



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:29 PM UTC

PDB ID : 4B7M / pdb_00004b7m
Title : H1N1 2009 Pandemic Influenza Virus: Resistance of the I223R Neuraminidase Mutant Explained by Kinetic and Structural Analysis
Authors : van der Vries, E.; Vachieri, S.G.; Xiong, X.; Liu, J.; Collins, P.J.; Walker, P.A.; Haire, L.F.; Hay, A.J.; Schutten, M.; Osterhaus, A.D.M.E.; Martin, S.R.; Boucher, C.A.B.; Skehel, J.J.; Gamblin, S.J.
Deposited on : 2012-08-21
Resolution : 2.50 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

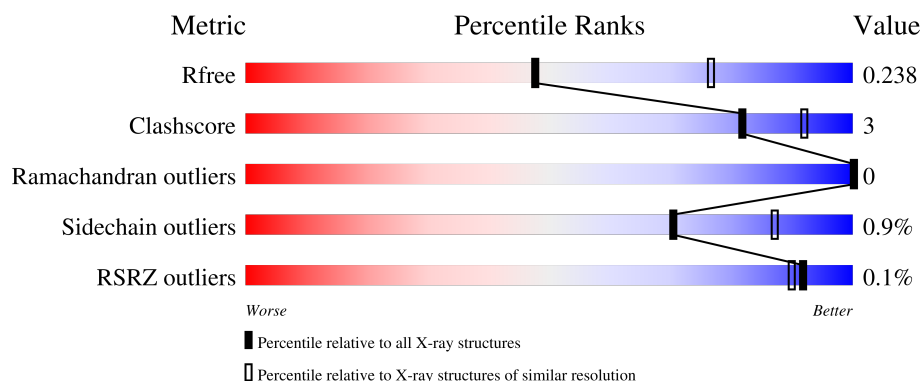
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

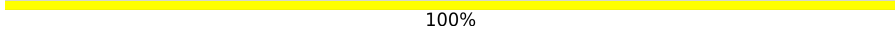
The reported resolution of this entry is 2.50 Å.

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.



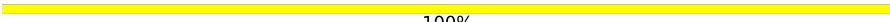
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	469	
1	B	469	
2	C	2	
2	D	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	2	 100%

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	B	521	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6367 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 NEURAMINIDASE.

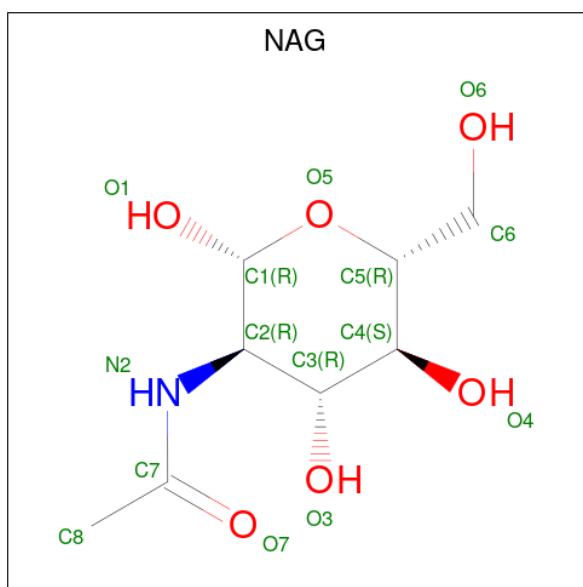
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2989	1875	516	577	21			
1	B	386	Total	C	N	O	S	0	0	0
			2989	1875	516	577	21			

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



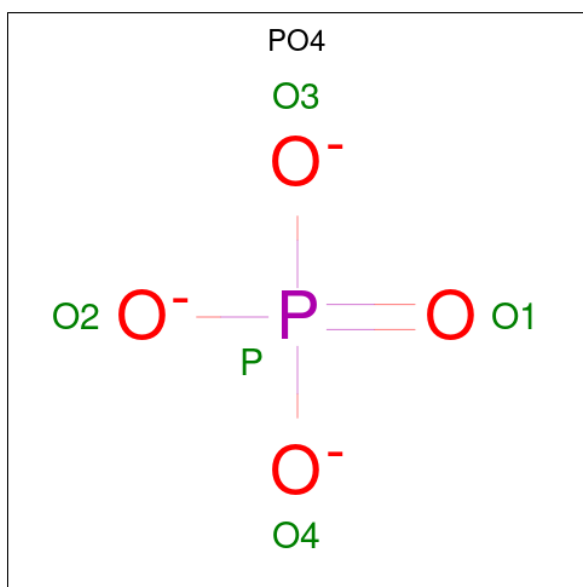
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O P	0	0
			5	4 1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total	O	0	0
			128	128		
6	B	113	Total	O	0	0
			113	113		



