



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 01:36 PM BST

PDB ID : 4BXS
Title : Crystal Structure of the Prothrombinase Complex from the Venom of Pseudonaja Textilis
Authors : Lechtenberg, B.C.; Murray-Rust, T.A.; Johnson, D.J.D.; Adams, T.E.; Krishnaswamy, S.; Camire, R.M.; Huntington, J.A.
Deposited on : 2013-07-15
Resolution : 3.32 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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

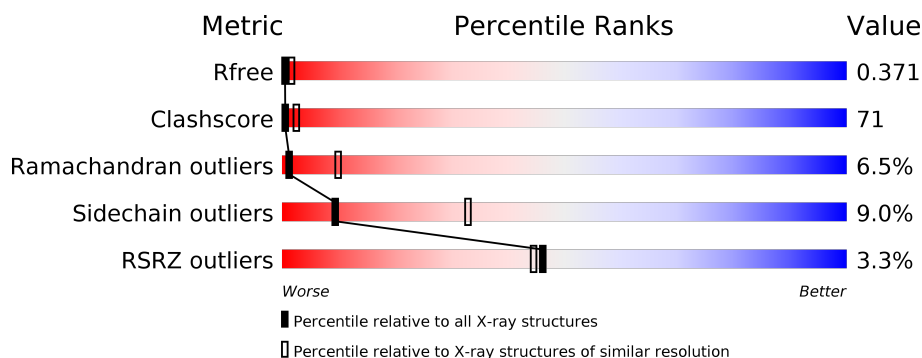
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	423	<div> <div>5%</div> <div> <div>36%</div> <div>20%</div> <div>•</div> <div>41%</div> </div> </div>
2	V	1430	<div> <div>2%</div> <div> <div>28%</div> <div>50%</div> <div>9%</div> <div>•</div> <div>12%</div> </div> </div>
3	B	2	<div> <div>50%</div> <div>50%</div> </div>
4	C	8	<div> <div>25%</div> <div>25%</div> <div>50%</div> </div>
5	D	2	<div> <div>100%</div> </div>
5	E	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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	E	1	X	-	-	-
6	NAG	V	1521	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11295 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 FACTOR X-LIKE PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1587	981	290	298	18			

- Molecule 2 is a protein called VENOM PROTHROMBIN ACTIVATOR PSEUTARIN-C NON-CATALYTIC SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	1262	Total	C	N	O	S	64	0	0
			9408	6020	1587	1766	35			

There are 3 discrepancies between the modelled and reference sequences:

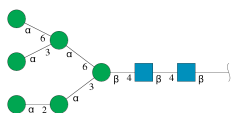
Chain	Residue	Modelled	Actual	Comment	Reference
V	50	LYS	GLU	conflict	UNP Q7SZN0
V	1287	LYS	SER	conflict	UNP Q7SZN0
V	1305	PHE	SER	conflict	UNP Q7SZN0

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



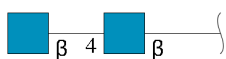
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



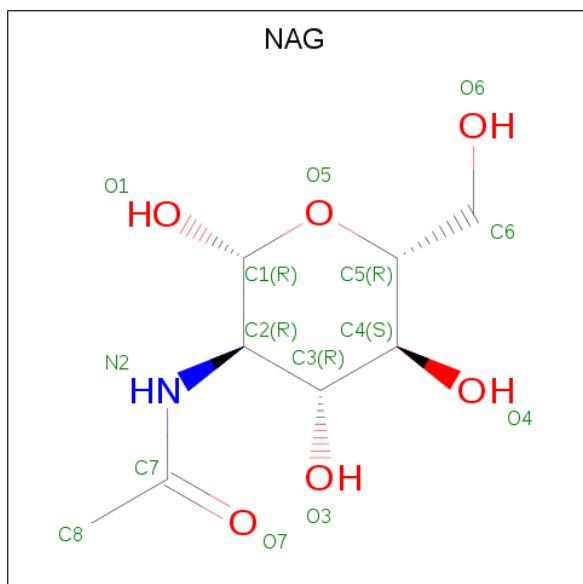
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	D	2	Total	C	N	O	0	0	0
			25	14	2	9			
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	V	2	Total 2	Ca 2	0	0

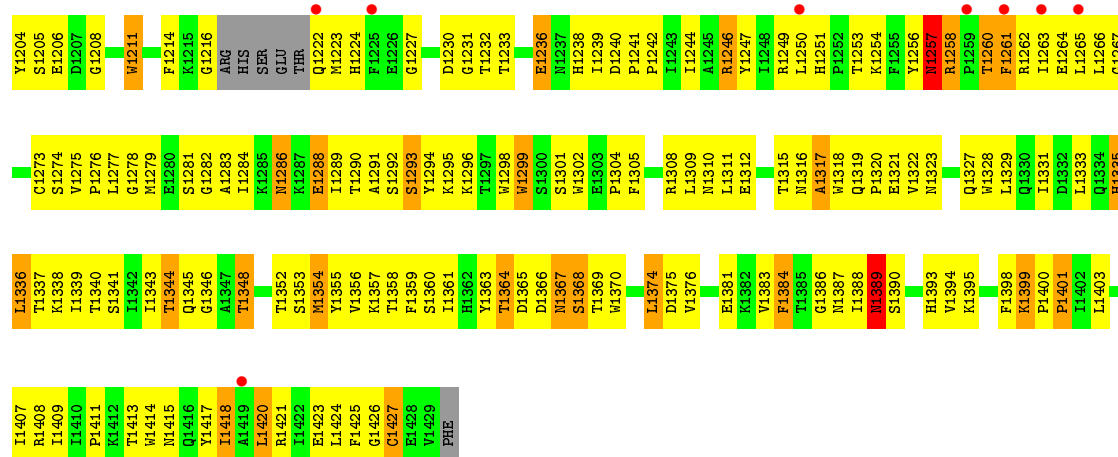
- Molecule 8 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	V	1	Total 1	Cu 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	7	Total 7	O 7	0	0
9	V	105	Total 105	O 105	0	0

