



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2021 – 08:10 PM JST

PDB ID : 7DEB
Title : Structure of an avian influenza H5 hemagglutinin from the influenza virus
A/duck/Eastern China/L0230/2010 (H5N2)
Authors : Sun, H.; Sun, H.; Song, J.; Zhang, W.; Qi, J.; Gao, G.F.; Liu, J.
Deposited on : 2020-11-03
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

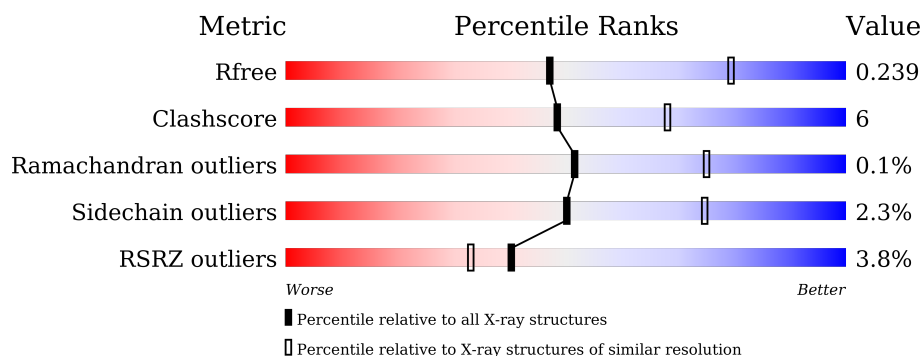
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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	505	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
1	B	505	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>
1	C	505	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
2	D	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
3	E	2	<div> <div></div> <div>100%</div> </div>
3	F	2	<div> <div></div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	2	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12488 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3946	2480	686	758	22			
1	B	494	Total	C	N	O	S	0	0	0
			3946	2480	686	758	22			
1	C	494	Total	C	N	O	S	0	0	0
			3946	2480	686	758	22			

- Molecule 2 is an oligosaccharide called 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	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

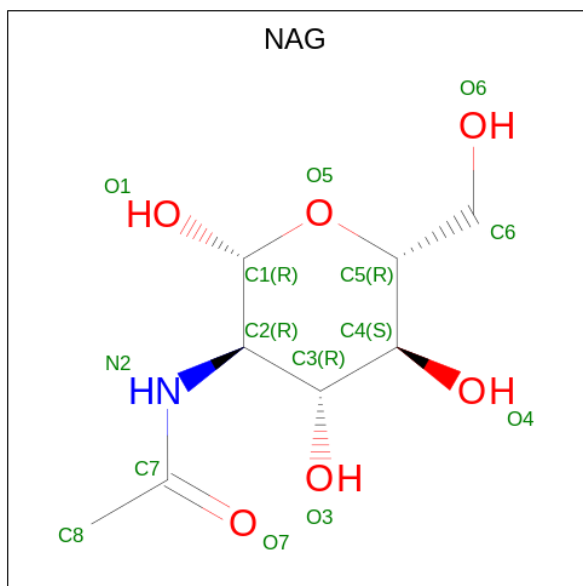
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

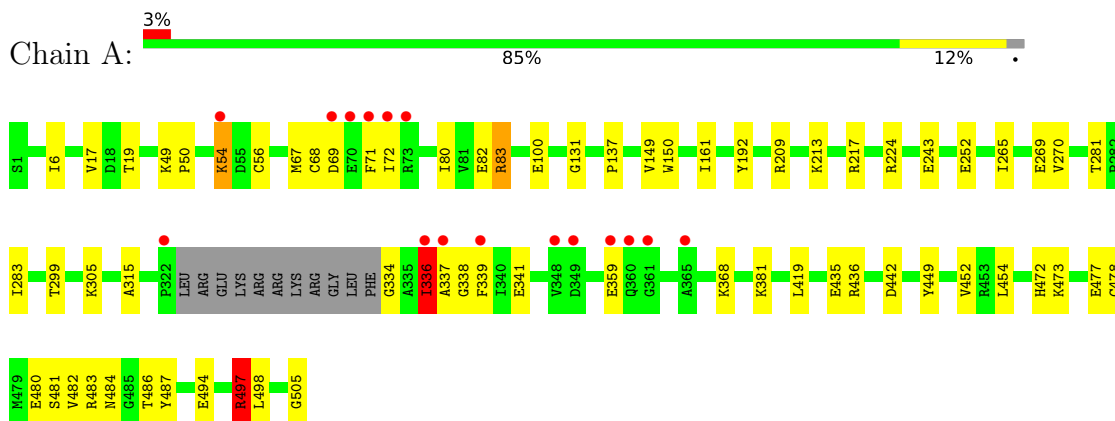
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total	O	0	0
			172	172		
5	B	181	Total	O	0	0
			181	181		
5	C	160	Total	O	0	0
			160	160		

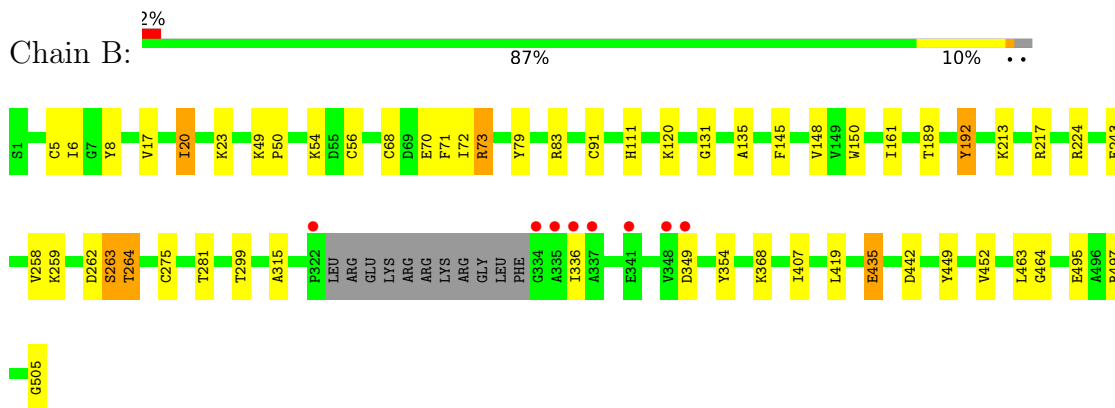
3 Residue-property plots [i](#)

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.

