



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:10 PM BST

PDB ID : 6CJX  
Title : Crystal structure of a Fc fragment LALA mutant (L234A, L235A) of human IgG1 (crystal form 2)  
Authors : Van, V.; Tolbert, W.D.; Pazgier, M.  
Deposited on : 2018-02-27  
Resolution : 2.44 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

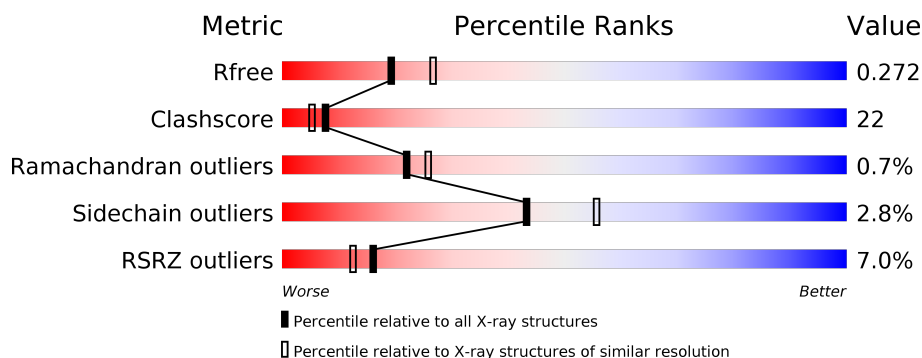
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	214	<div> <div>2%</div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
1	B	214	<div> <div>12%</div> <div>59%</div> <div>36%</div> <div>• •</div> </div>
2	C	8	<div> <div>13%</div> <div>75%</div> <div>13%</div> </div>
2	D	8	<div> <div>13%</div> <div>63%</div> <div>25%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3538 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.

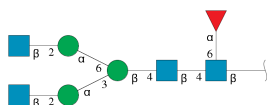
- Molecule 1 is a protein called Fc fragment of human IgG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1665	1059	280	319	7			
1	B	209	Total	C	N	O	S	0	0	0
			1672	1064	281	320	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ALA	LEU	engineered mutation	UNP Q6MZV7
A	235	ALA	LEU	engineered mutation	UNP Q6MZV7
B	234	ALA	LEU	engineered mutation	UNP Q6MZV7
B	235	ALA	LEU	engineered mutation	UNP Q6MZV7

- Molecule 2 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
2	C	8	Total	C	N	O	0	0	0
			99	56	4	39			
2	D	8	Total	C	N	O	0	0	0
			99	56	4	39			

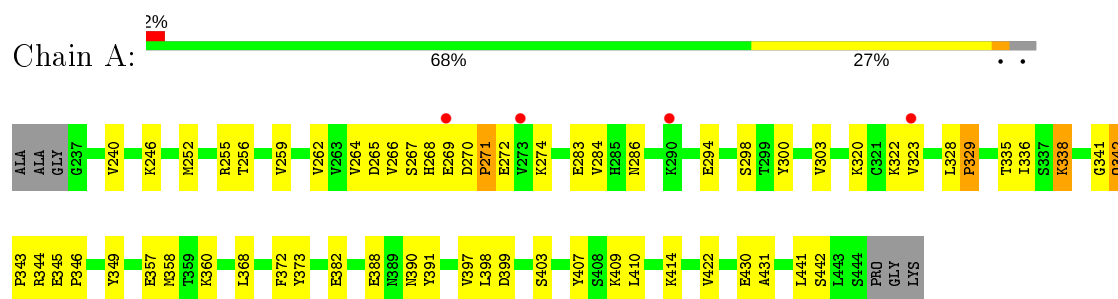
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		

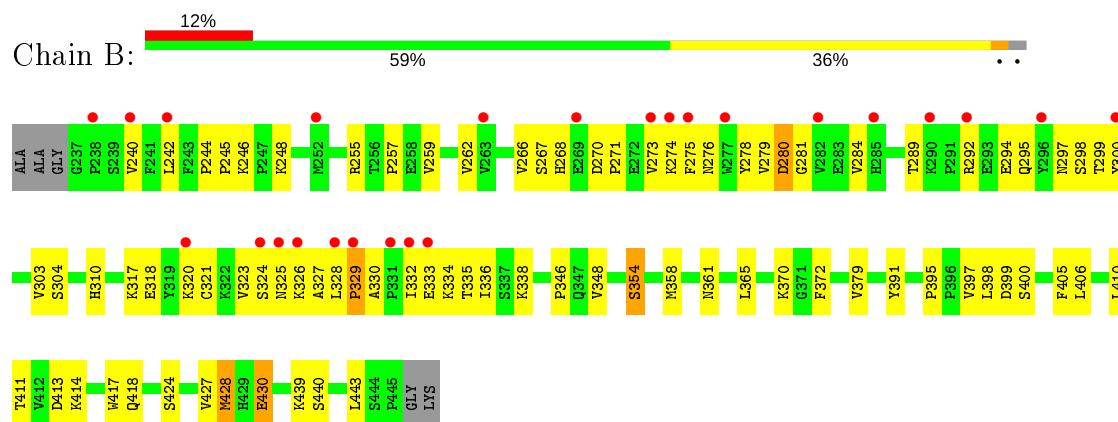
### 3 Residue-property plots

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.

