



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2020 – 11:23 AM EDT

PDB ID : 7K66
Title : Structure of Blood Coagulation Factor VIII in Complex with an Anti-C1 Domain Pathogenic Antibody Inhibitor
Authors : Childers, K.C.; Gish, J.; Jarvis, L.; Peters, S.; Garrels, C.; Smith, I.W.; Spencer, H.T.; Spiegel, P.C.
Deposited on : 2020-09-18
Resolution : 3.92 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
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) : 2.14.6

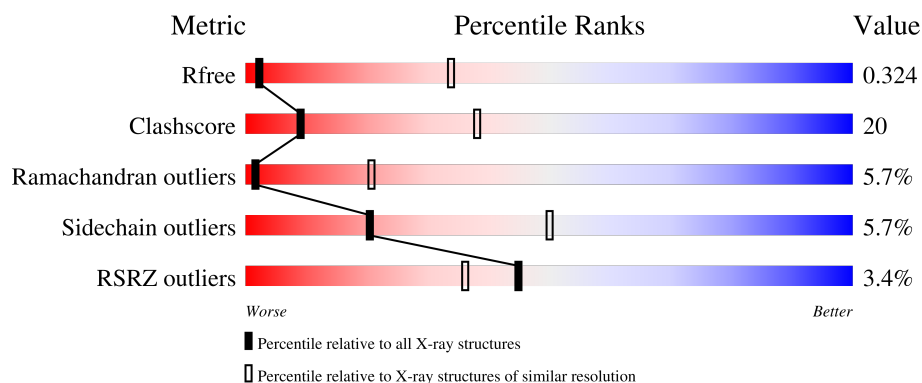
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 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	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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 on 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	1467	 2% 49% 33% 14%
2	B	223	 7% 45% 45% 5% 5%
3	C	213	 7% 59% 35% 5%
4	H	5	 100%
5	D	2	 100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13606 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 Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1265	Total	C	N	O	S	0	0	0
			10216	6562	1748	1854	52			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1627	ALA	-	linker	UNP P00451
A	1628	GLN	-	linker	UNP P00451
A	1629	ASN	-	linker	UNP P00451
A	1630	SER	-	linker	UNP P00451
A	1631	ARG	-	linker	UNP P00451
A	1632	PRO	-	linker	UNP P00451
A	1633	PRO	-	linker	UNP P00451
A	1634	SER	-	linker	UNP P00451
A	1635	ALA	-	linker	UNP P00451
A	1636	SER	-	linker	UNP P00451

- Molecule 2 is a protein called 2A9 heavy chain.

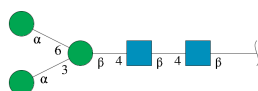
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1649	1048	266	327	8			

- Molecule 3 is a protein called 2A9 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1634	1019	271	335	9			

- 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-a

cetamido-2-deoxy-beta-D-glucopyranose.



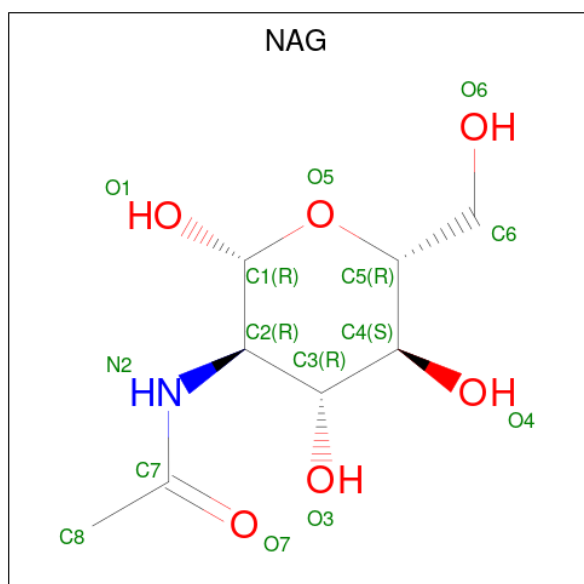
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 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
5	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cu	0	0
			1	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		

