



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:50 PM UTC

PDB ID : 4BXS / pdb_00004bxs
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

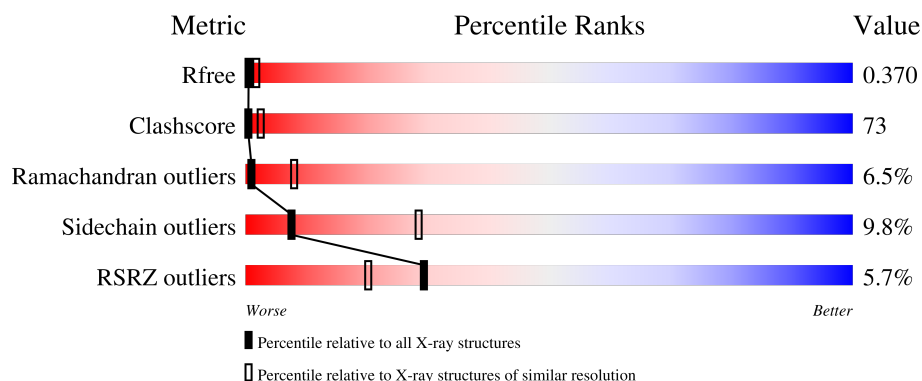
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



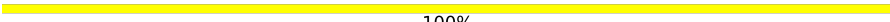
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	423	5% 35% 21% . 41%
2	V	1430	4% 27% 51% 10% . 12%
3	B	2	50% 50%
4	C	8	25% 62% 12%
5	D	2	100%

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Mol	Chain	Length	Quality of chain
5	E	2	 100%

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:

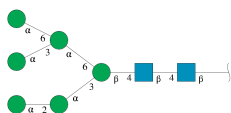
Chain	Residue	Modelled	Actual	Comment	Reference
V	50	LYS	GLU	conflict	UNP Q7SZN0
V	1287	LYS	SER	conflict	UNP Q7SZN0
V	1305	PHE	SER	conflict	UNP Q7SZN0

- 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.



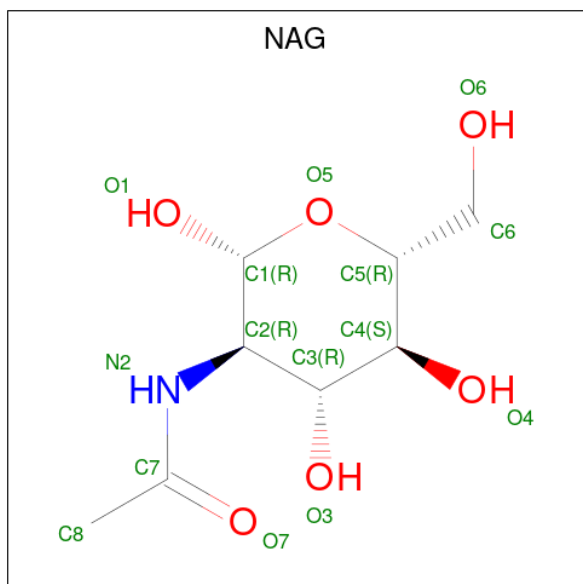
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	8	Total	C	N	O	0	0	0
			94	52	2	40			

- 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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

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

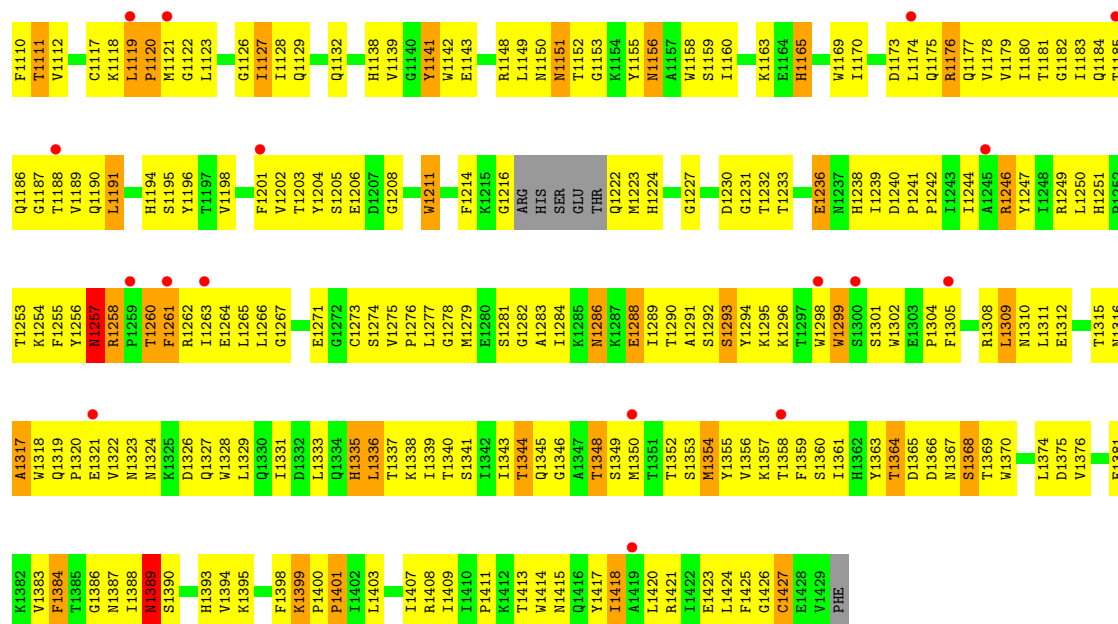
- Molecule 8 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 9 is water.

