



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 07:06 AM BST

PDB ID : 3CU7  
Title : Human Complement Component 5  
Authors : Fredslund, F.; Andersen, G.R.  
Deposited on : 2008-04-16  
Resolution : 3.10 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 : 2.13.1  
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

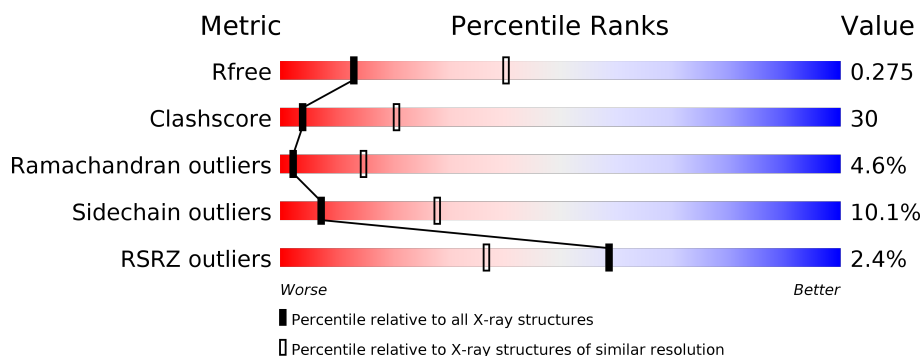
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	1676	<div> <div>3%</div> <div>45%</div> <div>44%</div> <div>8%</div> <div>...</div> </div>
1	B	1676	<div> <div>%</div> <div>42%</div> <div>39%</div> <div>6%</div> <div>12%</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>100%</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
2	NAG	D	2	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24655 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1625	Total	C	N	O	S	0	0	0
			12861	8239	2111	2458	53			
1	B	1481	Total	C	N	O	S	0	0	0
			11701	7493	1930	2232	46			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	802	ILE	VAL	SEE REMARK 999	UNP P01031
B	802	ILE	VAL	SEE REMARK 999	UNP P01031

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

- Molecule 3 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
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

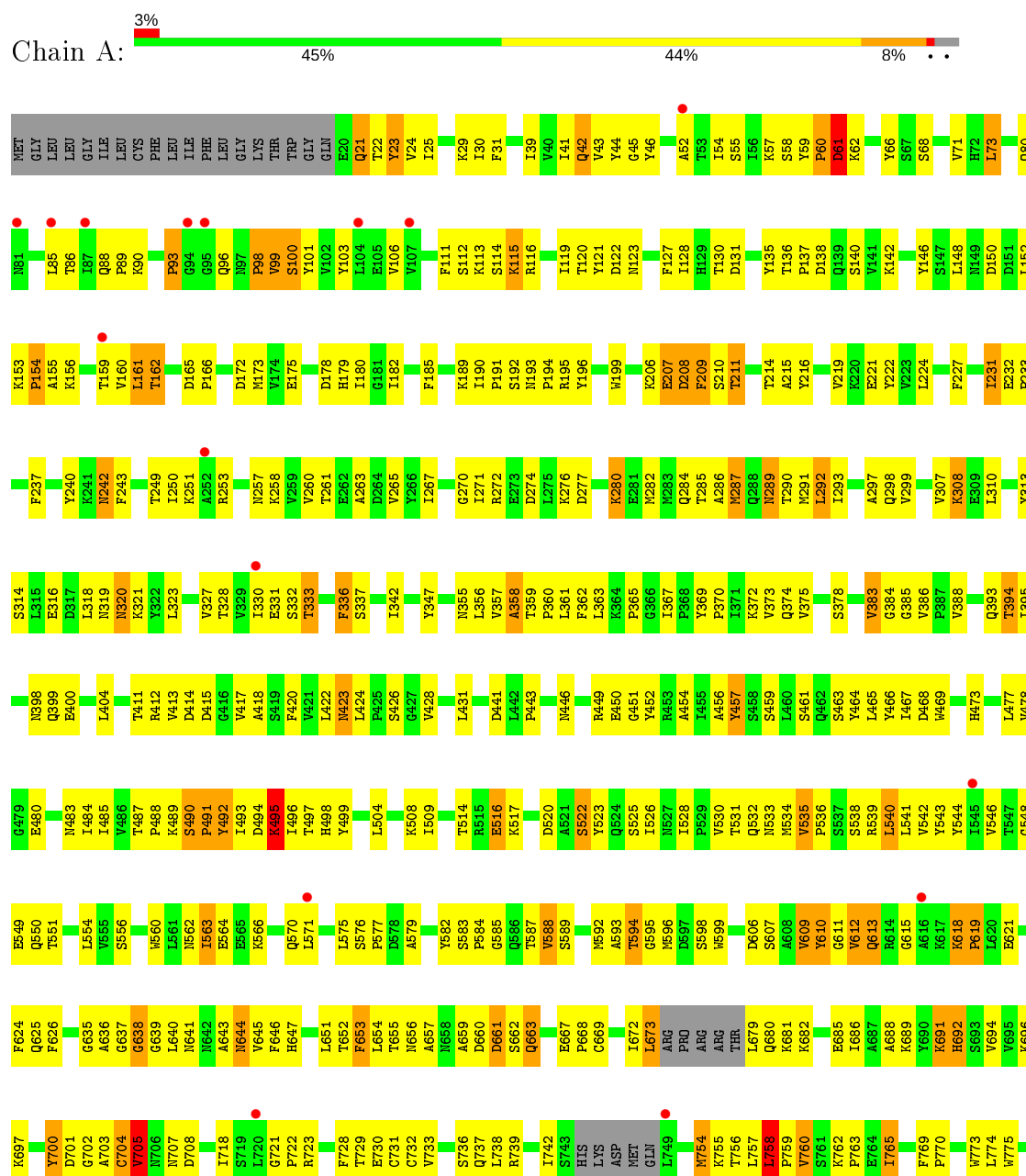
- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

