



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2023 – 05:10 pm GMT

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.

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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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

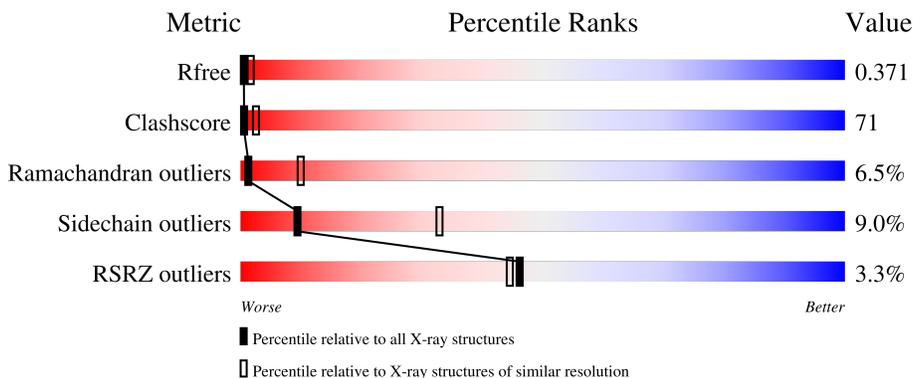
1 Overall quality at a glance

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.



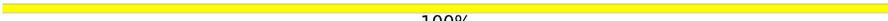
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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 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% 36% 20% 39%
2	V	1430	 2% 28% 50% 9% 11%
3	B	2	 50% 50%
4	C	8	 25% 25% 50%
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 i

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
			Total	C	N	O	S			
1	A	248	1587	981	290	298	18	0	0	0

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

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

There are 3 discrepancies between the modelled and reference sequences:

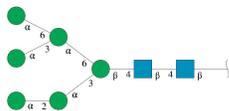
Chain	Residue	Modelled	Actual	Comment	Reference
V	50	LYS	GLU	conflict	UNP Q7SZN0
V	1287	LYS	SER	conflict	UNP Q7SZN0
V	1305	PHE	SER	conflict	UNP Q7SZN0

- 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
			Total	C	N	O			
3	B	2	24	14	1	9	0	0	0

- 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.



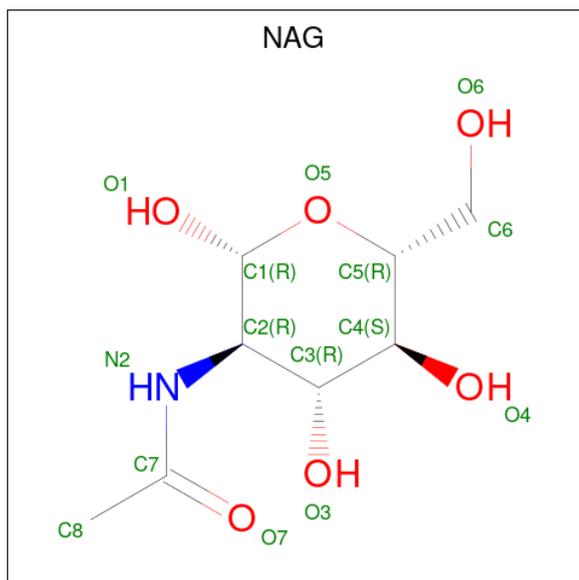
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	C	8	94	52	2	40	0	0	0

- 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
			Total	C	N	O			
5	D	2	25	14	2	9	0	0	0
5	E	2	28	16	2	10	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	V	2	Total Ca 2 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 Cu 1 1	0	0

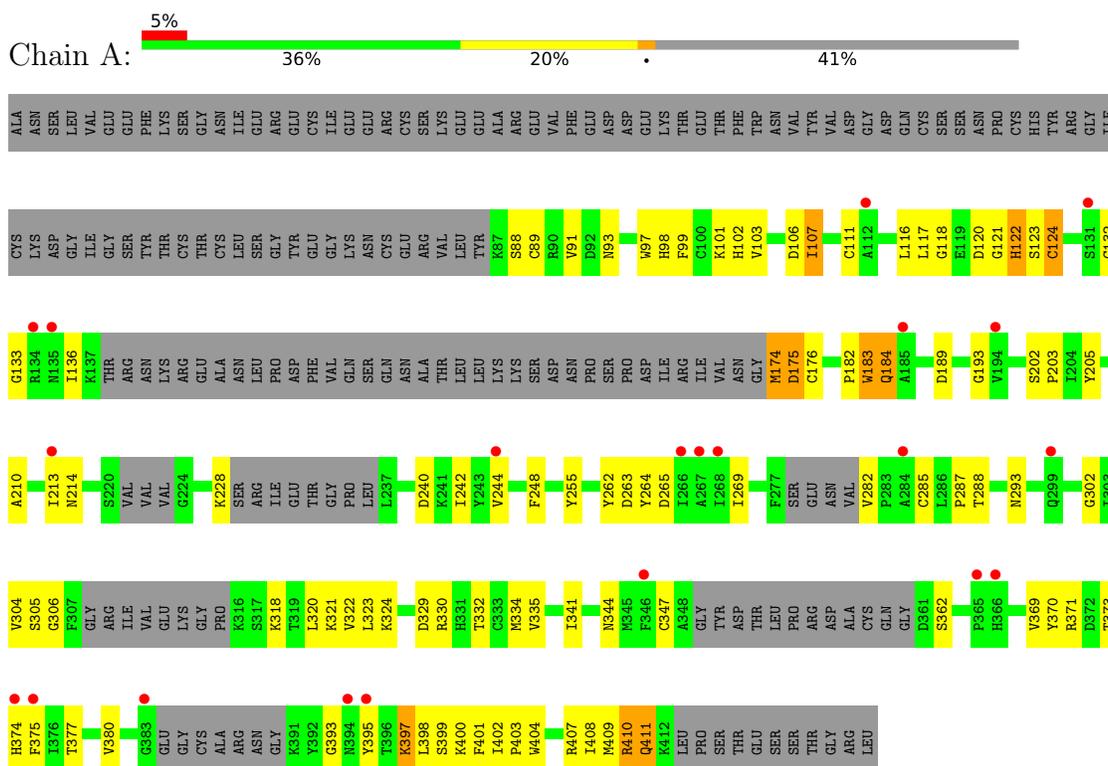
- Molecule 9 is water.

