



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:09 AM UTC

PDB ID : 2DTS / pdb_00002dts
Title : Crystal Structure of the Defucosylated Fc Fragment from Human Immunoglobulin G1
Authors : Matsumiya, S.; Yamaguchi, Y.; Saito, J.; Nagano, M.; Sasakawa, H.; Otaki, S.; Satoh, M.; Shitara, K.; Kato, K.
Deposited on : 2006-07-14
Resolution : 2.20 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

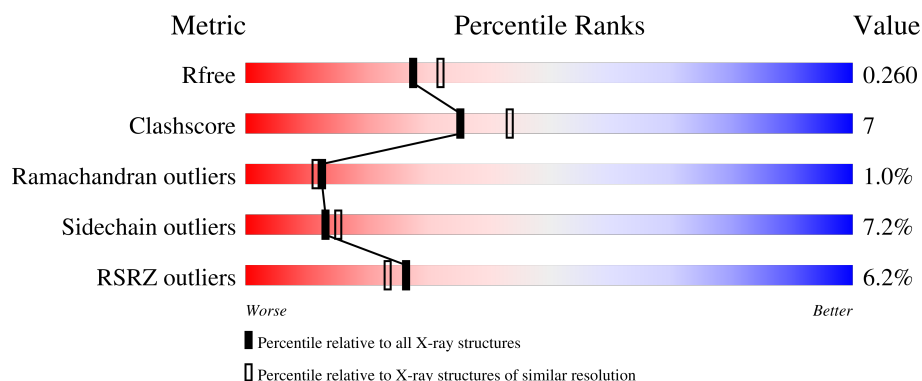
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

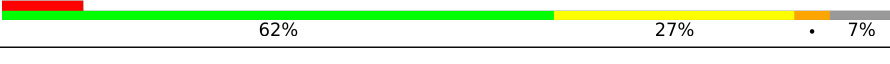
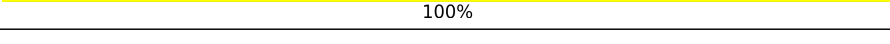
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	
1	B	223	
2	C	6	
3	D	7	

2 Entry composition [i](#)

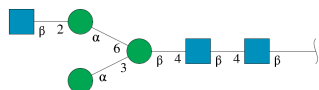
There are 4 unique types of molecules in this entry. The entry contains 3620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

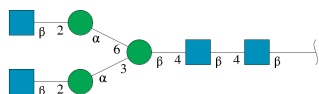
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1684	1073	283	322	6			
1	B	208	Total	C	N	O	S	0	0	0
			1664	1059	280	319	6			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			75	42	3	30			

- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	7	Total	C	N	O	0	0	0
			89	50	4	35			

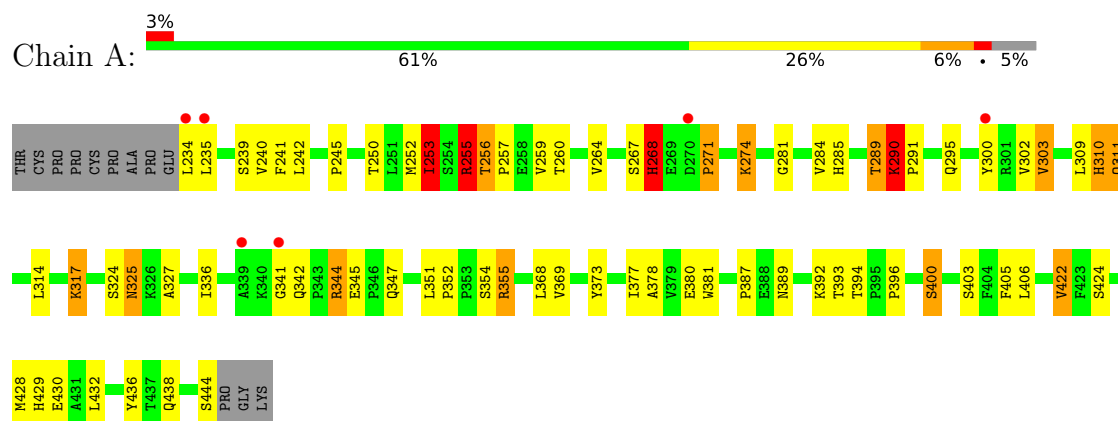
- Molecule 4 is water.

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

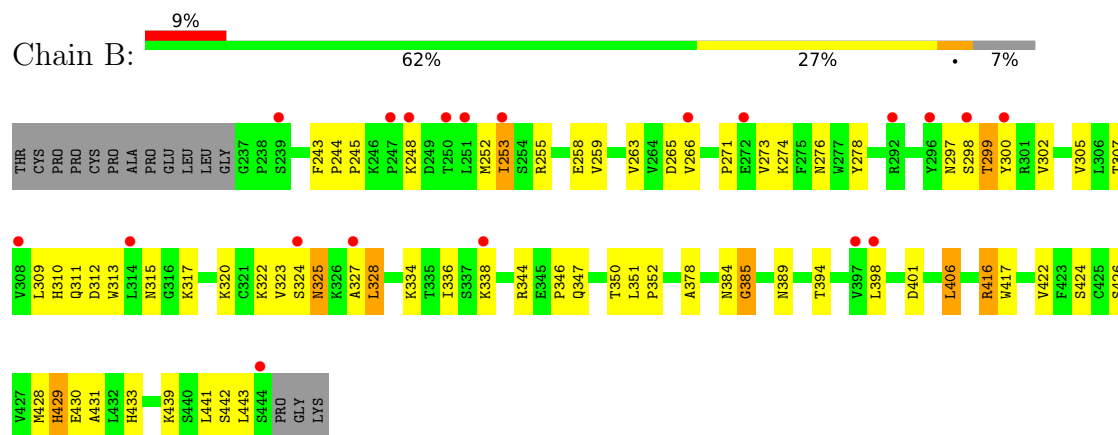
3 Residue-property plots [i](#)

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.