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

P1046	K1047	D1048	I1049	H1050	V1051	V1052	N1053	F1054	H1055	G1056	Q1057	L1058	F1059	E1062	G1063	R1064	E1065	D1066	N1067	Q1068	L1069	G1070	V1071	L1072	P1073	L1074	L1075	P1076	G1077	T1078	F1079	A1080	S1081	I1082	K1083	M1084	K1085	K1088	I1089	W1092	L1093	L1094	E1095	T1096	E1097	V1098	N1101	Q1102	E1103	R1104	G1105	M1106	Q1107	A1108	L1109										
F986	D987	E988	E989	K990	S991	K992	Y993	F994	P995	L995	SER	ASP	LYS	THR	C1002	GLU	GLY	GLY	LYS	LEU	ILE	GLY	VAL	GLN	S1011	L1012	E948	K949	D950	L951	L886	L887	Y888	K823	T824	R825	F826	K827	K828	A829	L830	F831	R832	S833	Y834	L835	D836	D837	T838	F839	Q840	T841	P842	G845	N911	F978	N979	N980	N981	G915	F982	F983	G1043	G1044	G1045
T854	L855	L858	L859	R860	L861	E862	R863	D864	D865	R866	L867	F871	K872	N873	L874	A875	S876	R877	F878	Y879	S880	L881	N881	H882	A883	K884	G885	L886	L887	Y888	S891	E892	G893	G894	R895	S896	D898	D899	K900	S901	P902	F905	K906	K907	D908	D909	A910	E978	F979	N980	N981	G915	F982	F983	G1043	G1044	G1045								
ASN	ARG	G793	N794	K795	R796	R797	Y798	Y799	D800	Y809	S810	F811	ILE	GLY	LYS	GLN	VAL	ARG	SER	GLY	GLY	GLY	GLN	HIS	THR	VAL	ARG	ALA	ALA	LYS	GLY	LEU	GLY	ASP	ALA	LEU	ALA	HIS	ALA	LYS	VAL	SER	ASP	ASP	GLY	GLY	ASN	ARG	PRO	ILE	ASN	PRO	ILE	ASN	GLY	GLN	THR	LEU	ARG	ASP	THR	ILE			
E669	D670	D673	L674	F675	L676	F679	L680	P681	Q611	S544	A545	V546	D482	D483	R484	R485	R486	D487	I488	A489	S490	G491	L492	I493	G494	P495	L496	T561	L562	N563	G564	K569	L573	R574	F575	H576	Q577	V580	V581	Q582	R583	H584	L585	V588	G589	T590	V591	D592	E593	I594	V595	P596	V597	H598	L599	S600									
GLU	GLN	LEU	MET	LYS	ALA	SER	MET	LEU	GLY	LEU	ARG	SER	PHE	LYS	GLY	LYS	VAL	LYS	VAL	GLU	VAL	VAL	ASN	PHE	THR	ALA	ALA	ALA	LYS	GLY	LEU	GLY	SER	ASP	ALA	LEU	ALA	HIS	ALA	LYS	VAL	SER	ASP	ASP	GLY	GLY	ASN	ARG	PRO	ILE	ASN	PRO	ILE	ASN	GLY	GLN	THR	LEU	ARG	ASP	THR	ILE			
G601	H602	T603	F604	L605	S606	K607	G608	K609	H610	S641	C540	K476	L477	I478	H479	S480	A481	V482	D483	R484	R485	R486	D487	I488	A489	S490	G491	L492	I493	G494	P495	L496	T561	L562	N563	G564	K569	L573	R574	F575	H576	Q577	V580	V581	Q582	R583	H584	L585	V588	G589	T590	V591	D592	E593	I594	V595	P596	V597	H598	L599	S600				
E331	T467	S266	W267	D270	K271	S272	W273	S274	R275	T276	V279	L280	S283	C221	L284	Y285	A286	K287	H288	I226	S227	W228	H229	L230	I231	G295	Y296	I299	K300	S301	S236	D302	E238	I239	F240	THR	LEU	THR	ARG	LYS	LEU	SER	PHE	ARG	GLY	LEU	K318	K319	Y320	K321	V325	V256	S257	T258	L259	N260	L261	V262	G263	C264					



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

Chain B: 50% 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% 62% 12%



- 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 , 0.370	Depositor DCC
R_{free} test set	2264 reflections (5.13%)	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)	0.34 , 192.1	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	0.87	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, CU, FUC, NAG, CA, BMA

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	0.28	0/1617	0.76	3/2210 (0.1%)
2	V	0.29	1/9671 (0.0%)	0.76	11/13230 (0.1%)
All	All	0.29	1/11288 (0.0%)	0.76	14/15440 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	657	TYR	C-N	5.51	1.41	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	670	ASP	O-C-N	-15.44	102.94	123.01
2	V	670	ASP	CA-C-N	11.26	137.75	120.75
2	V	670	ASP	C-N-CA	11.26	137.75	120.75
2	V	1095	GLU	N-CA-C	11.14	122.66	107.73
2	V	657	TYR	O-C-N	-8.87	112.42	122.09

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
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	123	0
2	V	9408	0	8230	1388	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	21	0
All	All	11295	0	9561	1507	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 73.

