



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 3, 2021 – 12:47 PM EDT

PDB ID : 3HS0  
Title : Cobra Venom Factor (CVF) in complex with human factor B  
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Deposited on : 2009-06-10  
Resolution : 3.00 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](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 : 2.23.2  
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) : 2.23.2



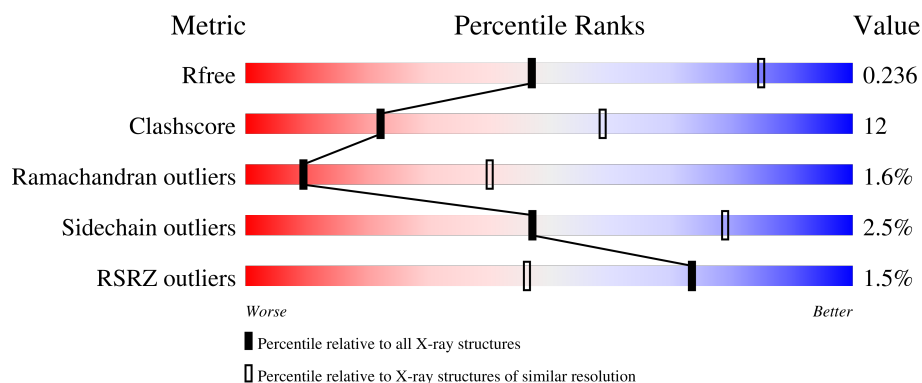
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*






The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	627	 77% 20% .
1	F	627	 76% 21% . .
2	B	252	 75% 17% . 8%
2	G	252	 72% 18% . 8%
3	C	379	 % 66% 26% . . 5%

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Mol	Chain	Length	Quality of chain
3	H	379	
4	D	741	
4	I	741	
5	E	2	
5	J	2	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	E	2	-	-	-	X
5	NAG	J	2	-	-	-	X



## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 30435 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 Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4794	3069	804	906	15			
1	F	617	Total	C	N	O	S	0	0	0
			4826	3085	811	915	15			

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1856	1194	311	346	5			
2	G	233	Total	C	N	O	S	0	0	0
			1856	1194	311	346	5			

- Molecule 3 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	359	Total	C	N	O	S	0	0	0
			2900	1831	484	566	19			
3	H	366	Total	C	N	O	S	0	0	0
			2957	1864	496	578	19			

- Molecule 4 is a protein called Complement factor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	699	Total	C	N	O	S	0	0	0
			5513	3474	954	1052	33			
4	I	704	Total	C	N	O	S	0	0	0
			5567	3506	972	1056	33			

There are 8 discrepancies between the modelled and reference sequences:



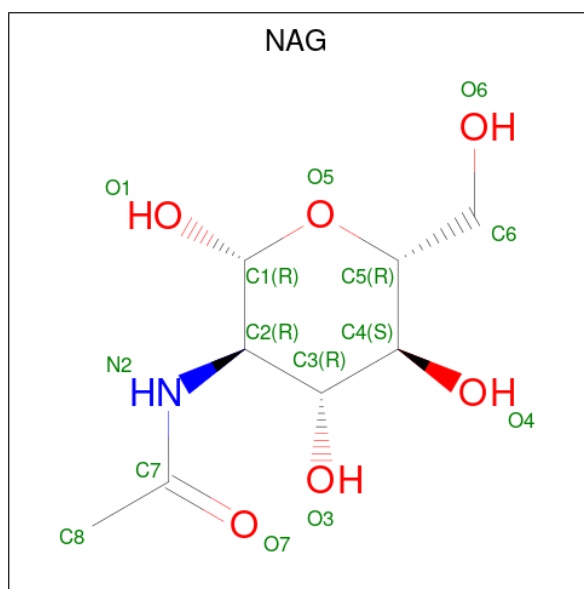
Chain	Residue	Modelled	Actual	Comment	Reference
D	254	GLY	ASP	engineered mutation	UNP P00751
D	260	ASP	ASN	engineered mutation	UNP P00751
D	740	ALA	-	insertion	UNP P00751
D	741	ALA	-	insertion	UNP P00751
I	254	GLY	ASP	engineered mutation	UNP P00751
I	260	ASP	ASN	engineered mutation	UNP P00751
I	740	ALA	-	insertion	UNP P00751
I	741	ALA	-	insertion	UNP P00751

- 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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	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<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0
7	I	1	Total Mg 1 1	0	0

- Molecule 8 is water.