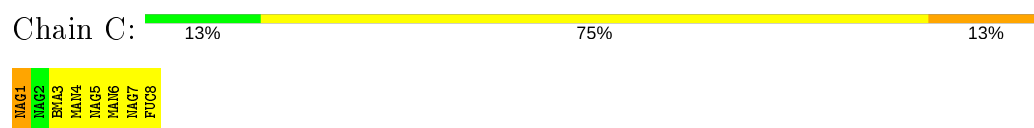
- Molecule 1: Fc fragment of human IgG1



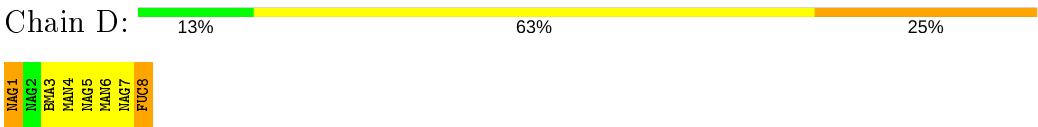
- Molecule 1: Fc fragment of human IgG1



- Molecule 2: 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



- Molecule 2: 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.00 Å 74.83 Å 145.77 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.75 – 2.44 46.45 – 2.44	Depositor EDS
% Data completeness (in resolution range)	91.2 (40.75-2.44) 91.5 (46.45-2.44)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.45 Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???), REFMAC	Depositor
R, $R_{free}$	0.216 , 0.264 0.215 , 0.272	Depositor DCC
$R_{free}$ test set	973 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.9	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 55.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3538	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2022e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, 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	0.64	0/1711	0.81	1/2330 (0.0%)
1	B	0.74	0/1719	0.79	0/2342
All	All	0.69	0/3430	0.80	1/4672 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	LEU	CB-CG-CD2	-6.30	100.29	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1665	0	1630	50	0
1	B	1672	0	1637	105	0
2	C	99	0	85	1	0
2	D	99	0	85	2	0
3	A	3	0	0	0	0
All	All	3538	0	3437	153	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 22.

