



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:45 AM UTC

PDB ID : 8F8X / pdb_00008f8x
Title : Crystal structure of Nb.X0 bound to the afucosylated human IgG1 fragment crystal form II
Authors : Goldgur, Y.; Ravetch, J.; Gupta, A.; Kao, K.; Oren, D.
Deposited on : 2022-11-22
Resolution : 2.60 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

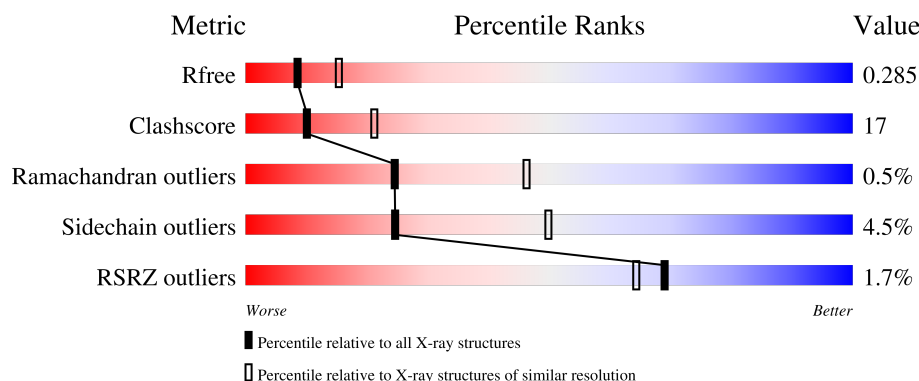
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	224	
1	B	224	
2	C	120	
2	D	120	
3	E	7	

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Mol	Chain	Length	Quality of chain
3	F	7	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5357 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 Uncharacterized protein DKFZp686C11235.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1657	1055	281	314	7			
1	B	207	Total	C	N	O	S	0	0	0
			1661	1057	282	315	7			

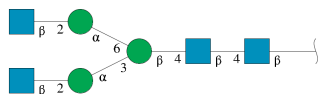
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	ARG	GLU	conflict	UNP Q6MZV7
B	382	ARG	GLU	conflict	UNP Q6MZV7

- Molecule 2 is a protein called Nb.X0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	120	Total	C	N	O	S	0	0	0
			923	578	162	179	4			
2	D	120	Total	C	N	O	S	0	0	0
			923	578	162	179	4			

- 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	E	7	Total	C	N	O		0	0	0
			89	50	4	35				

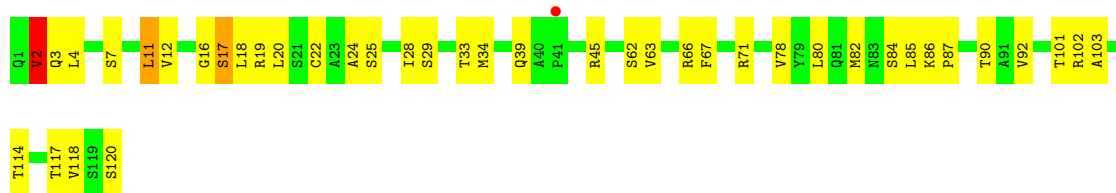
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	7	Total	C	N	O	0	0	0
			89	50	4	35			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	5	Total	O	0	0
			5	5		
4	C	3	Total	O	0	0
			3	3		



- 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



- 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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.58Å 92.23Å 76.50Å 90.00° 117.04° 90.00°	Depositor
Resolution (Å)	46.12 – 2.60 46.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.9 (46.12-2.60) 88.9 (46.12-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.215 , 0.285 0.214 , 0.285	Depositor DCC
R_{free} test set	2020 reflections (9.46%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5357	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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, MAN, BMA

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	0.67	1/1703 (0.1%)	0.99	13/2318 (0.6%)
1	B	0.58	1/1707 (0.1%)	1.01	14/2324 (0.6%)
2	C	0.55	1/945 (0.1%)	0.77	0/1280
2	D	0.54	1/945 (0.1%)	0.90	5/1280 (0.4%)
All	All	0.60	4/5300 (0.1%)	0.94	32/7202 (0.4%)