V1139	Q1068	ILE	Y942	A875	D808	SER	LYS	V546	S480	T406	F341	V273	F210
G140	L1069	GLY	S943	S876	T809	VAL	LYS	F547	A481	V407	S342	S274	A211
Y1141	G1070	VAL	G944	R877	S810	ALA	GLU	K548	D482	F408	S343	R275	N212
Y1142	G1071	GLN	Y945	P878	P811	GLU	GLU	D549	D483	T409	V344	T276	G213
E1143	L1072	L1011	N946	Y879	ILE	GLU	VAL	D550	R484	N410	D345	W279	T214
A1147	P1073	L1012	P947	S880	LYS	GLU	PRO	P851	T485	L411	R346	L280	L215
R1148	L1074	H1013	E948	L881	LYS	LEU	VAL	K552	R486	A412	R347		F216
L1149	L1075	T1014	R949	H882	SER	LYS	ASN	F553	D487	S413			D217
L1149	P1076	P1015	D950	A883	GLN	HIS	PHE	Y554	I488	R414	Y348	S283	Q219
N1150	G1077	VAL	R951	H884	VAL	THR	PRO	K555		P415	K349	L284	V285
N1151	T1078	ARG	R952	G885	ARG	ALA	VAL	S556	G491	Y416	A350	A266	A266
T1152	A1079	SER	R953	L886	SER	LEU	ASP	N557	L492	S417	Q351	K287	C221
G1153	F1079	ARG	G954	L887	ARG	LEU	PRO	V558	L493	T418	Y352	H288	A222
K1154	S1081	ALA	L955	Y888	ALA	LEU	GLU	L831	G494	Y419	L553	L289	Y223
Y1155	I1082	ALA	Y956		ALA	GLU	SER	G832	P495		D354	L289	Q290
N1156	K1083	P1022	G957	S891	R823	GLU	ASP	T633	L496	G422	N355	L290	D294
A1157	P1084	Q1023	P958	S892	T824	ASP	ALA	W634	L497	V423	F356	A291	H235
W1158	Q1024	GLY	R959	E893	7825	ALA	LEU	L635	Y498	S424	F357		I226
S1159	L1025	ALA	G994	G894	7826	HIS	ALA	L636	C499	V425	N358	Y294	S227
T1160	L1026	LYS	R995	R895	R827	ALA	LYS	S837	K500	S426	F359	G295	G295
	G1027	SER	R964	S896	R828	SER	GLU	S838	H501	K427	I360	Y296	H229
	L1028	ASP	G965	Y897	A829	ASP	LEU	W639	K502		G361		H229
	T1029	PRO	R966	D998	T830	PRO	GLY	G640	A503	E430	K362	I299	L230
	Q1030	ARG	R967	D898	7831	ARG	ILE	S641	L504	G431	K363	K300	G232
	L1031	ILE	D968	G894	R832	ILE	LEU	C642	S505	A432	K364	D301	W233
	K1032	ASP	R969	P902	S833	ASP	ASP	E843	VAL	I433	K365	C302	S234
	D1033	SER	Y970	F905	7834	SER	GLY	M644	LYS	Y434	K366	G303	S235
	E1034	ASN	R971	K906	L835	ASN	GLU	S645	G508	P438	F369	D306	S236
	N1035	GLY	R972	D908	D836	GLY	ASN	G647	V509	L438	R370	THR	P237
	V1036	ALA		K907	D837	ALA	PRO	M648	D510	GLU	K371	LEU	E238
	H1037	ASN	R977	D909	7838	ASN	ILE	R649	N511	ASN	R372	THR	I239
	H1038	PRO	E978	A910	7839	PRO	ILE	L850	K512	ILE		THR	F240
	H1039	GLN	F979	D910	Q840	PRO	GLN	R651	D514	T443	G375	ARG	S241
	R1040	ASP	Y980	N912	T841	ASP	PRD	F652	V515	H444	N376	LEU	V242
	L1041	ILE	N981	N912	P842	ILE	ILE	L851	E516	G445	PHE	LEU	H243
	M1042	ALA	R982	P913		ALA	ARG	D654	D591	K446	ARG	ARG	I244
	M1043	GLY	R983	N914	7848	GLY	GLU	A855	D592	A447		ARG	N245
	G1044	ARG	N984	G915	E849	ARG	GLN	M856	A519	V448	T381	GLU	G246
	P1045	ARG	Y985	T915	K850	ARG	GLN	Y857	F521	E449	Y382	LEU	Q247
	P1046	TYR	F986	Y917	H851	TYR	THR	D658	A522	P450		LEU	T248
	L1047	LEU	D987	T918	L852	LEU	GLU	P896	F521	Q451		M318	L249
	D1048	ARG	E988	Y919	G853	ARG	ASP	D659	A522	Q452		K319	E250
	I1049	THR	R989	V920	L854	THR	ASP		V523	V453		I320	Q251
	H1050	ILE	K990	N921	L855	ILE	GLU	E868	H598			K321	N252
	V1051	ASN	Q922	Q922		ASN	GLU	E869	D525	Y454		N322	H263
	V1052	ARG	V923	V923	T858	ARG	GLN	D870	D526			K321	H263
	N1053	GLY	P924	P924	T859	GLY	LEU	E526	E526			W323	Y254
	F1054	MET	P925	P925	R860	MET	LYS	D673	N527	T459		E324	K255
	H1055	ALA	R926	R926	A861	ALA	LYS	I674	K528	V460		Y325	V256
	G1056	LYS	S927	S927	E862	LYS	ALA	F675	S529	L461		F326	S257
	Q1057	SER			V863	SER	SER		T604			I327	T258
	T1058	ASP	T930	T930	D864	ASP	MET	I678	L605	E465		A328	I259
	L1059	LYS	D931	D931	D865	LYS	LEU	F679	S606	P466		A329	L260
		SER			V866		GLY	I680	G608	T467		E330	L261
		THR			V867		LEU	P681	H610	I474		E331	V262
	E1062	THR	E934	E934	I667	THR	LEU	P681	H610	I474		W334	V267
	G1063	C1002	K935	K935		ALA	ARG	S682	C540	I475		D355	
	A1064	GLU	W939	W939	F871	SER	SER	E883	S541	I476		D355	D270
	E1065	LYS			R872	PHE	LYS	VAL	N542	L477		Y336	L261
	N1067	LEU	Y941	Y941	L874		GLY	LVS	P543	H479		A337	M271
												P338	S272




