



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:44 PM BST

PDB ID : 4BSC  
Title : Human H7N9 Influenza Virus Haemagglutinin (with Asn-133 Glycosylation)  
in Complex with Human Receptor Analogue 6'-SLN  
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 : 2.55 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

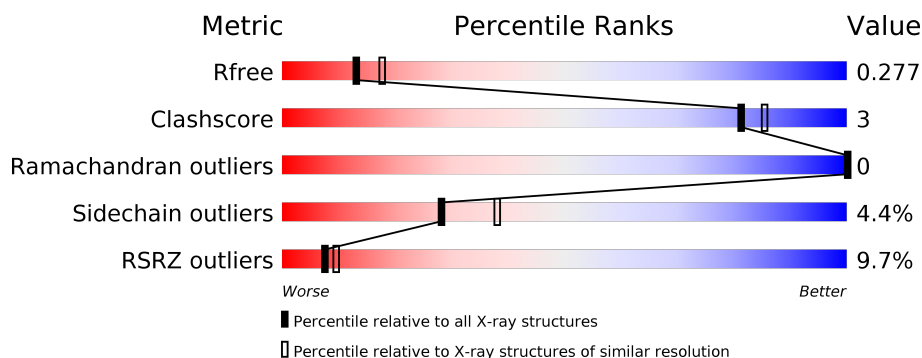
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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  $\geq 3$ , 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	<div> <div>6%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
2	B	177	<div> <div>16%</div> <div>85%</div> <div>10%</div> <div>..</div> </div>
3	C	3	<div> <div>33%</div> <div>67%</div> </div>
4	D	2	<div> <div>50%</div> <div>50%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	1	-	-	-	X
5	NAG	A	1319	-	-	-	X
5	NAG	A	1320	X	-	-	-
6	SO4	A	1325	-	-	-	X
6	SO4	A	1326	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4067 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
			Total	C	N	O	S			
1	A	317	2416	1500	437	464	15	0	0	1

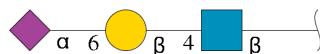
There are 3 discrepancies between the modelled and reference sequences:

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
			Total	C	N	O	S			
2	B	170	1379	851	241	280	7	0	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	46	25	2	19	0	0	0

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

- 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	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

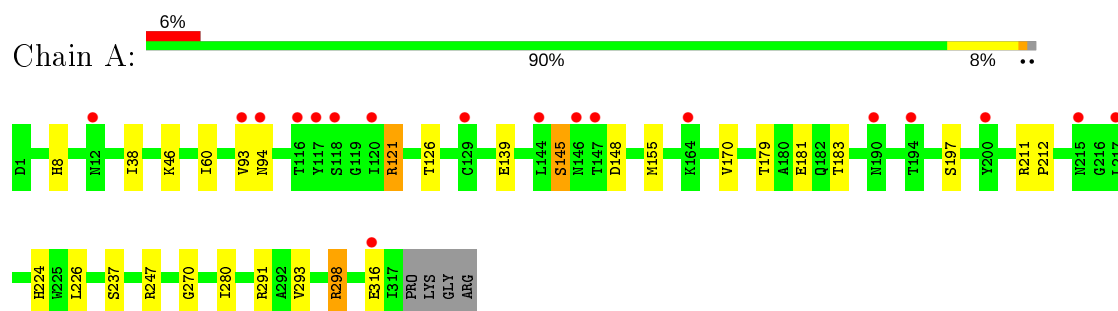
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	56	Total 56	O 56	0	0
7	B	21	Total 21	O 21	0	0