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	2
1	B	0	4
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	360	LYS	CE-NZ	12.12	1.85	1.49
1	B	314	LEU	CG-CD2	9.08	1.82	1.52
2	C	32	LYS	CE-NZ	-6.18	1.30	1.49
2	D	2	VAL	CB-CG1	-5.75	1.33	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	LEU	CA-CB-CG	12.81	161.14	116.30
1	B	344	ARG	CG-CD-NE	11.30	136.86	112.00
1	A	248	LYS	CD-CE-NZ	-9.40	81.82	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ARG	CB-CG-CD	-8.86	90.93	111.30
1	A	360	LYS	CB-CG-CD	8.03	129.76	111.30
1	B	274	LYS	CA-CB-CG	7.87	129.84	114.10
2	D	2	VAL	CG1-CB-CG2	-7.86	93.52	110.80
1	B	288	LYS	CB-CG-CD	7.77	129.18	111.30
1	A	326	LYS	CA-CB-CG	7.77	129.64	114.10
2	D	102	ARG	CA-CB-CG	7.49	129.09	114.10
1	B	274	LYS	CB-CA-C	-7.32	96.69	109.64
1	A	360	LYS	N-CA-C	7.30	121.08	110.28
1	B	438	GLN	CA-CB-CG	7.06	128.21	114.10
1	B	438	GLN	N-CA-C	6.95	120.92	110.14
1	A	417	TRP	CA-C-N	6.74	129.86	120.29
1	A	417	TRP	C-N-CA	6.74	129.86	120.29
1	A	253	ILE	CB-CA-C	-6.39	97.27	111.77
1	A	360	LYS	CD-CE-NZ	-6.05	92.55	111.90
2	D	102	ARG	CG-CD-NE	6.02	125.25	112.00
1	B	274	LYS	CB-CG-CD	-5.79	97.97	111.30
2	D	2	VAL	N-CA-C	5.60	116.93	109.37
1	B	314	LEU	CD1-CG-CD2	5.48	122.86	110.80
1	A	439	LYS	N-CA-CB	-5.43	101.92	110.77
1	B	344	ARG	CA-CB-CG	5.35	124.80	114.10
1	B	314	LEU	CB-CG-CD2	-5.34	94.68	110.70
2	D	102	ARG	CB-CG-CD	-5.28	99.15	111.30
1	B	438	GLN	CB-CA-C	-5.26	100.23	109.71
1	A	248	LYS	CB-CG-CD	-5.21	99.32	111.30
1	B	288	LYS	CG-CD-CE	5.19	123.24	111.30
1	A	317	LYS	CA-C-N	-5.18	115.17	122.94
1	A	317	LYS	C-N-CA	-5.18	115.17	122.94
1	A	439	LYS	CB-CG-CD	-5.15	99.44	111.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	GLU	Sidechain
1	A	355	ARG	Sidechain
1	B	255	ARG	Sidechain
1	B	274	LYS	Peptide
1	B	309	LEU	Peptide
1	B	438	GLN	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	1657	0	1630	59	1
1	B	1661	0	1632	70	1
2	C	923	0	884	19	0
2	D	923	0	884	38	0
3	E	89	0	76	1	0
3	F	89	0	76	1	0
4	A	7	0	0	1	0
4	B	5	0	0	1	0
4	C	3	0	0	1	0
All	All	5357	0	5182	182	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 17.