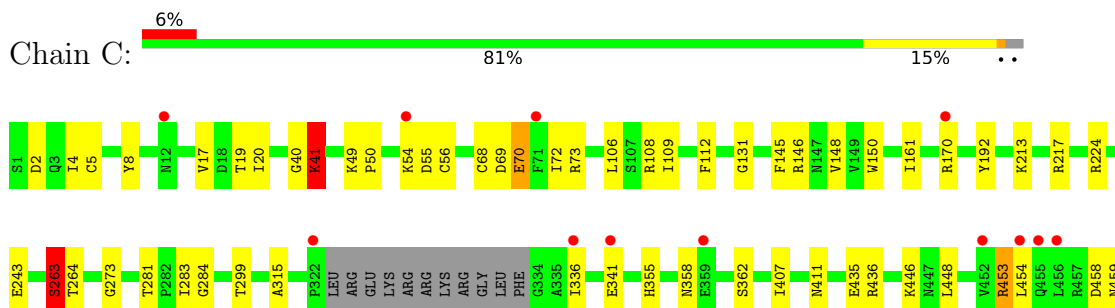
• Molecule 1: Hemagglutinin

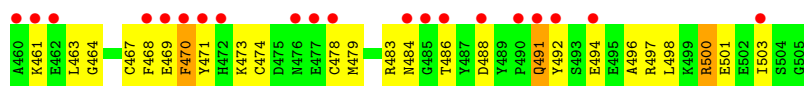


• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin





- Molecule 2: 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-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.96Å 164.86Å 230.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.58 – 2.60 46.58 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.58-2.60) 99.5 (46.58-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.61Å)	Xtriage
Refinement program	REFMAC 7.0.053	Depositor
R, R_{free}	0.206 , 0.238 0.207 , 0.239	Depositor DCC
R_{free} test set	5581 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12488	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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

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	0.38	2/4036 (0.0%)	0.59	9/5468 (0.2%)
1	B	0.34	0/4036	0.55	5/5468 (0.1%)
1	C	0.34	2/4036 (0.0%)	0.60	5/5468 (0.1%)
All	All	0.35	4/12108 (0.0%)	0.58	19/16404 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	ARG	CZ-NH2	6.10	1.41	1.33
1	A	497	ARG	CB-CG	5.96	1.68	1.52
1	C	170	ARG	CB-CG	-5.86	1.36	1.52
1	C	263	SER	CB-OG	-5.83	1.34	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	ARG	CG-CD-NE	-11.41	87.84	111.80
1	C	170	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	B	368	LYS	CD-CE-NZ	-9.49	89.88	111.70
1	C	41	LYS	CD-CE-NZ	7.27	128.42	111.70
1	A	359	GLU	CA-CB-CG	-7.18	97.61	113.40
1	B	349	ASP	CB-CA-C	-6.96	96.48	110.40
1	A	497	ARG	CG-CD-NE	6.35	125.14	111.80
1	C	491	GLN	CB-CA-C	-6.26	97.88	110.40
1	A	69	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	A	497	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	359	GLU	CB-CA-C	6.20	122.81	110.40
1	A	69	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	435	GLU	CB-CA-C	-6.01	98.37	110.40
1	B	349	ASP	CB-CG-OD1	-5.88	113.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	497	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	497	ARG	CA-CB-CG	5.07	124.55	113.40
1	A	82	GLU	C-N-CA	-5.06	109.05	121.70
1	B	20	ILE	CG1-CB-CG2	-5.01	100.38	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3946	0	3803	50	0
1	B	3946	0	3805	39	0
1	C	3946	0	3803	60	0
2	D	39	0	34	1	1
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
5	A	172	0	0	3	0
5	B	181	0	0	3	1
5	C	160	0	0	3	0
All	All	12488	0	11534	140	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 6.