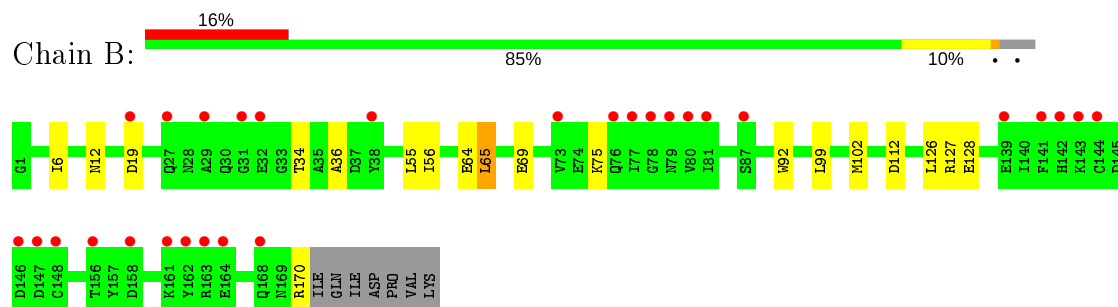
### 3 Residue-property plots

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: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



#### • Molecule 4: 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, $\alpha$ , $\beta$ , $\gamma$	116.11Å 116.11Å 296.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.06 – 2.55 50.05 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.06-2.55) 99.7 (50.05-2.55)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.52 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.220 , 0.280 0.223 , 0.277	Depositor DCC
$R_{free}$ test set	1293 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.017 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.010 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	0.93	EDS
Total number of atoms	4067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GAL, 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	0.35	0/2462	0.59	0/3328
2	B	0.34	0/1403	0.55	0/1890
All	All	0.35	0/3865	0.57	0/5218

There are no bond length outliers.

There are no bond angle outliers.

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	2416	0	2374	13	0
2	B	1379	0	1280	10	0
3	C	46	0	40	0	0
4	D	28	0	25	2	0
5	A	56	0	52	0	0
6	A	45	0	0	0	0
6	B	20	0	0	0	0
7	A	56	0	0	0	0
7	B	21	0	0	1	0
All	All	4067	0	3771	20	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 (20) 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:121:ARG:NH1	1:A:145:SER:O	2.30	0.63
1:A:38:ILE:HD12	1:A:280:ILE:HD12	1.80	0.62
2:B:56:ILE:HG22	2:B:56:ILE:O	2.08	0.52
1:A:293:VAL:HG11	2:B:65:LEU:HD13	1.91	0.52
1:A:139:GLU:OE1	1:A:247:ARG:HD3	2.12	0.50
1:A:60:ILE:HG21	1:A:170:VAL:HG21	1.97	0.47
2:B:75:LYS:HE3	4:D:1:NAG:H81	1.97	0.46
2:B:55:LEU:HD22	2:B:99:LEU:HD21	1.97	0.46
7:B:2010:HOH:O	4:D:1:NAG:H83	2.16	0.46
2:B:126:LEU:O	2:B:127:ARG:C	2.55	0.46
2:B:6:ILE:HD12	2:B:112:ASP:HA	1.99	0.44
1:A:298:ARG:HG2	2:B:92:TRP:CD2	2.53	0.43
1:A:211:ARG:HB3	1:A:212:PRO:HD2	2.00	0.43
2:B:19:ASP:HB2	2:B:36:ALA:HB2	2.02	0.42
1:A:93:VAL:HG21	1:A:224:HIS:NE2	2.36	0.41
1:A:46:LYS:NZ	1:A:270:GLY:O	2.53	0.41
1:A:179:THR:O	1:A:183:THR:HG23	2.21	0.40
1:A:155:MET:O	1:A:237:SER:HA	2.22	0.40
1:A:291:ARG:NH1	2:B:69:GLU:OE1	2.54	0.40
1:A:298:ARG:HG2	2:B:92:TRP:CE2	2.56	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	315/321 (98%)	299 (95%)	16 (5%)	0	100	100
2	B	168/177 (95%)	162 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	483/498 (97%)	461 (95%)	22 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	266/270 (98%)	255 (96%)	11 (4%)	30	41
2	B	145/152 (95%)	138 (95%)	7 (5%)	25	34
All	All	411/422 (97%)	393 (96%)	18 (4%)	28	38

