



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 07:18 AM BST

PDB ID : 5ESZ
Title : Crystal Structure of Broadly Neutralizing Antibody CH04, Isolated from Donor CH0219, in Complex with Scaffolded Trimeric HIV-1 Env V1V2 Domain from the Clade AE Strain A244
Authors : Gorman, J.; Yang, M.; Kwong, P.D.
Deposited on : 2015-11-17
Resolution : 4.19 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

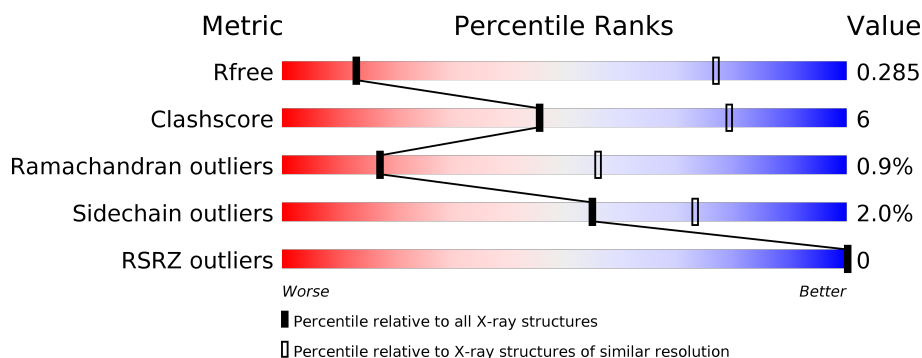
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.19 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	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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	244	
1	H	244	
2	B	215	
2	L	215	
3	C	222	
3	G	222	

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Mol	Chain	Length	Quality of chain
4	D	5	
5	E	2	
5	I	2	
6	F	6	
7	J	7	
8	K	4	

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	2	-	-	-	X
6	NAG	F	1	-	-	-	X
6	NAG	F	2	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9244 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 CH04 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	229	Total	C	N	O	S	0	0	0
			1735	1097	296	337	5			
1	A	212	Total	C	N	O	S	0	0	0
			1620	1026	276	313	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	219	GLY	-	expression tag	UNP A0A087WYE1
H	220	LEU	-	expression tag	UNP A0A087WYE1
H	221	GLU	-	expression tag	UNP A0A087WYE1
H	222	VAL	-	expression tag	UNP A0A087WYE1
H	223	LEU	-	expression tag	UNP A0A087WYE1
H	224	PHE	-	expression tag	UNP A0A087WYE1
A	219	GLY	-	expression tag	UNP A0A087WYE1
A	220	LEU	-	expression tag	UNP A0A087WYE1
A	221	GLU	-	expression tag	UNP A0A087WYE1
A	222	VAL	-	expression tag	UNP A0A087WYE1
A	223	LEU	-	expression tag	UNP A0A087WYE1
A	224	PHE	-	expression tag	UNP A0A087WYE1

- Molecule 2 is a protein called CH04 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1660	1039	288	329	4			
2	B	211	Total	C	N	O	S	0	0	0
			1636	1023	284	325	4			

- Molecule 3 is a protein called 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase,Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	163	Total 1199	C 749	N 217	O 225	S 8	0	0	0
3	G	142	Total 1072	C 665	N 197	O 203	S 7	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

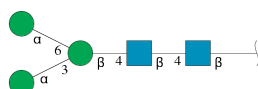
Chain	Residue	Modelled	Actual	Comment	Reference
C	111	SER	-	expression tag	UNP P44815
C	112	LEU	MET	conflict	UNP P44815
C	198	GLY	-	linker	UNP Q4QX31
C	199	GLY	-	linker	UNP Q4QX31
C	200	SER	-	linker	UNP Q4QX31
C	201	GLY	-	linker	UNP Q4QX31
C	?	-	ASP	deletion	UNP P44815
C	?	-	THR	deletion	UNP P44815
C	?	-	ASP	deletion	UNP P44815
C	?	-	MET	deletion	UNP P44815
C	?	-	GLN	deletion	UNP P44815
C	?	-	TYR	deletion	UNP P44815
C	317	GLY	-	expression tag	UNP P44815
C	318	LEU	-	expression tag	UNP P44815
C	319	GLU	-	expression tag	UNP P44815
C	320	VAL	-	expression tag	UNP P44815
C	321	LEU	-	expression tag	UNP P44815
C	322	PHE	-	expression tag	UNP P44815
C	323	GLN	-	expression tag	UNP P44815
G	111	SER	-	expression tag	UNP P44815
G	112	LEU	MET	conflict	UNP P44815
G	198	GLY	-	linker	UNP Q4QX31
G	199	GLY	-	linker	UNP Q4QX31
G	200	SER	-	linker	UNP Q4QX31
G	201	GLY	-	linker	UNP Q4QX31
G	?	-	ASP	deletion	UNP P44815
G	?	-	THR	deletion	UNP P44815
G	?	-	ASP	deletion	UNP P44815
G	?	-	MET	deletion	UNP P44815
G	?	-	GLN	deletion	UNP P44815
G	?	-	TYR	deletion	UNP P44815
G	317	GLY	-	expression tag	UNP P44815
G	318	LEU	-	expression tag	UNP P44815
G	319	GLU	-	expression tag	UNP P44815
G	320	VAL	-	expression tag	UNP P44815

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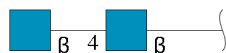
Chain	Residue	Modelled	Actual	Comment	Reference
G	321	LEU	-	expression tag	UNP P44815
G	322	PHE	-	expression tag	UNP P44815
G	323	GLN	-	expression tag	UNP P44815

- Molecule 4 is an oligosaccharide called 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.