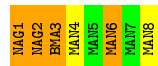
- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  50%



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  25%



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

Chain D:  100%



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

Chain E:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	115.31Å 115.31Å 429.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.81 – 3.32 89.81 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.1 (89.81-3.32) 99.1 (89.81-3.32)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.298 , 0.368 0.289 , 0.371	Depositor DCC
R_{free} test set	2241 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	86.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 116.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	11295	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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: BMA, NAG, CA, FUC, CU, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/1617	0.39	0/2210
2	V	0.23	0/9671	0.43	4/13230 (0.0%)
All	All	0.22	0/11288	0.43	4/15440 (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
2	V	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	670	ASP	O-C-N	-12.35	102.94	122.70
2	V	657	TYR	O-C-N	-6.42	112.42	122.70
2	V	670	ASP	C-N-CA	6.42	137.75	121.70
2	V	657	TYR	C-N-CA	5.43	135.28	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	V	657	TYR	Peptide
2	V	658	ASP	Peptide
2	V	668	GLU	Peptide
2	V	669	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	V	670	ASP	Mainchain

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	1587	0	1171	118	0
2	V	9408	0	8230	1343	0
3	B	24	0	22	4	0
4	C	94	0	79	11	0
5	D	25	0	21	0	0
5	E	28	0	25	3	0
6	V	14	0	13	3	0
7	V	2	0	0	0	0
8	V	1	0	0	0	0
9	A	7	0	0	0	0
9	V	105	0	0	19	0
All	All	11295	0	9561	1458	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 71.

The worst 5 of 1458 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:337:ALA:HB3	2:V:362:LYS:CD	1.25	1.60
2:V:1205:SER:CB	2:V:1211:TRP:HB3	1.32	1.55
2:V:337:ALA:CB	2:V:362:LYS:HD3	1.11	1.55
2:V:1094:LEU:HD23	2:V:1110:PHE:CD1	1.36	1.53
2:V:1309:LEU:HD12	2:V:1423:GLU:CB	1.33	1.52

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	232/423 (55%)	195 (84%)	27 (12%)	10 (4%)	2	18
2	V	1243/1430 (87%)	961 (77%)	196 (16%)	86 (7%)	1	9
All	All	1475/1853 (80%)	1156 (78%)	223 (15%)	96 (6%)	1	10

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ILE
1	A	305	SER
1	A	410	ARG
2	V	52	ARG
2	V	66	GLU

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	111/368 (30%)	106 (96%)	5 (4%)	27	60
2	V	878/1260 (70%)	794 (90%)	84 (10%)	8	30
All	All	989/1628 (61%)	900 (91%)	89 (9%)	9	33

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	877	ARG

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Mol	Chain	Res	Type
2	V	1030	MET
2	V	1364	THR
2	V	926	ARG
2	V	984	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	V	602	HIS
2	V	1037	HIS
2	V	1319	GLN
2	V	922	GLN
2	V	1055	HIS

