



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:49 AM UTC

PDB ID : 3V95 / pdb_00003v95
Title : Crystal structure of monoclonal human anti-rhesus D Fc and IgG1 t125(yb2/0) in the presence of EDTA
Authors : Menez, R.; A Stura, E.; Bourel, D.; Siberil, S.; Jorieux, S.; De Romeuf, C.; Ducancel, F.; Fridman, W.H.; Teillaud, J.L.
Deposited on : 2011-12-23
Resolution : 2.70 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

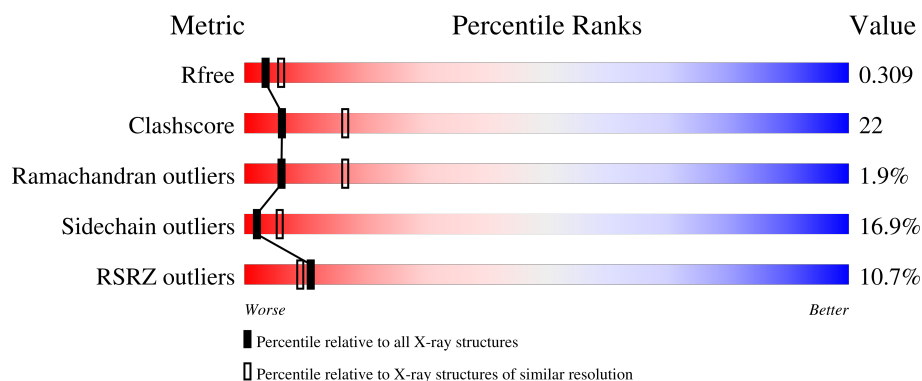
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	212	
1	B	212	
2	C	8	
2	D	8	

2 Entry composition [i](#)

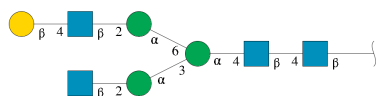
There are 4 unique types of molecules in this entry. The entry contains 3676 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	212	Total	C	N	O	S	0	0	0
			1689	1074	285	324	6			
1	B	209	Total	C	N	O	S	0	0	0
			1667	1062	280	319	6			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-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	C	8	Total	C	N	O	0	0	0
			100	56	4	40			
2	D	8	Total	C	N	O	0	0	0
			100	56	4	40			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

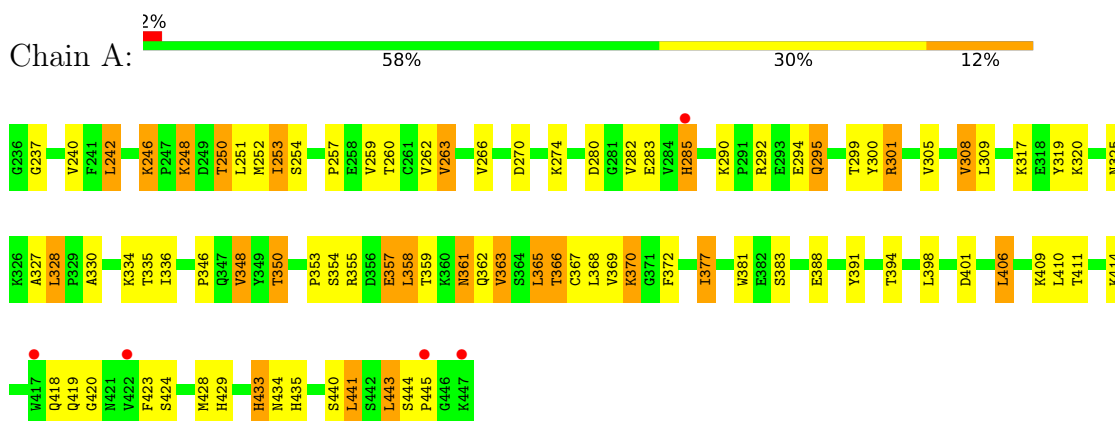
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	51	Total	O	0	0
			51	51		

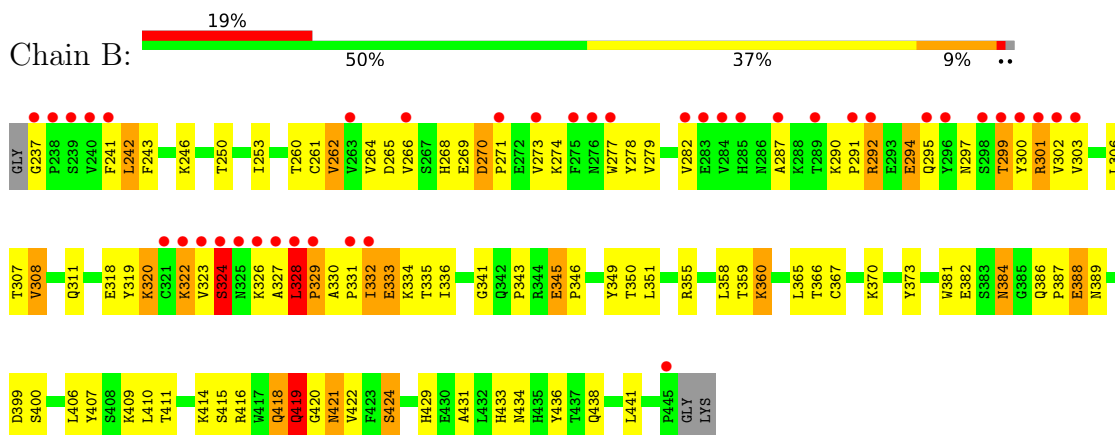
3 Residue-property plots [i](#)

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 1: Ig gamma-1 chain C region



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



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

Chain D:  62% 38%

NA61	NA62	MAN3	MAN4	NA65	GAL6	MAN7	NA68
------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.38Å 79.12Å 138.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.89 – 2.70 41.89 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.89-2.70) 99.8 (41.89-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.251 , 0.321 0.249 , 0.309	Depositor DCC
R_{free} test set	787 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3676	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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: GOL, NAG, MAN, GAL