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

Mol	Chain	Res	Type
1	A	8	HIS
1	A	94	ASN
1	A	121	ARG
1	A	126	THR
1	A	145	SER
1	A	148	ASP
1	A	181	GLU
1	A	197	SER
1	A	226	LEU
1	A	298	ARG
1	A	316	GLU
2	B	12	ASN
2	B	34	THR
2	B	64	GLU
2	B	65	LEU
2	B	102	MET
2	B	128	GLU
2	B	170	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
2	B	60	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 ⓘ

5 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	15,15,15	0.46	0	21,21,21	1.02	1 (4%)
3	GAL	C	2	3	11,11,12	0.32	0	15,15,17	0.65	0
3	SIA	C	3	3	17,20,21	0.35	0	21,28,31	1.09	2 (9%)
4	NAG	D	1	2,4	14,14,15	0.52	0	17,19,21	0.84	1 (5%)
4	NAG	D	2	4	14,14,15	0.55	0	17,19,21	0.74	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	C	1	3	-	4/6/26/26	0/1/1/1
3	GAL	C	2	3	-	0/2/19/22	0/1/1/1
3	SIA	C	3	3	-	4/14/34/38	0/1/1/1

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-C2-N2	-3.29	106.91	110.73
3	C	3	SIA	C4-C5-N5	-3.24	103.95	110.38
4	D	1	NAG	C1-O5-C5	2.38	115.42	112.19
3	C	3	SIA	C6-O6-C2	2.36	116.39	111.34

There are no chirality outliers.

All (10) torsion outliers are listed below:

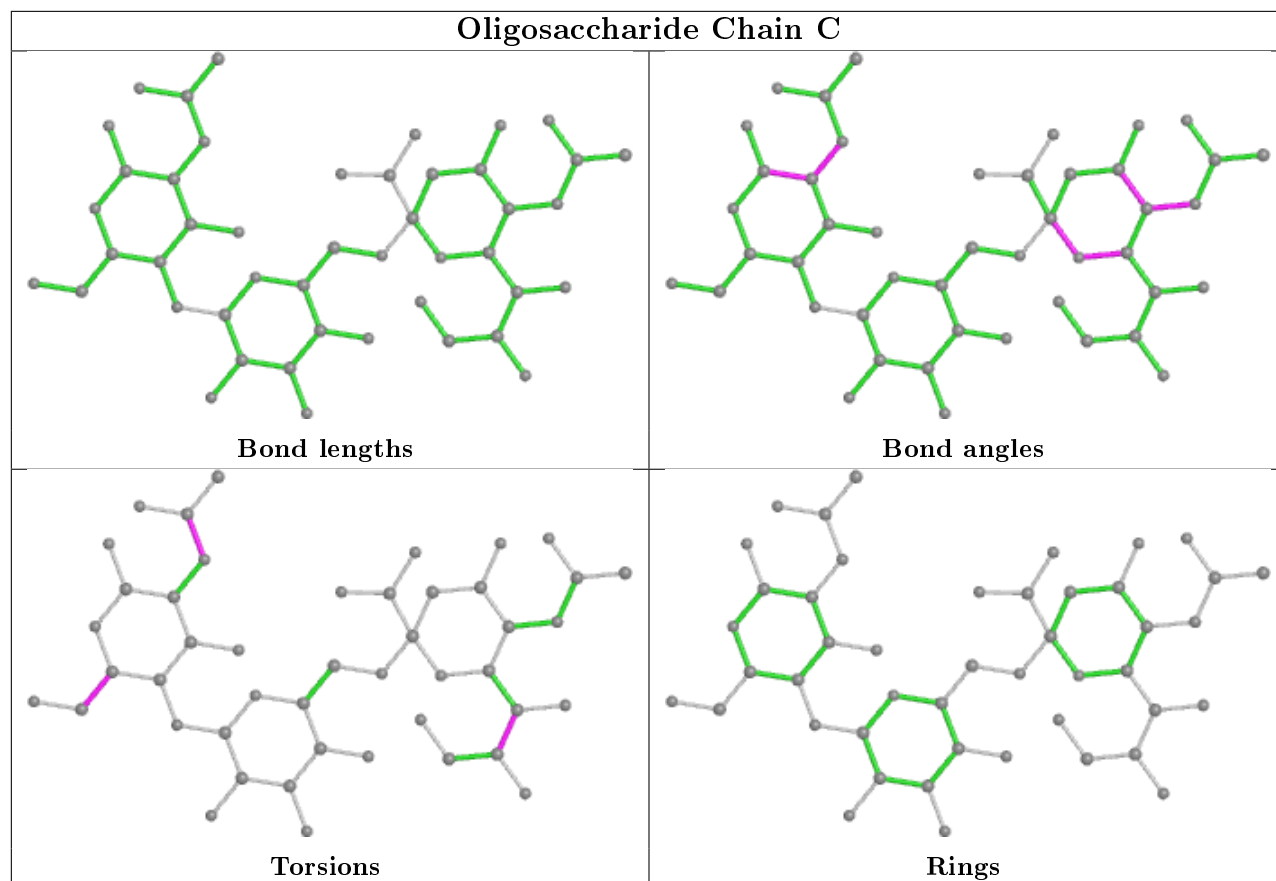
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6
3	C	3	SIA	O7-C7-C8-C9
3	C	3	SIA	C6-C7-C8-O8
3	C	1	NAG	C4-C5-C6-O6
3	C	3	SIA	O7-C7-C8-O8
3	C	3	SIA	C6-C7-C8-C9