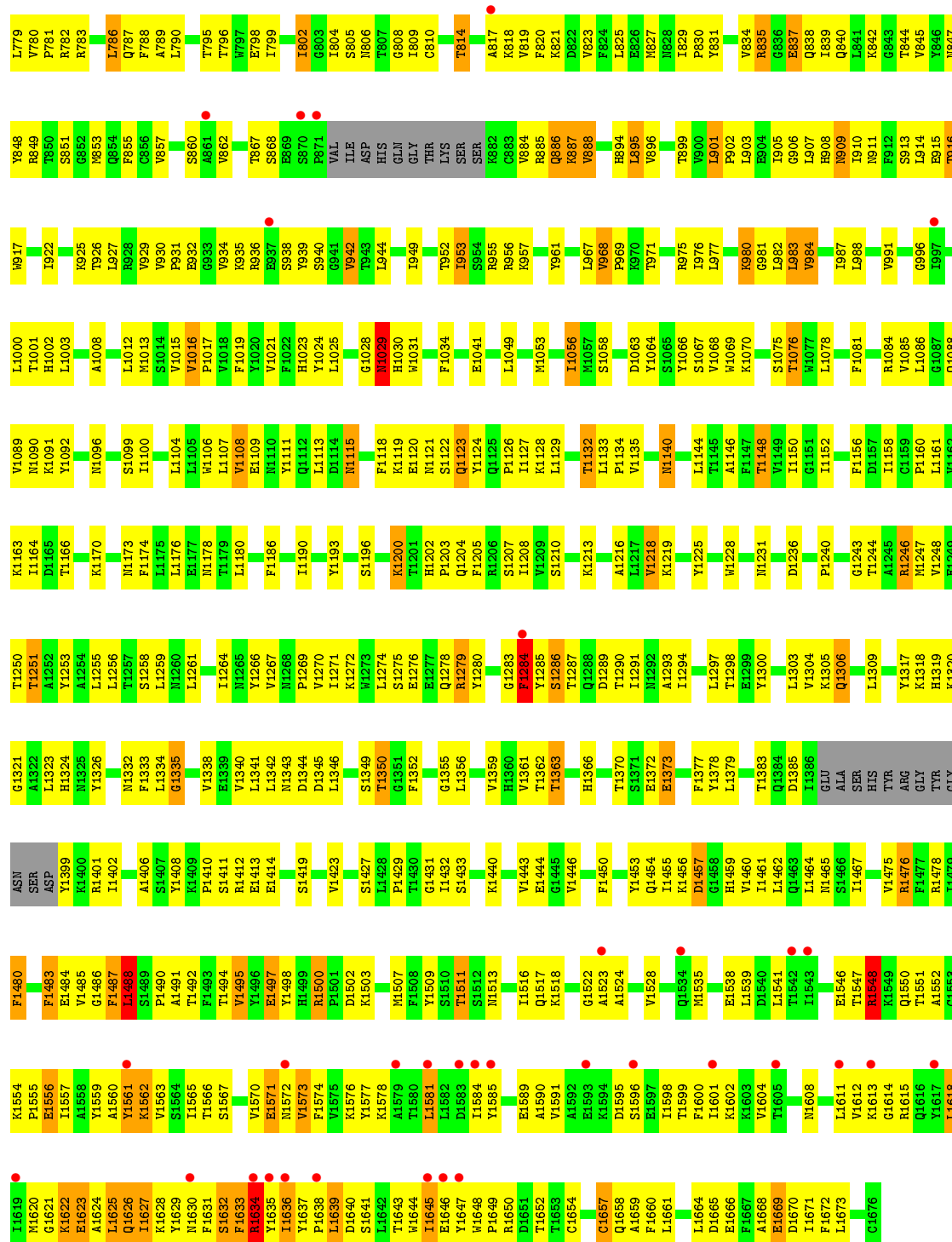
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Cd	0	0
			4	4		
4	A	5	Total	Cd	0	0
			5	5		