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 ⓘ

14 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	B	1	3,2	14,14,15	0.81	0	17,19,21	1.40	4 (23%)
3	FUC	B	2	3	10,10,11	0.71	0	14,14,16	0.66	0
4	NAG	C	1	2,4	14,14,15	0.51	0	17,19,21	0.87	1 (5%)
4	NAG	C	2	4	14,14,15	0.56	0	17,19,21	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	C	3	4	11,11,12	0.31	0	15,15,17	0.78	1 (6%)
4	MAN	C	4	4	11,11,12	0.64	0	15,15,17	0.63	0
4	MAN	C	5	4	11,11,12	0.70	0	15,15,17	0.76	0
4	MAN	C	6	4	11,11,12	0.63	0	15,15,17	0.88	1 (6%)
4	MAN	C	7	4	11,11,12	0.71	0	15,15,17	0.82	0
4	MAN	C	8	4	11,11,12	0.66	0	15,15,17	0.66	0
5	NAG	D	1	2,5	14,14,15	0.58	0	17,19,21	0.82	0
5	NAG	D	2	5	11,11,15	0.65	0	12,15,21	0.68	0
5	NAG	E	1	2,5	14,14,15	0.62	0	17,19,21	0.76	0
5	NAG	E	2	5	14,14,15	0.56	0	17,19,21	0.78	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	B	1	3,2	-	5/6/23/26	0/1/1/1
3	FUC	B	2	3	-	-	0/1/1/1
4	NAG	C	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
4	MAN	C	4	4	-	2/2/19/22	0/1/1/1
4	MAN	C	5	4	-	2/2/19/22	0/1/1/1
4	MAN	C	6	4	-	0/2/19/22	0/1/1/1
4	MAN	C	7	4	-	2/2/19/22	0/1/1/1
4	MAN	C	8	4	-	0/2/19/22	0/1/1/1
5	NAG	D	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	D	2	5	-	2/2/19/26	0/1/1/1
5	NAG	E	1	2,5	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	O5-C1-C2	-3.08	106.42	111.29
3	B	1	NAG	C4-C3-C2	2.69	114.96	111.02
4	C	1	NAG	O5-C5-C6	2.44	111.03	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	O5-C5-C4	-2.27	105.30	110.83
4	C	3	BMA	C1-C2-C3	2.18	112.34	109.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	1	NAG	C1

5 of 28 torsion outliers are listed below:

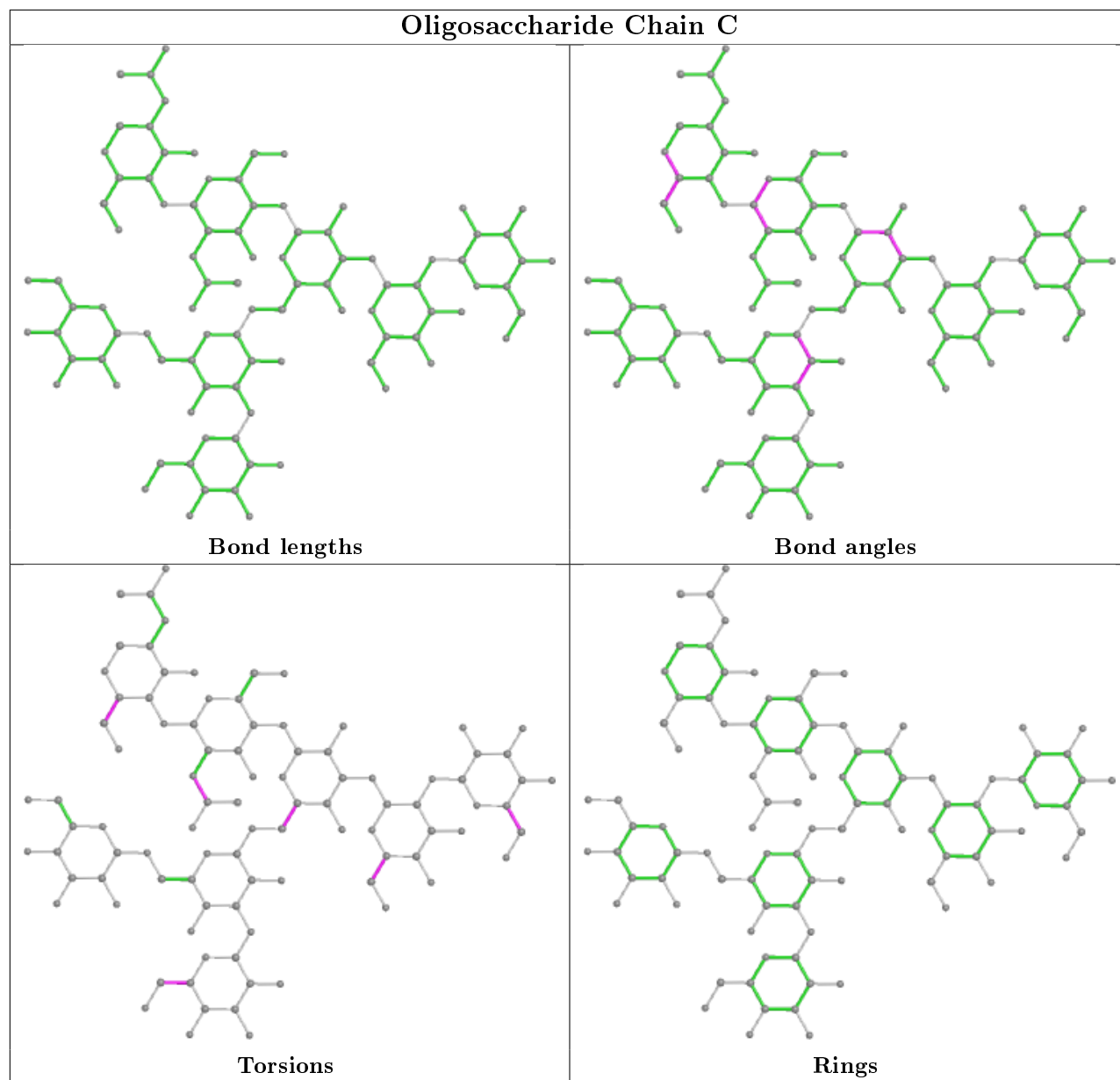
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C3-C2-N2-C7
4	C	3	BMA	C4-C5-C6-O6
4	C	5	MAN	O5-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6