All (182) 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:314:LEU:CD2	1:B:314:LEU:CG	1.82	1.57
1:A:360:LYS:CE	1:A:360:LYS:NZ	1.85	1.38
1:A:318:GLU:HG3	1:A:337:SER:HB2	1.43	0.99
1:B:314:LEU:CD2	1:B:314:LEU:CB	2.42	0.97
1:B:311:GLN:HA	1:B:314:LEU:HD22	1.45	0.97
2:D:2:VAL:CG1	2:D:28:ILE:HG21	1.98	0.93
1:B:314:LEU:CD2	1:B:314:LEU:HB3	2.04	0.86
1:A:318:GLU:HG3	1:A:337:SER:CB	2.08	0.83
1:B:312:ASP:HB3	1:B:317:LYS:HE2	1.60	0.83
1:B:350:THR:HB	1:B:441:LEU:HD22	1.59	0.83
2:D:90:THR:HG23	2:D:117:THR:HA	1.62	0.80
2:D:18:LEU:HD12	2:D:19:ARG:H	1.48	0.78
2:D:84:SER:HB3	2:D:86:LYS:HE2	1.66	0.77
1:B:424:SER:HB2	1:B:438:GLN:HE21	1.52	0.75
1:A:360:LYS:NZ	1:A:360:LYS:CD	2.51	0.74
1:A:280:ASP:OD1	1:A:317:LYS:HD2	1.87	0.73
1:A:379:VAL:HG23	1:A:427:VAL:HG12	1.71	0.72
2:D:63:VAL:HB	2:D:67:PHE:CD2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:LEU:HG	2:D:82:MET:HE3	1.71	0.72
1:B:272:GLU:N	1:B:272:GLU:OE2	2.21	0.71
1:B:424:SER:CB	1:B:438:GLN:HE21	2.04	0.71
1:B:349:TYR:HD2	1:B:368:LEU:HD23	1.57	0.70
2:C:51:ILE:HD13	2:C:71:ARG:HB2	1.74	0.70
1:A:318:GLU:CG	1:A:337:SER:HB2	2.21	0.69
1:A:348:VAL:HG22	1:A:369:VAL:HG22	1.74	0.68
2:D:34:MET:HE3	2:D:78:VAL:HB	1.75	0.68
1:A:312:ASP:OD2	1:A:317:LYS:HG3	1.94	0.68
1:A:337:SER:OG	4:A:501:HOH:O	2.11	0.68
2:D:67:PHE:HD1	2:D:82:MET:HA	1.60	0.67
2:D:28:ILE:HG13	2:D:29:SER:N	2.10	0.66
1:B:424:SER:HB2	1:B:438:GLN:NE2	2.12	0.65
1:B:262:VAL:HG22	1:B:303:VAL:HG22	1.80	0.64
1:B:274:LYS:HG3	1:B:324:SER:H	1.62	0.64
1:A:388:GLU:OE2	1:A:416:ARG:NH2	2.32	0.63
1:B:348:VAL:HG21	1:B:427:VAL:HG11	1.81	0.62
2:D:2:VAL:HG13	2:D:28:ILE:HG21	1.81	0.62
1:A:358:MET:HG3	1:A:363:VAL:HG11	1.82	0.61
1:B:360:LYS:HD2	1:B:361:ASN:H	1.65	0.61
2:C:44:GLU:OE1	2:C:44:GLU:N	2.29	0.59
2:D:18:LEU:HD12	2:D:19:ARG:N	2.17	0.59
2:D:67:PHE:CE1	2:D:82:MET:HB3	2.37	0.59
1:B:438:GLN:O	1:B:439:LYS:HD2	2.03	0.59
2:D:2:VAL:HG11	2:D:28:ILE:HG21	1.84	0.59
1:B:288:LYS:HG3	1:B:305:VAL:O	2.03	0.59
2:D:3:GLN:HA	2:D:3:GLN:OE1	2.02	0.59
2:D:101:THR:HG22	2:D:103:ALA:H	1.69	0.58
2:C:23:ALA:HA	2:C:77:THR:HG22	1.86	0.58
1:B:284:VAL:O	1:B:285:HIS:ND1	2.37	0.57
1:B:356:GLU:O	1:B:359:THR:HG23	2.04	0.57
2:C:101:THR:HG22	2:C:103:ALA:N	2.19	0.57
1:A:253:ILE:HG13	1:A:254:SER:N	2.17	0.57
1:A:274:LYS:HG2	1:A:324:SER:HB3	1.86	0.57
1:A:319:TYR:O	1:A:335:THR:HA	2.03	0.57
1:A:348:VAL:HG12	1:A:439:LYS:HG2	1.87	0.57
2:D:85:LEU:C	2:D:86:LYS:HD3	2.30	0.56
2:C:82:MET:HB3	2:C:85:LEU:HD21	1.87	0.56
1:B:274:LYS:HZ3	1:B:324:SER:CB	2.18	0.56
1:B:311:GLN:HA	1:B:314:LEU:CD2	2.30	0.56
2:C:12:VAL:O	2:C:118:VAL:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:GLY:C	2:D:85:LEU:HD12	2.31	0.55
3:E:2:NAG:H5	3:F:4:MAN:O4	2.07	0.55
1:A:424:SER:OG	1:A:438:GLN:NE2	2.39	0.55
1:A:310:HIS:CE1	1:A:311:GLN:HG3	2.42	0.55
1:A:382:ARG:HB2	1:A:424:SER:HB3	1.88	0.55
2:D:84:SER:HB3	2:D:86:LYS:CE	2.34	0.55
2:D:62:SER:O	2:D:66:ARG:NH1	2.39	0.55
1:B:312:ASP:HB3	1:B:317:LYS:CE	2.34	0.54
1:B:284:VAL:HG21	1:B:306:LEU:HD21	1.90	0.54
1:B:275:PHE:N	4:B:501:HOH:O	2.36	0.54
2:D:67:PHE:CD1	2:D:82:MET:HA	2.40	0.54
1:B:279:VAL:HG23	1:B:284:VAL:HG11	1.89	0.53
1:B:309:LEU:HD22	1:B:309:LEU:H	1.73	0.53
1:B:274:LYS:HZ3	1:B:324:SER:HB3	1.73	0.53
1:A:279:VAL:O	1:A:282:VAL:HG12	2.09	0.52
1:B:253:ILE:HD12	1:B:254:SER:N	2.25	0.52
1:A:360:LYS:HG3	1:A:362:GLN:H	1.73	0.52
1:B:283:GLU:HG2	1:B:285:HIS:CE1	2.44	0.52
2:D:101:THR:HG22	2:D:103:ALA:N	2.25	0.52
2:D:11:LEU:HD13	2:D:117:THR:O	2.10	0.52
1:B:312:ASP:HB2	1:B:319:TYR:OH	2.11	0.51
2:C:101:THR:HG22	2:C:103:ALA:H	1.75	0.51
1:B:274:LYS:CG	1:B:324:SER:H	2.24	0.51
1:A:272:GLU:O	1:A:325:ASN:ND2	2.44	0.51
1:B:314:LEU:HB3	1:B:314:LEU:HD23	1.88	0.51
1:A:390:ASN:OD1	1:A:411:THR:HB	2.11	0.50
1:B:311:GLN:CA	1:B:314:LEU:HD22	2.30	0.50
1:B:320:LYS:NZ	1:B:333:GLU:OE1	2.44	0.50
1:B:274:LYS:NZ	1:B:324:SER:HB3	2.27	0.50
1:B:296:TYR:O	2:C:33:THR:HG21	2.12	0.50
1:A:428:MET:HG2	1:A:436:TYR:HD1	1.77	0.50
2:D:4:LEU:HD23	2:D:24:ALA:HA	1.93	0.50
1:B:283:GLU:HG2	1:B:285:HIS:HE1	1.77	0.50
