



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:59 PM UTC

PDB ID : 4FIU / pdb_00004fiu
Title : The structure of hemagglutinin of H16 subtype influenza virus with V327G mutation
Authors : Lu, X.; Shi, Y.; Gao, F.; Xiao, H.; Wang, M.; Qi, J.; Gao, G.F.
Deposited on : 2012-06-11
Resolution : 2.00 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

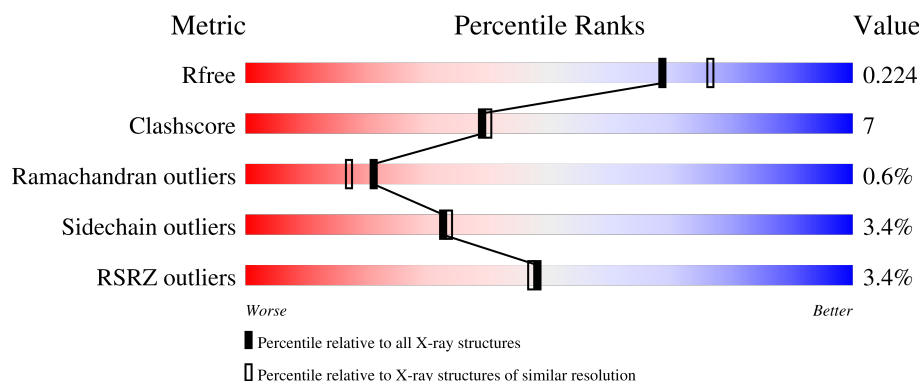
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	515	3% 83% 14% ..
1	B	515	4% 83% 14% ..
1	C	515	3% 86% 11% ..
2	D	2	100%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13742 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	509	Total	C	N	O	S	0	0	0
			4016	2507	715	776	18			
1	B	509	Total	C	N	O	S	0	0	0
			4016	2507	715	776	18			
1	C	509	Total	C	N	O	S	0	0	0
			4016	2507	715	776	18			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q5DL24
A	-4	HIS	-	expression tag	UNP Q5DL24
A	-3	HIS	-	expression tag	UNP Q5DL24
A	-2	HIS	-	expression tag	UNP Q5DL24
A	-1	HIS	-	expression tag	UNP Q5DL24
A	0	HIS	-	expression tag	UNP Q5DL24
A	1	ALA	-	SEE REMARK 999	UNP Q5DL24
A	2	ASP	-	SEE REMARK 999	UNP Q5DL24
A	3	GLY	-	SEE REMARK 999	UNP Q5DL24
A	4	ILE	-	SEE REMARK 999	UNP Q5DL24
A	5	GLN	-	SEE REMARK 999	UNP Q5DL24
A	326	GLY	VAL	engineered mutation	UNP Q5DL24
A	505	ARG	-	SEE REMARK 999	UNP Q5DL24
A	506	LEU	-	SEE REMARK 999	UNP Q5DL24
A	507	VAL	-	SEE REMARK 999	UNP Q5DL24
A	508	PRO	-	SEE REMARK 999	UNP Q5DL24
A	509	ARG	-	SEE REMARK 999	UNP Q5DL24
B	-5	HIS	-	expression tag	UNP Q5DL24
B	-4	HIS	-	expression tag	UNP Q5DL24
B	-3	HIS	-	expression tag	UNP Q5DL24
B	-2	HIS	-	expression tag	UNP Q5DL24
B	-1	HIS	-	expression tag	UNP Q5DL24
B	0	HIS	-	expression tag	UNP Q5DL24

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	SEE REMARK 999	UNP Q5DL24
B	2	ASP	-	SEE REMARK 999	UNP Q5DL24
B	3	GLY	-	SEE REMARK 999	UNP Q5DL24
B	4	ILE	-	SEE REMARK 999	UNP Q5DL24
B	5	GLN	-	SEE REMARK 999	UNP Q5DL24
B	326	GLY	VAL	engineered mutation	UNP Q5DL24
B	505	ARG	-	SEE REMARK 999	UNP Q5DL24
B	506	LEU	-	SEE REMARK 999	UNP Q5DL24
B	507	VAL	-	SEE REMARK 999	UNP Q5DL24
B	508	PRO	-	SEE REMARK 999	UNP Q5DL24
B	509	ARG	-	SEE REMARK 999	UNP Q5DL24
C	-5	HIS	-	expression tag	UNP Q5DL24
C	-4	HIS	-	expression tag	UNP Q5DL24
C	-3	HIS	-	expression tag	UNP Q5DL24
C	-2	HIS	-	expression tag	UNP Q5DL24
C	-1	HIS	-	expression tag	UNP Q5DL24
C	0	HIS	-	expression tag	UNP Q5DL24
C	1	ALA	-	SEE REMARK 999	UNP Q5DL24
C	2	ASP	-	SEE REMARK 999	UNP Q5DL24
C	3	GLY	-	SEE REMARK 999	UNP Q5DL24
C	4	ILE	-	SEE REMARK 999	UNP Q5DL24
C	5	GLN	-	SEE REMARK 999	UNP Q5DL24
C	326	GLY	VAL	engineered mutation	UNP Q5DL24
C	505	ARG	-	SEE REMARK 999	UNP Q5DL24
C	506	LEU	-	SEE REMARK 999	UNP Q5DL24
C	507	VAL	-	SEE REMARK 999	UNP Q5DL24
C	508	PRO	-	SEE REMARK 999	UNP Q5DL24
C	509	ARG	-	SEE REMARK 999	UNP Q5DL24

- Molecule 2 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
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

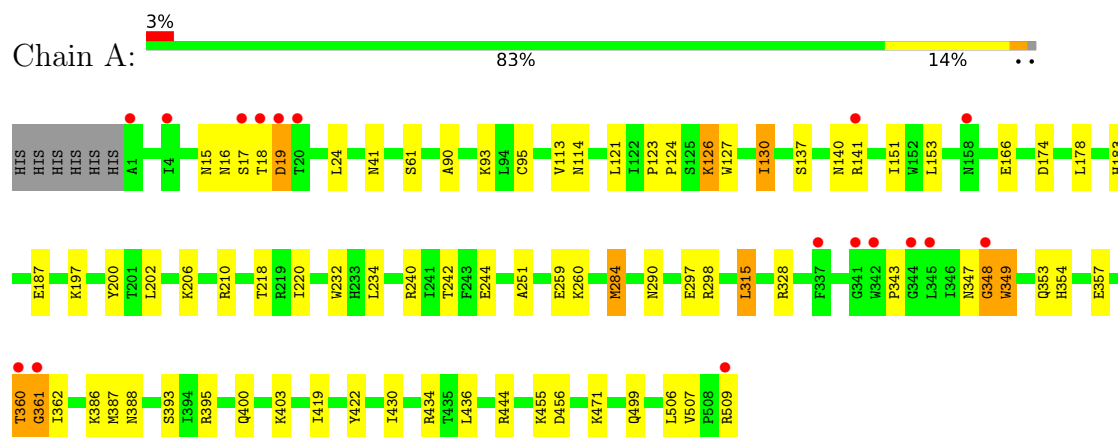
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	511	Total	O	0	0
			511	511		
4	B	528	Total	O	0	0
			528	528		
4	C	529	Total	O	0	0
			529	529		

