



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 04:44 PM BST

PDB ID : 5VOD
Title : Crystal structure of HCMV Pentamer in complex with neutralizing antibody 9I6
Authors : Malito, E.; Chandramouli, S.
Deposited on : 2017-05-02
Resolution : 5.90 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

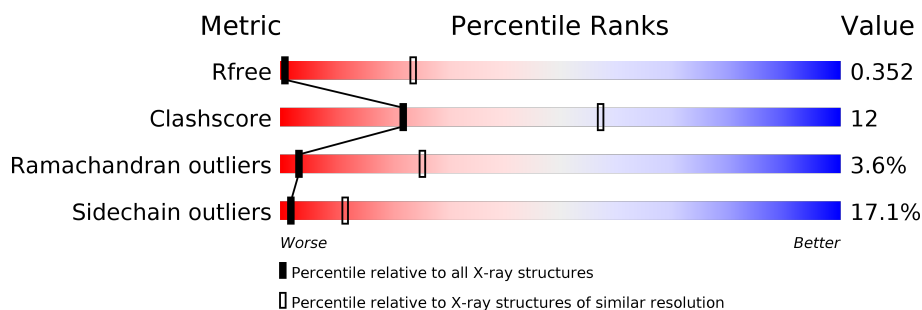
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.90 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	1016 (7.94-3.86)
Clashscore	141614	1042 (7.88-3.90)
Ramachandran outliers	138981	1011 (7.94-3.86)
Sidechain outliers	138945	1013 (7.94-3.82)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	725	63% 25% . . 8%
2	B	278	63% 21% . 15%
3	C	171	42% 31% . . 23%
4	D	252	45% 16% . 35%
5	E	129	59% 22% . 16%
6	H	288	32% 30% 7% 31%
7	L	241	44% 39% 9% 8%

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Mol	Chain	Length	Quality of chain
8	F	3	 33% 67%
8	G	3	 100%
8	K	3	 67% 33%
9	I	5	 20% 40% 40%
9	M	5	 20% 40% 40%
10	J	2	 100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14001 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	667	Total	C	N	O	S	0	0	0
			5358	3427	910	996	25			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	716	GLY	-	expression tag	UNP Q6SW67
A	717	SER	-	expression tag	UNP Q6SW67
A	718	GLY	-	expression tag	UNP Q6SW67
A	719	SER	-	expression tag	UNP Q6SW67
A	720	HIS	-	expression tag	UNP Q6SW67
A	721	HIS	-	expression tag	UNP Q6SW67
A	722	HIS	-	expression tag	UNP Q6SW67
A	723	HIS	-	expression tag	UNP Q6SW67
A	724	HIS	-	expression tag	UNP Q6SW67
A	725	HIS	-	expression tag	UNP Q6SW67

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1867	1188	326	345	8			

- Molecule 3 is a protein called Envelope glycoprotein UL128.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	131	Total	C	N	O	S	0	0	0
			1058	666	190	193	9			

- Molecule 4 is a protein called Envelope glycoprotein UL130.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	164	Total	C	N	O	S	0	0	0
			1337	854	234	241	8			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	215	GLY	-	expression tag	UNP F5HCP3
D	216	SER	-	expression tag	UNP F5HCP3
D	217	GLU	-	expression tag	UNP F5HCP3
D	218	ASN	-	expression tag	UNP F5HCP3
D	219	LEU	-	expression tag	UNP F5HCP3
D	220	TYR	-	expression tag	UNP F5HCP3
D	221	PHE	-	expression tag	UNP F5HCP3
D	222	GLN	-	expression tag	UNP F5HCP3
D	223	ALA	-	expression tag	UNP F5HCP3
D	224	GLY	-	expression tag	UNP F5HCP3
D	225	TRP	-	expression tag	UNP F5HCP3
D	226	SER	-	expression tag	UNP F5HCP3
D	227	HIS	-	expression tag	UNP F5HCP3
D	228	PRO	-	expression tag	UNP F5HCP3
D	229	GLN	-	expression tag	UNP F5HCP3
D	230	PHE	-	expression tag	UNP F5HCP3
D	231	GLU	-	expression tag	UNP F5HCP3
D	232	LYS	-	expression tag	UNP F5HCP3
D	233	GLY	-	expression tag	UNP F5HCP3
D	234	GLY	-	expression tag	UNP F5HCP3
D	235	GLY	-	expression tag	UNP F5HCP3
D	236	SER	-	expression tag	UNP F5HCP3
D	237	GLY	-	expression tag	UNP F5HCP3
D	238	GLY	-	expression tag	UNP F5HCP3
D	239	GLY	-	expression tag	UNP F5HCP3
D	240	SER	-	expression tag	UNP F5HCP3
D	241	GLY	-	expression tag	UNP F5HCP3
D	242	GLY	-	expression tag	UNP F5HCP3
D	243	GLY	-	expression tag	UNP F5HCP3
D	244	SER	-	expression tag	UNP F5HCP3
D	245	TRP	-	expression tag	UNP F5HCP3
D	246	SER	-	expression tag	UNP F5HCP3
D	247	HIS	-	expression tag	UNP F5HCP3
D	248	PRO	-	expression tag	UNP F5HCP3
D	249	GLN	-	expression tag	UNP F5HCP3
D	250	PHE	-	expression tag	UNP F5HCP3
D	251	GLU	-	expression tag	UNP F5HCP3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	252	LYS	-	expression tag	UNP F5HCP3

- Molecule 5 is a protein called Envelope glycoprotein UL131A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	108	Total	C	N	O	S	0	0	0
			893	557	168	166	2			