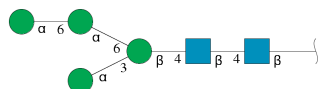
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



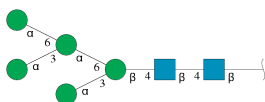
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
6	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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			
7	J	7	83	46	2	35	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

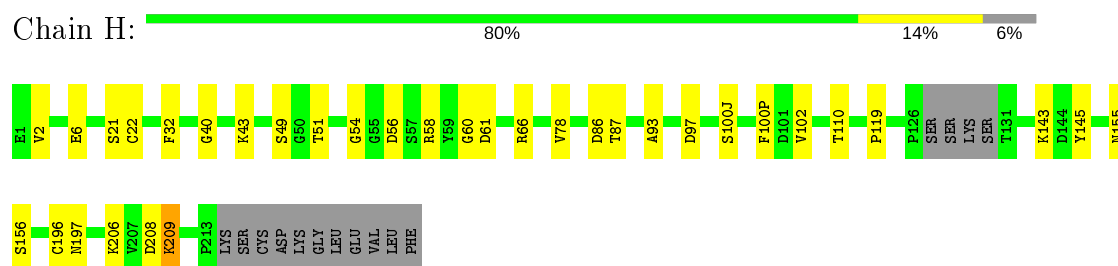


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	K	4	50	28	2	20	0	0	0

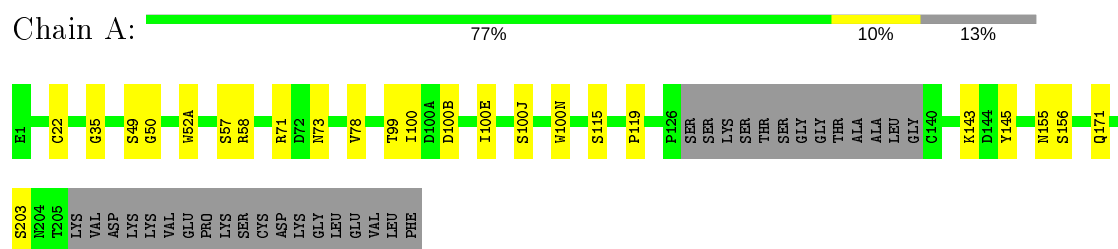
3 Residue-property plots [i](#)

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.