### 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.

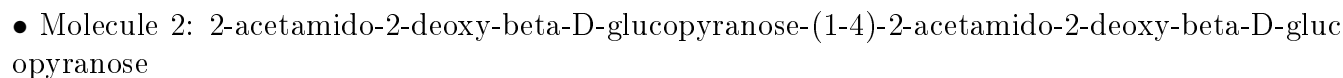
#### • Molecule 1: Complement C5





K1091	H1002	L925	Y848	L779	K697	Q625	E549	E480	Q393	Y313	E232	D151	Q80
Y1092	L1003	T926	R849	V780	Y700	F626	Q550	H461	T394	S314	F233	L152	N81
M1096	A1008	L927	T850	R781	D701	R782	L482	N482	I395	L315	F237	K153	L85
S1099	L1012	V929	G852	R783	A703	A636	I494	I495	Q398	D317	Y240	T86	T86
I1100	V1015	V930	Q854	L786	C704	Q638	V486	V487	N399	L318	K241	I87	I87
L1104	V1016	P931	F855	Q787	V705	Q639	P488	P488	Q399	L319	T159	Q88	Q88
W1106	P1017	E932	Q856	Q788	V706	L640	K489	K489	N562	N320	V160	P89	P89
W1107	V1018	V934	V857	A789	D708	N642	I563	S490	K561	Y322	T161	K90	K90
L1108	F1019	K935	S860	A643	I718	A643	E564	Y492	T411	L323	T249	Q91	Q91
E1109	V1020	R936	A644	V645	S719	V645	E565	I493	V413	T328	K251	L92	L92
H1110	F1022	E937	V862	T796	L720	H647	K566	D494	D414	V329	K252	P93	P93
H1111	H1023	Y938	C866	Q797	G721	H647	Q570	K495	G416	I330	R253	Q96	Q96
Q1112	Y1024	Y939	T867	Y798	R722	Y798	L571	I496	V417	D172	N257	N97	N97
L1113	L1025	S940	S868	I799	R723	R723	S576	T497	A418	K258	E262	P98	P98
D1114	G1028	Y942	E869	I802	F728	F653	L575	H498	S419	E175	V259	V99	V99
H1115	R1029	T943	S870	G803	I729	T652	S576	Y499	F420	T333	V260	S100	S100
F1118	H1030	I944	VAL	I804	T729	L654	P577	H499	L422	F336	T261	Y101	Y101
E1120	W1031	I949	I1E	N806	C731	N656	A579	L504	M423	I342	A263	Y103	Y103
N1121	F1034	T952	ASP	T807	C732	A657	Y582	K508	S426	Y347	D264	L104	L104
N1122	L1039	I953	HIS	G808	V733	N658	S583	I509	G427	Y350	Y265	V106	V106
Q1123	I1040	S954	GLN	I809	S736	A659	P584	T514	V428	P351	I267	Y107	Y107
Y1124	E1041	R955	THR	C810	Q737	D660	G585	R515	L431	N355	G270	F111	F111
Q1125	E1041	K956	LVS	T814	Q738	S662	Q586	E516	L431	L356	I271	K119	K119
P1126	L1049	R957	SER	T814	R739	Q663	Q586	K517	K436	V357	R272	P191	P191
I1127	L1049	R958	SER	A817	R742	E667	Y588	K517	P443	A358	E273	S192	S192
K1128	M1053	P959	K882	K818	S743	P668	S589	D820	M446	T359	D274	R195	R195
L1129	I1056	Y961	Q886	V819	HIS	C669	M592	A521	M446	P360	D277	P194	P194
T1132	M1057	V961	Q887	F820	LVS	F820	T594	S522	Y523	L361	K280	I119	I119
L1133	S1058	V968	V888	K821	ASP	A593	Q524	Q524	Y523	L361	E281	T120	T120
P1134	Y1059	P969	H894	V823	ASP	ASP	I526	I526	G451	F362	K282	Y121	Y121
Y1135	D1063	R970	H894	F824	GLN	ARG	D597	D597	R452	L363	K283	D122	D122
M1140	Y1064	T971	T899	L825	L749	ARG	S598	S598	R453	G366	E207	F127	F127
L1144	S1065	R975	V900	E825	G750	ARG	S598	S598	A454	Q284	D208	I128	I128
T1145	Y1066	Y976	L901	M827	R751	THR	V599	V599	R455	A286	S209	H129	H129
A1146	S1067	Y977	P902	N828	H753	Q680	D606	T531	I455	P368	E287	T130	T130
F1147	V1068	L977	L903	I829	W754	K681	S607	P532	A456	Y369	Q288	D131	D131
T1148	W1069	K980	E904	Y831	K755	R682	A608	N533	S458	I371	D289	Y135	Y135
W1149	K1070	V980	I905	V834	T756	L683	V609	M534	S459	K372	T290	T214	T214
G1151	S1075	L983	G906	R835	L757	E684	G611	P536	Y464	Q374	K291	A215	A215
I1152	T1076	V984	H908	G836	P759	E685	V612	P536	Y464	Q374	Y216	P137	P137
F1156	W1077	L987	I910	E837	V760	L686	Q613	S538	Y466	L293	Y219	D138	D138
D1157	L1078	L988	N911	Q838	T765	A688	G615	R539	I467	K297	K220	S140	S140
I1158	R1084	V991	F912	I839	A616	L689	A616	L541	V383	Q298	E221	V141	V141
G1159	Y1085	V991	S913	Q840	V690	K617	K617	V542	W469	V299	Y222	K142	K142
P1160	L1086	V991	L914	K942	K618	G991	Y543	Y543	G384	G384	V223	V223	V223
L1161	G1087	G996	E915	G843	H692	H692	P619	Y544	H473	V307	L224	Y146	Y146
V1162	Q1088	L1000	T916	T844	S693	S693	L650	I545	L477	K308	E309	S147	S147
K1163	W1089	T1001	W917	Y846	V694	V694	E621	V546	V478	P387	L310	N149	N149
I1164	N1090		I922	N947	W775	W775	F624	G548	G479	P388		D150	D150





