



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:18 PM UTC

PDB ID : 4BSA / pdb_00004bsa
Title : Crystal Structure of the Haemagglutinin (with Asn-133 Glycosylation) from an H7N9 Influenza Virus Isolated from Humans
Authors : Xiong, X.; Haire, L.F.; Martin, S.R.; Wharton, S.A.; Daniels, R.S.; Bennett, M.S.; McCauley, J.W.; Collins, P.J.; Walker, P.A.; Skehel, J.J.; Gamblin, S.J.
Deposited on : 2013-06-10
Resolution : 2.30 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

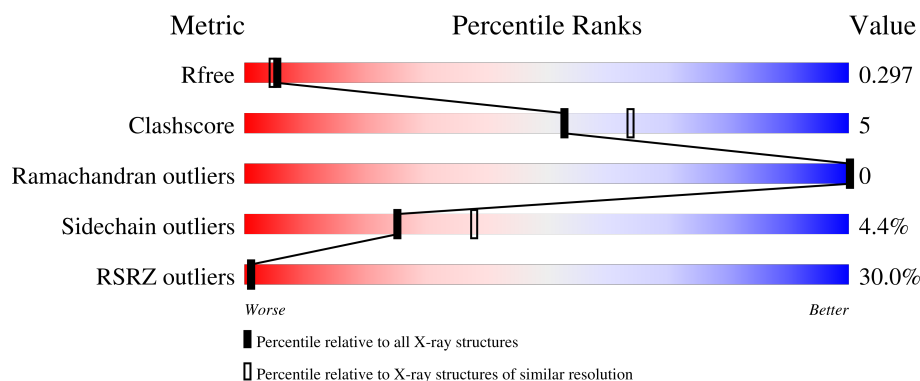
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	321	35% 86%12%..
2	B	177	19% 87%8%..
3	C	2	100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4216 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	317	Total	C	N	O	S	0	0	1
			2416	1500	437	464	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	LEU	VAL	SEE REMARK 999	UNP M4YV75
A	125	THR	ALA	SEE REMARK 999	UNP M4YV75
A	217	LEU	ILE	SEE REMARK 999	UNP M4YV75

- Molecule 2 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1379	851	241	280	7			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



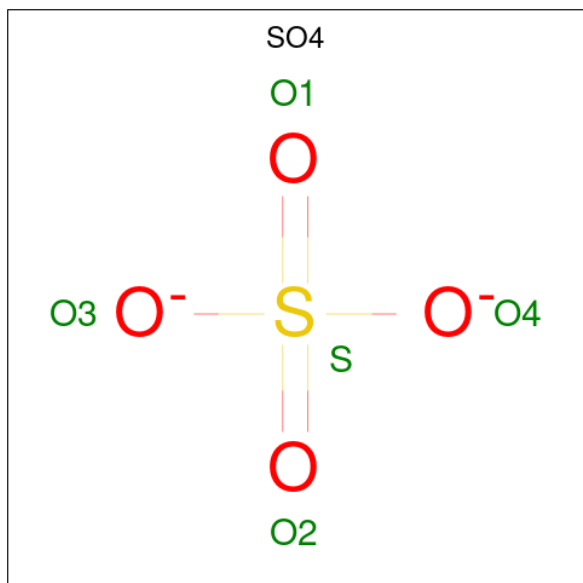
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

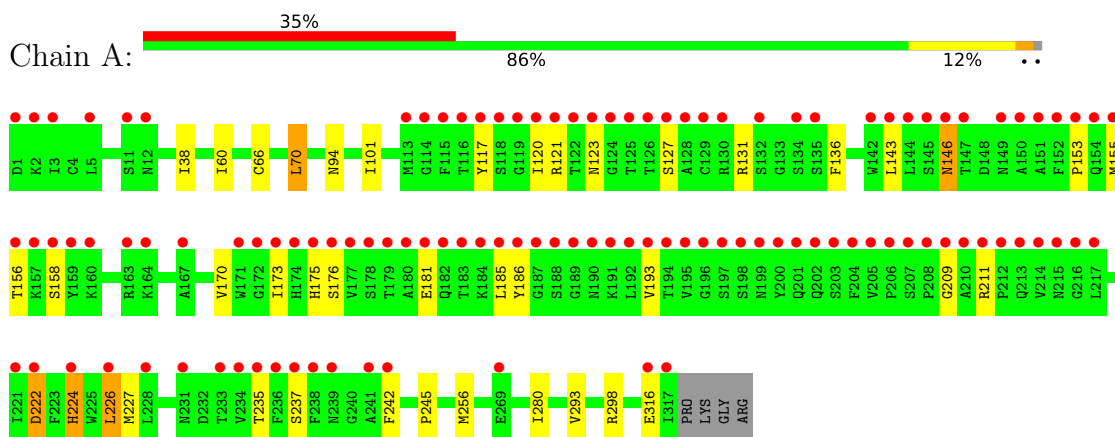
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	200	Total O 200 200	0	0
6	B	67	Total O 67 67	0	0