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	0.81	0/1736	1.07	6/2363 (0.3%)
1	B	0.86	1/1714 (0.1%)	1.02	5/2337 (0.2%)
All	All	0.83	1/3450 (0.0%)	1.05	11/4700 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308	VAL	C-O	-5.24	1.18	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	GLY	CA-C-N	6.51	126.48	119.78
1	A	237	GLY	C-N-CA	6.51	126.48	119.78
1	A	270	ASP	CA-C-N	5.82	125.52	119.64
1	A	270	ASP	C-N-CA	5.82	125.52	119.64
1	A	366	THR	N-CA-C	5.26	117.81	109.24
1	B	327	ALA	N-CA-C	-5.23	105.18	112.45
1	B	295	GLN	N-CA-C	5.20	115.16	108.34
1	B	328	LEU	CA-C-N	5.05	126.16	119.84
1	B	328	LEU	C-N-CA	5.05	126.16	119.84
1	B	324	SER	N-CA-C	5.05	121.56	110.80
1	A	348	VAL	N-CA-C	5.03	114.72	106.72

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	1689	0	1656	66	0
1	B	1667	0	1631	96	0
2	C	100	0	85	7	0
2	D	100	0	85	8	0
3	A	12	0	16	1	0
4	A	57	0	0	4	0
4	B	51	0	0	2	0
All	All	3676	0	3473	158	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 (158) 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:330:ALA:HB1	1:B:331:PRO:HD2	1.33	1.09
1:A:428:MET:HB2	1:A:435:HIS:O	1.70	0.92
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.53	0.91
1:B:237:GLY:HA2	1:B:328:LEU:HD12	1.54	0.90
1:B:328:LEU:HB2	1:B:329:PRO:HD2	1.54	0.89
1:A:253:ILE:H	1:A:253:ILE:HD12	1.43	0.81
1:B:264:VAL:HG12	1:B:265:ASP:N	1.96	0.81
1:B:241:PHE:CE1	2:D:2:NAG:H62	2.17	0.80
1:A:443:LEU:HD12	1:A:443:LEU:H	1.46	0.79
1:A:350:THR:HB	1:A:441:LEU:HD13	1.64	0.78
1:B:264:VAL:HG12	1:B:265:ASP:H	1.48	0.75
1:B:419:GLN:HE21	1:B:419:GLN:HA	1.51	0.75
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.24	0.72
1:B:328:LEU:CB	1:B:329:PRO:HD2	2.18	0.72
1:A:295:GLN:HE21	2:C:1:NAG:H62	1.55	0.72
1:A:409:LYS:HE2	4:A:646:HOH:O	1.89	0.72
1:B:301:ARG:HH11	1:B:301:ARG:HG3	1.53	0.72
1:B:264:VAL:CG1	1:B:265:ASP:H	2.02	0.71
1:B:241:PHE:HE1	2:D:2:NAG:H62	1.53	0.71
1:B:237:GLY:CA	1:B:328:LEU:HD12	2.21	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:VAL:HG22	1:B:332:ILE:HB	1.74	0.70
1:A:285:HIS:ND1	4:A:655:HOH:O	2.24	0.70
1:A:420:GLY:HA2	1:A:443:LEU:HD11	1.74	0.69
1:B:330:ALA:HB1	1:B:331:PRO:CD	2.17	0.69
1:B:328:LEU:CB	1:B:329:PRO:CD	2.71	0.69
1:A:369:VAL:HB	1:A:406:LEU:HD22	1.75	0.69
1:B:243:PHE:HE2	1:B:262:VAL:CG1	2.06	0.68
1:B:333:GLU:O	1:B:334:LYS:HG2	1.92	0.68
1:B:414:LYS:O	1:B:418:GLN:HG2	1.94	0.67
1:A:420:GLY:HA2	1:A:443:LEU:CD1	2.24	0.67
1:A:361:ASN:HD22	1:A:361:ASN:N	1.92	0.67
1:B:265:ASP:OD2	2:D:1:NAG:H83	1.95	0.67
1:A:253:ILE:H	1:A:253:ILE:CD1	2.07	0.66
1:A:325:ASN:OD1	1:A:327:ALA:HB3	1.96	0.66
1:A:354:SER:HB2	1:B:349:TYR:HB3	1.78	0.66
1:A:357:GLU:HG3	1:B:349:TYR:CZ	2.32	0.65
1:B:350:THR:HB	1:B:441:LEU:HD22	1.79	0.64
1:B:268:HIS:O	1:B:271:PRO:HD3	1.98	0.64
1:B:311:GLN:NE2	1:B:311:GLN:HA	2.12	0.64
1:A:346:PRO:HG3	1:A:372:PHE:HB3	1.80	0.63