All (140) 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:56:CYS:SG	1:B:68:CYS:SG	1.47	1.35
1:A:334:GLY:O	1:A:338:GLY:HA3	1.50	1.12
1:B:259:LYS:NZ	1:B:262:ASP:OD1	1.86	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLU:HA	1:A:483:ARG:HD2	1.46	0.96
1:A:54:LYS:HE3	1:A:83:ARG:HD2	1.48	0.96
1:A:83:ARG:NE	1:A:269:GLU:OE1	2.05	0.90
1:A:497:ARG:HE	1:A:498:LEU:HD21	1.33	0.90
1:C:494:GLU:HA	1:C:497:ARG:HG2	1.57	0.87
1:B:56:CYS:SG	1:B:68:CYS:CB	2.61	0.87
1:A:497:ARG:HE	1:A:498:LEU:CD2	1.88	0.85
1:A:213:LYS:O	1:A:217:ARG:NH2	2.13	0.81
1:B:263:SER:OG	1:B:264:THR:N	2.13	0.80
1:A:334:GLY:O	1:A:338:GLY:CA	2.30	0.78
1:A:472:HIS:HE2	1:A:487:TYR:HH	1.31	0.78
1:B:407:ILE:CD1	1:C:407:ILE:HG21	2.12	0.77
1:C:411:ASN:ND2	5:C:701:HOH:O	2.14	0.77
1:A:54:LYS:CE	1:A:83:ARG:HD2	2.13	0.77
1:C:213:LYS:O	1:C:217:ARG:NH2	2.18	0.77
1:B:407:ILE:HD11	1:C:407:ILE:HG21	1.65	0.76
1:C:496:ALA:O	1:C:500:ARG:HB2	1.89	0.73
1:B:213:LYS:O	1:B:217:ARG:NH2	2.22	0.73
1:A:68:CYS:HB2	1:A:71:PHE:HZ	1.53	0.73
1:A:472:HIS:NE2	1:A:487:TYR:OH	2.21	0.70
1:B:495:GLU:OE1	5:B:701:HOH:O	2.09	0.69
1:B:20:ILE:HG22	1:B:435:GLU:OE1	1.94	0.67
1:A:497:ARG:NE	1:A:498:LEU:HD21	2.08	0.65
1:B:259:LYS:CE	1:B:262:ASP:OD1	2.45	0.64
1:A:368:LYS:H	1:A:368:LYS:HE2	1.63	0.63
1:C:491:GLN:NE2	1:C:492:TYR:CZ	2.67	0.62
1:B:131:GLY:HA3	1:B:150:TRP:HB3	1.84	0.60
1:C:358:ASN:ND2	5:C:703:HOH:O	2.34	0.59
1:C:224:ARG:NH1	5:C:706:HOH:O	2.34	0.59
1:A:478:CYS:O	1:A:482:VAL:HG23	2.02	0.59
1:C:131:GLY:HA3	1:C:150:TRP:HB3	1.86	0.57
1:C:355:HIS:HE1	1:C:362:SER:HB2	1.70	0.57
1:B:70:GLU:HB3	1:B:72:ILE:HG23	1.87	0.57
1:A:484:ASN:OD1	1:A:486:THR:OG1	2.20	0.56
1:C:72:ILE:HG23	1:C:72:ILE:O	2.03	0.56
1:A:336:ILE:O	1:A:337:ALA:HB3	2.06	0.56
1:B:6:ILE:HD11	1:B:452:VAL:HG21	1.88	0.56
1:A:505:GLY:HA2	1:B:497:ARG:HH22	1.70	0.56
1:B:120:LYS:NZ	5:B:705:HOH:O	2.38	0.56
1:C:68:CYS:O	1:C:146:ARG:NH2	2.39	0.56
1:A:480:GLU:HB2	1:A:483:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LYS:HE3	1:A:83:ARG:CD	2.31	0.55
1:A:100:GLU:H	1:A:100:GLU:CD	2.10	0.55
1:C:494:GLU:CA	1:C:497:ARG:HG2	2.34	0.55
1:C:70:GLU:HB3	1:C:146:ARG:CZ	2.37	0.55
1:C:463:LEU:HD21	1:C:469:GLU:HB2	1.88	0.54
1:A:161:ILE:O	1:A:243:GLU:HA	2.07	0.54
1:B:145:PHE:HB2	1:B:148:VAL:HG12	1.90	0.54
1:C:488:ASP:HB3	1:C:491:GLN:HB2	1.90	0.53
1:C:497:ARG:HG3	1:C:498:LEU:N	2.22	0.53
1:C:4:ILE:HB	1:C:470:PHE:CZ	2.44	0.53
1:C:54:LYS:O	1:C:56:CYS:N	2.42	0.52
1:B:8:TYR:CZ	1:B:336:ILE:HG12	2.45	0.52
1:B:495:GLU:OE2	5:B:702:HOH:O	2.19	0.52
1:C:161:ILE:O	1:C:243:GLU:HA	2.10	0.52
1:C:263:SER:OG	1:C:264:THR:N	2.41	0.51
1:A:72:ILE:O	1:A:72:ILE:HG23	2.11	0.51
1:B:8:TYR:CE1	1:B:336:ILE:HG12	2.46	0.51
1:A:334:GLY:O	1:A:339:PHE:N	2.43	0.51
1:C:453:ARG:HH21	1:C:454:LEU:HD21	1.76	0.51
1:A:436:ARG:NH1	1:C:436:ARG:HG2	2.26	0.50
1:C:5:CYS:HA	1:C:467:CYS:HA	1.94	0.50
1:C:49:LYS:HG2	1:C:50:PRO:HD2	1.93	0.50
1:C:2:ASP:OD2	1:C:473:LYS:HD2	2.12	0.50
1:A:68:CYS:HB2	1:A:71:PHE:CZ	2.40	0.49
1:A:454:LEU:HD22	1:C:464:GLY:HA2	1.95	0.49
1:C:70:GLU:H	1:C:70:GLU:CD	2.13	0.49
1:C:458:ASP:O	1:C:500:ARG:NH1	2.45	0.49
1:C:494:GLU:OE2	1:C:497:ARG:NH2	2.34	0.48
1:A:149:VAL:HG23	1:A:252:GLU:HB2	1.96	0.48
1:A:19:THR:HB	1:A:435:GLU:HB2	1.96	0.47
1:A:68:CYS:CB	1:A:71:PHE:HZ	2.24	0.47
1:C:145:PHE:HB2	1:C:148:VAL:HG12	1.97	0.47
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.73	0.47
1:C:484:ASN:OD1	1:C:486:THR:OG1	2.24	0.47
1:C:463:LEU:HB2	1:C:467:CYS:O	2.16	0.46
1:A:49:LYS:HG2	1:A:50:PRO:HD2	1.97	0.46
2:D:2:NAG:H4	2:D:3:BMA:O2	2.14	0.46
1:A:67:MET:SD	1:A:137:PRO:HD2	2.56	0.46
1:A:270:VAL:HG21	1:A:283:ILE:HA	1.97	0.46
1:C:4:ILE:HB	1:C:470:PHE:HZ	1.80	0.46
1:C:106:LEU:HA	1:C:109:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:CYS:O	1:B:354:TYR:HA	2.16	0.45
1:C:109:ILE:HG21	1:C:112:PHE:HB2	1.97	0.45
1:B:161:ILE:O	1:B:243:GLU:HA	2.16	0.45
1:B:464:GLY:HA2	1:C:454:LEU:HD22	1.99	0.45
1:B:281:THR:HG22	1:B:299:THR:HG22	1.98	0.45
1:B:8:TYR:OH	1:B:336:ILE:HG23	2.17	0.44
1:C:8:TYR:CZ	1:C:336:ILE:HG23	2.53	0.44
1:C:501:GLU:HG2	1:C:501:GLU:O	2.18	0.44
1:C:491:GLN:NE2	1:C:492:TYR:OH	2.51	0.44
1:B:6:ILE:HG13	1:B:449:TYR:HA	1.99	0.44
1:A:131:GLY:HA3	1:A:150:TRP:HB3	1.99	0.43
1:A:481:SER:HB2	1:A:486:THR:O	2.18	0.43
1:A:494:GLU:HA	1:A:497:ARG:CB	2.48	0.43
1:B:54:LYS:O	1:B:83:ARG:HD2	2.18	0.43
1:C:41:LYS:H	1:C:284:GLY:HA2	1.82	0.43
1:B:505:GLY:HA3	1:C:497:ARG:NH1	2.33	0.43
1:A:6:ILE:HG13	1:A:449:TYR:HA	2.00	0.43
1:C:108:ARG:O	1:C:109:ILE:HD12	2.19	0.43
1:A:6:ILE:HD11	1:A:452:VAL:HG21	2.01	0.43
1:A:305:LYS:NZ	5:A:713:HOH:O	2.51	0.43
1:C:4:ILE:CG2	1:C:468:PHE:HB2	2.48	0.43
1:B:50:PRO:HB3	1:B:79:TYR:CE1	2.54	0.43
1:C:19:THR:HB	1:C:435:GLU:HB2	1.99	0.43
1:A:477:GLU:O	1:A:481:SER:HB3	2.19	0.43
1:B:336:ILE:HB	1:B:442:ASP:OD1	2.18	0.43
1:B:407:ILE:CD1	1:C:407:ILE:CG2	2.90	0.43
1:C:41:LYS:HD2	1:C:273:GLY:HA3	2.01	0.43
1:C:473:LYS:HA	1:C:473:LYS:HD3	1.64	0.43
1:C:40:GLY:HA2	1:C:283:ILE:O	2.19	0.43
1:C:479:MET:HB3	1:C:483:ARG:NH2	2.34	0.43
1:A:494:GLU:HA	1:A:497:ARG:HB3	2.01	0.42
1:C:281:THR:HG22	1:C:299:THR:HG22	2.01	0.42
1:A:224:ARG:NH1	5:A:711:HOH:O	2.51	0.42
1:A:281:THR:HG22	1:A:299:THR:HG22	2.01	0.42
1:C:17:VAL:HG21	1:C:315:ALA:HB2	2.00	0.42
1:A:224:ARG:NH2	5:A:716:HOH:O	2.53	0.42
1:B:495:GLU:OE2	1:B:495:GLU:N	2.27	0.42
1:C:341:GLU:H	1:C:341:GLU:HG3	1.59	0.42
1:A:336:ILE:HG13	1:A:442:ASP:HA	2.02	0.42
1:A:381:LYS:HG3	1:C:20:ILE:HG12	2.01	0.42
1:B:17:VAL:HG21	1:B:315:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:CYS:HB2	1:B:135:ALA:O	2.19	0.41
1:A:17:VAL:HG21	1:A:315:ALA:HB2	2.01	0.41
1:B:189:THR:HA	1:B:192:TYR:O	2.20	0.41
1:B:71:PHE:HA	1:B:73:ARG:NH1	2.36	0.41
1:A:80:ILE:HB	1:A:265:ILE:HG13	2.02	0.41
1:A:497:ARG:HH21	1:A:498:LEU:HD21	1.86	0.41
1:C:72:ILE:O	1:C:72:ILE:CG2	2.69	0.41
1:C:448:LEU:HD12	1:C:448:LEU:HA	1.83	0.41
1:C:459:ASN:O	1:C:471:TYR:HB2	2.21	0.40
1:B:111:HIS:HB3	1:B:258:VAL:HB	2.02	0.40
1:B:217:ARG:O	1:B:224:ARG:HD3	2.22	0.40
1:C:461:LYS:NZ	1:C:503:ILE:HD13	2.36	0.40
1:A:505:GLY:HA2	1:B:497:ARG:NH2	2.36	0.40
1:B:463:LEU:HD12	1:B:463:LEU:HA	1.92	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)
2:D:3:BMA:O6	5:B:879:HOH:O[4_545]	2.14	0.06