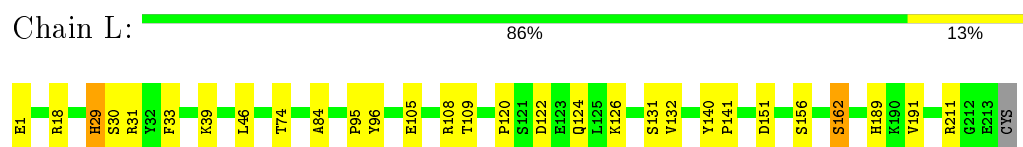
- Molecule 1: CH04 Heavy Chain



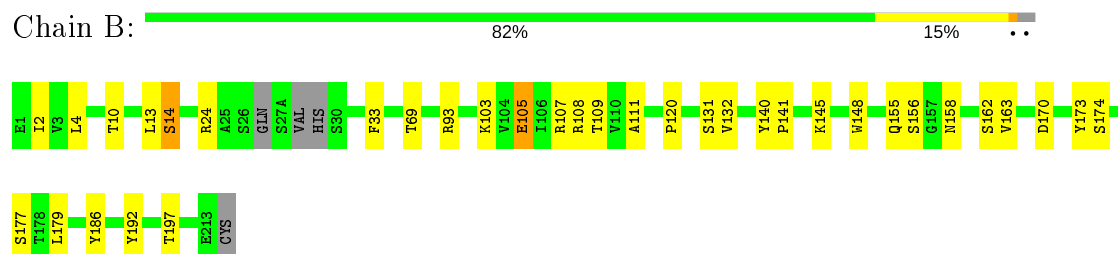
- Molecule 1: CH04 Heavy Chain



- Molecule 2: CH04 Light Chain

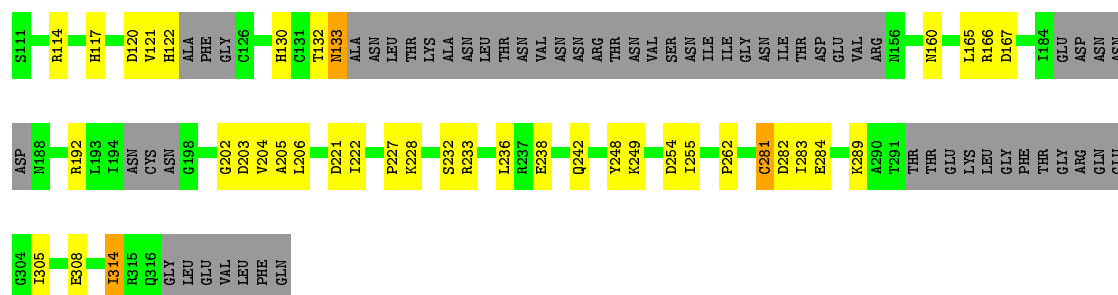


- Molecule 2: CH04 Light Chain



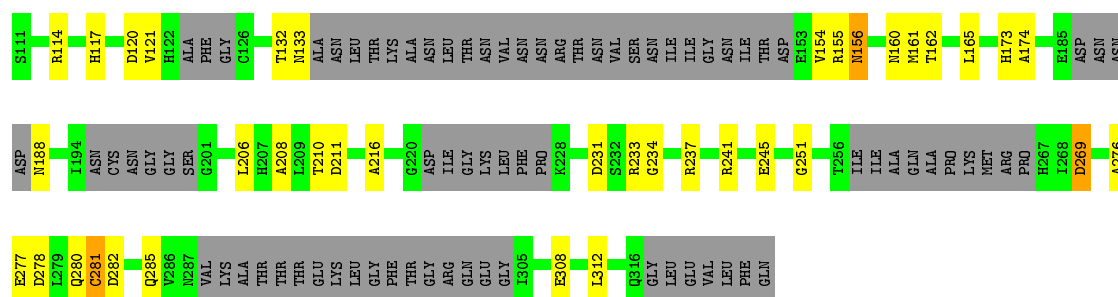
- Molecule 3: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase,Envelope glycoprotein gp160

Chain C: 



- Molecule 3: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase,Envelope glycoprotein gp160

Chain G: 



- Molecule 4: 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 D: 



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

Chain E: 



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

Chain I: 



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

Chain F:  67% 33%




- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  25% 25% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	116.72Å 116.72Å 249.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.77 – 4.19 47.77 – 4.19	Depositor EDS
% Data completeness (in resolution range)	92.3 (47.77-4.19) 92.3 (47.77-4.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 4.14Å)	Xtriage
Refinement program	PHENIX (dev_2243: ???)	Depositor
R, R_{free}	0.252 , 0.282 0.262 , 0.285	Depositor DCC
R_{free} test set	667 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , -62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.299 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	9244	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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	0.28	0/1664	0.50	0/2264
1	H	0.28	0/1780	0.51	0/2420
2	B	0.27	0/1672	0.52	0/2268
2	L	0.27	0/1699	0.50	0/2308
3	C	0.29	0/1208	0.50	0/1628
3	G	0.29	0/1076	0.47	0/1443
All	All	0.28	0/9099	0.50	0/12331

There are no bond length outliers.

There are no bond angle outliers.

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	1620	0	1542	18	0
1	H	1735	0	1665	20	0
2	B	1636	0	1575	19	0
2	L	1660	0	1601	16	0
3	C	1199	0	1179	23	1
3	G	1072	0	1050	22	0
4	D	61	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	28	0	25	1	0
5	I	28	0	25	5	0
6	F	72	0	61	3	0
7	J	83	0	70	2	0
8	K	50	0	43	4	0
All	All	9244	0	8888	116	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 6.

The worst 5 of 116 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)
5:I:1:NAG:O3	5:I:1:NAG:O7	1.99	0.79
3:G:117:HIS:NE2	3:G:308:GLU:OE1	2.18	0.77
3:C:281:CYS:SG	3:C:282:ASP:N	2.56	0.76
3:C:282:ASP:OD2	3:C:283:ILE:N	2.22	0.72
1:A:143:LYS:NZ	1:A:171:GLN:OE1	2.23	0.71

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)
3:C:114:ARG:NH2	3:C:284:GLU:O[3_475]	2.17	0.03

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	208/244 (85%)	201 (97%)	7 (3%)	0	100	100
1	H	225/244 (92%)	220 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	206/215 (96%)	197 (96%)	8 (4%)	1 (0%)	29	68
2	L	212/215 (99%)	202 (95%)	8 (4%)	2 (1%)	17	56
3	C	151/222 (68%)	117 (78%)	29 (19%)	5 (3%)	4	30
3	G	126/222 (57%)	103 (82%)	21 (17%)	2 (2%)	9	45
All	All	1128/1362 (83%)	1040 (92%)	78 (7%)	10 (1%)	17	56

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	30	SER
3	C	166	ARG
3	C	221	ASP
3	C	222	ILE
3	C	262	PRO

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	178/204 (87%)	178 (100%)	0	100	100
1	H	190/204 (93%)	188 (99%)	2 (1%)	73	84
2	B	181/186 (97%)	177 (98%)	4 (2%)	52	70
2	L	184/186 (99%)	179 (97%)	5 (3%)	44	66
3	C	121/183 (66%)	117 (97%)	4 (3%)	38	61
3	G	111/183 (61%)	107 (96%)	4 (4%)	35	60
All	All	965/1146 (84%)	946 (98%)	19 (2%)	55	73

