



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:41 AM UTC

PDB ID : 4X99 / pdb_00004x99
Title : Immunoglobulin Fc heterodimers variant
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Deposited on : 2014-12-11
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

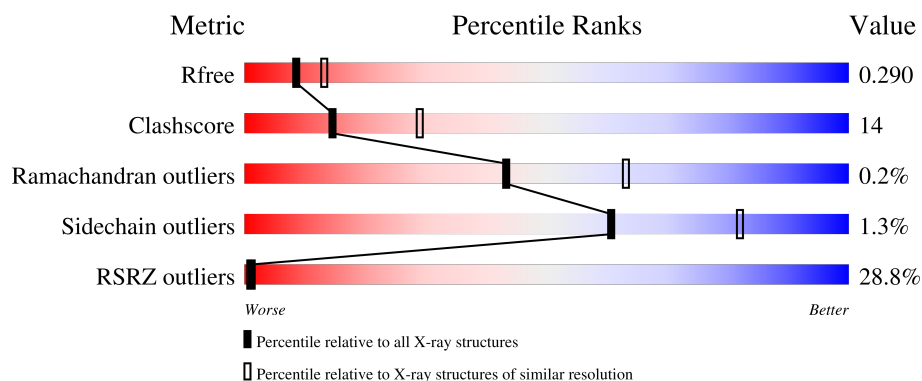
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	 13% 71% 21% 7%
2	B	223	 40% 65% 26% 8%
3	C	8	 62% 38%
3	D	8	 38% 62%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3502 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1663	1057	279	320	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	CYS	TYR	engineered mutation	UNP P01857
A	360	GLU	LYS	engineered mutation	UNP P01857
A	409	TRP	LYS	engineered mutation	UNP P01857

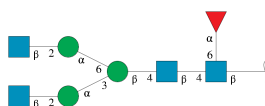
- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	205	Total	C	N	O	S	0	0	0
			1600	1018	273	302	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	347	ARG	GLN	engineered mutation	UNP P01857
B	354	CYS	SER	engineered mutation	UNP P01857
B	399	VAL	ASP	engineered mutation	UNP P01857
B	405	THR	PHE	engineered mutation	UNP P01857

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

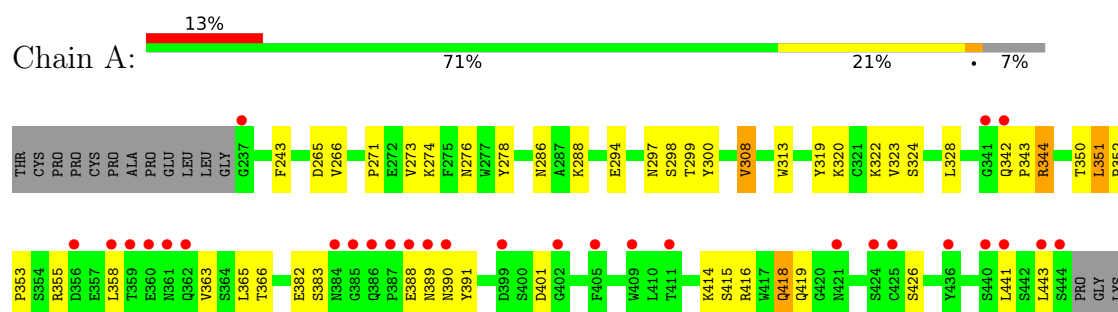
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	11	Total	O	0	0
			11	11		

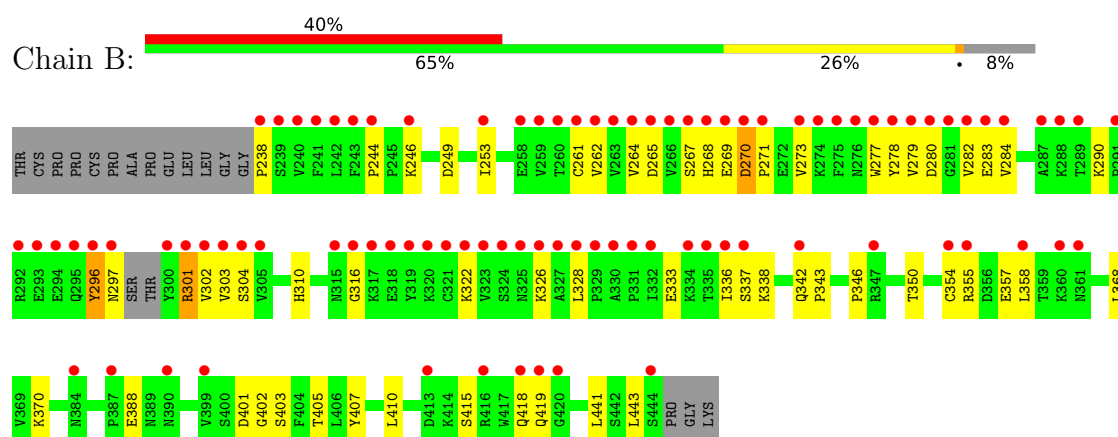
3 Residue-property plots [i](#)