- Molecule 6 is a protein called Fab 9I6 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	199	Total	C	N	O	S	13	0	0
			1511	965	247	292	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	MET	-	initiating methionine	PDB ?
H	246	SER	-	expression tag	UNP S6B291
H	247	SER	-	expression tag	UNP S6B291
H	248	GLY	-	expression tag	UNP S6B291
H	249	LEU	-	expression tag	UNP S6B291
H	250	GLU	-	expression tag	UNP S6B291
H	251	VAL	-	expression tag	UNP S6B291
H	252	LEU	-	expression tag	UNP S6B291
H	253	PHE	-	expression tag	UNP S6B291
H	254	GLN	-	expression tag	UNP S6B291
H	255	GLY	-	expression tag	UNP S6B291
H	256	PRO	-	expression tag	UNP S6B291
H	257	LEU	-	expression tag	UNP S6B291
H	258	GLY	-	expression tag	UNP S6B291
H	259	SER	-	expression tag	UNP S6B291
H	260	ALA	-	expression tag	UNP S6B291
H	261	TRP	-	expression tag	UNP S6B291
H	262	SER	-	expression tag	UNP S6B291
H	263	HIS	-	expression tag	UNP S6B291
H	264	PRO	-	expression tag	UNP S6B291
H	265	GLN	-	expression tag	UNP S6B291
H	266	PHE	-	expression tag	UNP S6B291
H	267	GLU	-	expression tag	UNP S6B291
H	268	LYS	-	expression tag	UNP S6B291
H	269	GLY	-	expression tag	UNP S6B291

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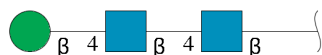
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Chain	Residue	Modelled	Actual	Comment	Reference
H	270	GLY	-	expression tag	UNP S6B291
H	271	GLY	-	expression tag	UNP S6B291
H	272	SER	-	expression tag	UNP S6B291
H	273	GLY	-	expression tag	UNP S6B291
H	274	GLY	-	expression tag	UNP S6B291
H	275	GLY	-	expression tag	UNP S6B291
H	276	SER	-	expression tag	UNP S6B291
H	277	GLY	-	expression tag	UNP S6B291
H	278	GLY	-	expression tag	UNP S6B291
H	279	GLY	-	expression tag	UNP S6B291
H	280	SER	-	expression tag	UNP S6B291
H	281	TRP	-	expression tag	UNP S6B291
H	282	SER	-	expression tag	UNP S6B291
H	283	HIS	-	expression tag	UNP S6B291
H	284	PRO	-	expression tag	UNP S6B291
H	285	GLN	-	expression tag	UNP S6B291
H	286	PHE	-	expression tag	UNP S6B291
H	287	GLU	-	expression tag	UNP S6B291
H	288	LYS	-	expression tag	UNP S6B291

- Molecule 7 is a protein called Fab 9I6 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	221	Total	C	N	O	S	53	0	0
			1710	1063	293	345	9			

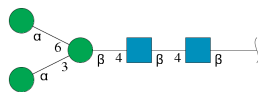
- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
8	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
8	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



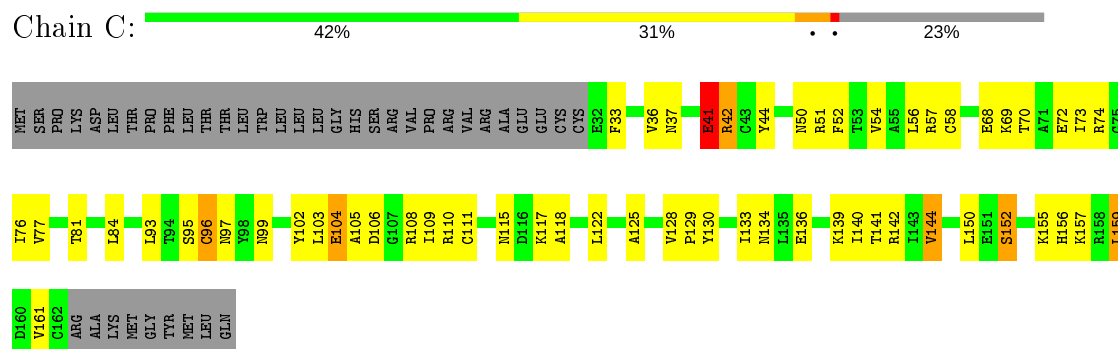
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
9	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

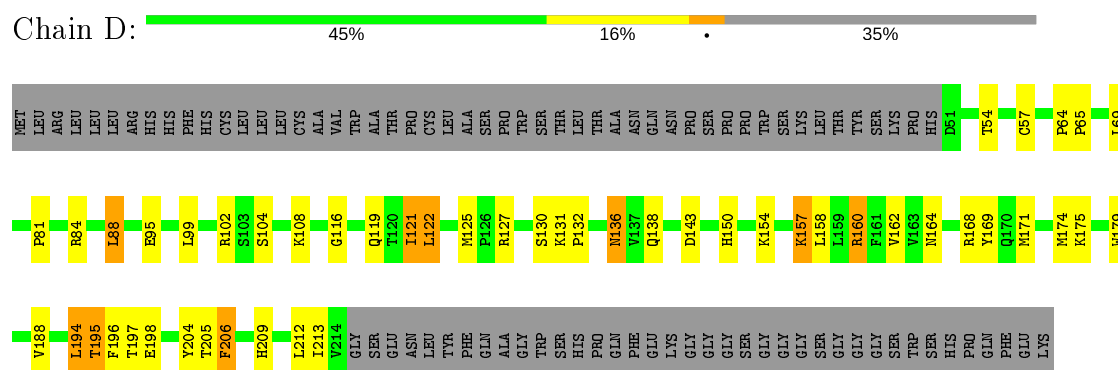


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

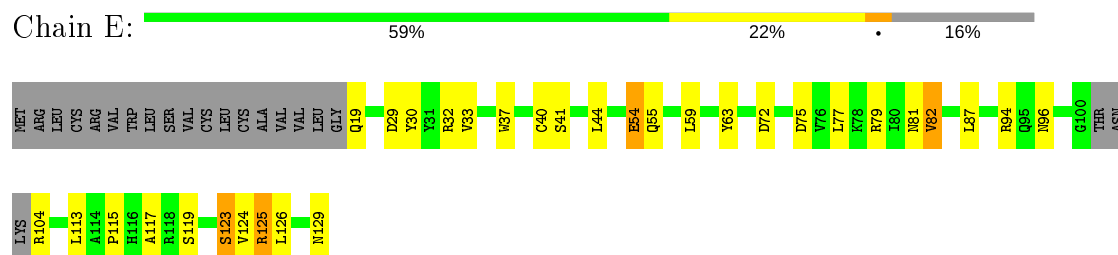
- Molecule 3: Envelope glycoprotein UL128