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

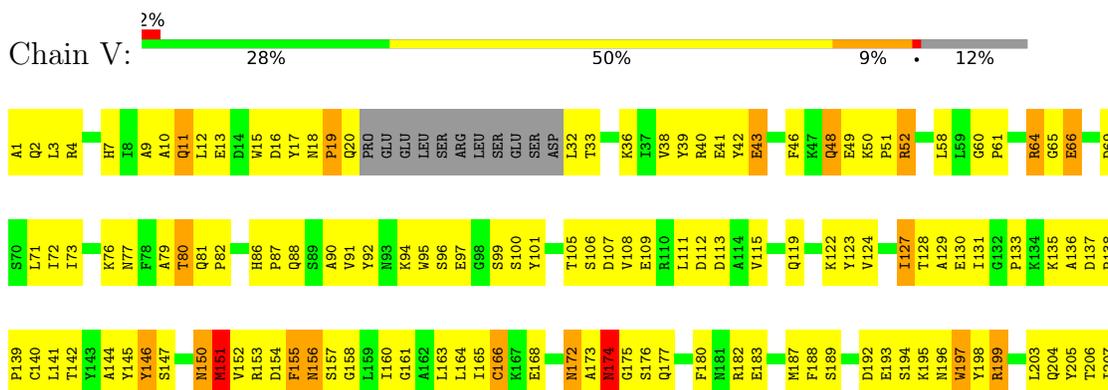
3 Residue-property plots [i](#)

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.