The worst 5 of 1507 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:337:ALA:CB	2:V:362:LYS:HD3	1.11	1.55
2:V:1205:SER:CB	2:V:1211:TRP:HB3	1.32	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

5.3.1 Protein backbone

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	15
2	V	1243/1430 (87%)	961 (77%)	196 (16%)	86 (7%)	1	7
All	All	1475/1853 (80%)	1156 (78%)	223 (15%)	96 (6%)	1	8

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

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%)	24	53
2	V	878/1260 (70%)	786 (90%)	92 (10%)	6	25
All	All	989/1628 (61%)	892 (90%)	97 (10%)	7	28

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	1013	HIS

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Mol	Chain	Res	Type
2	V	1120	PRO
2	V	1030	MET
2	V	1079	PHE
2	V	1176	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
2	V	1057	GLN
2	V	1184	GLN
2	V	1067	ASN
2	V	1151	ASN
2	V	1224	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	0.82	0	17,19,21	1.41	4 (23%)
3	FUC	B	2	3	10,10,11	0.71	0	14,14,16	0.63	0
4	NAG	C	1	4,2	14,14,15	0.50	0	17,19,21	0.77	0
4	NAG	C	2	4	14,14,15	0.53	0	17,19,21	0.81	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	0.30	0	15,15,17	0.67	0
4	MAN	C	4	4	11,11,12	0.62	0	15,15,17	0.53	0
4	MAN	C	5	4	11,11,12	0.68	0	15,15,17	0.65	0
4	MAN	C	6	4	11,11,12	0.61	0	15,15,17	0.72	0
4	MAN	C	7	4	11,11,12	0.69	0	15,15,17	0.68	0
4	MAN	C	8	4	11,11,12	0.64	0	15,15,17	0.55	0
5	NAG	D	1	5,2	14,14,15	0.56	0	17,19,21	0.80	0
5	NAG	D	2	5	11,11,15	0.62	0	13,15,21	0.62	0
5	NAG	E	1	5,2	14,14,15	0.61	0	17,19,21	0.71	0
5	NAG	E	2	5	14,14,15	0.54	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	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	4,2	-	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	5,2	-	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	5,2	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	O5-C1-C2	-3.15	106.42	111.29
3	B	1	NAG	C4-C3-C2	2.69	114.96	111.02
3	B	1	NAG	O5-C5-C4	-2.27	105.30	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	C2-N2-C7	2.17	125.80	122.90
4	C	2	NAG	O5-C1-C2	-2.17	107.94	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	1	NAG	C1

5 of 27 torsion outliers are listed below:

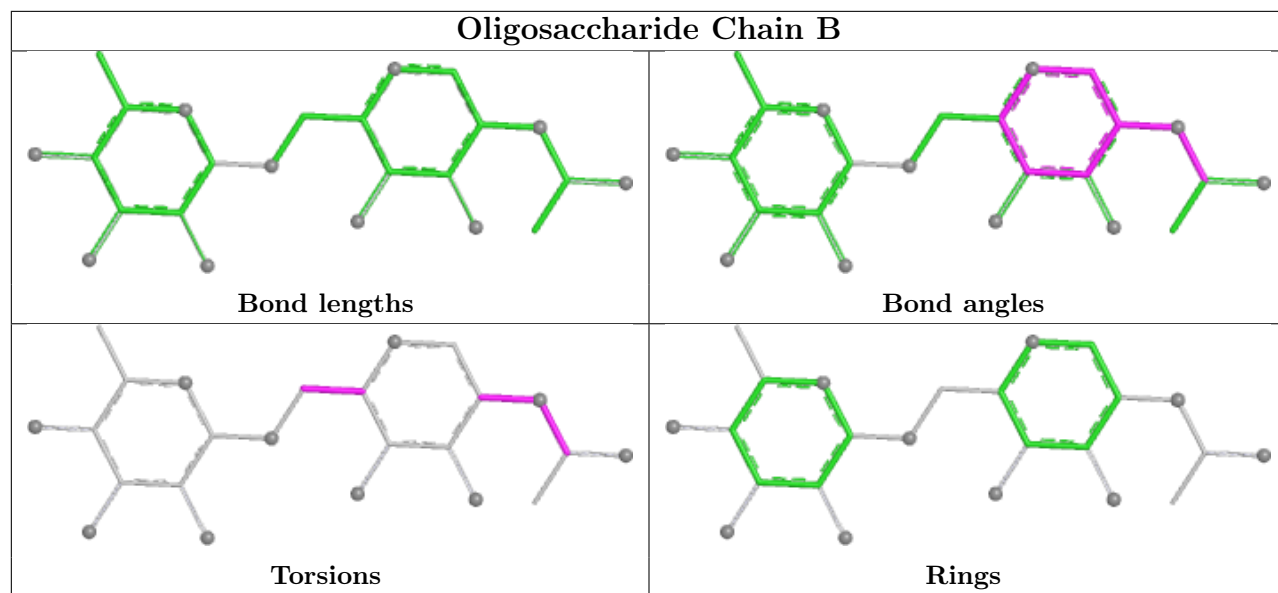
Mol	Chain	Res	Type	Atoms
3	B	1	NAG	C1-C2-N2-C7
5	E	2	NAG	C3-C2-N2-C7
4	C	3	BMA	C4-C5-C6-O6
4	C	5	MAN	O5-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6

