



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:27 AM UTC

PDB ID : 4DAG / pdb_00004dag
Title : Structure of the Human Metapneumovirus Fusion Protein with Neutralizing Antibody Identifies a Pneumovirus Antigenic Site
Authors : Jardetzky, T.S.; Wen, X.
Deposited on : 2012-01-12
Resolution : 3.39 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

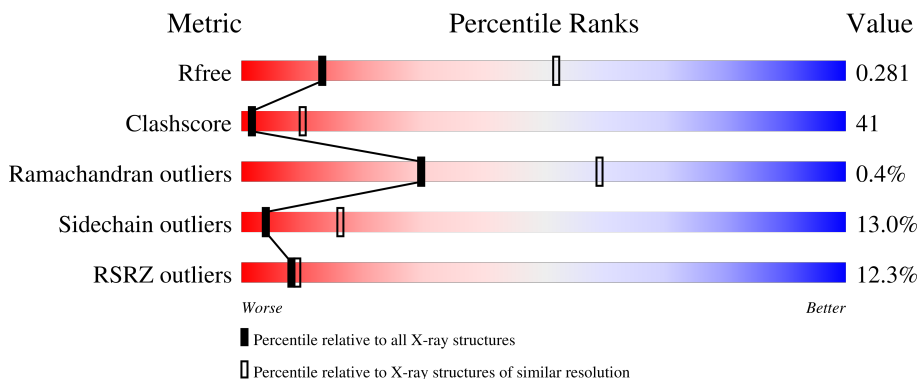
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	415	
2	H	220	
3	L	213	
4	B	5	
4	C	5	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6064 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	2740	1707	473	540	20	0	0	0

- Molecule 2 is a protein called Neutralizing Antibody DS7 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	220	1621	1021	272	319	9	0	0	0

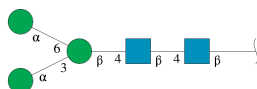
- Molecule 3 is a protein called Neutralizing Antibody DS7 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	213	1581	985	259	330	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	233	MET	-	expression tag	UNP Q8N5F4

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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
			Total	C	N	O			
4	B	5	61	34	2	25	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	C	5	61	34	2	25	0	0	0

K218
K219
V220

- Molecule 3: Neutralizing Antibody DS7 light chain

Chain L: 4% 39% 54% 7%

E21 L22 A23 L24 I25 Q26 V30 S31 V32 P34 A38 S39 I40 S43 C44 D45 K46 L47 C48 D49 K50 Y51 A52 S53 W54 Y55 Q56 Q57 K58 P59 S62 P63 V64 L65 V66 L67 Y68 Q69 D70 S71 E72 R73 P74 S75 G76 I77 P78 E79 R80 F81 S82 G83 T89

T93 I94 S95 G96 A99 E102 Y106 C107 Q108 A109 W110 D111 S112 S113 T114 A115 V116 F117 M118 G119 G120 T121 T122 L123 L126 G127 Y128 A132 K133 P133 S134 V135 T136 L137 F138 P139 P140 S141 E142 E143 E144 L145 Q146 R147 N148 K149 A150 T151 L152 V153 R153 C154 F154 L155 I156 S157 D158 F159

Y160 A167 W168 K169 S173 P174 V175 K176 V179 E180 T181 T182 T183 P184 S185 K186 Q187 S188 M189 N190 Y191 Y192 A193 A194 S195 S196 Y197 L198 S199 L200 T201 P202 E203 Q204 M205 K206 S207 S210 Q214 G219 S220 T221 A227 P228 T229 E230 C231 S232 M233

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

Chain B: 60% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain C: 20% 80%

MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	258.96Å 258.96Å 167.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.85 – 3.39 44.85 – 3.39	Depositor EDS
% Data completeness (in resolution range)	78.8 (44.85-3.39) 78.4 (44.85-3.39)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.40Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.260 , 0.289 0.245 , 0.281	Depositor DCC
R_{free} test set	1855 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6064	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: MAN, BMA, 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	0.63	0/2776	1.21	23/3785 (0.6%)
2	H	0.76	0/1659	1.25	15/2260 (0.7%)
3	L	0.64	0/1618	1.14	10/2211 (0.5%)
All	All	0.67	0/6053	1.20	48/8256 (0.6%)