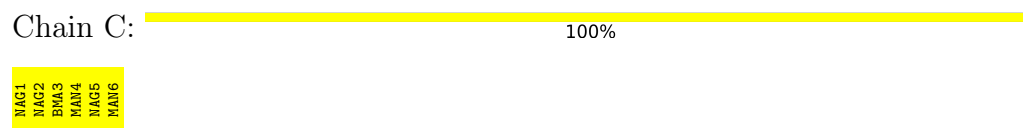
• Molecule 1: Ig gamma-1 chain C region



• Molecule 1: Ig gamma-1 chain C region



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

Chain D:

71%

29%

NAG1	NAG2	MAN3	MAN4	NAG5	MAN6	NAG7
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.47Å 77.69Å 143.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.20) 98.3 (50.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.192 , 0.251 0.206 , 0.260	Depositor DCC
R_{free} test set	1434 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.1	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	0.92	EDS
Total number of atoms	3620	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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, 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	2.08	57/1730 (3.3%)	1.56	21/2357 (0.9%)
1	B	1.71	26/1710 (1.5%)	1.50	14/2330 (0.6%)
All	All	1.91	83/3440 (2.4%)	1.53	35/4687 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	THR	C-O	11.53	1.37	1.24
1	A	256	THR	N-CA	-9.65	1.37	1.46
1	A	430	GLU	CD-OE1	9.37	1.43	1.25
1	A	290	LYS	CB-CG	8.83	1.78	1.52
1	A	377	ILE	C-O	8.69	1.33	1.23
1	B	244	PRO	C-O	8.34	1.33	1.24
1	A	392	LYS	C-O	8.05	1.33	1.23
1	B	352	PRO	CA-C	7.95	1.59	1.52
1	A	444	SER	N-CA	7.41	1.60	1.46
1	A	268	HIS	ND1-CE1	-7.40	1.25	1.32
1	A	271	PRO	C-O	-7.07	1.16	1.23
1	A	387	PRO	N-CA	-7.01	1.38	1.46
1	A	394	THR	CA-CB	6.91	1.64	1.53
1	B	325	ASN	N-CA	6.80	1.53	1.46
1	A	284	VAL	C-O	-6.78	1.15	1.23
1	B	243	PHE	CA-C	-6.76	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	TRP	CA-C	-6.75	1.44	1.52
1	A	403	SER	N-CA	6.55	1.53	1.45
1	A	396	PRO	N-CA	-6.55	1.39	1.47
1	B	406	LEU	CG-CD1	6.54	1.74	1.52
1	A	259	VAL	N-CA	-6.47	1.38	1.46
1	B	347	GLN	CD-NE2	6.44	1.46	1.33
1	A	290	LYS	CD-CE	6.40	1.71	1.52
1	B	433	HIS	CA-C	6.39	1.60	1.52
1	A	369	VAL	CA-CB	6.37	1.62	1.54
1	A	256	THR	C-O	-6.35	1.19	1.24
1	A	345	GLU	N-CA	-6.34	1.36	1.46
1	B	378	ALA	CA-CB	-6.32	1.41	1.53
1	B	385	GLY	N-CA	6.28	1.54	1.45
1	A	268	HIS	CA-CB	6.21	1.63	1.53
1	A	310	HIS	C-O	6.15	1.31	1.24
1	A	268	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	432	LEU	CA-C	-5.93	1.45	1.52
1	A	256	THR	CA-CB	5.93	1.61	1.52
1	B	347	GLN	C-O	-5.91	1.16	1.23
1	A	253	ILE	CA-CB	5.90	1.62	1.54
1	B	398	LEU	CA-C	-5.89	1.45	1.52
1	A	245	PRO	C-O	-5.89	1.16	1.23
1	B	429	HIS	C-O	-5.86	1.16	1.23
1	A	295	GLN	CA-C	-5.86	1.45	1.52
1	B	441	LEU	C-O	-5.86	1.17	1.23
1	A	354	SER	C-O	-5.85	1.17	1.23
1	A	257	PRO	C-O	-5.81	1.17	1.23
1	A	347	GLN	CD-NE2	5.76	1.45	1.33
1	B	320	LYS	CA-C	5.75	1.59	1.52
1	A	436	TYR	C-O	-5.63	1.16	1.23
1	B	351	LEU	CA-C	-5.58	1.47	1.52
1	B	401	ASP	C-O	-5.55	1.16	1.24