NAG1  
NAG2

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

NAG1  
NAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.26 Å   144.26 Å   241.00 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	29.29 – 3.10 29.29 – 3.11	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.29-3.10) 97.4 (29.29-3.11)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 3.11 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.236 , 0.281 0.230 , 0.275	Depositor DCC
$R_{free}$ test set	5010 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.3	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 91.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.468 for h,-h-k,-l 0.009 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CD

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	0.26	0/13137	0.47	1/17820 (0.0%)
1	B	0.26	0/11954	0.47	1/16219 (0.0%)
All	All	0.26	0/25091	0.47	2/34039 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1488	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	1488	LEU	CA-CB-CG	5.05	126.91	115.30

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	12861	0	12817	794	0
1	B	11701	0	11669	700	0
2	C	28	0	25	2	0
2	D	28	0	25	2	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	0	0
All	All	24655	0	24562	1484	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 30.

The worst 5 of 1484 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:1538:GLU:HG2	1:A:1539:LEU:HG	1.31	1.12
1:A:253:ARG:HH22	1:A:257:ASN:HA	1.13	1.11
1:B:253:ARG:HH22	1:B:257:ASN:HA	1.12	1.10
1:A:1279:ARG:HG3	1:A:1284:PHE:HB2	1.30	1.08
1:B:1279:ARG:HG3	1:B:1284:PHE:HB2	1.31	1.06

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	1615/1676 (96%)	1282 (79%)	257 (16%)	76 (5%)	2	14
1	B	1471/1676 (88%)	1191 (81%)	214 (14%)	66 (4%)	2	15
All	All	3086/3352 (92%)	2473 (80%)	471 (15%)	142 (5%)	2	15

5 of 142 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	PRO
1	A	261	THR
1	A	308	LYS

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Mol	Chain	Res	Type
1	A	336	PHE
1	A	490	SER

### 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	1441/1484 (97%)	1294 (90%)	147 (10%)	7	27
1	B	1314/1484 (88%)	1183 (90%)	131 (10%)	7	28
All	All	2755/2968 (93%)	2477 (90%)	278 (10%)	7	28

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1500	ARG
1	B	116	ARG
1	B	1338	VAL
1	A	1548	ARG
1	A	1626	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1459	HIS
1	B	80	GLN
1	B	1234	HIS
1	A	1463	GLN
1	A	1626	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$
2	NAG	C	1	1,2	14,14,15	0.51	0	17,19,21	0.77	0
2	NAG	C	2	2	14,14,15	0.48	0	17,19,21	0.85	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.51	0	17,19,21	0.77	0
2	NAG	D	2	2	14,14,15	0.49	0	17,19,21	0.87	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	2.23	115.22	112.19
2	D	2	NAG	C1-O5-C5	2.16	115.12	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