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	8
3	L	0	4
All	All	0	12

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	118	GLY	N-CA-C	-9.11	96.96	110.90
1	A	420	ILE	N-CA-C	8.74	120.51	112.29
1	A	66	LEU	N-CA-C	8.22	122.65	108.02
1	A	316	SER	N-CA-C	-8.17	96.56	109.23
2	H	143	GLY	N-CA-C	-8.12	104.56	115.36

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ILE	Peptide
1	A	145	ASN	Peptide
1	A	185	ALA	Peptide
1	A	66	LEU	Peptide
1	A	68	LYS	Peptide

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	2740	0	2604	239	0
2	H	1621	0	1596	127	0
3	L	1581	0	1519	134	0
4	B	61	0	50	1	0
4	C	61	0	52	5	0
All	All	6064	0	5821	483	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 41.

The worst 5 of 483 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:45:THR:HG22	1:A:272:GLN:HG2	1.38	1.06
2:H:34:MET:HE3	2:H:78:LEU:HD22	1.44	0.99
3:L:47:LEU:O	3:L:50:LYS:N	1.97	0.97
1:A:314:ALA:N	1:A:315:GLY:HA2	1.80	0.97
1:A:39:LEU:HB2	1:A:278:VAL:HG23	1.46	0.96

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	377/415 (91%)	327 (87%)	48 (13%)	2 (0%)	24	54
2	H	218/220 (99%)	204 (94%)	13 (6%)	1 (0%)	24	54
3	L	211/213 (99%)	197 (93%)	14 (7%)	0	100	100
All	All	806/848 (95%)	728 (90%)	75 (9%)	3 (0%)	30	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	MET
2	H	141	SER
1	A	162	VAL

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	279/347 (80%)	243 (87%)	36 (13%)	4	16
2	H	182/182 (100%)	156 (86%)	26 (14%)	3	13
3	L	178/178 (100%)	157 (88%)	21 (12%)	5	20
All	All	639/707 (90%)	556 (87%)	83 (13%)	4	16

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	187	LEU
3	L	95	SER
2	H	193	VAL
3	L	64	VAL
3	L	123	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	204	GLN
3	L	146	GLN
1	A	412	ASN
1	A	342	ASN
3	L	26	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

10 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
4	NAG	B	1	4,1	14,14,15	2.33	6 (42%)	17,19,21	1.31	3 (17%)
4	NAG	B	2	4	14,14,15	2.34	6 (42%)	17,19,21	1.26	3 (17%)
4	BMA	B	3	4	11,11,12	2.44	4 (36%)	15,15,17	1.39	3 (20%)
4	MAN	B	4	4	11,11,12	2.51	4 (36%)	15,15,17	1.15	1 (6%)
4	MAN	B	5	4	11,11,12	2.58	5 (45%)	15,15,17	1.13	0
4	NAG	C	1	4,1	14,14,15	2.22	5 (35%)	17,19,21	1.69	4 (23%)
4	NAG	C	2	4	14,14,15	2.42	6 (42%)	17,19,21	1.61	3 (17%)
4	BMA	C	3	4	11,11,12	2.56	6 (54%)	15,15,17	1.98	4 (26%)
4	MAN	C	4	4	11,11,12	2.29	4 (36%)	15,15,17	1.13	1 (6%)
4	MAN	C	5	4	11,11,12	2.40	3 (27%)	15,15,17	2.17	7 (46%)

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	B	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	BMA	B	3	4	-	1/2/19/22	0/1/1/1
4	MAN	B	4	4	-	2/2/19/22	1/1/1/1
4	MAN	B	5	4	-	2/2/19/22	1/1/1/1
4	NAG	C	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
4	MAN	C	4	4	-	1/2/19/22	1/1/1/1
4	MAN	C	5	4	-	2/2/19/22	0/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5	MAN	O5-C5	6.63	1.56	1.43
4	C	4	MAN	O5-C5	6.12	1.55	1.43
4	B	4	MAN	O5-C5	4.93	1.53	1.43
4	C	3	BMA	C4-C3	-4.89	1.39	1.52
4	C	2	NAG	C7-N2	4.84	1.50	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3	BMA	C1-C2-C3	-5.29	101.95	109.64
4	C	5	MAN	C1-O5-C5	4.15	117.75	112.19
4	C	1	NAG	C2-N2-C7	-4.02	117.51	122.90
4	C	5	MAN	O2-C2-C3	3.37	117.13	110.15
4	C	5	MAN	O6-C6-C5	3.31	122.61	111.33