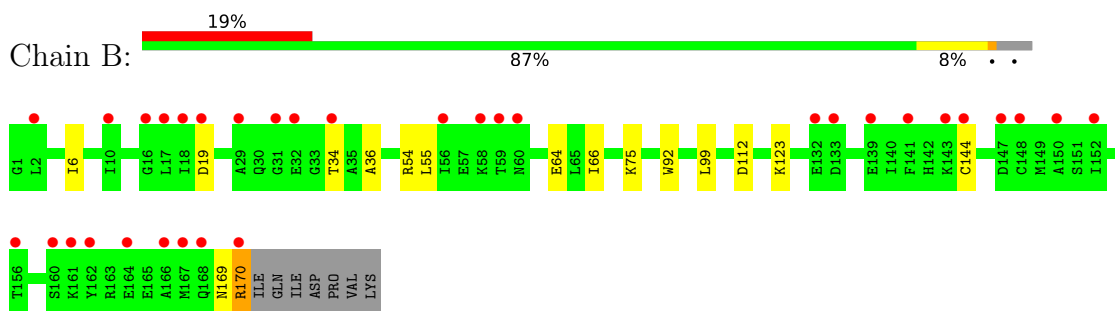
3 Residue-property plots [i](#)

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.

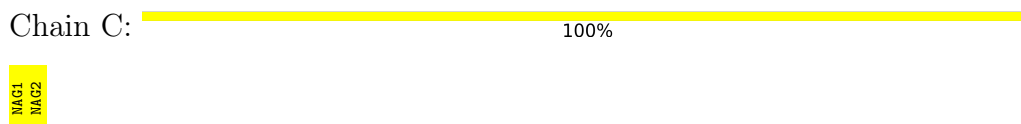
• Molecule 1: HEMAGGLUTININ



• Molecule 2: HEMAGGLUTININ



• Molecule 3: 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	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	116.13Å 116.13Å 295.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.13 – 2.30 58.13 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (58.13-2.30) 98.9 (58.13-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.250 , 0.296 0.251 , 0.297	Depositor DCC
R_{free} test set	1725 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.018 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.008 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4216	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage'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: NAG, SO4

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	0.48	1/2462 (0.0%)	0.70	0/3328
2	B	0.45	0/1403	0.74	0/1890
All	All	0.47	1/3865 (0.0%)	0.71	0/5218

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	316	GLU	C-N	-7.00	1.23	1.33

There are no bond angle outliers.

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	2416	0	2374	32	0
2	B	1379	0	1280	7	0
3	C	28	0	25	2	0
4	A	56	0	52	0	0
5	A	50	0	0	0	0
5	B	20	0	0	0	0
6	A	200	0	0	13	1
6	B	67	0	0	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4216	0	3731	38	2

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 5.