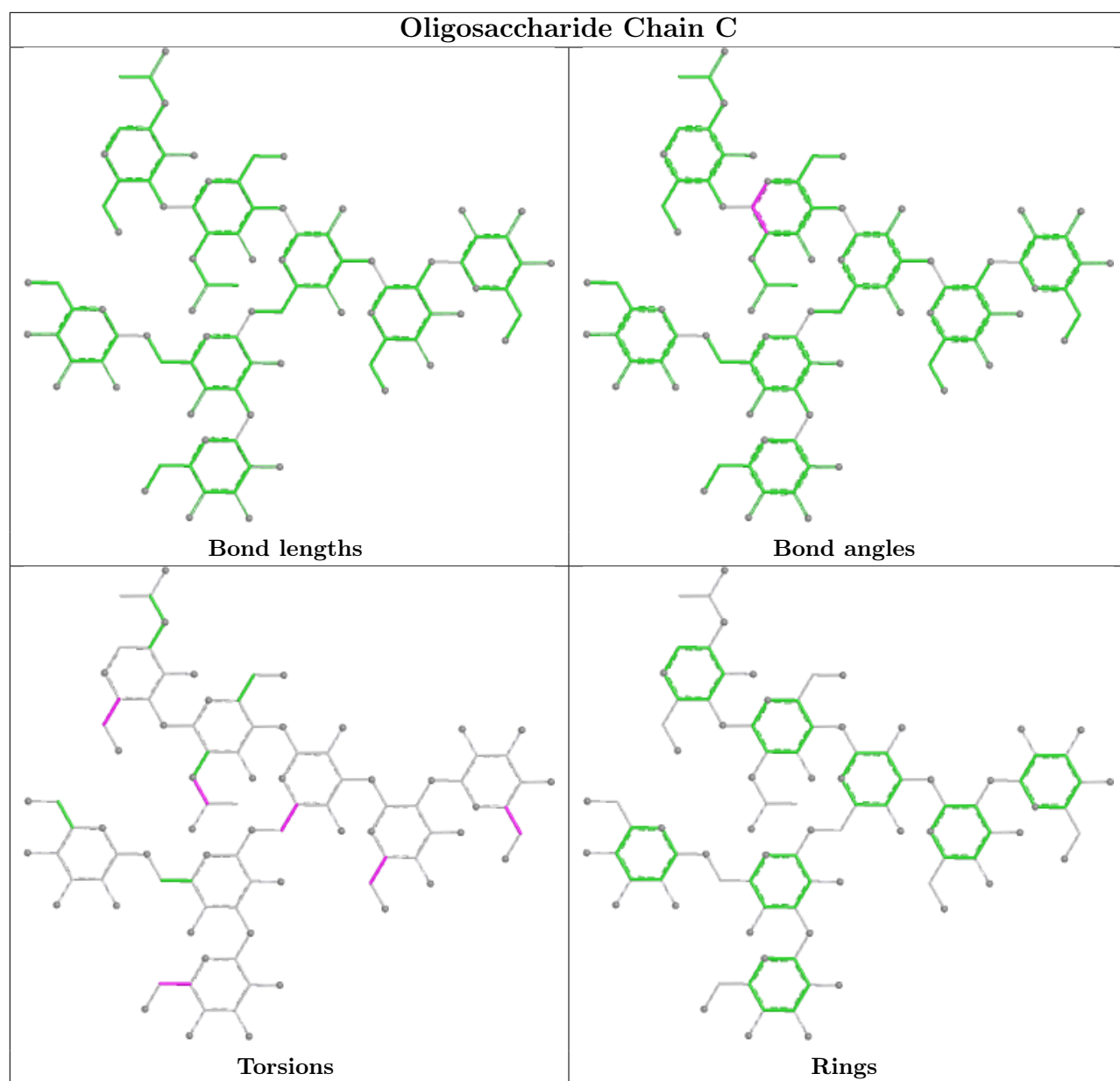
There are no ring outliers.