1	A	303	VAL	CA-CB	5.51	1.61	1.54
1	A	368	LEU	CA-CB	5.48	1.60	1.53
1	A	240	VAL	C-O	-5.40	1.18	1.24
1	A	239	SER	CA-C	-5.39	1.46	1.52
1	B	417	TRP	CA-C	5.39	1.59	1.52
1	A	355	ARG	CG-CD	5.38	1.68	1.52
1	A	311	GLN	CG-CD	5.37	1.65	1.52
1	B	426	SER	CB-OG	-5.34	1.31	1.42
1	A	394	THR	N-CA	5.32	1.53	1.45
1	B	312	ASP	C-O	5.30	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	LEU	CA-C	-5.30	1.46	1.52
1	A	268	HIS	CE1-NE2	-5.30	1.27	1.32
1	A	405	PHE	C-O	-5.29	1.17	1.23
1	B	406	LEU	CG-CD2	-5.28	1.35	1.52
1	A	260	THR	C-O	-5.27	1.17	1.24
1	A	255	ARG	C-N	5.26	1.38	1.33
1	A	240	VAL	CA-CB	5.19	1.60	1.54
1	A	380	GLU	N-CA	-5.19	1.39	1.45
1	A	345	GLU	C-O	-5.18	1.17	1.24
1	B	430	GLU	C-O	-5.17	1.18	1.24
1	A	373	TYR	C-O	-5.16	1.18	1.24
1	B	351	LEU	C-O	5.16	1.31	1.24
1	A	302	VAL	N-CA	5.14	1.52	1.46
1	A	314	LEU	C-O	-5.14	1.17	1.24
1	B	324	SER	CA-C	5.10	1.58	1.52
1	B	346	PRO	C-O	-5.10	1.17	1.23
1	A	424	SER	C-O	-5.10	1.17	1.23
1	A	241	PHE	CA-C	-5.08	1.46	1.52
1	A	256	THR	CA-C	5.05	1.58	1.52
1	A	264	VAL	C-O	-5.05	1.17	1.23
1	B	324	SER	N-CA	5.05	1.52	1.46
1	A	317	LYS	N-CA	5.02	1.52	1.45
1	B	248	LYS	N-CA	5.01	1.52	1.46
1	A	378	ALA	C-O	-5.01	1.18	1.24
1	A	429	HIS	C-O	5.00	1.30	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	THR	CA-C-N	9.68	130.44	119.99
1	A	256	THR	C-N-CA	9.68	130.44	119.99
1	A	400	SER	N-CA-C	9.31	123.67	111.75
1	B	328	LEU	CA-C-N	8.23	127.80	119.24
1	B	328	LEU	C-N-CA	8.23	127.80	119.24
1	B	315	ASN	N-CA-C	7.75	122.31	113.01
1	B	253	ILE	N-CA-C	7.51	120.44	111.05
1	A	268	HIS	N-CA-C	-7.46	103.17	111.82
1	B	253	ILE	CB-CA-C	-6.94	101.41	112.16
1	B	394	THR	CA-C-N	-6.80	113.37	120.38
1	B	394	THR	C-N-CA	-6.80	113.37	120.38
1	A	393	THR	OG1-CB-CG2	-6.62	96.07	109.30
1	A	311	GLN	CB-CA-C	-6.42	100.14	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	VAL	CB-CA-C	6.19	119.37	110.33
1	A	281	GLY	N-CA-C	-6.13	107.20	115.36
1	A	267	SER	CA-C-N	6.08	129.55	120.31
1	A	267	SER	C-N-CA	6.08	129.55	120.31
1	A	389	ASN	N-CA-C	6.06	120.67	113.16
1	A	289	THR	CB-CA-C	5.90	119.48	109.75
1	A	250	THR	OG1-CB-CG2	-5.82	97.66	109.30
1	A	444	SER	CA-C-O	5.60	130.32	120.80
1	A	342	GLN	N-CA-C	-5.35	103.04	109.72
1	A	392	LYS	CA-C-O	5.24	126.88	120.60
1	B	313	TRP	N-CA-C	-5.23	105.49	111.14
1	A	352	PRO	CA-C-N	5.22	125.14	119.76
1	A	352	PRO	C-N-CA	5.22	125.14	119.76
1	A	268	HIS	CB-CA-C	5.21	120.68	110.67
1	A	422	VAL	N-CA-C	5.21	116.08	108.58
1	B	416	ARG	CG-CD-NE	-5.10	100.79	112.00
1	B	351	LEU	CA-C-N	-5.09	115.14	120.38
1	B	351	LEU	C-N-CA	-5.09	115.14	120.38
1	B	265	ASP	N-CA-C	5.06	118.58	111.90
1	A	341	GLY	CA-C-O	-5.06	118.23	122.33
1	B	244	PRO	CA-C-N	5.02	124.95	119.78
1	B	244	PRO	C-N-CA	5.02	124.95	119.78