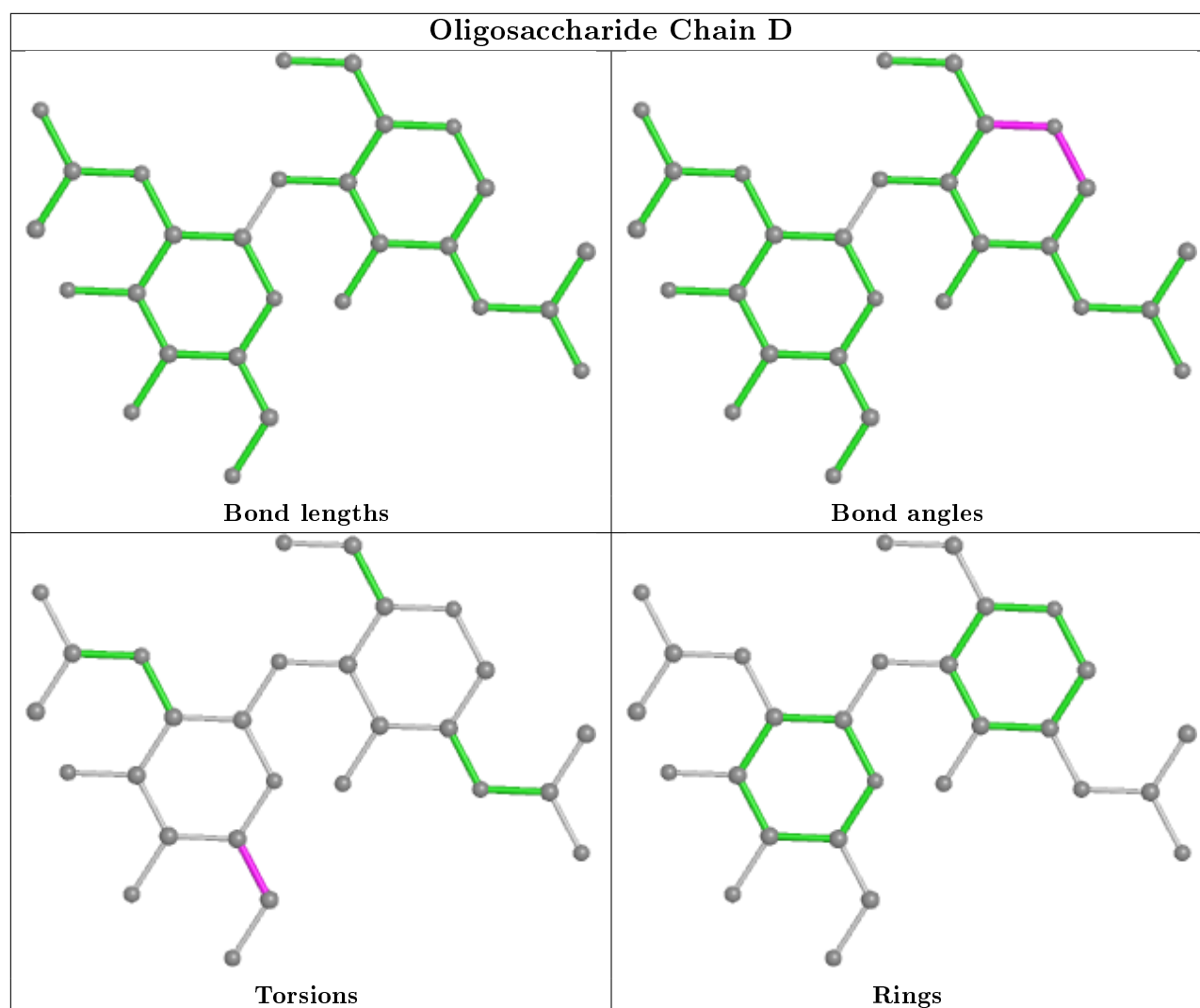
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	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 ⓘ