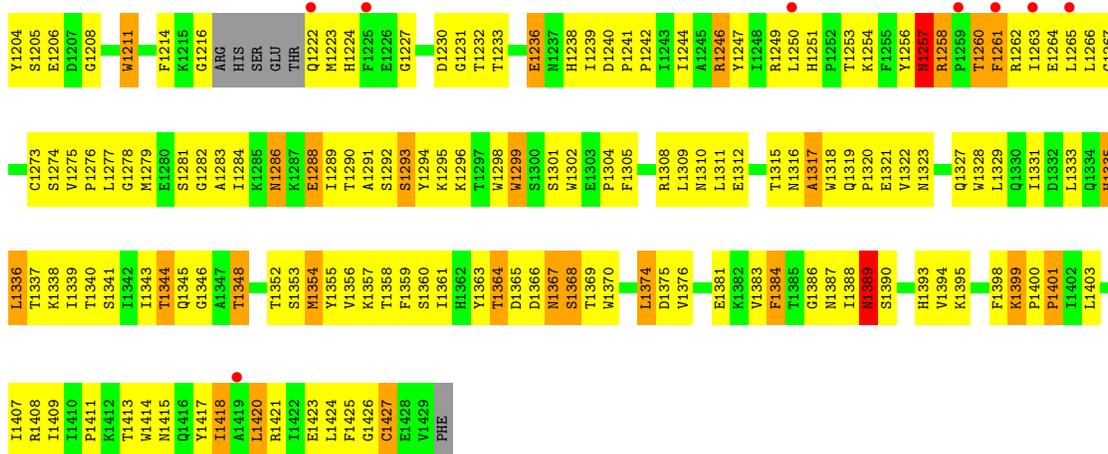
• Molecule 1: FACTOR X-LIKE PROTEASE



• Molecule 2: VENOM PROTHROMBIN ACTIVATOR PSEUTARIN-C NON-CATALYTIC SUB-UNIT



V1139	Q1068	I1E	Y942	A875	D808	SER	LYS	M615	V546	S480	T406	F341	V273	F210	
G1140	L1069	GLY	S943	S876	Y809	VAL	LYS	L616	K947	A481	V407	S342	S274	M11	
Y1141	G1070	VAL	G944	R877	S810	ALA	GLU	F617	K548	V482	F408	S343	R275	A211	
W1142	G1071	GLN	Y945	P878	P811	GLU	GLU	P618	D549	D483	R409	D483	T276	M12	
E1143	L1072	S1011	N946	P879	I1E	GLU	VAL	D550	W484	W484	N410	V344	R277	G213	
	P1073	L1012	N947	S880	GLY	GLU	PRO	S620	P651	T485	L411	D345	W279	T214	
	L1074	H1013	E948	L881	LYS	LEU	VAL	G625	K552	R486	A412	R346	L280	L215	
	L1075	T1014	H882	H882	SER	LYS	ASN	T626	F553	D487	S413	R347	L281	F216	
	P1076	P1015	K950	A883	GLN	HIS	PHE	G625	Y554	L488	R414	Y348	D217	D217	
	G1077	H1016	H884	H884	VAL	THR	VAL	T627	K656	G491	P415	K349	L284	V18	
	T1078	A1017	H952	G885	ARG	ALA	PRO	M628	S556	A350	Y416	A350	Q219	Q219	
	F1079	M1018	S953	L886	SER	LEU	ASP	D629	N557	L492	S417	K287	A286	A286	
	A1080	M1019	G954	L887	ARG	ALA	PRO	N630	Y568	L493	Y418	K287	C221	C221	
	S1081	G1020	L955	Y888	ALA	LEU	GLU	L681		G494	Y419	L553	H288	A222	
	I1082	I1021	I956	G991	ALA	GLU	SER	G632	T561	P495	Y419	D354	H288	A222	
	K1083	K1083	G957	S891	K823	GLU	ASP	T633	L562	L496	C422	N355	L289	D224	
	M1084	Y1023	P958	S892	T824	ASP	ALA	W634	N563	L497	Y423	F356	Q290	D224	
	K1085	Q1024	E893	E893	T825	ALA	LEU	L635	G564	W498	W423	S357	A291	H235	
		L1025	F826	G894	F826	HIS	ALA	L636		C499	W425	N358	Y284	I226	
	K1088	Q1026	K827	R895	K827	ALA	LYS	S637	R569	K500	W425	F359	G295	S227	
	I1089	G1027	K828	S896	R828	SER	GLY	S638	H501	H501	K427	I360	G295	S227	
	W1092	L1028	G965	F905	A829	PRO	LEU	W639	V581	G508	P438	K367	Y296	H229	
	L1093	T1029	N966	K906	L835	ASP	GLY	G640	H574	V509	E430	G361	I299	L230	
	E1095	M1030	F831	D898	D837	ALA	ASN	S641	F575	A503	G431	K362	K300	I231	
	I1096	I1031	D968	D899	F831	ARG	LEU	C642	H576	L504	4432	Y364	D301	G232	
	E1097	K1032	K969	P902	S883	ASP	ASP	E643	G577	S505	I433	K365	C302	W233	
	E1097	D1033	N970	F905	Y834	SER	ASP	M644		LYS	Y434	K366	G303	S234	
	E1097	M1035	N971	K907	L835	ASN	GLU	N646	V581	G508	P438	A367	D306	S236	
	I1172	V1036	R972	K907	D836	SER	GLY	N646	H582	V509	F368	V369	THR	E238	
	M1101	H1037	R977	D908	D837	ALA	ASN	M648	H584	Q510	R370	R370	I239	E238	
	Q1102	H1038	R978	D909	F839	ARG	PRO	R649	H584	N511	Q371	R371	F240	E238	
	Q1103	H1039	F979	A910	Q840	ASN	ILE	R649	L585		ASN	Q371	THR	E238	
	R1104	H1039	N980	A910	Q840	PRO	ILE	L650	V588	D514	L443	Y372	ARG	E238	
	Q1105	L1040	L981	M912	P842	ASP	GLN	R651	V588	V515	T443	G375	LYS	F242	
	M1106	M1042	F982	P913	P842	ILE	PRO	F652	T590	V515	H444	N376	LEU	H243	
	L1107	M1043	F983	N914	Y648	ALA	ARG	L653	E516	V515	Q445	F377	SER	F244	
	A1108	G1044	H984	G915	E849	ALA	ARG	D654	V591	O517	K446	PHE	N245	N245	
	L1109	P1045	Y985	T916	K850	GLY	GLU	A655	D592	H518	A447	ARG	G246	G246	
	Q1110	G1045	F986	T917	H851	ARG	GLN	M656	E593	A519	V446	GLU	Q247	Q247	
	T1111	K1047	D987	T918	L852	TYR	THR	Y657	I594	E449	E449	Y382	LEU	T248	
	Q1184	D1048	E988	Y919	G853	LEU	GLU	D658	V595	F521	P450		M318	L249	
	T1185	I1049	F989	Y920	L854	ARG	ASP	D659	P596	A522	Q451		K319	E250	
	Q1186	H1050	K990	Y921	L855	THR	ASP	E668	H598	V523	W463		M320	Q251	
	G1187	V1051	S991	Q922	L855	ILE	GLU	E669	H598	F524	W463		K321	Q251	
	T1188	M1052	N992	V923	L858	ASN	GLU	D670	L599	D525	Y454		N322	H253	
	Y1189	M1053	Y993	P924	L859	ARG	GLN	D670	S600	E526	Y454		W323	H254	
	Q1190	F1054	F994	P925	R860	GLU	LEU	D673	G601	N527	T459		W324	Y254	
	L1191	H1055	P995	R926	A861	LYS	MET	I674	H602	K528	W460		E324	K255	
		G1056	LYS	S927	E862	ALA	ALA	F675	T603	S529	L461		F326	V256	
		Q1057	SER	S927	E862	ALA	ALA	F675	F604	W530	L392		I327	S257	
		T1058	ASP	T930	V863	SER	SER	L605	L605	Y531	E465		A328	T258	
	I1127	F1059	L931	D931	D864	LEU	MET	I678	S606		F466		A329	I259	
	L1128	SER	L931	D931	D865	LEU	LEU	F679	K607	T467	T467		E330	N260	
	Q1129	THR	E934	E934	V866	GLY	GLY	I680	G608		T474		E331	L261	
	L1130	C1002	K935	K935	L667	LEU	LEU	P681	K609	Y539	1474		E331	V262	
	S1131	R1064	C1002	K935	L667	ARG	ARG	S682	H610	C540	T475		W334	G267	
	Q1132	E1065	GLU	W939	F871	SER	SER	E883	G611	S541	K476		D385	V267	
	L1133	D1066	LYS	N939	K872	PHE	PHE	VAL	D612	N542	L477		A336	I267	
		M1067	LEU	Y941	L874	LYS	GLY	LYS	L614	W807	H479		Y337	D270	
														M271	S272
														P338	