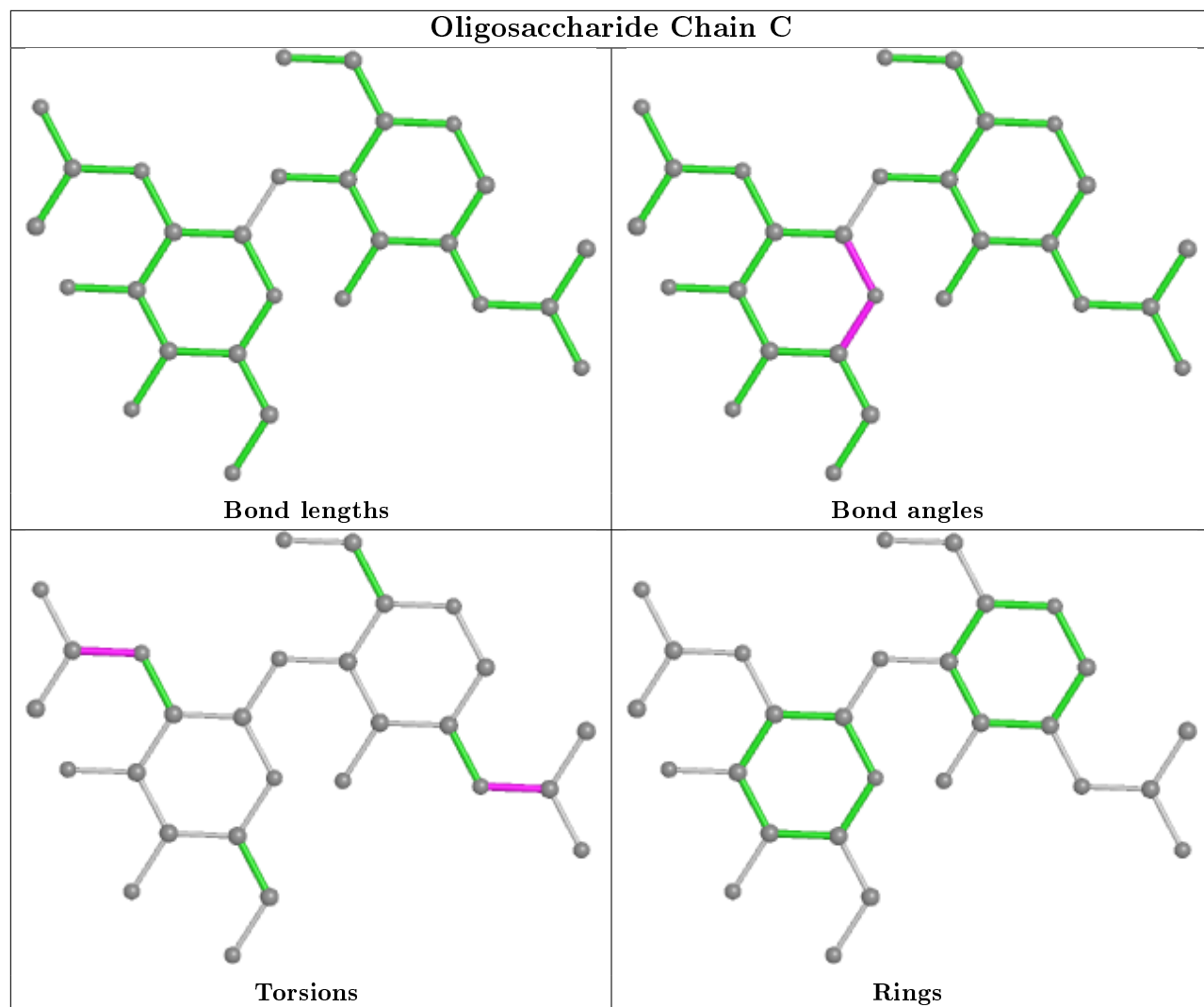
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2

There are no ring outliers.