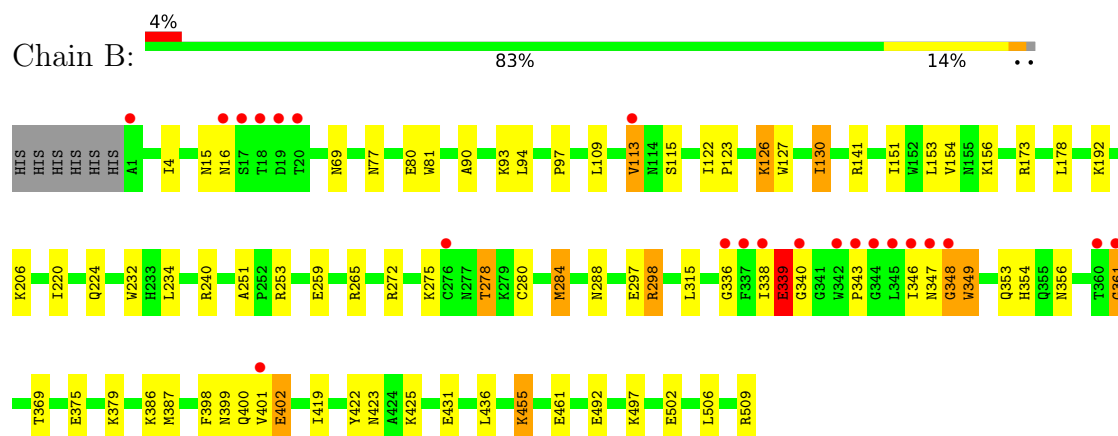
3 Residue-property plots [i](#)

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.

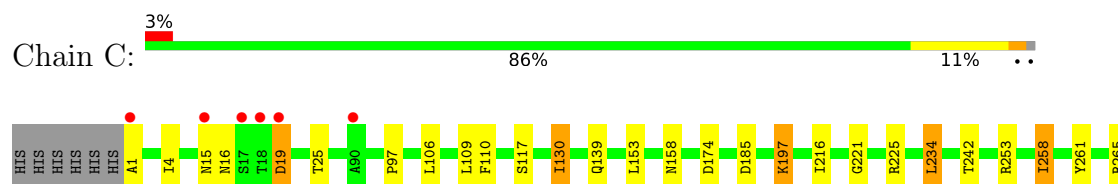
- Molecule 1: hemagglutinin

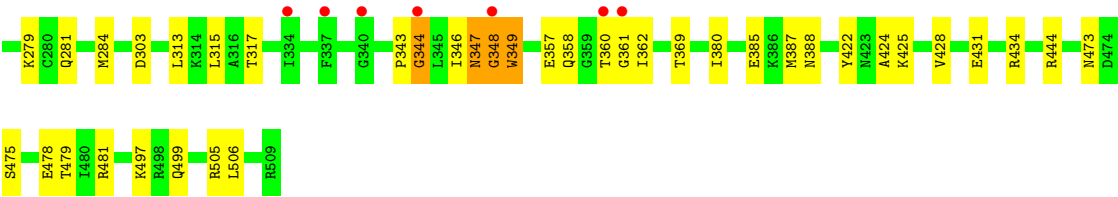


- Molecule 1: hemagglutinin



- Molecule 1: hemagglutinin





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



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



● Molecule 2: 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.07Å 240.78Å 69.48Å 90.00° 119.68° 90.00°	Depositor
Resolution (Å)	42.50 – 2.00 42.50 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.50-2.00) 98.3 (42.50-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.87 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.193 , 0.228 0.189 , 0.224	Depositor DCC
R_{free} test set	6661 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.068 for -h-l,k,h 0.068 for l,k,-h-l 0.039 for h,-k,-h-l 0.038 for -h-l,-k,l 0.036 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13742	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.49	0/4099	0.83	5/5551 (0.1%)
1	B	0.49	0/4099	0.82	3/5551 (0.1%)
1	C	0.49	0/4099	0.81	4/5551 (0.1%)
All	All	0.49	0/12297	0.82	12/16653 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	TRP	N-CA-C	6.87	120.64	109.59
1	C	362	ILE	N-CA-C	6.33	118.59	108.85
1	B	340	GLY	N-CA-C	-6.29	106.64	115.32
1	B	455	LYS	CB-CA-C	-6.08	109.55	116.54
1	C	349	TRP	N-CA-C	5.97	119.27	109.72
1	B	349	TRP	N-CA-C	5.89	119.01	109.40
1	A	362	ILE	N-CA-C	5.74	116.74	108.48
1	C	344	GLY	N-CA-C	5.39	118.75	112.50
1	A	347	ASN	N-CA-C	5.29	118.69	111.39
1	C	347	ASN	N-CA-C	5.11	118.45	111.39
1	A	183	HIS	CA-C-N	5.09	125.02	119.78
1	A	183	HIS	C-N-CA	5.09	125.02	119.78

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	4016	0	3897	61	0
1	B	4016	0	3897	64	0
1	C	4016	0	3897	47	0
2	D	28	0	25	1	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	1	0
4	A	511	0	0	26	0
4	B	528	0	0	29	0
4	C	529	0	0	24	0
All	All	13742	0	11805	164	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 7.