- 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)	Xtrriage
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	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 116.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: CU, CA, FUC, BMA, NAG, 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($^{\circ}$)	Ideal($^{\circ}$)
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 [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	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: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 [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	1094	LEU

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Mol	Chain	Res	Type
2	V	1258	ARG
2	V	1102	GLN
2	V	1156	ASN
2	V	1288	GLU

Sometimes 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	1151	ASN
2	V	1286	ASN
2	V	1156	ASN
2	V	1222	GLN
2	V	1323	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	2,3	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	2,3	-	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:

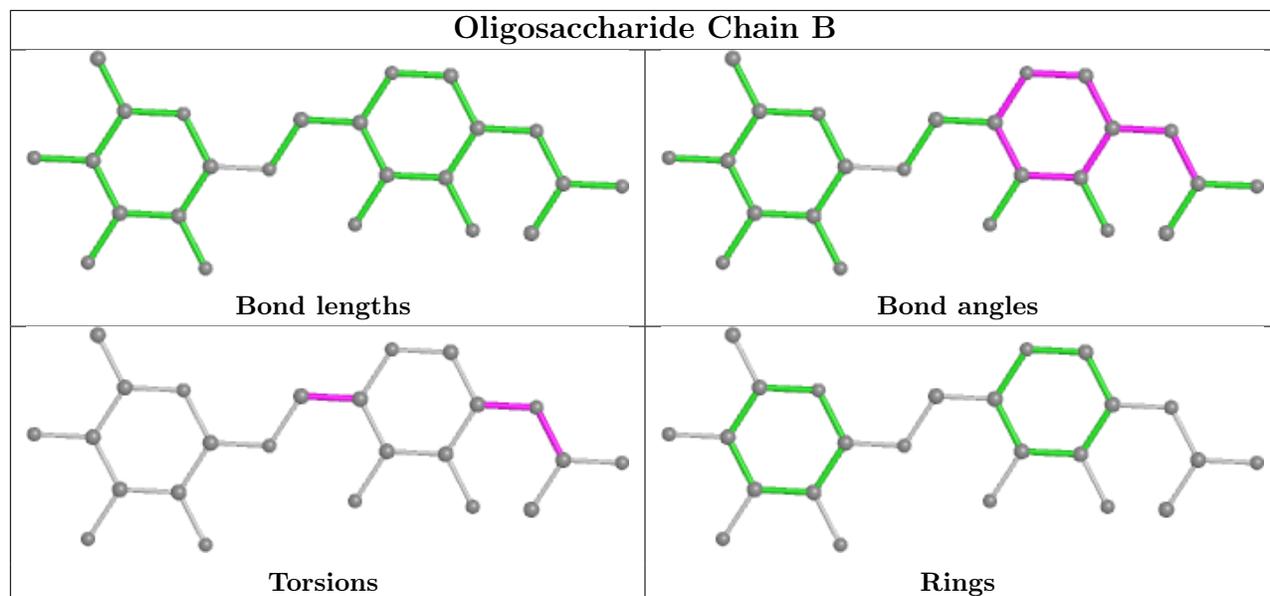
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C3-C2-N2-C7
4	C	3	BMA	C4-C5-C6-O6
4	C	5	MAN	O5-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6

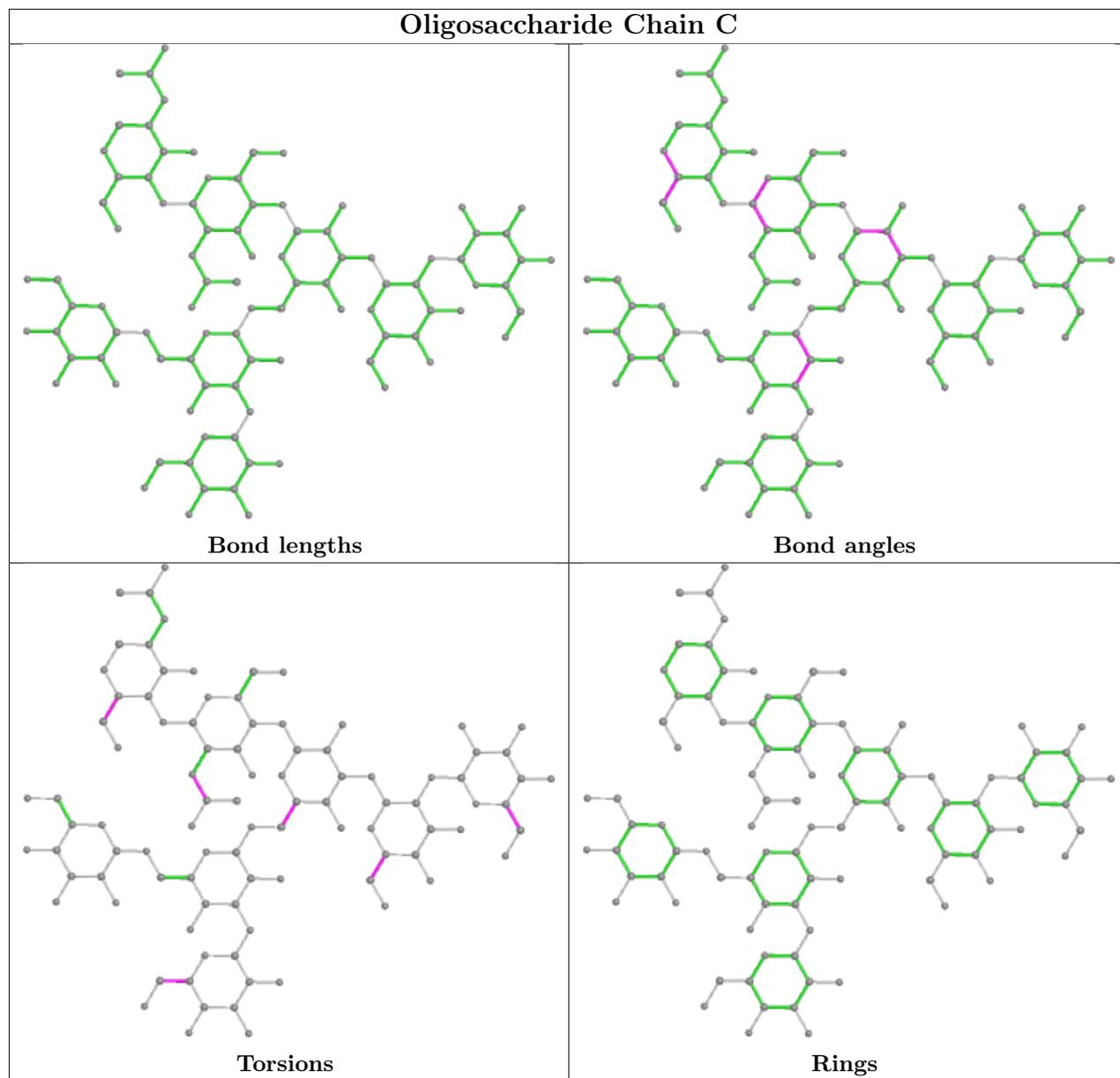
There are no ring outliers.