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	192	ARG
3	C	314	ILE

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Mol	Chain	Res	Type
2	B	14	SER
3	C	133	ASN
2	B	33	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	70	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

26 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	$\# Z > 2$
4	NAG	D	1	4	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	D	2	4	14,14,15	0.20	0	17,19,21	0.44	0
4	BMA	D	3	4	11,11,12	0.63	0	15,15,17	0.71	0
4	MAN	D	4	4	11,11,12	1.10	1 (9%)	15,15,17	1.74	5 (33%)
4	MAN	D	5	4	11,11,12	0.52	0	15,15,17	1.01	2 (13%)
5	NAG	E	1	3,5	14,14,15	0.54	0	17,19,21	0.79	0
5	NAG	E	2	5	14,14,15	0.33	0	17,19,21	0.36	0
6	NAG	F	1	3,6	14,14,15	0.88	1 (7%)	17,19,21	0.68	0
6	NAG	F	2	6	14,14,15	0.23	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	F	3	6	11,11,12	0.96	0	15,15,17	1.44	1 (6%)
6	MAN	F	4	6	11,11,12	0.97	1 (9%)	15,15,17	1.41	4 (26%)
6	MAN	F	5	6	11,11,12	0.67	0	15,15,17	1.08	2 (13%)
6	MAN	F	6	6	11,11,12	1.12	1 (9%)	15,15,17	1.41	2 (13%)
5	NAG	I	1	3,5	14,14,15	1.01	1 (7%)	17,19,21	1.36	1 (5%)
5	NAG	I	2	5	14,14,15	0.20	0	17,19,21	0.67	1 (5%)
7	NAG	J	1	3,7	14,14,15	0.47	0	17,19,21	0.75	0
7	NAG	J	2	7	14,14,15	0.31	0	17,19,21	0.59	0
7	BMA	J	3	7	11,11,12	1.04	1 (9%)	15,15,17	1.48	3 (20%)
7	MAN	J	4	7	11,11,12	0.68	0	15,15,17	1.16	1 (6%)
7	MAN	J	5	7	11,11,12	0.94	1 (9%)	15,15,17	1.47	3 (20%)
7	MAN	J	6	7	11,11,12	0.66	0	15,15,17	0.99	1 (6%)
7	MAN	J	7	7	11,11,12	1.18	1 (9%)	15,15,17	1.00	1 (6%)
8	NAG	K	1	8	14,14,15	0.33	0	17,19,21	0.37	0
8	NAG	K	2	8	14,14,15	0.33	0	17,19,21	0.52	0
8	BMA	K	3	8	11,11,12	1.07	0	15,15,17	1.14	2 (13%)
8	MAN	K	4	8	11,11,12	1.05	1 (9%)	15,15,17	1.34	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
4	NAG	D	1	4	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1
6	NAG	F	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	3/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	MAN	F	4	6	-	0/2/19/22	0/1/1/1
6	MAN	F	5	6	-	2/2/19/22	0/1/1/1
6	MAN	F	6	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
7	NAG	J	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	4/6/23/26	0/1/1/1
7	BMA	J	3	7	-	2/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	0/1/1/1
7	MAN	J	5	7	-	1/2/19/22	0/1/1/1
7	MAN	J	6	7	-	1/2/19/22	0/1/1/1
7	MAN	J	7	7	-	1/2/19/22	1/1/1/1
8	NAG	K	1	8	-	2/6/23/26	0/1/1/1
8	NAG	K	2	8	-	4/6/23/26	0/1/1/1
8	BMA	K	3	8	-	0/2/19/22	0/1/1/1
8	MAN	K	4	8	-	0/2/19/22	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	7	MAN	C1-C2	3.50	1.60	1.52
5	I	1	NAG	C1-C2	3.44	1.57	1.52
4	D	4	MAN	C1-C2	2.90	1.58	1.52
7	J	5	MAN	C1-C2	2.82	1.58	1.52
6	F	4	MAN	C1-C2	2.77	1.58	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	NAG	C1-O5-C5	5.12	119.13	112.19
7	J	5	MAN	C1-O5-C5	3.99	117.59	112.19
8	K	4	MAN	C1-O5-C5	3.90	117.47	112.19
7	J	3	BMA	C1-C2-C3	3.84	114.38	109.67
4	D	4	MAN	O5-C1-C2	3.49	116.16	110.77

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	3	BMA	C4-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
6	F	6	MAN	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	F	5	MAN	O5-C5-C6-O6