All (153) 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:328:LEU:CD2	1:B:332:ILE:HD13	1.50	1.41
1:B:328:LEU:HD21	1:B:332:ILE:CD1	1.51	1.39
1:A:294:GLU:HG2	1:A:300:TYR:CE2	1.74	1.21
1:B:275:PHE:CE2	1:B:289:THR:HG23	1.85	1.12
1:B:266:VAL:HG12	1:B:300:TYR:H	1.05	1.11
1:B:275:PHE:HE2	1:B:289:THR:CG2	1.63	1.10
1:B:275:PHE:HE2	1:B:289:THR:HG23	0.93	1.06
1:A:338:LYS:NZ	1:A:430:GLU:OE2	1.91	1.02
1:B:266:VAL:CG1	1:B:300:TYR:H	1.71	1.01
1:B:271:PRO:HG2	1:B:292:ARG:HH22	1.20	1.01
1:B:271:PRO:HB2	1:B:292:ARG:NH2	1.76	1.00
1:B:275:PHE:CE2	1:B:289:THR:CG2	2.44	0.98
1:B:328:LEU:HD21	1:B:332:ILE:HD13	1.11	0.96
1:A:294:GLU:HG2	1:A:300:TYR:HE2	1.22	0.94
1:B:281:GLY:N	1:B:320:LYS:HE3	1.83	0.93
1:B:328:LEU:HD23	1:B:332:ILE:HD13	1.49	0.92
1:B:338:LYS:NZ	1:B:430:GLU:OE1	2.04	0.90
1:B:266:VAL:HG12	1:B:300:TYR:N	1.85	0.90
1:B:271:PRO:CB	1:B:292:ARG:NH2	2.36	0.89
1:A:240:VAL:HG11	1:A:323:VAL:HG11	1.54	0.88
1:B:328:LEU:CD2	1:B:332:ILE:CD1	2.26	0.87
1:B:328:LEU:HD21	1:B:332:ILE:HD11	1.55	0.87
1:A:358:MET:O	1:A:414:LYS:NZ	2.09	0.85
1:A:268:HIS:NE2	1:A:298:SER:O	2.10	0.84
1:B:328:LEU:HD12	1:B:329:PRO:CD	2.08	0.83
1:B:271:PRO:CG	1:B:292:ARG:HH22	1.91	0.82
1:B:295:GLN:HE22	1:B:297:ASN:HB2	1.45	0.82
1:B:271:PRO:HB2	1:B:292:ARG:HH21	1.41	0.81
1:B:278:TYR:HB2	1:B:320:LYS:HD2	1.63	0.80
1:B:271:PRO:HG2	1:B:292:ARG:NH2	1.96	0.80
1:B:281:GLY:H	1:B:320:LYS:HE3	1.44	0.79
1:B:266:VAL:HG11	1:B:300:TYR:CD1	2.18	0.78
1:B:274:LYS:HG2	1:B:275:PHE:N	1.97	0.78
1:A:294:GLU:HG2	1:A:300:TYR:CD2	2.20	0.77
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.68	0.76
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.67	0.75
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.67	0.74
1:B:328:LEU:HD12	1:B:329:PRO:HD2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LYS:HB2	1:A:335:THR:HG22	1.71	0.73
1:B:266:VAL:CG1	1:B:300:TYR:N	2.48	0.71
1:A:294:GLU:CG	1:A:300:TYR:HE2	2.00	0.70
1:B:417:TRP:CE2	1:B:443:LEU:HD13	2.26	0.70
1:B:275:PHE:CE2	1:B:289:THR:HG21	2.24	0.69
1:B:295:GLN:NE2	1:B:299:THR:OG1	2.26	0.69
1:B:358:MET:O	1:B:414:LYS:NZ	2.22	0.69
1:B:271:PRO:O	1:B:292:ARG:NH2	2.25	0.69
1:A:344:ARG:NH2	1:A:403:SER:HB3	2.08	0.68
1:A:266:VAL:HG13	1:A:300:TYR:HB2	1.76	0.68
1:B:271:PRO:CG	1:B:292:ARG:NH2	2.53	0.68
1:B:266:VAL:HG11	1:B:300:TYR:HD1	1.59	0.67
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.31	0.66
1:B:328:LEU:HD12	1:B:329:PRO:N	2.09	0.66
1:B:244:PRO:O	1:B:246:LYS:NZ	2.29	0.65
1:B:398:LEU:HD23	1:B:399:ASP:N	2.12	0.64
1:B:240:VAL:HG13	1:B:334:LYS:HE2	1.81	0.63
1:B:242:LEU:HD22	1:B:336:ILE:HG12	1.81	0.62
1:B:418:GLN:HA	1:B:443:LEU:CD2	2.29	0.62
1:B:271:PRO:C	1:B:292:ARG:NH2	2.54	0.62
1:B:266:VAL:HG22	1:B:267:SER:O	2.00	0.61
1:B:279:VAL:HG23	1:B:284:VAL:HG21	1.82	0.61
1:B:271:PRO:C	1:B:292:ARG:HH21	2.05	0.60
1:A:328:LEU:HD23	1:A:329:PRO:HD2	1.84	0.60
1:B:295:GLN:NE2	1:B:297:ASN:HB2	2.15	0.59
1:B:328:LEU:HD12	1:B:328:LEU:C	2.23	0.58
1:B:262:VAL:HG22	1:B:303:VAL:CG2	2.32	0.58
1:A:390:ASN:O	1:A:410:LEU:HD12	2.03	0.58
1:B:318:GLU:HG3	1:B:335:THR:CG2	2.34	0.58
1:B:294:GLU:HA	1:B:300:TYR:HA	1.87	0.57
1:A:272:GLU:OE2	1:A:272:GLU:N	2.38	0.57
1:A:266:VAL:CG1	1:A:300:TYR:HB2	2.34	0.57
1:A:344:ARG:HH21	1:A:403:SER:CB	2.18	0.56
1:B:271:PRO:CB	1:B:292:ARG:HH21	2.09	0.56
1:A:267:SER:OG	1:A:269:GLU:OE2	2.19	0.55
1:B:273:VAL:HA	1:B:324:SER:O	2.06	0.55
1:A:252:MET:CE	1:A:255:ARG:HD2	2.37	0.55
1:A:270:ASP:OD2	1:A:270:ASP:N	2.38	0.55
1:B:328:LEU:O	1:B:329:PRO:C	2.44	0.54
1:B:399:ASP:OD1	1:B:400:SER:N	2.39	0.54
1:A:264:VAL:HG11	2:C:1:NAG:O4	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD13	1:A:407:TYR:CE2	2.42	0.54
1:B:257:PRO:CD	1:B:310:HIS:CE1	2.91	0.54
1:A:320:LYS:CB	1:A:335:THR:HG22	2.38	0.54
1:B:266:VAL:HG22	1:B:267:SER:N	2.24	0.53
1:B:257:PRO:HD3	1:B:310:HIS:CE1	2.43	0.53
1:B:328:LEU:O	1:B:329:PRO:O	2.26	0.53
1:B:240:VAL:HG11	1:B:332:ILE:CG2	2.38	0.53
1:B:270:ASP:HB3	1:B:326:LYS:HE3	1.90	0.53
1:A:398:LEU:HD23	1:A:399:ASP:N	2.25	0.52
1:B:318:GLU:HG3	1:B:335:THR:HG21	1.91	0.52
1:B:398:LEU:HD23	1:B:399:ASP:O	2.09	0.52
1:B:297:ASN:HD21	2:D:8:FUC:H5	1.75	0.52
1:B:328:LEU:HG	1:B:330:ALA:O	2.10	0.52
1:A:264:VAL:HG12	1:A:265:ASP:H	1.76	0.51
1:A:349:TYR:HB3	1:B:354:SER:HB2	1.92	0.51
1:B:417:TRP:NE1	1:B:443:LEU:HD13	2.26	0.51
1:A:360:LYS:O	1:A:414:LYS:HE2	2.10	0.51
1:A:382:GLU:HA	1:A:388:GLU:H	1.76	0.50
2:D:1:NAG:H61	2:D:8:FUC:O2	2.11	0.50
1:B:398:LEU:C	1:B:398:LEU:HD23	2.32	0.50
1:B:418:GLN:HA	1:B:443:LEU:HD22	1.94	0.50
1:A:344:ARG:HH21	1:A:403:SER:HB3	1.74	0.49
1:B:348:VAL:HG12	1:B:439:LYS:HG3	1.94	0.49
1:B:406:LEU:HD12	1:B:406:LEU:C	2.34	0.48
1:B:398:LEU:CD2	1:B:399:ASP:O	2.62	0.48
1:B:279:VAL:CG2	1:B:284:VAL:HG21	2.43	0.47
1:A:357:GLU:OE1	1:B:370:LYS:NZ	2.37	0.47
1:B:257:PRO:CD	1:B:310:HIS:HE1	2.28	0.47
1:A:397:VAL:HG11	1:B:395:PRO:HD3	1.97	0.46
1:B:321:CYS:O	1:B:333:GLU:HA	2.14	0.46
1:A:262:VAL:HG23	1:A:303:VAL:HG12	1.97	0.46
1:A:294:GLU:CG	1:A:300:TYR:CE2	2.68	0.46
1:B:443:LEU:HD12	1:B:443:LEU:HA	1.67	0.46
1:B:275:PHE:HD1	1:B:323:VAL:HG23	1.80	0.46
1:B:379:VAL:HG22	1:B:427:VAL:HG22	1.96	0.46
1:B:275:PHE:CD2	1:B:304:SER:HB3	2.50	0.46
1:A:256:THR:O	1:A:256:THR:HG23	2.15	0.46
1:B:245:PRO:HD3	1:B:259:VAL:HG22	1.97	0.46
1:B:268:HIS:NE2	1:B:298:SER:O	2.49	0.46
1:A:264:VAL:HG12	1:A:265:ASP:N	2.31	0.45
1:A:342:GLN:HA	1:A:343:PRO:HD3	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLY:HA3	1:A:373:TYR:HE2	1.80	0.45
1:A:391:TYR:HA	1:A:409:LYS:O	2.17	0.45
1:B:273:VAL:HG22	1:B:325:ASN:HB2	1.98	0.45
1:B:294:GLU:HB2	1:B:300:TYR:CD2	2.53	0.44
1:B:294:GLU:HB2	1:B:300:TYR:CE2	2.53	0.44
1:A:341:GLY:HA3	1:A:373:TYR:CE2	2.52	0.44
1:B:424:SER:OG	1:B:440:SER:OG	2.35	0.44
1:A:267:SER:O	1:A:271:PRO:HB3	2.17	0.43
1:B:273:VAL:CG1	1:B:323:VAL:HG22	2.48	0.43
1:A:259:VAL:HG13	1:A:336:ILE:HD11	1.99	0.43
1:A:283:GLU:HG2	1:A:284:VAL:N	2.33	0.43
1:B:266:VAL:HG11	1:B:300:TYR:N	2.32	0.43
1:A:269:GLU:OE2	1:A:269:GLU:N	2.51	0.43
1:A:267:SER:OG	1:A:268:HIS:N	2.52	0.43
1:B:240:VAL:HG11	1:B:332:ILE:HG21	2.01	0.42
1:B:361:ASN:OD1	1:B:361:ASN:N	2.53	0.42
1:A:422:VAL:HA	1:A:442:SER:HB3	2.01	0.42
1:B:266:VAL:HG11	1:B:300:TYR:CB	2.49	0.42
1:B:295:GLN:HE22	1:B:297:ASN:CB	2.24	0.42
1:B:270:ASP:OD1	1:B:327:ALA:HB2	2.19	0.42
1:B:280:ASP:OD1	1:B:317:LYS:HG2	2.19	0.42
1:B:276:ASN:HB3	1:B:278:TYR:CE2	2.55	0.42
1:B:248:LYS:HG3	1:B:428:MET:CE	2.50	0.41
1:B:248:LYS:HG3	1:B:428:MET:HE3	2.02	0.41
1:A:267:SER:OG	1:A:269:GLU:N	2.48	0.41
1:B:275:PHE:CD1	1:B:323:VAL:HG23	2.56	0.41
1:A:284:VAL:HG22	1:A:286:ASN:OD1	2.20	0.41
1:B:397:VAL:CG2	1:B:405:PHE:CE2	3.04	0.41
1:A:345:GLU:HG3	1:A:431:ALA:O	2.21	0.41
1:A:283:GLU:HG2	1:A:284:VAL:H	1.86	0.41
1:B:391:TYR:HB3	1:B:410:LEU:HD12	2.03	0.41
1:B:266:VAL:HG12	1:B:299:THR:HA	2.03	0.40
1:B:248:LYS:HD2	1:B:255:ARG:NH1	2.37	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	206/214 (96%)	191 (93%)	13 (6%)	2 (1%)	15	16
1	B	207/214 (97%)	195 (94%)	11 (5%)	1 (0%)	29	34
All	All	413/428 (96%)	386 (94%)	24 (6%)	3 (1%)	22	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	329	PRO
1	A	329	PRO
1	A	271	PRO