1:B:436:TYR:OH	1:B:438:GLN:NE2	2.33	0.62
1:B:419:GLN:HE21	1:B:419:GLN:CA	2.12	0.62
1:B:287:ALA:HB2	1:B:306:LEU:HD12	1.80	0.62
1:B:297:ASN:OD1	1:B:299:THR:HB	1.98	0.62
1:A:361:ASN:ND2	4:A:602:HOH:O	2.32	0.61
1:B:243:PHE:CE2	1:B:262:VAL:CG1	2.83	0.61
1:A:295:GLN:NE2	1:A:301:ARG:HG2	2.16	0.61
1:B:388:GLU:OE2	1:B:416:ARG:NH1	2.33	0.60
1:A:369:VAL:HB	1:A:406:LEU:CD2	2.33	0.58
1:A:253:ILE:HD12	1:A:253:ILE:N	2.16	0.58
1:B:382:GLU:HA	1:B:388:GLU:H	1.69	0.57
1:B:266:VAL:HG13	1:B:300:TYR:HB2	1.85	0.57
1:B:294:GLU:HA	1:B:300:TYR:HA	1.87	0.56
1:B:301:ARG:HG3	1:B:301:ARG:NH1	2.15	0.56
1:B:290:LYS:HD3	1:B:303:VAL:HB	1.88	0.56
1:A:283:GLU:HG2	4:A:655:HOH:O	2.05	0.55
1:B:270:ASP:N	1:B:271:PRO:HD3	2.23	0.54
1:B:274:LYS:HB3	1:B:324:SER:HB2	1.89	0.54
1:B:323:VAL:HG23	1:B:323:VAL:O	2.07	0.53
1:A:357:GLU:HG3	1:B:349:TYR:CE2	2.44	0.53
1:B:333:GLU:O	1:B:334:LYS:CG	2.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:THR:HG22	1:A:251:LEU:HG	1.91	0.53
1:A:355:ARG:O	1:A:358:LEU:HD22	2.08	0.53
1:B:241:PHE:CZ	2:D:2:NAG:H62	2.44	0.53
1:B:330:ALA:CB	1:B:331:PRO:HD2	2.22	0.52
1:A:406:LEU:C	1:A:406:LEU:HD23	2.34	0.52
1:B:433:HIS:O	1:B:434:ASN:HB2	2.10	0.52
2:C:8:NAG:C1	2:C:8:NAG:H82	2.40	0.52
1:B:264:VAL:CG1	1:B:265:ASP:N	2.59	0.51
1:A:246:LYS:HB2	2:C:6:GAL:H61	1.92	0.51
1:B:301:ARG:HH11	1:B:301:ARG:CG	2.23	0.51
1:B:242:LEU:HD23	1:B:260:THR:O	2.10	0.51
1:B:264:VAL:HG11	2:D:2:NAG:O5	2.11	0.51
1:B:311:GLN:HA	1:B:311:GLN:HE21	1.76	0.50
1:A:424:SER:HA	1:A:440:SER:HA	1.93	0.50
1:B:311:GLN:HE21	1:B:311:GLN:CA	2.24	0.50
1:B:262:VAL:HG21	1:B:301:ARG:NH1	2.27	0.49
1:B:359:THR:C	1:B:360:LYS:HG2	2.37	0.49
1:B:420:GLY:O	1:B:421:ASN:C	2.55	0.49
1:A:246:LYS:HD2	2:C:6:GAL:H61	1.94	0.49
1:A:266:VAL:O	1:A:300:TYR:HB2	2.13	0.49
1:B:355:ARG:O	1:B:358:LEU:HB2	2.13	0.48
1:B:359:THR:O	1:B:360:LYS:HG2	2.14	0.48
1:A:414:LYS:O	1:A:418:GLN:HG2	2.12	0.48
1:A:383:SER:HB2	1:A:423:PHE:CD2	2.48	0.48
1:B:242:LEU:HD13	1:B:336:ILE:HB	1.95	0.48
1:A:320:LYS:HE3	3:A:510:GOL:H2	1.96	0.47
1:A:242:LEU:HD13	1:A:336:ILE:HB	1.95	0.47
1:B:268:HIS:O	1:B:271:PRO:CD	2.62	0.47
2:C:8:NAG:C1	2:C:8:NAG:C8	2.92	0.47
1:B:418:GLN:O	1:B:419:GLN:C	2.57	0.47
1:A:424:SER:HB3	1:A:440:SER:HB3	1.96	0.47
1:A:358:LEU:O	1:A:414:LYS:NZ	2.46	0.47
1:B:311:GLN:NE2	1:B:311:GLN:CA	2.77	0.47
1:B:290:LYS:HG2	1:B:291:PRO:O	2.16	0.46
1:B:320:LYS:N	1:B:320:LYS:HD2	2.30	0.46
1:B:306:LEU:HD23	1:B:308:VAL:HG22	1.98	0.46
1:A:363:VAL:HG22	1:A:414:LYS:HA	1.98	0.45
1:B:266:VAL:HG13	1:B:300:TYR:CB	2.46	0.45
1:B:278:TYR:HB2	1:B:320:LYS:HD3	1.98	0.45
1:B:429:HIS:CD2	1:B:431:ALA:H	2.34	0.45
1:A:444:SER:N	1:A:445:PRO:HD3	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:GLU:HA	1:B:346:PRO:HD3	1.88	0.45
1:B:355:ARG:HA	1:B:358:LEU:HD12	1.98	0.45
1:A:366:THR:OG1	1:B:407:TYR:OH	2.23	0.44
1:B:301:ARG:HH22	2:D:2:NAG:H2	1.82	0.44
