



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 10:37 AM UTC

PDB ID : 4GKO / pdb_00004gko
Title : Crystal structure of the calcium²⁺-bound human IgE-Fc(epsilon)3-4 bound to its B cell receptor derCD23
Authors : Yuan, D.; Sutton, B.J.; Dhaliwal, B.
Deposited on : 2012-08-13
Resolution : 3.30 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

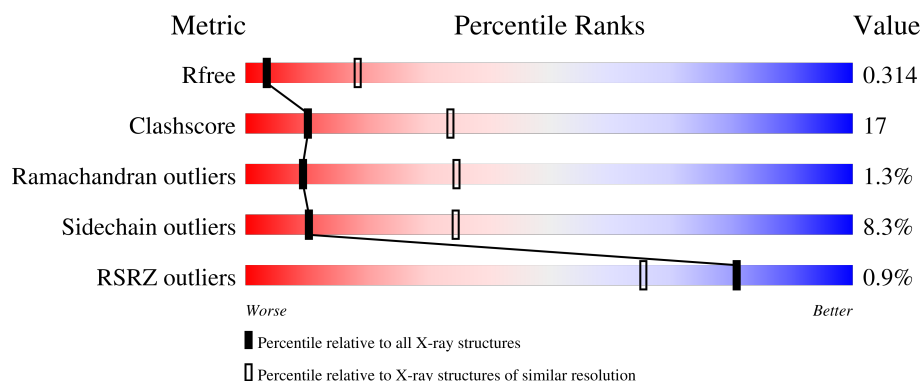
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



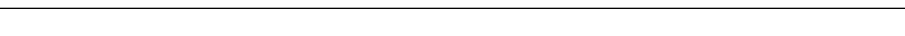
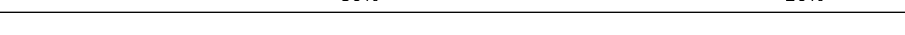
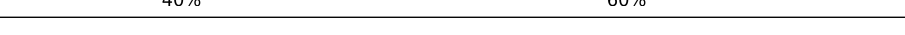
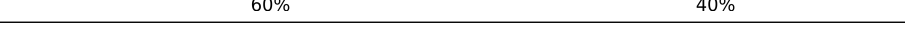
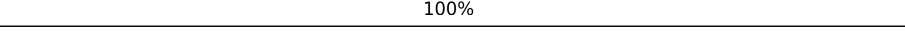
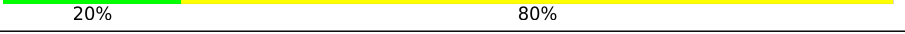
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	223	60% 30% 6%
1	B	223	69% 21% 7%
1	C	223	2% 50% 32% 6% 12%
1	D	223	55% 26% 15%
1	E	223	2% 58% 19% 19%

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Mol	Chain	Length	Quality of chain
1	F	223	
2	G	143	
2	H	143	
2	I	143	
2	J	143	
2	K	143	
2	L	143	
3	M	5	
3	N	5	
3	O	5	
3	P	5	
3	Q	5	
3	R	5	

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
3	NAG	O	1	-	-	X	-
3	MAN	O	5	-	-	X	-
3	NAG	Q	1	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16217 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 Ig epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1647	1032	301	308	6			
1	B	207	Total	C	N	O	S	0	0	0
			1642	1029	303	304	6			
1	C	197	Total	C	N	O	S	0	1	0
			1565	981	284	294	6			
1	D	189	Total	C	N	O	S	0	0	0
			1499	944	272	277	6			
1	E	180	Total	C	N	O	S	0	0	0
			1414	882	261	266	5			
1	F	197	Total	C	N	O	S	0	0	0
			1570	980	292	292	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	-	expression tag	UNP P01854
A	326	ASP	-	expression tag	UNP P01854
A	327	PRO	-	expression tag	UNP P01854
A	371	GLN	ASN	conflict	UNP P01854
A	383	GLN	ASN	conflict	UNP P01854
B	325	ALA	-	expression tag	UNP P01854
B	326	ASP	-	expression tag	UNP P01854
B	327	PRO	-	expression tag	UNP P01854
B	371	GLN	ASN	conflict	UNP P01854
B	383	GLN	ASN	conflict	UNP P01854
C	325	ALA	-	expression tag	UNP P01854
C	326	ASP	-	expression tag	UNP P01854
C	327	PRO	-	expression tag	UNP P01854
C	371	GLN	ASN	conflict	UNP P01854
C	383	GLN	ASN	conflict	UNP P01854
D	325	ALA	-	expression tag	UNP P01854
D	326	ASP	-	expression tag	UNP P01854