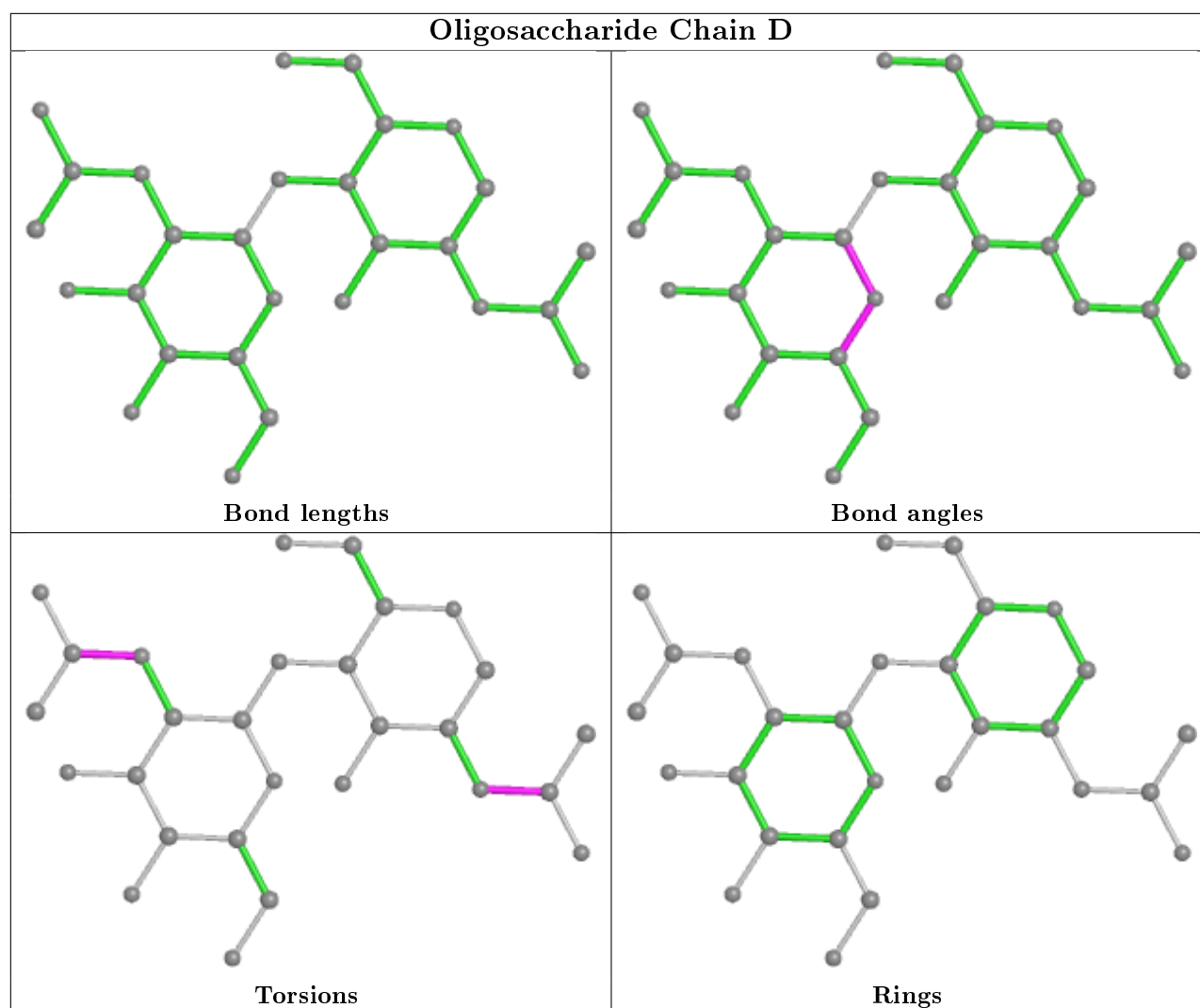
2 monomers are involved in 4 short contacts:

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

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	$\# Z  > 2$
3	NAG	A	2003	1	14,14,15	0.58	0	17,19,21	0.98	1 (5%)
3	NAG	B	2003	1	14,14,15	0.61	0	17,19,21	1.14	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
3	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2003	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2003	NAG	O5-C1-C2	2.68	115.52	111.29
3	B	2003	NAG	O5-C5-C6	2.08	110.47	107.20
3	A	2003	NAG	O5-C1-C2	2.06	114.54	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2003	NAG	C8-C7-N2-C2
3	A	2003	NAG	O7-C7-N2-C2
3	B	2003	NAG	C8-C7-N2-C2
3	B	2003	NAG	O7-C7-N2-C2

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, 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	1625/1676 (96%)	0.17	50 (3%) 49 26	73, 136, 224, 290	0
1	B	1481/1676 (88%)	0.10	25 (1%) 70 49	75, 131, 205, 267	0
All	All	3106/3352 (92%)	0.14	75 (2%) 59 37	73, 133, 215, 290	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	871	PRO	10.0
1	B	871	PRO	6.1
1	A	1534	GLN	4.9
1	A	1635	TYR	4.1
1	B	1518	LYS	4.1