1:B:243:PHE:HE2	1:B:262:VAL:HG13	1.80	0.44
1:B:301:ARG:NH2	2:D:2:NAG:H2	2.33	0.44
1:A:246:LYS:HD2	2:C:6:GAL:C6	2.47	0.44
1:A:361:ASN:N	1:A:361:ASN:ND2	2.62	0.44
1:A:308:VAL:HG22	1:A:319:TYR:CE2	2.52	0.44
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.53	0.44
1:B:381:TRP:HA	1:B:424:SER:O	2.18	0.44
1:A:257:PRO:HG2	1:A:308:VAL:O	2.18	0.44
1:A:388:GLU:OE2	1:A:388:GLU:HA	2.17	0.43
1:A:391:TYR:C	1:A:391:TYR:CD2	2.96	0.43
1:B:328:LEU:HB3	1:B:329:PRO:CD	2.46	0.43
1:A:274:LYS:HB3	1:A:274:LYS:HE3	1.76	0.43
1:A:259:VAL:HG23	1:A:308:VAL:HG21	1.99	0.43
1:B:384:ASN:C	1:B:386:GLN:H	2.26	0.43
1:B:406:LEU:HD12	1:B:406:LEU:C	2.44	0.43
1:A:248:LYS:O	1:A:252:MET:HG3	2.18	0.43
1:A:294:GLU:HB2	1:A:300:TYR:CE1	2.54	0.43
1:A:319:TYR:O	1:A:335:THR:HA	2.19	0.43
1:A:363:VAL:O	1:A:411:THR:HA	2.19	0.42
1:A:388:GLU:HB3	1:A:410:LEU:HD13	2.01	0.42
1:A:409:LYS:NZ	1:B:399:ASP:OD1	2.50	0.42
1:B:268:HIS:C	1:B:271:PRO:HD3	2.43	0.42
1:A:377:ILE:HG13	1:A:429:HIS:HB2	2.02	0.42
1:A:368:LEU:HD12	1:A:369:VAL:N	2.35	0.42
1:B:241:PHE:HB2	1:B:262:VAL:HG13	2.01	0.42
1:A:260:THR:HG23	1:A:305:VAL:HG22	2.02	0.42
1:A:328:LEU:HD13	1:A:330:ALA:O	2.19	0.42
1:A:353:PRO:HD3	1:A:365:LEU:HD12	2.02	0.42
1:B:292:ARG:HB3	1:B:302:VAL:HG22	2.02	0.42
1:B:360:LYS:NZ	4:B:615:HOH:O	2.51	0.42
1:A:348:VAL:O	1:A:348:VAL:HG12	2.19	0.42
1:A:246:LYS:H	2:C:6:GAL:C6	2.33	0.41
1:B:341:GLY:O	1:B:343:PRO:HD3	2.20	0.41
1:B:351:LEU:HD12	1:B:366:THR:HG21	2.01	0.41
1:A:401:ASP:OD2	1:A:401:ASP:C	2.62	0.41
1:B:266:VAL:CG2	1:B:271:PRO:HB3	2.50	0.41
1:B:278:TYR:HA	1:B:282:VAL:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASP:OD1	1:A:317:LYS:HG3	2.20	0.41
1:A:354:SER:CB	1:B:349:TYR:HB3	2.50	0.41
1:B:246:LYS:HZ3	2:D:6:GAL:H2	1.86	0.41
1:B:308:VAL:HG13	1:B:319:TYR:OH	2.20	0.41
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.56	0.41
1:B:386:GLN:HA	1:B:387:PRO:HD3	1.90	0.41
1:A:433:HIS:O	1:A:434:ASN:HB2	2.21	0.41
1:B:278:TYR:O	1:B:320:LYS:HD2	2.21	0.41
1:B:343:PRO:HA	1:B:373:TYR:O	2.21	0.41
1:A:370:LYS:HB2	1:A:370:LYS:HE3	1.76	0.40
1:B:415:SER:O	1:B:419:GLN:HG2	2.21	0.40
1:A:240:VAL:HG22	1:A:263:VAL:HG13	2.02	0.40
1:B:360:LYS:O	1:B:414:LYS:HD3	2.21	0.40
1:B:320:LYS:HD2	1:B:320:LYS:H	1.87	0.40
1:B:322:LYS:NZ	4:B:642:HOH:O	2.54	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	210/212 (99%)	200 (95%)	7 (3%)	3 (1%)	9	23
1	B	207/212 (98%)	180 (87%)	22 (11%)	5 (2%)	4	12
All	All	417/424 (98%)	380 (91%)	29 (7%)	8 (2%)	6	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	324	SER
1	A	292	ARG
1	A	419	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	421	ASN
1	B	419	GLN
1	A	377	ILE
1	B	270	ASP
1	B	329	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	196/196 (100%)	163 (83%)	33 (17%)	2	6
1	B	194/196 (99%)	161 (83%)	33 (17%)	2	6
All	All	390/392 (100%)	324 (83%)	66 (17%)	2	6