17 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	$\# Z  > 2$
6	SO4	B	1174	-	4,4,4	0.35	0	6,6,6	0.13	0
6	SO4	A	1327	-	4,4,4	0.36	0	6,6,6	0.10	0
5	NAG	A	1318	1	14,14,15	0.47	0	17,19,21	1.19	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	A	1330	-	4,4,4	0.35	0	6,6,6	0.15	0
6	SO4	A	1328	-	4,4,4	0.35	0	6,6,6	0.17	0
6	SO4	B	1173	-	4,4,4	0.34	0	6,6,6	0.17	0
6	SO4	A	1326	-	4,4,4	0.35	0	6,6,6	0.09	0
5	NAG	A	1319	1	14,14,15	0.60	0	17,19,21	1.73	1 (5%)
5	NAG	A	1320	1	14,14,15	0.46	0	17,19,21	1.38	1 (5%)
6	SO4	A	1325	-	4,4,4	0.37	0	6,6,6	0.12	0
6	SO4	A	1331	-	4,4,4	0.36	0	6,6,6	0.12	0
6	SO4	B	1175	-	4,4,4	0.37	0	6,6,6	0.08	0
6	SO4	A	1324	-	4,4,4	0.33	0	6,6,6	0.06	0
6	SO4	A	1329	-	4,4,4	0.36	0	6,6,6	0.17	0
5	NAG	A	1317	1	14,14,15	0.52	0	17,19,21	1.17	1 (5%)
6	SO4	B	1176	-	4,4,4	0.33	0	6,6,6	0.10	0
6	SO4	A	1332	-	4,4,4	0.33	0	6,6,6	0.13	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
5	NAG	A	1317	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1320	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	A	1318	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1319	1	-	1/6/23/26	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(°)
5	A	1319	NAG	C1-O5-C5	6.44	120.92	112.19
5	A	1320	NAG	C1-O5-C5	4.89	118.82	112.19
5	A	1317	NAG	C4-C3-C2	3.12	115.59	111.02
5	A	1318	NAG	O5-C1-C2	-2.79	106.88	111.29
5	A	1318	NAG	C1-O5-C5	2.72	115.88	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1320	NAG	C1