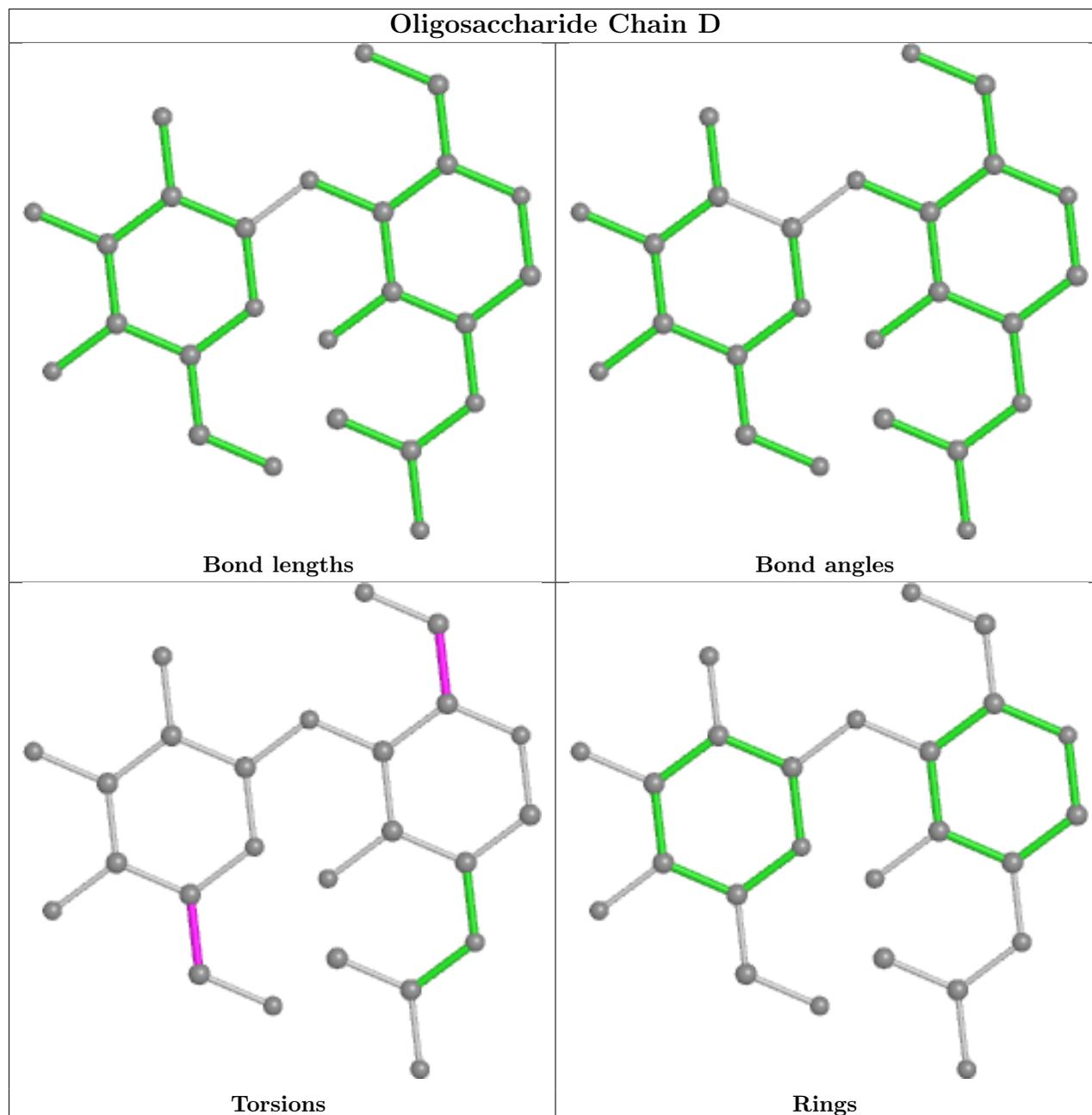
9 monomers are involved in 18 short contacts:

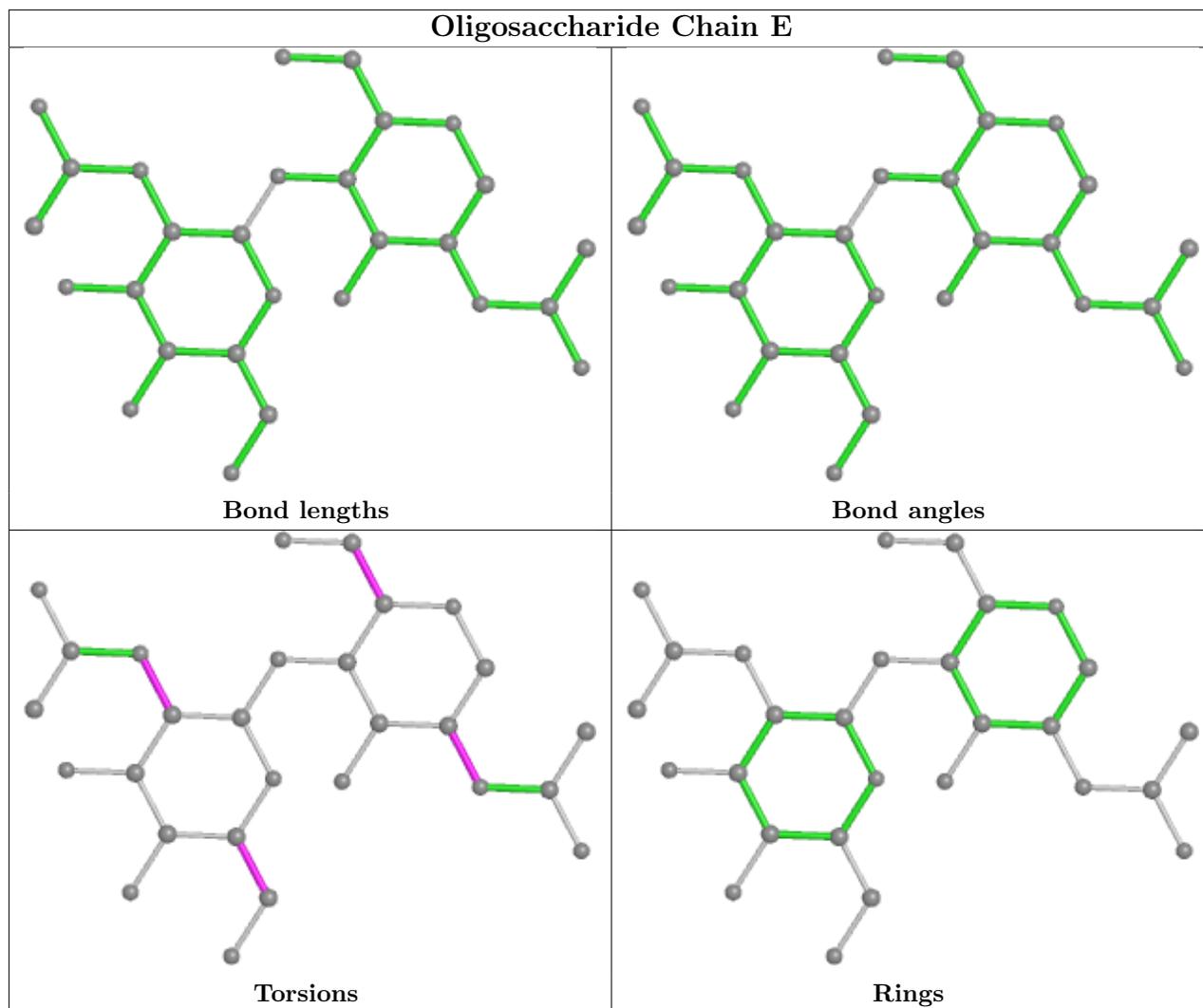
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	NAG	2	0
3	B	1	NAG	4	0
4	C	8	MAN	1	0
4	C	4	MAN	2	0
4	C	1	NAG	5	0
4	C	6	MAN	1	0
4	C	3	BMA	2	0
5	E	1	NAG	1	0
4	C	2	NAG	3	0

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	0.53	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.