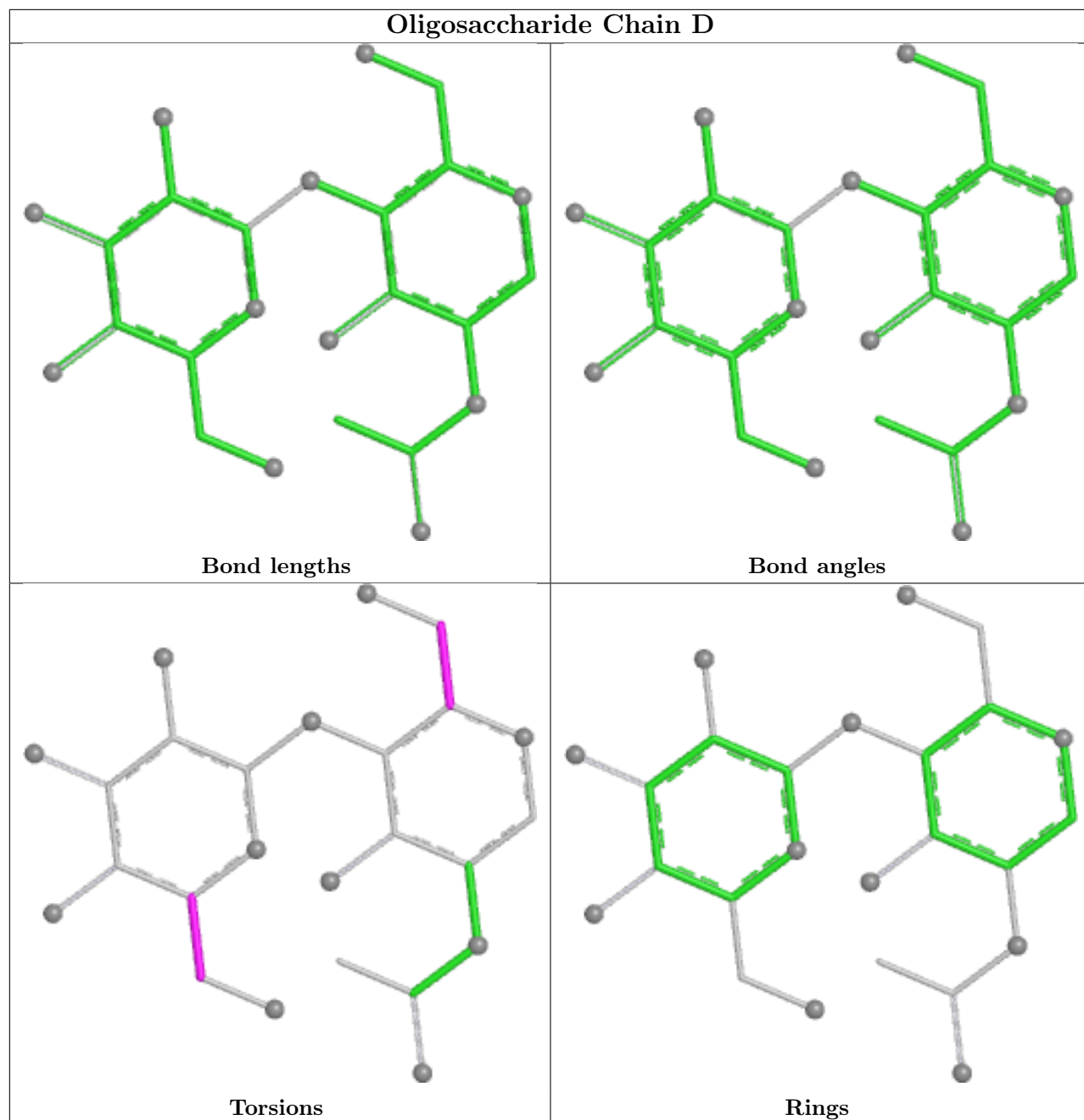
9 monomers are involved in 18 short contacts:

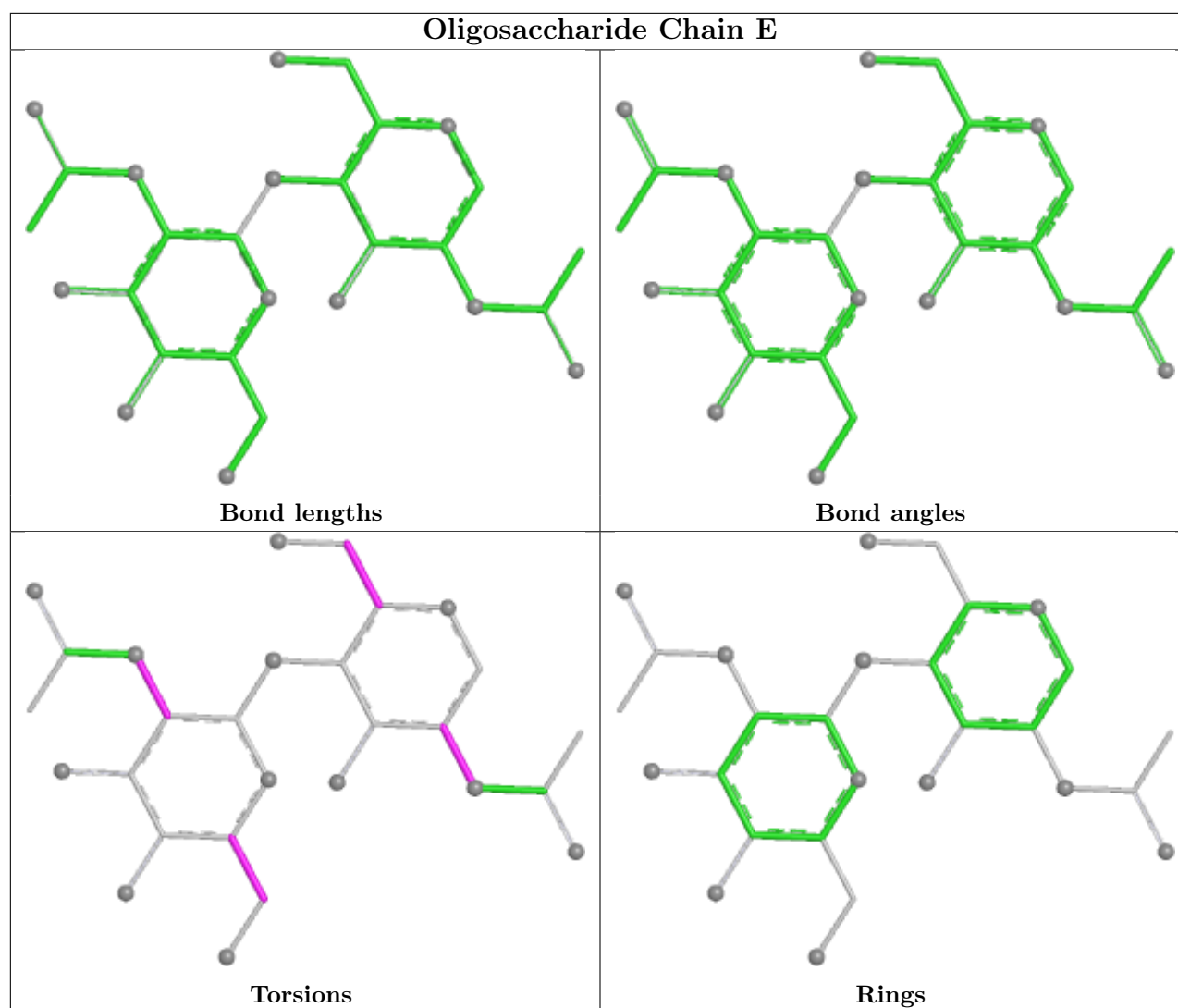
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	4	MAN	2	0
4	C	3	BMA	1	0
3	B	1	NAG	4	0
4	C	6	MAN	1	0
5	E	1	NAG	1	0
5	E	2	NAG	2	0
4	C	8	MAN	1	0
4	C	1	NAG	6	0
4	C	2	NAG	3	0

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	0.52	0	17,19,21	0.73	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	4/6/23/26	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 (4) 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	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%)	0.61	21 (8%) 16 13	82, 154, 205, 249	0
2	V	1249/1430 (87%)	0.45	64 (5%) 33 22	65, 122, 172, 255	0
All	All	1497/1853 (80%)	0.48	85 (5%) 29 20	65, 126, 185, 255	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	1119	LEU	4.4
1	A	87	LYS	4.2
2	V	885	GLY	4.1
2	V	639	TRP	3.9
2	V	1121	MET	3.8

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.

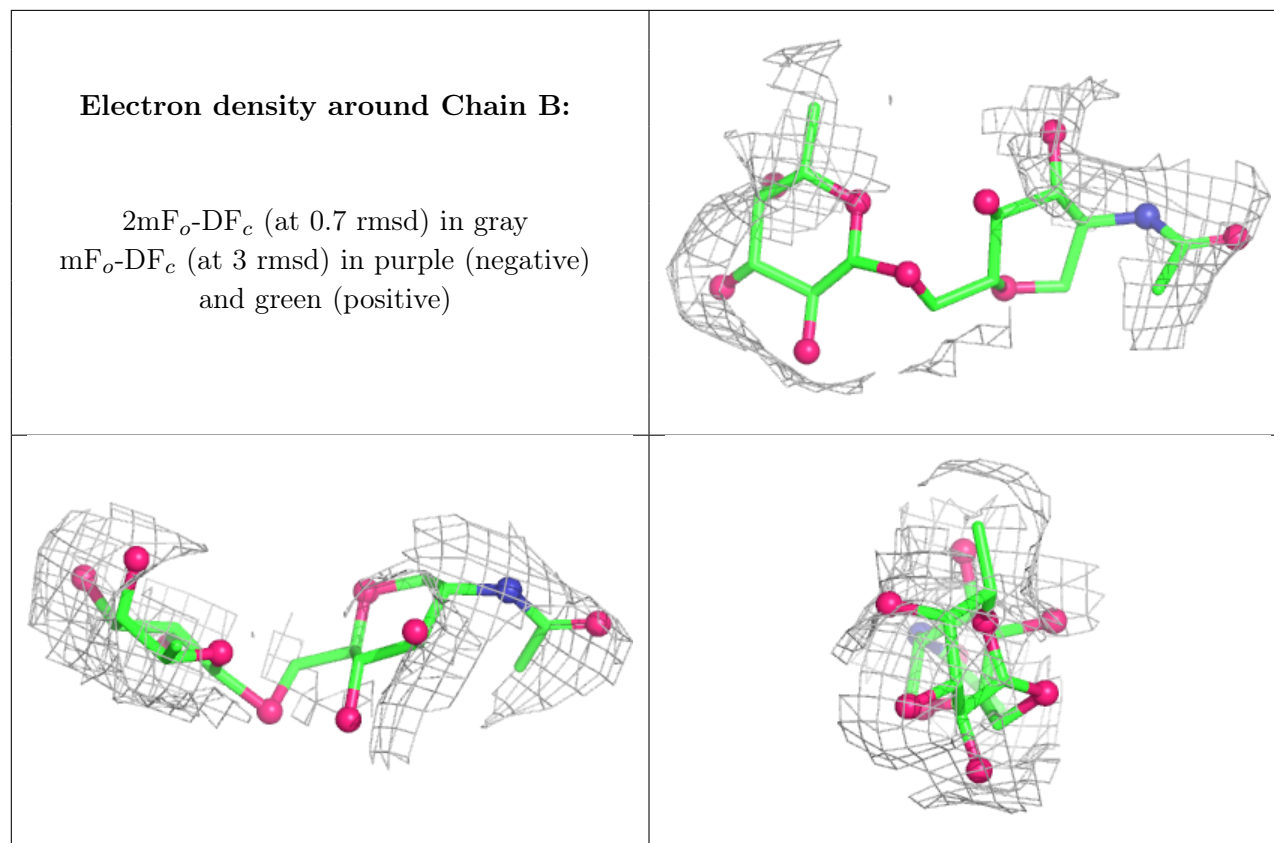
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	1	14/15	-	-	170,211,254,267	0
3	FUC	B	2	10/11	-	-	174,220,248,281	0
5	NAG	E	2	14/15	0.39	0.12	166,195,234,249	0
4	NAG	C	2	14/15	-	-	100,114,135,135	0
4	BMA	C	3	11/12	-	-	120,126,151,159	0