All (164) 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:206:LYS:HG3	4:B:932:HOH:O	1.64	0.96
1:A:41:ASN:ND2	4:A:1126:HOH:O	2.00	0.94
1:A:187:GLU:OE1	4:A:1199:HOH:O	1.84	0.94
1:C:478:GLU:OE2	4:C:1218:HOH:O	1.87	0.93
1:B:288:ASN:ND2	4:B:991:HOH:O	2.01	0.89
1:A:19:ASP:N	4:A:781:HOH:O	2.08	0.86
1:A:499:GLN:NE2	4:A:1120:HOH:O	2.09	0.84
1:B:141:ARG:NH2	4:B:873:HOH:O	2.08	0.81
1:C:19:ASP:OD1	4:C:927:HOH:O	1.99	0.80
1:C:385:GLU:OE2	4:C:1000:HOH:O	1.99	0.79
1:B:298:ARG:NH1	4:B:708:HOH:O	2.16	0.79
1:A:114:ASN:ND2	4:A:873:HOH:O	2.16	0.79
1:A:386:LYS:NZ	4:A:934:HOH:O	2.15	0.79
1:B:122:ILE:O	4:B:908:HOH:O	1.98	0.79
1:C:434:ARG:NH1	4:C:1202:HOH:O	2.16	0.78
3:C:603:NAG:O4	4:C:1158:HOH:O	1.98	0.76
1:B:284:MET:HG3	1:B:297:GLU:HB2	1.71	0.73
1:C:388:ASN:OD1	4:C:1082:HOH:O	2.06	0.73
1:C:109:LEU:HB2	4:C:1005:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:GLU:OE1	4:B:1125:HOH:O	2.07	0.72
1:A:353:GLN:NE2	4:A:1177:HOH:O	1.85	0.72
1:A:240:ARG:NH1	4:A:1202:HOH:O	2.23	0.71
1:B:278:THR:HG22	1:B:280:CYS:H	1.53	0.71
1:A:499:GLN:OE1	4:A:1096:HOH:O	2.09	0.71
1:A:290:ASN:OD1	4:A:1117:HOH:O	2.08	0.70
1:B:375:GLU:O	4:B:865:HOH:O	2.10	0.68
1:C:344:GLY:O	4:C:1210:HOH:O	2.11	0.68
1:C:434:ARG:NH1	4:C:848:HOH:O	2.22	0.68
1:B:354:HIS:CE1	1:B:361:GLY:HA2	2.28	0.68
1:B:206:LYS:N	4:B:932:HOH:O	2.25	0.67
1:C:139:GLN:NE2	4:C:794:HOH:O	2.25	0.67
1:A:354:HIS:CE1	1:A:361:GLY:HA2	2.30	0.67
1:C:106:LEU:O	4:C:1005:HOH:O	2.13	0.67
1:B:398:PHE:HB3	1:B:402:GLU:HG3	1.77	0.66
1:B:343:PRO:HD2	1:B:348:GLY:HA3	1.77	0.66
1:C:357:GLU:OE2	4:C:724:HOH:O	2.15	0.65
1:C:444:ARG:NH1	4:C:805:HOH:O	2.06	0.65
1:C:158:ASN:OD1	4:C:829:HOH:O	2.15	0.64
1:B:80:GLU:OE1	4:B:834:HOH:O	2.14	0.64
1:B:141:ARG:NE	4:B:1170:HOH:O	2.25	0.64
1:B:115:SER:HB3	1:B:259:GLU:HB3	1.78	0.64
1:A:15:ASN:OD1	1:A:16:ASN:N	2.30	0.63
1:B:15:ASN:OD1	1:B:16:ASN:N	2.30	0.63
1:C:431:GLU:OE2	1:C:434:ARG:NH2	2.31	0.63
1:C:16:ASN:ND2	4:C:911:HOH:O	1.97	0.61
1:B:90:ALA:O	1:B:93:LYS:NZ	2.33	0.60
1:C:106:LEU:HD12	4:C:1005:HOH:O	2.01	0.60
1:A:141:ARG:NH2	4:A:1100:HOH:O	2.33	0.60
1:A:15:ASN:OD1	4:A:1181:HOH:O	2.16	0.60
1:A:353:GLN:HA	1:A:361:GLY:O	2.02	0.59
1:C:15:ASN:OD1	1:C:16:ASN:N	2.31	0.59
1:A:343:PRO:HD3	1:A:349:TRP:CE2	2.38	0.59
1:B:156:LYS:NZ	4:B:1077:HOH:O	2.34	0.59
1:B:77:ASN:ND2	4:B:1142:HOH:O	2.02	0.58
1:B:387:MET:HG3	1:C:422:TYR:CE1	2.38	0.58
1:C:110:PHE:HD2	4:C:1005:HOH:O	1.86	0.58
1:B:298:ARG:NH1	4:B:726:HOH:O	2.36	0.57
1:C:130:ILE:HG21	1:C:153:LEU:HD22	1.85	0.57
1:A:130:ILE:HG21	1:A:153:LEU:HD22	1.88	0.56
1:A:114:ASN:CG	4:A:873:HOH:O	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:LYS:NZ	4:C:1108:HOH:O	2.39	0.56
1:B:509:ARG:HD3	4:B:1055:HOH:O	2.06	0.56
1:B:379:LYS:NZ	1:B:431:GLU:OE1	2.39	0.55
1:A:395:ARG:HB2	4:A:1062:HOH:O	2.07	0.54
1:A:360:THR:HG22	1:A:361:GLY:HA3	1.89	0.54
1:C:343:PRO:HD3	1:C:349:TRP:CE2	2.42	0.54
1:B:356:ASN:HB2	4:B:858:HOH:O	2.08	0.54
1:B:253:ARG:HG2	4:B:908:HOH:O	2.07	0.54
1:B:338:ILE:HG23	1:B:339:GLU:H	1.73	0.53
1:A:419:ILE:HG21	1:B:419:ILE:HD13	1.91	0.53
1:A:200:TYR:OH	1:A:244:GLU:OE2	2.26	0.53
1:A:298:ARG:O	1:A:393:SER:OG	2.19	0.52
1:B:502:GLU:OE2	4:B:910:HOH:O	2.19	0.52
1:A:206:LYS:NZ	4:A:1032:HOH:O	2.43	0.52
1:B:379:LYS:HB2	4:B:865:HOH:O	2.10	0.52
1:C:117:SER:HB3	4:C:1138:HOH:O	2.08	0.52
1:B:343:PRO:HD2	1:B:348:GLY:CA	2.40	0.52
1:B:130:ILE:HG21	1:B:153:LEU:HD22	1.92	0.51
1:C:265:ARG:NH2	4:C:893:HOH:O	2.32	0.51
1:A:284:MET:HG3	1:A:297:GLU:HB2	1.93	0.51
1:A:357:GLU:HG3	4:A:839:HOH:O	2.10	0.51
1:A:400:GLN:NE2	4:A:1137:HOH:O	2.42	0.51
1:A:422:TYR:CE1	1:C:387:MET:HG3	2.46	0.51
1:C:258:ILE:HG13	1:C:261:TYR:CD1	2.47	0.50
1:A:90:ALA:O	1:A:93:LYS:HE2	2.12	0.50
1:A:343:PRO:HD2	1:A:348:GLY:HA3	1.94	0.50
1:B:278:THR:CG2	1:B:280:CYS:H	2.25	0.49