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	HIS	Sidechain

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	1684	0	1655	26	1
1	B	1664	0	1630	23	0
2	C	75	0	64	0	0
3	D	89	0	76	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	57	0	0	4	0
4	B	51	0	0	0	0
All	All	3620	0	3425	51	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (51) 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:A:290:LYS:CB	1:A:290:LYS:CG	1.78	1.55
1:A:290:LYS:HE2	1:A:291:PRO:O	1.70	0.90
1:A:268:HIS:ND1	4:A:456:HOH:O	2.13	0.81
1:A:290:LYS:CE	1:A:291:PRO:O	2.32	0.77
1:B:429:HIS:CD2	1:B:431:ALA:H	2.06	0.73
1:A:344:ARG:HG2	1:A:344:ARG:HH11	1.59	0.67
1:A:234:LEU:HD13	4:A:456:HOH:O	1.94	0.66
1:A:290:LYS:CG	1:A:290:LYS:CA	2.74	0.64
1:A:268:HIS:CE1	4:A:456:HOH:O	2.50	0.64
1:B:263:VAL:HG21	1:B:323:VAL:HG11	1.78	0.64
1:A:290:LYS:C	1:A:290:LYS:HG3	2.23	0.64
1:A:252:MET:HB2	1:A:255:ARG:HG3	1.80	0.63
1:B:245:PRO:HD3	1:B:259:VAL:HG12	1.82	0.62
1:B:429:HIS:HD2	1:B:431:ALA:H	1.47	0.62
1:B:252:MET:HG3	1:B:428:MET:HE1	1.84	0.60
1:B:422:VAL:HG22	1:B:442:SER:OG	2.01	0.59
1:A:325:ASN:HD21	1:A:327:ALA:HB3	1.68	0.59
3:D:7:NAG:O3	3:D:7:NAG:H83	2.05	0.57
1:A:290:LYS:CG	1:A:290:LYS:C	2.79	0.56
1:A:234:LEU:N	1:A:234:LEU:HD12	2.20	0.56
1:B:266:VAL:HG21	1:B:302:VAL:HG23	1.89	0.55
1:A:252:MET:HG3	1:A:428:MET:HE1	1.90	0.54
1:A:310:HIS:CD2	1:A:310:HIS:H	2.25	0.54
1:B:263:VAL:CG2	1:B:323:VAL:HG11	2.39	0.53
1:B:273:VAL:HG12	1:B:325:ASN:OD1	2.08	0.53
1:A:235:LEU:HD12	1:A:235:LEU:O	2.10	0.52
1:B:252:MET:HB2	1:B:255:ARG:HG3	1.92	0.51
1:B:278:TYR:CD1	1:B:278:TYR:N	2.78	0.51
1:B:389:ASN:OD1	1:B:389:ASN:N	2.39	0.51
1:B:309:LEU:HB3	1:B:311:GLN:OE1	2.12	0.49
1:A:271:PRO:HB3	1:A:300:TYR:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LEU:C	1:A:406:LEU:HD12	2.38	0.49
1:A:290:LYS:HG3	1:A:290:LYS:O	2.13	0.49
1:B:274:LYS:HE2	1:B:276:ASN:HD21	1.78	0.48
1:A:274:LYS:HG2	1:A:324:SER:HB2	1.96	0.47
1:A:336:ILE:HA	4:A:473:HOH:O	2.16	0.45
1:B:297:ASN:OD1	1:B:299:THR:HG22	2.16	0.45
1:A:355:ARG:HG2	1:A:355:ARG:HH11	1.83	0.43
1:B:258:GLU:HG3	1:B:305:VAL:HG13	2.01	0.43
1:B:350:THR:HG23	1:B:439:LYS:HG2	2.01	0.42
1:A:253:ILE:HD12	1:A:253:ILE:HA	1.93	0.42
1:A:344:ARG:HG2	1:A:344:ARG:NH1	2.31	0.41
1:B:266:VAL:HB	1:B:300:TYR:HB2	2.02	0.41
1:B:336:ILE:HG21	1:B:336:ILE:HD13	1.64	0.41
1:A:309:LEU:O	1:A:310:HIS:C	2.62	0.41
1:B:276:ASN:HB2	1:B:322:LYS:HB3	2.02	0.41
1:A:234:LEU:N	1:A:234:LEU:CD1	2.84	0.41
1:B:297:ASN:O	1:B:299:THR:N	2.54	0.41
3:D:1:NAG:H61	3:D:2:NAG:H82	2.03	0.41
1:B:266:VAL:HG11	1:B:271:PRO:HA	2.03	0.40
1:B:310:HIS:CD2	1:B:310:HIS:H	2.38	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:HIS:NE2	1:A:285:HIS:ND1[4_456]	1.67	0.53

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	209/223 (94%)	205 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	206/223 (92%)	193 (94%)	9 (4%)	4 (2%)	6	4
All	All	415/446 (93%)	398 (96%)	13 (3%)	4 (1%)	12	11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	SER
1	B	327	ALA
1	B	385	GLY
1	B	443	LEU

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	196/206 (95%)	180 (92%)	16 (8%)	10	12
1	B	194/206 (94%)	182 (94%)	12 (6%)	16	20
All	All	390/412 (95%)	362 (93%)	28 (7%)	13	15

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ILE
1	A	255	ARG
1	A	256	THR
1	A	268	HIS
1	A	274	LYS
1	A	289	THR
1	A	290	LYS
1	A	303	VAL
1	A	311	GLN
1	A	317	LYS
1	A	325	ASN
1	A	344	ARG