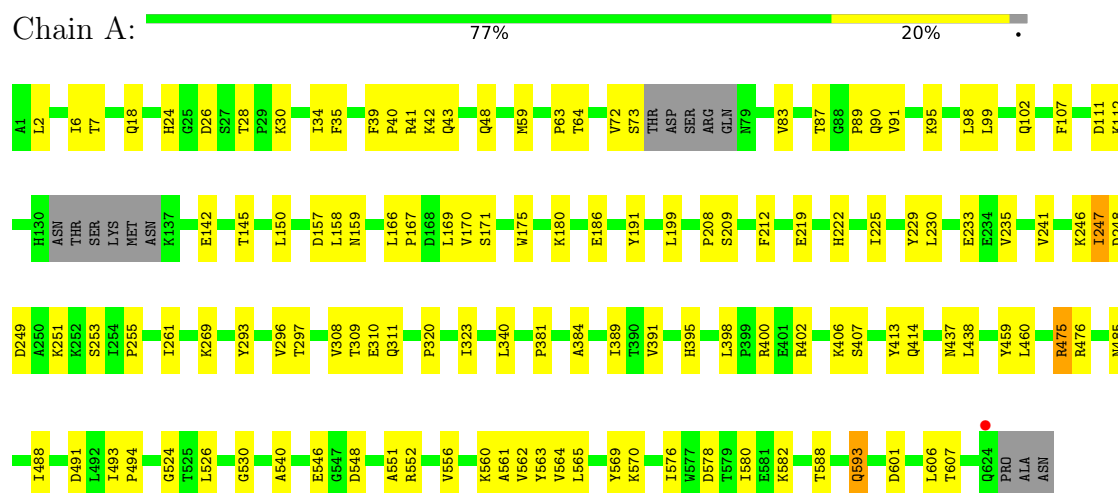
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total O 2 2	0	0
8	C	1	Total O 1 1	0	0
8	D	1	Total O 1 1	0	0
8	F	2	Total O 2 2	0	0
8	H	1	Total O 1 1	0	0
8	I	1	Total O 1 1	0	0



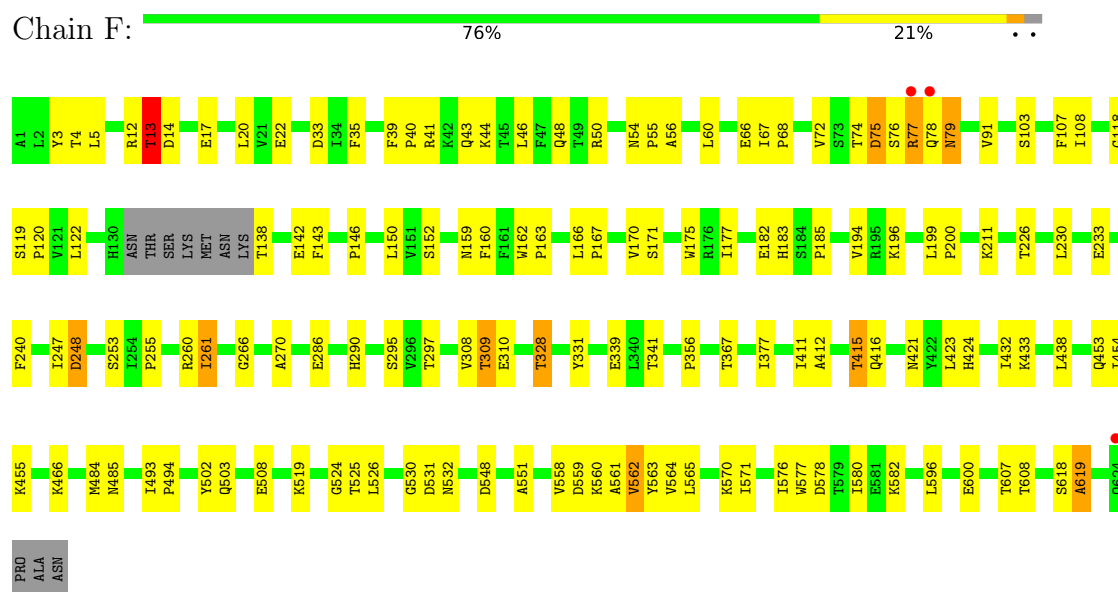
### 3 Residue-property plots

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: Cobra venom factor



#### • Molecule 1: Cobra venom factor



#### • Molecule 2: Cobra venom factor



[illegible][illegible]