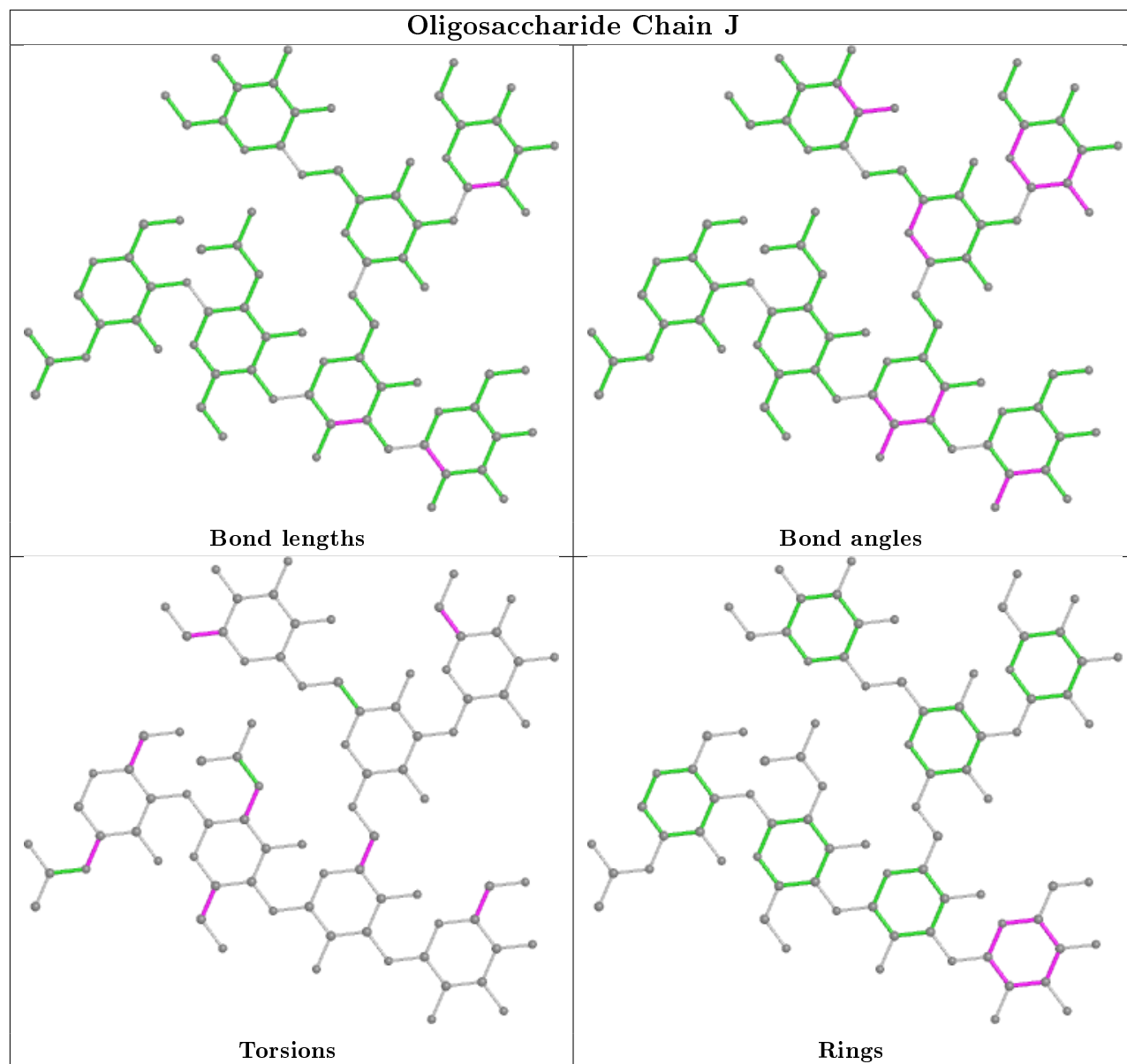
All (1) ring outliers are listed below:

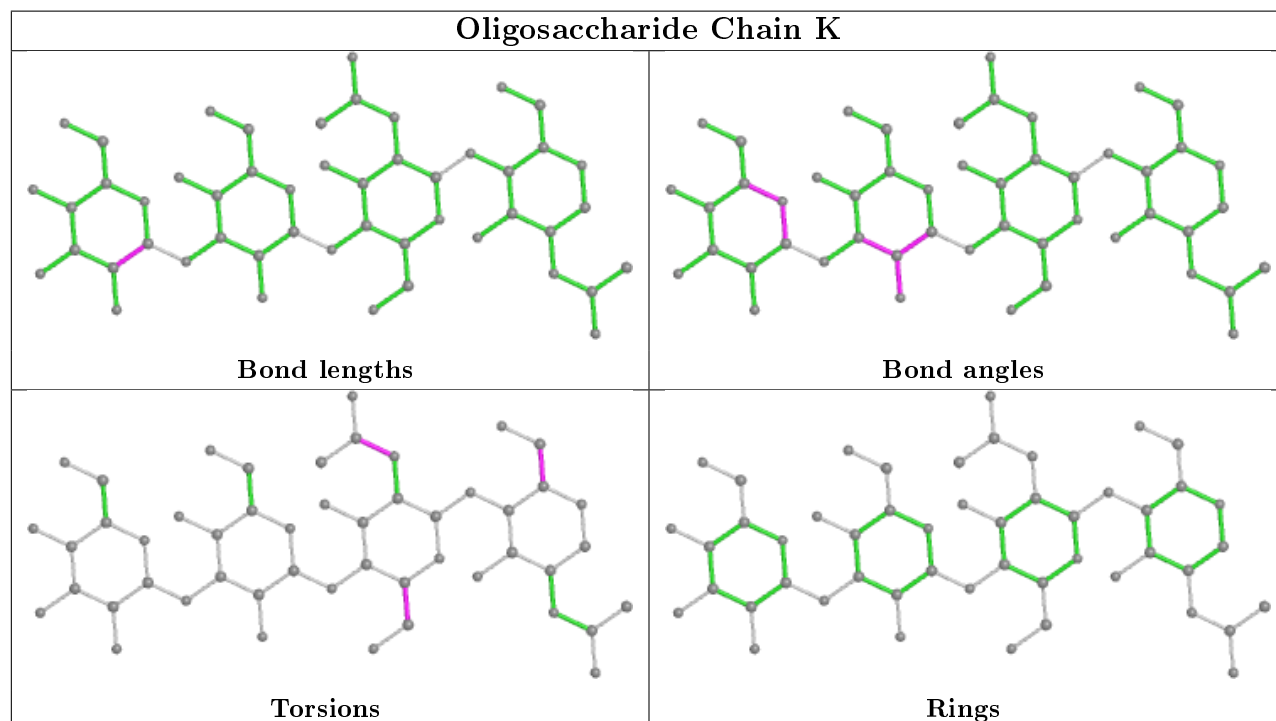
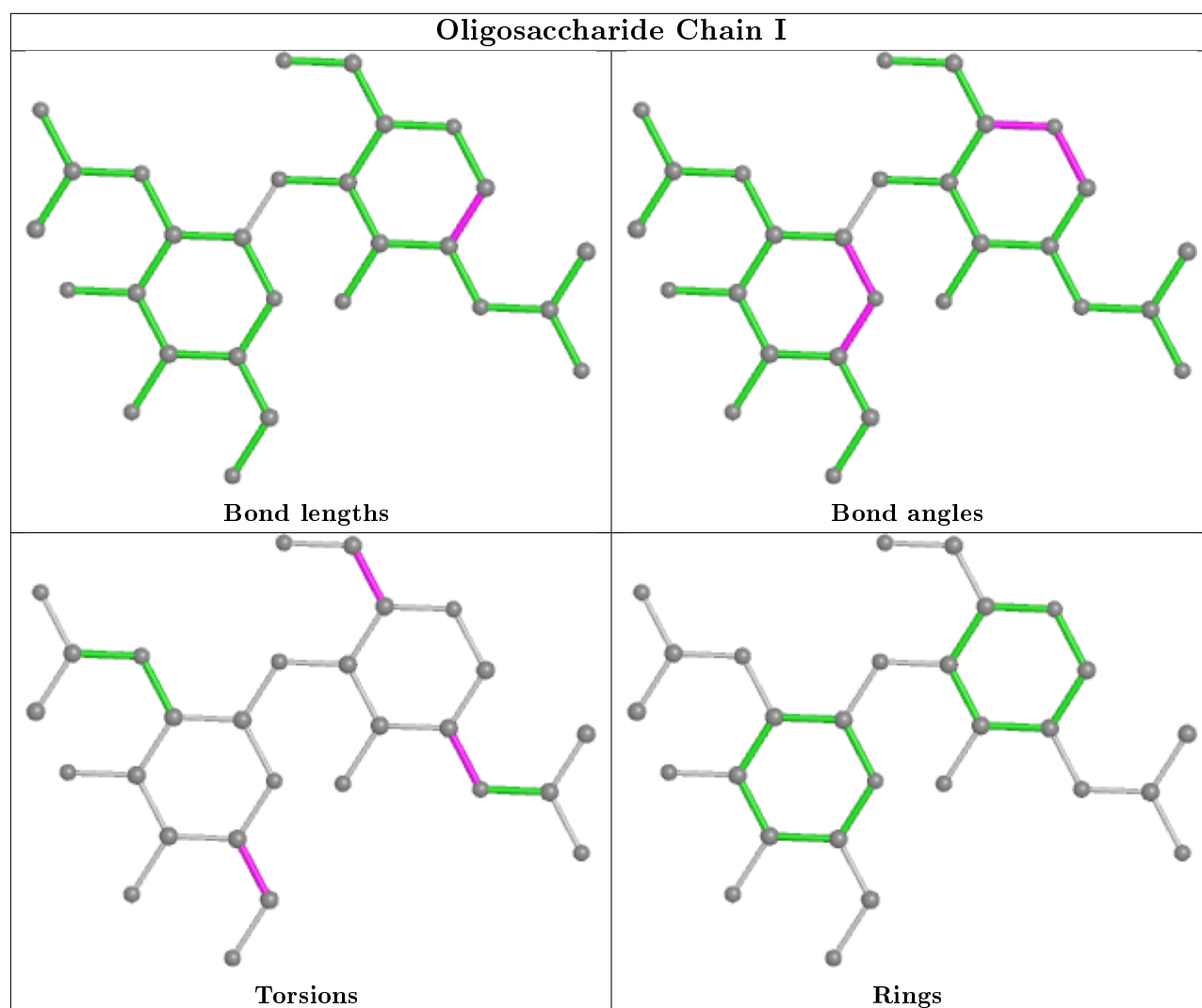
Mol	Chain	Res	Type	Atoms
7	J	7	MAN	C1-C2-C3-C4-C5-O5