WORLD WIDE
PDB
PROTEIN DATA BANK



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

Chain E:

100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.58Å 162.47Å 118.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.78 – 2.50 95.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	71.9 (95.78-2.50) 93.3 (95.78-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.237 0.213 , 0.238	Depositor DCC
R_{free} test set	1862 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.885	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 21.3	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	6367	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.49% 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: PO4, NAG, CA

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	0.59	0/3071	0.72	1/4173 (0.0%)
1	B	0.59	0/3071	0.72	1/4173 (0.0%)
All	All	0.59	0/6142	0.72	2/8346 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	GLN	N-CA-C	6.50	118.36	111.28
1	B	227	GLN	N-CA-C	6.11	117.94	111.28

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	2989	0	2816	14	0
1	B	2989	0	2814	16	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
3	A	28	0	26	4	0
3	B	14	0	13	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	128	0	0	0	0
6	B	113	0	0	1	0
All	All	6367	0	5744	30	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 3.

All (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:HD22	3:A:521:NAG:H83	1.32	0.93
1:B:229:SER:HB2	1:B:347:LYS:HE2	1.68	0.75
1:B:216:ILE:HD11	1:B:263:ILE:HG13	1.76	0.67
1:B:229:SER:HB2	1:B:347:LYS:CE	2.31	0.60
1:A:278:GLU:HB3	1:A:347:LYS:HD3	1.88	0.56
1:A:204:ALA:HB3	1:A:216:ILE:HD12	1.91	0.53
1:A:195:ILE:HG12	1:A:204:ALA:HB2	1.91	0.53
1:A:219:TRP:CD1	1:A:220:ARG:HG2	2.45	0.52
1:A:235:ASN:HD22	3:A:521:NAG:C8	2.13	0.52
1:B:235:ASN:OD1	3:B:521:NAG:O5	2.29	0.49
1:B:258:ILE:HG12	1:B:263:ILE:HD13	1.95	0.48
1:A:402:TYR:HB2	1:A:425:GLU:OE1	2.14	0.47
1:B:443:ILE:HD12	1:B:445:PHE:HE1	1.79	0.47
1:A:235:ASN:ND2	3:A:521:NAG:H83	2.15	0.47
1:A:393:ILE:HG22	1:A:394:VAL:HG23	1.98	0.46
1:B:322:PHE:HB2	1:B:327:ARG:HD2	1.98	0.46
1:B:219:TRP:CD1	1:B:220:ARG:HG2	2.52	0.45
1:A:308:GLN:OE1	3:A:521:NAG:H81	2.16	0.44
1:B:193:ILE:HG12	1:B:206:LEU:HG	1.99	0.44
1:B:300:ASN:ND2	1:B:316:TYR:HB3	2.33	0.43
1:B:441:SER:HB2	1:B:459:ASP:OD1	2.19	0.43
1:A:122:ILE:HD12	1:A:423:TRP:HB3	2.00	0.43
1:B:140:LEU:HB2	6:B:2020:HOH:O	2.19	0.43
1:B:320:GLY:HA3	1:B:385:ASN:HB3	2.01	0.42
1:A:428:ARG:NH2	1:A:463:LEU:HG	2.34	0.42
1:A:443:ILE:HD12	1:A:445:PHE:HE1	1.85	0.42
1:B:122:ILE:HD12	1:B:423:TRP:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ILE:HG22	1:B:310:LEU:HD22	2.03	0.41
1:A:121:PHE:CG	1:A:229:SER:HA	2.57	0.40
1:B:393:ILE:HG22	1:B:394:VAL:HG23	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	384/469 (82%)	364 (95%)	20 (5%)	0	100	100
1	B	384/469 (82%)	366 (95%)	18 (5%)	0	100	100
All	All	768/938 (82%)	730 (95%)	38 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	333/408 (82%)	329 (99%)	4 (1%)	63	83
1	B	333/408 (82%)	331 (99%)	2 (1%)	78	91
All	All	666/816 (82%)	660 (99%)	6 (1%)	70	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	ILE
1	A	231	CYS
1	A	248	ASP
1	A	441	SER
1	B	231	CYS
1	B	344	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	221	ASN
1	A	309	ASN
1	A	325	ASN
1	A	341	ASN
1	B	308	GLN
1	B	325	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	C	1	2,1	14,14,15	0.54	0	17,19,21	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	2	2	14,14,15	0.44	0	17,19,21	1.19	2 (11%)
2	NAG	D	1	2,1	14,14,15	0.64	0	17,19,21	1.12	1 (5%)
2	NAG	D	2	2	14,14,15	0.52	0	17,19,21	0.95	0
2	NAG	E	1	2,1	14,14,15	0.50	0	17,19,21	1.05	1 (5%)
2	NAG	E	2	2	14,14,15	0.64	0	17,19,21	1.21	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	3.28	116.58	112.19
2	D	1	NAG	O5-C1-C2	-3.17	106.39	111.29
2	E	2	NAG	C4-C3-C2	3.08	115.53	111.02
2	C	1	NAG	O5-C1-C2	-2.50	107.43	111.29
2	E	1	NAG	O5-C1-C2	-2.44	107.52	111.29
2	E	2	NAG	C1-O5-C5	2.40	115.41	112.19
2	C	2	NAG	C1-C2-N2	2.39	114.20	110.43