### 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	194/196 (99%)	189 (97%)	5 (3%)	46	58
1	B	195/196 (100%)	189 (97%)	6 (3%)	40	52
All	All	389/392 (99%)	378 (97%)	11 (3%)	43	56

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	LYS
1	A	274	LYS
1	A	322	LYS

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Mol	Chain	Res	Type
1	A	338	LYS
1	A	342	GLN
1	B	280	ASP
1	B	354	SER
1	B	411	THR
1	B	413	ASP
1	B	428	MET
1	B	430	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	295	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

16 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	C	1	1,2	14,14,15	1.05	1 (7%)	17,19,21	1.17	1 (5%)
2	NAG	C	2	2	14,14,15	0.34	0	17,19,21	0.56	0
2	BMA	C	3	2	11,11,12	1.22	1 (9%)	15,15,17	2.27	7 (46%)
2	MAN	C	4	2	11,11,12	1.33	2 (18%)	15,15,17	1.87	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	5	2	14,14,15	0.49	0	17,19,21	1.85	3 (17%)
2	MAN	C	6	2	11,11,12	1.23	1 (9%)	15,15,17	1.22	1 (6%)
2	NAG	C	7	2	14,14,15	1.35	2 (14%)	17,19,21	1.05	1 (5%)
2	FUC	C	8	2	10,10,11	1.29	1 (10%)	14,14,16	1.47	2 (14%)
2	NAG	D	1	1,2	14,14,15	0.80	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	D	2	2	14,14,15	0.44	0	17,19,21	0.33	0
2	BMA	D	3	2	11,11,12	1.33	1 (9%)	15,15,17	2.03	5 (33%)
2	MAN	D	4	2	11,11,12	1.34	3 (27%)	15,15,17	1.78	4 (26%)
2	NAG	D	5	2	14,14,15	0.31	0	17,19,21	1.61	2 (11%)
2	MAN	D	6	2	11,11,12	1.49	2 (18%)	15,15,17	1.25	3 (20%)
2	NAG	D	7	2	14,14,15	0.82	1 (7%)	17,19,21	1.11	1 (5%)
2	FUC	D	8	2	10,10,11	2.47	3 (30%)	14,14,16	1.82	4 (28%)