1:B:416:ARG:O	1:B:421:ASN:HB2	2.12	0.49
1:A:393:THR:HG22	1:A:408:SER:OG	2.12	0.49
2:D:80:LEU:HD23	2:D:82:MET:HE2	1.94	0.49
1:B:286:ASN:O	1:B:286:ASN:ND2	2.45	0.49
1:B:274:LYS:NZ	1:B:324:SER:CB	2.76	0.49
1:A:320:LYS:HE2	1:A:335:THR:OG1	2.12	0.49
1:A:279:VAL:HG22	1:A:319:TYR:CE1	2.48	0.49
1:B:349:TYR:CD2	1:B:368:LEU:HD23	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LYS:HD2	1:B:323:VAL:HA	1.95	0.48
1:B:320:LYS:HG3	1:B:335:THR:OG1	2.12	0.48
1:B:418:GLN:HA	1:B:443:LEU:CD2	2.44	0.48
2:D:39:GLN:HB2	2:D:45:ARG:HA	1.95	0.47
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.95	0.47
1:A:284:VAL:HG21	1:A:306:LEU:HD11	1.96	0.47
1:A:412:VAL:HG11	1:A:423:PHE:CE2	2.48	0.47
1:B:240:VAL:HG22	1:B:263:VAL:HG22	1.97	0.47
1:A:322:LYS:HE3	1:A:331:PRO:HG2	1.95	0.47
1:A:360:LYS:HE2	1:A:361:ASN:HB2	1.95	0.47
1:B:338:LYS:NZ	1:B:430:GLU:OE2	2.47	0.47
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.50	0.47
2:C:72:ASP:OD1	2:C:75:LYS:N	2.44	0.47
2:C:19:ARG:NE	4:C:201:HOH:O	2.32	0.46
1:B:269:GLU:HG2	2:C:31:TYR:CE2	2.50	0.46
2:D:4:LEU:HD23	2:D:4:LEU:HA	1.69	0.46
1:B:278:TYR:HE1	1:B:322:LYS:HD3	1.81	0.46
2:C:90:THR:HA	2:C:116:VAL:O	2.15	0.46
2:C:37:TYR:OH	2:C:98:ASP:OD2	2.32	0.46
1:A:414:LYS:O	1:A:418:GLN:HG3	2.16	0.46
1:A:270:ASP:O	1:A:270:ASP:CG	2.59	0.46
1:B:252:MET:HG2	1:B:428:MET:HE1	1.97	0.45
1:B:424:SER:CB	1:B:438:GLN:NE2	2.76	0.45
1:B:310:HIS:O	1:B:314:LEU:HD13	2.16	0.45
1:A:328:LEU:HA	1:A:328:LEU:HD23	1.66	0.45
2:C:85:LEU:C	2:C:86:LYS:HD3	2.41	0.45
1:A:310:HIS:CG	1:A:311:GLN:N	2.83	0.45
1:A:438:GLN:HG3	1:A:439:LYS:N	2.30	0.45
1:A:290:LYS:HE2	1:A:303:VAL:CG1	2.47	0.45
1:A:354:SER:HB3	1:B:349:TYR:HB3	1.99	0.45
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.52	0.44
1:A:413:ASP:O	1:A:416:ARG:N	2.49	0.44
1:B:250:THR:O	1:B:314:LEU:HD11	2.18	0.44
2:D:12:VAL:O	2:D:118:VAL:HA	2.18	0.44
2:D:17:SER:HA	2:D:82:MET:O	2.17	0.44
1:A:296:TYR:O	2:D:33:THR:OG1	2.32	0.44
1:A:332:ILE:HD13	2:C:106:TYR:CE1	2.52	0.44
2:C:68:THR:OG1	2:C:81:GLN:HB3	2.18	0.43
1:A:355:ARG:C	1:A:357:GLU:H	2.26	0.43
1:B:274:LYS:HD2	1:B:323:VAL:CA	2.48	0.43
1:A:306:LEU:HD23	1:A:307:THR:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:O	1:A:311:GLN:N	2.52	0.43
1:B:267:SER:OG	1:B:268:HIS:N	2.50	0.43
1:B:360:LYS:HD2	1:B:360:LYS:HA	1.79	0.43
1:B:309:LEU:O	1:B:311:GLN:N	2.51	0.43
1:A:355:ARG:C	1:A:357:GLU:N	2.76	0.43
2:D:11:LEU:HA	2:D:117:THR:O	2.18	0.43
1:A:320:LYS:HD3	1:A:333:GLU:CD	2.44	0.42
1:A:360:LYS:HG3	1:A:361:ASN:N	2.35	0.42
2:D:34:MET:HG3	2:D:71:ARG:CZ	2.49	0.42
1:B:284:VAL:C	1:B:285:HIS:ND1	2.78	0.42
2:D:87:PRO:HA	2:D:118:VAL:CG1	2.50	0.42
1:B:247:PRO:O	1:B:251:LEU:HD23	2.20	0.42
2:D:18:LEU:O	2:D:82:MET:HG3	2.18	0.42
1:B:275:PHE:CD2	1:B:304:SER:HB2	2.55	0.42
1:B:390:ASN:O	1:B:410:LEU:HD12	2.19	0.42
2:D:92:VAL:HA	2:D:114:THR:O	2.19	0.42
1:B:356:GLU:OE1	1:B:356:GLU:C	2.63	0.42
2:D:28:ILE:H	2:D:28:ILE:HG23	1.37	0.42
1:B:273:VAL:HG23	1:B:274:LYS:O	2.20	0.42
1:B:338:LYS:HG2	1:B:339:ALA:O	2.20	0.42
2:D:90:THR:HG23	2:D:117:THR:CA	2.43	0.42
1:A:290:LYS:HE2	1:A:303:VAL:HG11	2.02	0.41
1:B:344:ARG:NH2	1:B:401:ASP:OD2	2.53	0.41
2:C:2:VAL:CG1	2:C:112:GLN:HE22	2.34	0.41
1:B:275:PHE:CE2	1:B:304:SER:HB2	2.55	0.41
1:A:271:PRO:HB2	1:A:292:ARG:CZ	2.50	0.41
2:C:84:SER:O	2:C:86:LYS:HE2	2.20	0.41
1:A:311:GLN:O	1:A:315:ASN:N	2.54	0.41
2:D:16:GLY:O	2:D:85:LEU:HD12	2.20	0.41
1:A:406:LEU:HD12	1:A:406:LEU:C	2.46	0.41
2:D:20:LEU:HG	2:D:82:MET:CE	2.47	0.41
1:A:414:LYS:HB3	1:A:414:LYS:HE2	1.80	0.41
1:A:279:VAL:HG22	1:A:319:TYR:HE1	1.85	0.40
2:C:18:LEU:HD23	2:C:18:LEU:HA	1.83	0.40
1:A:270:ASP:OD1	1:A:325:ASN:CG	2.64	0.40
1:A:358:MET:HG3	1:A:363:VAL:CG1	2.49	0.40
1:A:377:ILE:HG12	1:A:378:ALA:N	2.37	0.40
1:B:406:LEU:C	1:B:406:LEU:HD12	2.47	0.40
1:B:250:THR:HB	1:B:314:LEU:HD12	2.02	0.40
1:B:253:ILE:H	1:B:253:ILE:HG13	1.57	0.40
1:A:369:VAL:HG12	1:A:372:PHE:CD1	2.57	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:382:ARG:NH2	1:B:254:SER:OG[4_555]	2.07	0.13