1:B:173:ARG:NH1	4:B:923:HOH:O	2.45	0.49
1:C:358:GLN:OE1	1:C:473:ASN:HB2	2.13	0.49
1:A:17:SER:HA	4:A:1020:HOH:O	2.13	0.49
1:A:328:ARG:O	1:A:444:ARG:NH2	2.46	0.49
1:B:353:GLN:HA	1:B:361:GLY:O	2.13	0.48
1:A:18:THR:HA	4:A:781:HOH:O	2.13	0.48
1:B:492:GLU:HB2	1:C:505:ARG:HE	1.79	0.48
1:B:497:LYS:NZ	4:B:981:HOH:O	2.46	0.48
1:B:343:PRO:HD3	1:B:349:TRP:NE1	2.28	0.48
1:C:185:ASP:OD1	1:C:225:ARG:NH1	2.47	0.48
1:A:178:LEU:HD23	1:A:232:TRP:HB3	1.95	0.47
1:A:387:MET:HG3	1:B:422:TYR:CE1	2.49	0.47
1:A:259:GLU:OE2	4:A:1000:HOH:O	2.20	0.47
1:C:1:ALA:N	4:C:1190:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:SER:HB3	1:A:93:LYS:HG2	1.96	0.47
1:B:69:ASN:N	4:B:928:HOH:O	2.46	0.47
1:A:114:ASN:HB2	1:A:260:LYS:HB3	1.97	0.47
1:B:127:TRP:CZ2	1:B:251:ALA:HB1	2.49	0.47
1:A:218:THR:HG23	4:A:1072:HOH:O	2.14	0.46
1:B:192:LYS:NZ	4:B:1053:HOH:O	2.45	0.46
1:B:275:LYS:NZ	4:B:1218:HOH:O	2.48	0.46
1:B:253:ARG:HD2	4:B:973:HOH:O	2.16	0.46
1:C:197:LYS:HB2	4:C:1098:HOH:O	2.15	0.46
1:C:317:THR:HG22	1:C:380:ILE:HD11	1.98	0.46
1:C:347:ASN:N	1:C:348:GLY:HA2	2.31	0.46
1:A:18:THR:C	4:A:781:HOH:O	2.55	0.45
1:C:343:PRO:HD2	1:C:348:GLY:HA3	1.97	0.45
1:B:173:ARG:CZ	4:B:923:HOH:O	2.65	0.45
1:B:343:PRO:HD3	1:B:349:TRP:CE2	2.51	0.45
1:B:399:ASN:OD1	1:B:402:GLU:HG2	2.17	0.45
1:A:130:ILE:HD12	1:A:130:ILE:HA	1.80	0.45
1:C:313:LEU:HB3	1:C:428:VAL:HG21	1.99	0.44
1:A:315:LEU:HD22	4:A:733:HOH:O	2.17	0.44
4:B:865:HOH:O	1:C:25:THR:HG22	2.16	0.44
1:B:130:ILE:HG13	1:B:154:VAL:O	2.16	0.44
1:A:388:ASN:OD1	4:A:819:HOH:O	2.21	0.44
1:B:401:VAL:HG13	4:B:1177:HOH:O	2.17	0.44
1:A:24:LEU:HD22	1:A:430:ILE:HG12	1.98	0.44
1:A:202:LEU:HD12	1:A:210:ARG:O	2.18	0.44
1:A:400:GLN:O	1:A:403:LYS:NZ	2.48	0.44
1:B:386:LYS:HD2	1:C:425:LYS:HD3	2.01	0.43
1:B:97:PRO:HG2	1:B:224:GLN:HB2	2.00	0.43
1:B:497:LYS:HD3	1:B:497:LYS:HA	1.80	0.43
1:A:290:ASN:ND2	4:A:994:HOH:O	2.49	0.43
1:A:124:PRO:HG3	1:A:151:ILE:HD11	1.99	0.43
1:A:140:ASN:HD21	1:A:141:ARG:CZ	2.31	0.43
1:A:174:ASP:HB3	1:A:234:LEU:HD11	1.99	0.43
1:A:242:THR:HG23	1:B:220:ILE:HD13	2.00	0.43
1:B:423:ASN:OD1	4:B:1018:HOH:O	2.21	0.42
1:A:386:LYS:HD2	1:B:425:LYS:HD3	2.01	0.42
1:B:81:TRP:CZ2	1:B:113:VAL:HG13	2.54	0.42
1:B:178:LEU:HD23	1:B:232:TRP:HB3	2.01	0.42
1:B:278:THR:HG22	1:B:280:CYS:N	2.30	0.42
1:A:127:TRP:CZ2	1:A:251:ALA:HB1	2.55	0.42
1:A:354:HIS:O	1:A:360:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ARG:HD2	4:A:1121:HOH:O	2.20	0.42
1:B:346:ILE:HD11	1:B:369:THR:HG23	2.01	0.42
1:C:346:ILE:HD11	1:C:369:THR:HG23	2.02	0.42
1:B:173:ARG:NH2	4:B:923:HOH:O	2.52	0.42
1:A:455:LYS:HB3	1:A:456:ASP:H	1.65	0.41
1:A:220:ILE:HG21	1:C:242:THR:HG21	2.02	0.41
1:C:253:ARG:NH2	4:C:1149:HOH:O	2.44	0.41
1:B:15:ASN:ND2	1:B:336:GLY:HA2	2.35	0.41
1:C:97:PRO:HB3	1:C:221:GLY:HA3	2.03	0.41
1:C:424:ALA:O	1:C:428:VAL:HG23	2.20	0.41
1:C:475:SER:O	1:C:479:THR:HG23	2.20	0.41
1:A:166:GLU:HG3	2:D:1:NAG:H82	2.02	0.41
1:A:95:CYS:HB2	1:A:137:SER:O	2.21	0.41
1:A:123:PRO:HG2	1:A:126:LYS:HB2	2.03	0.41
1:C:281:GLN:HB2	4:C:873:HOH:O	2.21	0.41
1:B:347:ASN:N	1:B:348:GLY:HA2	2.37	0.40
1:C:174:ASP:HB3	1:C:234:LEU:HD22	2.02	0.40
1:A:360:THR:CG2	1:A:361:GLY:HA3	2.52	0.40
1:C:478:GLU:OE1	1:C:481:ARG:NH2	2.51	0.40
1:B:123:PRO:O	1:B:126:LYS:HB2	2.22	0.40
1:B:151:ILE:HD11	1:B:253:ARG:HG3	2.03	0.40
1:C:279:LYS:HB2	1:C:303:ASP:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/515 (98%)	493 (97%)	11 (2%)	3 (1%)	21	17
1	B	507/515 (98%)	488 (96%)	16 (3%)	3 (1%)	21	17
1	C	507/515 (98%)	488 (96%)	16 (3%)	3 (1%)	21	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1521/1545 (98%)	1469 (97%)	43 (3%)	9 (1%)	21	17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	348	GLY
1	B	339	GLU
1	B	361	GLY
1	C	19	ASP
1	C	361	GLY
1	A	361	GLY
1	B	348	GLY
1	C	348	GLY