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	490/505 (97%)	472 (96%)	17 (4%)	1 (0%)	47	71
1	B	490/505 (97%)	473 (96%)	17 (4%)	0	100	100
1	C	490/505 (97%)	470 (96%)	20 (4%)	0	100	100
All	All	1470/1515 (97%)	1415 (96%)	54 (4%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	ILE

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	435/445 (98%)	425 (98%)	10 (2%)	50	75
1	B	435/445 (98%)	427 (98%)	8 (2%)	59	80
1	C	435/445 (98%)	423 (97%)	12 (3%)	43	69
All	All	1305/1335 (98%)	1275 (98%)	30 (2%)	50	75

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	56	CYS
1	A	83	ARG
1	A	192	TYR
1	A	209	ARG
1	A	336	ILE
1	A	341	GLU
1	A	419	LEU
1	A	473	LYS
1	A	497	ARG
1	B	23	LYS
1	B	49	LYS
1	B	73	ARG
1	B	192	TYR
1	B	263	SER
1	B	264	THR
1	B	275	CYS
1	B	419	LEU
1	C	41	LYS
1	C	69	ASP
1	C	70	GLU
1	C	73	ARG

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Mol	Chain	Res	Type
1	C	192	TYR
1	C	263	SER
1	C	446	LYS
1	C	453	ARG
1	C	470	PHE
1	C	474	CYS
1	C	478	CYS
1	C	500	ARG

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

Mol	Chain	Res	Type
1	B	360	GLN
1	C	491	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 ⓘ

7 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	D	1	2,1	14,14,15	0.25	0	17,19,21	1.04	1 (5%)
2	NAG	D	2	2	14,14,15	0.64	0	17,19,21	0.71	0
2	BMA	D	3	2	11,11,12	1.08	1 (9%)	15,15,17	1.61	3 (20%)

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	0.28	0	17,19,21	0.74	1 (5%)
3	NAG	E	2	3	14,14,15	0.24	0	17,19,21	0.72	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.22	0	17,19,21	0.85	1 (5%)
3	NAG	F	2	3	14,14,15	0.20	0	17,19,21	0.71	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
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BMA	C1-C2	2.89	1.58	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	3.62	117.09	112.19
2	D	3	BMA	O2-C2-C3	-3.37	103.38	110.14
2	D	3	BMA	C1-O5-C5	3.22	116.56	112.19
3	F	1	NAG	C1-O5-C5	3.05	116.32	112.19
3	F	2	NAG	C1-O5-C5	2.67	115.81	112.19
2	D	3	BMA	C1-C2-C3	-2.66	106.39	109.67
3	E	1	NAG	C1-O5-C5	2.62	115.74	112.19
3	E	2	NAG	C1-O5-C5	2.49	115.57	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