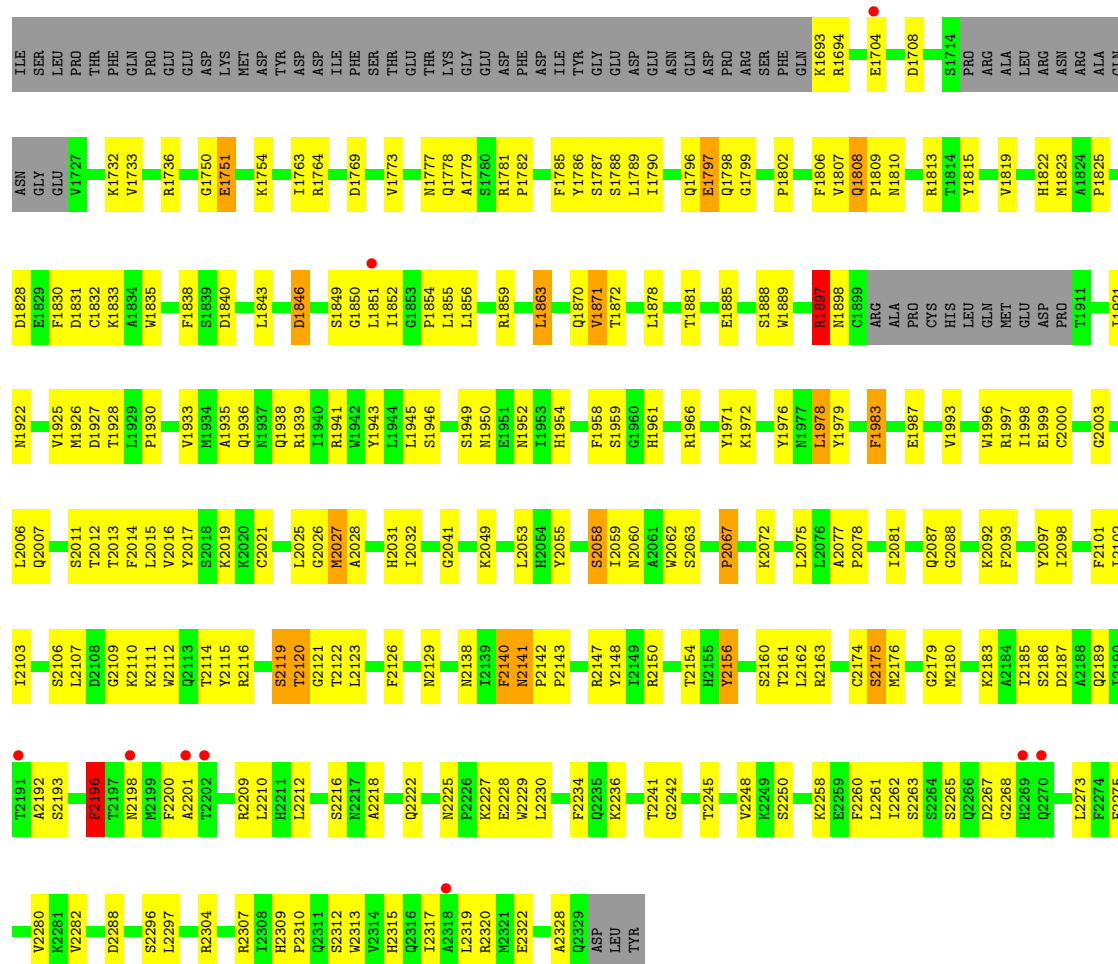
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	0
			1	1		