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	204/224 (91%)	197 (97%)	6 (3%)	1 (0%)	24	46
1	B	205/224 (92%)	197 (96%)	7 (3%)	1 (0%)	24	46
2	C	118/120 (98%)	115 (98%)	2 (2%)	1 (1%)	16	34
2	D	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
All	All	645/688 (94%)	626 (97%)	16 (2%)	3 (0%)	24	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	310	HIS
1	A	310	HIS
2	C	4	LEU

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	193/208 (93%)	189 (98%)	4 (2%)	47	73
1	B	193/208 (93%)	182 (94%)	11 (6%)	18	40
2	C	95/95 (100%)	91 (96%)	4 (4%)	26	52
2	D	95/95 (100%)	88 (93%)	7 (7%)	13	29
All	All	576/606 (95%)	550 (96%)	26 (4%)	24	50

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	VAL
1	A	310	HIS
1	A	399	ASP
1	A	427	VAL
1	B	239	SER
1	B	253	ILE
1	B	273	VAL
1	B	282	VAL
1	B	304	SER
1	B	309	LEU
1	B	365	LEU
1	B	412	VAL
1	B	424	SER
1	B	440	SER
1	B	443	LEU
2	C	11	LEU
2	C	18	LEU
2	C	25	SER
2	C	64	LYS
2	D	2	VAL
2	D	7	SER
2	D	11	LEU
2	D	17	SER
2	D	22	CYS
2	D	25	SER
2	D	120	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	ASN

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Mol	Chain	Res	Type
1	A	438	GLN
1	B	286	ASN
1	B	325	ASN
1	B	438	GLN
2	C	5	GLN
2	C	73	ASN
2	C	76	ASN
2	C	112	GLN
2	D	81	GLN
2	D	115	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 ⓘ

14 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	E	1	3,1	14,14,15	0.53	0	17,19,21	0.62	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.52	0
3	BMA	E	3	3	11,11,12	0.86	1 (9%)	15,15,17	1.22	1 (6%)
3	MAN	E	4	3	11,11,12	1.82	4 (36%)	15,15,17	0.71	0
3	NAG	E	5	3	14,14,15	0.42	0	17,19,21	0.53	0
3	MAN	E	6	3	11,11,12	1.27	1 (9%)	15,15,17	0.87	0
3	NAG	E	7	3	14,14,15	0.59	0	17,19,21	1.15	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.20	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	2	3	14,14,15	0.68	1 (7%)	17,19,21	0.45	0
3	BMA	F	3	3	11,11,12	0.79	0	15,15,17	1.40	3 (20%)
3	MAN	F	4	3	11,11,12	1.01	1 (9%)	15,15,17	1.20	1 (6%)
3	NAG	F	5	3	14,14,15	0.59	0	17,19,21	0.66	1 (5%)
3	MAN	F	6	3	11,11,12	1.19	2 (18%)	15,15,17	1.30	1 (6%)
3	NAG	F	7	3	14,14,15	0.36	0	17,19,21	0.96	1 (5%)

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	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	NAG	E	5	3	-	2/6/23/26	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	NAG	E	7	3	-	1/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	NAG	F	5	3	-	4/6/23/26	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
3	NAG	F	7	3	-	4/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	6	MAN	C4-C3	3.52	1.61	1.52
3	E	4	MAN	O5-C5	2.91	1.49	1.43
3	E	4	MAN	O5-C1	-2.71	1.39	1.43
3	F	6	MAN	C4-C3	2.53	1.58	1.52
3	E	3	BMA	C1-C2	2.43	1.58	1.52
3	E	4	MAN	C4-C5	2.42	1.58	1.53
3	F	2	NAG	O5-C1	2.20	1.47	1.43
3	F	6	MAN	O5-C5	2.14	1.47	1.43
3	F	4	MAN	C4-C5	2.14	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	MAN	C4-C3	2.02	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	MAN	O2-C2-C3	-4.05	101.77	110.15
3	E	7	NAG	C1-O5-C5	3.94	117.47	112.19
3	F	6	MAN	O2-C2-C3	-3.86	102.15	110.15
3	F	7	NAG	C1-O5-C5	3.47	116.84	112.19
3	F	3	BMA	C1-O5-C5	3.24	116.53	112.19
3	E	3	BMA	C1-O5-C5	2.65	115.73	112.19
3	F	3	BMA	O2-C2-C3	-2.63	104.71	110.15
3	F	3	BMA	C1-C2-C3	2.20	112.85	109.64
3	F	5	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	5	NAG	C8-C7-N2-C2
3	E	5	NAG	O7-C7-N2-C2
3	F	5	NAG	C8-C7-N2-C2
3	F	5	NAG	O7-C7-N2-C2
3	F	7	NAG	C8-C7-N2-C2
3	F	7	NAG	O7-C7-N2-C2
3	F	5	NAG	C4-C5-C6-O6
3	F	5	NAG	O5-C5-C6-O6
3	E	7	NAG	C1-C2-N2-C7
3	F	7	NAG	C4-C5-C6-O6
3	F	7	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