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	438/444 (99%)	425 (97%)	13 (3%)	36	38
1	B	438/444 (99%)	417 (95%)	21 (5%)	23	21
1	C	438/444 (99%)	427 (98%)	11 (2%)	42	45
All	All	1314/1332 (99%)	1269 (97%)	45 (3%)	32	33

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	VAL
1	A	121	LEU
1	A	126	LYS
1	A	130	ILE
1	A	197	LYS
1	A	284	MET
1	A	315	LEU

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Mol	Chain	Res	Type
1	A	360	THR
1	A	436	LEU
1	A	471	LYS
1	A	506	LEU
1	A	507	VAL
1	A	509	ARG
1	B	4	ILE
1	B	94	LEU
1	B	109	LEU
1	B	113	VAL
1	B	126	LYS
1	B	130	ILE
1	B	234	LEU
1	B	240	ARG
1	B	265	ARG
1	B	272	ARG
1	B	278	THR
1	B	284	MET
1	B	298	ARG
1	B	315	LEU
1	B	339	GLU
1	B	400	GLN
1	B	402	GLU
1	B	436	LEU
1	B	455	LYS
1	B	461	GLU
1	B	506	LEU
1	C	4	ILE
1	C	130	ILE
1	C	197	LYS
1	C	216	ILE
1	C	234	LEU
1	C	258	ILE
1	C	284	MET
1	C	315	LEU
1	C	360	THR
1	C	499	GLN
1	C	506	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	149	ASN
1	A	347	ASN
1	A	370	GLN
1	A	499	GLN
1	B	114	ASN
1	B	370	GLN
1	C	390	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 ⓘ

6 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	0.56	0	17,19,21	0.83	0
2	NAG	D	2	2	14,14,15	0.43	0	17,19,21	1.37	2 (11%)
2	NAG	E	1	2,1	14,14,15	0.48	0	17,19,21	0.93	1 (5%)
2	NAG	E	2	2	14,14,15	0.55	0	17,19,21	0.46	0
2	NAG	F	1	2,1	14,14,15	0.59	0	17,19,21	0.62	0
2	NAG	F	2	2	14,14,15	0.55	0	17,19,21	0.78	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
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	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(°)
2	D	2	NAG	C1-O5-C5	4.36	118.02	112.19
2	E	1	NAG	C1-O5-C5	2.56	115.62	112.19
2	D	2	NAG	C6-C5-C4	-2.30	107.37	113.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

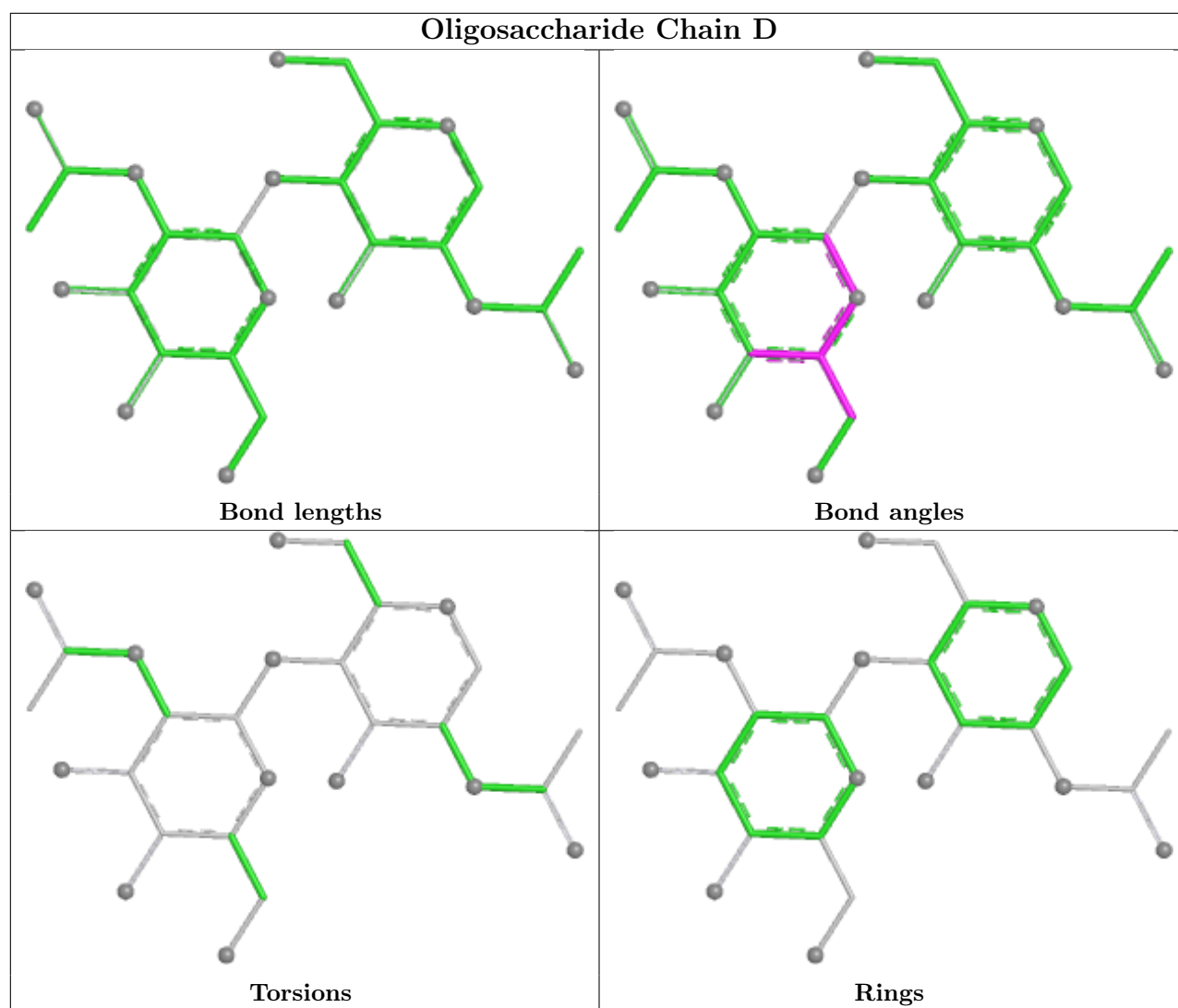
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6

