Full wwPDB X-ray Structure Validation Report (i)

May 16, 2023 – 10:28 pm BST

PDB ID	:	8AHN
Title	:	Sin Nombre virus Gn in complex with Fab SNV-42
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Deposited on	:	2022-07-22
Resolution	:	1.80 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 (i) 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 (1)) were used in the production of this report:

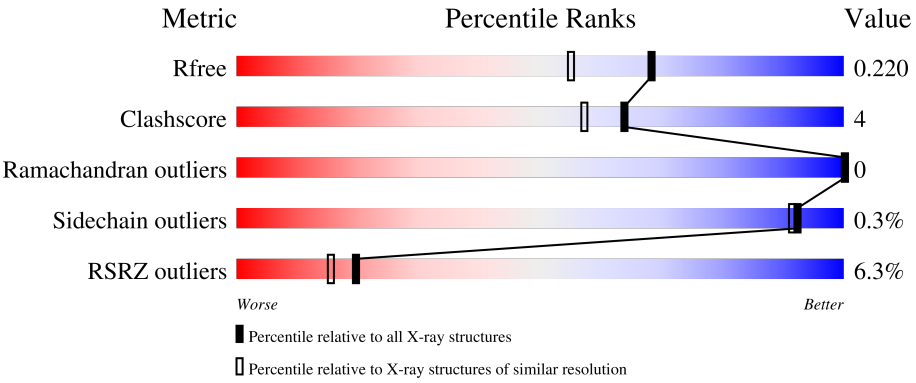
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	356	12% 74% 14% 12%
2	L	217	91% 6% .
3	H	223	% 94% . .
4	B	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6622 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 Envelope polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	3	0
			2443	1556	398	467	22			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	GLY	-	linker	PDB ?
A	87	GLY	-	linker	PDB ?
A	88	SER	-	linker	PDB ?
A	89	GLY	-	linker	PDB ?
A	273	LEU	VAL	variant	UNP K9MNN9
A	378	GLY	-	expression tag	UNP K9MNN9
A	379	THR	-	expression tag	UNP K9MNN9
A	380	LYS	-	expression tag	UNP K9MNN9
A	381	HIS	-	expression tag	UNP K9MNN9
A	382	HIS	-	expression tag	UNP K9MNN9
A	383	HIS	-	expression tag	UNP K9MNN9
A	384	HIS	-	expression tag	UNP K9MNN9
A	385	HIS	-	expression tag	UNP K9MNN9
A	386	HIS	-	expression tag	UNP K9MNN9

- Molecule 2 is a protein called Fab SNV-42 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	10	0
			1648	1035	272	337	4			

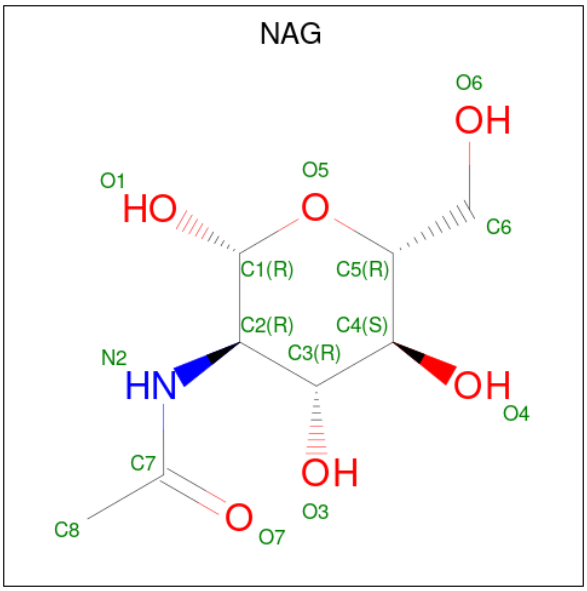
- Molecule 3 is a protein called Fab SNV-42 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	14	0
			1728	1088	290	344	6			

- Molecule 4 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
4	B	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