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Mol	Chain	Res	Type
1	A	351	LEU
1	A	400	SER
1	A	422	VAL
1	A	438	GLN
1	B	253	ILE
1	B	299	THR
1	B	307	THR
1	B	317	LYS
1	B	328	LEU
1	B	334	LYS
1	B	338	LYS
1	B	344	ARG
1	B	384	ASN
1	B	406	LEU
1	B	416	ARG
1	B	424	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	HIS
1	A	315	ASN
1	A	325	ASN
1	A	361	ASN
1	A	418	GLN
1	B	276	ASN
1	B	310	HIS
1	B	347	GLN
1	B	390	ASN
1	B	418	GLN
1	B	421	ASN
1	B	429	HIS
1	B	434	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 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	2,1	14,14,15	1.10	2 (14%)	17,19,21	1.78	6 (35%)
2	NAG	C	2	2	14,14,15	1.27	2 (14%)	17,19,21	2.32	6 (35%)
2	BMA	C	3	2	11,11,12	1.27	1 (9%)	15,15,17	2.22	7 (46%)
2	MAN	C	4	2	11,11,12	0.77	0	15,15,17	2.19	5 (33%)
2	NAG	C	5	2	14,14,15	1.30	2 (14%)	17,19,21	2.71	8 (47%)
2	MAN	C	6	2	11,11,12	1.06	1 (9%)	15,15,17	1.57	3 (20%)
3	NAG	D	1	3,1	14,14,15	0.64	0	17,19,21	0.98	0
3	NAG	D	2	3	14,14,15	0.60	0	17,19,21	1.58	3 (17%)
3	BMA	D	3	3	11,11,12	0.63	0	15,15,17	1.88	4 (26%)
3	MAN	D	4	3	11,11,12	0.82	0	15,15,17	1.42	3 (20%)
3	NAG	D	5	3	14,14,15	0.94	0	17,19,21	1.78	5 (29%)
3	MAN	D	6	3	11,11,12	0.60	0	15,15,17	2.27	5 (33%)
3	NAG	D	7	3	14,14,15	0.87	0	17,19,21	1.66	4 (23%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	C1-C2	3.31	1.56	1.52
2	C	3	BMA	C4-C5	-2.91	1.46	1.53
2	C	5	NAG	C4-C3	2.74	1.59	1.52
2	C	6	MAN	C1-C2	2.63	1.58	1.52
2	C	1	NAG	O5-C1	-2.61	1.39	1.43
2	C	2	NAG	O5-C1	-2.10	1.40	1.43
2	C	5	NAG	O5-C5	-2.08	1.39	1.43
2	C	1	NAG	C1-C2	2.01	1.55	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	NAG	O3-C3-C2	-6.17	96.59	109.40
3	D	6	MAN	C1-O5-C5	5.91	120.11	112.19
2	C	4	MAN	C1-O5-C5	5.35	119.36	112.19
2	C	2	NAG	C2-N2-C7	5.31	130.02	122.90
3	D	3	BMA	C1-O5-C5	5.27	119.24	112.19
2	C	5	NAG	O3-C3-C4	5.03	122.24	110.38
2	C	3	BMA	O3-C3-C4	-4.96	98.69	110.38
2	C	2	NAG	C1-C2-N2	4.80	118.00	110.43
3	D	2	NAG	C1-O5-C5	3.83	117.31	112.19
2	C	2	NAG	O7-C7-N2	3.70	128.51	121.98
2	C	5	NAG	O4-C4-C3	3.62	118.91	110.38
2	C	6	MAN	O2-C2-C3	3.56	117.52	110.15
2	C	1	NAG	O7-C7-C8	-3.35	116.08	122.05
3	D	5	NAG	O3-C3-C2	-3.33	102.49	109.40
2	C	5	NAG	C2-N2-C7	-3.20	118.61	122.90
2	C	4	MAN	C1-C2-C3	3.19	114.28	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	O5-C5-C6	3.10	113.69	107.66
3	D	7	NAG	O5-C5-C6	3.07	113.64	107.66
3	D	6	MAN	O2-C2-C1	3.01	116.11	109.22
2	C	4	MAN	O4-C4-C5	3.00	116.72	109.32
3	D	4	MAN	C1-O5-C5	2.99	116.20	112.19
3	D	7	NAG	C2-N2-C7	-2.96	118.93	122.90
2	C	5	NAG	C1-C2-N2	-2.96	105.77	110.43
3	D	5	NAG	O5-C1-C2	-2.92	106.77	111.29
2	C	5	NAG	C1-O5-C5	2.92	116.10	112.19
2	C	1	NAG	O4-C4-C5	-2.89	102.21	109.32
3	D	7	NAG	C1-C2-N2	-2.88	105.89	110.43
3	D	6	MAN	O3-C3-C4	2.86	117.12	110.38
3	D	2	NAG	O3-C3-C2	-2.86	103.46	109.40
3	D	2	NAG	C2-N2-C7	-2.82	119.12	122.90
2	C	5	NAG	C6-C5-C4	2.80	119.90	113.02
2	C	2	NAG	C8-C7-N2	-2.78	111.50	116.12
3	D	7	NAG	O4-C4-C3	2.77	116.89	110.38
3	D	5	NAG	C8-C7-N2	2.74	120.67	116.12
2	C	1	NAG	O3-C3-C2	2.74	115.08	109.40
2	C	4	MAN	O3-C3-C4	-2.70	104.02	110.38
2	C	6	MAN	C1-O5-C5	2.66	115.75	112.19
2	C	3	BMA	C1-O5-C5	2.60	115.67	112.19
2	C	3	BMA	O6-C6-C5	-2.58	102.56	111.33
3	D	3	BMA	O4-C4-C5	2.54	115.59	109.32
2	C	6	MAN	O3-C3-C2	2.39	114.94	110.05
3	D	3	BMA	O3-C3-C2	2.37	114.89	110.05
3	D	4	MAN	C1-C2-C3	2.35	113.07	109.64
3	D	6	MAN	C1-C2-C3	-2.35	106.22	109.64
3	D	4	MAN	O4-C4-C3	-2.31	104.92	110.38
2	C	3	BMA	O4-C4-C5	-2.28	103.70	109.32
3	D	5	NAG	C1-C2-N2	2.27	114.02	110.43
2	C	3	BMA	O3-C3-C2	2.25	114.64	110.05
2	C	4	MAN	O5-C5-C6	2.22	111.98	107.66
3	D	6	MAN	O5-C5-C6	2.21	111.95	107.66
2	C	5	NAG	C4-C3-C2	-2.18	107.82	111.02
2	C	3	BMA	O2-C2-C1	-2.15	104.30	109.22
2	C	1	NAG	C8-C7-N2	2.14	119.66	116.12
2	C	1	NAG	C6-C5-C4	-2.12	107.81	113.02
2	C	2	NAG	O4-C4-C3	2.11	115.35	110.38
3	D	3	BMA	C1-C2-C3	-2.08	106.62	109.64
2	C	2	NAG	C6-C5-C4	-2.03	108.04	113.02
3	D	5	NAG	O4-C4-C5	-2.02	104.35	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-C2-N2	-2.02	107.26	110.43

There are no chirality outliers.