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

Continued on next page...

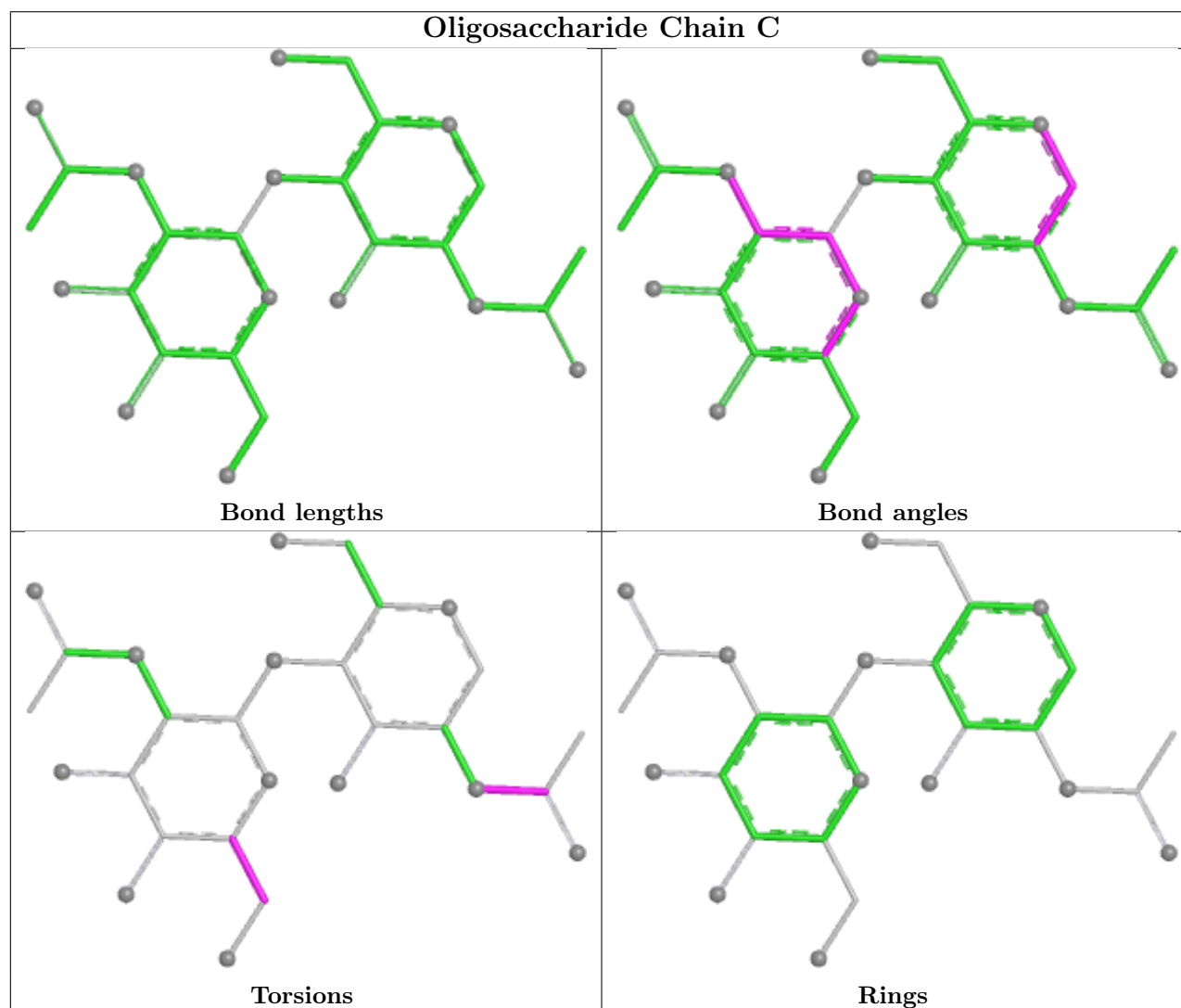
Continued from previous page...

