1.40	1.43
3	E	3	BMA	O5-C1	-2.02	1.40	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	NAG	C2-N2-C7	4.79	129.32	122.90
3	E	5	NAG	C2-N2-C7	4.77	129.29	122.90
3	D	6	MAN	C1-O5-C5	4.66	118.43	112.19
3	E	6	MAN	O2-C2-C3	-4.52	100.78	110.15
3	D	4	MAN	O2-C2-C3	-3.81	102.26	110.15
3	D	6	MAN	O2-C2-C3	-3.71	102.46	110.15
3	D	8	FUC	C1-C2-C3	-3.38	104.72	109.64
3	D	8	FUC	C2-C3-C4	-3.15	105.32	110.86
3	D	1	NAG	C1-O5-C5	3.08	116.32	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	MAN	O2-C2-C3	-2.90	104.15	110.15
3	E	5	NAG	C1-C2-N2	2.78	114.82	110.43
3	D	3	BMA	O2-C2-C3	-2.67	104.62	110.15
3	D	6	MAN	O5-C5-C6	-2.52	102.77	107.66
3	D	6	MAN	C1-C2-C3	2.45	113.21	109.64
3	E	1	NAG	C1-O5-C5	2.31	115.28	112.19
3	D	8	FUC	O2-C2-C1	2.31	114.51	109.22
3	D	8	FUC	O2-C2-C3	2.12	114.54	110.15
3	D	6	MAN	O6-C6-C5	-2.04	104.39	111.33

There are no chirality outliers.

All (27) torsion outliers are listed below:

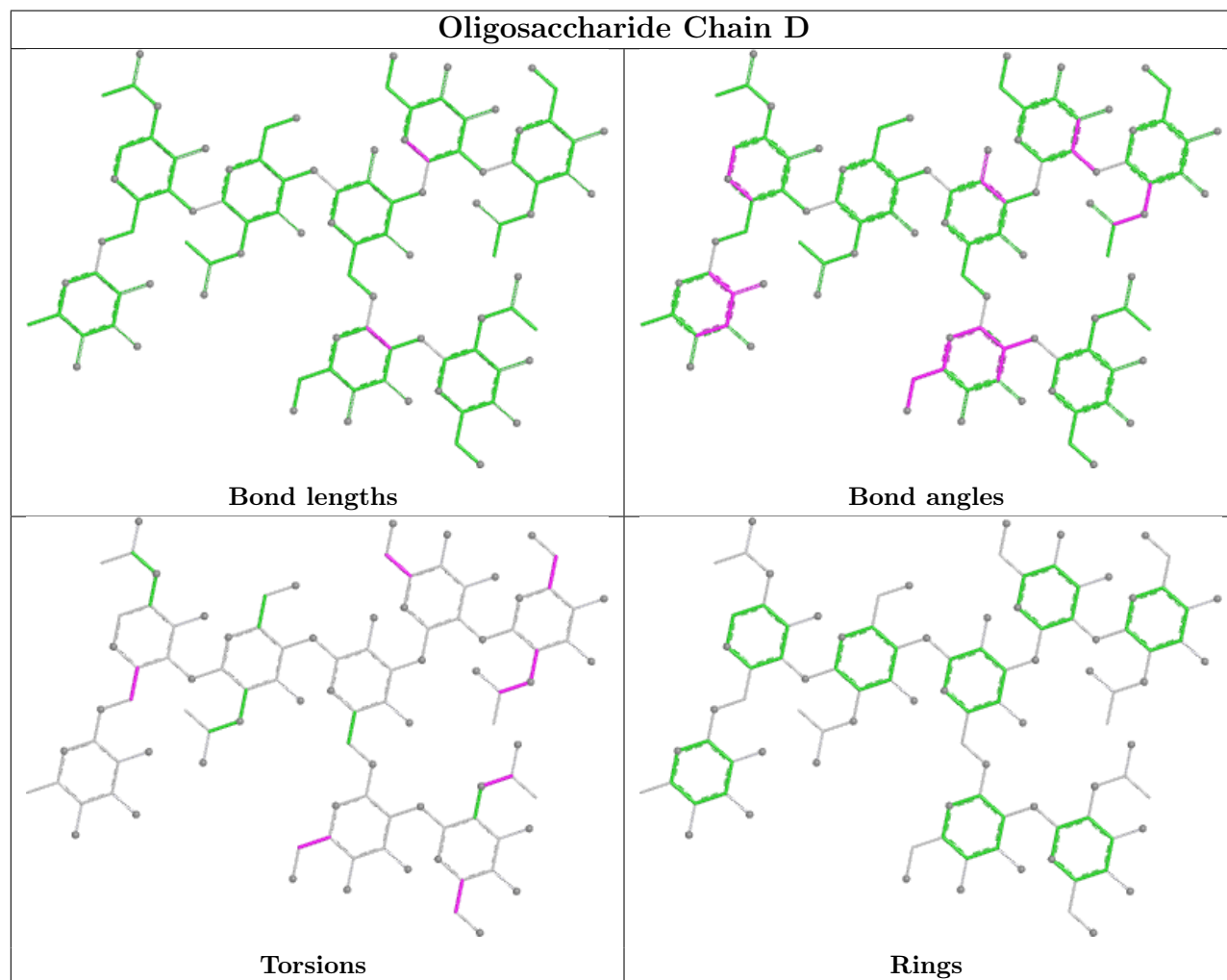
Mol	Chain	Res	Type	Atoms
3	E	4	MAN	C4-C5-C6-O6