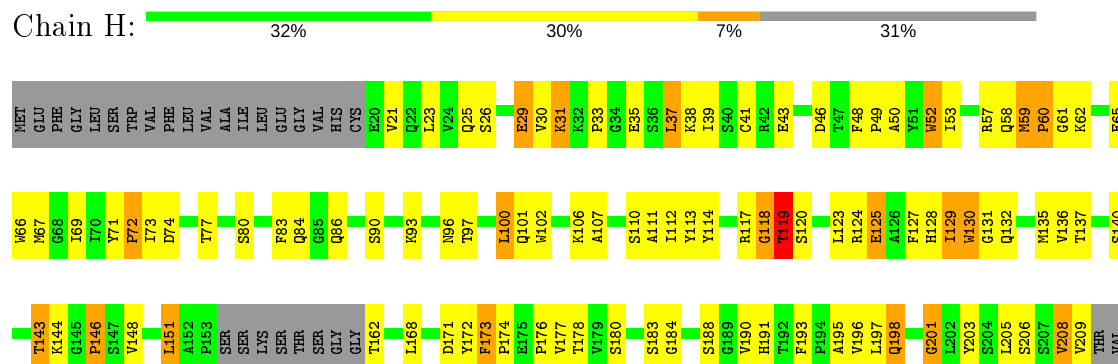
- Molecule 4: Envelope glycoprotein UL130

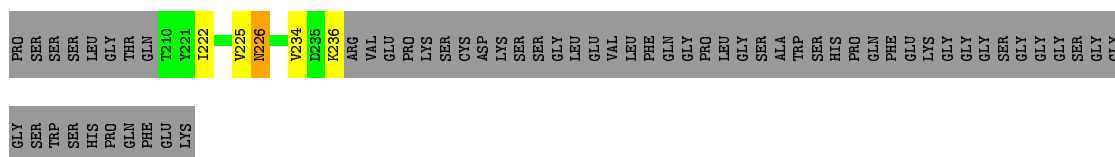


- Molecule 5: Envelope glycoprotein UL131A



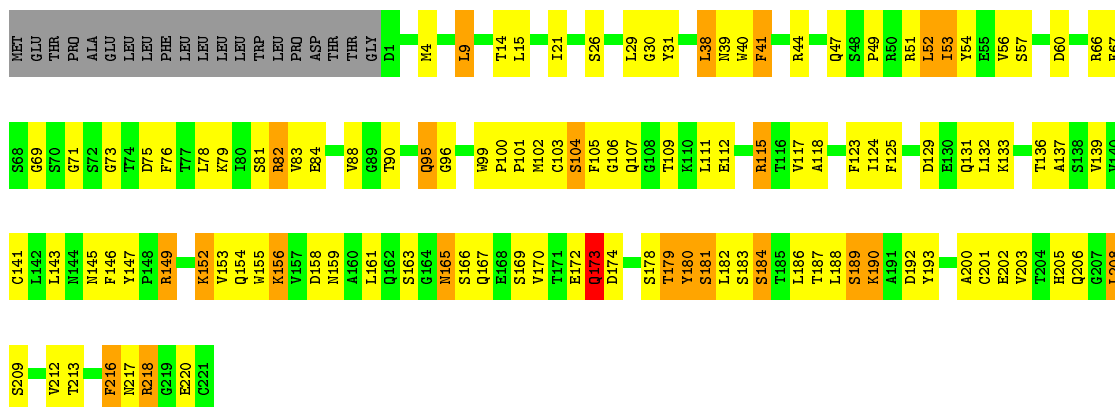
- Molecule 6: Fab 9I6 heavy chain





• Molecule 7: Fab 9I6 light chain

Chain L: 44% 39% 9% 8%



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 33% 67%



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 67% 33%



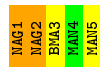
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 20% 40% 40%



- Molecule 9: alpha-D-mannopyranose-(1-3)-[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 M:



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	148.26 Å 208.82 Å 267.98 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.71 – 5.90 89.76 – 5.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.71-5.90) 99.9 (89.76-5.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 5.76 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.258 , 0.299 0.291 , 0.352	Depositor DCC
R_{free} test set	505 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	276.9	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 264.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	14001	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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, 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	0.47	0/5484	0.76	1/7473 (0.0%)
2	B	0.53	0/1913	0.74	0/2612
3	C	0.52	0/1080	0.82	0/1461
4	D	0.49	0/1373	0.80	1/1865 (0.1%)
5	E	0.40	0/912	0.63	0/1233
6	H	0.56	0/1550	0.90	0/2112
7	L	0.61	0/1748	0.89	0/2370
All	All	0.51	0/14060	0.79	2/19126 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	136	ASN	C-N-CA	6.59	138.18	121.70
1	A	177	TRP	C-N-CA	5.26	134.86	121.70