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	1	NAG	1	0
8	K	4	MAN	2	0
6	F	1	NAG	2	0
5	I	1	NAG	5	0
6	F	2	NAG	1	0
8	K	3	BMA	1	0
7	J	2	NAG	1	0
5	E	2	NAG	1	0
8	K	2	NAG	2	0
6	F	3	BMA	1	0
4	D	4	MAN	1	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 ⓘ

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	212/244 (86%)	-0.37	0 100 100	68, 86, 109, 122	0
1	H	229/244 (93%)	-0.59	0 100 100	15, 57, 89, 124	0
2	B	211/215 (98%)	-0.37	0 100 100	67, 95, 122, 148	0
2	L	214/215 (99%)	-0.57	0 100 100	49, 65, 96, 120	0
3	C	163/222 (73%)	-0.41	0 100 100	7, 39, 114, 152	0
3	G	142/222 (63%)	-0.22	0 100 100	65, 93, 115, 130	0
All	All	1171/1362 (85%)	-0.44	0 100 100	7, 78, 113, 152	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

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	0.67	0.45	66,68,72,72	0
6	NAG	F	1	14/15	0.71	0.42	60,60,63,65	0
4	MAN	D	5	11/12	0.75	0.38	60,60,60,61	0
6	NAG	F	2	14/15	0.76	0.51	63,71,77,80	0
8	NAG	K	2	14/15	0.80	0.34	69,72,75,75	0
6	BMA	F	3	11/12	0.80	0.26	65,69,72,72	0

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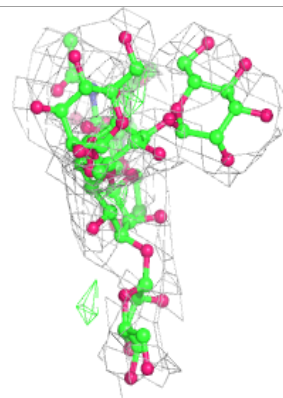
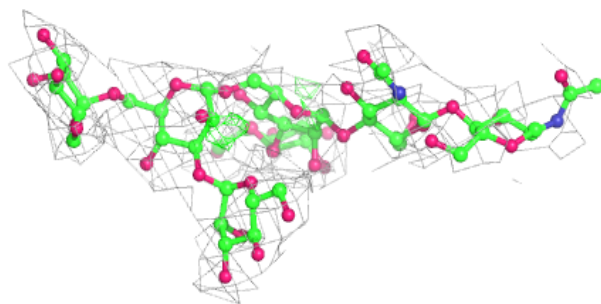
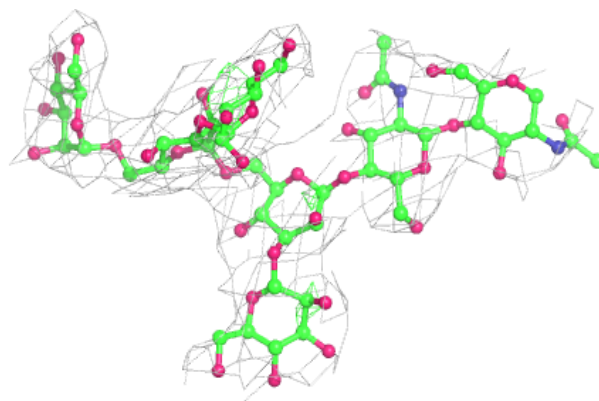
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MAN	F	4	11/12	0.83	0.25	62,63,64,64	0
5	NAG	I	2	14/15	0.84	0.30	63,66,70,70	0
8	NAG	K	1	14/15	0.85	0.38	66,69,76,77	0
6	MAN	F	5	11/12	0.85	0.29	63,64,64,65	0
7	MAN	J	6	11/12	0.86	0.32	60,60,60,60	0
7	MAN	J	7	11/12	0.87	0.23	66,66,69,69	0
7	MAN	J	4	11/12	0.88	0.18	60,60,61,62	0
5	NAG	E	1	14/15	0.88	0.38	60,60,62,63	0
6	MAN	F	6	11/12	0.90	0.22	72,72,73,73	0
5	NAG	I	1	14/15	0.90	0.17	60,60,65,70	0
4	BMA	D	3	11/12	0.90	0.17	60,60,60,61	0
4	NAG	D	2	14/15	0.90	0.27	60,61,62,62	0
8	BMA	K	3	11/12	0.90	0.18	65,69,71,72	0
4	MAN	D	4	11/12	0.90	0.19	63,63,66,68	0
4	NAG	D	1	14/15	0.90	0.30	60,61,66,67	0
7	BMA	J	3	11/12	0.91	0.19	60,61,63,65	0
7	NAG	J	2	14/15	0.91	0.20	60,60,60,60	0
7	MAN	J	5	11/12	0.91	0.22	63,64,65,65	0
8	MAN	K	4	11/12	0.92	0.17	60,60,61,62	0
7	NAG	J	1	14/15	0.96	0.19	60,64,74,75	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.