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	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	NAG	C	5	2	-	2/6/23/26	0/1/1/1
2	MAN	C	6	2	-	2/2/19/22	0/1/1/1
2	NAG	C	7	2	-	2/6/23/26	0/1/1/1
2	FUC	C	8	2	-	-	0/1/1/1
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
2	NAG	D	5	2	-	1/6/23/26	0/1/1/1
2	MAN	D	6	2	-	2/2/19/22	0/1/1/1
2	NAG	D	7	2	-	2/6/23/26	0/1/1/1
2	FUC	D	8	2	-	-	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8	FUC	O5-C1	5.74	1.52	1.43
2	D	8	FUC	C1-C2	4.30	1.62	1.52
2	C	7	NAG	O5-C1	-4.27	1.36	1.43
2	C	1	NAG	O5-C1	-3.39	1.38	1.43
2	D	6	MAN	O5-C1	-3.20	1.38	1.43
2	C	6	MAN	O5-C1	-3.09	1.38	1.43
2	C	8	FUC	C1-C2	3.08	1.59	1.52
2	C	4	MAN	C4-C5	2.84	1.59	1.53
2	D	1	NAG	C1-C2	2.76	1.56	1.52
2	D	6	MAN	C4-C5	2.65	1.58	1.53
2	D	8	FUC	O5-C5	2.57	1.49	1.43
2	D	4	MAN	C2-C3	-2.55	1.48	1.52
2	D	3	BMA	C4-C5	2.49	1.58	1.53
2	C	4	MAN	C2-C3	-2.20	1.49	1.52
2	C	3	BMA	O4-C4	-2.16	1.37	1.43
2	D	4	MAN	O5-C1	-2.14	1.40	1.43
2	C	7	NAG	C1-C2	2.14	1.55	1.52
2	D	7	NAG	C1-C2	2.09	1.55	1.52
2	D	4	MAN	O5-C5	2.05	1.47	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	NAG	C1-O5-C5	5.60	119.78	112.19
2	D	5	NAG	C1-O5-C5	4.83	118.73	112.19
2	C	3	BMA	C3-C4-C5	4.74	118.70	110.24
2	D	8	FUC	C1-O5-C5	4.56	123.11	112.78
2	C	4	MAN	C1-O5-C5	4.34	118.07	112.19
2	D	3	BMA	C3-C4-C5	4.30	117.91	110.24
2	D	4	MAN	C1-O5-C5	4.14	117.80	112.19
2	C	6	MAN	O2-C2-C3	-3.81	102.51	110.14
2	D	1	NAG	C1-O5-C5	3.79	117.33	112.19
2	C	5	NAG	C3-C4-C5	3.77	116.96	110.24
2	D	3	BMA	O5-C1-C2	-3.57	105.26	110.77
2	C	8	FUC	C1-C2-C3	3.47	113.93	109.67
2	C	4	MAN	C3-C4-C5	3.42	116.34	110.24
2	C	1	NAG	C1-O5-C5	-3.34	107.67	112.19
2	D	5	NAG	C3-C4-C5	3.28	116.09	110.24
2	D	7	NAG	C4-C3-C2	3.17	115.67	111.02
2	C	7	NAG	C4-C3-C2	3.13	115.60	111.02
2	C	3	BMA	O5-C1-C2	-3.12	105.95	110.77
2	D	4	MAN	O2-C2-C3	-2.98	104.18	110.14
2	C	4	MAN	O2-C2-C3	-2.88	104.37	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	FUC	O5-C1-C2	2.86	115.19	110.77
2	D	8	FUC	C1-C2-C3	2.76	113.06	109.67
2	C	3	BMA	C1-C2-C3	-2.75	106.29	109.67
2	D	8	FUC	O2-C2-C1	2.72	114.71	109.15
2	C	3	BMA	O2-C2-C3	-2.69	104.75	110.14
2	C	3	BMA	O4-C4-C5	-2.67	102.66	109.30
2	D	3	BMA	O3-C3-C2	2.49	114.75	109.99
2	C	5	NAG	O5-C5-C4	2.48	116.86	110.83
2	D	4	MAN	C3-C4-C5	2.42	114.56	110.24
2	D	4	MAN	O5-C1-C2	-2.36	107.12	110.77
2	D	8	FUC	O5-C5-C4	2.34	113.72	109.52
2	D	3	BMA	O2-C2-C3	-2.32	105.48	110.14
2	D	6	MAN	O2-C2-C1	2.32	113.90	109.15
2	D	6	MAN	O2-C2-C3	-2.29	105.54	110.14
2	D	6	MAN	C1-O5-C5	2.21	115.18	112.19
2	C	3	BMA	O6-C6-C5	-2.19	103.77	111.29
2	D	3	BMA	C2-C3-C4	2.09	114.52	110.89
2	C	4	MAN	O5-C5-C4	2.07	115.87	110.83
2	C	3	BMA	C2-C3-C4	2.04	114.42	110.89

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	7	NAG	O5-C5-C6-O6
2	D	6	MAN	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	6	MAN	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	7	NAG	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
2	C	6	MAN	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	7	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	7	NAG	C4-C5-C6-O6