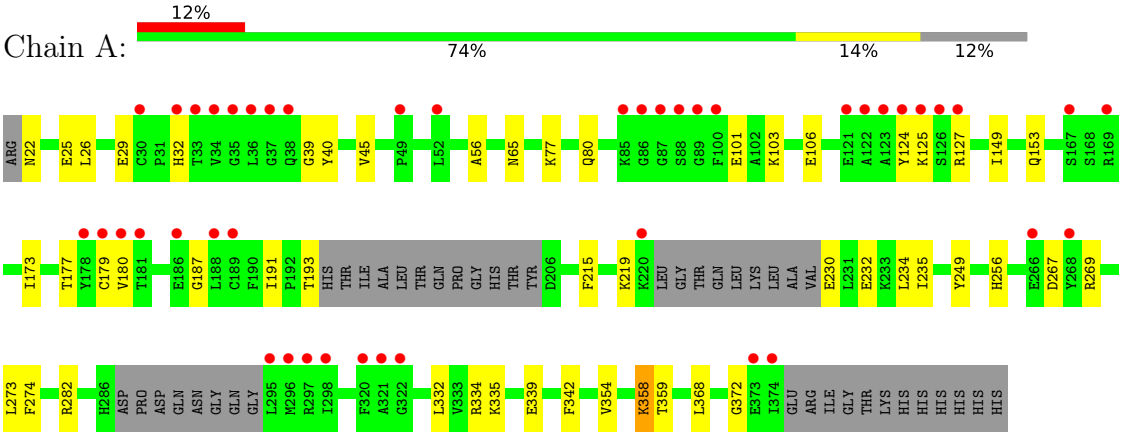
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	237	Total O 237 237	0	0
6	L	240	Total O 240 240	0	0
6	H	284	Total O 284 284	0	0

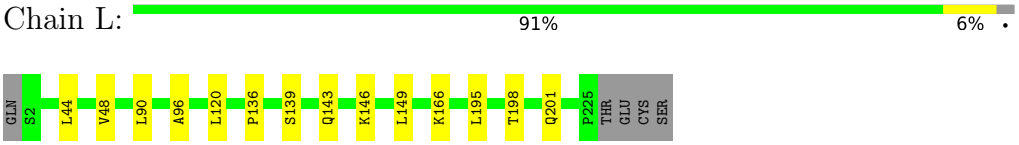
3 Residue-property plots (i)

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.

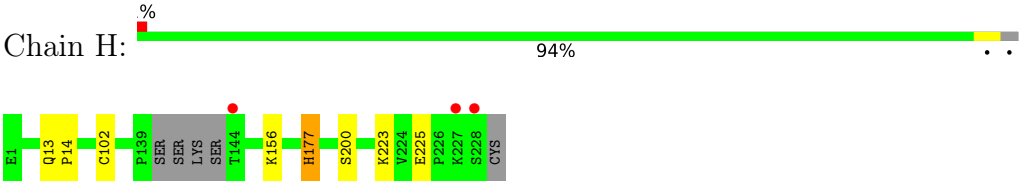
• Molecule 1: Envelope polyprotein



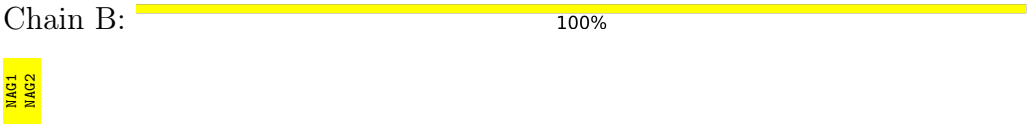
• Molecule 2: Fab SNV-42 light chain



• Molecule 3: Fab SNV-42 heavy chain



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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	88.93Å 146.42Å 157.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.62 – 1.80 46.62 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.62-1.80) 99.9 (46.62-1.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.190 , 0.221 0.188 , 0.220	Depositor DCC
R_{free} test set	4846 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6622	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.41	0/2493	0.64	1/3385 (0.0%)
2	L	0.44	0/1689	0.60	0/2312
3	H	0.46	1/1768 (0.1%)	0.65	0/2406
All	All	0.43	1/5950 (0.0%)	0.63	1/8103 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	102	CYS	CB-SG	-6.59	1.71	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	358	LYS	CD-CE-NZ	-6.58	96.57	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2443	0	2430	34	0
2	L	1648	0	1593	9	0
3	H	1728	0	1675	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	28	0	25	0	0
5	A	14	0	13	1	0
6	A	237	0	0	6	0
6	H	284	0	0	4	1
6	L	240	0	0	2	0
All	All	6622	0	5736	49	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 4.