S1576	D1485	K1344	GLU
Y1577	Y1486	GLN	ILE
I1578	P1487		GLN
I1579		Y1349	MET
T1580	I1490		PRO
			THR
P1589	A1493	S1355	HIS
H1590	C1494	T1356	LYS
E1591	E1495	M1357	
D1592		T1358	D1250
E1593	V1498	I1359	L1251
C1594			
Q1595	Y1502	L1365	D1254
	K1503	T1366	
F1599	T1504	G1367	D1261
Q1600	K1505	F1368	
K1601	L1506	L1369	I1266
L1602	L1507		
C1603	I1508	D1383	R1269
L1613	I1509		
		S1387	V1281
F1616	Q1512	R1388	E1282
	M1515		T1283
T1620	D1516	M1395	K1284
	I1517		L1285
	Y1518	M1406	
	M1519	K1407	V1291
	M1520	V1426	G1297
	D1521	G1427	
	V1522	Q1430	M1301
	H1539		T1305
	Q1540	K1435	F1306
	Y1541		
		D1443	Q1310
	Q1544		L1311
	R1546	C1446	GLN
	K1546	T1447	GLU
	C1547		LYS
	Q1548	H1451	ALA
	E1549		ASN
	A1550	K1454	
	L1551		V1317
	L1552	T1462	C1318
	K1553	I1464	
	K1554		
	V1555	A1471	
	M1556		
	D1557	T1474	HIS
	D1558	C1475	LEU
	Y1559	S1476	ASN
		I1477	ALA
		L1478	MET
	M1562		GLY
		H1480	
	L1569	K1481	K1338
		E1482	G1339
	D1573		
	K1574	R1483	
	T1575	T1484	A1341

K1581		Y1349	GLU
R1587	L1580	V1353	ILE
W1588	C1603	D1354	GLN
P1589	D1604	S1355	MET
	D1605	T1356	PRO
Q1600	S1610	M1357	THR
K1601	T1614		HIS
L1602	T1620	D1361	LYS
C1603		T1366	D1250
D1604		G1367	L1251
D1605		L1416	W1252
S1610		F1424	L1253
T1614		Q1430	D1254
T1620		K1435	T1255
		G1446	T1256
		H1451	L1259
		K1454	F1260
		R1469	D1261
		L1478	R1267
		I1484	Y1268
		Y1500	
		E1511	T1280
		G1514	
		I1517	T1289
		Y1518	T1290
		D1531	Y1291
		I1542	T1292
		S1543	
		R1545	G1297
		C1547	K1298
		L1553	M1301
		W1562	
		L1569	T1305
		P1570	F1306
		I1579	
		T1580	L1311
			Q1312
			E1313
			K1314
			A1315
			M1316
			V1317
			K1320
			I1330
			H1331
			L1332
			W1333
			ALA
			MET
			GLY
			ALA
			LYS
			G1339
			A1340



[illegible]

Chain I:





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

Chain E: 100%

MAG1  
MAG2

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

Chain J: 100%

MAG1  
MAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.03Å 136.97Å 283.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.88 – 3.00 34.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.88-3.00) 99.8 (34.88-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 3.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.189 , 0.243 0.179 , 0.236	Depositor DCC
$R_{free}$ test set	2093 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.0	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	30435	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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: NAG, MG

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	0.27	0/4902	0.46	0/6668
1	F	0.27	0/4935	0.49	2/6715 (0.0%)
2	B	0.27	0/1894	0.46	0/2570
2	G	0.28	0/1894	0.51	1/2570 (0.0%)
3	C	0.26	0/2950	0.51	1/3989 (0.0%)
3	H	0.26	0/3009	0.47	0/4071
4	D	0.26	0/5636	0.48	2/7629 (0.0%)
4	I	0.25	0/5691	0.46	0/7699
All	All	0.26	0/30911	0.48	6/41911 (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	F	1	0
3	C	0	1
All	All	1	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1553	LEU	N-CA-C	5.97	127.12	111.00
1	F	13	THR	C-N-CA	5.71	135.96	121.70
4	D	739	LEU	CA-CB-CG	5.49	127.93	115.30
2	G	917	GLY	N-CA-C	5.23	126.18	113.10
1	F	13	THR	CA-C-N	5.19	128.62	117.20



All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	13	THR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	1551	LEU	Peptide

## 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	4794	0	4801	90	0
1	F	4826	0	4826	111	0
2	B	1856	0	1900	37	0
2	G	1856	0	1900	40	0
3	C	2900	0	2851	101	0
3	H	2957	0	2900	62	0
4	D	5513	0	5376	153	0
4	I	5567	0	5446	160	0
5	E	28	0	25	0	0
5	J	28	0	25	0	0
6	A	14	0	13	2	0
6	C	14	0	13	0	0
6	D	28	0	26	0	0
6	F	14	0	13	0	0
6	H	14	0	13	0	0
6	I	14	0	13	0	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	I	1	0	0	0	0
8	A	2	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	2	0	0	0	0
8	H	1	0	0	0	0
8	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30435	0	30141	711	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 12.