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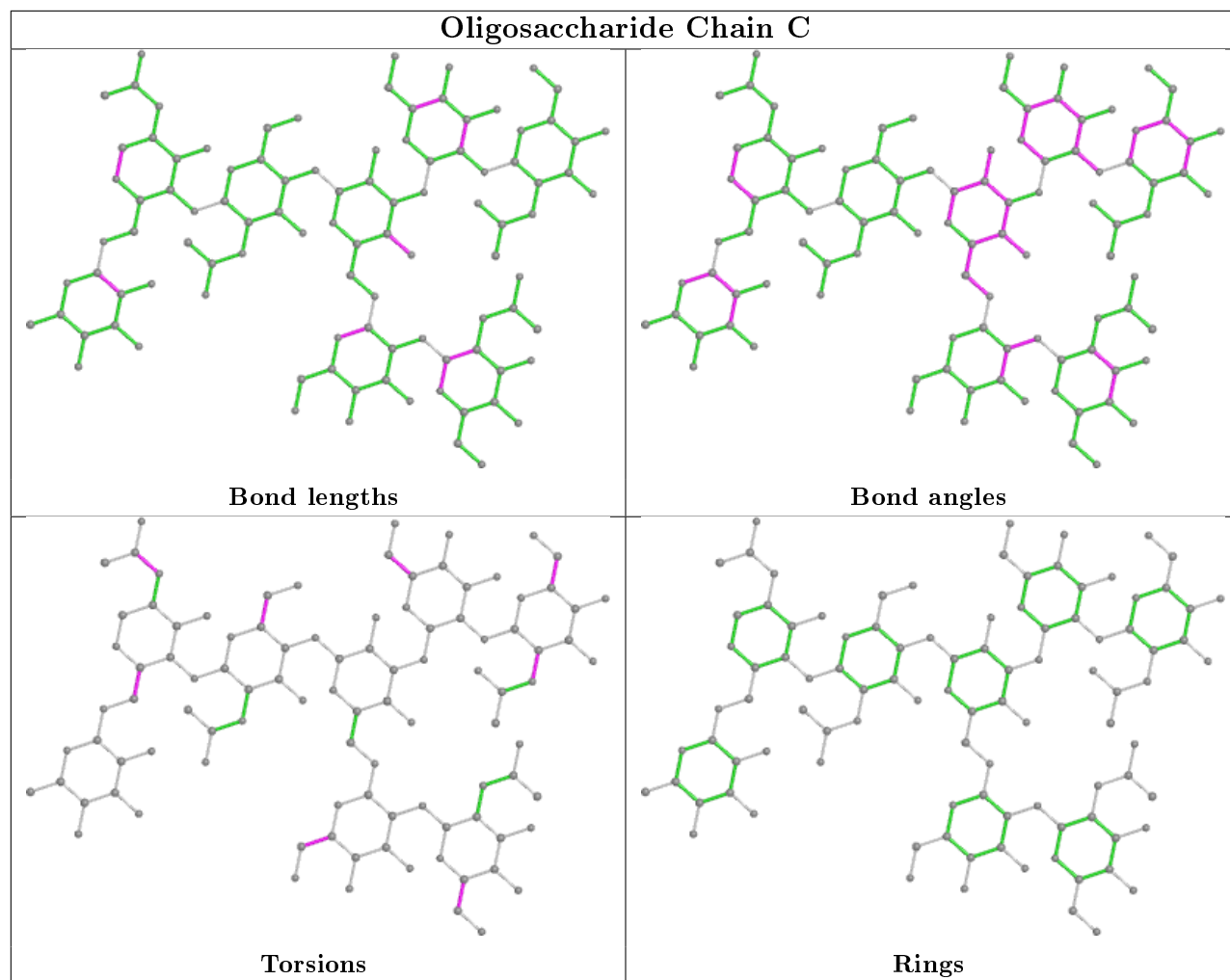
Mol	Chain	Res	Type	Atoms
2	C	4	MAN	O5-C5-C6-O6
2	D	6	MAN	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6
2	C	5	NAG	C3-C2-N2-C7
2	D	5	NAG	C3-C2-N2-C7
2	C	5	NAG	O5-C5-C6-O6
2	D	2	NAG	C1-C2-N2-C7