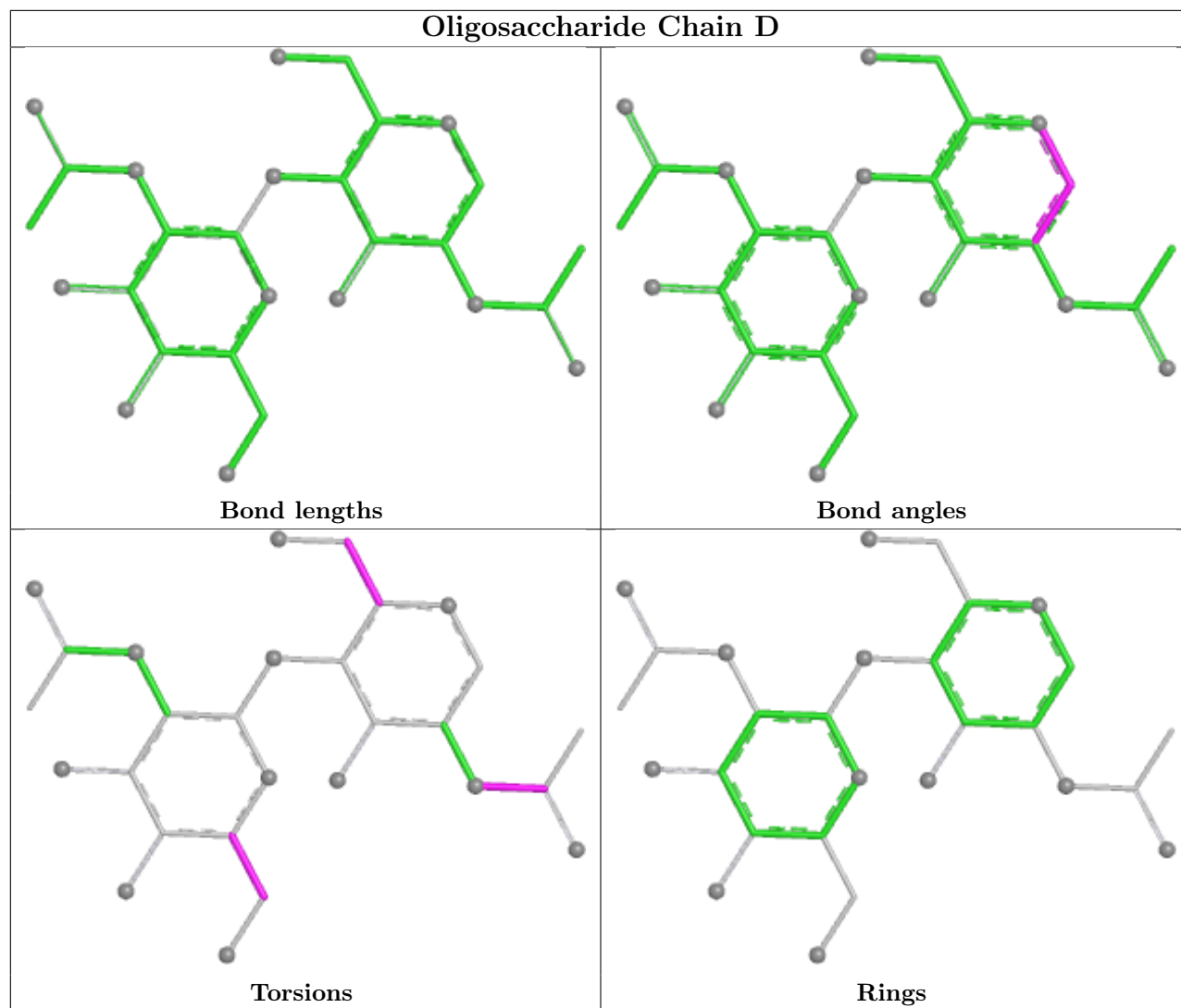
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6