3	D	7	NAG	O5-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	D	7	NAG	C4-C5-C6-O6
3	E	7	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	5	NAG	C8-C7-N2-C2
3	D	5	NAG	O7-C7-N2-C2
3	D	7	NAG	C8-C7-N2-C2
3	D	7	NAG	O7-C7-N2-C2
3	E	5	NAG	C8-C7-N2-C2
3	E	5	NAG	O7-C7-N2-C2
3	E	7	NAG	C8-C7-N2-C2
3	E	7	NAG	O7-C7-N2-C2
3	E	7	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	D	5	NAG	C4-C5-C6-O6
3	E	5	NAG	C3-C2-N2-C7
3	E	6	MAN	O5-C5-C6-O6
3	D	5	NAG	O5-C5-C6-O6
3	D	5	NAG	C1-C2-N2-C7
3	E	5	NAG	C1-C2-N2-C7
3	D	5	NAG	C3-C2-N2-C7
3	E	3	BMA	O5-C5-C6-O6
3	D	6	MAN	O5-C5-C6-O6

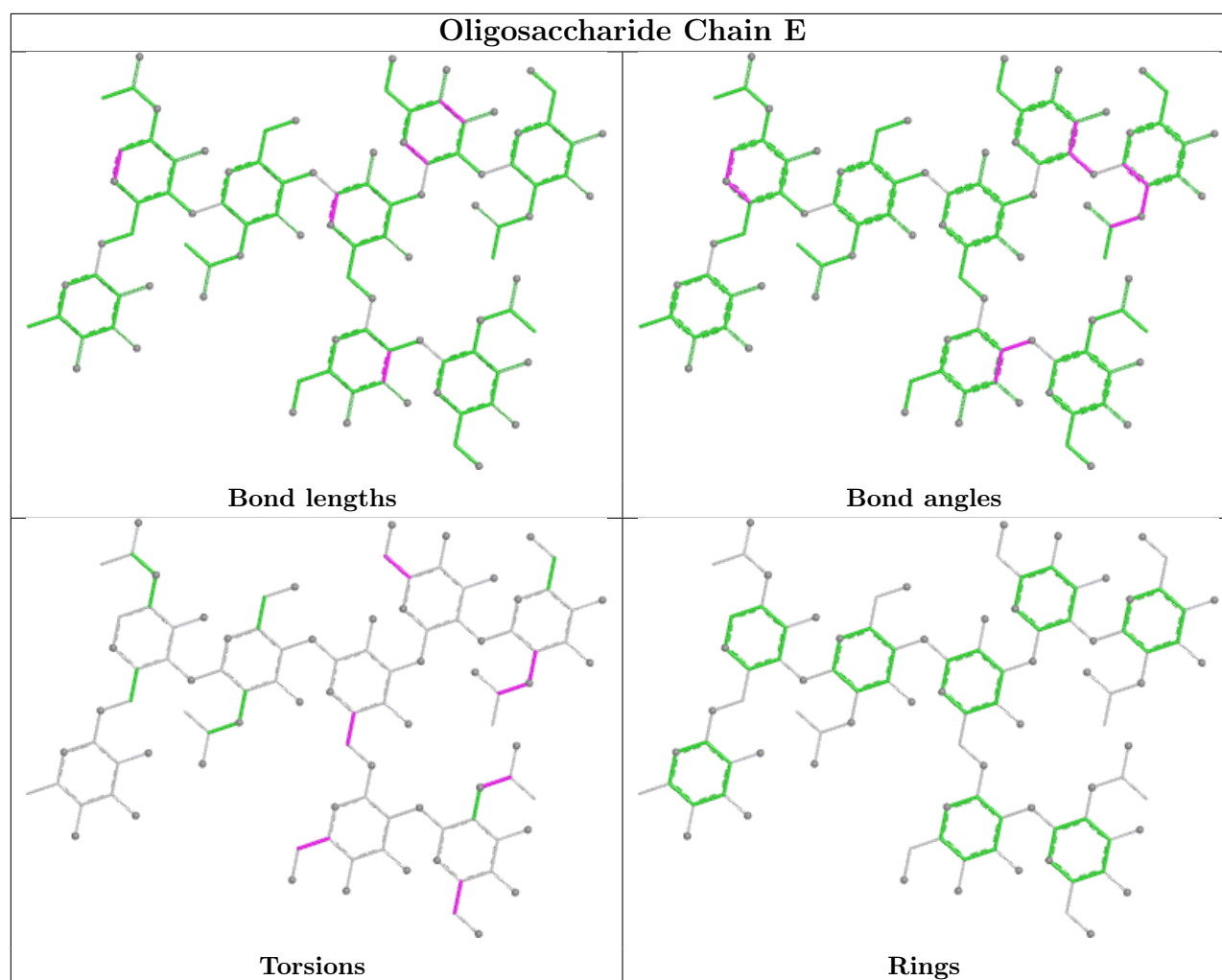
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	NAG	1	0
3	D	5	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](#)

2 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	$\# Z > 2$
4	NAG	C	1001	2	14,14,15	1.74	2 (14%)	17,19,21	1.50	4 (23%)
4	NAG	C	1002	2	14,14,15	0.52	0	17,19,21	0.42	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
4	NAG	C	1001	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1002	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1001	NAG	O5-C1	-4.37	1.36	1.43