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: Ig gamma-1 chain C region



- Molecule 2: Ig gamma-1 chain C region



- 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



- 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-mannopyra

nose-(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:  38% 62%

MAG1	MAG2	EMA3	MAM4	MAG5	MAM6	MAG7	FUC8
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4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.77Å 152.77Å 109.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.63 – 2.50 44.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.63-2.50) 93.4 (44.63-2.50)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.62 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.248 , 0.283 0.267 , 0.290	Depositor DCC
R_{free} test set	2000 reflections (7.48%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3502	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, 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	0.74	0/1710	1.03	7/2333 (0.3%)
2	B	0.79	2/1642 (0.1%)	1.17	14/2241 (0.6%)
All	All	0.77	2/3352 (0.1%)	1.10	21/4574 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	270	ASP	C-N	6.22	1.41	1.33
2	B	301	ARG	C-N	6.20	1.42	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	268	HIS	CB-CA-C	-17.46	88.87	111.40
2	B	268	HIS	N-CA-C	-7.86	100.78	111.55
2	B	246	LYS	CA-C-N	7.38	126.92	119.24
2	B	246	LYS	C-N-CA	7.38	126.92	119.24
1	A	243	PHE	CA-C-N	7.20	127.80	120.38
1	A	243	PHE	C-N-CA	7.20	127.80	120.38
2	B	270	ASP	CA-C-N	-6.07	113.53	119.90
2	B	270	ASP	C-N-CA	-6.07	113.53	119.90
2	B	296	TYR	CB-CA-C	-5.80	109.91	116.63
2	B	244	PRO	CA-C-N	5.62	125.59	120.03
2	B	244	PRO	C-N-CA	5.62	125.59	120.03
2	B	290	LYS	CA-C-N	-5.53	112.93	119.84
2	B	290	LYS	C-N-CA	-5.53	112.93	119.84
2	B	402	GLY	N-CA-C	-5.21	108.89	115.08
2	B	273	VAL	N-CA-C	5.15	116.00	108.53
2	B	303	VAL	N-CA-C	5.13	116.05	107.18
1	A	391	TYR	N-CA-C	-5.11	101.99	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	LEU	CA-C-N	5.06	124.24	118.97
1	A	328	LEU	C-N-CA	5.06	124.24	118.97
1	A	351	LEU	CA-C-N	5.04	125.57	120.38
1	A	351	LEU	C-N-CA	5.04	125.57	120.38

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	1663	0	1614	30	0
2	B	1600	0	1555	50	0
3	C	99	0	83	7	0
3	D	99	0	85	10	0
4	A	30	0	0	1	0
4	B	11	0	0	1	0
All	All	3502	0	3337	95	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 14.