All (49) 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:219:LYS:HD3	1:A:232:GLU:HG2	1.56	0.86
1:A:179:CYS:SG	6:A:697:HOH:O	2.44	0.76
1:A:65:ASN:ND2	6:A:503:HOH:O	2.20	0.73
1:A:101:GLU:OE2	1:A:103:LYS:NZ	2.22	0.69
3:H:200[A]:SER:OG	6:H:301:HOH:O	2.10	0.67
1:A:56:ALA:O	6:A:501:HOH:O	2.12	0.67
1:A:22:ASN:N	6:A:506:HOH:O	2.30	0.65
2:L:139:SER:O	2:L:143:GLN:HG3	1.98	0.64
1:A:267:ASP:OD2	1:A:269:ARG:NH2	2.32	0.62
3:H:177:HIS:HE1	6:H:511:HOH:O	1.83	0.61
3:H:223:LYS:HE2	3:H:225:GLU:OE2	2.01	0.61
3:H:200[B]:SER:OG	6:H:302:HOH:O	2.16	0.58
2:L:149[B]:LEU:HD12	2:L:195:LEU:HD23	1.87	0.56
1:A:193:THR:HG22	1:A:372:GLY:HA2	1.88	0.55
1:A:77:LYS:HD3	1:A:106:GLU:CD	2.29	0.53
2:L:198:THR:OG1	2:L:201:GLN:HG3	2.08	0.53
1:A:234:LEU:HG	1:A:274:PHE:CZ	2.45	0.52
1:A:25:GLU:HG2	1:A:173:ILE:HD12	1.93	0.51
3:H:13[B]:GLN:HG2	3:H:14:PRO:HD2	1.93	0.51
1:A:219:LYS:CD	1:A:232:GLU:HG2	2.36	0.50
1:A:29:GLU:HG3	1:A:177:THR:HG21	1.93	0.50
2:L:146:LYS:HD2	3:H:156[B]:LYS:HZ1	1.74	0.50
2:L:90:LEU:HD11	2:L:120[B]:LEU:HD21	1.94	0.50
2:L:136:PRO:HA	2:L:149[B]:LEU:HD23	1.93	0.50
6:L:464:HOH:O	3:H:177:HIS:HD2	1.95	0.49
1:A:334:ARG:NH2	6:H:308:HOH:O	2.45	0.49
1:A:32:HIS:HB3	1:A:180:VAL:HA	1.95	0.48
1:A:230:GLU:HG2	1:A:232:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:44[B]:LEU:HD23	2:L:96:ALA:HB2	1.94	0.48
1:A:282:ARG:NH1	6:A:514:HOH:O	2.46	0.48
1:A:187:GLY:O	6:A:502:HOH:O	2.20	0.47
1:A:273:LEU:HG	1:A:368:LEU:HD13	1.96	0.47
1:A:29:GLU:HG3	1:A:177:THR:CG2	2.45	0.46
2:L:166:LYS:HE3	2:L:166:LYS:HB2	1.69	0.46
1:A:39:GLY:HA2	1:A:127:ARG:HH12	1.81	0.45
1:A:354:VAL:O	1:A:358:LYS:HD3	2.17	0.45
1:A:335:LYS:HE3	1:A:339:GLU:OE1	2.18	0.43
1:A:40:TYR:O	1:A:256:HIS:HA	2.19	0.42
1:A:334:ARG:HD3	1:A:334:ARG:HA	1.74	0.42
1:A:282:ARG:NH1	5:A:401:NAG:O6	2.43	0.42
1:A:332:LEU:HD23	1:A:359:THR:HG22	2.02	0.41
1:A:124:TYR:HD2	1:A:125:LYS:HG3	1.85	0.41
1:A:149:ILE:HD11	1:A:215:PHE:CZ	2.56	0.41
1:A:26:LEU:HD12	1:A:45:VAL:HG12	2.03	0.41
1:A:39:GLY:HA2	1:A:127:ARG:NH1	2.36	0.40
1:A:235:ILE:HD11	1:A:249:TYR:CE2	2.55	0.40
1:A:80:GLN:HA	1:A:342:PHE:O	2.21	0.40
1:A:191:ILE:HD13	1:A:191:ILE:HG21	1.89	0.40
2:L:48[B]:VAL:HG12	6:L:402:HOH:O	2.22	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)
6:H:578:HOH:O	6:H:578:HOH:O[2_765]	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	309/356 (87%)	300 (97%)	9 (3%)	0	100 100
2	L	220/217 (101%)	214 (97%)	6 (3%)	0	100 100
3	H	228/223 (102%)	224 (98%)	4 (2%)	0	100 100
All	All	757/796 (95%)	738 (98%)	19 (2%)	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	279/311 (90%)	278 (100%)	1 (0%)	91 89
2	L	187/182 (103%)	187 (100%)	0	100 100
3	H	193/184 (105%)	192 (100%)	1 (0%)	88 87
All	All	659/677 (97%)	657 (100%)	2 (0%)	92 91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
3	H	177	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	171	GLN
3	H	177	HIS
3	H	205	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)