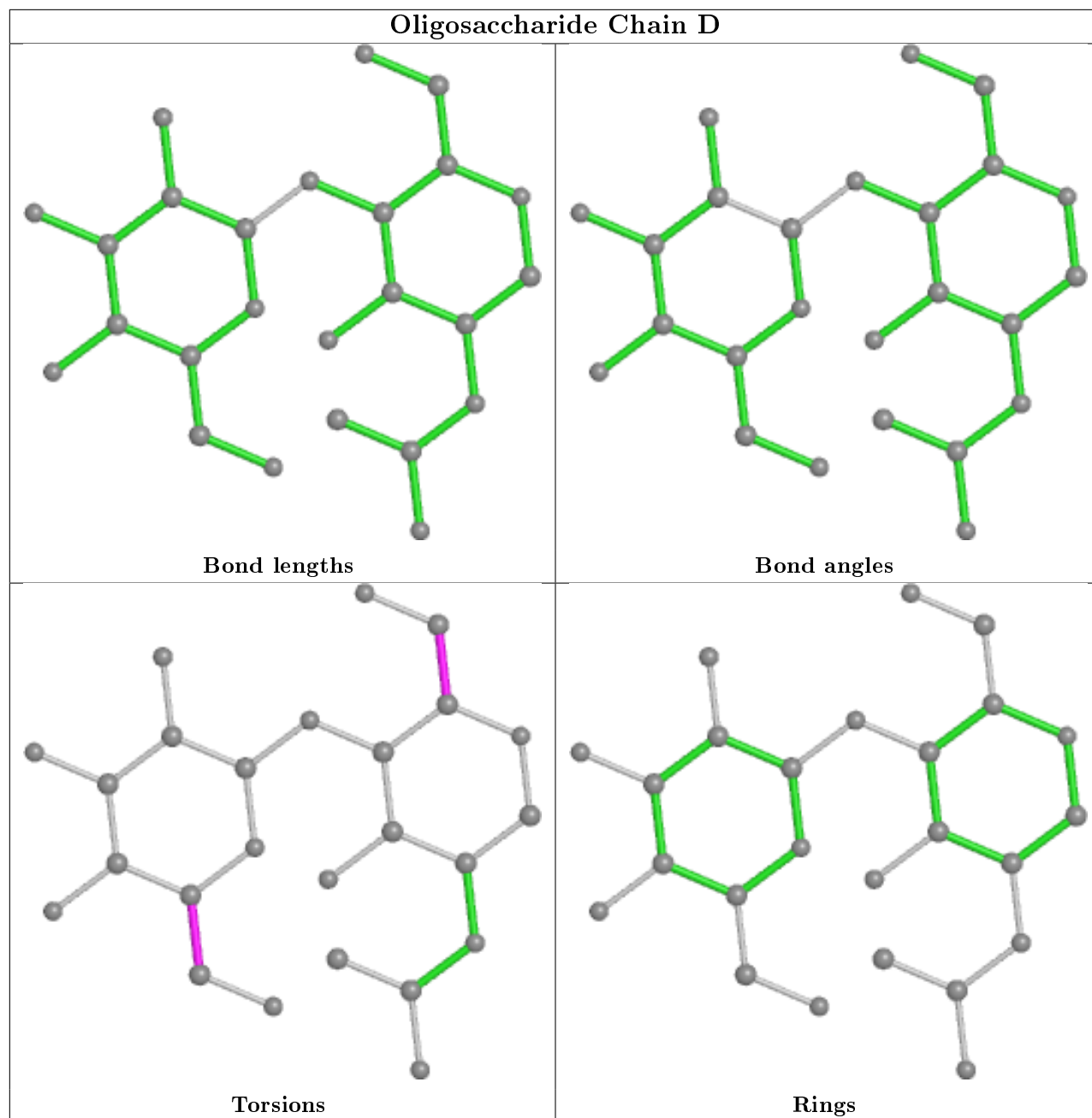
There are no ring outliers.