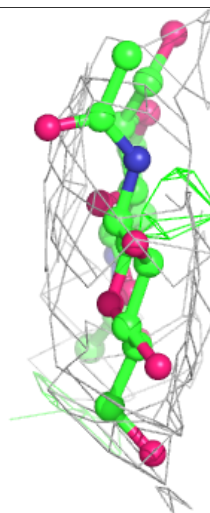
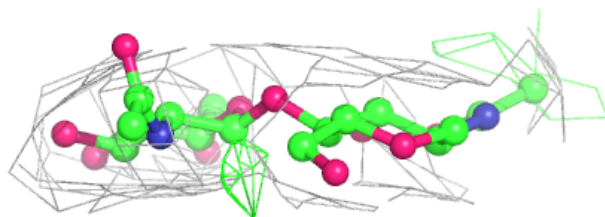
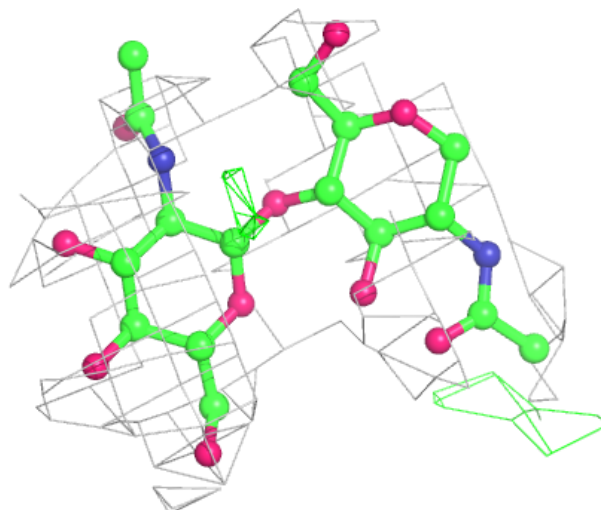
Electron density around Chain J:

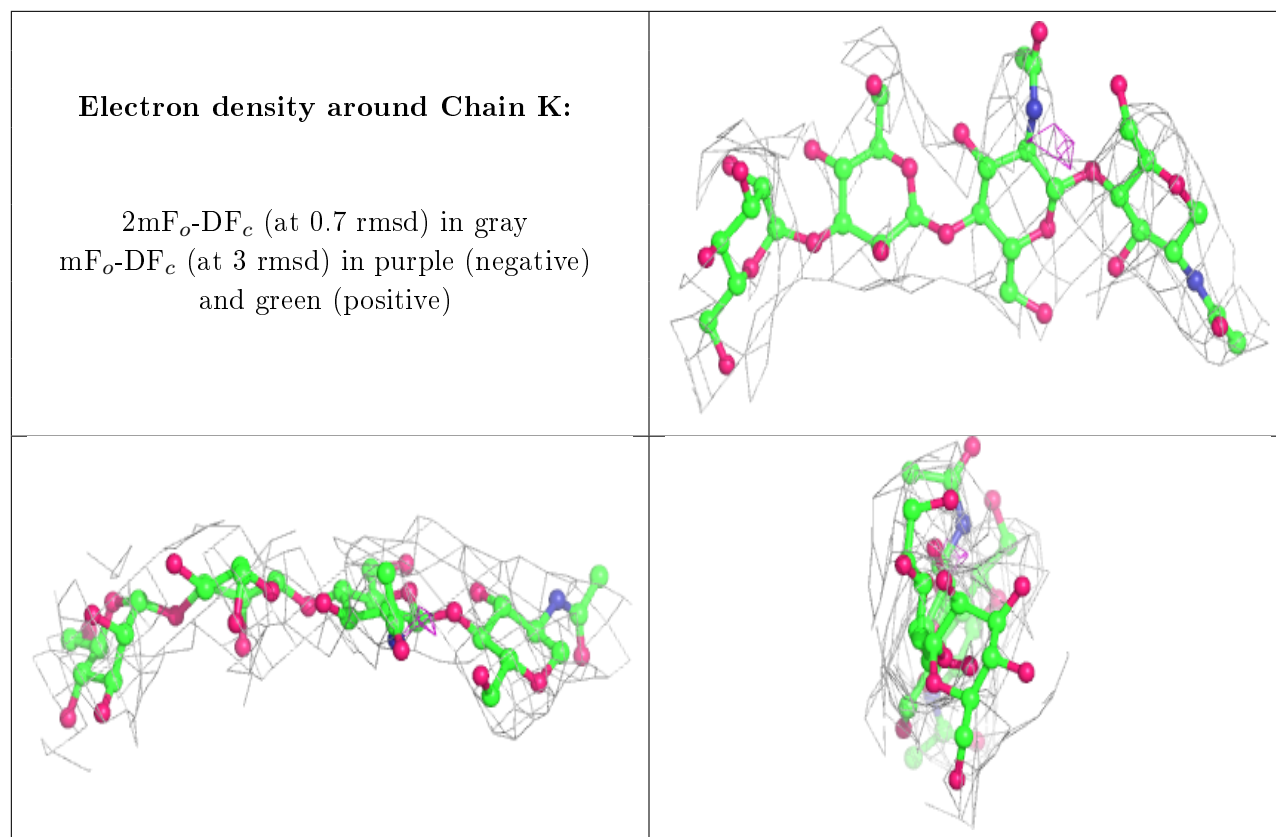
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.