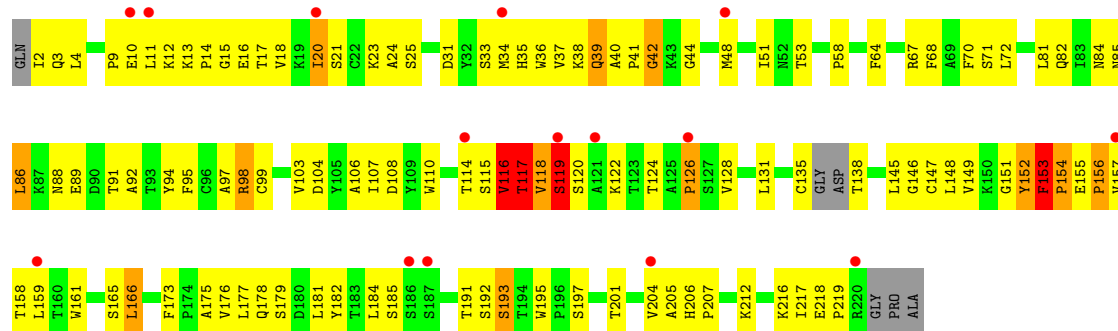
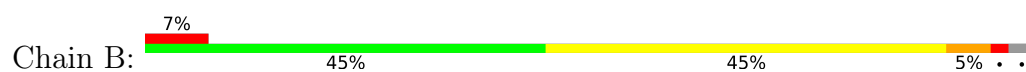
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	O	0	0
			1	1		



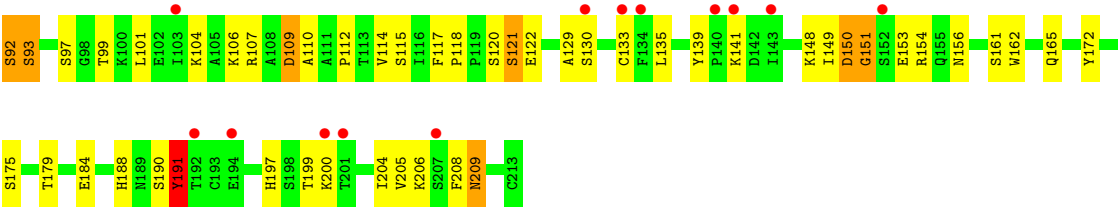


• Molecule 2: 2A9 heavy chain



• Molecule 3: 2A9 light chain





● Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



● Molecule 5: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.72Å 116.72Å 371.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.49 – 3.92 49.49 – 3.92	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.49-3.92) 97.7 (49.49-3.92)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.226 , 0.322 0.238 , 0.324	Depositor DCC
R_{free} test set	1991 reflections (8.50%)	wwPDB-VP
Wilson B-factor (Å ²)	147.6	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 125.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13606	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: ZN, BMA, NAG, CA, CU, MAN

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	0.28	0/10502	0.50	0/14238
2	B	0.31	0/1693	0.59	3/2312 (0.1%)
3	C	0.27	0/1672	0.52	0/2269
All	All	0.29	0/13867	0.52	3/18819 (0.0%)

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	1
2	B	0	4
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	VAL	N-CA-C	-6.30	93.99	111.00
2	B	119	SER	N-CA-C	-5.96	94.91	111.00
2	B	119	SER	CA-C-N	-5.40	105.31	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	HIS	Peptide
2	B	117	THR	Peptide

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Mol	Chain	Res	Type	Group
2	B	119	SER	Mainchain
2	B	120	SER	Peptide
2	B	153	PHE	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	10216	0	9961	347	0
2	B	1649	0	1593	133	0
3	C	1634	0	1560	68	0
4	H	61	0	51	2	0
5	D	28	0	25	0	0
6	A	14	0	13	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
10	B	1	0	0	0	0
All	All	13606	0	13203	540	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 20.

The worst 5 of 540 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)
2:B:91:THR:CB	2:B:117:THR:HG21	1.03	1.48
2:B:91:THR:CB	2:B:117:THR:CG2	1.98	1.40
2:B:91:THR:OG1	2:B:117:THR:CG2	1.68	1.38
2:B:91:THR:CA	2:B:117:THR:HG21	1.57	1.34
2:B:91:THR:CA	2:B:117:THR:CG2	2.07	1.33