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	LEU
1	A	246	LYS
1	A	248	LYS
1	A	250	THR
1	A	253	ILE
1	A	254	SER
1	A	262	VAL
1	A	263	VAL
1	A	282	VAL
1	A	285	HIS
1	A	290	LYS
1	A	295	GLN
1	A	299	THR
1	A	301	ARG
1	A	308	VAL
1	A	309	LEU
1	A	328	LEU
1	A	334	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	350	THR
1	A	357	GLU
1	A	358	LEU
1	A	359	THR
1	A	361	ASN
1	A	362	GLN
1	A	363	VAL
1	A	365	LEU
1	A	370	LYS
1	A	394	THR
1	A	398	LEU
1	A	406	LEU
1	A	433	HIS
1	A	441	LEU
1	A	443	LEU
1	B	242	LEU
1	B	250	THR
1	B	253	ILE
1	B	262	VAL
1	B	269	GLU
1	B	273	VAL
1	B	279	VAL
1	B	292	ARG
1	B	294	GLU
1	B	299	THR
1	B	301	ARG
1	B	307	THR
1	B	318	GLU
1	B	320	LYS
1	B	322	LYS
1	B	326	LYS
1	B	328	LEU
1	B	332	ILE
1	B	333	GLU
1	B	335	THR
1	B	345	GLU
1	B	360	LYS
1	B	370	LYS
1	B	384	ASN
1	B	388	GLU
1	B	389	ASN
1	B	400	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	409	LYS
1	B	411	THR
1	B	418	GLN
1	B	419	GLN
1	B	422	VAL
1	B	424	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN
1	A	311	GLN
1	A	347	GLN
1	A	361	ASN
1	A	386	GLN
1	A	421	ASN
1	B	285	HIS
1	B	295	GLN
1	B	311	GLN
1	B	325	ASN
1	B	390	ASN
1	B	419	GLN
1	B	429	HIS
1	B	438	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	0.52	0	17,19,21	1.52	2 (11%)
2	NAG	C	2	2	14,14,15	0.73	0	17,19,21	1.78	6 (35%)
2	MAN	C	3	2	11,11,12	0.76	0	15,15,17	2.69	4 (26%)
2	MAN	C	4	2	11,11,12	0.70	0	15,15,17	1.02	1 (6%)
2	NAG	C	5	2	14,14,15	0.48	0	17,19,21	1.17	1 (5%)
2	GAL	C	6	2	11,11,12	0.48	0	15,15,17	2.54	6 (40%)
2	MAN	C	7	2	11,11,12	0.64	0	15,15,17	1.96	8 (53%)
2	NAG	C	8	2	14,14,15	0.51	0	17,19,21	2.44	6 (35%)
2	NAG	D	1	1,2	14,14,15	0.68	0	17,19,21	1.25	2 (11%)
2	NAG	D	2	2	14,14,15	0.79	0	17,19,21	1.52	3 (17%)
2	MAN	D	3	2	11,11,12	0.55	0	15,15,17	1.69	3 (20%)
2	MAN	D	4	2	11,11,12	0.57	0	15,15,17	2.74	2 (13%)
2	NAG	D	5	2	14,14,15	0.47	0	17,19,21	2.98	7 (41%)
2	GAL	D	6	2	11,11,12	0.67	0	15,15,17	1.20	2 (13%)
2	MAN	D	7	2	11,11,12	0.74	0	15,15,17	1.31	3 (20%)
2	NAG	D	8	2	14,14,15	0.73	0	17,19,21	1.33	2 (11%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	1/2/19/22	0/1/1/1
2	NAG	D	5	2	-	4/6/23/26	0/1/1/1
2	GAL	D	6	2	-	1/2/19/22	0/1/1/1
2	MAN	D	7	2	-	2/2/19/22	0/1/1/1
2	NAG	D	8	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	MAN	C1-O5-C5	9.55	124.99	112.19
2	D	5	NAG	C1-O5-C5	8.51	123.59	112.19
2	C	3	MAN	C1-O5-C5	8.43	123.48	112.19
2	C	6	GAL	C1-O5-C5	7.22	121.86	112.19
2	C	8	NAG	C1-O5-C5	6.39	120.76	112.19
2	C	8	NAG	C2-N2-C7	5.25	129.94	122.90
2	D	5	NAG	C2-N2-C7	5.09	129.72	122.90
2	C	2	NAG	O4-C4-C3	4.21	120.29	110.38
2	D	3	MAN	C1-O5-C5	4.20	117.82	112.19
2	C	3	MAN	C1-C2-C3	4.15	115.68	109.64
2	C	1	NAG	C1-C2-N2	4.10	116.89	110.43
2	D	2	NAG	C4-C3-C2	3.96	116.82	111.02
2	C	6	GAL	O3-C3-C4	-3.54	102.04	110.38
2	D	5	NAG	C4-C3-C2	-3.46	105.94	111.02
2	C	6	GAL	C1-C2-C3	-3.44	104.64	109.64
2	D	8	NAG	C1-O5-C5	3.26	116.56	112.19
2	D	3	MAN	C1-C2-C3	3.23	114.35	109.64
2	D	5	NAG	O5-C5-C4	3.23	118.68	110.83
2	C	4	MAN	C1-O5-C5	3.18	116.45	112.19
2	D	2	NAG	O4-C4-C3	3.14	117.77	110.38
2	C	1	NAG	O5-C5-C6	3.05	113.60	107.66
2	C	7	MAN	O3-C3-C2	2.92	116.01	110.05
2	C	7	MAN	C1-C2-C3	-2.91	105.41	109.64
2	D	1	NAG	C4-C3-C2	2.87	115.23	111.02
2	D	7	MAN	O2-C2-C3	2.80	115.95	110.15
2	C	8	NAG	C8-C7-N2	2.73	120.65	116.12
2	D	6	GAL	C1-O5-C5	2.70	115.80	112.19
2	D	5	NAG	C1-C2-N2	2.68	114.65	110.43
2	C	2	NAG	C1-C2-N2	-2.65	106.25	110.43
2	C	2	NAG	C2-N2-C7	-2.60	119.42	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	NAG	O5-C5-C6	2.59	112.70	107.66
2	C	7	MAN	C2-C3-C4	-2.58	106.33	110.86
2	D	1	NAG	C1-O5-C5	2.58	115.64	112.19
2	C	7	MAN	C1-O5-C5	2.49	115.53	112.19
2	C	2	NAG	O3-C3-C2	-2.47	104.28	109.40
2	C	8	NAG	O5-C1-C2	2.46	115.10	111.29
2	C	7	MAN	O2-C2-C1	-2.45	103.61	109.22
2	C	6	GAL	O2-C2-C3	2.42	115.16	110.15
2	D	6	GAL	C1-C2-C3	2.42	113.16	109.64
2	C	5	NAG	C1-O5-C5	2.38	115.38	112.19
2	D	8	NAG	C3-C4-C5	-2.37	105.94	110.23
2	C	8	NAG	C4-C3-C2	-2.33	107.60	111.02
2	C	7	MAN	O4-C4-C5	2.32	115.05	109.32
2	D	5	NAG	O4-C4-C3	-2.29	104.97	110.38
2	D	2	NAG	O3-C3-C4	-2.27	105.02	110.38
2	C	6	GAL	O4-C4-C3	-2.24	105.09	110.38
2	C	2	NAG	C4-C3-C2	-2.23	107.75	111.02
2	D	3	MAN	C6-C5-C4	-2.22	107.57	113.02
2	D	5	NAG	O3-C3-C2	2.20	113.96	109.40
2	D	4	MAN	O5-C1-C2	2.18	116.00	110.79
2	D	7	MAN	C1-C2-C3	2.16	112.79	109.64
2	C	3	MAN	O5-C5-C4	2.16	116.08	110.83
2	C	2	NAG	C1-O5-C5	2.16	115.08	112.19
2	C	6	GAL	C6-C5-C4	-2.14	107.76	113.02
2	C	7	MAN	C3-C4-C5	-2.07	106.47	110.23
2	C	7	MAN	O3-C3-C4	2.04	115.19	110.38
2	D	7	MAN	O2-C2-C1	2.02	113.84	109.22
2	C	3	MAN	C6-C5-C4	-2.00	108.11	113.02