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

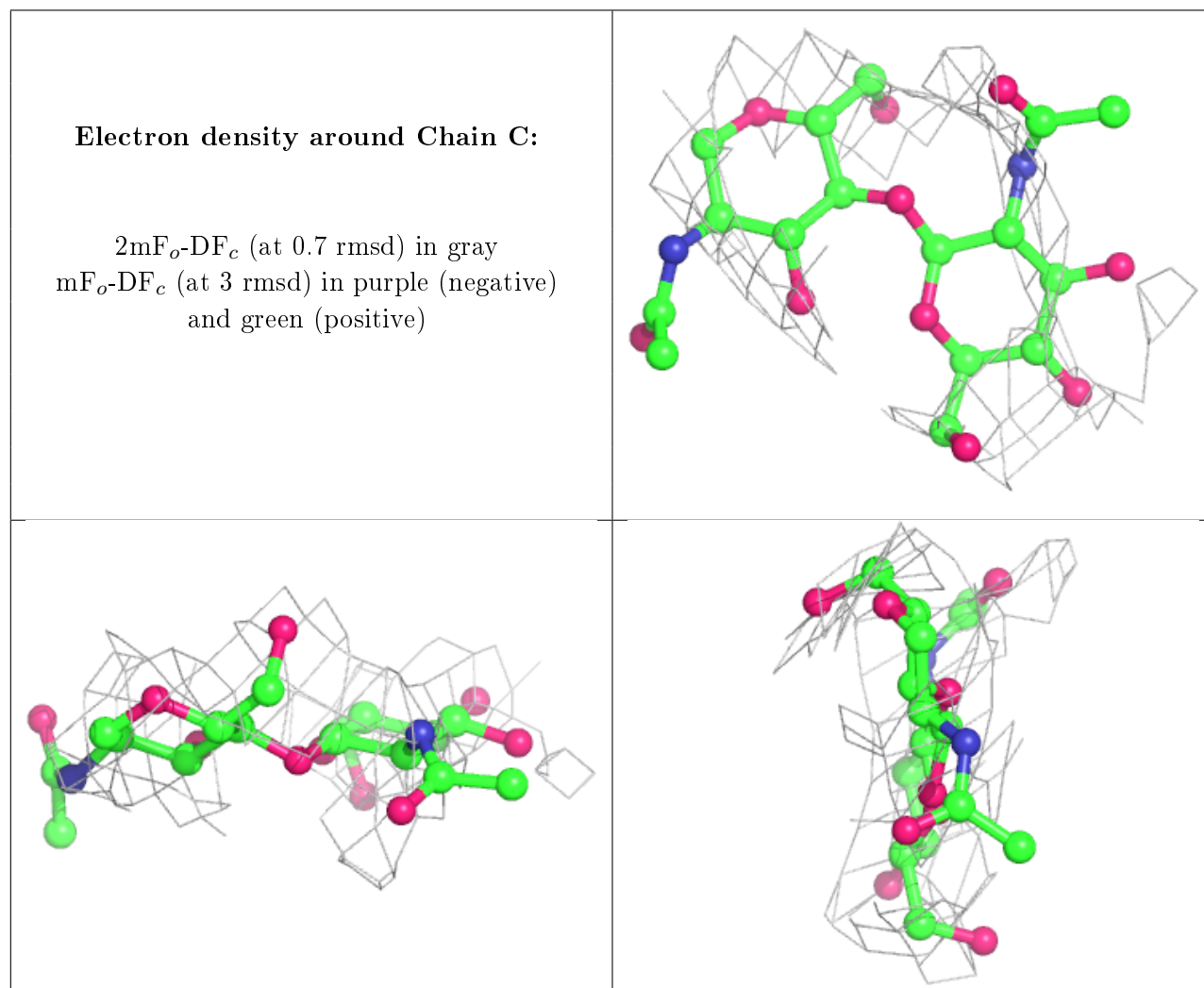
There are no non-standard protein/DNA/RNA residues in this entry.