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1249/1467 (85%)	962 (77%)	222 (18%)	65 (5%)	2	22
2	B	213/223 (96%)	139 (65%)	58 (27%)	16 (8%)	1	16
3	C	211/213 (99%)	149 (71%)	48 (23%)	14 (7%)	1	18
All	All	1673/1903 (88%)	1250 (75%)	328 (20%)	95 (6%)	1	21

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	187	ARG
1	A	250	HIS
1	A	265	PRO
1	A	291	PRO

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	1118/1301 (86%)	1048 (94%)	70 (6%)	18	47
2	B	186/189 (98%)	179 (96%)	7 (4%)	33	59
3	C	186/186 (100%)	178 (96%)	8 (4%)	29	56
All	All	1490/1676 (89%)	1405 (94%)	85 (6%)	20	50

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1708	ASP
1	A	1888	SER
3	C	52	SER
1	A	1736	ARG
1	A	1840	ASP

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

Mol	Chain	Res	Type
1	A	317	HIS
1	A	2007	GLN
2	B	35	HIS
2	B	88	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 ⓘ

7 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	D	1	1,5	14,14,15	1.33	1 (7%)	17,19,21	1.26	1 (5%)
5	NAG	D	2	5	14,14,15	1.25	1 (7%)	17,19,21	1.24	1 (5%)
4	NAG	H	1	1,4	14,14,15	0.39	0	17,19,21	0.59	0
4	NAG	H	2	4	14,14,15	0.35	0	17,19,21	0.48	0
4	BMA	H	3	4	11,11,12	0.94	0	15,15,17	1.58	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	H	4	4	11,11,12	1.14	2 (18%)	15,15,17	1.17	2 (13%)
4	MAN	H	5	4	11,11,12	0.93	1 (9%)	15,15,17	1.53	2 (13%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1	NAG	O5-C1	4.72	1.51	1.43
5	D	2	NAG	O5-C1	3.95	1.50	1.43
4	H	4	MAN	C1-C2	2.60	1.58	1.52
4	H	5	MAN	O5-C5	2.52	1.48	1.43
4	H	4	MAN	O5-C5	2.15	1.47	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	5	MAN	C1-O5-C5	4.66	118.51	112.19
5	D	1	NAG	C1-O5-C5	4.54	118.34	112.19
4	H	3	BMA	C3-C4-C5	3.46	116.41	110.24
5	D	2	NAG	C1-O5-C5	3.01	116.27	112.19
4	H	4	MAN	C1-O5-C5	2.99	116.25	112.19

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	D	2	NAG	O5-C5-C6-O6
4	H	4	MAN	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	4	MAN	O5-C5-C6-O6