The worst 5 of 711 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)
3:H:1469:ARG:HG2	3:H:1469:ARG:HH11	1.10	1.12
4:D:714:ARG:HG2	4:D:714:ARG:HH11	1.17	1.07
4:I:705:ARG:HB3	4:I:707:LYS:HG2	1.37	1.04
4:D:699:VAL:HG23	4:D:707:LYS:HD2	1.42	1.01
1:F:13:THR:HG23	1:F:14:ASP:CB	1.89	1.01

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	607/627 (97%)	577 (95%)	26 (4%)	4 (1%)	22	60
1	F	613/627 (98%)	571 (93%)	36 (6%)	6 (1%)	15	53
2	B	231/252 (92%)	218 (94%)	13 (6%)	0	100	100
2	G	231/252 (92%)	218 (94%)	12 (5%)	1 (0%)	34	72
3	C	353/379 (93%)	318 (90%)	29 (8%)	6 (2%)	9	39
3	H	362/379 (96%)	333 (92%)	24 (7%)	5 (1%)	11	43
4	D	687/741 (93%)	608 (88%)	63 (9%)	16 (2%)	6	30
4	I	694/741 (94%)	605 (87%)	65 (9%)	24 (4%)	3	20
All	All	3778/3998 (94%)	3448 (91%)	268 (7%)	62 (2%)	9	40



5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	ILE
4	D	44	TYR
4	D	46	VAL
4	D	344	PRO
4	D	505	VAL

### 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	535/548 (98%)	529 (99%)	6 (1%)	73	90
1	F	539/548 (98%)	528 (98%)	11 (2%)	55	83
2	B	210/227 (92%)	200 (95%)	10 (5%)	25	62
2	G	210/227 (92%)	202 (96%)	8 (4%)	33	69
3	C	329/345 (95%)	314 (95%)	15 (5%)	27	64
3	H	335/345 (97%)	326 (97%)	9 (3%)	44	77
4	D	610/643 (95%)	596 (98%)	14 (2%)	50	80
4	I	615/643 (96%)	605 (98%)	10 (2%)	62	86
All	All	3383/3526 (96%)	3300 (98%)	83 (2%)	47	79

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

Mol	Chain	Res	Type
2	G	851	LYS
3	H	1478	LEU
2	G	918	THR
3	H	1311	LEU
4	I	216	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	593	GLN
4	D	47	GLN
4	D	601	GLN
1	F	473	GLN
4	I	468	GLN

### 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 ⓘ

4 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	E	1	4,5	14,14,15	0.52	0	17,19,21	1.84	5 (29%)
5	NAG	E	2	5	14,14,15	0.49	0	17,19,21	1.09	2 (11%)
5	NAG	J	1	4,5	14,14,15	0.44	0	17,19,21	1.14	1 (5%)
5	NAG	J	2	5	14,14,15	0.49	0	17,19,21	1.30	2 (11%)

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	E	1	4,5	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	1	4,5	-	4/6/23/26	0/1/1/1
5	NAG	J	2	5	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C1-O5-C5	4.52	118.31	112.19
5	J	2	NAG	O5-C5-C6	4.28	113.92	107.20
5	J	1	NAG	C1-O5-C5	3.18	116.50	112.19
5	E	1	NAG	C3-C4-C5	2.81	115.26	110.24
5	E	1	NAG	C2-N2-C7	2.80	126.90	122.90