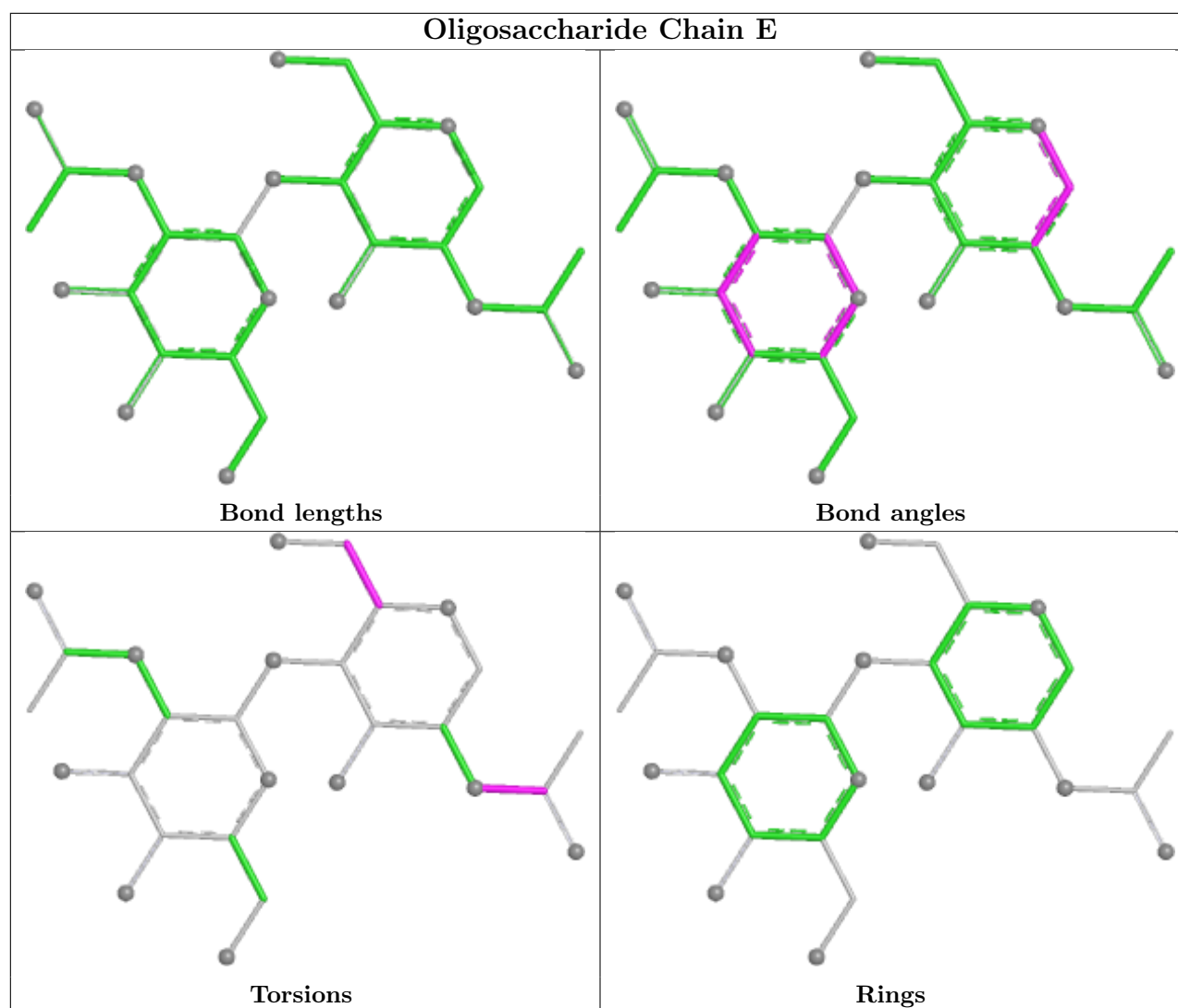
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	521	1	14,14,15	0.76	1 (7%)	17,19,21	1.34	1 (5%)
4	PO4	A	1469	-	4,4,4	0.96	0	6,6,6	0.46	0
3	NAG	A	501	1	14,14,15	0.70	0	17,19,21	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	521	1	14,14,15	0.51	0	17,19,21	0.91	1 (5%)
4	PO4	B	1469	-	4,4,4	0.97	0	6,6,6	0.56	0
4	PO4	A	1470	-	4,4,4	0.98	0	6,6,6	0.46	0
4	PO4	B	1470	-	4,4,4	0.95	0	6,6,6	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	501	1	-	4/6/23/26	0/1/1/1
3	NAG	A	521	1	-	4/6/23/26	0/1/1/1
3	NAG	B	521	1	1/1/5/7	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	521	NAG	C1-C2	2.07	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	521	NAG	C2-N2-C7	-3.80	117.81	122.90
3	B	521	NAG	O5-C1-C2	-2.17	107.94	111.29
3	A	501	NAG	C1-O5-C5	2.12	115.03	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	521	NAG	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	521	NAG	C4-C5-C6-O6
3	A	501	NAG	C8-C7-N2-C2
3	A	501	NAG	O7-C7-N2-C2
3	A	521	NAG	C8-C7-N2-C2
3	A	521	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	521	NAG	C8-C7-N2-C2
3	B	521	NAG	O7-C7-N2-C2
3	B	521	NAG	O5-C5-C6-O6
3	A	521	NAG	C4-C5-C6-O6
3	A	501	NAG	O5-C5-C6-O6
3	A	501	NAG	C4-C5-C6-O6
3	A	521	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	521	NAG	4	0
3	B	521	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	386/469 (82%)	-0.19	0 100 100	12, 15, 22, 28	0
1	B	386/469 (82%)	-0.15	1 (0%) 90 87	12, 15, 22, 33	0
All	All	772/938 (82%)	-0.17	1 (0%) 92 90	12, 15, 22, 33	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	CYS	2.8