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1318	NAG	C4-C5-C6-O6
5	A	1317	NAG	C4-C5-C6-O6
5	A	1318	NAG	O5-C5-C6-O6
5	A	1317	NAG	O5-C5-C6-O6
5	A	1320	NAG	C4-C5-C6-O6
5	A	1320	NAG	O5-C5-C6-O6
5	A	1319	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	317/321 (98%)	0.54	18 (5%) 23 28	31, 56, 97, 109	0
2	B	170/177 (96%)	1.05	29 (17%) 1 1	29, 76, 114, 121	0
All	All	487/498 (97%)	0.72	47 (9%) 7 9	29, 61, 106, 121	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	THR	3.8
1	A	190	ASN	3.8
2	B	143	LYS	3.7
2	B	73	VAL	3.6
2	B	161	LYS	3.5
2	B	80	VAL	3.5
2	B	141	PHE	3.4
2	B	27	GLN	3.4
1	A	120	ILE	3.3
1	A	118	SER	3.1
1	A	144	LEU	3.0
1	A	117	TYR	3.0
2	B	156	THR	2.9
2	B	81	ILE	2.8
1	A	146	ASN	2.8
2	B	78	GLY	2.8
2	B	147	ASP	2.8
2	B	32	GLU	2.7
2	B	29	ALA	2.7
2	B	77	ILE	2.7
1	A	94	ASN	2.7
1	A	93	VAL	2.6
1	A	129	CYS	2.6
2	B	168	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	31	GLY	2.6
1	A	316	GLU	2.5
2	B	164	GLU	2.5
2	B	163	ARG	2.5
1	A	194	THR	2.4
2	B	79	ASN	2.4
2	B	146	ASP	2.4
1	A	12	ASN	2.3
2	B	142	HIS	2.3
2	B	87	SER	2.3
1	A	215	ASN	2.3
2	B	148	CYS	2.3
1	A	116	THR	2.2
2	B	38	TYR	2.2
1	A	200	TYR	2.2
2	B	158	ASP	2.2
1	A	164	LYS	2.1
2	B	162	TYR	2.1
2	B	139	GLU	2.1
2	B	19	ASP	2.1
2	B	76	GLN	2.1
1	A	217	LEU	2.1
2	B	144	CYS	2.0