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

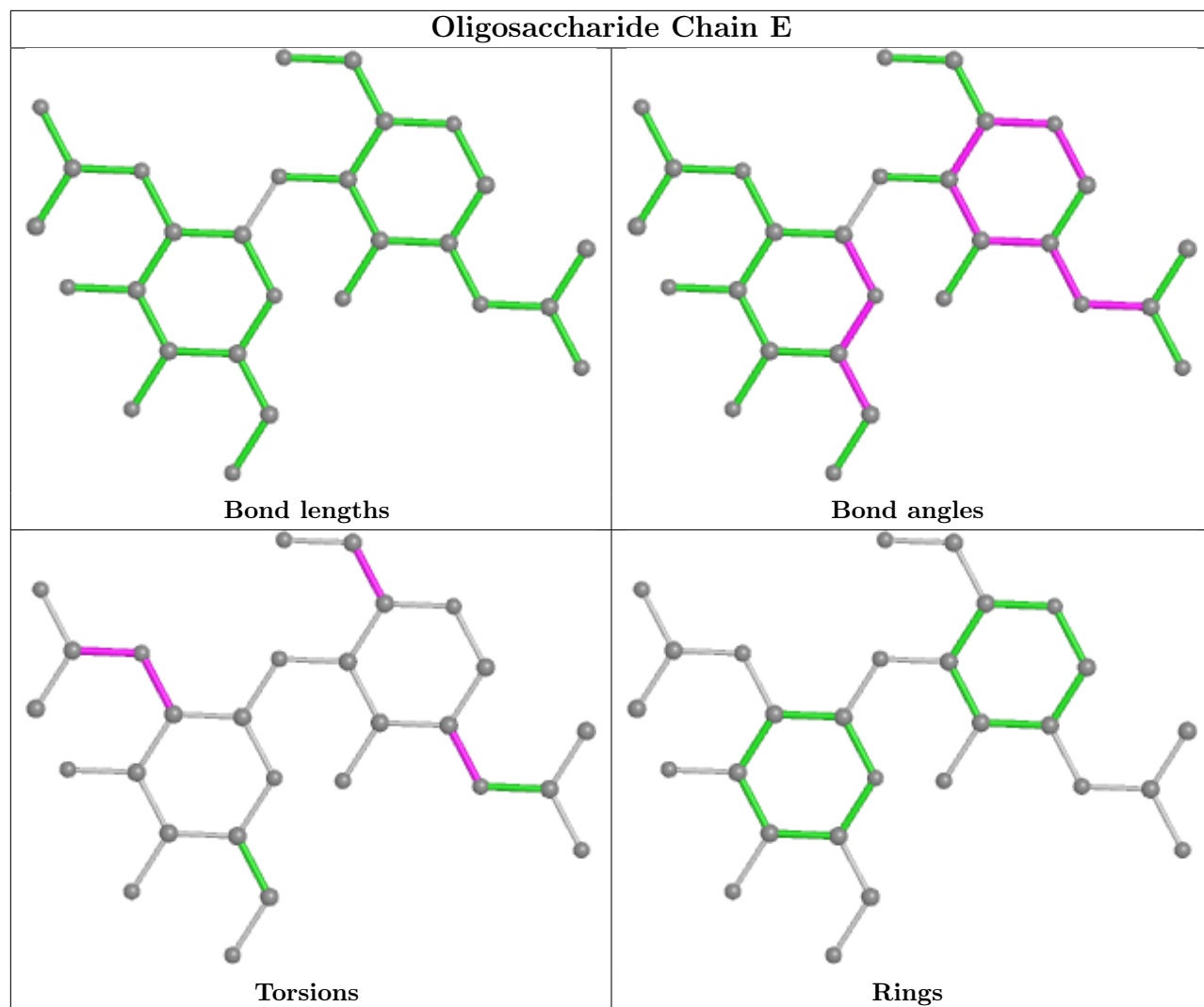
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C3-C2-N2-C7
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2

There are no ring outliers.