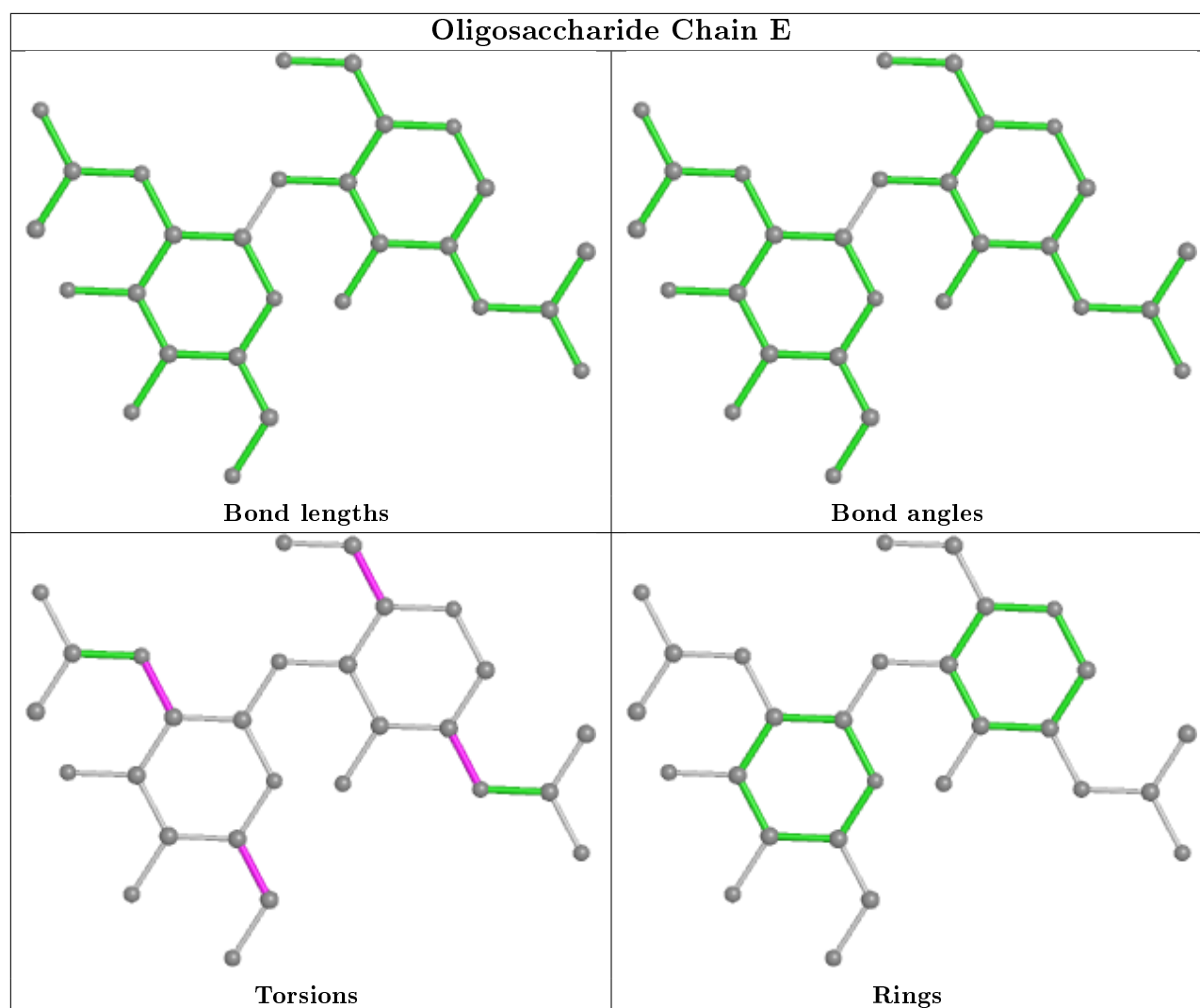
9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	4	MAN	2	0
5	E	2	NAG	2	0
4	C	2	NAG	3	0
4	C	1	NAG	5	0
5	E	1	NAG	1	0
4	C	6	MAN	1	0
4	C	3	BMA	2	0
4	C	8	MAN	1	0
3	B	1	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	V	1521	2	14,14,15	0.53	0	17,19,21	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	V	1521	2	1/1/5/7	5/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	V	1521	NAG	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	V	1521	NAG	C8-C7-N2-C2
6	V	1521	NAG	O7-C7-N2-C2
6	V	1521	NAG	O5-C5-C6-O6
6	V	1521	NAG	C1-C2-N2-C7
6	V	1521	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	V	1521	NAG	3	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, 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	248/423 (58%)	0.30	21 (8%) 10 11	82, 154, 205, 249	0
2	V	1249/1430 (87%)	0.06	29 (2%) 60 59	65, 122, 172, 255	0
All	All	1497/1853 (80%)	0.10	50 (3%) 46 44	65, 126, 185, 255	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	375	PHE	4.9
2	V	1263	ILE	4.8
2	V	1188	THR	4.4
1	A	366	HIS	3.8
2	V	1201	PHE	3.7