All (26) torsion outliers are listed below:

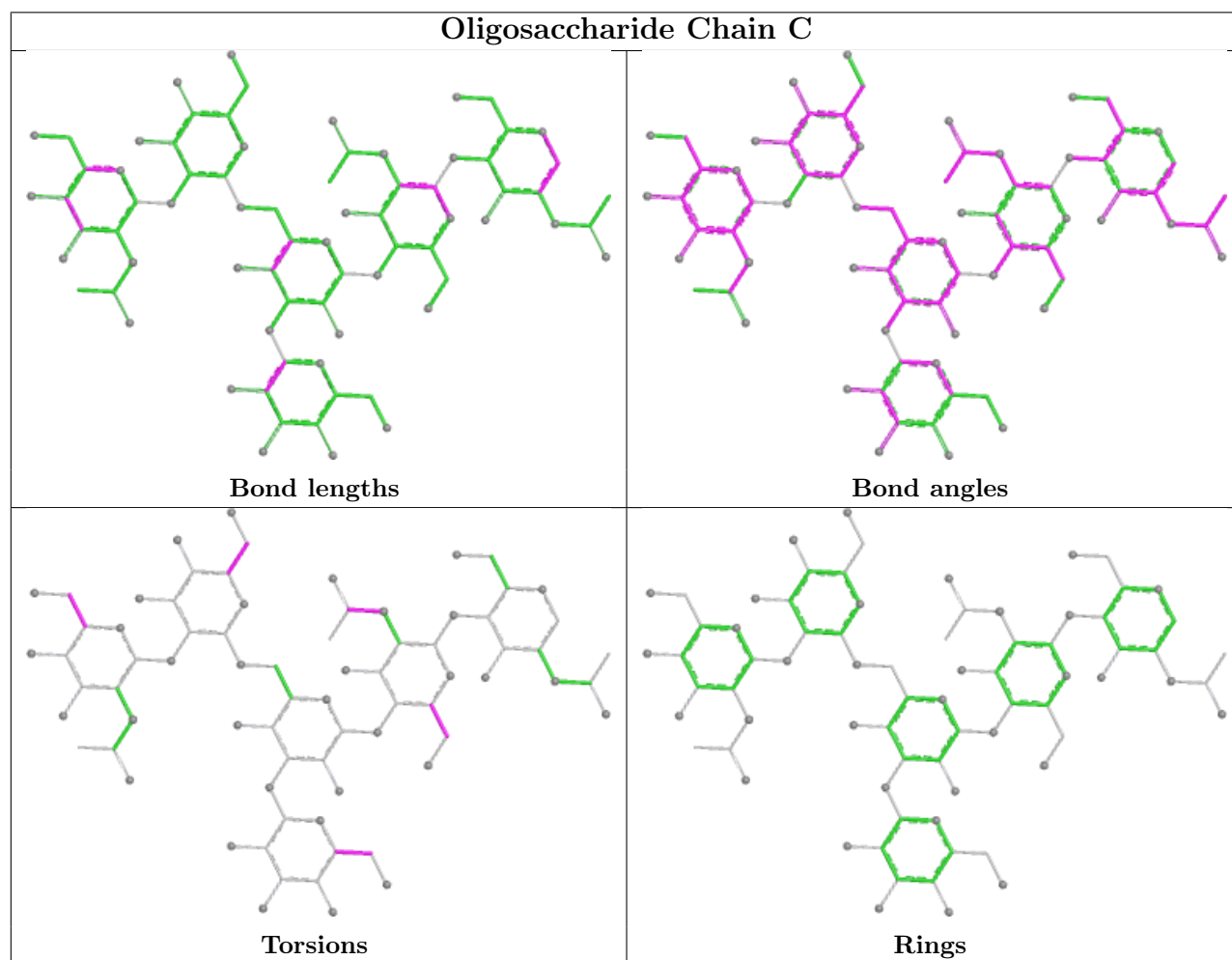
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	5	NAG	C8-C7-N2-C2
3	D	5	NAG	O7-C7-N2-C2
3	D	7	NAG	C8-C7-N2-C2
3	D	7	NAG	O7-C7-N2-C2
2	C	4	MAN	O5-C5-C6-O6
3	D	6	MAN	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
3	D	7	NAG	C4-C5-C6-O6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