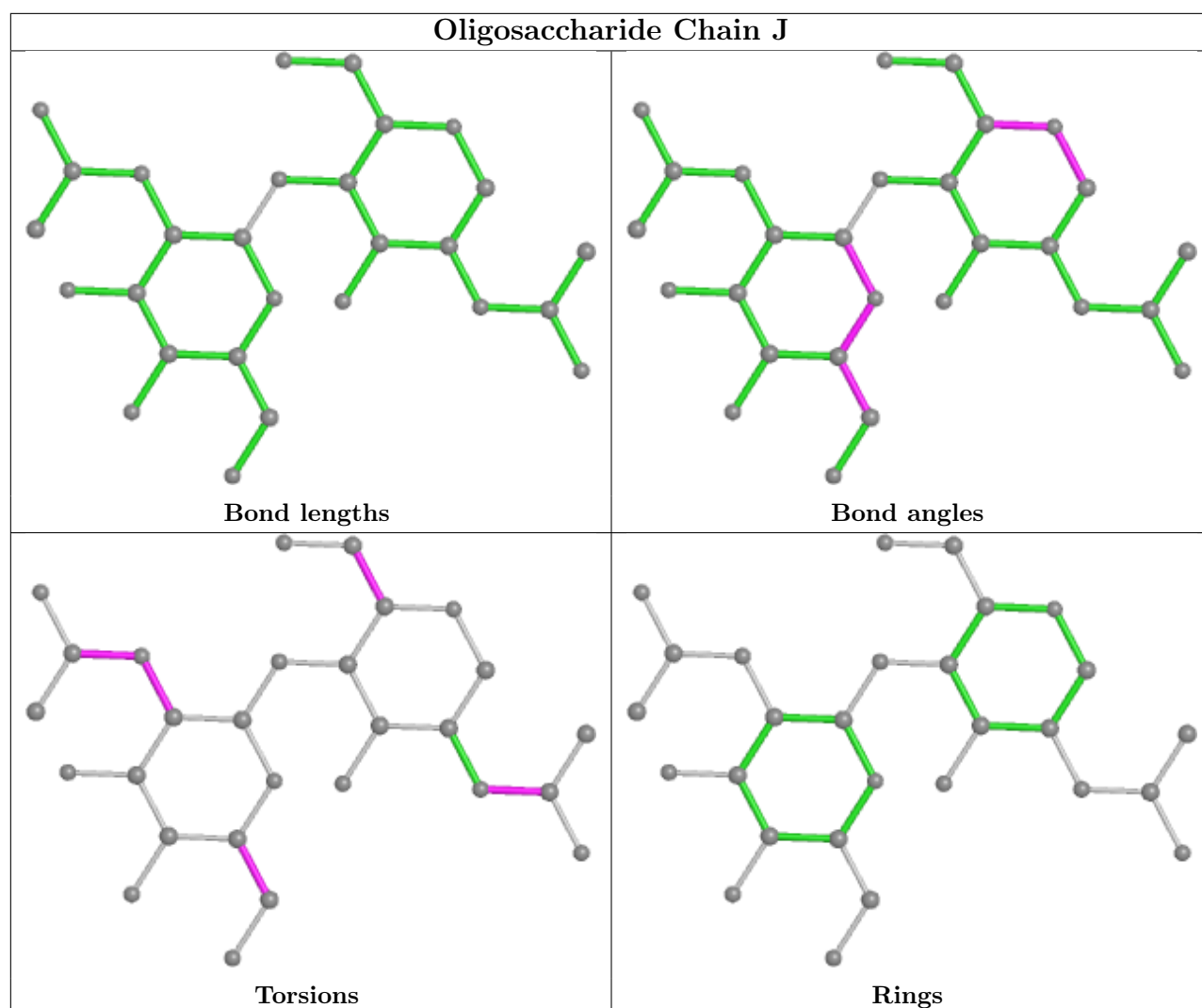
No monomer is involved in short contacts.

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](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	I	9117	4	14,14,15	0.45	0	17,19,21	1.10	1 (5%)
6	NAG	D	9353	4	14,14,15	0.47	0	17,19,21	0.89	1 (5%)
6	NAG	F	9187	1	14,14,15	0.44	0	17,19,21	1.41	3 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	9187	1	14,14,15	0.45	0	17,19,21	1.21	2 (11%)
6	NAG	H	9324	3	14,14,15	0.46	0	17,19,21	0.82	0
6	NAG	D	9117	4	14,14,15	0.37	0	17,19,21	2.43	4 (23%)
6	NAG	C	9324	3	14,14,15	0.52	0	17,19,21	1.01	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
6	NAG	I	9117	4	-	4/6/23/26	0/1/1/1
6	NAG	D	9353	4	-	2/6/23/26	0/1/1/1
6	NAG	F	9187	1	-	3/6/23/26	0/1/1/1
6	NAG	A	9187	1	-	3/6/23/26	0/1/1/1
6	NAG	H	9324	3	-	3/6/23/26	0/1/1/1
6	NAG	D	9117	4	-	4/6/23/26	0/1/1/1
6	NAG	C	9324	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	9117	NAG	C1-O5-C5	8.51	123.73	112.19
6	F	9187	NAG	C1-O5-C5	3.79	117.33	112.19
6	A	9187	NAG	C1-O5-C5	3.39	116.79	112.19
6	I	9117	NAG	C1-O5-C5	3.37	116.76	112.19
6	C	9324	NAG	C1-O5-C5	3.20	116.52	112.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	9187	NAG	C8-C7-N2-C2
6	A	9187	NAG	O7-C7-N2-C2
6	C	9324	NAG	C8-C7-N2-C2
6	C	9324	NAG	O7-C7-N2-C2
6	D	9117	NAG	C8-C7-N2-C2