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3	BMA	C4-C5-C6-O6
4	C	5	MAN	C4-C5-C6-O6
4	C	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	3	BMA	O5-C5-C6-O6
4	B	4	MAN	O5-C5-C6-O6

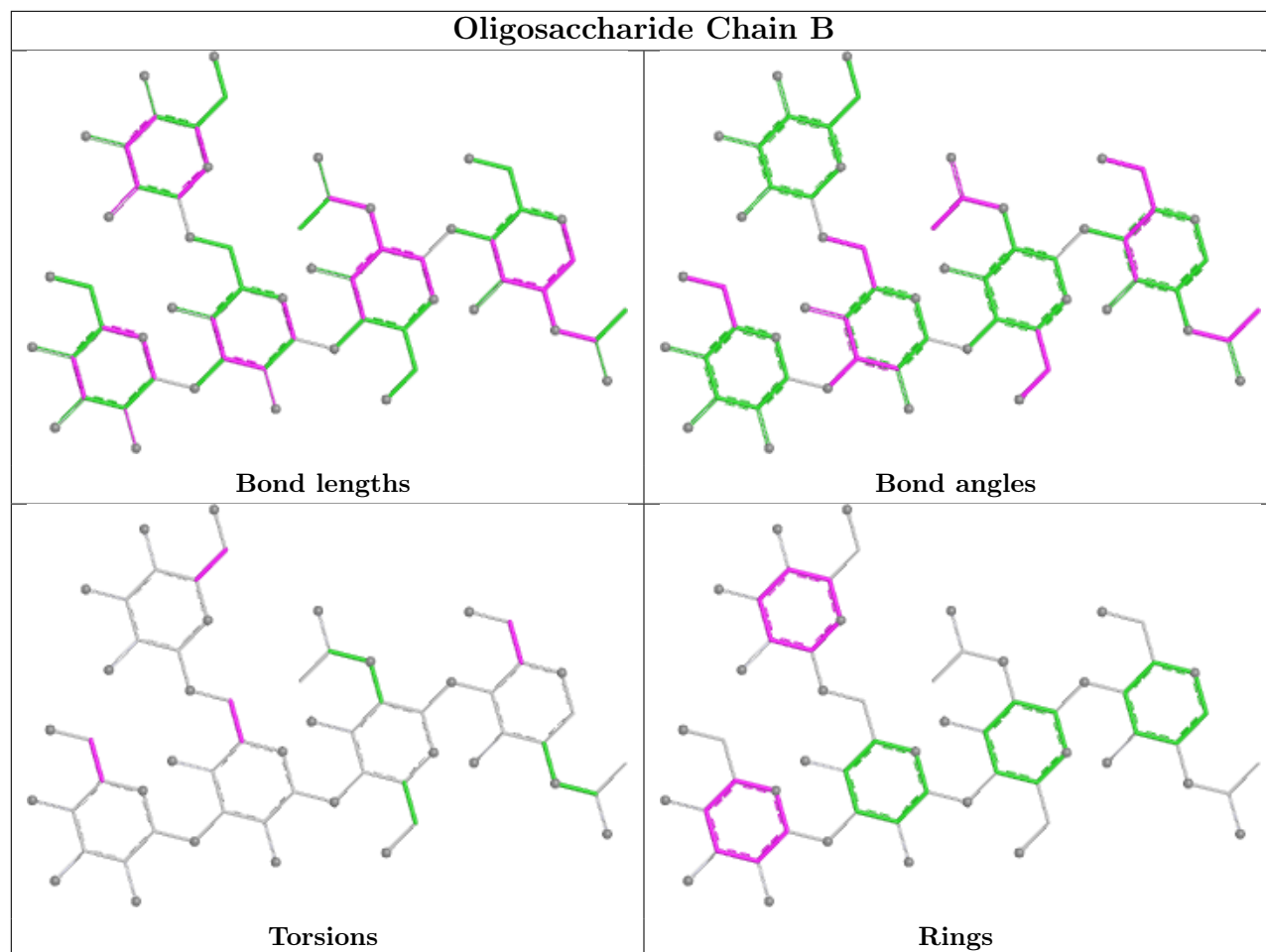
All (3) ring outliers are listed below:

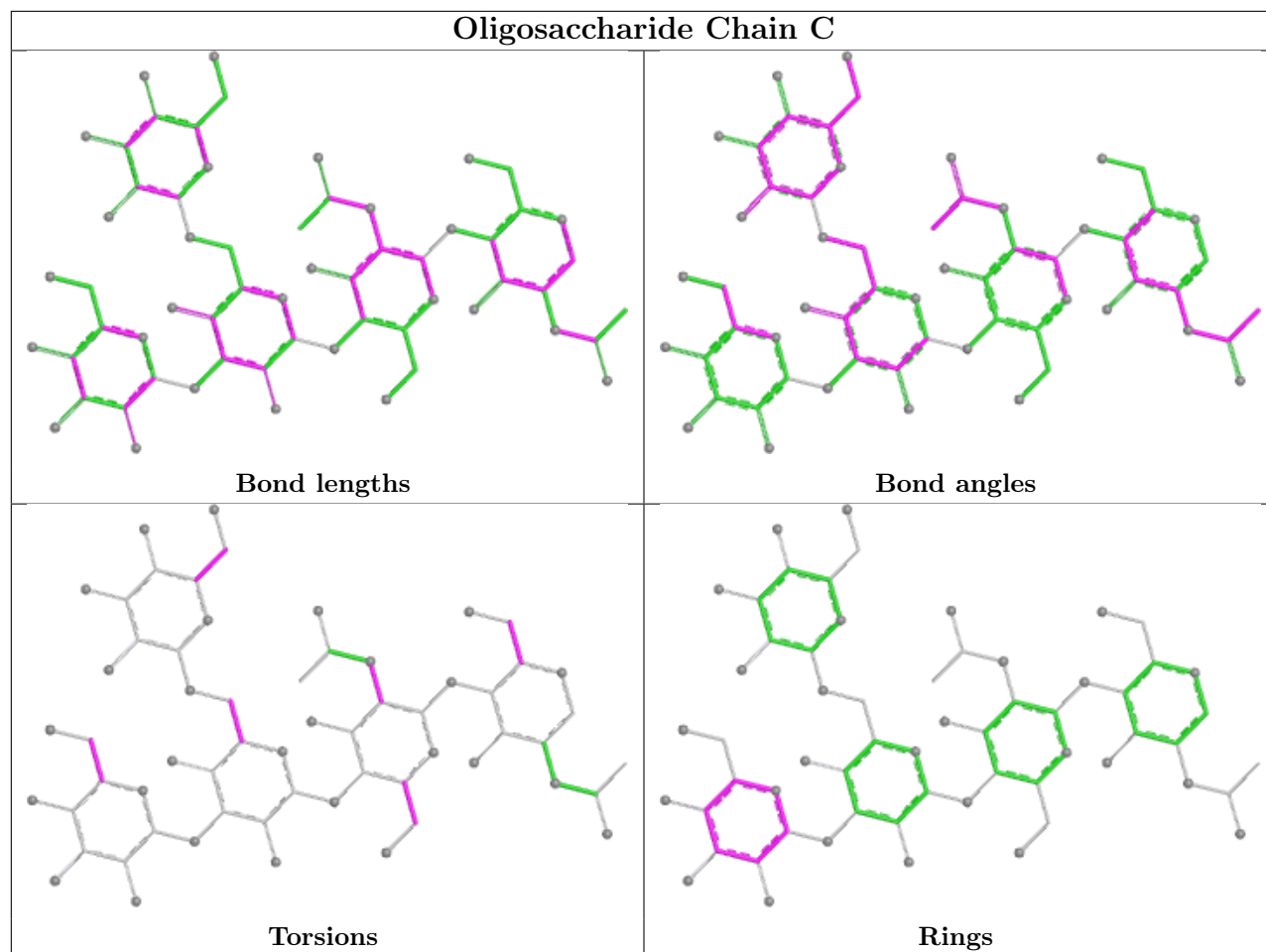
Mol	Chain	Res	Type	Atoms
4	C	4	MAN	C1-C2-C3-C4-C5-O5
4	B	5	MAN	C1-C2-C3-C4-C5-O5
4	B	4	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3	BMA	3	0
4	C	5	MAN	1	0
4	B	3	BMA	1	0
4	B	4	MAN	1	0
4	C	2	NAG	3	0
4	C	1	NAG	2	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 [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	383/415 (92%)	1.15	81 (21%) 2 4	55, 111, 158, 178	0
2	H	220/220 (100%)	0.24	10 (4%) 38 28	44, 69, 135, 193	0
3	L	213/213 (100%)	0.40	9 (4%) 40 29	45, 86, 125, 181	0
All	All	816/848 (96%)	0.71	100 (12%) 8 9	44, 91, 152, 193	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	SER	8.4
1	A	181	LYS	7.3
1	A	66	LEU	7.2
1	A	195	GLN	6.6
1	A	67	ILE	5.9

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.