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	5358	0	5309	99	1
2	B	1867	0	1859	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1058	0	1050	42	0
4	D	1337	0	1312	28	0
5	E	893	0	851	16	0
6	H	1511	0	1477	69	0
7	L	1710	0	1644	74	0
8	F	39	0	34	1	0
8	G	39	0	34	0	0
8	K	39	0	34	1	0
9	I	61	0	52	2	0
9	M	61	0	52	2	0
10	J	28	0	25	2	0
All	All	14001	0	13733	325	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 325 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)
6:H:52:TRP:HA	6:H:71:TYR:CE1	1.84	1.11
6:H:53:ILE:HG12	6:H:72:PRO:HD3	1.27	1.11
6:H:225:VAL:HB	6:H:234:VAL:HB	1.43	0.98
6:H:52:TRP:HA	6:H:71:TYR:HE1	1.16	0.96
3:C:103:LEU:HG	3:C:109:ILE:HG12	1.48	0.95

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:TRP:NE1	1:A:483:GLU:OE2[8_534]	1.81	0.39

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	661/725 (91%)	598 (90%)	47 (7%)	16 (2%)	6	33
2	B	235/278 (84%)	214 (91%)	19 (8%)	2 (1%)	17	56
3	C	129/171 (75%)	107 (83%)	14 (11%)	8 (6%)	1	16
4	D	162/252 (64%)	155 (96%)	6 (4%)	1 (1%)	25	65
5	E	104/129 (81%)	100 (96%)	4 (4%)	0	100	100
6	H	193/288 (67%)	138 (72%)	35 (18%)	20 (10%)	0	8
7	L	219/241 (91%)	161 (74%)	43 (20%)	15 (7%)	1	15
All	All	1703/2084 (82%)	1473 (86%)	168 (10%)	62 (4%)	3	25

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	PRO
1	A	297	PHE
3	C	41	GLU
6	H	46	ASP
6	H	118	GLY

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	607/655 (93%)	512 (84%)	95 (16%)	2	14
2	B	204/238 (86%)	172 (84%)	32 (16%)	2	14
3	C	118/154 (77%)	93 (79%)	25 (21%)	1	6
4	D	150/222 (68%)	129 (86%)	21 (14%)	3	17
5	E	95/114 (83%)	78 (82%)	17 (18%)	2	10
6	H	168/238 (71%)	136 (81%)	32 (19%)	1	8
7	L	195/213 (92%)	154 (79%)	41 (21%)	1	6
All	All	1537/1834 (84%)	1274 (83%)	263 (17%)	2	11

5 of 263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	203	ASN
3	C	150	LEU
7	L	112	GLU
2	B	231	GLU
3	C	51	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	480	HIS
3	C	99	ASN
7	L	98	HIS
1	A	512	HIS
1	A	181	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 ⓘ

21 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	$\# Z > 2$
8	NAG	F	1	1,8	14,14,15	0.60	0	17,19,21	1.59	3 (17%)
8	NAG	F	2	8	14,14,15	0.46	0	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	F	3	8	11,11,12	0.71	0	15,15,17	1.28	2 (13%)
8	NAG	G	1	1,8	14,14,15	0.53	0	17,19,21	1.28	2 (11%)
8	NAG	G	2	8	14,14,15	0.64	0	17,19,21	1.76	3 (17%)
8	BMA	G	3	8	11,11,12	0.57	0	15,15,17	0.79	1 (6%)
9	NAG	I	1	1,9	14,14,15	0.31	0	17,19,21	0.77	0
9	NAG	I	2	9	14,14,15	0.54	0	17,19,21	2.77	6 (35%)
9	BMA	I	3	9	11,11,12	0.49	0	15,15,17	1.00	1 (6%)
9	MAN	I	4	9	11,11,12	0.62	0	15,15,17	1.44	1 (6%)
9	MAN	I	5	9	11,11,12	0.58	0	15,15,17	1.27	2 (13%)
10	NAG	J	1	10,4	14,14,15	0.65	0	17,19,21	1.57	4 (23%)
10	NAG	J	2	10	14,14,15	0.74	0	17,19,21	1.47	2 (11%)
8	NAG	K	1	8,4	14,14,15	0.35	0	17,19,21	1.64	2 (11%)
8	NAG	K	2	8	14,14,15	0.39	0	17,19,21	0.97	0
8	BMA	K	3	8	11,11,12	0.56	0	15,15,17	1.26	2 (13%)
9	NAG	M	1	9,5	14,14,15	0.29	0	17,19,21	1.31	2 (11%)
9	NAG	M	2	9	14,14,15	0.26	0	17,19,21	1.13	2 (11%)
9	BMA	M	3	9	11,11,12	0.49	0	15,15,17	1.20	2 (13%)
9	MAN	M	4	9	11,11,12	0.42	0	15,15,17	0.85	0
9	MAN	M	5	9	11,11,12	0.57	0	15,15,17	1.90	1 (6%)

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
8	NAG	F	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	3/6/23/26	0/1/1/1
8	BMA	F	3	8	-	1/2/19/22	0/1/1/1
8	NAG	G	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	G	2	8	-	0/6/23/26	0/1/1/1
8	BMA	G	3	8	-	2/2/19/22	0/1/1/1
9	NAG	I	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	I	2	9	-	1/6/23/26	0/1/1/1
9	BMA	I	3	9	-	1/2/19/22	0/1/1/1
9	MAN	I	4	9	-	1/2/19/22	0/1/1/1
9	MAN	I	5	9	-	1/2/19/22	0/1/1/1
10	NAG	J	1	10,4	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	J	2	10	-	1/6/23/26	0/1/1/1
8	NAG	K	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	K	2	8	-	2/6/23/26	0/1/1/1
8	BMA	K	3	8	-	0/2/19/22	0/1/1/1
9	NAG	M	1	9,5	-	0/6/23/26	0/1/1/1
9	NAG	M	2	9	-	2/6/23/26	0/1/1/1
9	BMA	M	3	9	-	1/2/19/22	0/1/1/1
9	MAN	M	4	9	-	0/2/19/22	0/1/1/1
9	MAN	M	5	9	-	1/2/19/22	1/1/1/1