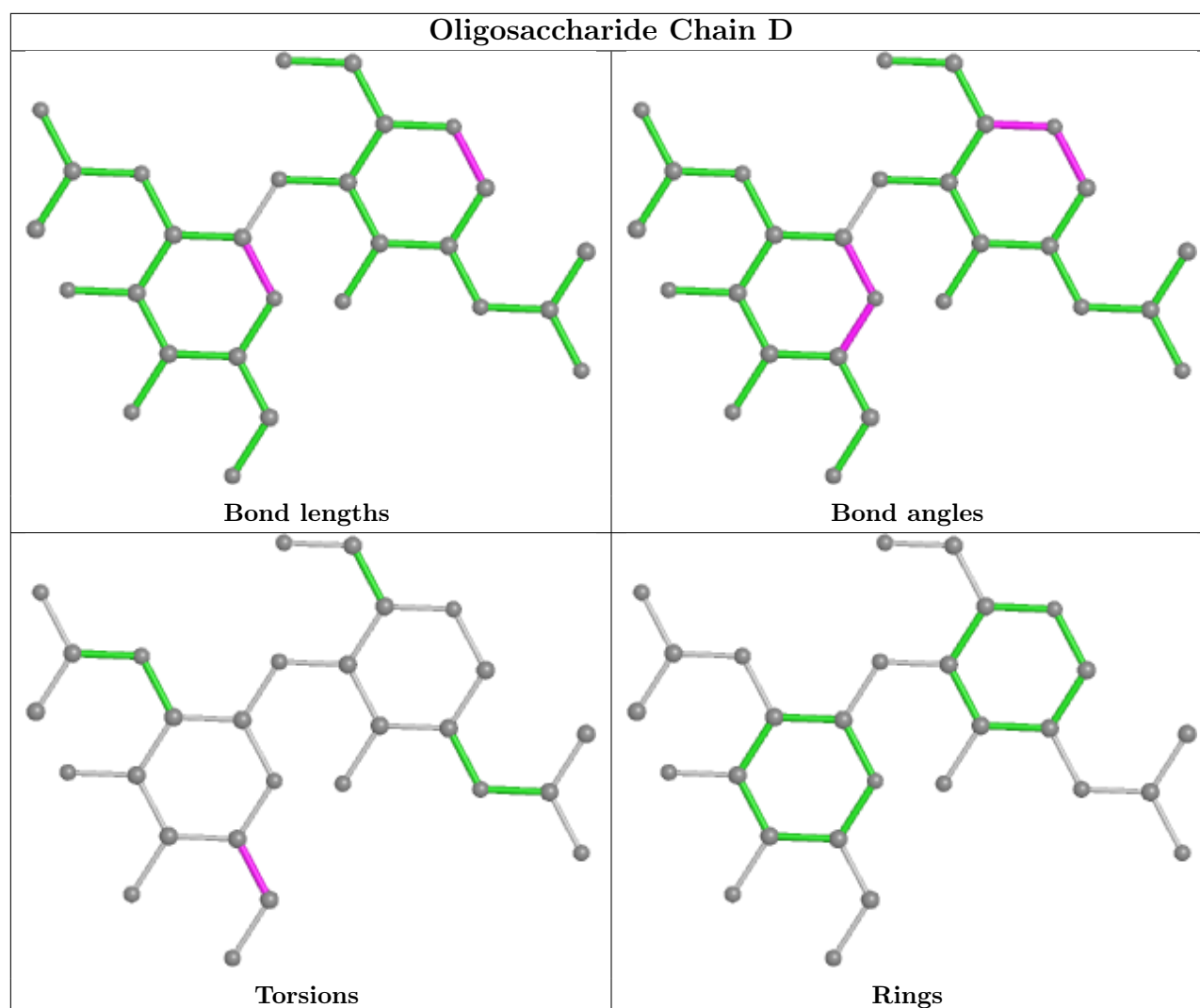
All (2) ring outliers are listed below:

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

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	NAG	1	0
4	H	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](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
6	NAG	A	2401	1	14,14,15	0.53	0	17,19,21	0.52	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
6	NAG	A	2401	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2401	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	1265/1467 (86%)	0.03	28 (2%) 62 52	73, 137, 194, 330	1 (0%)
2	B	217/223 (97%)	0.42	15 (6%) 16 13	30, 172, 220, 233	0
3	C	213/213 (100%)	0.36	14 (6%) 18 14	99, 156, 232, 243	0
All	All	1695/1903 (89%)	0.12	57 (3%) 45 36	30, 142, 212, 330	1 (0%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	THR	7.1
1	A	28	ASP	4.6
1	A	26	HIS	4.3
2	B	186	SER	4.1
1	A	44	SER	3.8

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.