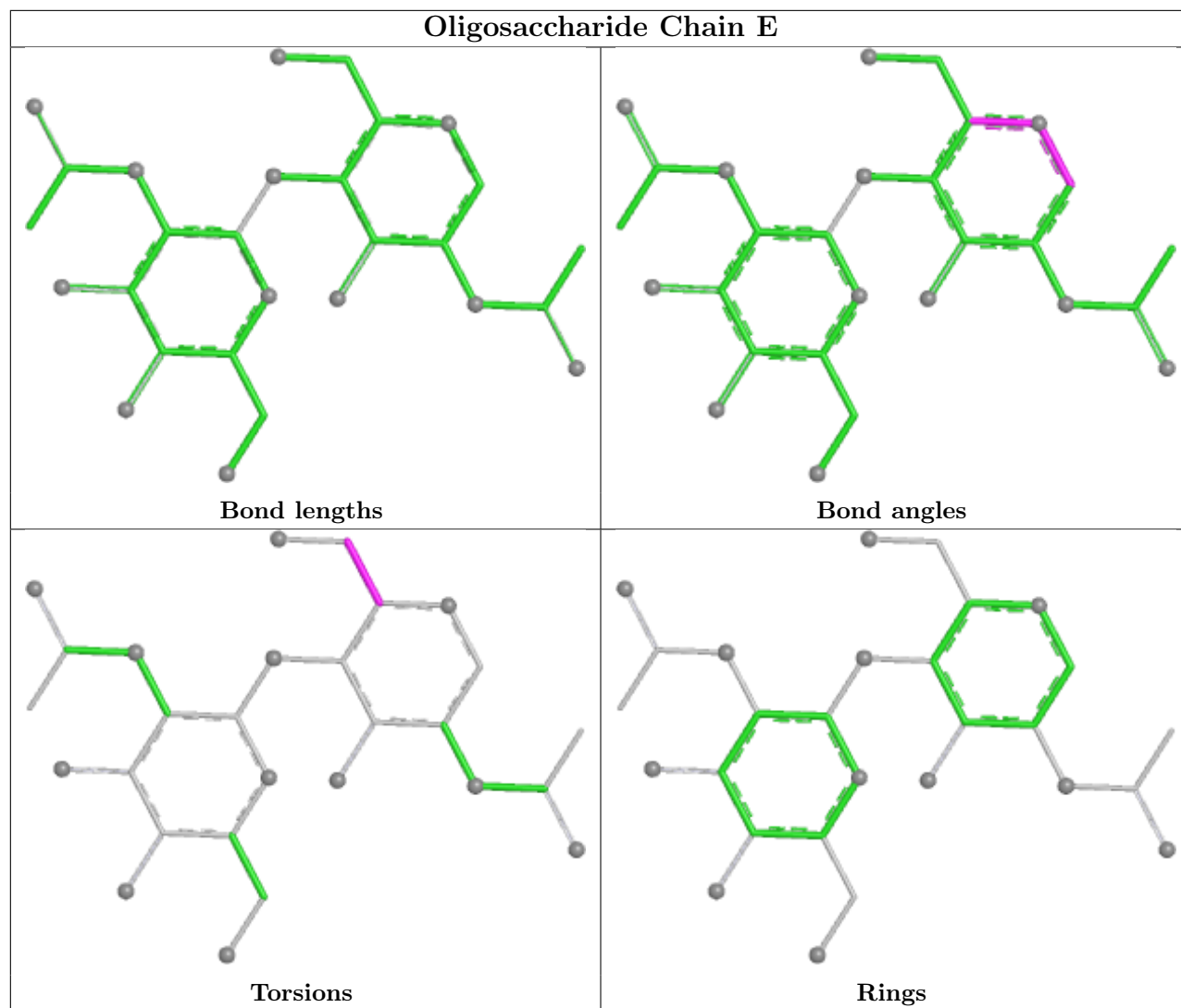
There are no ring outliers.

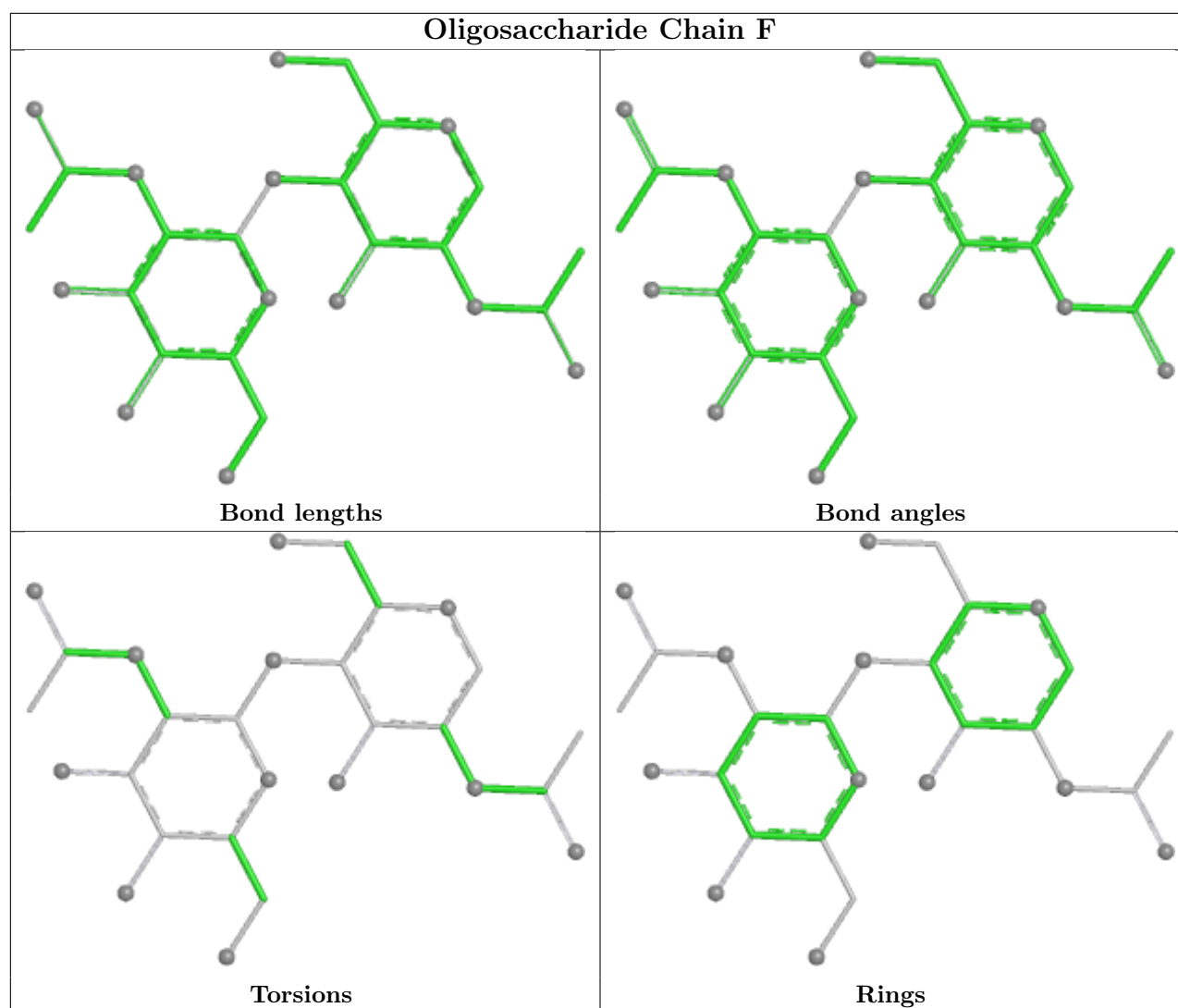
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	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](#)