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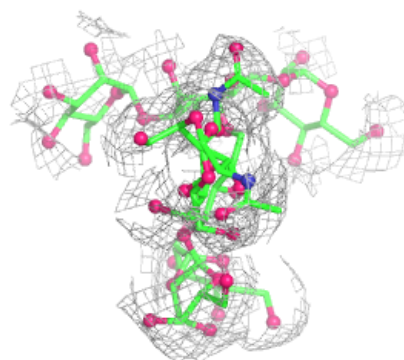
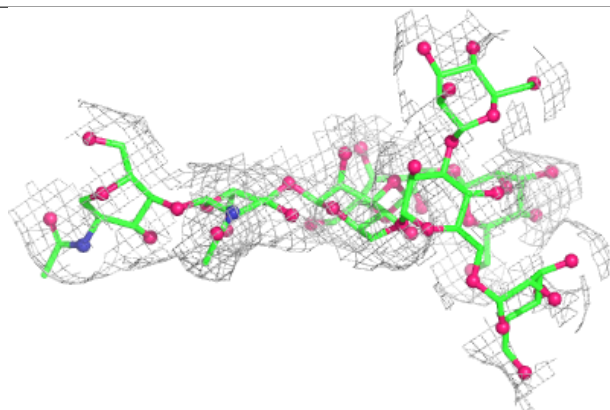
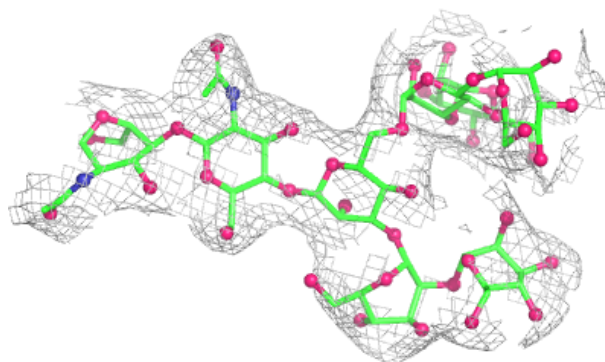
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	C	4	11/12	-	-	122,131,153,163	0
4	MAN	C	5	11/12	-	-	124,154,178,181	0
4	MAN	C	6	11/12	-	-	89,146,182,203	0
4	MAN	C	7	11/12	-	-	99,147,176,234	0
4	MAN	C	8	11/12	-	-	166,216,232,241	0
4	NAG	C	1	14/15	0.50	0.11	109,122,134,138	0
5	NAG	D	1	14/15	0.89	0.09	123,145,212,220	0
5	NAG	D	2	11/15	0.91	0.10	171,180,203,215	0
5	NAG	E	1	14/15	0.92	0.12	132,201,219,237	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.