All (95) 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:B:278:TYR:CE1	2:B:283:GLU:HB2	1.30	1.56
2:B:278:TYR:CE1	2:B:283:GLU:CB	2.23	1.20
2:B:267:SER:HB2	2:B:271:PRO:HG2	1.33	1.05
1:A:265:ASP:OD1	3:C:1:NAG:O7	1.83	0.96
2:B:278:TYR:HE1	2:B:283:GLU:HB2	1.28	0.94
3:C:4:MAN:H4	3:C:5:NAG:H83	1.50	0.94
2:B:278:TYR:CD1	2:B:283:GLU:CA	2.55	0.90
2:B:278:TYR:CZ	2:B:283:GLU:HB2	2.06	0.88
2:B:267:SER:O	2:B:271:PRO:HD2	1.75	0.87
2:B:278:TYR:CD1	2:B:283:GLU:HB2	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1:NAG:H62	3:D:8:FUC:H5	1.59	0.83
1:A:350:THR:HB	1:A:441:LEU:HD13	1.61	0.81
2:B:269:GLU:C	2:B:271:PRO:HD3	2.06	0.81
2:B:278:TYR:HD1	2:B:282:VAL:C	1.90	0.79
1:A:294:GLU:OE2	1:A:298:SER:HA	1.84	0.77
2:B:278:TYR:CD1	2:B:283:GLU:N	2.55	0.75
2:B:253:ILE:H	2:B:253:ILE:HD12	1.52	0.74
3:C:4:MAN:O2	3:C:5:NAG:H83	1.87	0.73
2:B:278:TYR:CD1	2:B:283:GLU:HA	2.21	0.73
2:B:278:TYR:HD1	2:B:283:GLU:N	1.87	0.72
3:D:1:NAG:H62	3:D:8:FUC:C5	2.21	0.70
1:A:418:GLN:HA	1:A:443:LEU:HD22	1.75	0.69
2:B:278:TYR:CD1	2:B:283:GLU:CB	2.69	0.69
3:D:1:NAG:C6	3:D:8:FUC:H5	2.23	0.68
3:C:4:MAN:H4	3:C:5:NAG:C8	2.22	0.68
3:D:4:MAN:H4	3:D:5:NAG:H4	1.78	0.66
1:A:415:SER:O	1:A:419:GLN:HG3	1.96	0.66
3:D:4:MAN:O3	3:D:5:NAG:H61	1.96	0.65
1:A:274:LYS:HB3	1:A:324:SER:HB2	1.79	0.65
1:A:353:PRO:HB3	1:A:363:VAL:HG13	1.79	0.64
1:A:355:ARG:HA	1:A:358:LEU:HD12	1.79	0.64
2:B:265:ASP:OD1	3:D:1:NAG:H83	1.98	0.63
2:B:279:VAL:O	2:B:280:ASP:HB2	2.01	0.61
1:A:308:VAL:HG11	1:A:313:TRP:HB2	1.83	0.60
2:B:354:CYS:SG	2:B:357:GLU:HB2	2.42	0.60
3:C:4:MAN:C4	3:C:5:NAG:H83	2.30	0.59
2:B:279:VAL:O	2:B:279:VAL:HG23	2.02	0.58
2:B:262:VAL:CG1	2:B:301:ARG:HH21	2.17	0.57
1:A:308:VAL:HG22	1:A:319:TYR:CE1	2.40	0.57
2:B:267:SER:HB2	2:B:271:PRO:CG	2.21	0.57
2:B:261:CYS:HB2	2:B:277:TRP:CH2	2.41	0.55
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.88	0.54
1:A:350:THR:CB	1:A:441:LEU:HD13	2.35	0.54
2:B:418:GLN:HA	2:B:443:LEU:HD22	1.90	0.54
1:A:388:GLU:OE2	1:A:416:ARG:NH1	2.40	0.54
2:B:322:LYS:HG3	2:B:333:GLU:HG2	1.90	0.54
3:C:4:MAN:O2	3:C:5:NAG:O6	2.27	0.53
3:D:7:NAG:O7	3:D:7:NAG:O3	2.26	0.53
3:D:5:NAG:O7	3:D:5:NAG:H5	2.08	0.53
2:B:316:GLY:O	2:B:337:SER:HB2	2.10	0.51
3:D:1:NAG:C6	3:D:8:FUC:C5	2.85	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:PRO:HB2	2:B:328:LEU:HD11	1.93	0.50
2:B:278:TYR:CE1	2:B:283:GLU:CA	2.84	0.50
1:A:297:ASN:OD1	1:A:299:THR:OG1	2.27	0.50
1:A:344:ARG:HH12	1:A:401:ASP:CG	2.21	0.48
2:B:238:PRO:HA	2:B:264:VAL:O	2.14	0.48
2:B:338:LYS:HE3	4:B:606:HOH:O	2.13	0.48
1:A:351:LEU:HB2	1:A:366:THR:HB	1.95	0.48
2:B:262:VAL:HG11	2:B:301:ARG:HH21	1.77	0.48
2:B:355:ARG:HA	2:B:358:LEU:HD12	1.96	0.48
2:B:296:TYR:O	2:B:297:ASN:C	2.56	0.48
2:B:278:TYR:CD1	2:B:282:VAL:C	2.81	0.47
3:D:6:MAN:O3	3:D:7:NAG:N2	2.48	0.47
1:A:308:VAL:CG1	1:A:313:TRP:HB2	2.44	0.47
1:A:271:PRO:HD2	4:A:628:HOH:O	2.15	0.47
2:B:388:GLU:HG2	2:B:410:LEU:HD11	1.95	0.47
2:B:253:ILE:H	2:B:253:ILE:CD1	2.24	0.47
2:B:401:ASP:HB3	2:B:403:SER:H	1.80	0.47
2:B:337:SER:O	2:B:338:LYS:C	2.57	0.47
1:A:358:LEU:O	1:A:414:LYS:NZ	2.23	0.47
2:B:346:PRO:HA	2:B:370:LYS:O	2.17	0.45
2:B:326:LYS:C	2:B:328:LEU:H	2.24	0.45
2:B:350:THR:OG1	2:B:441:LEU:HD22	2.17	0.45
1:A:382:GLU:OE1	1:A:426:SER:OG	2.35	0.44
2:B:262:VAL:HG13	2:B:301:ARG:HH21	1.82	0.44
1:A:286:ASN:O	1:A:288:LYS:NZ	2.37	0.44
2:B:368:LEU:HD13	2:B:407:TYR:CZ	2.53	0.44
1:A:342:GLN:HA	1:A:343:PRO:HD3	1.91	0.44
1:A:276:ASN:HB2	1:A:322:LYS:HB3	2.01	0.43
2:B:283:GLU:HG2	2:B:284:VAL:N	2.34	0.43
1:A:353:PRO:HD3	1:A:365:LEU:HD23	2.01	0.43
1:A:383:SER:HB2	1:A:388:GLU:OE1	2.19	0.43
2:B:269:GLU:C	2:B:271:PRO:CD	2.85	0.42
2:B:415:SER:O	2:B:419:GLN:HG3	2.19	0.42
1:A:308:VAL:HG22	1:A:319:TYR:CZ	2.54	0.42
1:A:278:TYR:CD1	1:A:320:LYS:HD2	2.55	0.42
2:B:277:TRP:NE1	2:B:304:SER:OG	2.53	0.42
2:B:336:ILE:O	2:B:337:SER:HB3	2.20	0.41
2:B:249:ASP:O	2:B:310:HIS:HE1	2.03	0.41
1:A:389:ASN:O	1:A:390:ASN:HB2	2.20	0.41
1:A:273:VAL:HG13	1:A:323:VAL:HG13	2.03	0.41
1:A:351:LEU:HA	1:A:352:PRO:HD2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:GLN:OE1	2:B:343:PRO:HD2	2.20	0.41
2:B:277:TRP:HZ2	2:B:304:SER:HB3	1.86	0.40
3:C:1:NAG:O7	3:C:1:NAG:C3	2.70	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	206/223 (92%)	200 (97%)	6 (3%)	0	100	100
2	B	201/223 (90%)	188 (94%)	12 (6%)	1 (0%)	24	43
All	All	407/446 (91%)	388 (95%)	18 (4%)	1 (0%)	43	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	270	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/206 (94%)	191 (98%)	3 (2%)	57	80
2	B	183/206 (89%)	181 (99%)	2 (1%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	377/412 (92%)	372 (99%)	5 (1%)	61 82