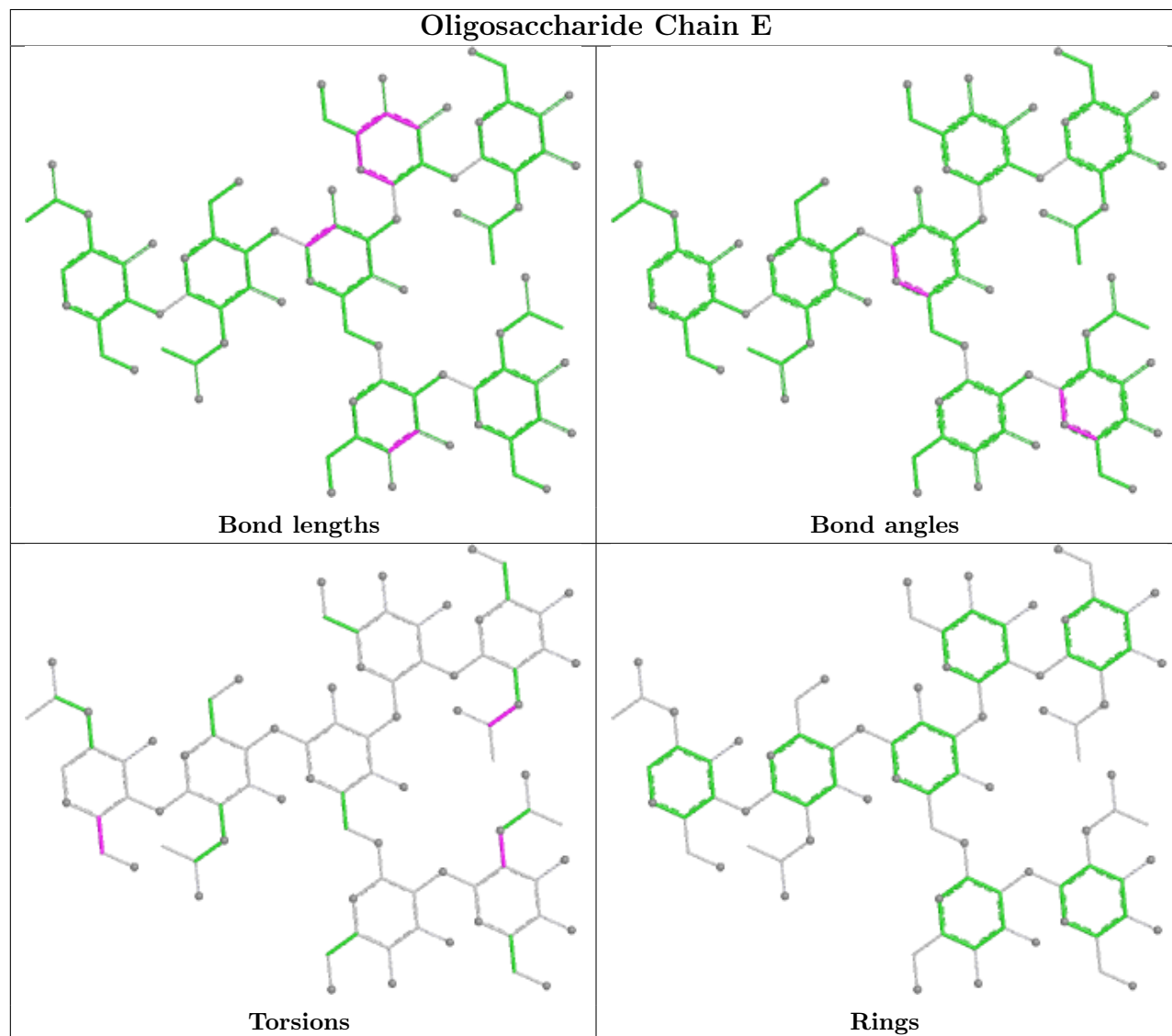
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	MAN	1	0