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	5	MAN	C1-O5-C5	6.85	121.47	112.19
9	I	2	NAG	O5-C1-C2	-6.67	100.75	111.29
9	I	2	NAG	C1-C2-N2	5.72	120.26	110.49
8	K	1	NAG	O5-C1-C2	-5.37	102.81	111.29
10	J	2	NAG	C1-O5-C5	5.15	119.17	112.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	G	1	NAG	C3-C2-N2-C7
9	I	2	NAG	C1-C2-N2-C7
9	M	2	NAG	C3-C2-N2-C7
8	G	3	BMA	C4-C5-C6-O6
8	F	2	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	5	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 8 short contacts:

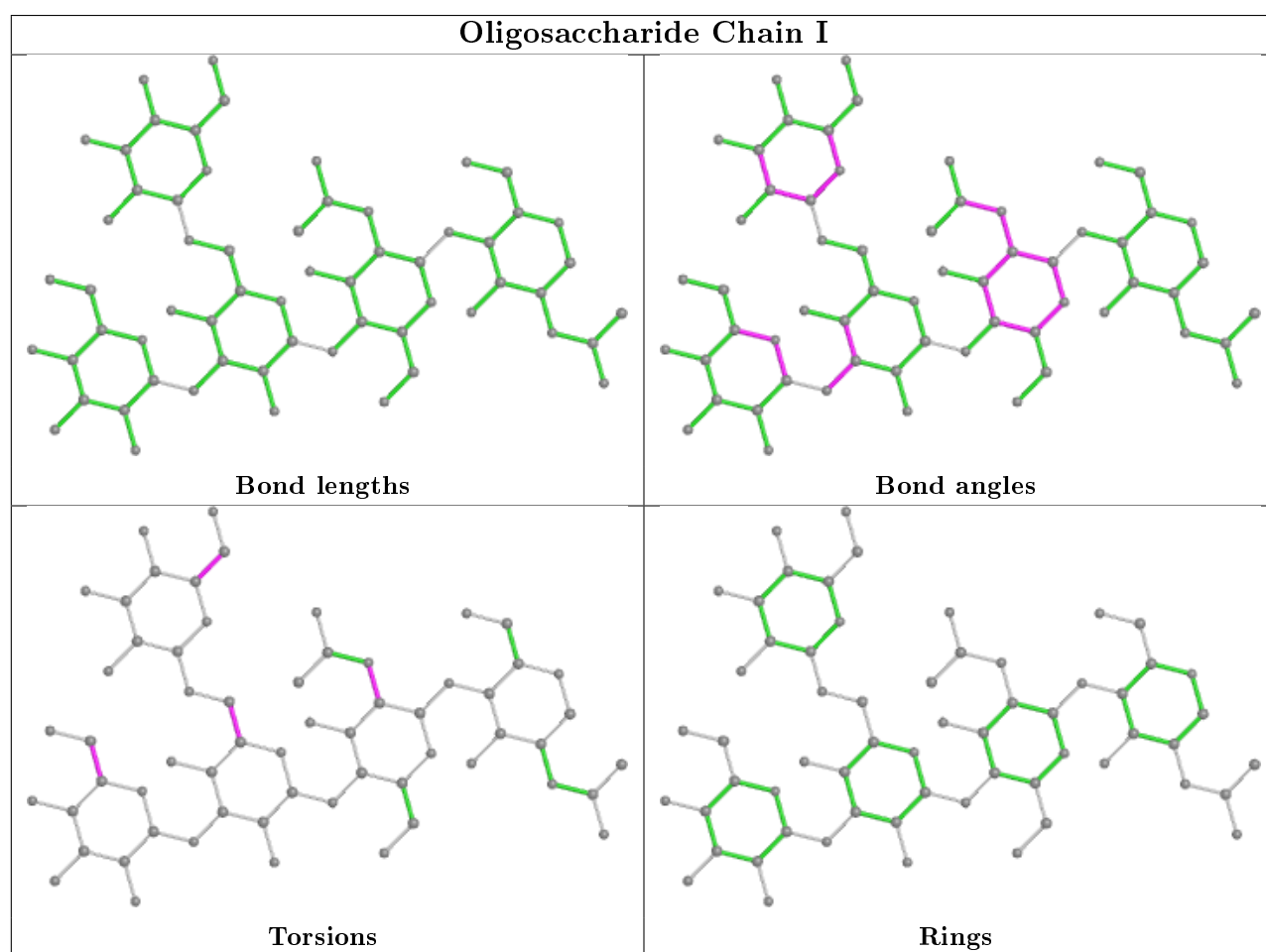
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	5	MAN	2	0
8	F	2	NAG	1	0