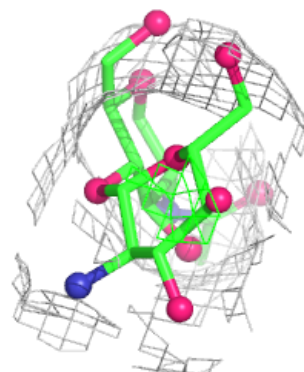
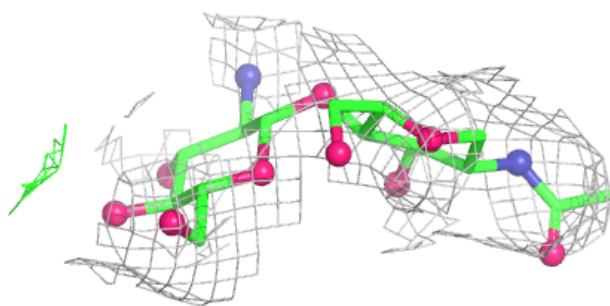
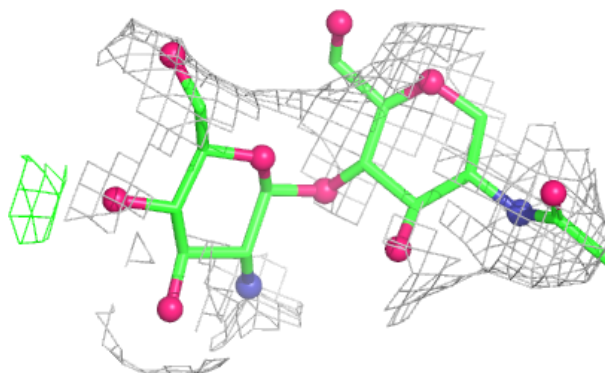


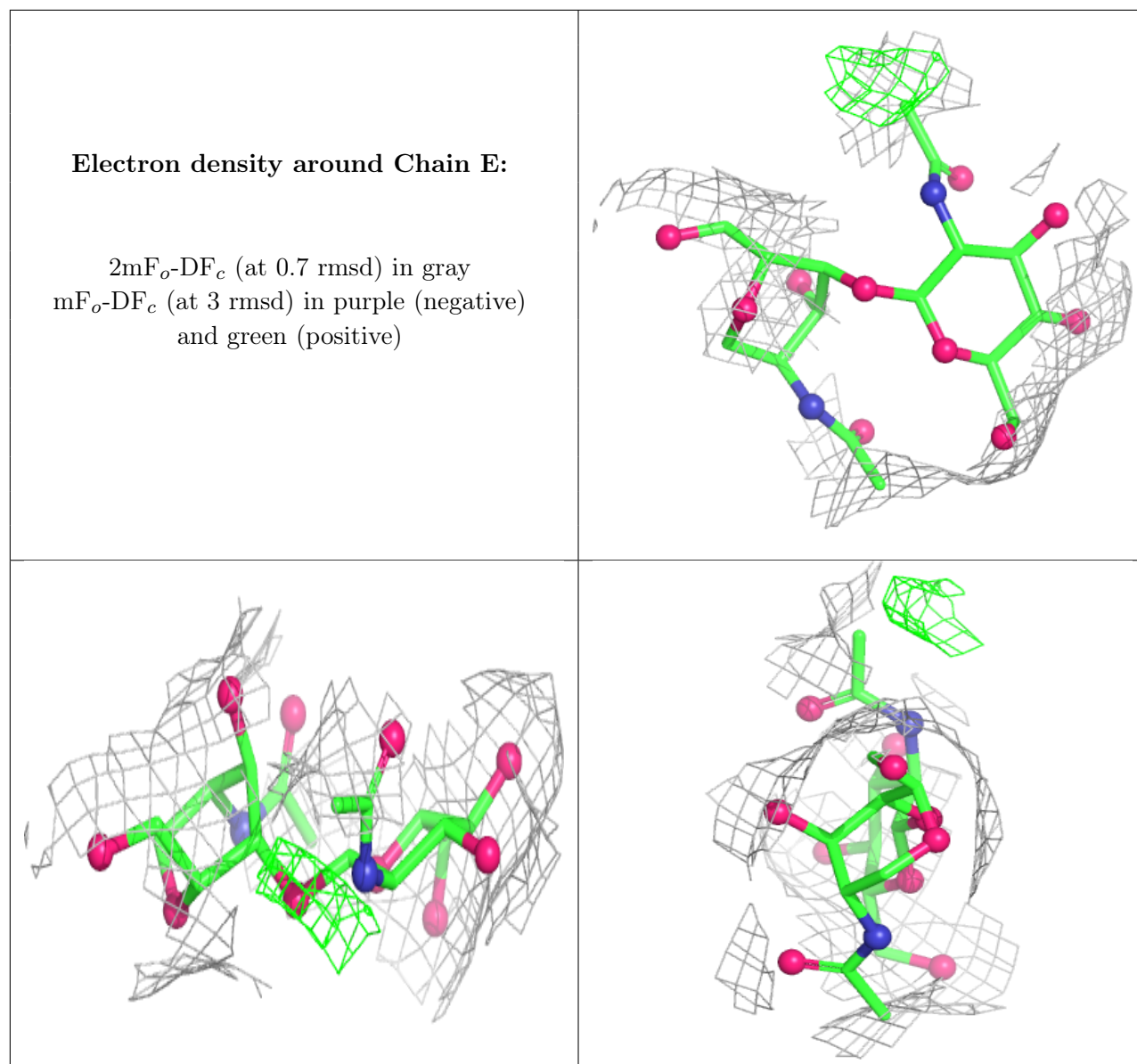
Electron density around Chain C:

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

**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	0.52	0.13	152,206,263,286	0
8	CU	V	2432	1/1	0.97	0.05	124,124,124,124	0
7	CA	V	2431	1/1	0.99	0.06	105,105,105,105	0
7	CA	V	2430	1/1	0.99	0.03	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.