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	VAL
1	A	344	ARG
1	A	418	GLN
2	B	302	VAL
2	B	405	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	HIS
2	B	435	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	C	1	1,3	14,14,15	1.36	2 (14%)	17,19,21	1.84	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	2	3	14,14,15	1.31	2 (14%)	17,19,21	1.35	3 (17%)
3	BMA	C	3	3	11,11,12	1.57	2 (18%)	15,15,17	1.49	2 (13%)
3	MAN	C	4	3	11,11,12	1.38	1 (9%)	15,15,17	2.03	6 (40%)
3	NAG	C	5	3	14,14,15	0.99	1 (7%)	17,19,21	2.00	5 (29%)
3	MAN	C	6	3	11,11,12	1.92	4 (36%)	15,15,17	2.12	3 (20%)
3	NAG	C	7	3	14,14,15	1.39	3 (21%)	17,19,21	1.50	4 (23%)
3	FUC	C	8	3	10,10,11	1.81	5 (50%)	14,14,16	1.10	0
3	NAG	D	1	2,3	14,14,15	0.79	0	17,19,21	0.82	0
3	NAG	D	2	3	14,14,15	0.95	1 (7%)	17,19,21	1.36	2 (11%)
3	BMA	D	3	3	11,11,12	1.24	1 (9%)	15,15,17	2.09	4 (26%)
3	MAN	D	4	3	11,11,12	0.79	0	15,15,17	1.75	3 (20%)
3	NAG	D	5	3	14,14,15	1.45	4 (28%)	17,19,21	1.84	4 (23%)
3	MAN	D	6	3	11,11,12	1.01	1 (9%)	15,15,17	1.63	3 (20%)
3	NAG	D	7	3	14,14,15	1.02	1 (7%)	17,19,21	1.46	3 (17%)
3	FUC	D	8	3	10,10,11	1.15	1 (10%)	14,14,16	1.45	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
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	NAG	C	5	3	-	3/6/23/26	0/1/1/1
3	MAN	C	6	3	-	2/2/19/22	0/1/1/1
3	NAG	C	7	3	-	2/6/23/26	0/1/1/1
3	FUC	C	8	3	-	-	0/1/1/1
3	NAG	D	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1
3	NAG	D	7	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	D	8	3	-	-	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C1-C2	-3.33	1.47	1.52
3	C	6	MAN	O3-C3	-3.32	1.34	1.43
3	C	8	FUC	O5-C1	-3.12	1.38	1.43
3	C	6	MAN	O5-C1	-3.03	1.38	1.43
3	D	5	NAG	C3-C2	3.00	1.58	1.52
3	C	7	NAG	O4-C4	-2.91	1.35	1.43
3	C	2	NAG	O5-C1	-2.68	1.39	1.43
3	D	2	NAG	C1-C2	-2.67	1.48	1.52
3	C	3	BMA	O2-C2	-2.66	1.37	1.43
3	D	8	FUC	C4-C5	-2.58	1.46	1.52
3	D	3	BMA	C4-C3	-2.51	1.45	1.52
3	C	6	MAN	C2-C3	-2.49	1.48	1.52
3	D	5	NAG	C4-C5	2.37	1.58	1.53
3	C	3	BMA	O3-C3	-2.34	1.37	1.43
3	C	5	NAG	C3-C2	-2.32	1.47	1.52
3	C	7	NAG	C4-C5	-2.31	1.48	1.53
3	D	5	NAG	C1-C2	2.29	1.55	1.52
3	C	8	FUC	C4-C5	-2.24	1.47	1.52
3	D	7	NAG	C1-C2	-2.21	1.49	1.52
3	C	6	MAN	C4-C5	-2.20	1.48	1.53
3	C	8	FUC	O4-C4	-2.15	1.37	1.43
3	C	8	FUC	O2-C2	-2.15	1.38	1.43
3	D	5	NAG	O5-C5	2.14	1.47	1.43
3	C	2	NAG	C1-C2	-2.12	1.49	1.52
3	D	6	MAN	O5-C1	2.12	1.47	1.43
3	C	7	NAG	C1-C2	-2.07	1.49	1.52
3	C	4	MAN	O2-C2	-2.05	1.39	1.43
3	C	8	FUC	O3-C3	-2.03	1.37	1.43
3	C	1	NAG	C7-N2	-2.01	1.27	1.34

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6	MAN	C1-O5-C5	6.06	120.30	112.19
3	D	3	BMA	C1-O5-C5	5.37	119.39	112.19
3	D	5	NAG	C1-O5-C5	5.21	119.17	112.19
3	C	1	NAG	C1-O5-C5	4.86	118.70	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	NAG	C1-O5-C5	4.76	118.56	112.19
3	D	4	MAN	O5-C5-C6	-4.60	98.70	107.66
3	D	3	BMA	C1-C2-C3	-4.20	103.52	109.64
3	D	7	NAG	C1-O5-C5	4.09	117.67	112.19
3	C	5	NAG	C1-C2-N2	-4.00	104.12	110.43
3	C	5	NAG	O5-C1-C2	3.56	116.81	111.29
3	C	4	MAN	O5-C5-C6	-3.56	100.73	107.66
3	D	2	NAG	O5-C1-C2	-3.38	106.06	111.29
3	C	4	MAN	C1-O5-C5	3.31	116.62	112.19
3	C	6	MAN	O5-C5-C6	-3.31	101.23	107.66
3	C	2	NAG	O5-C1-C2	-3.28	106.22	111.29
3	D	6	MAN	O2-C2-C1	3.27	116.72	109.22
3	D	6	MAN	O5-C5-C6	3.21	113.90	107.66
3	C	3	BMA	C1-O5-C5	3.20	116.48	112.19
3	C	7	NAG	O5-C1-C2	-3.19	106.36	111.29
3	C	1	NAG	O5-C1-C2	-3.13	106.45	111.29
3	C	1	NAG	C4-C3-C2	-3.07	106.52	111.02
3	C	4	MAN	C3-C4-C5	-2.75	105.25	110.23
3	C	4	MAN	O2-C2-C3	-2.75	104.46	110.15
3	D	7	NAG	O5-C1-C2	-2.73	107.06	111.29
3	D	2	NAG	C2-N2-C7	-2.66	119.34	122.90
3	D	4	MAN	O2-C2-C1	-2.64	103.19	109.22
3	D	7	NAG	C2-N2-C7	-2.63	119.38	122.90
3	C	7	NAG	C2-N2-C7	-2.55	119.48	122.90
3	D	8	FUC	C6-C5-C4	-2.52	108.47	113.08
3	D	8	FUC	C3-C4-C5	-2.47	106.05	109.81
3	D	5	NAG	C3-C4-C5	-2.46	105.77	110.23
3	D	3	BMA	C6-C5-C4	-2.32	107.32	113.02
3	C	6	MAN	C6-C5-C4	-2.24	107.51	113.02
3	C	4	MAN	O5-C5-C4	-2.23	105.40	110.83
3	D	4	MAN	C1-O5-C5	2.22	115.16	112.19
3	D	6	MAN	C1-O5-C5	-2.21	109.22	112.19
3	C	5	NAG	C4-C3-C2	-2.21	107.78	111.02
3	C	7	NAG	C1-C2-N2	-2.20	106.97	110.43
3	D	3	BMA	O4-C4-C3	-2.18	105.23	110.38
3	C	2	NAG	C1-O5-C5	2.18	115.11	112.19
3	C	5	NAG	C3-C4-C5	2.17	114.16	110.23
3	D	5	NAG	C2-N2-C7	2.16	125.79	122.90
3	D	8	FUC	C1-C2-C3	-2.16	106.50	109.64
3	D	8	FUC	O4-C4-C5	-2.15	104.98	109.74
3	D	5	NAG	O7-C7-N2	2.09	125.68	121.98
3	C	4	MAN	O4-C4-C3	-2.07	105.49	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	O2-C2-C1	-2.07	104.49	109.22
3	C	7	NAG	O5-C5-C6	2.05	111.66	107.66
3	C	1	NAG	C3-C4-C5	-2.03	106.56	110.23
3	C	2	NAG	C6-C5-C4	-2.02	108.06	113.02