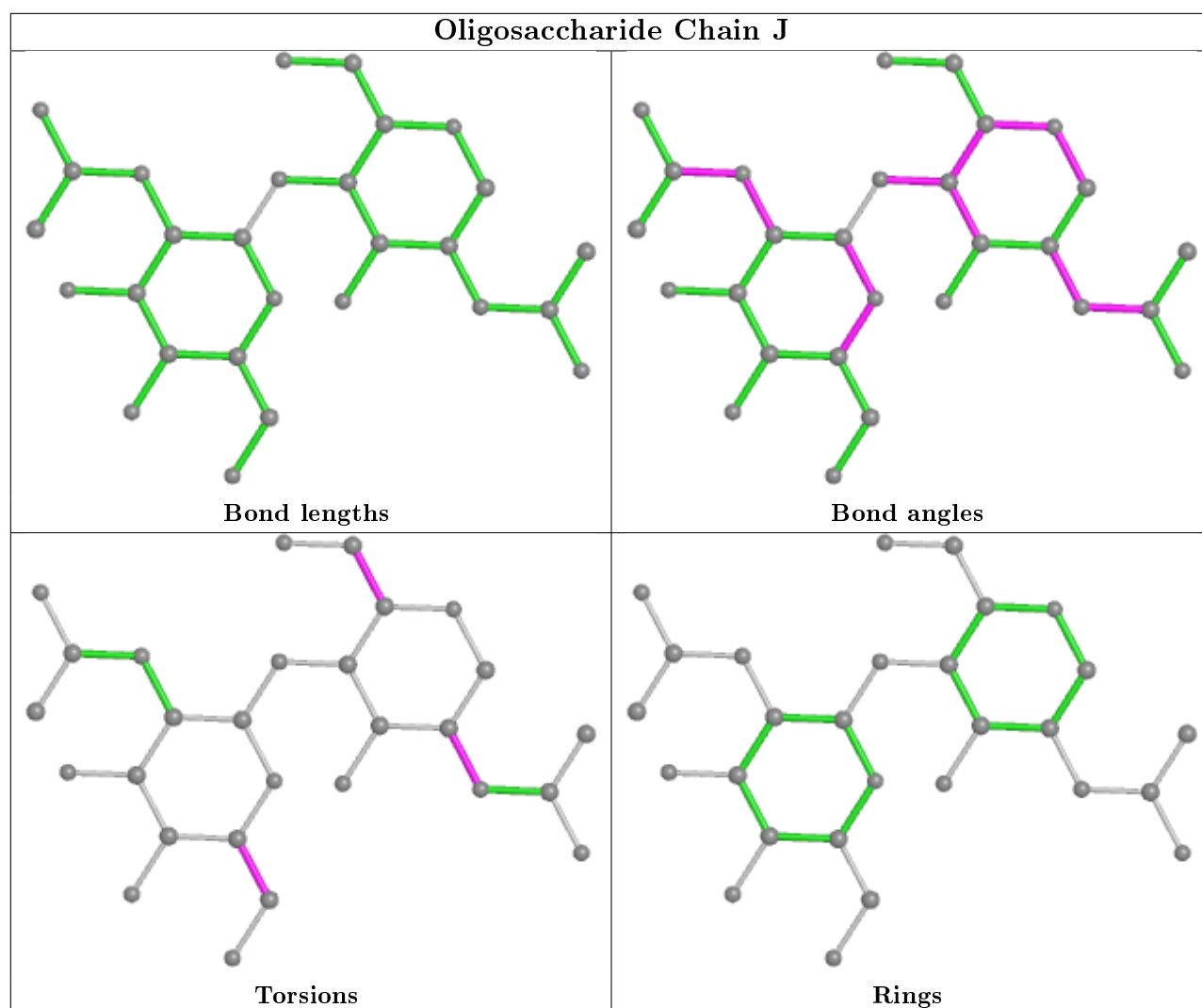
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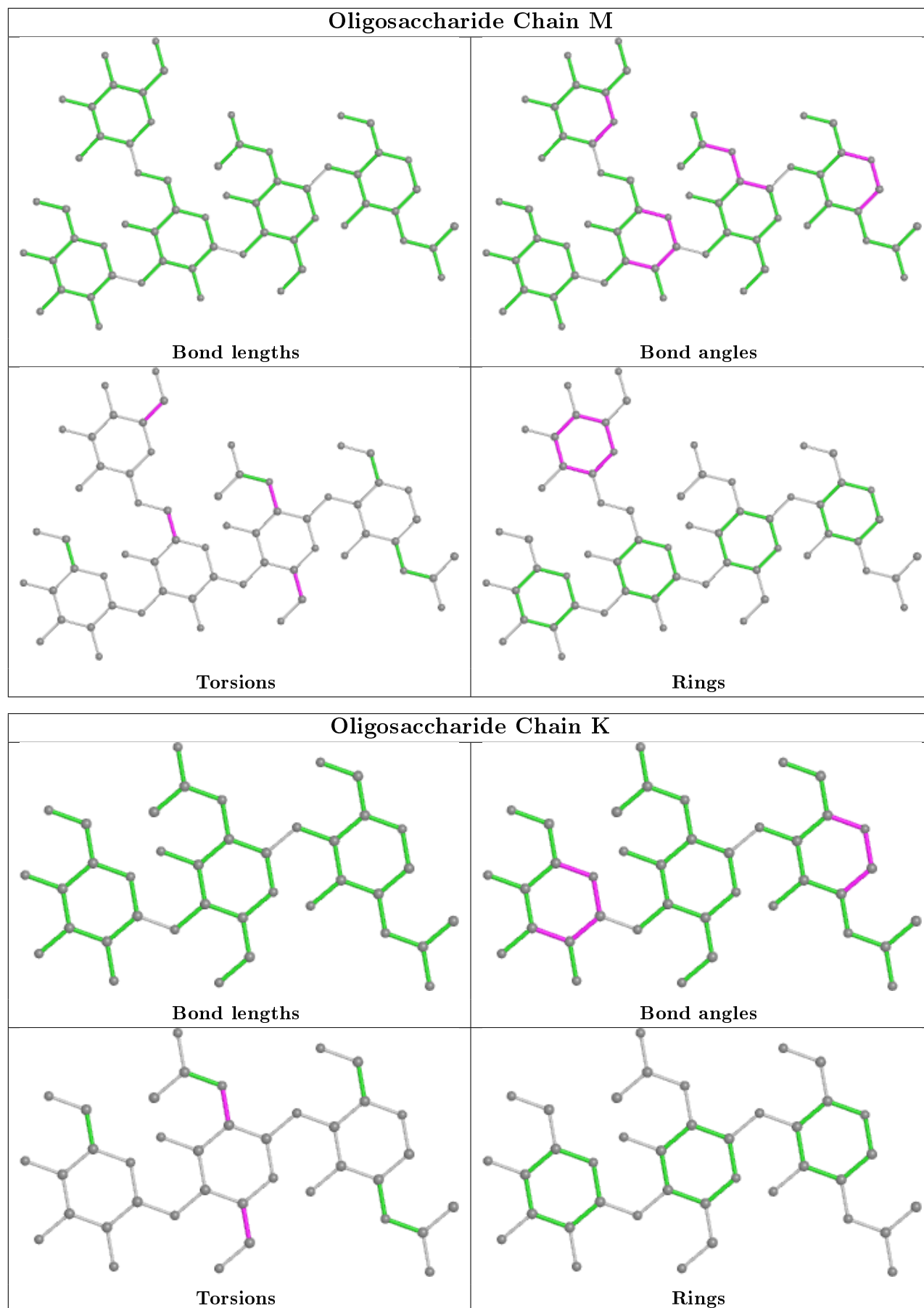
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	3	BMA	1	0
10	J	2	NAG	1	0
10	J	1	NAG	2	0
9	M	1	NAG	1	0
8	K	2	NAG	1	0
9	I	3	BMA	2	0
8	K	1	NAG	1	0
9	M	2	NAG	2	0