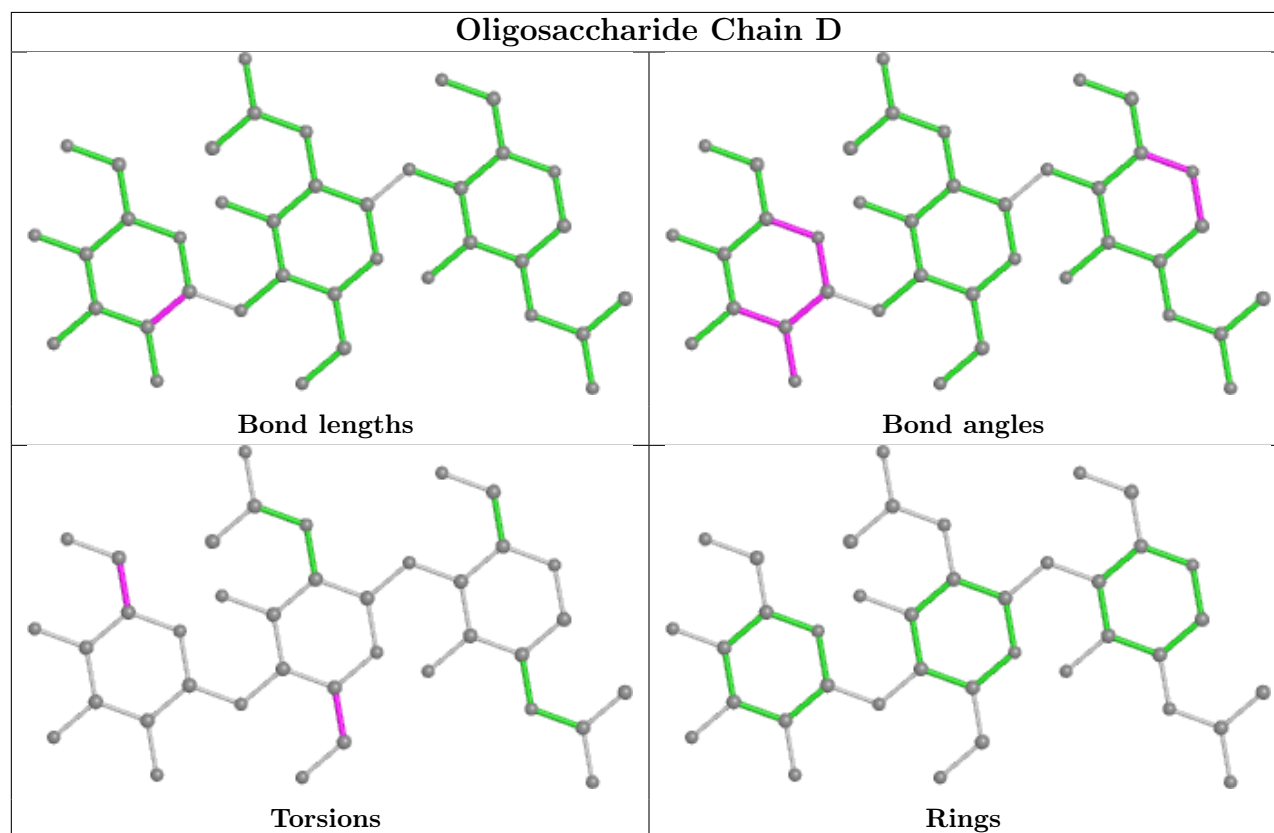
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

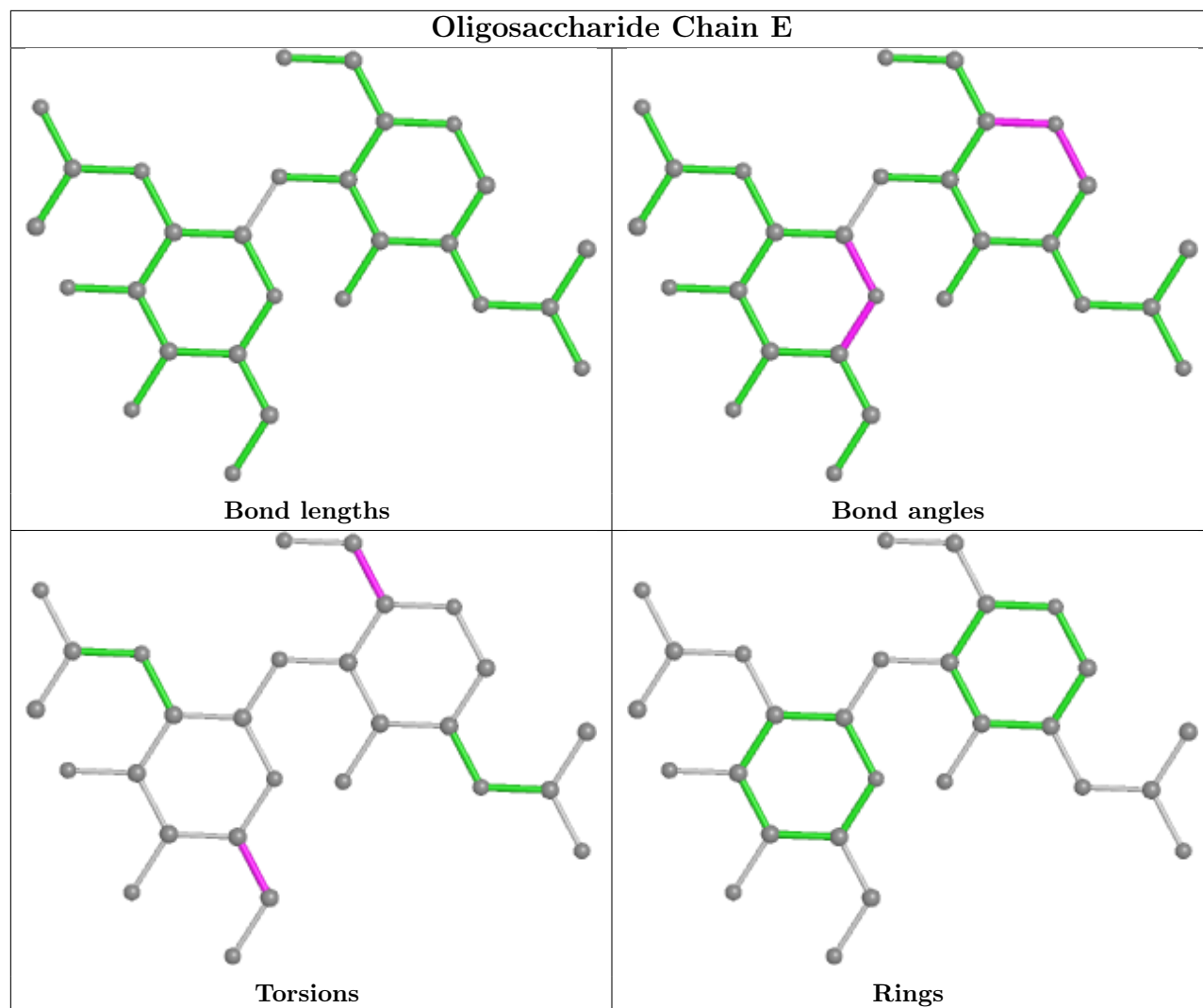
There are no ring outliers.