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

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

6.3 Carbohydrates [i](#)

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

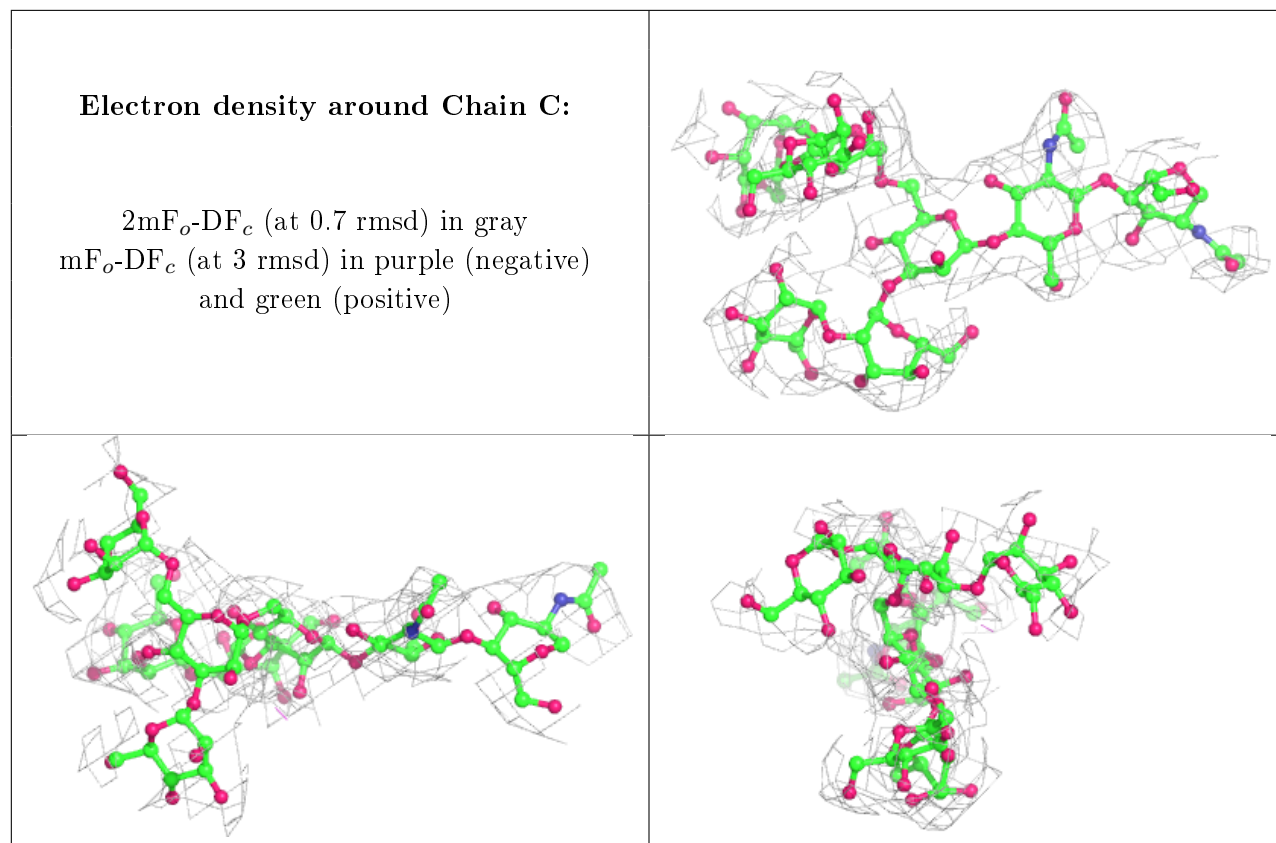
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	E	2	14/15	0.77	0.15	166,195,234,249	0
5	NAG	E	1	14/15	0.82	0.13	132,201,219,237	0
3	FUC	B	2	10/11	0.83	0.15	174,220,248,281	0
4	MAN	C	8	11/12	0.86	0.34	166,216,232,241	0
3	NAG	B	1	14/15	0.86	0.10	170,211,254,267	0

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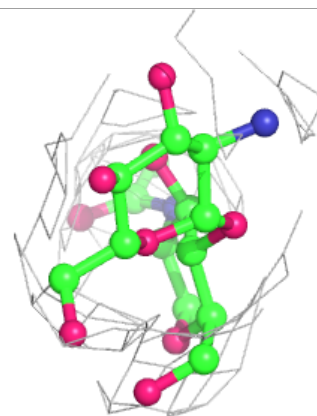
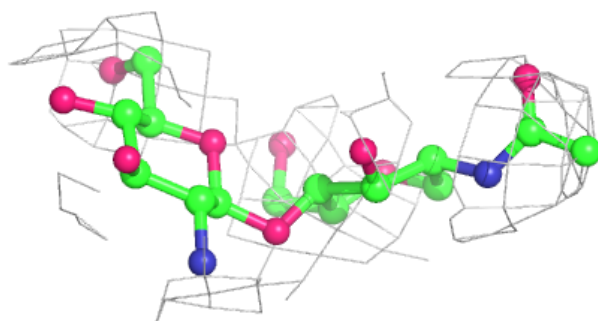
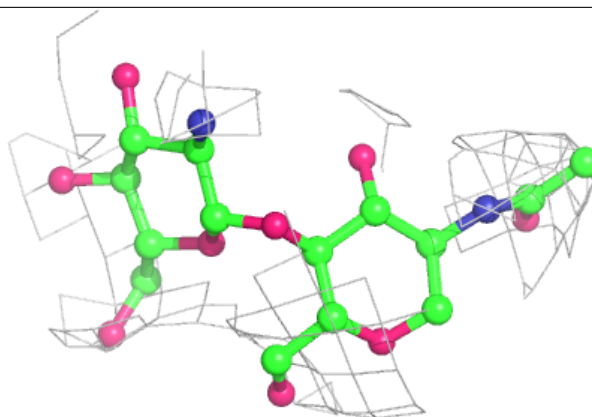
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	C	7	11/12	0.87	0.29	99,147,176,234	0
5	NAG	D	2	11/15	0.89	0.41	171,180,203,215	0
5	NAG	D	1	14/15	0.92	0.27	123,145,212,220	0
4	MAN	C	4	11/12	0.93	0.21	122,131,153,163	0
4	MAN	C	6	11/12	0.93	0.16	89,146,182,203	0
4	MAN	C	5	11/12	0.95	0.24	124,154,178,181	0
4	BMA	C	3	11/12	0.95	0.15	120,126,151,159	0
4	NAG	C	2	14/15	0.96	0.18	100,114,135,135	0
4	NAG	C	1	14/15	0.96	0.17	109,122,134,138	0