All (38) 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:211:ARG:HD3	6:A:2113:HOH:O	1.95	0.66
1:A:38:ILE:HD12	1:A:280:ILE:HD12	1.78	0.63
1:A:121:ARG:NH1	1:A:146:ASN:O	2.32	0.63
1:A:101:ILE:HD13	1:A:227:MET:HE3	1.81	0.62
1:A:222:ASP:HB3	6:A:2128:HOH:O	2.00	0.61
1:A:173:ILE:HD11	6:A:2110:HOH:O	2.03	0.59
1:A:298:ARG:HG2	2:B:92:TRP:CE2	2.40	0.56
1:A:242:PHE:CD2	6:A:2136:HOH:O	2.53	0.55
1:A:226:LEU:HD22	1:A:226:LEU:C	2.32	0.54
1:A:170:VAL:O	1:A:245:PRO:HB3	2.07	0.54
2:B:169:ASN:O	2:B:170:ARG:C	2.51	0.53
1:A:298:ARG:HG2	2:B:92:TRP:CD2	2.46	0.51
6:B:2027:HOH:O	3:C:1:NAG:H83	2.09	0.51
1:A:66:CYS:O	1:A:70:LEU:HD13	2.11	0.50
1:A:185:LEU:HA	6:A:2089:HOH:O	2.11	0.50
1:A:235:THR:HG23	6:A:2105:HOH:O	2.12	0.50
1:A:131:ARG:NH1	1:A:136:PHE:O	2.45	0.49
1:A:193:VAL:HB	6:A:2110:HOH:O	2.12	0.49
1:A:175:HIS:HA	6:A:2111:HOH:O	2.12	0.48
1:A:256:MET:HE1	1:A:293:VAL:HB	1.95	0.48
1:A:173:ILE:HB	1:A:222:ASP:HB2	1.97	0.46
1:A:224:HIS:CE1	6:A:2128:HOH:O	2.69	0.46
2:B:6:ILE:HD12	2:B:112:ASP:HA	1.97	0.46
1:A:38:ILE:CD1	1:A:280:ILE:HD12	2.45	0.45
1:A:117:TYR:CE1	1:A:143:LEU:HD11	2.53	0.44
2:B:75:LYS:HE3	3:C:1:NAG:H81	2.00	0.44
1:A:209:GLY:O	1:A:211:ARG:NH1	2.49	0.44
1:A:158:SER:N	6:A:2106:HOH:O	2.51	0.43
1:A:123:ASN:N	1:A:123:ASN:OD1	2.51	0.43
1:A:175:HIS:NE2	1:A:222:ASP:OD1	2.52	0.42
1:A:60:ILE:HG21	1:A:170:VAL:HG21	2.00	0.42
2:B:19:ASP:HB3	2:B:36:ALA:HB2	2.02	0.42
2:B:55:LEU:HD22	2:B:99:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:VAL:HA	1:A:237:SER:O	2.21	0.41
1:A:143:LEU:HD12	6:A:2136:HOH:O	2.21	0.41
1:A:176:SER:HB3	1:A:181:GLU:HB2	2.03	0.41
1:A:158:SER:HB2	6:A:2105:HOH:O	2.21	0.40
1:A:153:PRO:HG2	6:A:2103:HOH:O	2.21	0.40

All (2) 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:A:2029:HOH:O	6:A:2031:HOH:O[6_555]	1.84	0.36
6:B:2044:HOH:O	6:B:2046:HOH:O[3_655]	2.13	0.07

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	315/321 (98%)	300 (95%)	15 (5%)	0	100	100
2	B	168/177 (95%)	164 (98%)	4 (2%)	0	100	100
All	All	483/498 (97%)	464 (96%)	19 (4%)	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	266/270 (98%)	255 (96%)	11 (4%)	27	41
2	B	145/152 (95%)	138 (95%)	7 (5%)	23	35
All	All	411/422 (97%)	393 (96%)	18 (4%)	25	38

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	94	ASN
1	A	120	ILE
1	A	127	SER
1	A	146	ASN
1	A	155	MET
1	A	156	THR
1	A	186	TYR
1	A	222	ASP
1	A	224	HIS
1	A	226	LEU
2	B	34	THR
2	B	54	ARG
2	B	64	GLU
2	B	66	ILE
2	B	123	LYS
2	B	144	CYS
2	B	170	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	174	HIS
1	A	201	GLN
1	A	263	GLN
1	A	287	ASN
2	B	12	ASN
2	B	62	GLN
2	B	154	ASN
2	B	155	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 ⓘ

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	$\# Z > 2$
3	NAG	C	1	3,2	14,14,15	0.52	0	17,19,21	0.91	0
3	NAG	C	2	3	14,14,15	0.56	0	17,19,21	0.83	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	C	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C4-C3-C2	2.09	114.08	111.02

There are no chirality outliers.