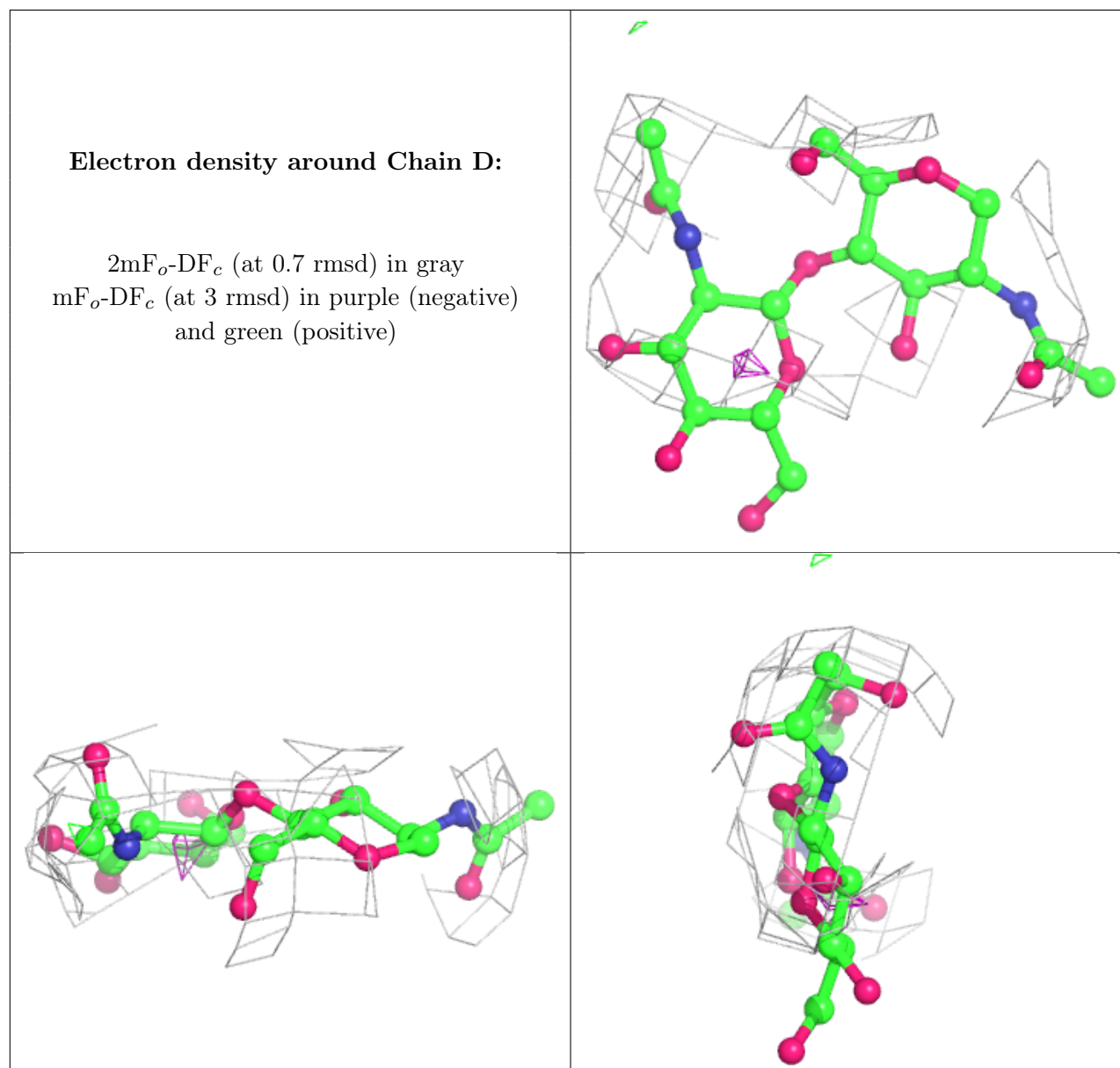
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	H	3	11/12	0.70	0.21	179,186,197,202	0
5	NAG	D	2	14/15	0.71	0.31	194,209,214,215	0
4	MAN	H	4	11/12	0.78	0.39	171,188,202,202	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	H	2	14/15	0.88	0.17	150,171,185,185	0
5	NAG	D	1	14/15	0.89	0.21	164,200,213,214	0
4	MAN	H	5	11/12	0.89	0.20	167,182,186,189	0
4	NAG	H	1	14/15	0.90	0.23	138,150,158,160	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	A	2401	14/15	0.80	0.25	167,182,194,195	0
9	ZN	A	2404	1/1	0.96	0.23	137,137,137,137	0
7	CU	A	2402	1/1	0.98	0.26	133,133,133,133	0
8	CA	A	2403	1/1	0.99	0.20	141,141,141,141	0

6.5 Other polymers [i](#)

There are no such residues in this entry.