There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	9187	NAG	2	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 [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, 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	613/627 (97%)	-0.67	1 (0%) 95 87	31, 68, 125, 182	0
1	F	617/627 (98%)	-0.61	3 (0%) 91 75	37, 75, 132, 187	0
2	B	233/252 (92%)	-0.73	0 100 100	34, 63, 111, 123	0
2	G	233/252 (92%)	-0.71	0 100 100	33, 66, 115, 151	0
3	C	359/379 (94%)	-0.42	3 (0%) 86 65	40, 94, 210, 291	0
3	H	366/379 (96%)	-0.62	2 (0%) 91 75	33, 81, 135, 216	0
4	D	699/741 (94%)	-0.36	25 (3%) 42 17	35, 88, 189, 233	0
4	I	704/741 (95%)	-0.33	25 (3%) 42 17	37, 91, 191, 244	0
All	All	3824/3998 (95%)	-0.52	59 (1%) 73 46	31, 79, 168, 291	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	16	GLY	8.8
4	I	30	GLY	6.8
4	I	51	CYS	6.4
4	I	50	THR	5.9
4	I	29	GLU	5.6

### 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](#)

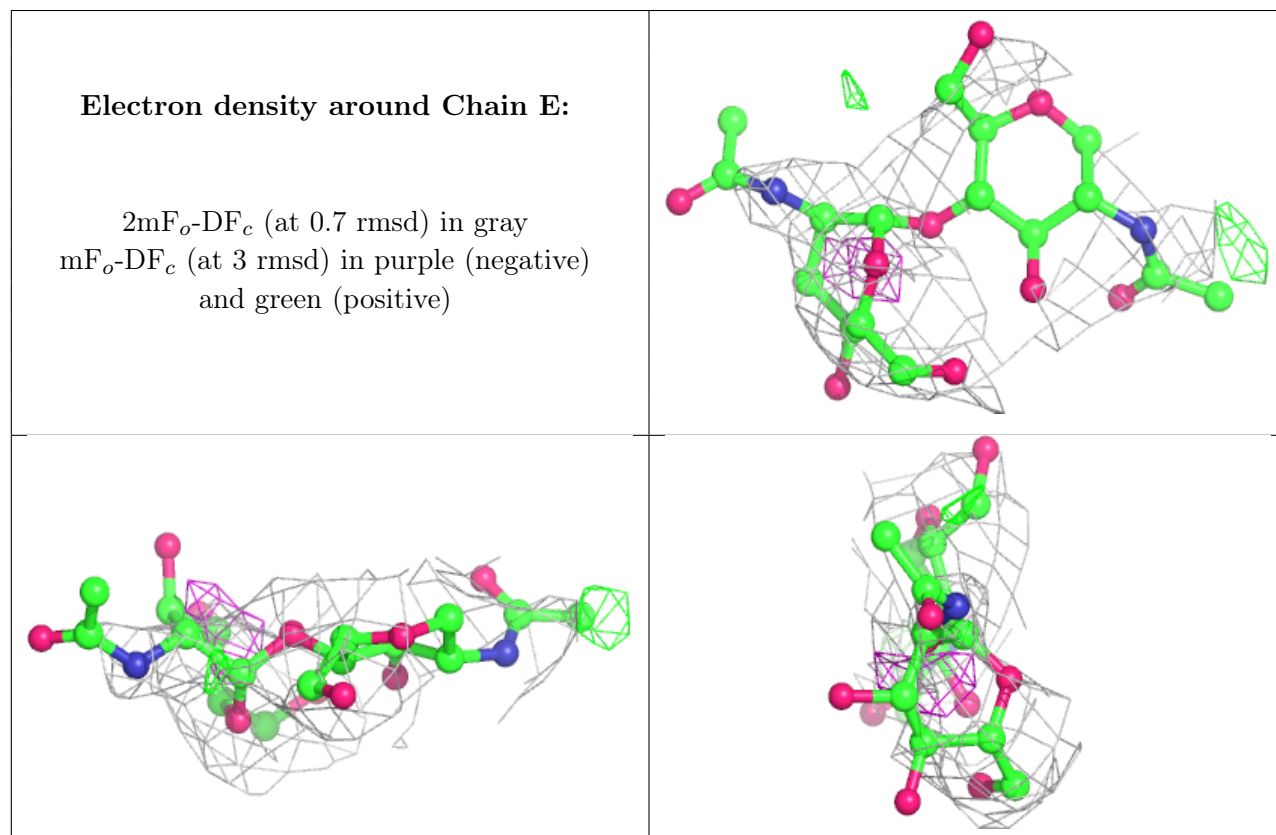
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