4	C	1001	NAG	C1-C2	4.17	1.58	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1001	NAG	C4-C3-C2	3.88	116.70	111.02
4	C	1001	NAG	O5-C5-C4	-2.79	104.04	110.83
4	C	1001	NAG	C2-N2-C7	2.41	126.12	122.90
4	C	1001	NAG	C1-C2-N2	-2.07	107.17	110.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1001	NAG	O5-C5-C6-O6
4	C	1001	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1001	NAG	1	0
4	C	1002	NAG	1	0

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	212/223 (95%)	0.90	28 (13%) 7 5	58, 84, 114, 148	0
1	B	213/223 (95%)	0.81	22 (10%) 12 9	52, 77, 111, 127	0
2	C	171/177 (96%)	0.73	12 (7%) 22 19	56, 78, 114, 137	0
All	All	596/623 (95%)	0.82	62 (10%) 11 9	52, 80, 114, 148	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	GLU	5.0
2	C	47	SER	4.4
2	C	46	GLU	4.0
2	C	42	TRP	3.9
1	B	382	GLU	3.7
1	B	232	PRO	3.6
1	A	234	LEU	3.6
1	B	434	ASN	3.5
1	A	235	LEU	3.3
2	C	29	CYS	3.2
1	A	233	GLU	3.1
1	A	397	VAL	3.1
1	B	302	VAL	3.1
1	A	407	TYR	3.1