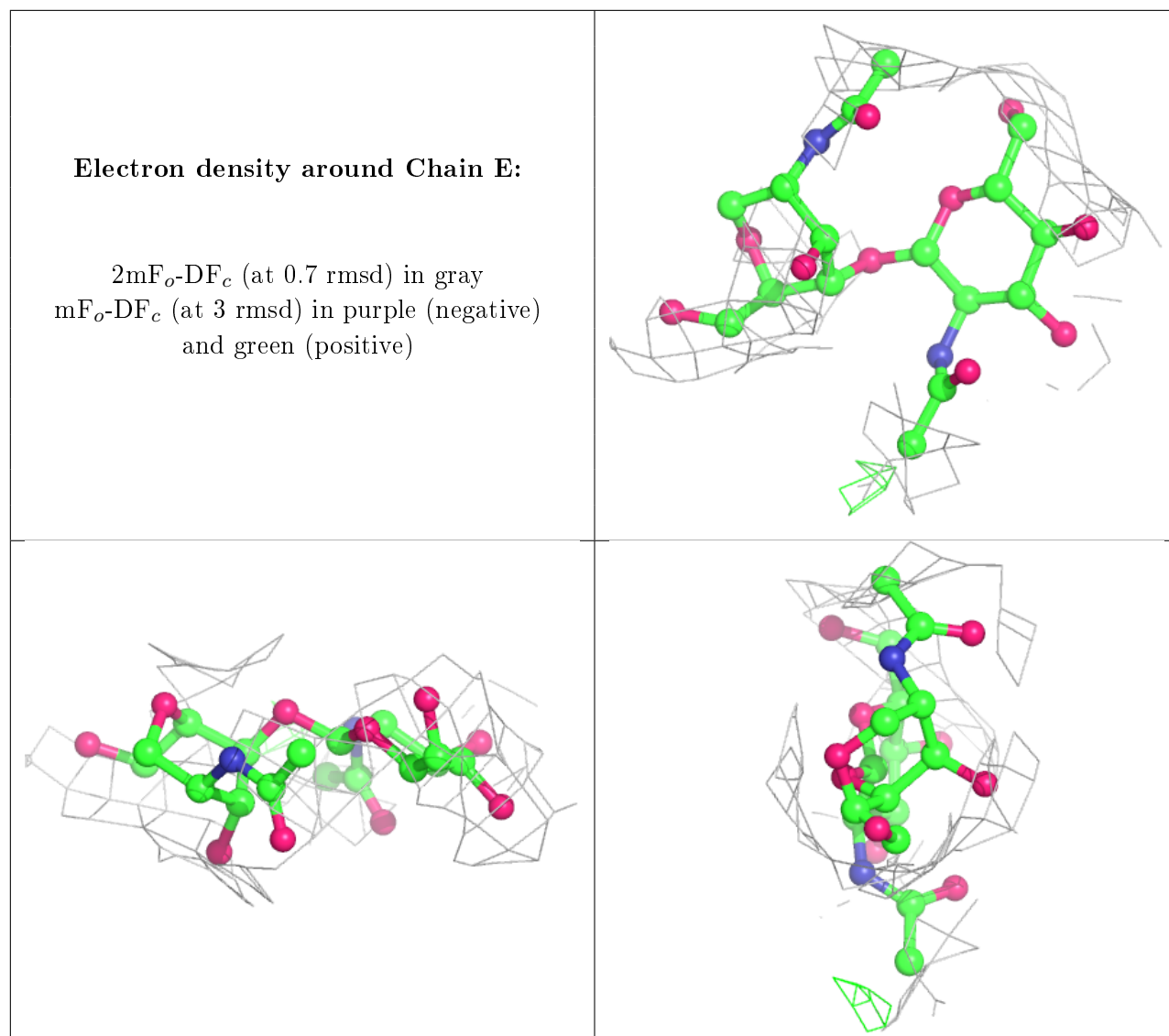
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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(Å ²)	Q<0.9
6	NAG	V	1521	14/15	0.81	0.32	152,206,263,286	0
8	CU	V	2432	1/1	0.98	0.11	124,124,124,124	0
7	CA	V	2430	1/1	0.99	0.12	88,88,88,88	0
7	CA	V	2431	1/1	0.99	0.08	105,105,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.