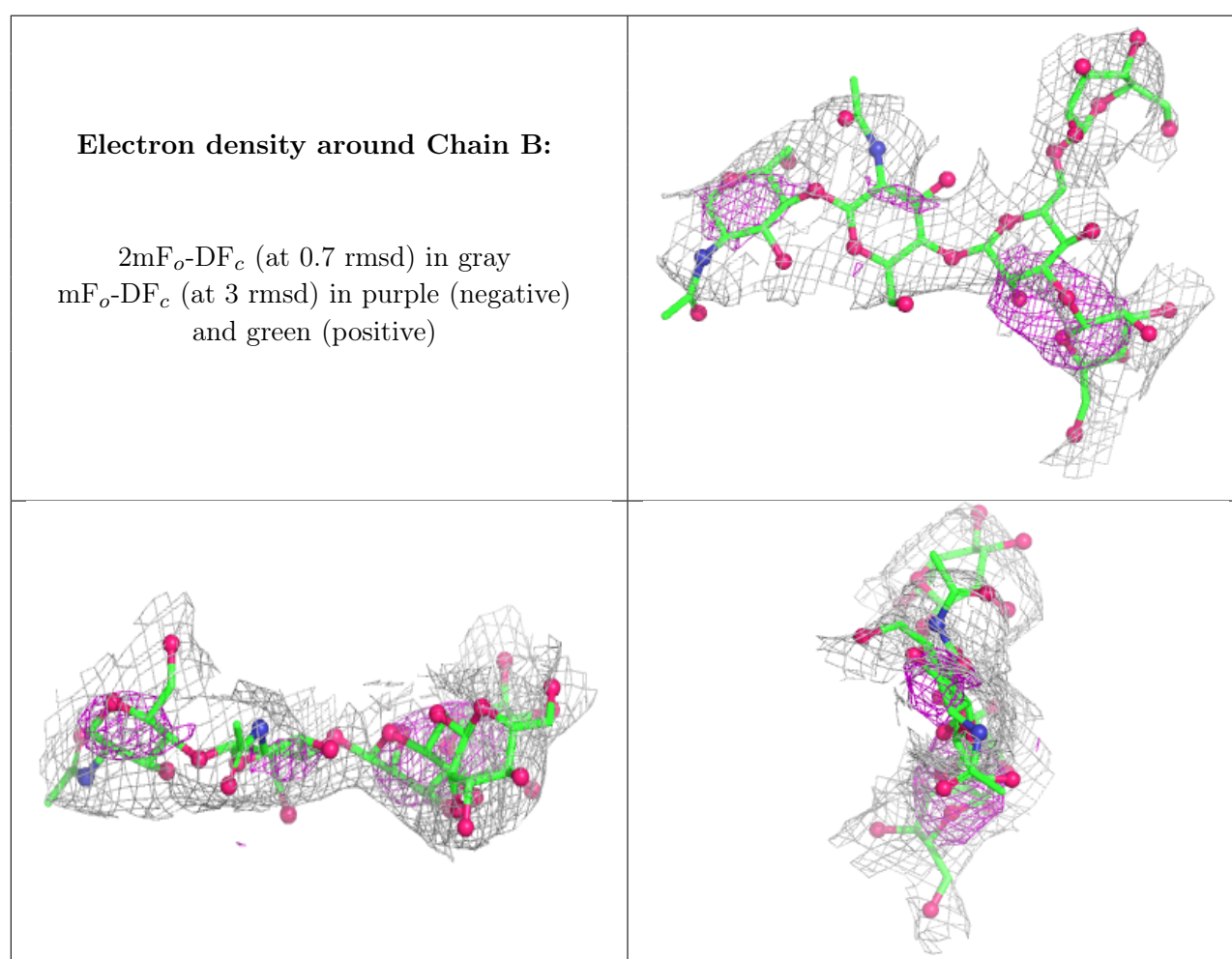
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	1	14/15	-	-	127,144,158,169	0
4	NAG	B	2	14/15	-	-	138,164,173,178	0
4	BMA	B	3	11/12	-	-	175,182,187,190	0