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	$\# Z > 2$
3	NAG	A	603	1	14,14,15	0.66	1 (7%)	17,19,21	1.20	1 (5%)
3	NAG	C	603	1	14,14,15	0.66	1 (7%)	17,19,21	1.86	2 (11%)
3	NAG	B	603	1	14,14,15	0.58	0	17,19,21	1.37	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	A	603	1	-	0/6/23/26	0/1/1/1
3	NAG	C	603	1	-	0/6/23/26	0/1/1/1
3	NAG	B	603	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	NAG	C1-C2	2.05	1.55	1.52
3	A	603	NAG	C1-C2	2.01	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	NAG	C1-O5-C5	6.45	120.83	112.19
3	B	603	NAG	C1-O5-C5	4.49	118.21	112.19
3	A	603	NAG	C1-O5-C5	3.85	117.35	112.19
3	C	603	NAG	O5-C1-C2	2.37	114.96	111.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	NAG	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	509/515 (98%)	0.23	17 (3%) 49 48	7, 18, 32, 62	0
1	B	509/515 (98%)	0.28	22 (4%) 40 39	6, 18, 32, 64	0
1	C	509/515 (98%)	0.22	13 (2%) 57 56	7, 18, 32, 63	0
All	All	1527/1545 (98%)	0.24	52 (3%) 48 47	6, 18, 32, 64	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	GLY	5.0
1	B	348	GLY	4.8
1	C	17	SER	4.3
1	C	348	GLY	4.1
1	B	18	THR	4.0
1	A	18	THR	3.8
1	A	19	ASP	3.6
1	B	17	SER	3.6
1	A	361	GLY	3.6
1	B	361	GLY	3.6
1	B	19	ASP	3.6
1	A	344	GLY	3.5
1	A	337	PHE	3.4
1	B	338	ILE	3.2
1	C	360	THR	3.2
1	B	343	PRO	3.2
1	C	344	GLY	3.2
1	C	361	GLY	3.1
1	C	18	THR	3.1
1	B	344	GLY	3.1
1	C	340	GLY	3.1
1	B	337	PHE	3.1
1	A	360	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	3.0
1	B	1	ALA	3.0
1	B	401	VAL	2.9
1	A	17	SER	2.8
1	C	15	ASN	2.7
1	B	360	THR	2.7
1	C	1	ALA	2.6
1	A	4	ILE	2.6
1	C	19	ASP	2.6
1	C	90	ALA	2.5
1	A	158	ASN	2.4
1	B	347	ASN	2.4
1	B	340	GLY	2.4
1	B	345	LEU	2.4
1	A	141	ARG	2.3
1	B	276	CYS	2.3
1	B	20	THR	2.3
1	A	345	LEU	2.3
1	B	336	GLY	2.3
1	B	16	ASN	2.2
1	C	337	PHE	2.2
1	C	334	ILE	2.2
1	A	509	ARG	2.2
1	B	113	VAL	2.2
1	A	20	THR	2.2
1	A	341	GLY	2.2
1	B	346	ILE	2.1
1	A	342	TRP	2.0
1	B	342	TRP	2.0

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

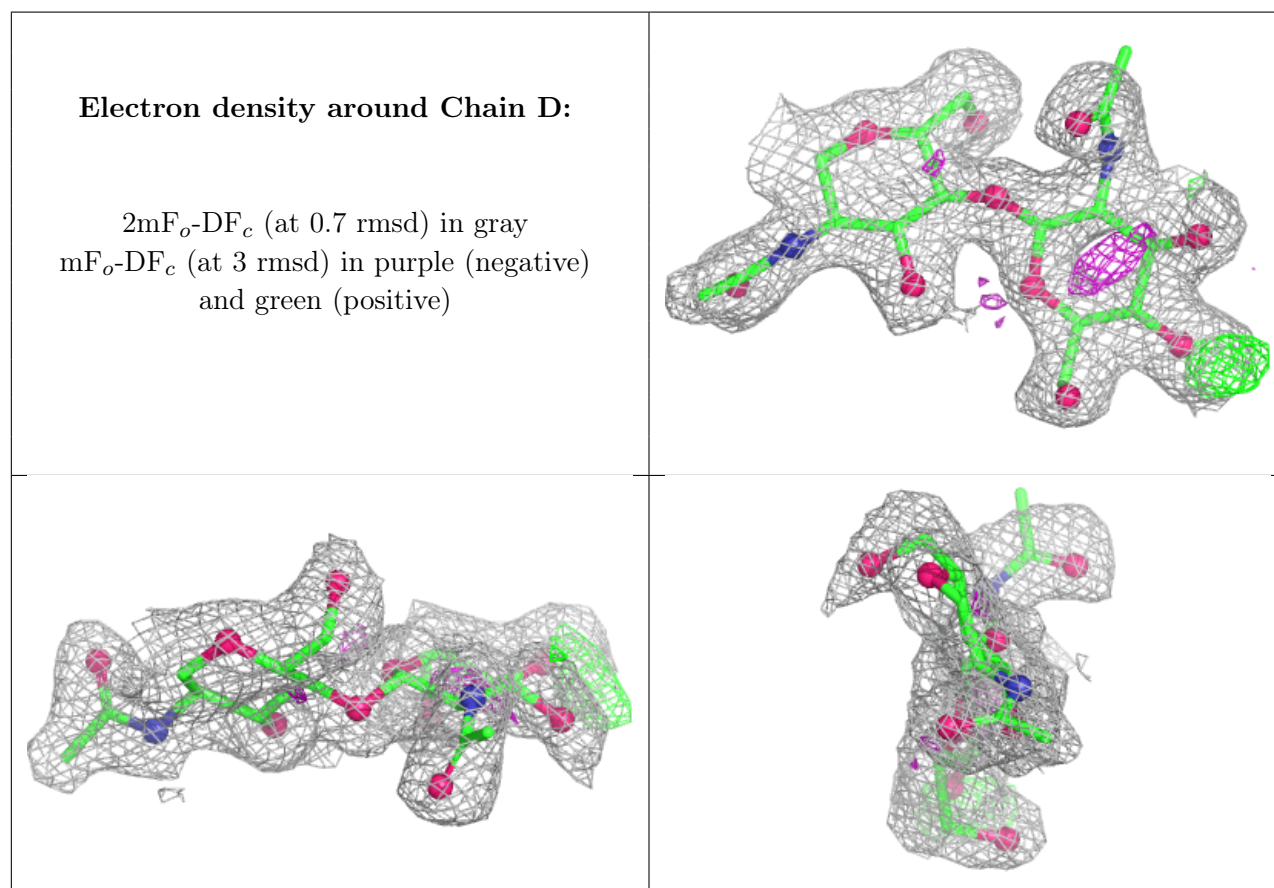
There are no non-standard protein/DNA/RNA residues in this entry.