2 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	0.70	1 (7%)	17,19,21	0.80	0
4	NAG	B	2	4	14,14,15	0.47	0	17,19,21	0.90	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	B	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	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)
4	B	1	NAG	C1-C2	2.08	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2	NAG	O3-C3-C2	-2.13	105.05	109.47

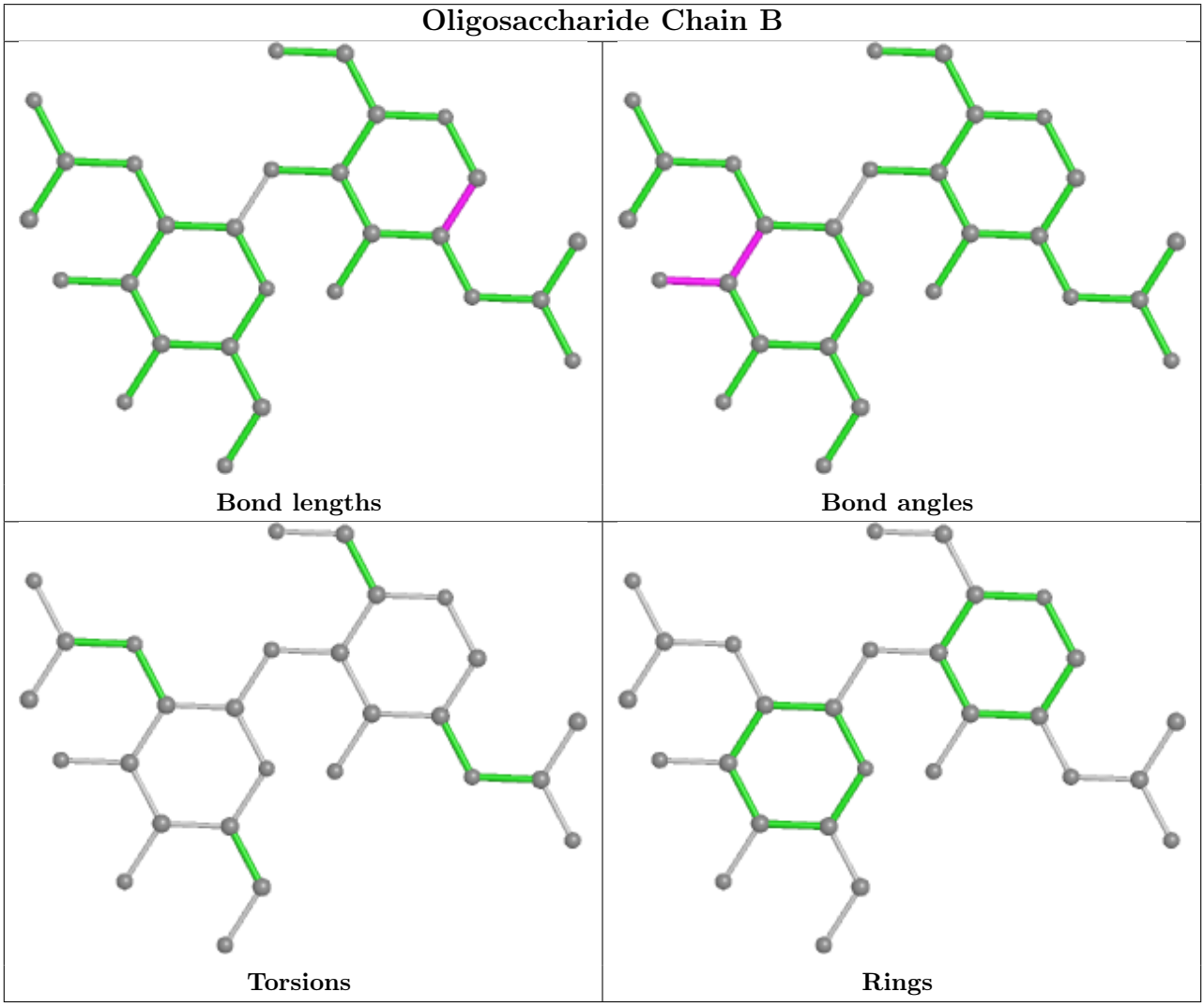
There are no chirality outliers.