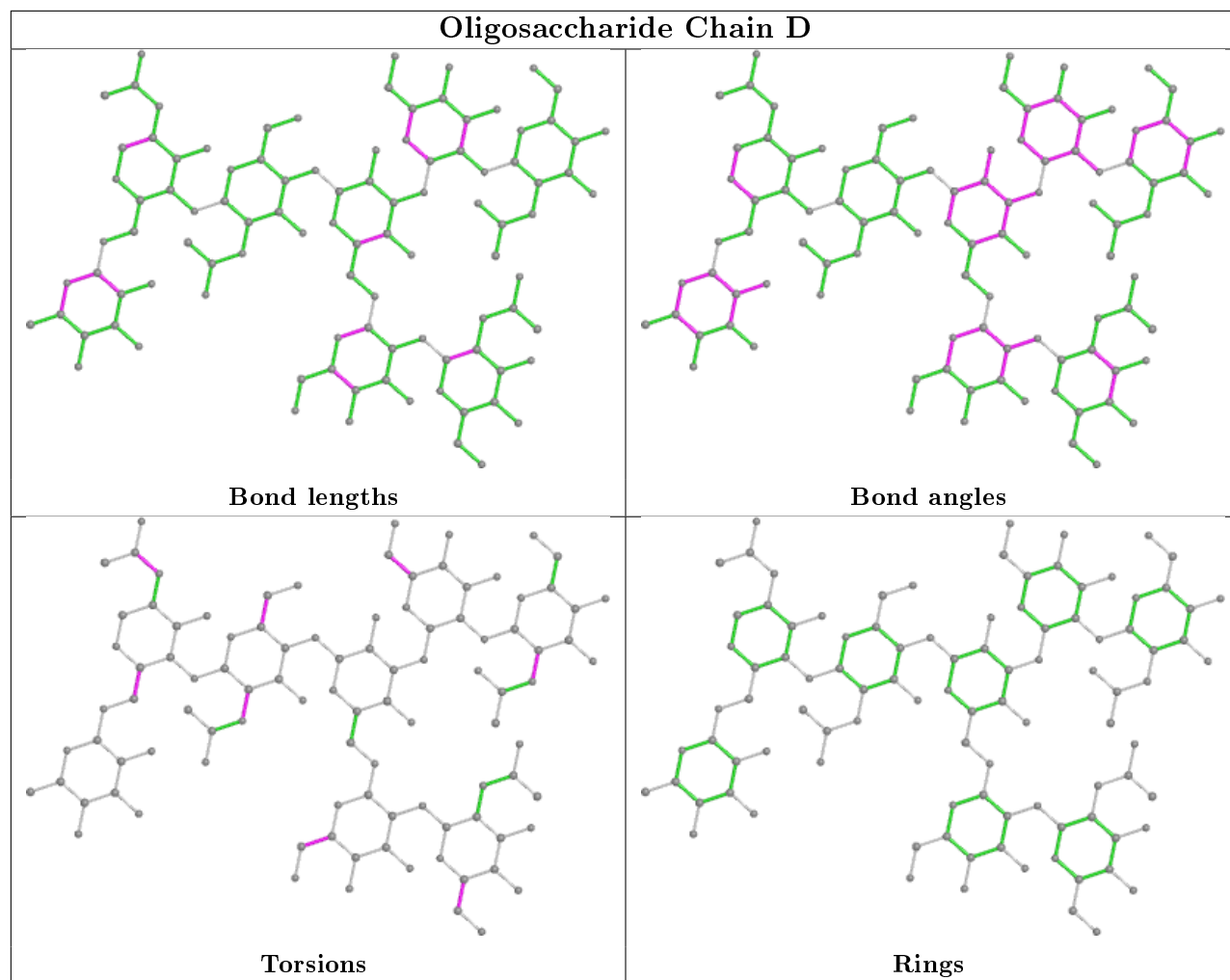
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	8	FUC	2	0
2	C	1	NAG	1	0
2	D	1	NAG	1	0

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





## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	208/214 (97%)	-0.03	4 (1%) 66 63	45, 76, 120, 185	0
1	B	209/214 (97%)	0.43	25 (11%) 4 2	41, 86, 172, 221	0
All	All	417/428 (97%)	0.20	29 (6%) 16 12	41, 79, 166, 221	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	GLU	6.0
1	B	333	GLU	5.6
1	B	324	SER	5.6
1	B	326	LYS	5.2
1	B	329	PRO	4.7
1	B	238	PRO	4.5
1	B	275	PHE	3.4
1	B	331	PRO	3.3
1	B	274	LYS	3.2
1	B	240	VAL	3.1
1	A	273	VAL	3.0
1	B	292	ARG	3.0
1	B	325	ASN	2.9
1	B	277	TRP	2.9
1	B	242	LEU	2.8
1	A	269	GLU	2.8
1	B	273	VAL	2.5
1	B	290	LYS	2.4
1	B	332	ILE	2.4
1	B	263	VAL	2.3
1	B	282	VAL	2.3
1	B	320	LYS	2.2
1	B	300	TYR	2.2
1	B	285	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	328	LEU	2.2
1	B	252	MET	2.2
1	A	323	VAL	2.1
1	A	290	LYS	2.1
1	B	296	TYR	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](#)

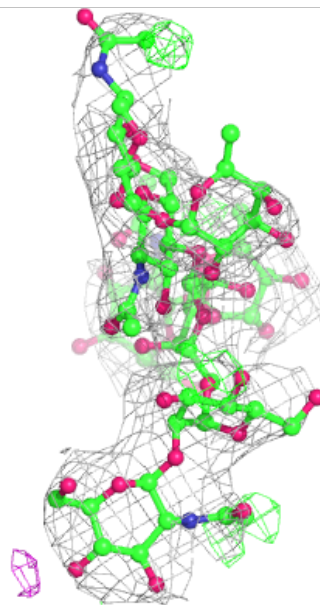
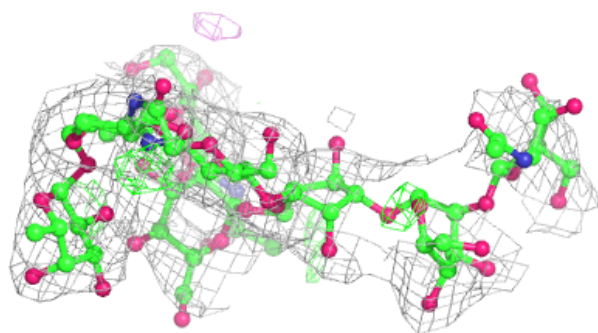
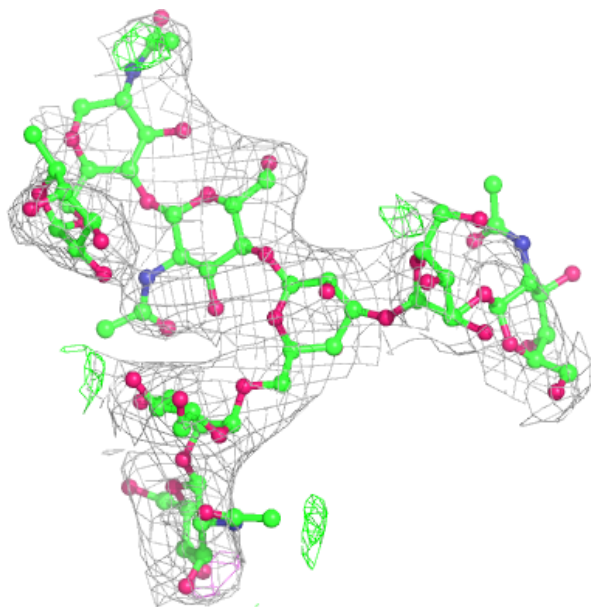
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