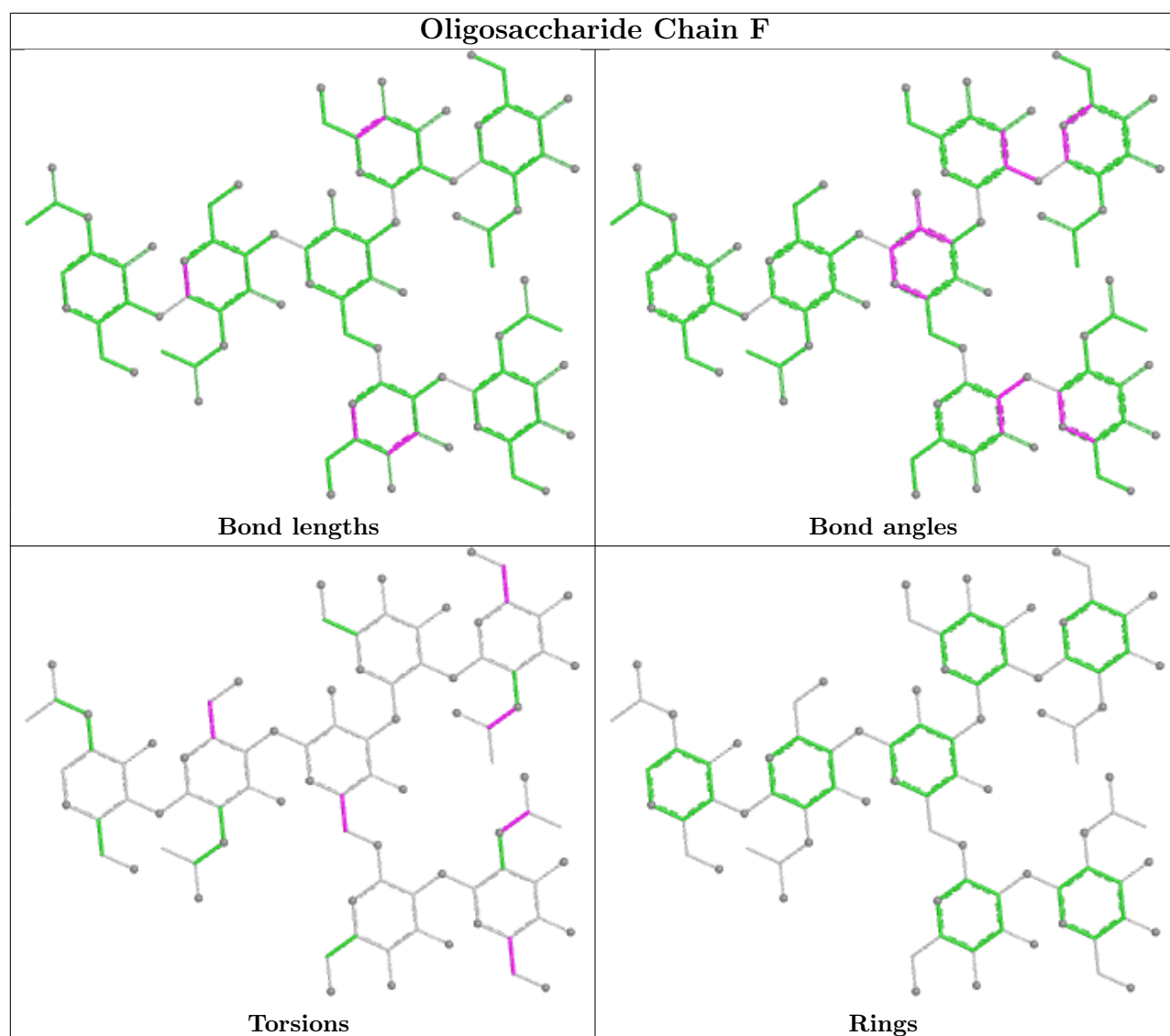
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0

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	206/224 (91%)	0.25	5 (2%) 59 54	53, 79, 103, 114	0
1	B	207/224 (92%)	0.22	5 (2%) 59 54	57, 82, 98, 105	0
2	C	120/120 (100%)	-0.06	0 100 100	48, 61, 83, 101	0
2	D	120/120 (100%)	0.27	1 (0%) 82 80	61, 91, 117, 134	0
All	All	653/688 (94%)	0.19	11 (1%) 69 64	48, 79, 103, 134	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	CYS	3.6
1	A	282	VAL	3.4
1	B	310	HIS	3.3
1	A	310	HIS	2.8
1	A	309	LEU	2.8
2	D	41	PRO	2.6
1	A	281	GLY	2.4
1	B	325	ASN	2.3
1	A	412	VAL	2.1
1	B	323	VAL	2.1
1	B	441	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

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,

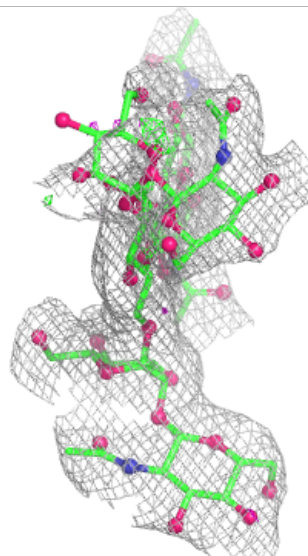
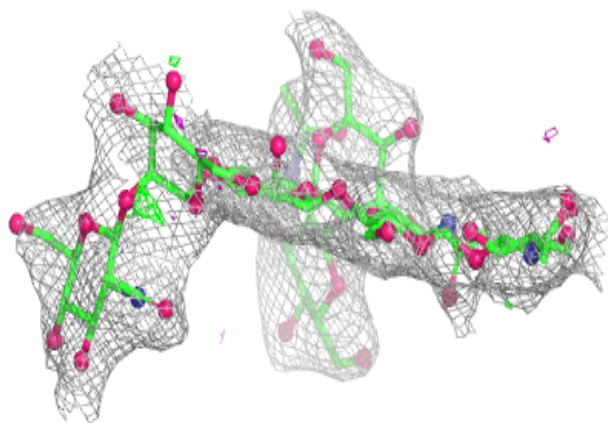
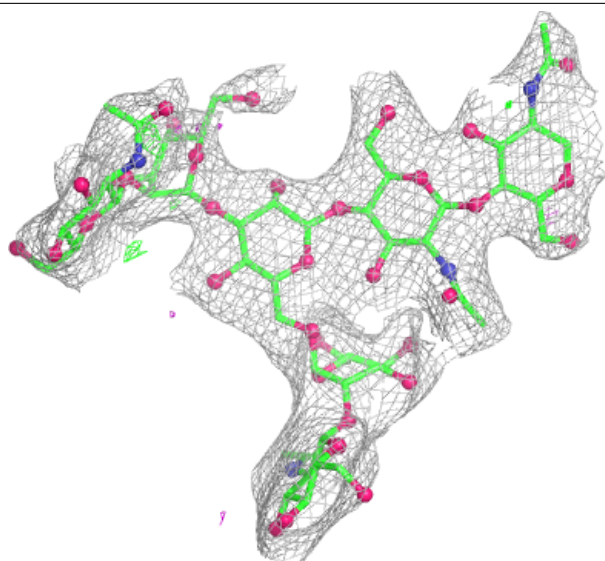
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