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

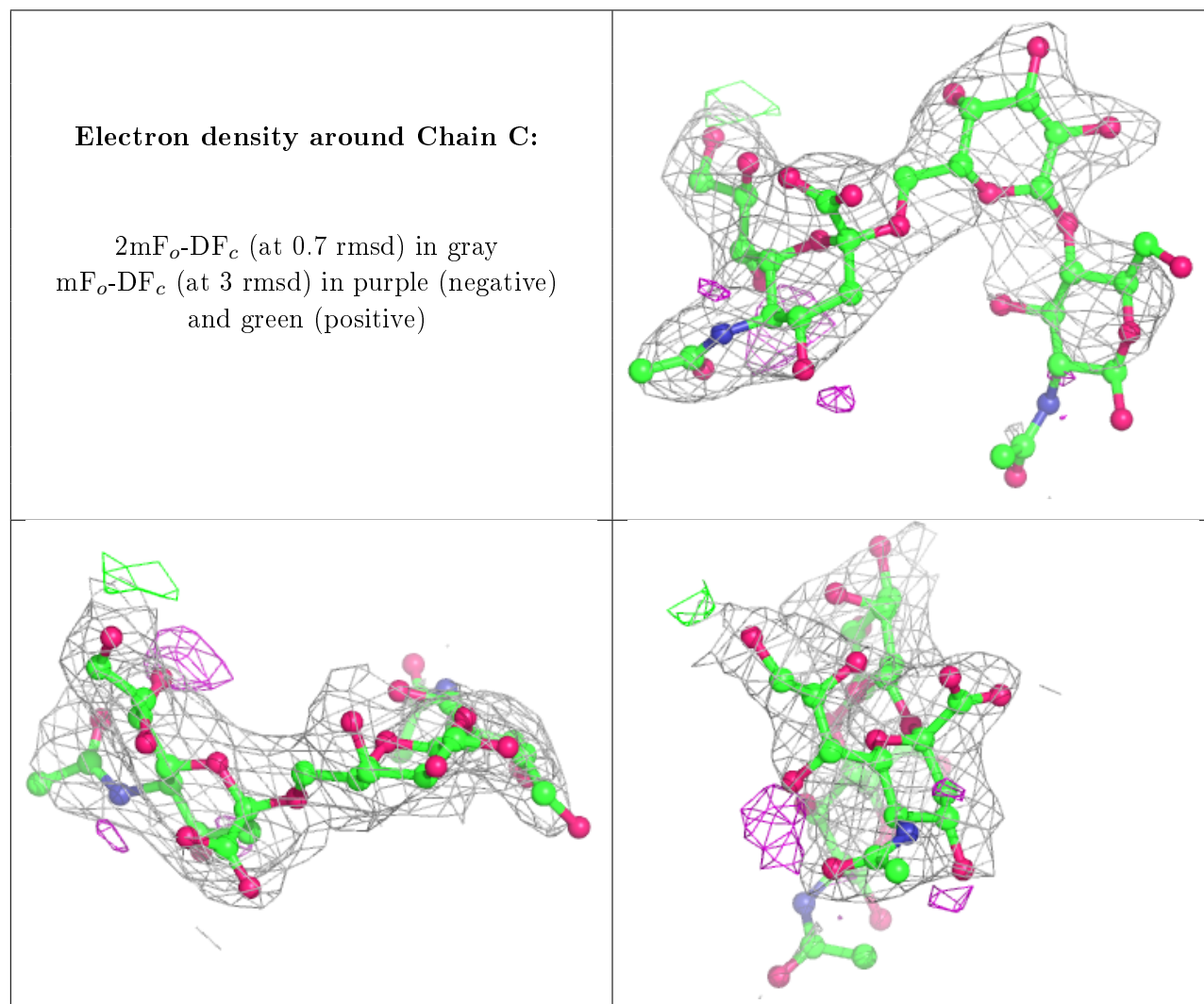
There are no non-standard protein/DNA/RNA residues in this entry.