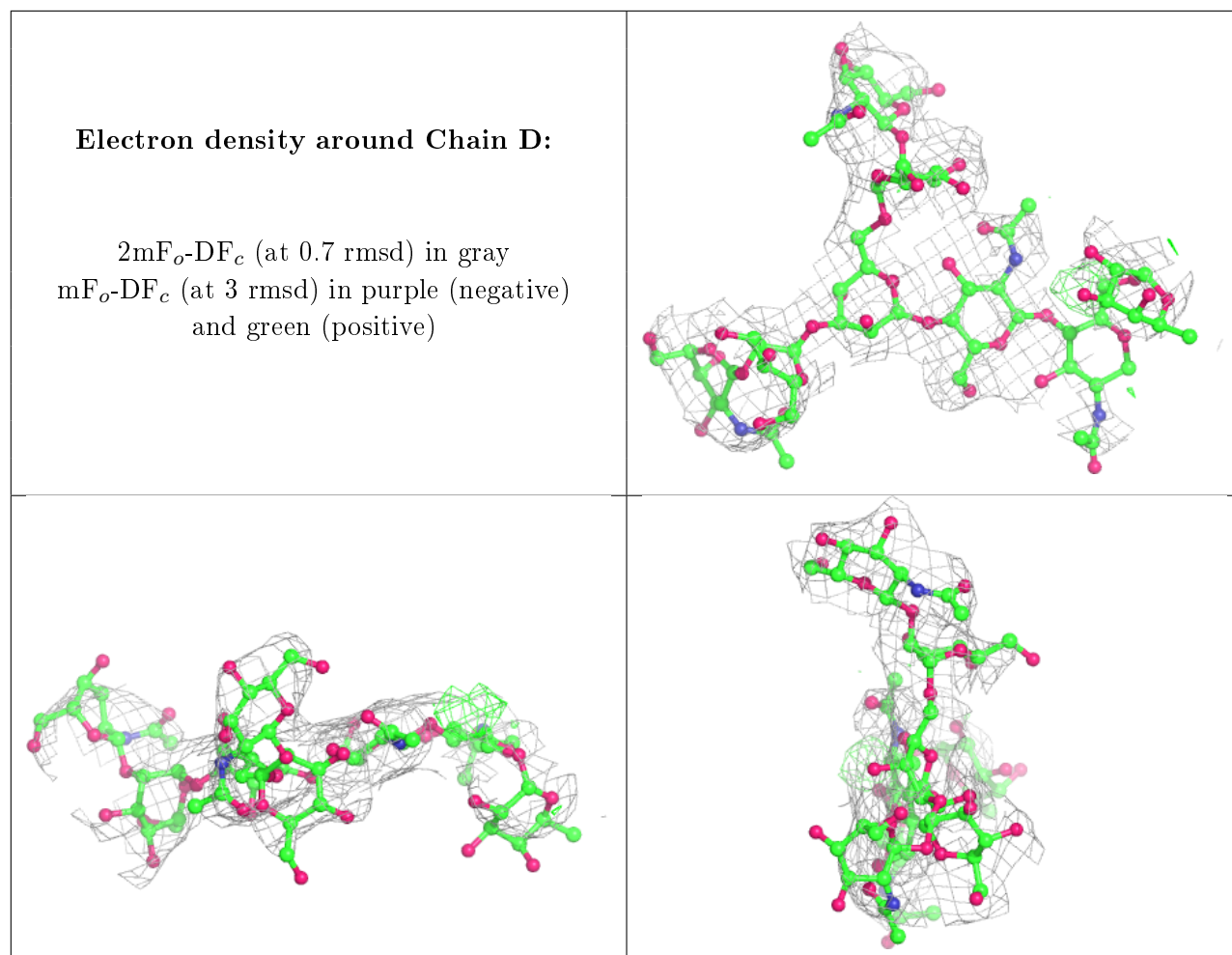
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	C	5	14/15	0.65	0.26	176,195,207,212	0
2	FUC	D	8	10/11	0.73	0.30	187,207,220,232	0
2	MAN	D	4	11/12	0.82	0.09	160,170,177,188	0
2	NAG	C	1	14/15	0.82	0.15	110,119,133,135	0
2	NAG	D	1	14/15	0.83	0.14	133,156,173,186	0
2	MAN	D	6	11/12	0.83	0.15	140,148,165,167	0
2	FUC	C	8	10/11	0.83	0.30	131,140,149,150	0
2	BMA	D	3	11/12	0.85	0.15	135,160,171,180	0
2	NAG	D	5	14/15	0.85	0.24	170,196,201,202	0
2	BMA	C	3	11/12	0.86	0.14	120,128,145,148	0
2	MAN	C	4	11/12	0.87	0.12	153,159,169,184	0
2	NAG	C	7	14/15	0.87	0.20	109,125,158,160	0
2	NAG	D	7	14/15	0.90	0.13	138,155,159,160	0
2	NAG	D	2	14/15	0.92	0.14	140,151,161,169	0
2	MAN	C	6	11/12	0.93	0.15	118,128,135,142	0
2	NAG	C	2	14/15	0.95	0.14	103,115,141,141	0

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

**Electron density around Chain C:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.