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C3-C2-N2-C7
3	D	5	NAG	C1-C2-N2-C7
3	D	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	C	6	MAN	O5-C5-C6-O6
3	D	6	MAN	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	C	6	MAN	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	C	5	NAG	C8-C7-N2-C2
3	C	5	NAG	O7-C7-N2-C2
3	C	7	NAG	O5-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6
3	C	7	NAG	C4-C5-C6-O6
3	D	5	NAG	C4-C5-C6-O6
3	D	7	NAG	C4-C5-C6-O6
3	D	7	NAG	C3-C2-N2-C7
3	C	5	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 17 short contacts:

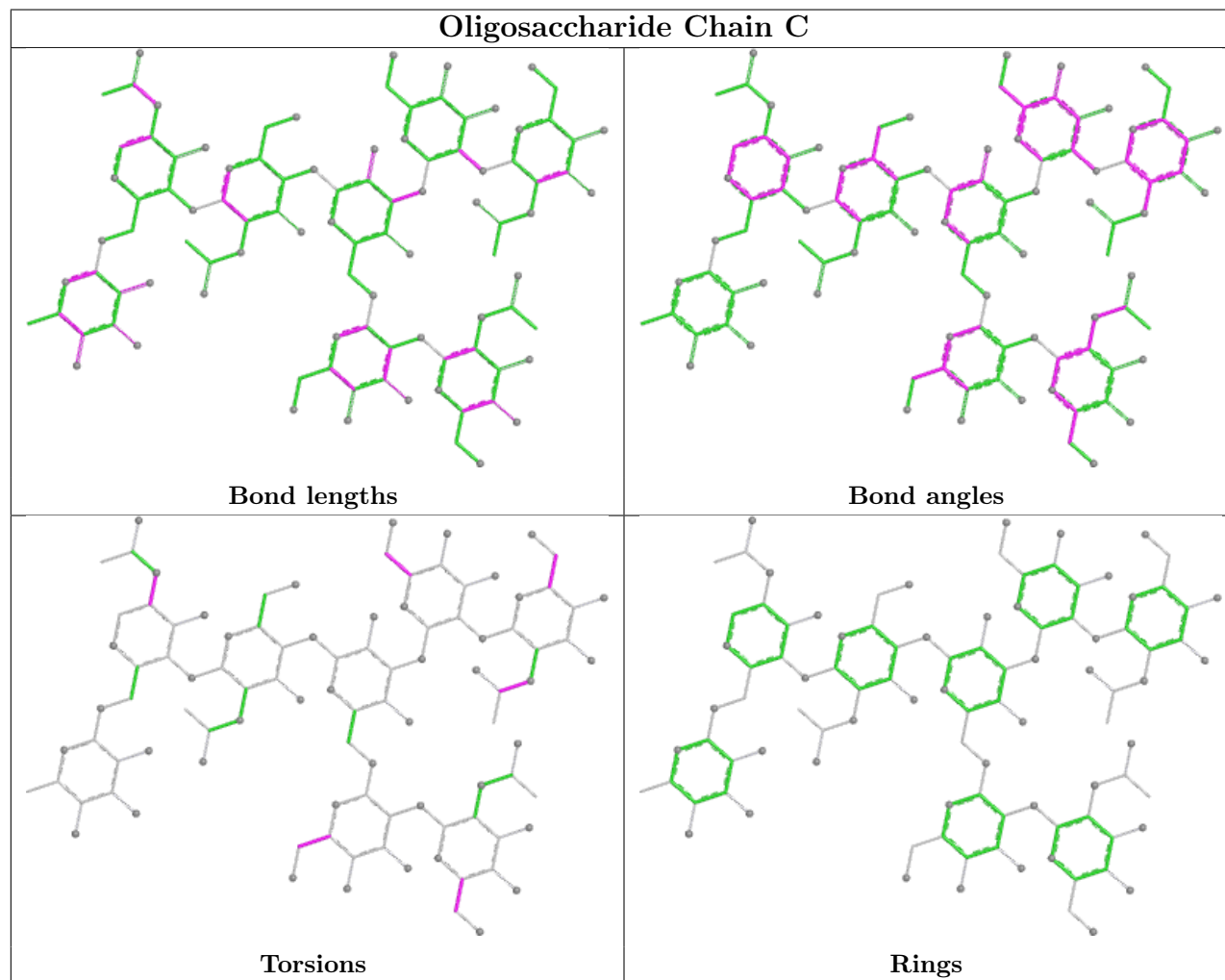
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	MAN	5	0
3	D	7	NAG	2	0
3	D	8	FUC	4	0
3	D	5	NAG	3	0
3	D	1	NAG	5	0
3	C	5	NAG	5	0
3	D	4	MAN	2	0