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

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

6.3 Carbohydrates [i](#)

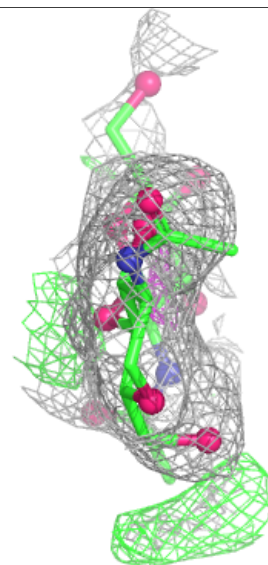
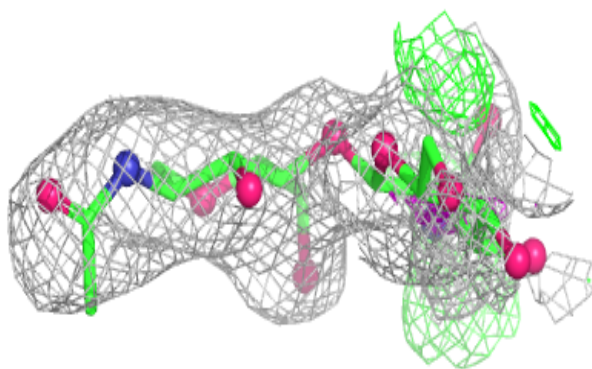
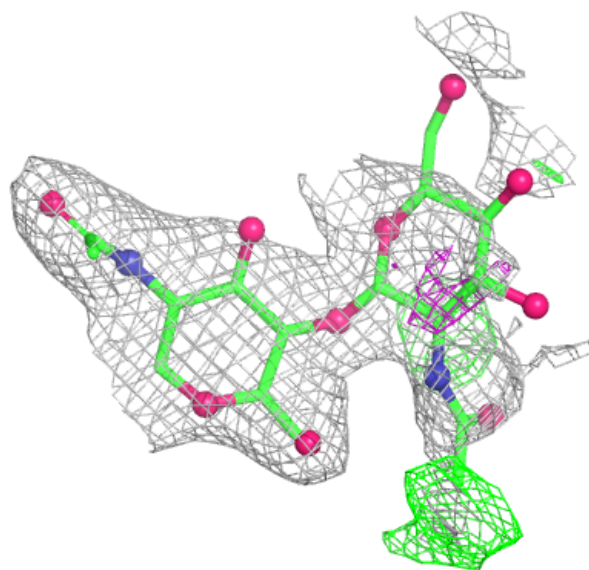
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.31	0.21	51,53,55,55	0
2	NAG	E	2	14/15	0.44	0.20	51,53,53,54	0
2	NAG	D	2	14/15	0.64	0.17	49,51,52,53	0
2	NAG	E	1	14/15	0.75	0.14	41,43,45,48	0
2	NAG	D	1	14/15	0.75	0.14	36,41,43,46	0
2	NAG	C	1	14/15	0.82	0.11	37,39,42,47	0

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

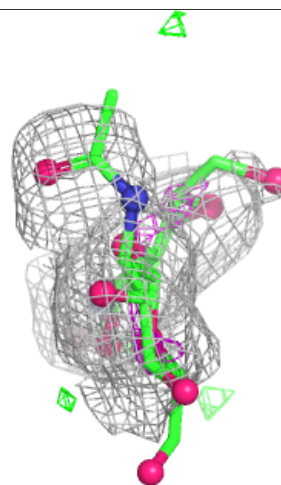
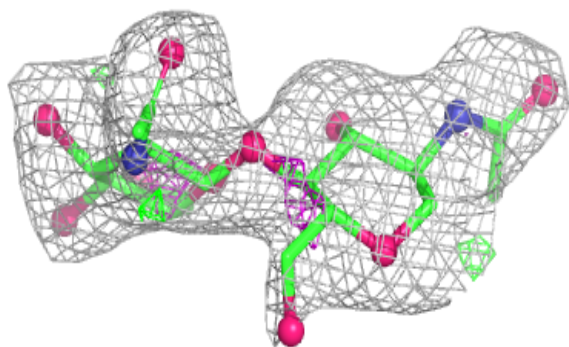
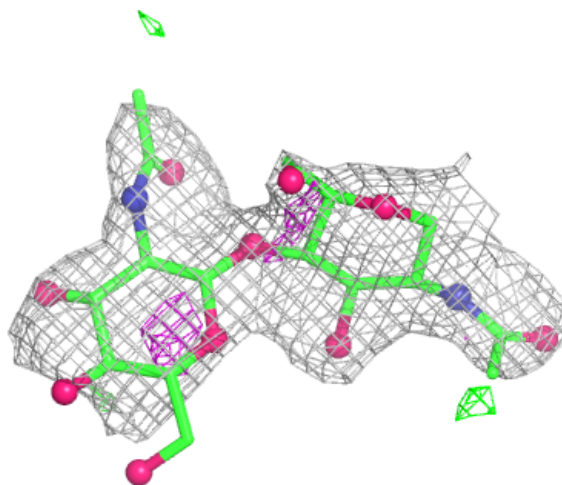
Electron density around Chain C:

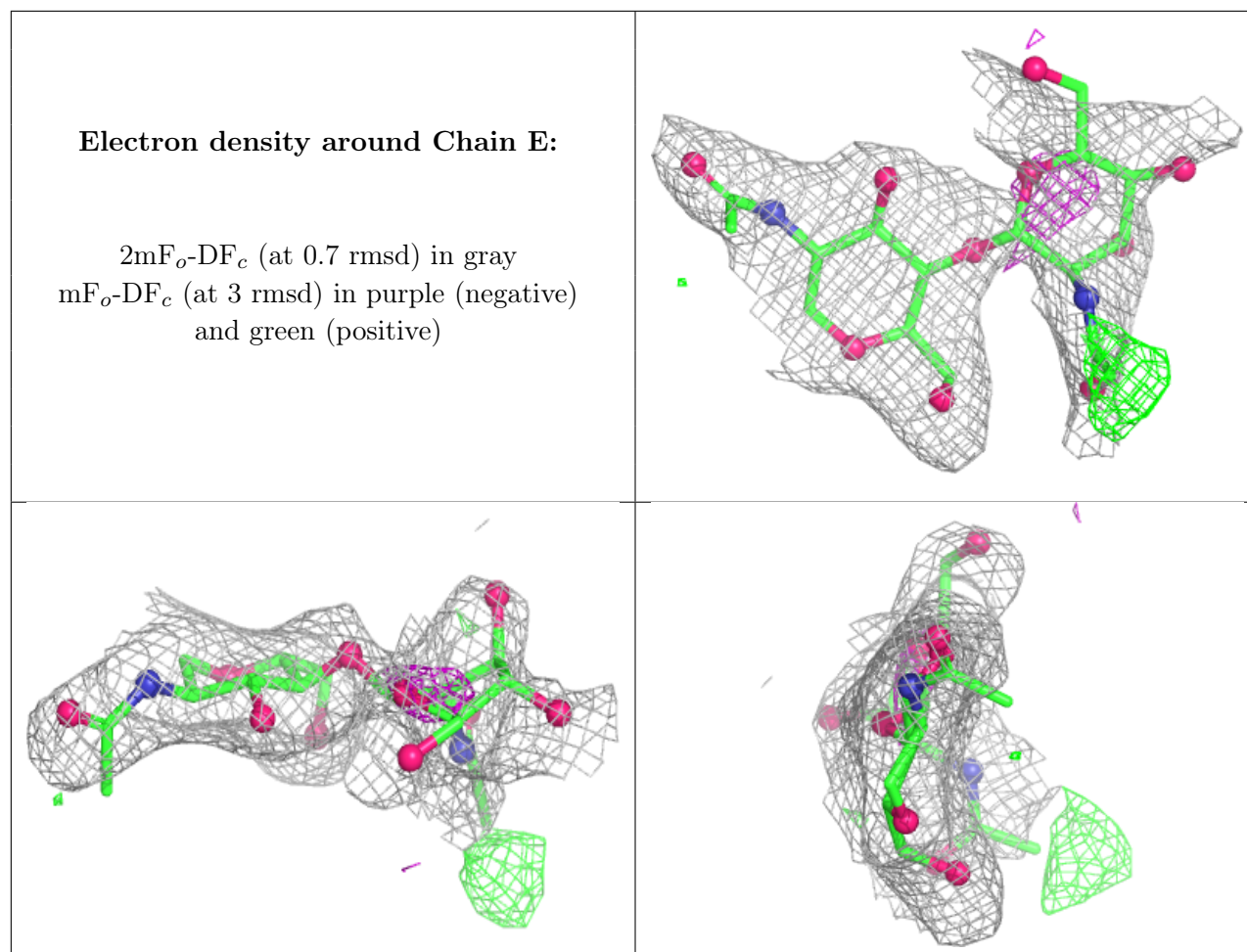
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
3	NAG	A	521	14/15	0.62	0.15	32,34,36,36	0
3	NAG	B	521	14/15	0.68	0.20	28,29,30,30	0
3	NAG	A	501	14/15	0.78	0.12	30,31,32,33	0
4	PO4	B	1469	5/5	0.95	0.08	28,29,29,29	0
5	CA	B	1471	1/1	0.95	0.03	17,17,17,17	0
4	PO4	B	1470	5/5	0.97	0.08	21,21,21,21	0
4	PO4	A	1470	5/5	0.97	0.07	17,17,17,17	0
4	PO4	A	1469	5/5	0.98	0.09	20,20,21,21	0
5	CA	A	1471	1/1	0.99	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.