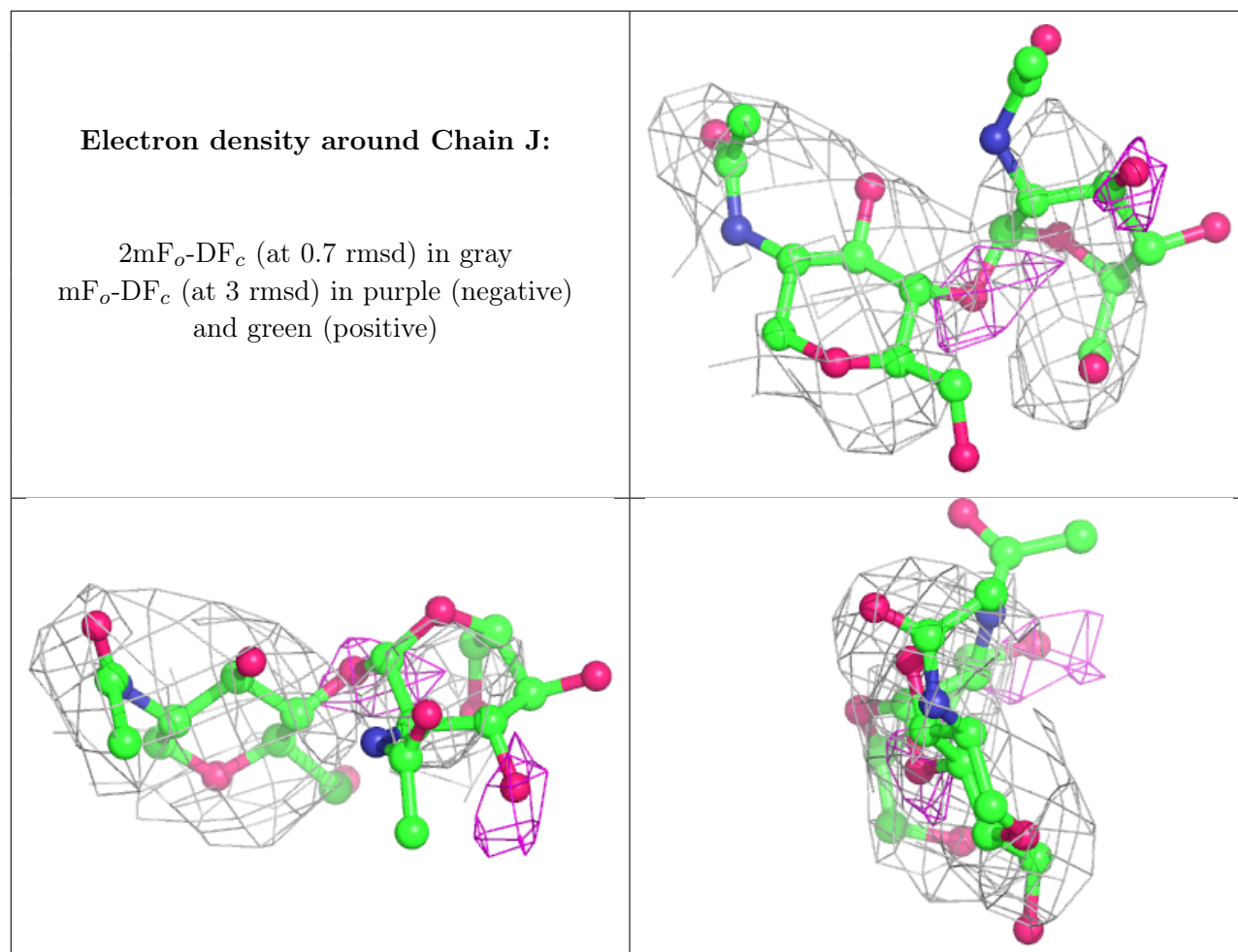
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	E	2	14/15	0.64	0.49	161,168,182,183	0
5	NAG	J	2	14/15	0.66	0.63	173,184,194,201	0
5	NAG	J	1	14/15	0.80	0.26	126,139,157,173	0
5	NAG	E	1	14/15	0.86	0.25	136,146,153,163	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	NAG	H	9324	14/15	0.76	0.36	129,140,144,146	0
6	NAG	C	9324	14/15	0.82	0.25	111,123,130,134	0
6	NAG	F	9187	14/15	0.87	0.30	106,116,125,127	0
6	NAG	D	9353	14/15	0.88	0.31	122,136,142,146	0
7	MG	A	628	1/1	0.89	0.07	105,105,105,105	0
6	NAG	I	9117	14/15	0.92	0.38	116,129,142,143	0
6	NAG	D	9117	14/15	0.93	0.22	98,117,131,132	0
6	NAG	A	9187	14/15	0.94	0.19	87,102,110,114	0
7	MG	F	628	1/1	0.97	0.04	73,73,73,73	0
7	MG	I	742	1/1	0.97	0.13	97,97,97,97	0
7	MG	D	742	1/1	0.98	0.10	107,107,107,107	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.