1	A	405	PHE	3.1
1	B	290	LYS	3.0
1	B	234	LEU	3.0
1	A	423	PHE	3.0
1	B	399	ASP	3.0
1	B	296	TYR	2.9
1	A	321	CYS	2.8
1	A	410	LEU	2.8
1	A	247	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	25	VAL	2.7
1	A	391	TYR	2.6
1	B	272	GLU	2.6
1	A	381	TRP	2.6
1	B	381	TRP	2.6
1	A	241	PHE	2.6
1	A	327	ALA	2.6
1	A	255	ARG	2.5
1	B	303	VAL	2.5
1	B	287	ALA	2.5
1	B	243	PHE	2.5
1	A	323	VAL	2.5
1	A	269	GLU	2.4
1	B	425	CYS	2.4
1	B	389	ASN	2.4
1	B	247	PRO	2.4
1	B	291	PRO	2.4
1	B	407	TYR	2.4
1	A	266	VAL	2.4
1	A	363	VAL	2.4
2	C	10	VAL	2.3
2	C	62	THR	2.3
1	B	387	PRO	2.3
2	C	43	PHE	2.3
1	A	236	GLY	2.2
2	C	72	GLN	2.2
1	A	316	GLY	2.2
1	A	330	ALA	2.2
1	A	332	ILE	2.2
1	A	282	VAL	2.2
1	B	315	ASN	2.2
2	C	55	SER	2.2
1	B	265	ASP	2.1
1	A	420	GLY	2.1
2	C	56	TYR	2.1
1	A	264	VAL	2.0
1	A	244	PRO	2.0
2	C	11	PHE	2.0
1	B	246	LYS	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](#)

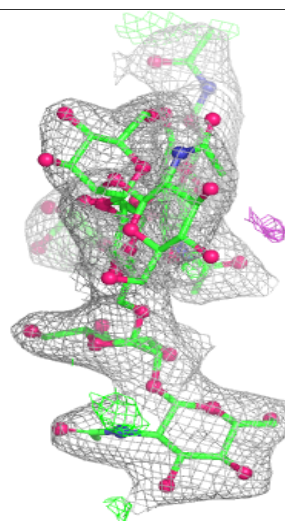
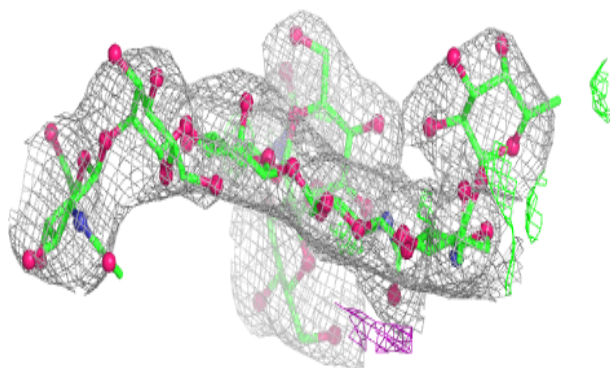
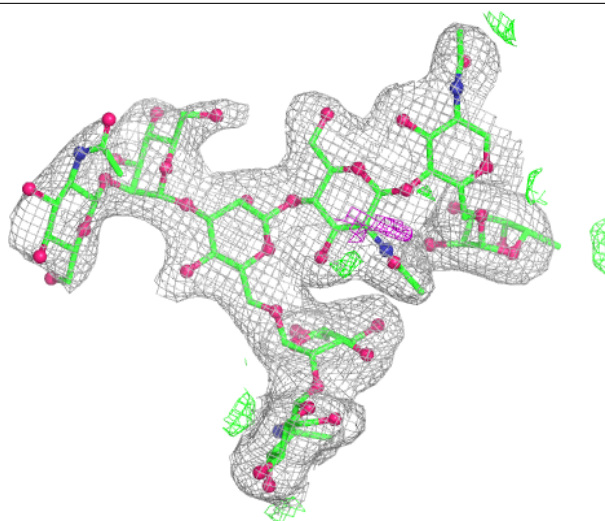
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