There are no torsion outliers.

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)

1 ligand is 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	$\#\|Z\|>2$
5	NAG	A	401	1	14,14,15	0.95	1 (7%)	17,19,21	1.12	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
5	NAG	A	401	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	NAG	O5-C1	-2.76	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	401	NAG	C1-O5-C5	-3.25	107.79	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	NAG	C8-C7-N2-C2
5	A	401	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	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, 95^{th} 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	314/356 (88%)	0.74	44 (14%) 2 2	24, 45, 70, 78	0
2	L	212/217 (97%)	-0.26	0 100 100	19, 29, 45, 50	0
3	H	218/223 (97%)	-0.18	3 (1%) 75 72	20, 28, 42, 60	0
All	All	744/796 (93%)	0.18	47 (6%) 20 15	19, 33, 64, 78	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	TYR	11.5
1	A	181	THR	9.5
1	A	34	VAL	8.0
1	A	36	LEU	7.5
1	A	86	GLY	6.7
1	A	180	VAL	6.3
1	A	125	LYS	5.9
1	A	123	ALA	5.8
1	A	38	GLN	5.5
1	A	88	SER	5.4
3	H	228	SER	5.2
1	A	33	THR	5.0
1	A	295	LEU	4.7
1	A	87	GLY	4.3
1	A	100	PHE	4.1
1	A	266	GLU	4.0
1	A	85	LYS	3.8
1	A	179	CYS	3.8
1	A	321	ALA	3.7
1	A	35	GLY	3.5
1	A	189	CYS	3.4
1	A	126	SER	3.4
1	A	186	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	188	LEU	3.3
1	A	122	ALA	3.1
1	A	178	TYR	3.0
3	H	227	LYS	3.0
1	A	89	GLY	3.0
1	A	220	LYS	3.0
1	A	37	GLY	2.8
1	A	167	SER	2.8
1	A	374	ILE	2.8
1	A	127	ARG	2.8
1	A	121	GLU	2.7
3	H	144	THR	2.6
1	A	52	LEU	2.4
1	A	320	PHE	2.4
1	A	169	ARG	2.4
1	A	30	CYS	2.4
1	A	298	ILE	2.3
1	A	32	HIS	2.3
1	A	49	PRO	2.2
1	A	296	MET	2.2
1	A	268	TYR	2.1
1	A	373	GLU	2.1
1	A	297	ARG	2.1
1	A	322	GLY	2.1

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, 95^{th} 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.