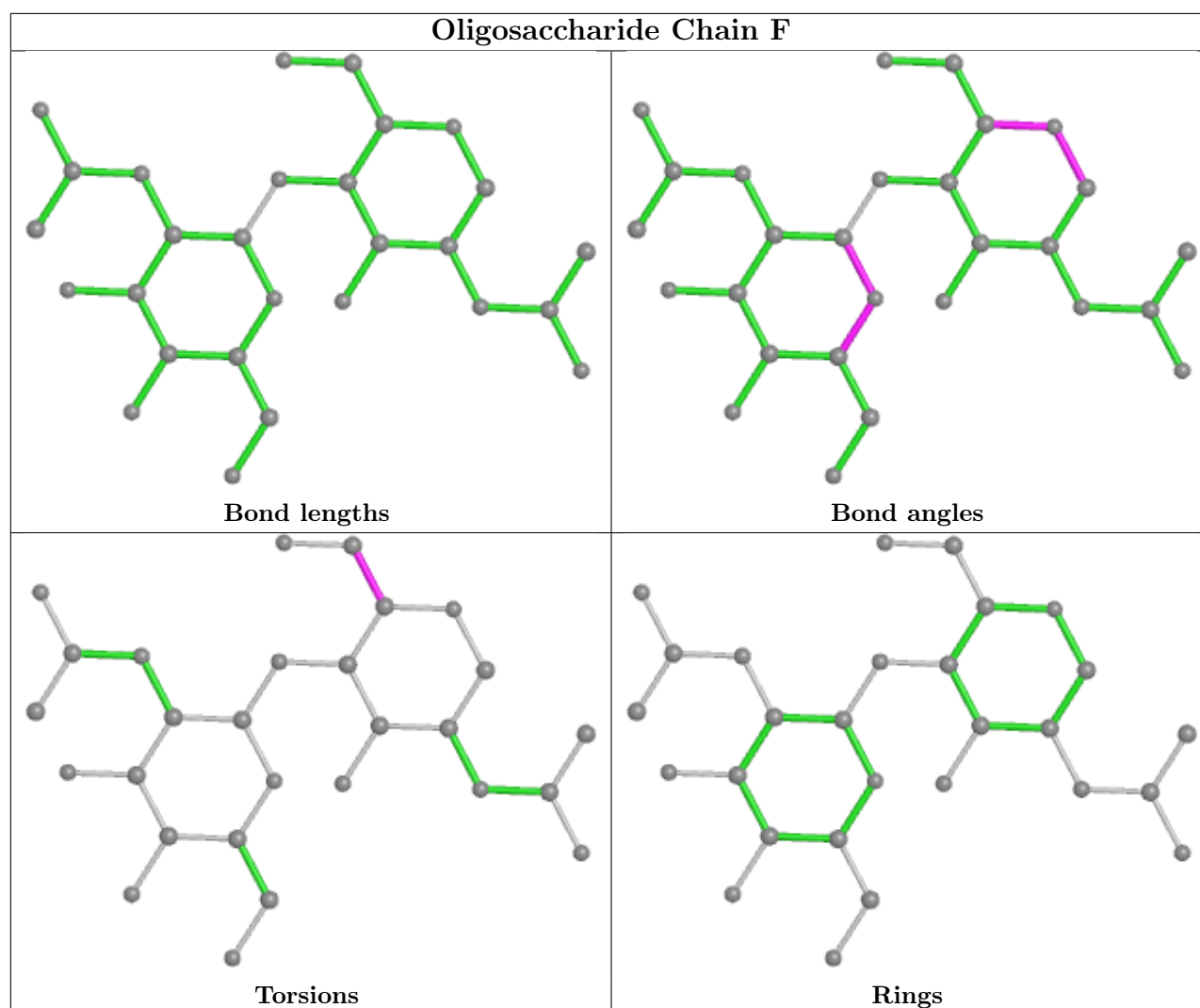
2 monomers are involved in 2 short contacts:

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

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](#)