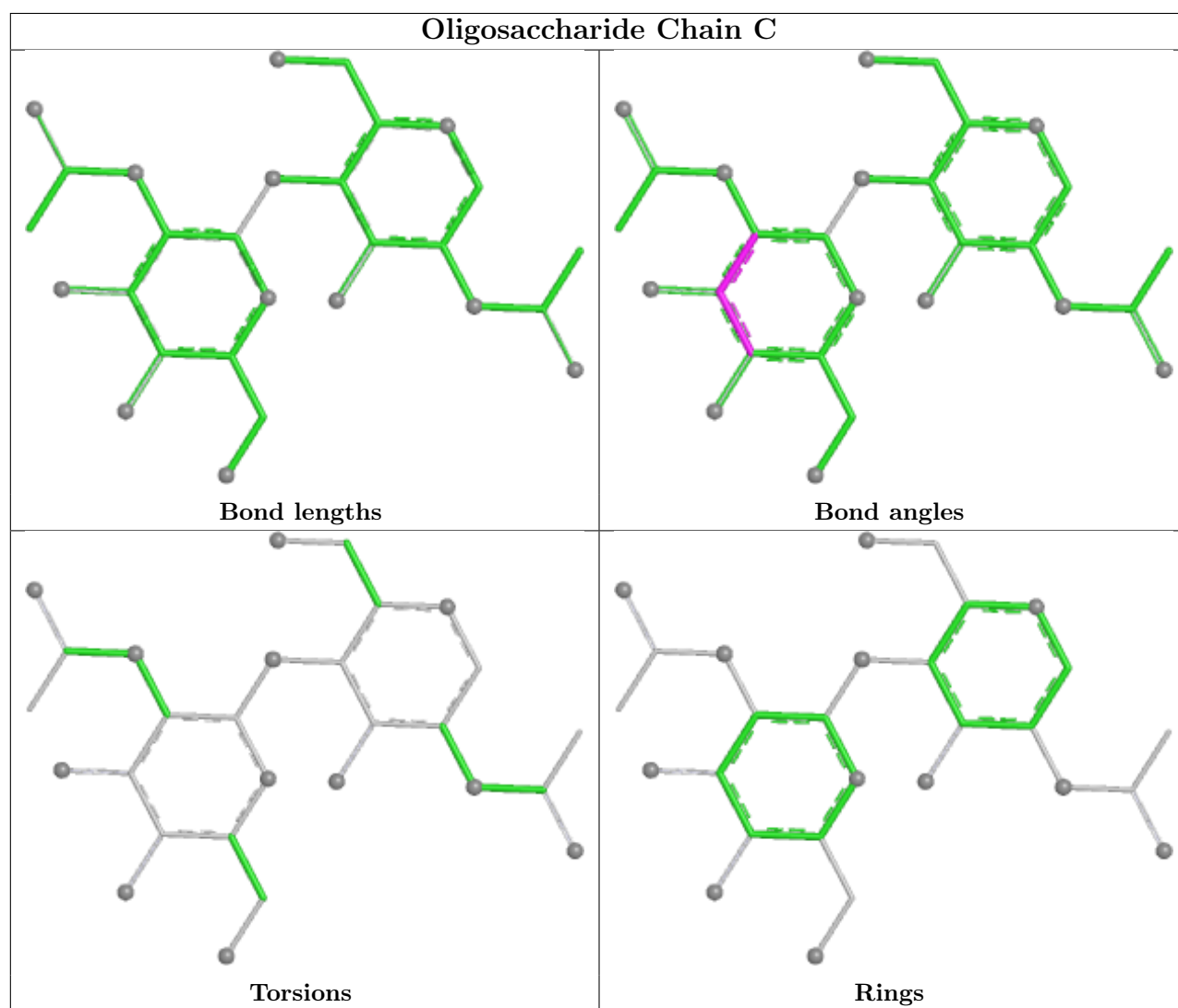
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	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](#)