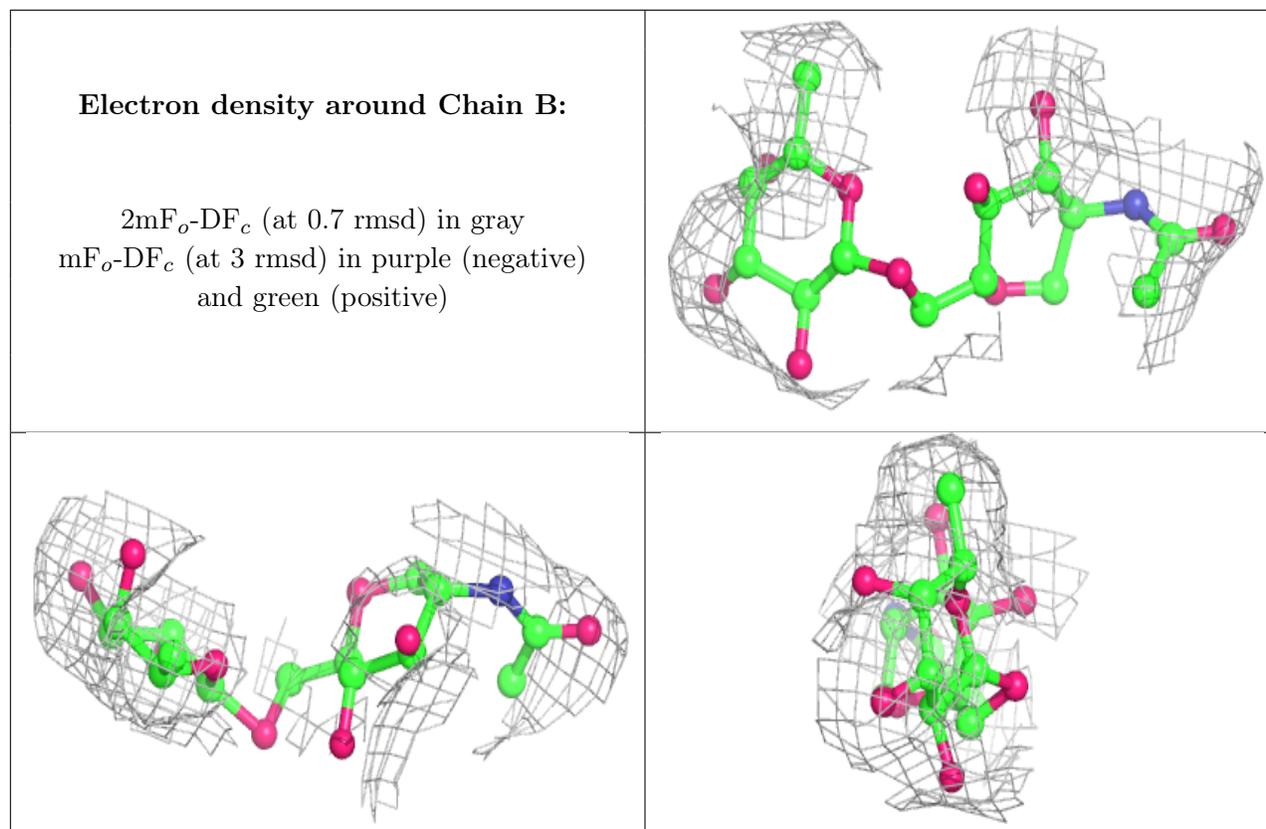
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	E	2	14/15	0.77	0.15	166,195,234,249	0
5	NAG	E	1	14/15	0.82	0.13	132,201,219,237	0
3	FUC	B	2	10/11	0.83	0.15	174,220,248,281	0
3	NAG	B	1	14/15	0.86	0.10	170,211,254,267	0
4	MAN	C	8	11/12	0.86	0.34	166,216,232,241	0

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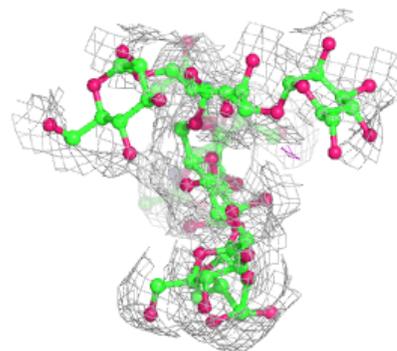
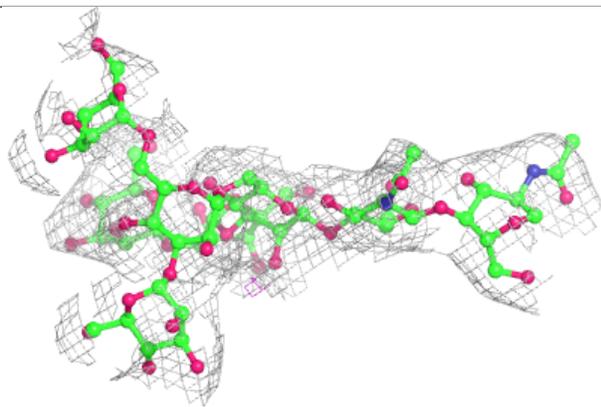
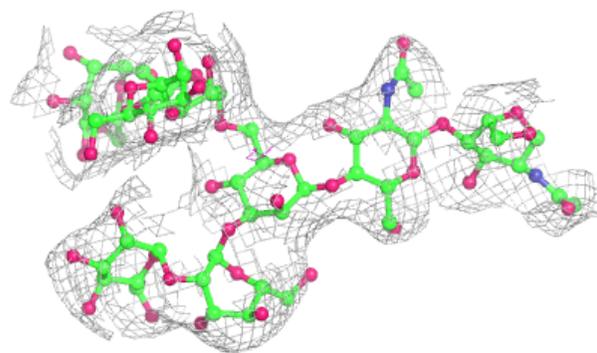
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	C	7	11/12	0.87	0.29	99,147,176,234	0
5	NAG	D	2	11/15	0.89	0.41	171,180,203,215	0
5	NAG	D	1	14/15	0.92	0.27	123,145,212,220	0
4	MAN	C	4	11/12	0.93	0.21	122,131,153,163	0
4	MAN	C	6	11/12	0.93	0.16	89,146,182,203	0
4	MAN	C	5	11/12	0.95	0.24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