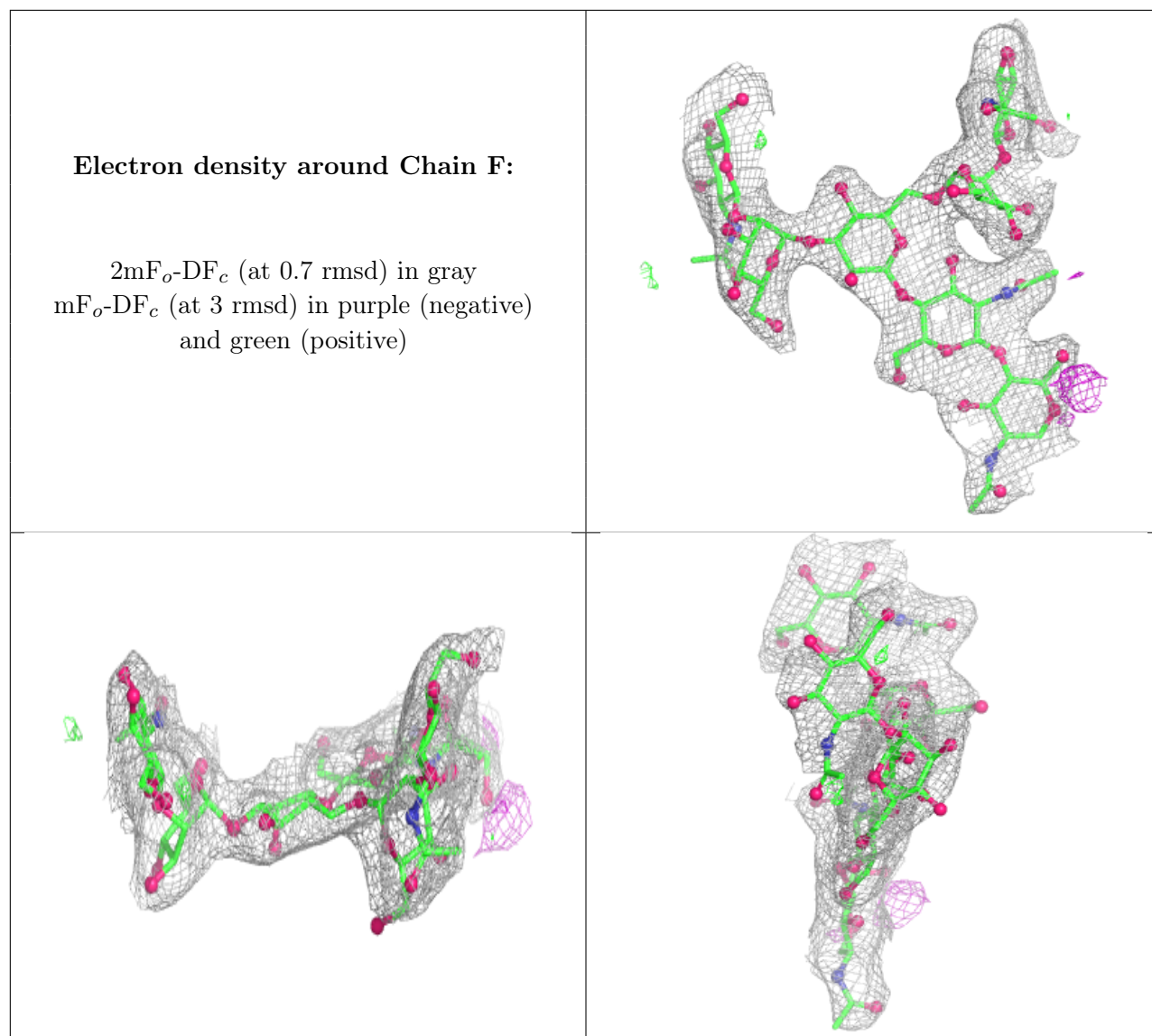
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	5	14/15	0.75	0.14	106,111,113,114	0
3	MAN	E	4	11/12	0.78	0.14	89,96,101,101	0
3	NAG	E	5	14/15	0.79	0.11	94,100,103,105	0
3	NAG	F	1	14/15	0.88	0.10	66,69,72,72	0
3	BMA	F	3	11/12	0.89	0.09	78,84,91,94	0
3	NAG	E	1	14/15	0.89	0.12	73,80,88,91	0
3	NAG	E	7	14/15	0.90	0.09	72,81,84,90	0
3	MAN	F	4	11/12	0.91	0.08	94,100,104,108	0
3	NAG	F	7	14/15	0.91	0.07	73,77,81,82	0
3	BMA	E	3	11/12	0.92	0.07	76,79,84,90	0
3	MAN	E	6	11/12	0.92	0.07	75,78,81,81	0
3	MAN	F	6	11/12	0.93	0.06	76,80,85,89	0
3	NAG	E	2	14/15	0.93	0.09	70,73,77,78	0
3	NAG	F	2	14/15	0.96	0.06	66,72,79,84	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 E:

$2mF_o-DF_c$ (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.