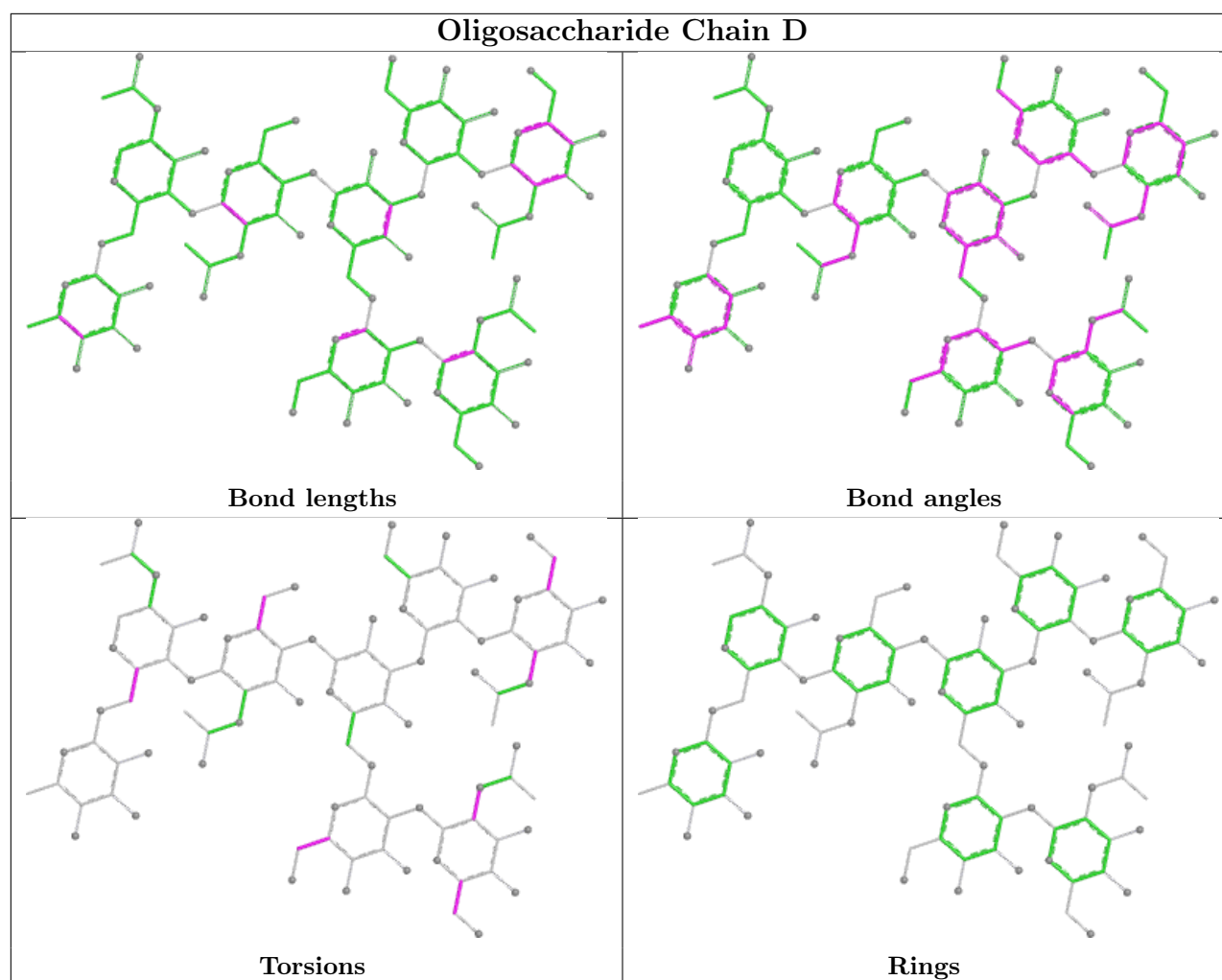
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	6	MAN	1	0
3	C	1	NAG	2	0