3 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	$\# Z > 2$
4	NAG	C	601	1	14,14,15	0.57	0	17,19,21	0.78	1 (5%)
4	NAG	B	601	1	14,14,15	0.59	0	17,19,21	0.76	1 (5%)
4	NAG	A	601	1	14,14,15	0.50	0	17,19,21	0.80	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
4	NAG	C	601	1	-	0/6/23/26	0/1/1/1
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C1-O5-C5	2.99	116.24	112.19
4	C	601	NAG	C1-O5-C5	2.86	116.06	112.19
4	B	601	NAG	C1-O5-C5	2.78	115.96	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	NAG	O5-C5-C6-O6
4	B	601	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	494/505 (97%)	-0.24	16 (3%) 47 40	25, 43, 98, 133	0
1	B	494/505 (97%)	-0.36	8 (1%) 72 68	25, 41, 69, 111	0
1	C	494/505 (97%)	-0.07	32 (6%) 18 14	25, 44, 104, 126	0
All	All	1482/1515 (97%)	-0.22	56 (3%) 40 33	25, 43, 96, 133	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	470	PHE	5.5
1	B	336	ILE	5.3
1	C	468	PHE	5.2
1	A	72	ILE	4.9
1	C	322	PRO	4.3
1	C	336	ILE	4.1
1	C	486	THR	4.0
1	A	322	PRO	3.7
1	A	71	PHE	3.6
1	C	492	TYR	3.5
1	C	456	LEU	3.5
1	A	359	GLU	3.4
1	A	70	GLU	3.4
1	C	491	GLN	3.4
1	C	490	PRO	3.4
1	C	484	ASN	3.2
1	C	476	ASN	3.2
1	B	322	PRO	3.2
1	A	349	ASP	3.2
1	C	71	PHE	3.2
1	A	336	ILE	3.2
1	C	485	GLY	3.1
1	A	69	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	337	ALA	3.0
1	C	488	ASP	2.9
1	A	365	ALA	2.8
1	C	469	GLU	2.8
1	C	460	ALA	2.8
1	B	349	ASP	2.7
1	B	335	ALA	2.7
1	B	334	GLY	2.7
1	B	341	GLU	2.6
1	C	472	HIS	2.6
1	C	452	VAL	2.6
1	C	454	LEU	2.6
1	C	359	GLU	2.6
1	A	73	ARG	2.6
1	C	471	TYR	2.5
1	C	12	ASN	2.5
1	A	348	VAL	2.5
1	C	462	GLU	2.5
1	C	503	ILE	2.4
1	A	361	GLY	2.4
1	C	477	GLU	2.4
1	A	337	ALA	2.3
1	C	478	CYS	2.3
1	C	494	GLU	2.2
1	A	360	GLN	2.2
1	C	455	GLN	2.2
1	A	54	LYS	2.1
1	C	341	GLU	2.1
1	A	339	PHE	2.1
1	C	461	LYS	2.1
1	B	348	VAL	2.0
1	C	170	ARG	2.0
1	C	54	LYS	2.0

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

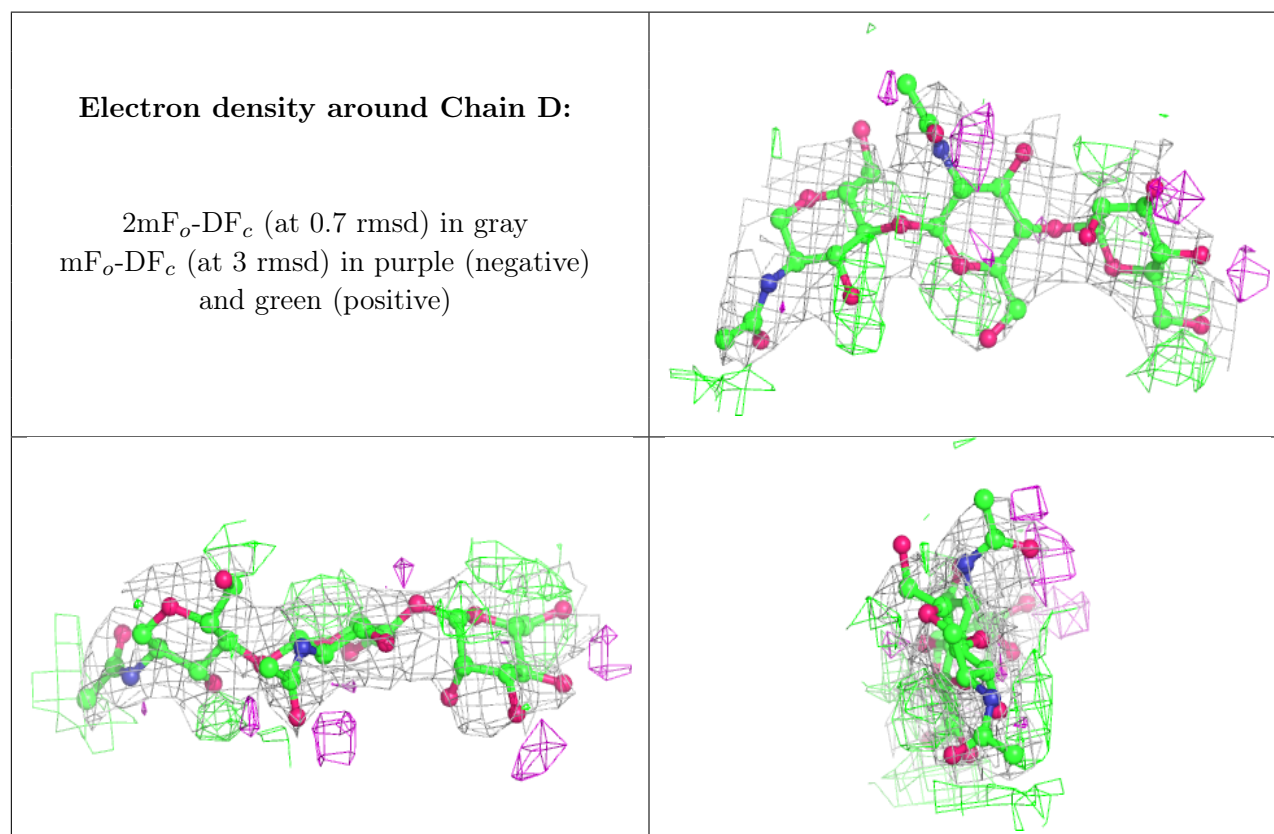
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