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	8	NAG	C1-C2-N2-C7
2	D	2	NAG	O5-C5-C6-O6
2	D	7	MAN	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	8	NAG	O5-C5-C6-O6
2	D	5	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	7	MAN	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

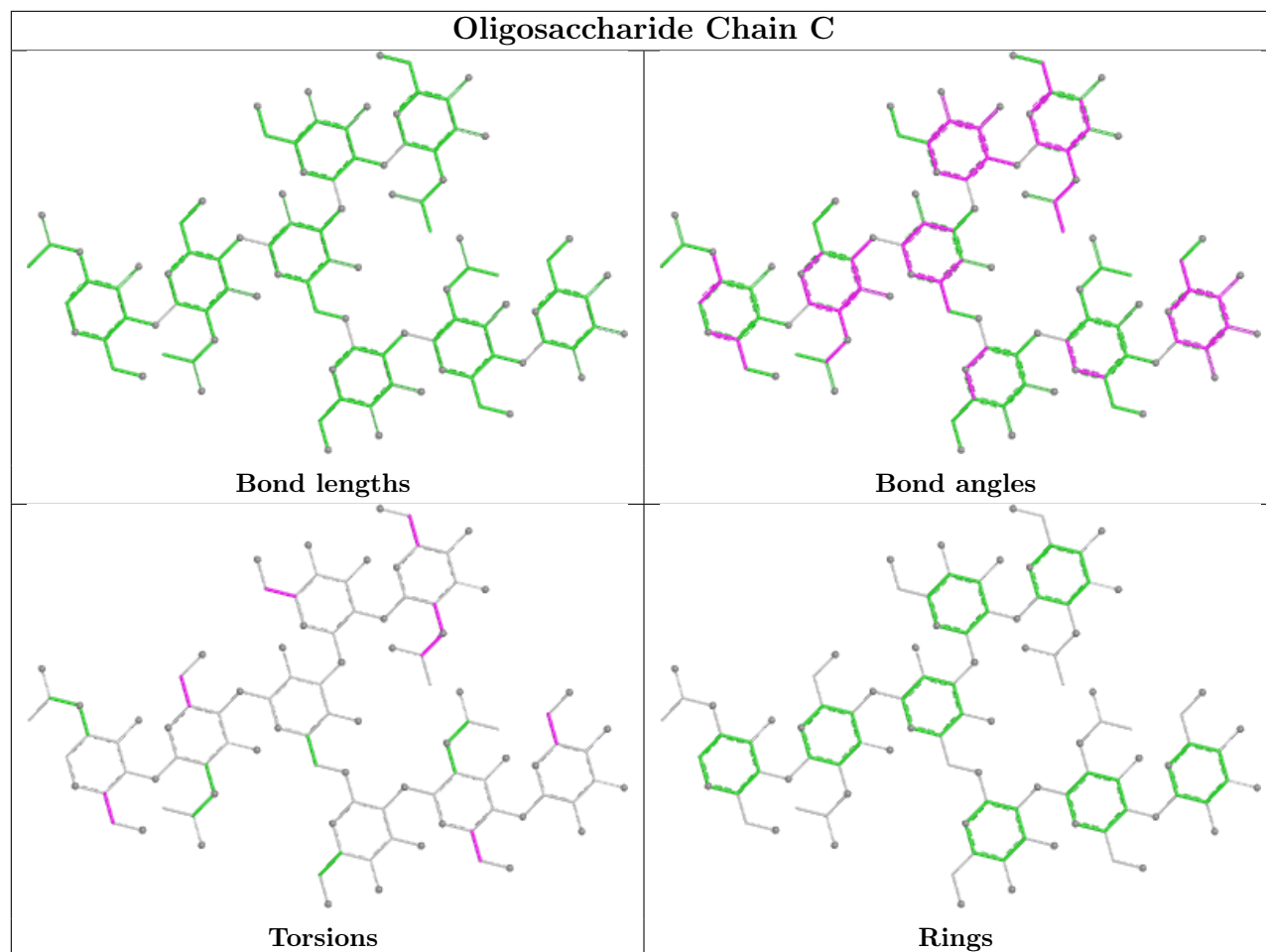
Mol	Chain	Res	Type	Atoms
2	C	8	NAG	C4-C5-C6-O6
2	C	8	NAG	C8-C7-N2-C2
2	C	8	NAG	O7-C7-N2-C2
2	C	5	NAG	O5-C5-C6-O6
2	D	5	NAG	C4-C5-C6-O6
2	C	5	NAG	C4-C5-C6-O6
2	C	6	GAL	O5-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6
2	C	7	MAN	C4-C5-C6-O6
2	D	6	GAL	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	5	NAG	C1-C2-N2-C7
2	D	5	NAG	C3-C2-N2-C7

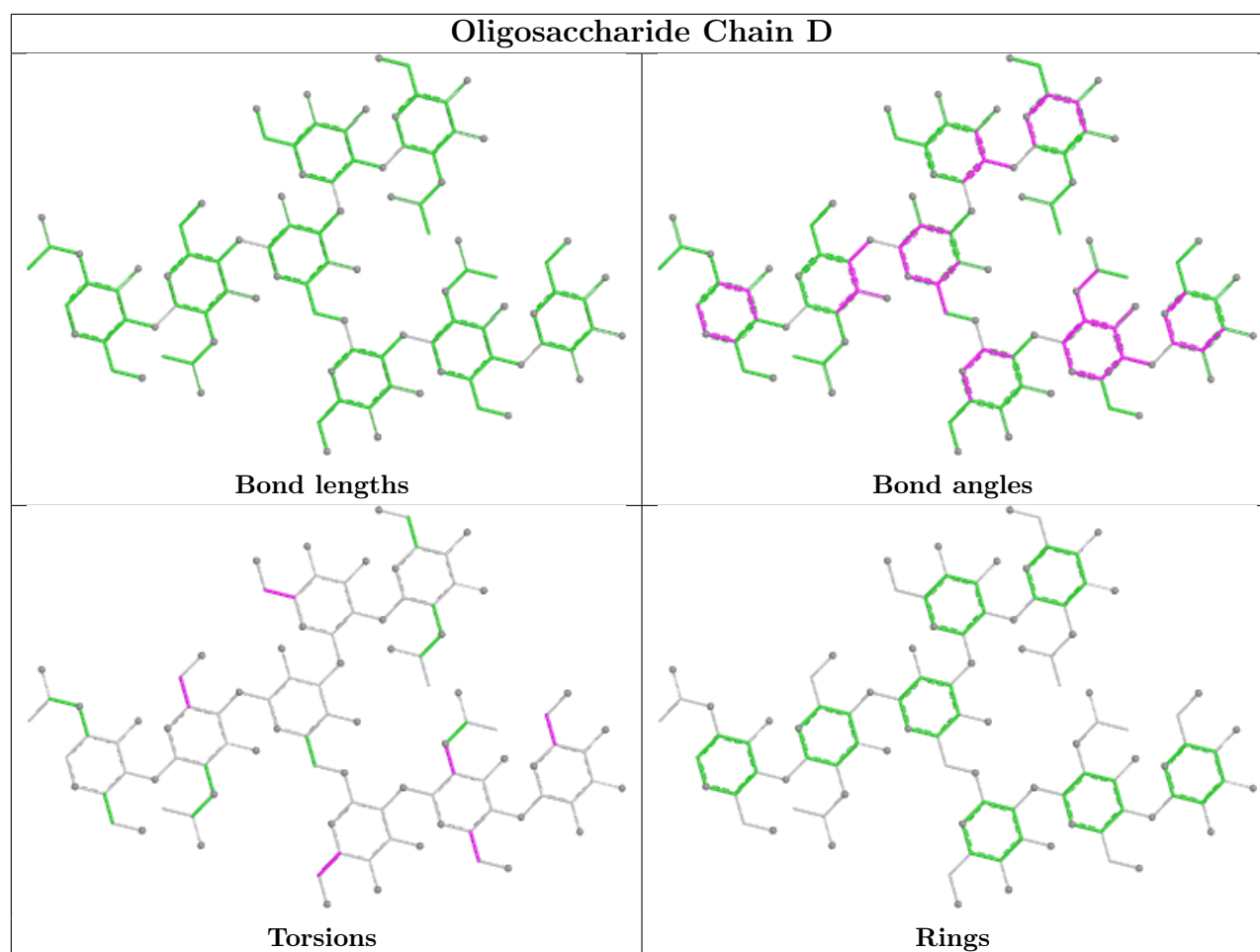
There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	6	GAL	1	0
2	D	2	NAG	6	0
2	C	6	GAL	4	0
2	D	1	NAG	1	0
2	C	1	NAG	1	0
2	C	8	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](#)