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, 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	208/223 (93%)	0.94	29 (13%) 6 5	39, 52, 82, 95	0
2	B	205/223 (91%)	2.26	90 (43%) 0 0	37, 71, 109, 132	0
All	All	413/446 (92%)	1.59	119 (28%) 1 1	37, 59, 104, 132	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	302	VAL	12.3
2	B	300	TYR	9.8
2	B	303	VAL	7.8
2	B	241	PHE	7.7
2	B	240	VAL	7.5
2	B	273	VAL	6.6
2	B	330	ALA	6.5
2	B	331	PRO	6.5
2	B	268	HIS	6.5
2	B	263	VAL	6.4
2	B	278	TYR	6.1
2	B	295	GLN	5.8
2	B	336	ILE	5.7
2	B	324	SER	5.6
2	B	266	VAL	5.6
2	B	296	TYR	5.5
2	B	269	GLU	5.5
2	B	264	VAL	5.4
2	B	262	VAL	5.3
2	B	332	ILE	5.2
2	B	243	PHE	5.1
2	B	328	LEU	5.0
2	B	327	ALA	5.0
2	B	281	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	294	GLU	4.9
2	B	242	LEU	4.8
2	B	270	ASP	4.7
2	B	323	VAL	4.7
2	B	277	TRP	4.6
2	B	267	SER	4.5
2	B	275	PHE	4.4
2	B	291	PRO	4.4
2	B	329	PRO	4.3
2	B	326	LYS	4.2
2	B	335	THR	4.2
2	B	319	TYR	4.0
2	B	260	THR	4.0
2	B	279	VAL	4.0
2	B	274	LYS	3.9
2	B	292	ARG	3.9
2	B	282	VAL	3.9
2	B	301	ARG	3.8
2	B	444	SER	3.7
2	B	361	ASN	3.7
2	B	347	ARG	3.7
2	B	271	PRO	3.7
1	A	387	PRO	3.7
2	B	293	GLU	3.6
2	B	304	SER	3.6
2	B	320	LYS	3.6
2	B	419	GLN	3.6
2	B	321	CYS	3.5
1	A	361	ASN	3.4
2	B	337	SER	3.4
2	B	360	LYS	3.4
2	B	276	ASN	3.4
1	A	441	LEU	3.4
1	A	341	GLY	3.3
2	B	239	SER	3.3
2	B	238	PRO	3.3
2	B	342	GLN	3.3
2	B	253	ILE	3.2
2	B	384	ASN	3.2
2	B	258	GLU	3.2
2	B	334	LYS	3.2
2	B	387	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	284	VAL	3.2
2	B	305	VAL	3.2
2	B	354	CYS	3.2
1	A	384	ASN	3.1
1	A	362	GLN	3.1
1	A	388	GLU	3.1
2	B	390	ASN	3.0
2	B	288	LYS	3.0
2	B	416	ARG	3.0
1	A	360	GLU	3.0
1	A	440	SER	2.9
2	B	259	VAL	2.9
1	A	389	ASN	2.8
1	A	409	TRP	2.8
1	A	359	THR	2.8
2	B	358	LEU	2.8
1	A	356	ASP	2.8
1	A	402	GLY	2.8
1	A	405	PHE	2.8
1	A	237	GLY	2.7
1	A	386	GLN	2.7
2	B	399	VAL	2.7
2	B	316	GLY	2.6
2	B	283	GLU	2.6
2	B	297	ASN	2.6
1	A	444	SER	2.5
2	B	287	ALA	2.5
1	A	385	GLY	2.5
1	A	358	LEU	2.5
2	B	322	LYS	2.5
2	B	355	ARG	2.5
1	A	436	TYR	2.5
1	A	342	GLN	2.5
2	B	317	LYS	2.5
1	A	421	ASN	2.4
2	B	261	CYS	2.4
2	B	325	ASN	2.4
1	A	390	ASN	2.4
2	B	413	ASP	2.4
2	B	246	LYS	2.4
1	A	411	THR	2.3
2	B	280	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	244	PRO	2.3
2	B	265	ASP	2.2
2	B	418	GLN	2.2
1	A	399	ASP	2.1
2	B	420	GLY	2.1
1	A	443	LEU	2.0
2	B	315	ASN	2.0
2	B	318	GLU	2.0
1	A	424	SER	2.0
1	A	425	CYS	2.0
2	B	289	THR	2.0

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

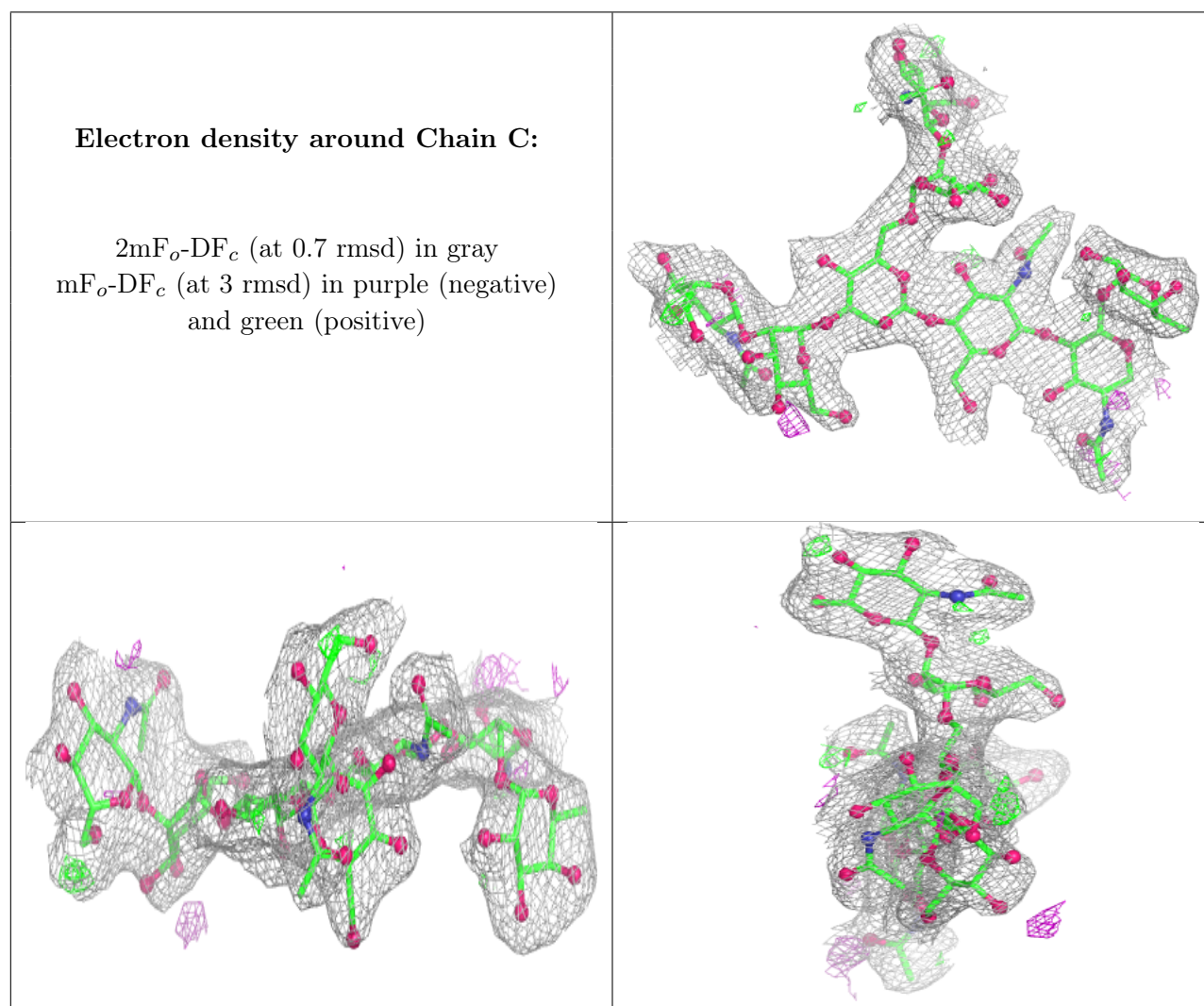
There are no non-standard protein/DNA/RNA residues in this entry.