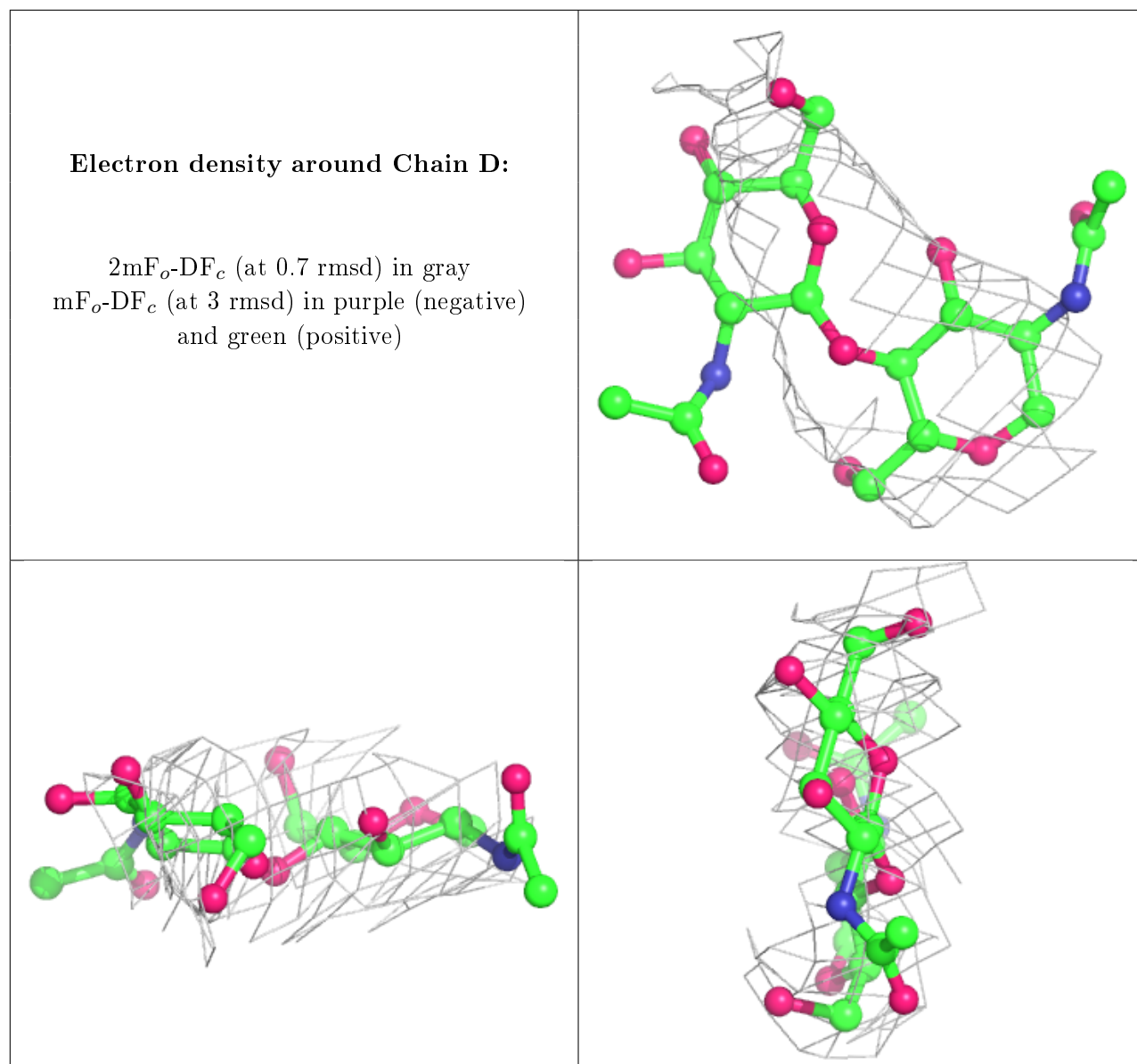
### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
2	NAG	D	2	14/15	0.58	0.51	251,259,262,262	0
2	NAG	C	2	14/15	0.79	0.24	249,258,261,262	0
2	NAG	C	1	14/15	0.81	0.32	257,259,270,271	0
2	NAG	D	1	14/15	0.89	0.38	263,269,274,275	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(Å <sup>2</sup> )	Q<0.9
4	CD	A	2006	1/1	0.68	0.18	189,189,189,189	0
4	CD	A	2008	1/1	0.72	0.11	282,282,282,282	0
4	CD	B	2005	1/1	0.75	0.20	181,181,181,181	0
4	CD	B	2006	1/1	0.76	0.20	183,183,183,183	0
4	CD	B	2007	1/1	0.78	0.13	264,264,264,264	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	2003	14/15	0.81	0.56	246,252,259,262	0
3	NAG	A	2003	14/15	0.85	0.25	215,223,233,237	0
4	CD	A	2007	1/1	0.94	0.21	184,184,184,184	0
4	CD	A	2004	1/1	0.95	0.35	123,123,123,123	1
4	CD	A	2005	1/1	0.97	0.16	243,243,243,243	0
4	CD	B	2004	1/1	0.99	0.18	239,239,239,239	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.