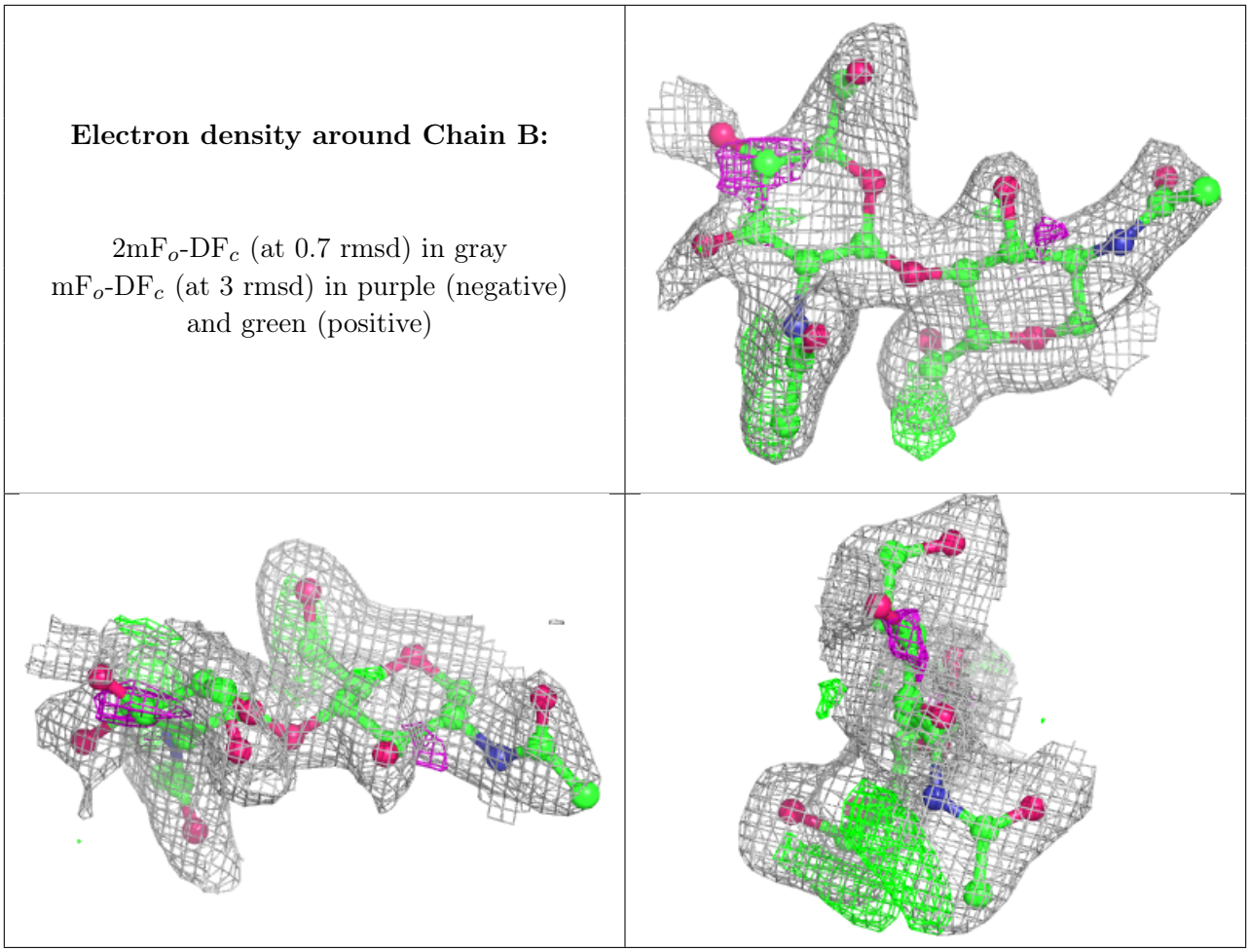
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	B	2	14/15	0.62	0.33	48,54,67,72	0
4	NAG	B	1	14/15	0.79	0.24	41,50,56,68	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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



6.4 Ligands

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, 95^{th} 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
5	NAG	A	401	14/15	0.78	0.25	43,51,69,77	0

6.5 Other polymers

There are no such residues in this entry.