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	$\# Z > 2$
3	GOL	A	510	-	5,5,5	0.50	0	5,5,5	0.59	0
3	GOL	A	509	-	5,5,5	0.39	0	5,5,5	0.35	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	GOL	A	510	-	-	2/4/4/4	-
3	GOL	A	509	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	510	GOL	C1-C2-C3-O3
3	A	510	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	510	GOL	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

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	212/212 (100%)	0.12	5 (2%) 59 56	11, 31, 52, 78	1 (0%)
1	B	209/212 (98%)	0.80	40 (19%) 3 3	11, 43, 75, 86	1 (0%)
All	All	421/424 (99%)	0.46	45 (10%) 11 9	11, 34, 73, 86	2 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	275	PHE	3.9
1	B	332	ILE	3.7
1	B	285	HIS	3.6
1	B	237	GLY	3.6
1	B	238	PRO	3.5
1	B	300	TYR	3.3
1	B	302	VAL	3.3
1	B	327	ALA	3.3
1	B	239	SER	3.1
1	B	263	VAL	3.0
1	B	295	GLN	3.0
1	B	299	THR	3.0
1	B	289	THR	2.9
1	B	331	PRO	2.9
1	B	301	ARG	2.9
1	B	445	PRO	2.9
1	B	325	ASN	2.8
1	B	303	VAL	2.8
1	B	324	SER	2.8
1	B	298	SER	2.7
1	B	283	GLU	2.7
1	A	445	PRO	2.7
1	B	266	VAL	2.7
1	B	284	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	277	TRP	2.7
1	B	323	VAL	2.6
1	B	296	TYR	2.6
1	B	287	ALA	2.5
1	A	422	VAL	2.5
1	B	273	VAL	2.4
1	B	328	LEU	2.4
1	A	417	TRP	2.4
1	B	322	LYS	2.4
1	A	447	LYS	2.4
1	B	291	PRO	2.3
1	B	329	PRO	2.3
1	B	282	VAL	2.3
1	B	326	LYS	2.3
1	B	240	VAL	2.2
1	B	292	ARG	2.1
1	A	285	HIS	2.1
1	B	271	PRO	2.1
1	B	276	ASN	2.1
1	B	321	CYS	2.1
1	B	241	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

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

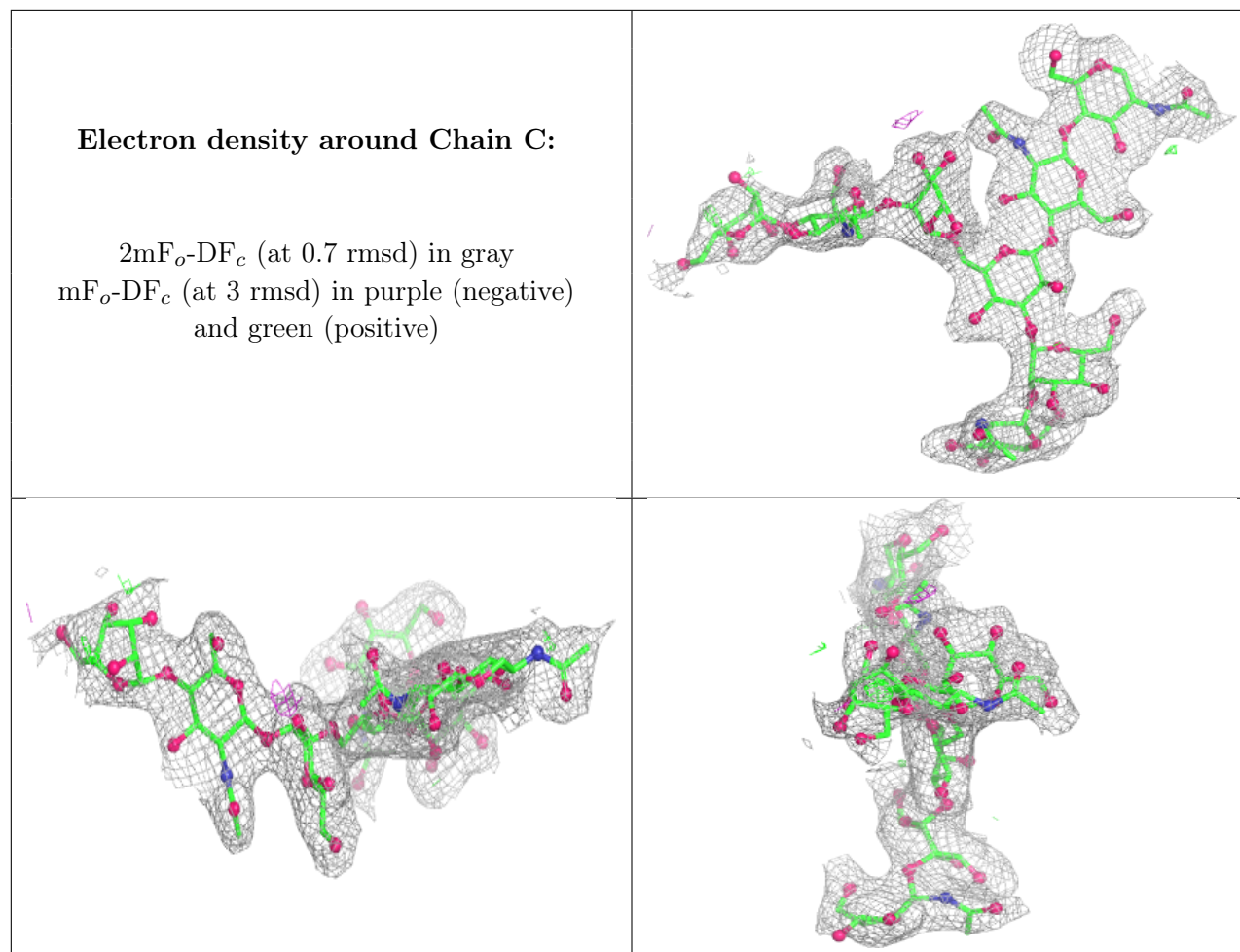
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	1	14/15	0.59	0.21	79,82,83,83	0
2	NAG	D	2	14/15	0.61	0.22	78,82,82,82	0
2	NAG	D	8	14/15	0.73	0.16	75,76,78,78	0
2	GAL	C	6	11/12	0.75	0.21	34,36,37,37	11
2	NAG	C	8	14/15	0.77	0.11	58,61,63,64	0
2	MAN	D	7	11/12	0.79	0.15	73,73,74,75	0
2	MAN	D	3	11/12	0.79	0.14	60,71,73,74	0