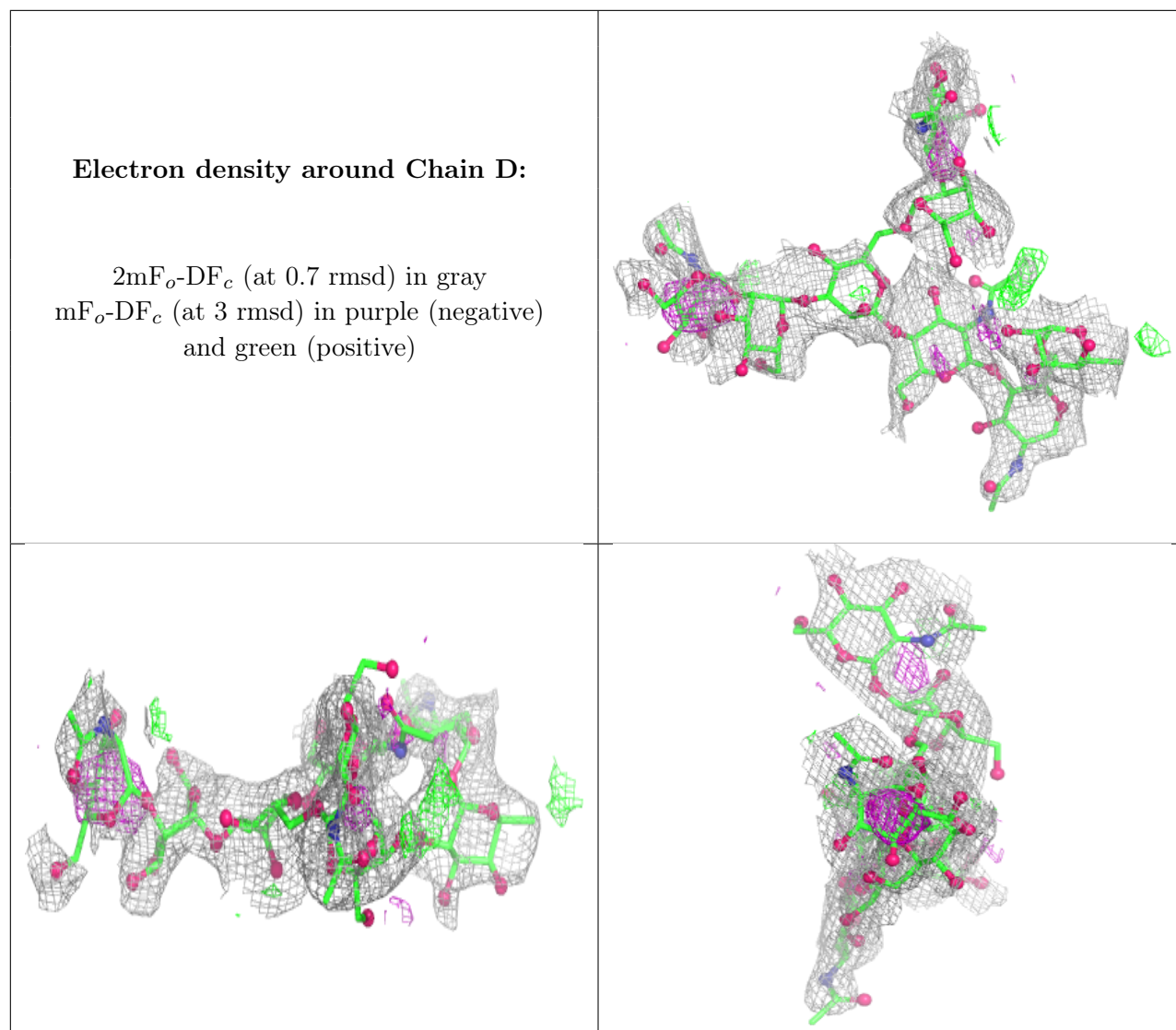
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	5	14/15	0.24	0.26	97,105,112,113	0
3	FUC	D	8	10/11	0.30	0.30	97,104,108,109	0
3	MAN	D	6	11/12	0.49	0.24	94,101,106,108	0
3	NAG	D	2	14/15	0.49	0.30	103,106,111,112	0
3	BMA	D	3	11/12	0.56	0.22	97,104,109,110	0
3	MAN	D	4	11/12	0.59	0.21	92,100,105,106	0
3	NAG	D	7	14/15	0.62	0.20	96,101,106,107	0
3	NAG	C	5	14/15	0.68	0.18	74,83,91,91	0
3	NAG	D	1	14/15	0.71	0.19	95,109,112,113	0
3	MAN	C	4	11/12	0.85	0.14	73,79,87,87	0
3	NAG	C	7	14/15	0.87	0.13	53,59,66,70	0
3	NAG	C	1	14/15	0.89	0.12	44,49,54,54	0
3	MAN	C	6	11/12	0.91	0.11	56,58,64,75	0
3	NAG	C	2	14/15	0.91	0.11	43,51,57,59	0
3	FUC	C	8	10/11	0.92	0.11	48,52,56,59	0
3	BMA	C	3	11/12	0.93	0.09	50,56,62,71	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.





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.