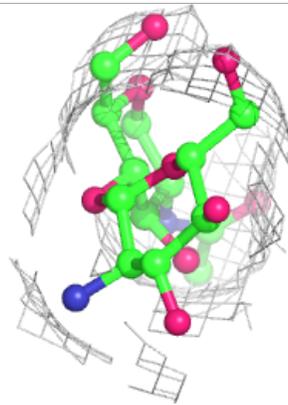
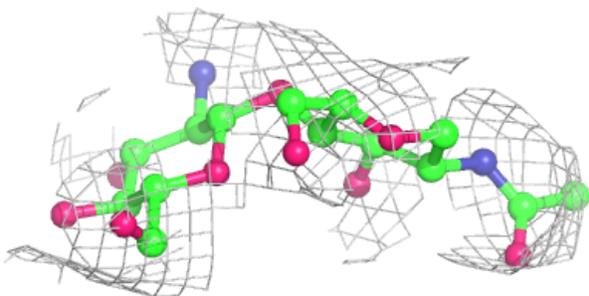
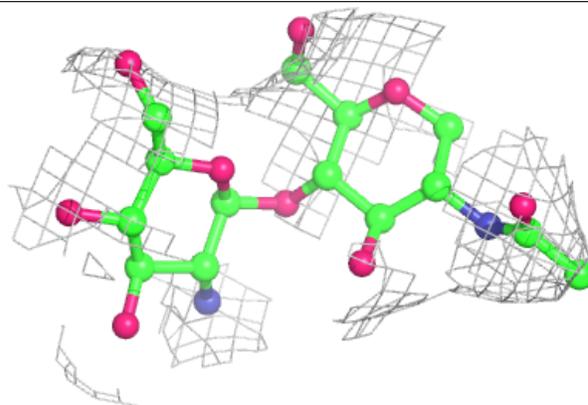


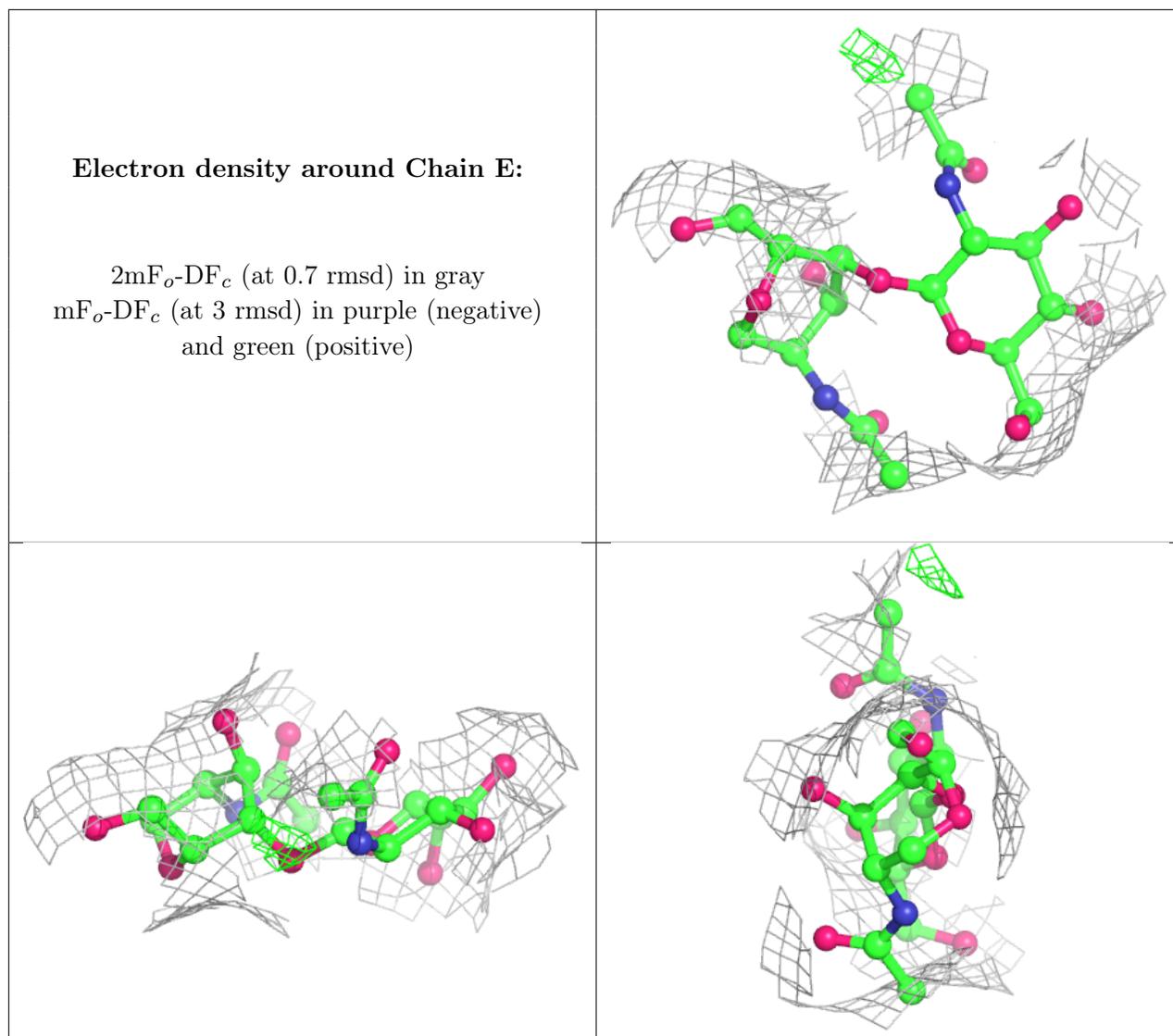
Electron density around Chain C:

$2mF_o-DF_c$ (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(\AA^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	2431	1/1	0.99	0.08	105,105,105,105	0
7	CA	V	2430	1/1	0.99	0.12	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.