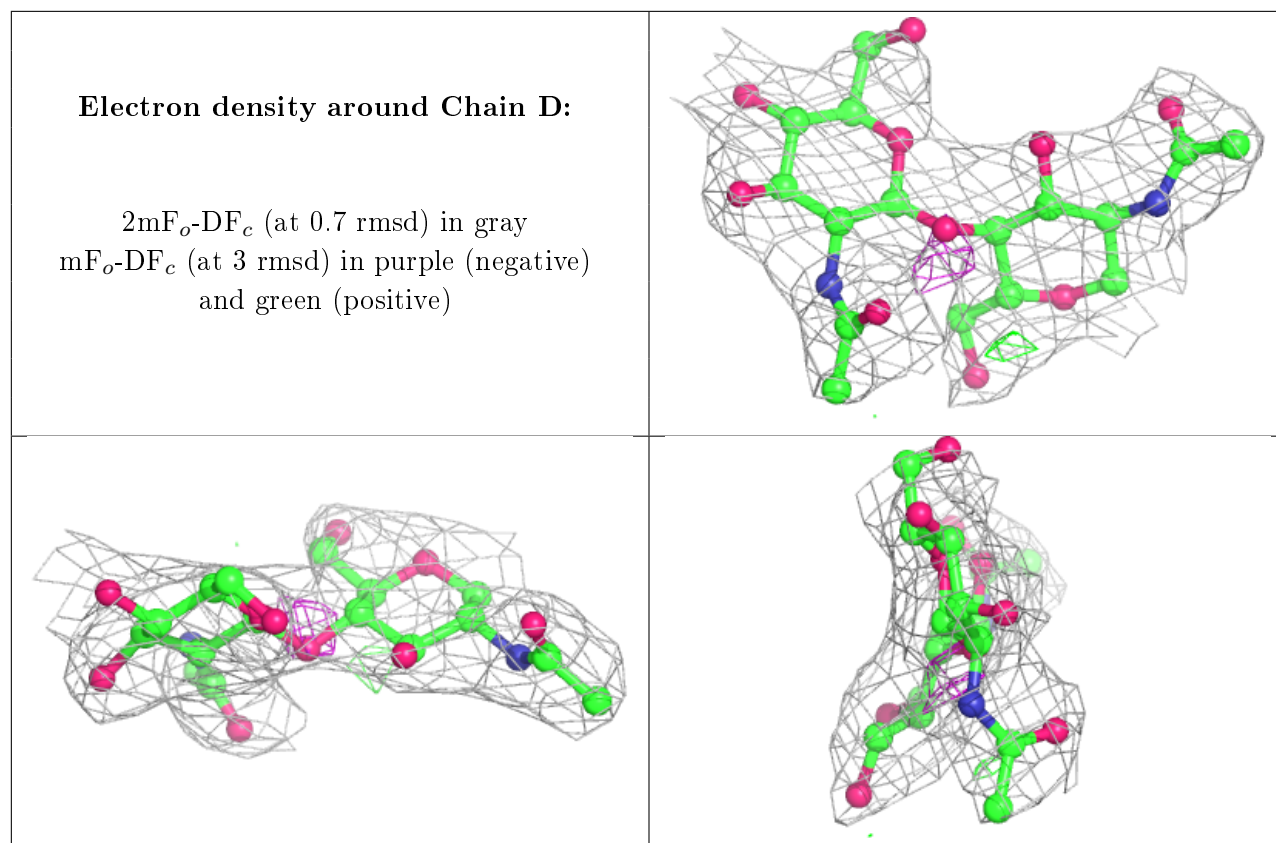
## 6.3 Carbohydrates [i](#)

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<sup>th</sup> 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	C	1	15/15	0.76	0.54	109,115,119,119	0
3	GAL	C	2	11/12	0.84	0.22	79,95,102,105	0
4	NAG	D	1	14/15	0.89	0.15	52,63,68,74	0
4	NAG	D	2	14/15	0.89	0.17	68,77,84,85	0
3	SIA	C	3	20/21	0.93	0.24	59,66,78,79	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, 95<sup>th</sup> 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
6	SO4	A	1326	5/5	0.63	0.44	126,129,133,135	0
6	SO4	A	1325	5/5	0.66	0.49	114,116,120,122	0
5	NAG	A	1317	14/15	0.73	0.39	73,81,85,85	0
5	NAG	A	1319	14/15	0.76	0.49	83,92,97,99	0
6	SO4	B	1176	5/5	0.77	0.39	104,106,117,120	3
5	NAG	A	1320	14/15	0.81	0.28	78,85,89,91	0
6	SO4	A	1330	5/5	0.82	0.40	104,104,109,111	0
6	SO4	A	1327	5/5	0.83	0.45	114,115,119,120	0
6	SO4	B	1173	5/5	0.84	0.30	108,112,114,115	0
5	NAG	A	1318	14/15	0.84	0.52	78,91,102,106	0
6	SO4	B	1175	5/5	0.85	0.27	99,100,105,109	0
6	SO4	A	1324	5/5	0.88	0.51	128,129,132,133	0
6	SO4	A	1329	5/5	0.88	0.24	84,91,95,96	0
6	SO4	A	1328	5/5	0.89	0.27	86,91,98,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	B	1174	5/5	0.91	0.23	86,89,91,97	0
6	SO4	A	1331	5/5	0.92	0.28	84,85,88,88	0
6	SO4	A	1332	5/5	0.94	0.40	104,105,105,106	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.