18 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
4	NAG	A	403	1	14,14,15	0.47	0	17,19,21	0.95	1 (5%)
5	SO4	B	1174	-	4,4,4	0.42	0	6,6,6	0.11	0
5	SO4	A	1323	-	4,4,4	0.45	0	6,6,6	0.09	0
5	SO4	A	1321	-	4,4,4	0.46	0	6,6,6	0.13	0
5	SO4	A	1320	-	4,4,4	0.43	0	6,6,6	0.09	0
5	SO4	B	1173	-	4,4,4	0.44	0	6,6,6	0.17	0
4	NAG	A	1123	1	14,14,15	0.51	0	17,19,21	1.41	2 (11%)
5	SO4	A	1319	-	4,4,4	0.43	0	6,6,6	0.10	0
5	SO4	B	1172	-	4,4,4	0.46	0	6,6,6	0.13	0
5	SO4	A	1325	-	4,4,4	0.43	0	6,6,6	0.14	0
5	SO4	A	1324	-	4,4,4	0.45	0	6,6,6	0.15	0
5	SO4	A	1326	-	4,4,4	0.44	0	6,6,6	0.14	0
5	SO4	B	1171	-	4,4,4	0.46	0	6,6,6	0.13	0
5	SO4	A	1318	-	4,4,4	0.44	0	6,6,6	0.09	0
4	NAG	A	404	1	14,14,15	0.48	0	17,19,21	0.94	1 (5%)
5	SO4	A	1317	-	4,4,4	0.45	0	6,6,6	0.07	0
5	SO4	A	1322	-	4,4,4	0.45	0	6,6,6	0.20	0
4	NAG	A	405	1	14,14,15	0.37	0	17,19,21	1.82	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	A	403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	404	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1123	1	-	2/6/23/26	0/1/1/1
4	NAG	A	405	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	NAG	C1-O5-C5	6.39	120.75	112.19
4	A	1123	NAG	C1-O5-C5	4.85	118.68	112.19
4	A	403	NAG	C1-O5-C5	2.45	115.48	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	NAG	O7-C7-C8	-2.29	117.98	122.05
4	A	1123	NAG	C1-C2-N2	2.07	113.69	110.43

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1123	NAG	O5-C5-C6-O6
4	A	1123	NAG	C4-C5-C6-O6
4	A	403	NAG	C4-C5-C6-O6
4	A	403	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