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.

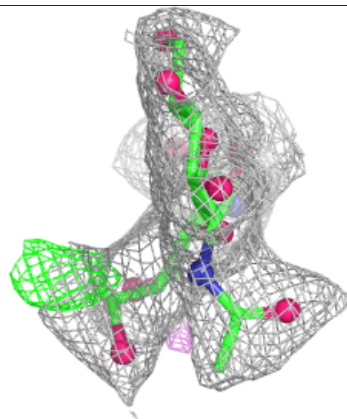
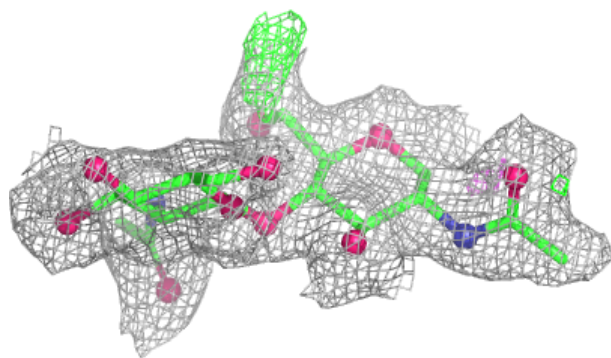
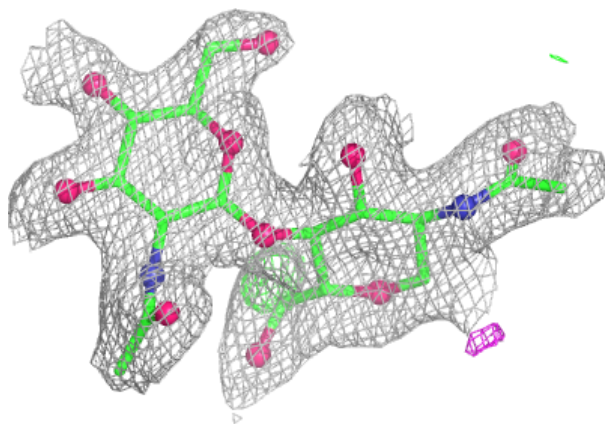
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	2	14/15	0.76	0.15	26,36,42,44	0
2	NAG	F	2	14/15	0.86	0.13	25,29,35,43	0
2	NAG	E	2	14/15	0.88	0.11	29,35,39,41	0
2	NAG	E	1	14/15	0.91	0.08	25,27,32,33	0
2	NAG	F	1	14/15	0.92	0.09	23,25,27,28	0
2	NAG	D	1	14/15	0.92	0.09	18,25,32,32	0

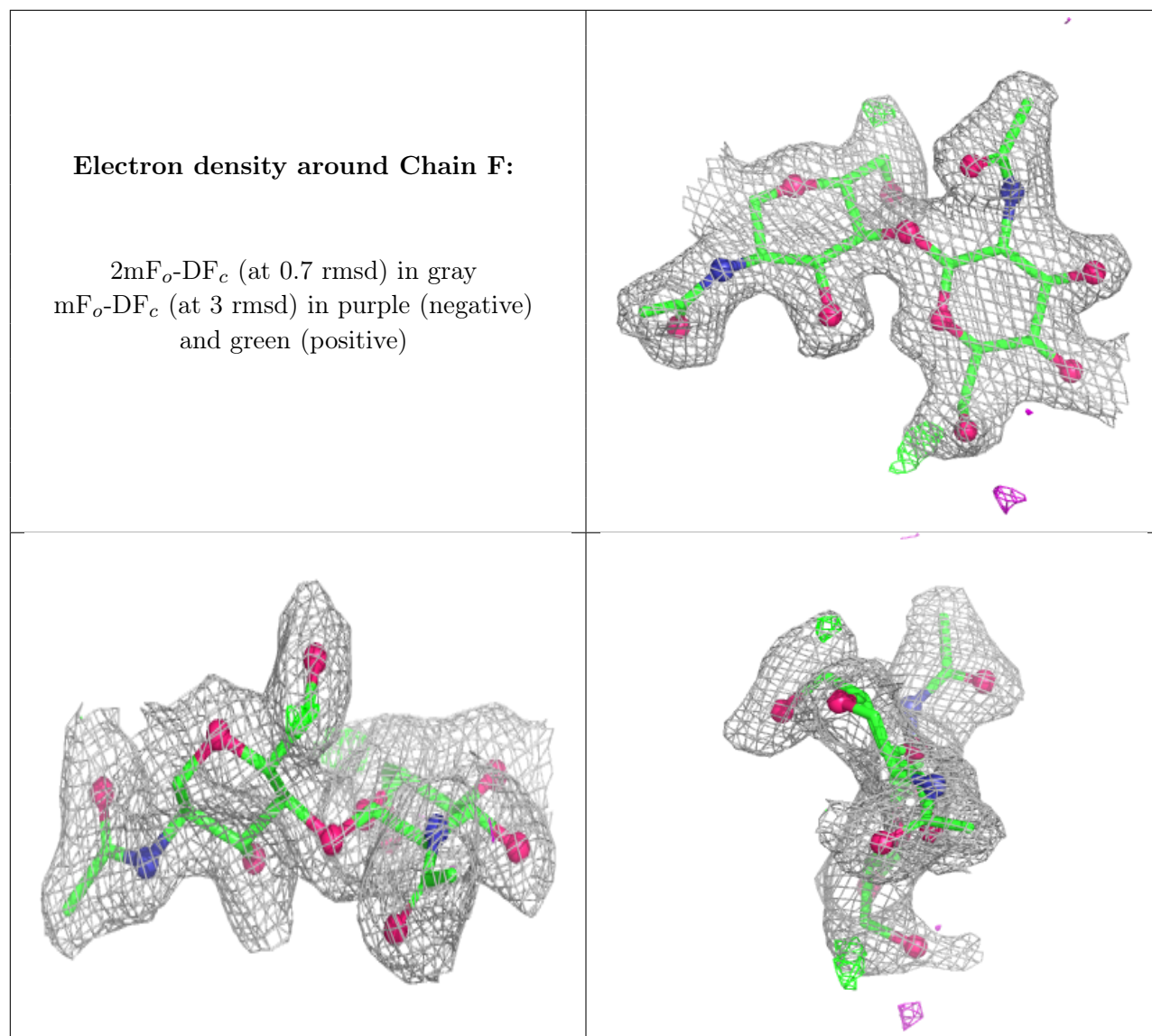
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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(Å ²)	Q<0.9
3	NAG	B	603	14/15	0.73	0.15	33,40,47,51	0
3	NAG	C	603	14/15	0.82	0.12	29,38,42,47	0
3	NAG	A	603	14/15	0.83	0.12	25,34,39,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.