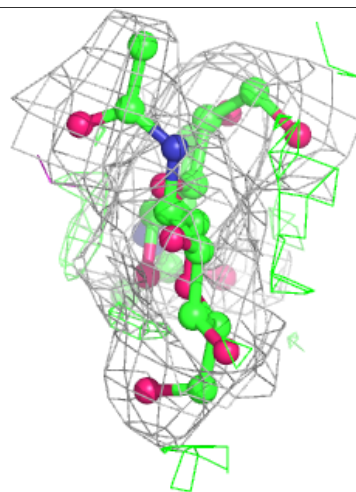
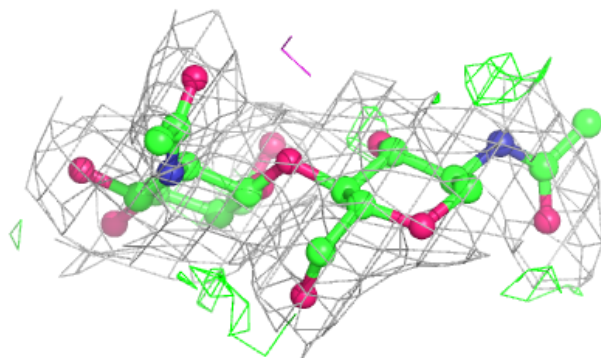
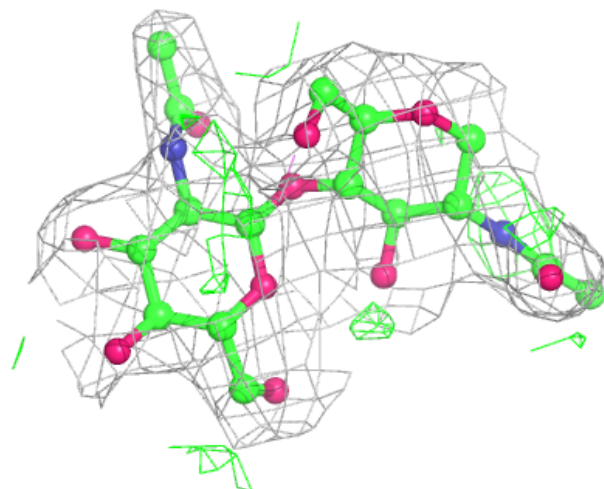
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	2	14/15	0.68	0.44	81,109,124,125	0
2	BMA	D	3	11/12	0.80	0.25	37,82,93,95	0
2	NAG	D	2	14/15	0.85	0.25	46,66,81,88	0
3	NAG	E	2	14/15	0.86	0.18	46,81,90,98	0
2	NAG	D	1	14/15	0.91	0.16	43,58,76,79	0
3	NAG	F	1	14/15	0.92	0.24	44,75,94,117	0
3	NAG	E	1	14/15	0.92	0.13	51,57,68,70	0

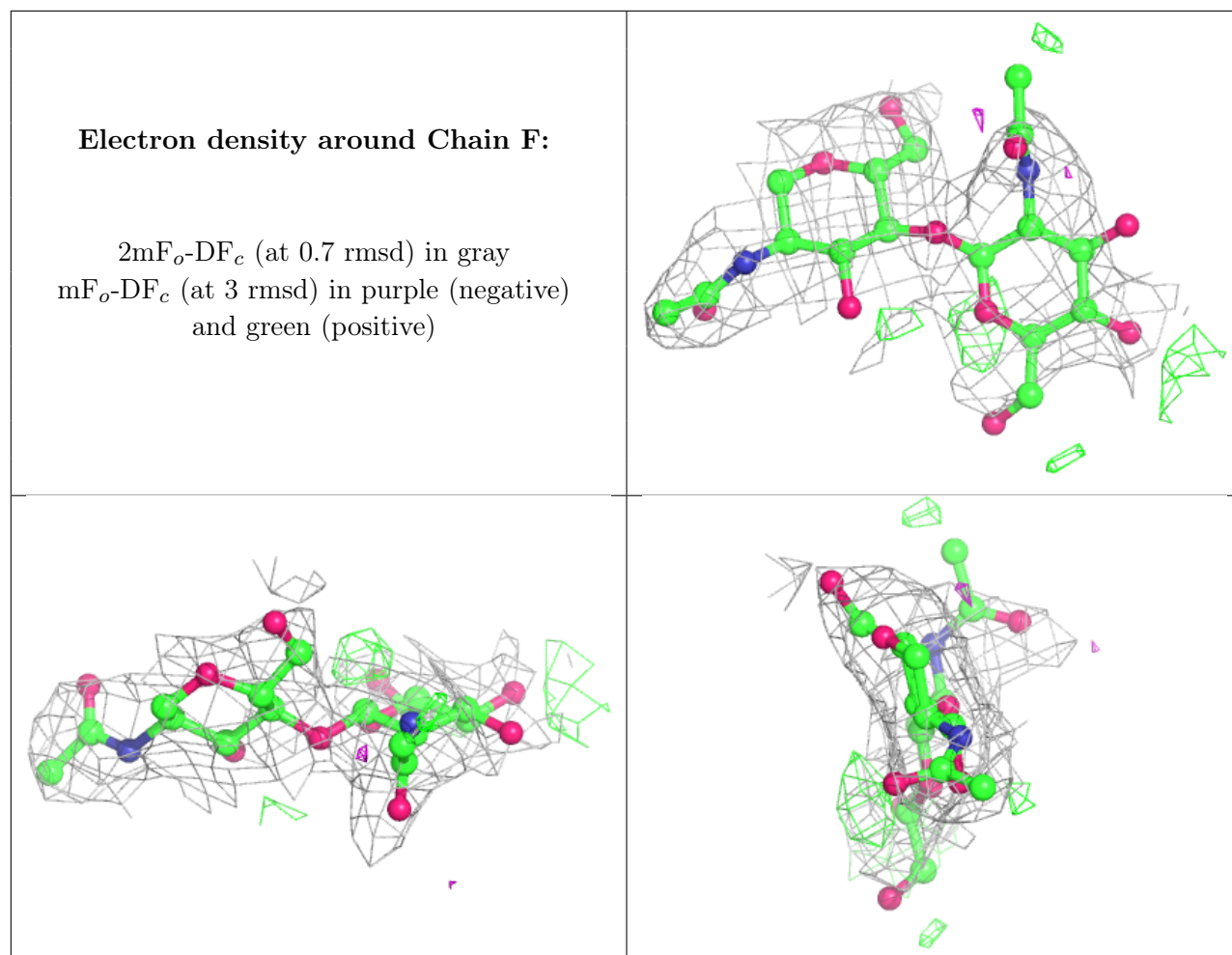
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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](#)

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(\AA^2)	Q<0.9
4	NAG	B	601	14/15	0.79	0.24	62,87,105,106	0
4	NAG	A	601	14/15	0.83	0.20	61,93,100,106	0
4	NAG	C	601	14/15	0.84	0.22	73,94,108,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.