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	317/321 (98%)	1.64	113 (35%)  	20, 47, 125, 152	0
2	B	170/177 (96%)	1.10	33 (19%)  	18, 61, 102, 110	0
All	All	487/498 (97%)	1.45	146 (29%)  	18, 50, 118, 152	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	GLY	8.5
1	A	192	LEU	7.5
1	A	189	GLY	7.5
1	A	214	VAL	7.0
1	A	204	PHE	6.9
1	A	205	VAL	6.9
1	A	217	LEU	6.8
1	A	185	LEU	6.7
1	A	195	VAL	6.5
1	A	190	ASN	6.5
1	A	191	LYS	6.4
1	A	216	GLY	6.3
1	A	193	VAL	6.3
1	A	194	THR	6.3
1	A	215	ASN	6.0
1	A	210	ALA	5.9
1	A	237	SER	5.6
1	A	212	PRO	5.5
1	A	235	THR	5.4
1	A	197	SER	5.4
1	A	239	ASN	5.4
1	A	236	PHE	5.2
1	A	203	SER	5.2
1	A	122	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	186	TYR	5.1
1	A	151	ALA	5.0
1	A	206	PRO	5.0
1	A	213	GLN	4.9
1	A	211	ARG	4.9
1	A	208	PRO	4.8
1	A	200	TYR	4.8
1	A	242	PHE	4.8
1	A	198	SER	4.8
1	A	179	THR	4.7
1	A	120	ILE	4.7
1	A	180	ALA	4.7
1	A	187	GLY	4.6
2	B	141	PHE	4.5
1	A	178	SER	4.4
1	A	158	SER	4.3
1	A	201	GLN	4.3
1	A	1	ASP	4.3
1	A	129	CYS	4.3
1	A	209	GLY	4.2
1	A	153	PRO	4.2
1	A	241	ALA	4.2
1	A	234	VAL	4.1
1	A	183	THR	4.1
1	A	238	PHE	4.0
1	A	118	SER	4.0
2	B	59	THR	4.0
1	A	188	SER	4.0
1	A	177	VAL	4.0
1	A	147	THR	4.0
2	B	170	ARG	3.9
1	A	176	SER	3.9
1	A	207	SER	3.9
1	A	119	GLY	3.9
1	A	184	LYS	3.8
2	B	58	LYS	3.8
1	A	154	GLN	3.7
1	A	128	ALA	3.6
1	A	152	PHE	3.5
1	A	173	ILE	3.5
1	A	202	GLN	3.5
1	A	114	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	115	PHE	3.5
1	A	182	GLN	3.4
1	A	149	ASN	3.4
1	A	233	THR	3.3
1	A	156	THR	3.2
1	A	155	MET	3.2
1	A	117	TYR	3.2
1	A	157	LYS	3.2
1	A	123	ASN	3.2
2	B	2	LEU	3.1
2	B	156	THR	3.1
1	A	174	HIS	3.1
1	A	142	TRP	3.1
1	A	134	SER	3.1
1	A	222	ASP	3.1
1	A	124	GLY	3.1
1	A	12	ASN	3.0
2	B	29	ALA	3.0
1	A	125	THR	3.0
1	A	132	SER	2.9
1	A	199	ASN	2.9
1	A	143	LEU	2.9
1	A	144	LEU	2.9
1	A	181	GLU	2.9
1	A	175	HIS	2.8
2	B	164	GLU	2.8
2	B	31	GLY	2.8
1	A	121	ARG	2.8
1	A	116	THR	2.8
2	B	34	THR	2.8
1	A	146	ASN	2.8
2	B	144	CYS	2.7
1	A	224	HIS	2.7
2	B	56	ILE	2.7
1	A	127	SER	2.7
1	A	11	SER	2.6
1	A	145	SER	2.6
2	B	161	LYS	2.6
1	A	226	LEU	2.5
1	A	126	THR	2.5
1	A	135	SER	2.5
1	A	221	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	139	GLU	2.5
2	B	17	LEU	2.5
1	A	167	ALA	2.5
2	B	168	GLN	2.5
1	A	113	MET	2.4
1	A	160	LYS	2.4
1	A	171	TRP	2.4
2	B	133	ASP	2.4
2	B	143	LYS	2.4
2	B	162	TYR	2.4
1	A	150	ALA	2.3
1	A	231	ASN	2.3
2	B	19	ASP	2.3
2	B	167	MET	2.3
2	B	60	ASN	2.3
1	A	159	TYR	2.3
1	A	316	GLU	2.3
2	B	160	SER	2.3
1	A	3	ILE	2.3
2	B	152	ILE	2.3
1	A	172	GLY	2.2
2	B	150	ALA	2.2
2	B	148	CYS	2.2
2	B	10	ILE	2.2
2	B	18	ILE	2.2
1	A	5	LEU	2.2
2	B	147	ASP	2.2
2	B	166	ALA	2.2
1	A	163	ARG	2.1
2	B	32	GLU	2.1
1	A	130	ARG	2.1
1	A	228	LEU	2.1
2	B	16	GLY	2.1
1	A	2	LYS	2.1
1	A	269	GLU	2.0
1	A	317	ILE	2.0
1	A	164	LYS	2.0
2	B	132	GLU	2.0