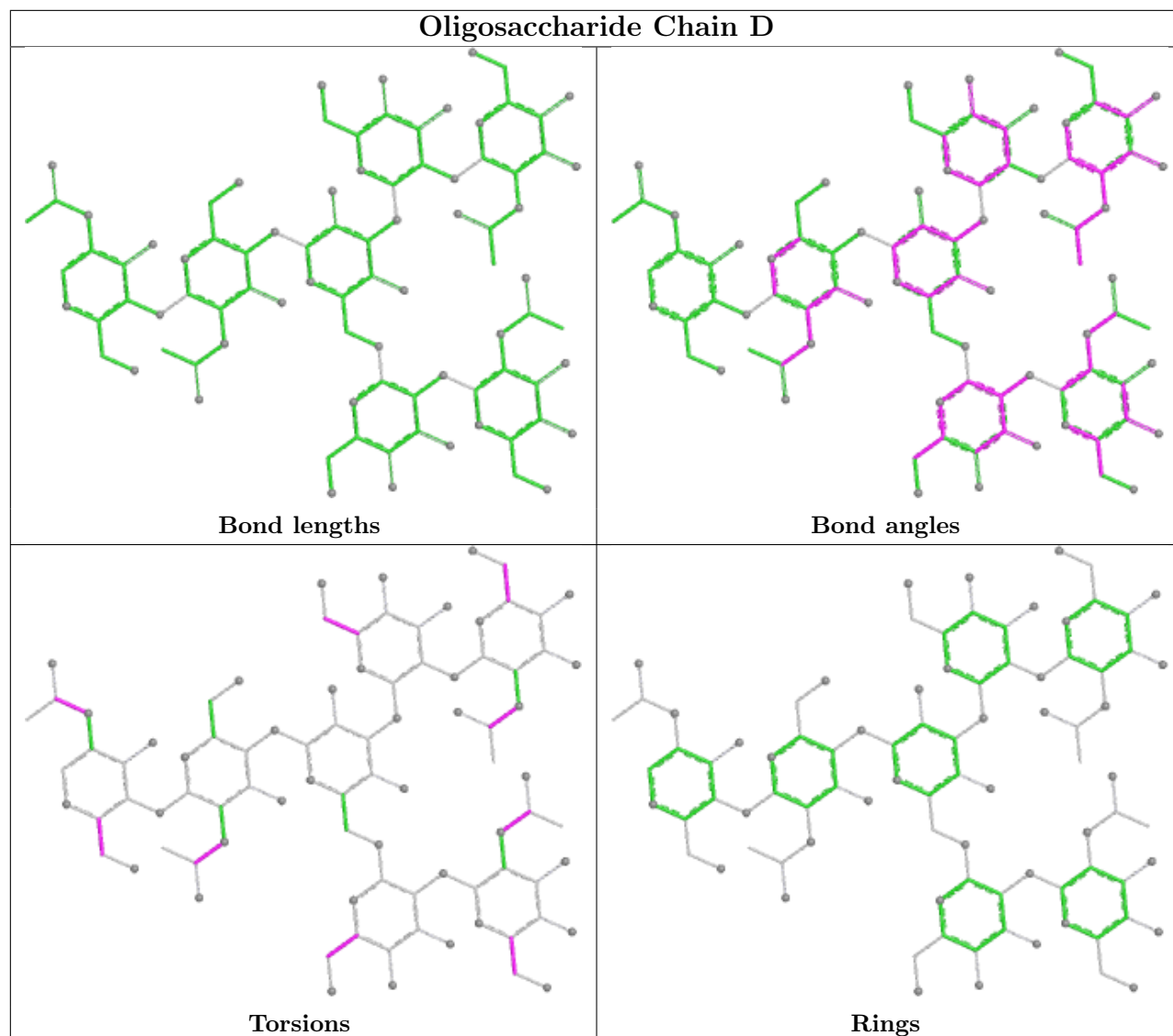
There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
3	D	1	NAG	1	0
3	D	7	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, 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	211/223 (94%)	0.45	6 (2%) 55 52	25, 40, 50, 63	0
1	B	208/223 (93%)	0.90	20 (9%) 13 11	29, 39, 48, 56	0
All	All	419/446 (93%)	0.67	26 (6%) 26 23	25, 40, 49, 63	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	LEU	3.6
1	B	251	LEU	3.1
1	B	327	ALA	2.8
1	B	250	THR	2.6
1	B	300	TYR	2.6
1	B	292	ARG	2.6
1	B	253	ILE	2.5
1	A	300	TYR	2.5
1	B	296	TYR	2.5
1	B	314	LEU	2.5
1	A	270	ASP	2.4
1	B	247	PRO	2.3
1	B	398	LEU	2.3
1	B	298	SER	2.3
1	B	338	LYS	2.3
1	B	397	VAL	2.2
1	A	234	LEU	2.2
1	B	324	SER	2.2
1	B	266	VAL	2.2
1	A	341	GLY	2.2
1	B	272	GLU	2.1
1	B	239	SER	2.1
1	B	248	LYS	2.1
1	A	339	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	308	VAL	2.0
1	B	444	SER	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](#)

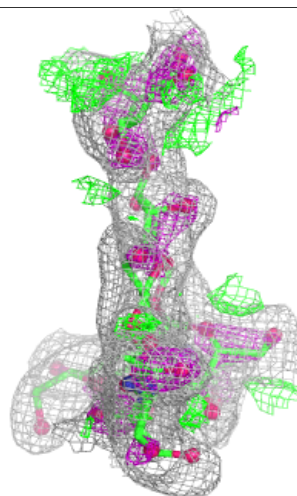
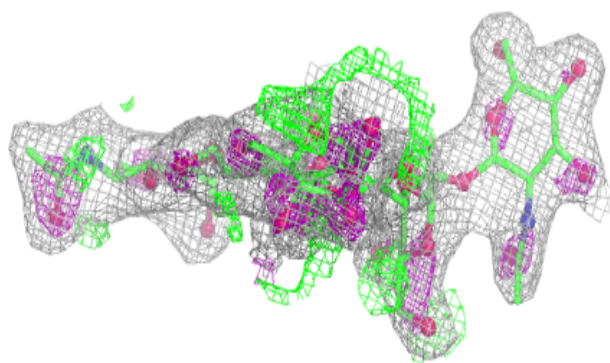
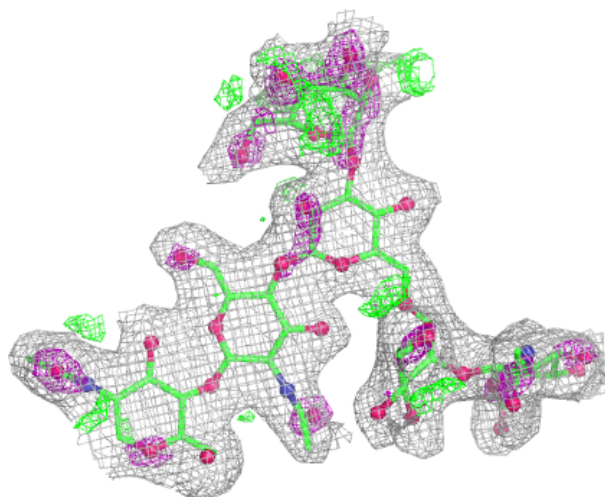
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