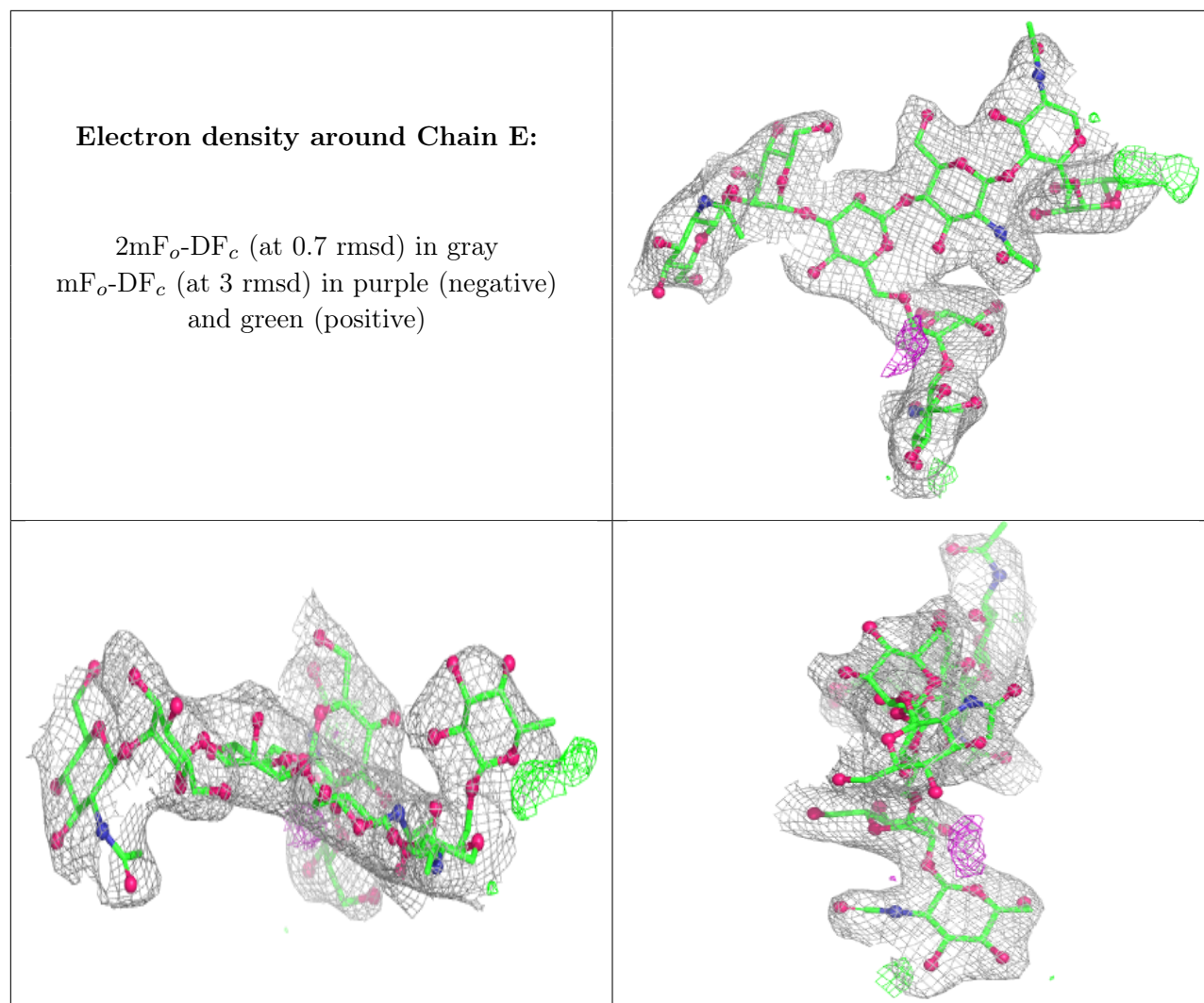
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	E	5	14/15	0.60	0.12	108,116,126,126	0
3	FUC	E	8	10/11	0.65	0.14	96,104,114,122	0
3	NAG	D	5	14/15	0.68	0.12	120,136,145,146	0
3	FUC	D	8	10/11	0.76	0.14	91,93,104,105	0
3	NAG	E	7	14/15	0.78	0.14	71,84,90,91	0
3	NAG	D	7	14/15	0.79	0.13	68,79,86,100	0
3	MAN	E	4	11/12	0.81	0.10	88,100,106,106	0
3	MAN	D	4	11/12	0.81	0.12	90,106,116,121	0
3	MAN	E	6	11/12	0.87	0.09	74,83,89,90	0
3	BMA	E	3	11/12	0.90	0.07	70,77,88,92	0
3	MAN	D	6	11/12	0.90	0.09	69,75,80,81	0
3	NAG	E	1	14/15	0.91	0.09	79,93,104,106	0
3	NAG	D	2	14/15	0.92	0.09	55,60,69,75	0
3	NAG	D	1	14/15	0.93	0.10	59,69,80,83	0
3	BMA	D	3	11/12	0.94	0.06	61,77,85,97	0
3	NAG	E	2	14/15	0.96	0.07	66,75,84,91	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 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($\text{\AA}^2$)	Q<0.9
4	NAG	C	1001	14/15	0.90	0.12	62,74,92,99	0
4	NAG	C	1002	14/15	0.94	0.09	61,74,83,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.