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](#)

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

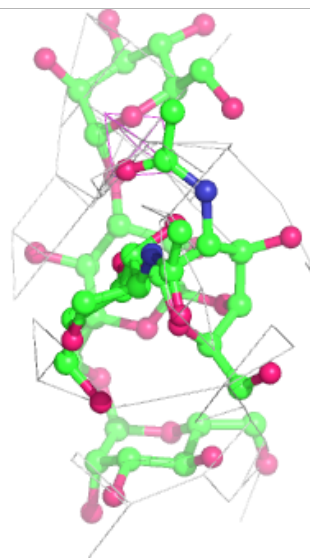
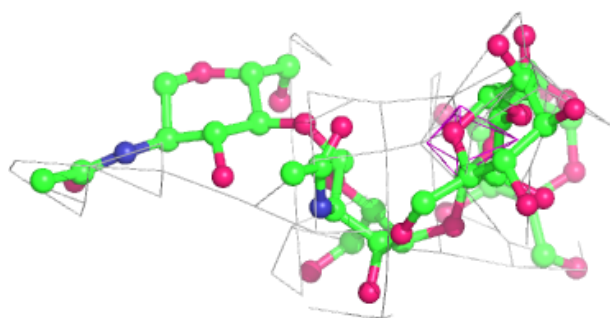
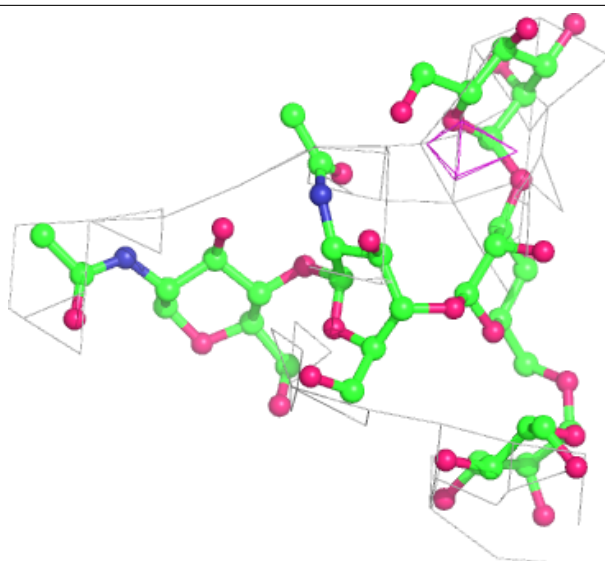
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

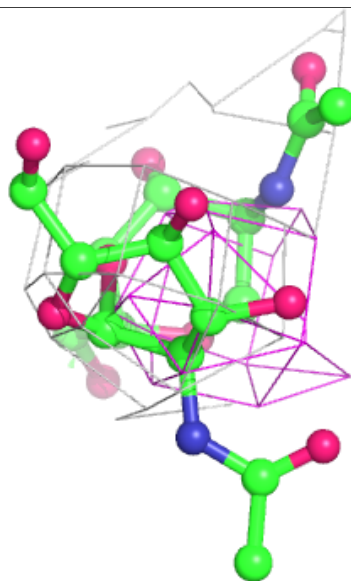
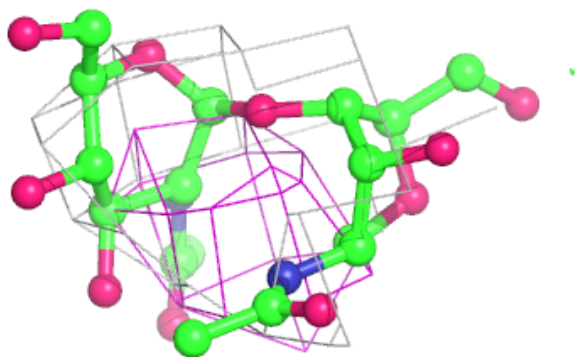
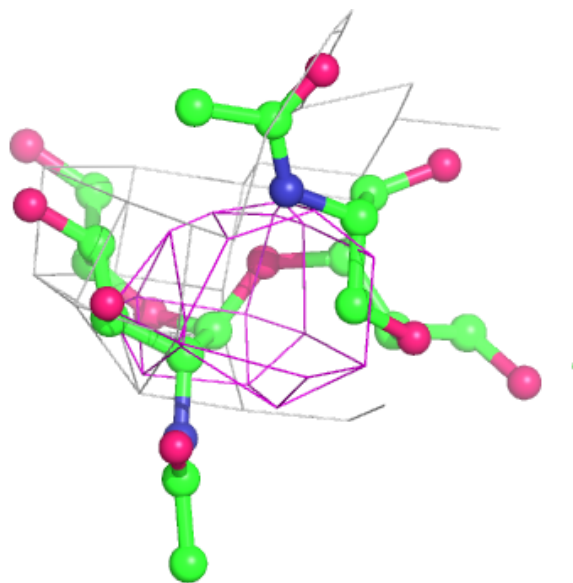
Electron density around Chain I:

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



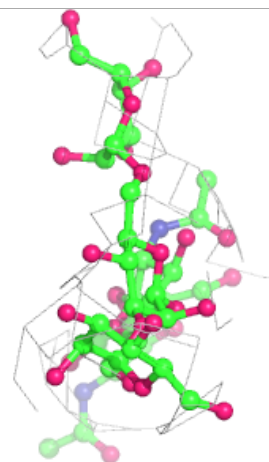
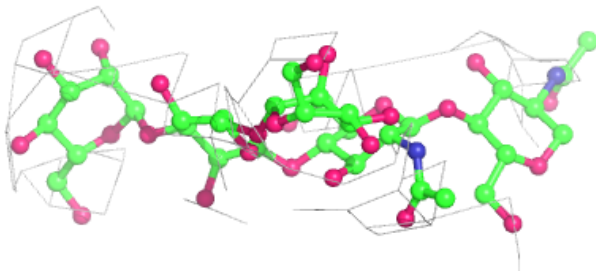
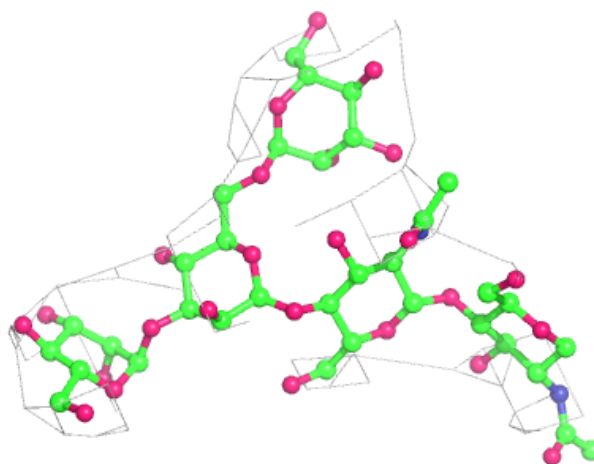
Electron density around Chain J:

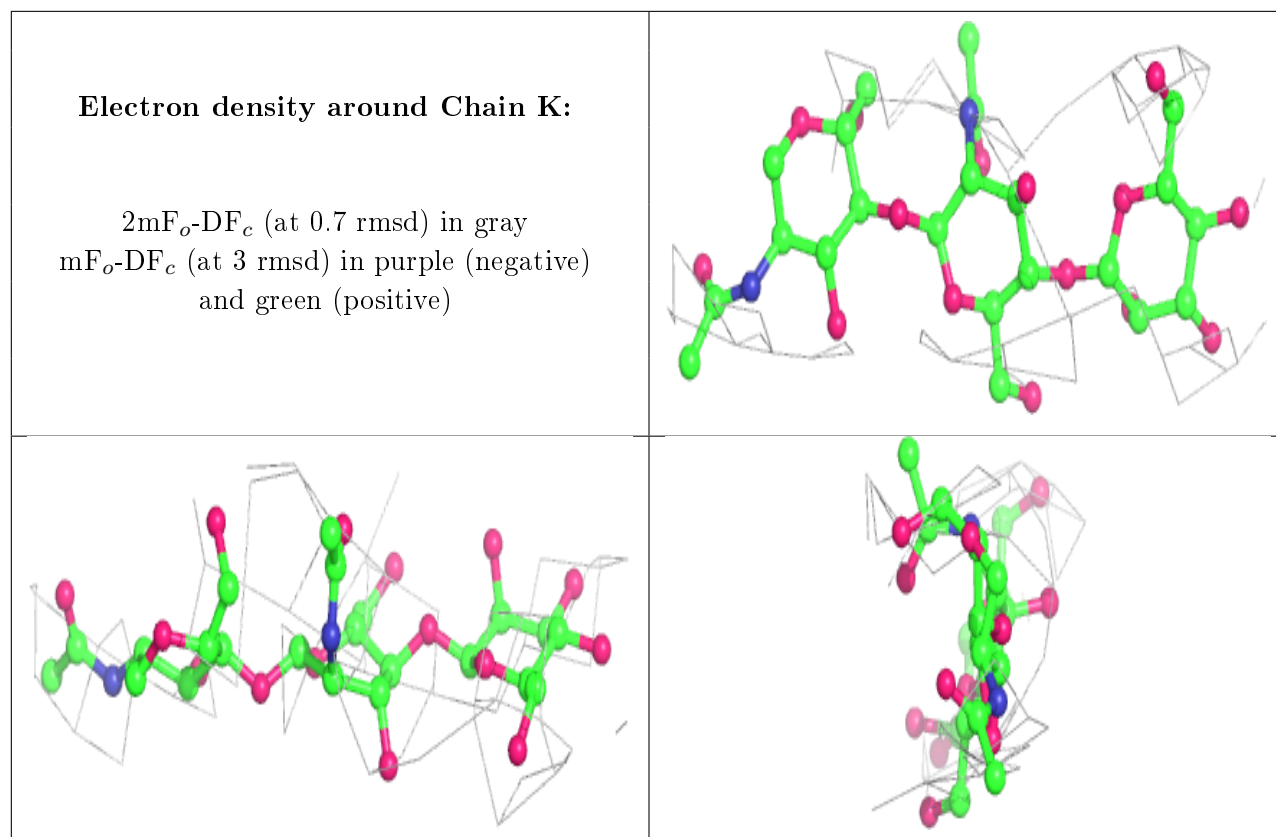
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain M:

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





6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.