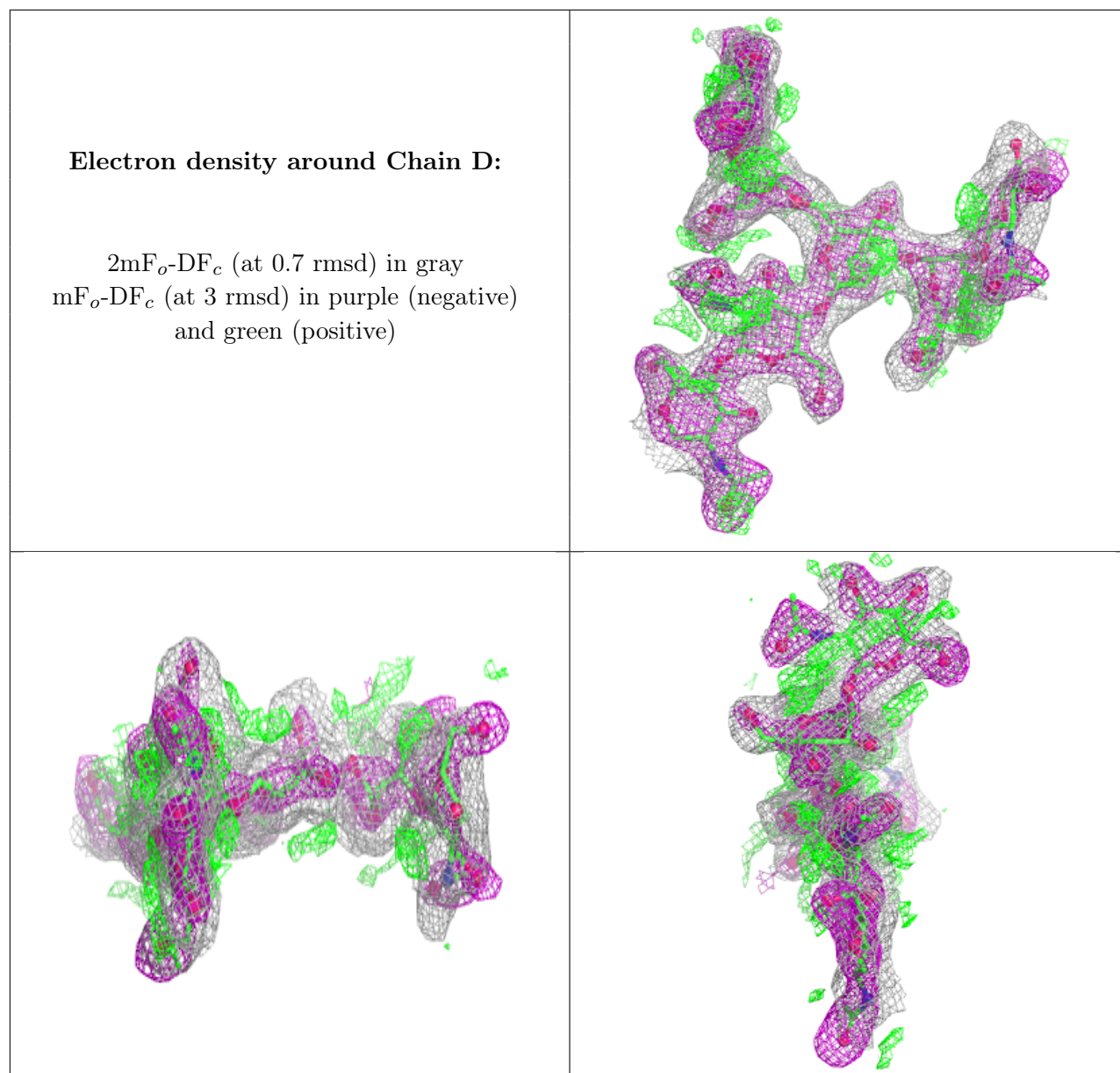
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	5	14/15	0.49	0.18	37,38,40,40	0
3	NAG	D	1	14/15	0.65	0.17	26,32,35,35	0
3	MAN	D	6	11/12	0.67	0.15	26,30,35,37	0
3	NAG	D	2	14/15	0.69	0.16	29,33,36,37	0
3	MAN	D	4	11/12	0.72	0.14	28,30,31,35	0
3	BMA	D	3	11/12	0.74	0.13	27,30,33,35	0
2	MAN	C	6	11/12	0.78	0.14	30,33,35,42	0
3	NAG	D	7	14/15	0.79	0.15	15,24,31,35	0
2	NAG	C	1	14/15	0.83	0.12	28,34,43,44	0
2	NAG	C	2	14/15	0.84	0.12	33,40,44,49	0
2	MAN	C	4	11/12	0.86	0.11	36,40,43,45	0
2	NAG	C	5	14/15	0.88	0.12	34,43,50,51	0
2	BMA	C	3	11/12	0.90	0.09	30,32,36,41	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.