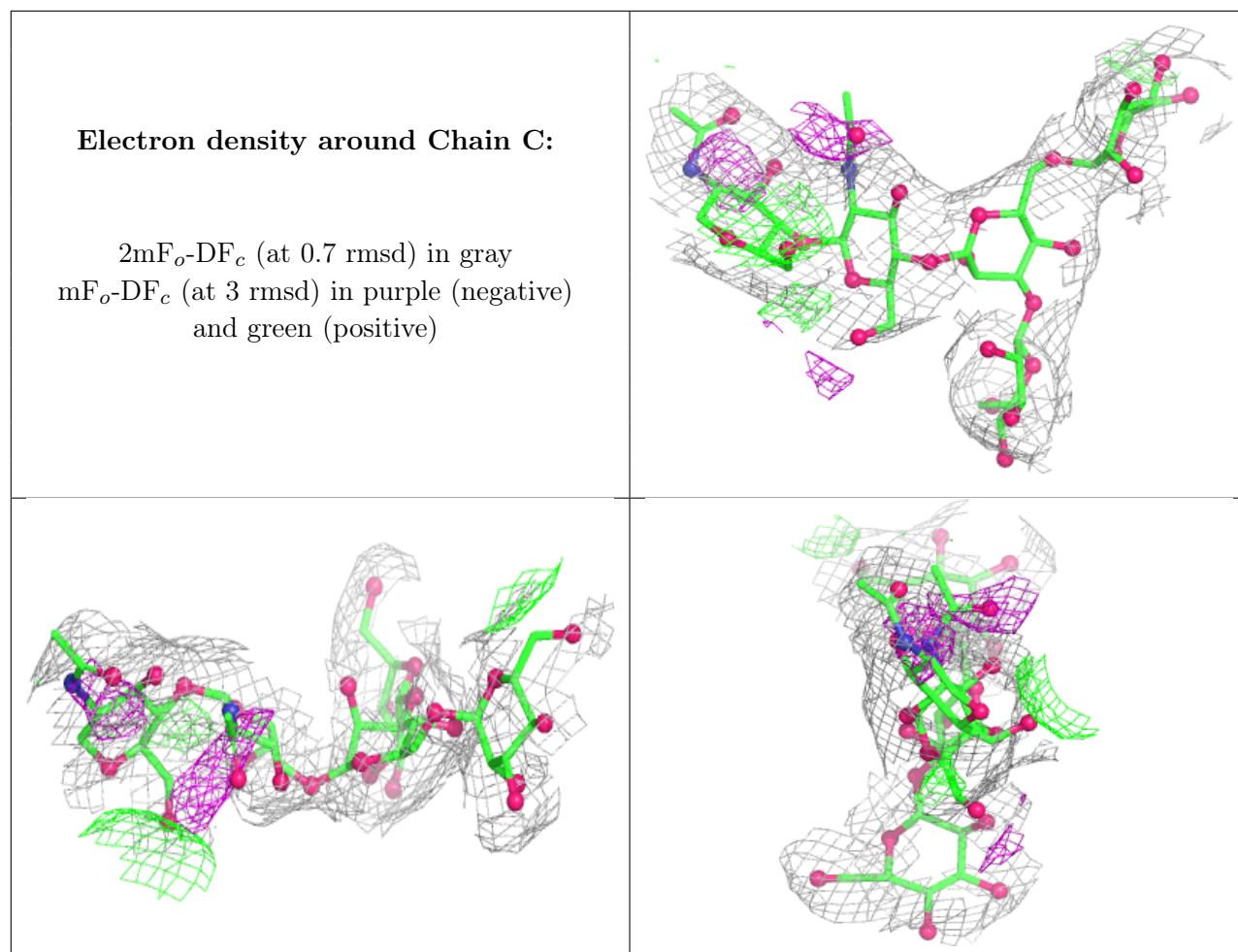
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	B	4	11/12	-	-	138,167,189,189	0
4	MAN	B	5	11/12	-	-	144,162,175,175	0
4	NAG	C	1	14/15	-	-	40,48,70,91	0
4	NAG	C	2	14/15	-	-	97,123,150,163	0
4	BMA	C	3	11/12	-	-	143,148,164,185	0
4	MAN	C	4	11/12	-	-	105,158,187,207	0
4	MAN	C	5	11/12	-	-	124,151,190,240	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.





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.