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

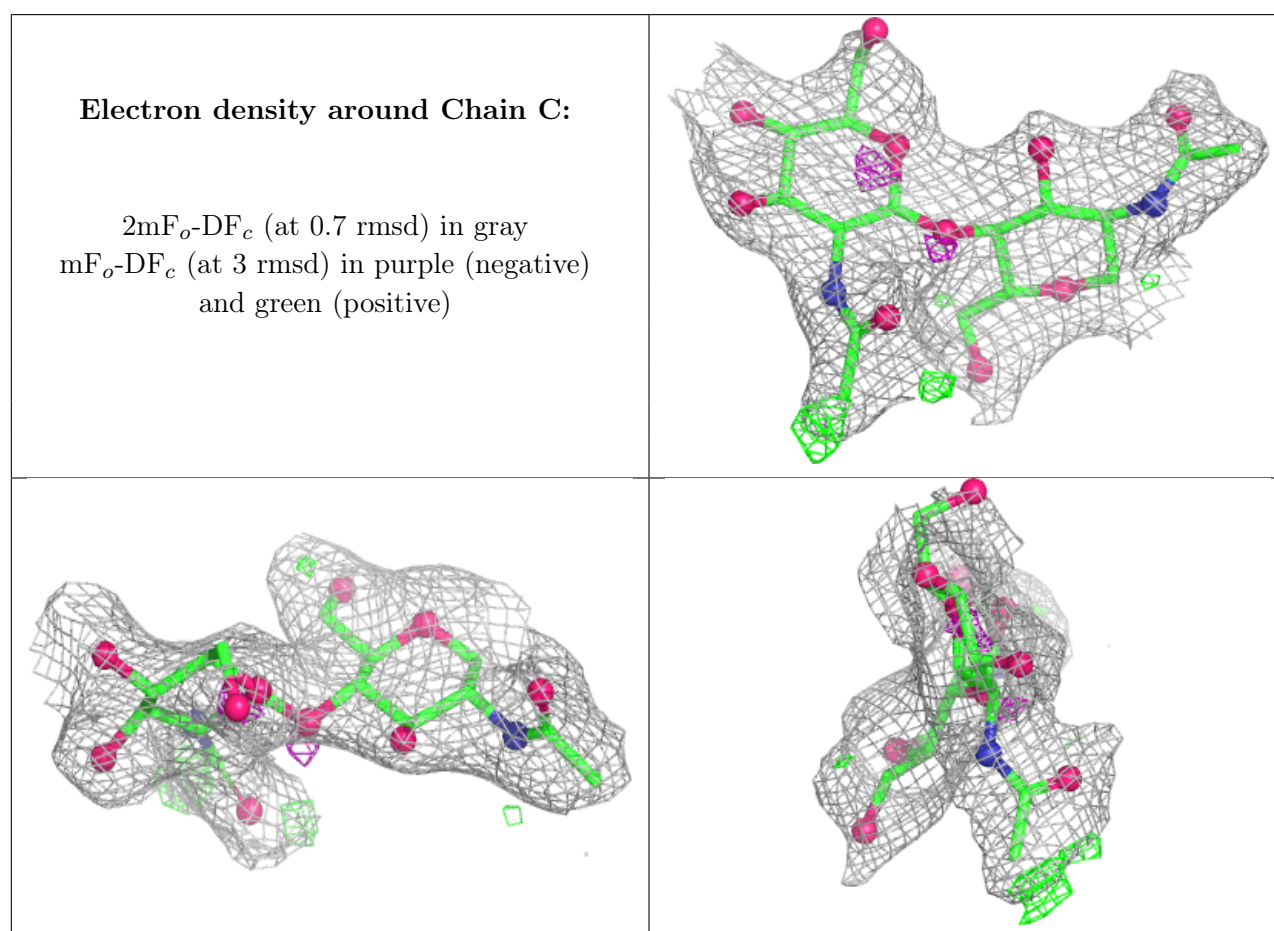
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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	C	2	14/15	0.68	0.17	58,64,68,69	0
3	NAG	C	1	14/15	0.84	0.12	38,46,53,56	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($\text{\AA}^2$)	Q<0.9
4	NAG	A	405	14/15	0.59	0.19	59,70,73,76	0
5	SO4	A	1319	5/5	0.59	0.16	108,108,111,112	0
4	NAG	A	404	14/15	0.62	0.19	59,71,75,76	0
5	SO4	B	1171	5/5	0.64	0.16	86,87,92,92	0
5	SO4	A	1317	5/5	0.65	0.13	92,94,95,96	0
5	SO4	A	1323	5/5	0.66	0.17	97,105,105,107	0
4	NAG	A	403	14/15	0.68	0.17	56,67,70,71	0
4	NAG	A	1123	14/15	0.68	0.17	49,57,62,62	0
5	SO4	A	1321	5/5	0.70	0.18	83,84,90,92	0
5	SO4	A	1320	5/5	0.72	0.15	112,116,119,119	0
5	SO4	A	1325	5/5	0.73	0.15	89,91,93,93	0
5	SO4	B	1174	5/5	0.73	0.22	95,99,115,115	3
5	SO4	A	1324	5/5	0.74	0.14	90,92,95,95	0
5	SO4	B	1172	5/5	0.74	0.14	78,80,81,82	0
5	SO4	A	1326	5/5	0.74	0.15	99,101,103,105	0
5	SO4	A	1322	5/5	0.76	0.19	65,66,71,71	0
5	SO4	B	1173	5/5	0.77	0.18	72,72,75,76	0
5	SO4	A	1318	5/5	0.77	0.17	115,116,118,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.