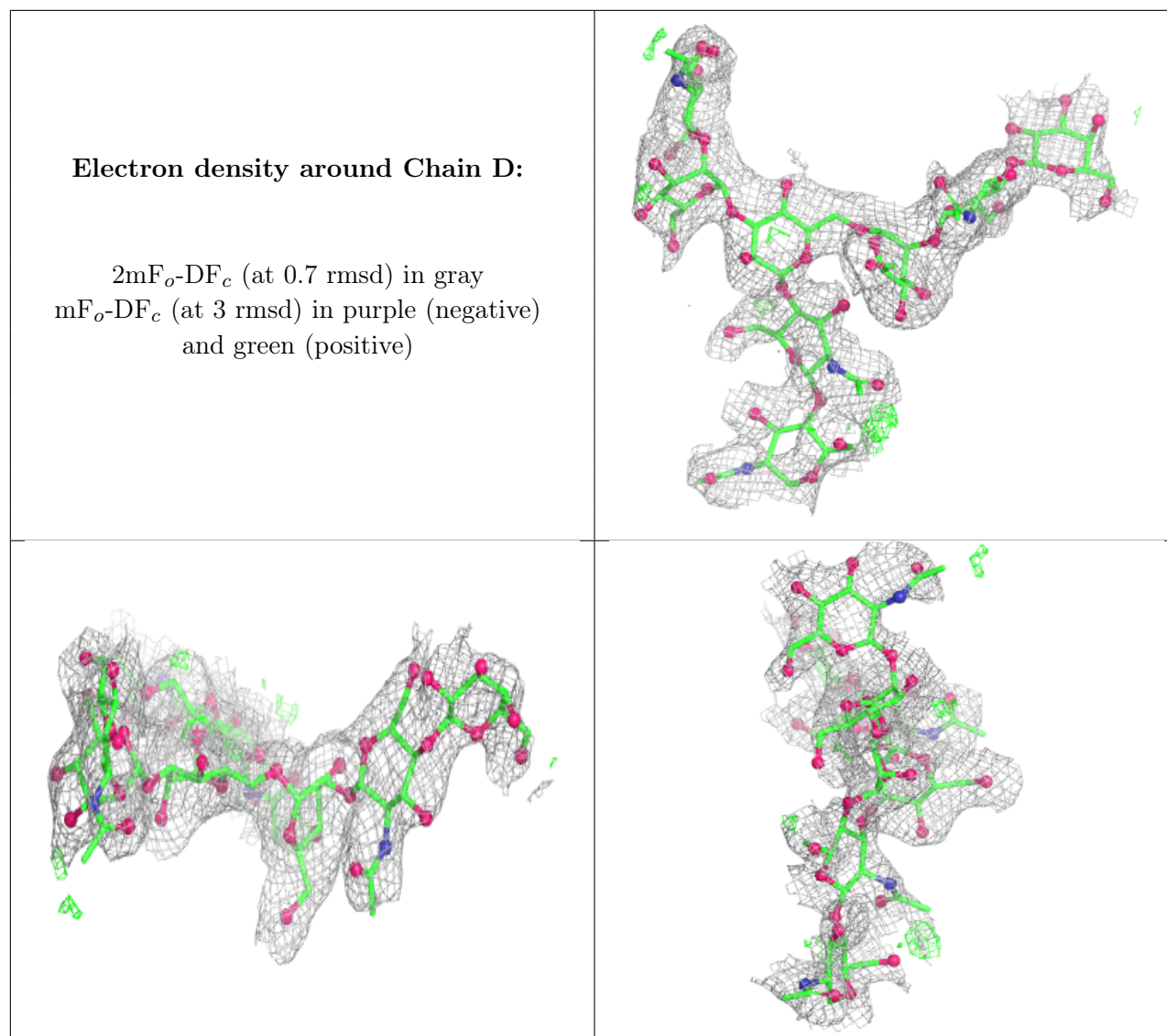
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	5	14/15	0.83	0.14	47,51,55,56	0
2	MAN	C	7	11/12	0.87	0.10	43,44,47,53	0
2	MAN	D	4	11/12	0.89	0.10	52,54,55,56	0
2	GAL	D	6	11/12	0.89	0.17	42,45,46,46	11
2	MAN	C	4	11/12	0.90	0.08	33,35,36,36	0
2	NAG	C	2	14/15	0.90	0.12	29,31,34,34	0
2	MAN	C	3	11/12	0.90	0.09	34,35,41,42	0
2	NAG	C	1	14/15	0.91	0.08	23,27,29,29	0
2	NAG	C	5	14/15	0.92	0.09	34,37,44,44	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](#)

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	GOL	A	509	6/6	0.65	0.15	89,90,90,91	0
3	GOL	A	510	6/6	0.72	0.16	48,49,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.