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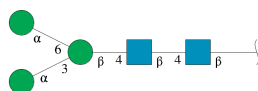
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Chain	Residue	Modelled	Actual	Comment	Reference
D	327	PRO	-	expression tag	UNP P01854
D	371	GLN	ASN	conflict	UNP P01854
D	383	GLN	ASN	conflict	UNP P01854
E	325	ALA	-	expression tag	UNP P01854
E	326	ASP	-	expression tag	UNP P01854
E	327	PRO	-	expression tag	UNP P01854
E	371	GLN	ASN	conflict	UNP P01854
E	383	GLN	ASN	conflict	UNP P01854
F	325	ALA	-	expression tag	UNP P01854
F	326	ASP	-	expression tag	UNP P01854
F	327	PRO	-	expression tag	UNP P01854
F	371	GLN	ASN	conflict	UNP P01854
F	383	GLN	ASN	conflict	UNP P01854

- Molecule 2 is a protein called Low affinity immunoglobulin epsilon Fc receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	135	Total	C	N	O	S	0	0	0
			1083	680	193	199	11			
2	H	133	Total	C	N	O	S	0	0	0
			1071	672	191	197	11			
2	I	134	Total	C	N	O	S	0	0	0
			1078	677	192	198	11			
2	J	135	Total	C	N	O	S	0	0	0
			1083	680	193	199	11			
2	K	135	Total	C	N	O	S	0	0	0
			1082	679	193	199	11			
2	L	136	Total	C	N	O	S	0	0	0
			1089	683	194	201	11			

- Molecule 3 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.



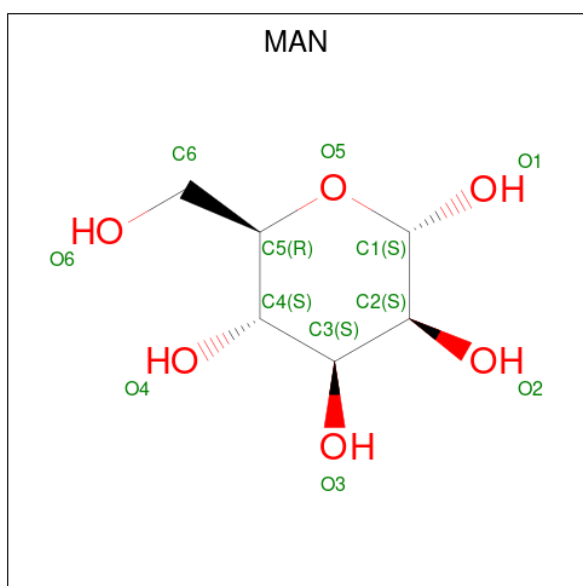
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	N	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	O	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	P	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	Q	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	R	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		

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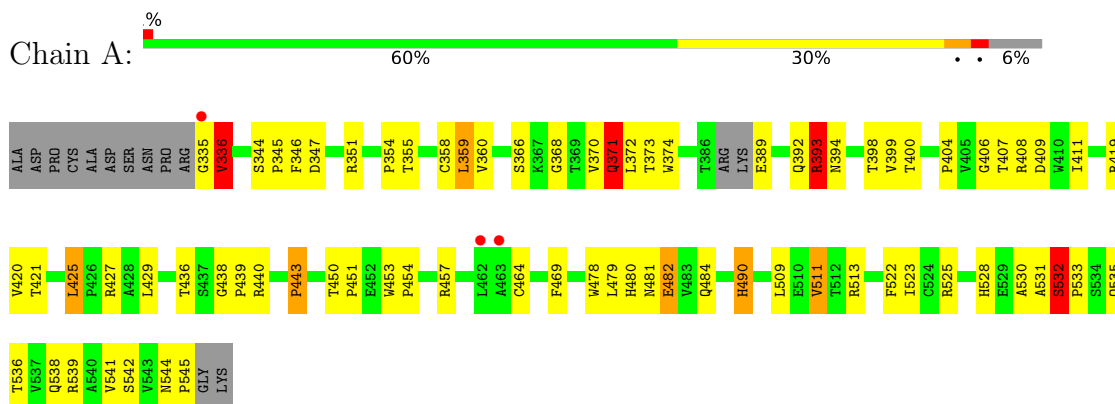
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total 1	Ca 1	0	0
5	J	1	Total 1	Ca 1	0	0
5	K	1	Total 1	Ca 1	0	0
5	L	1	Total 1	Ca 1	0	0

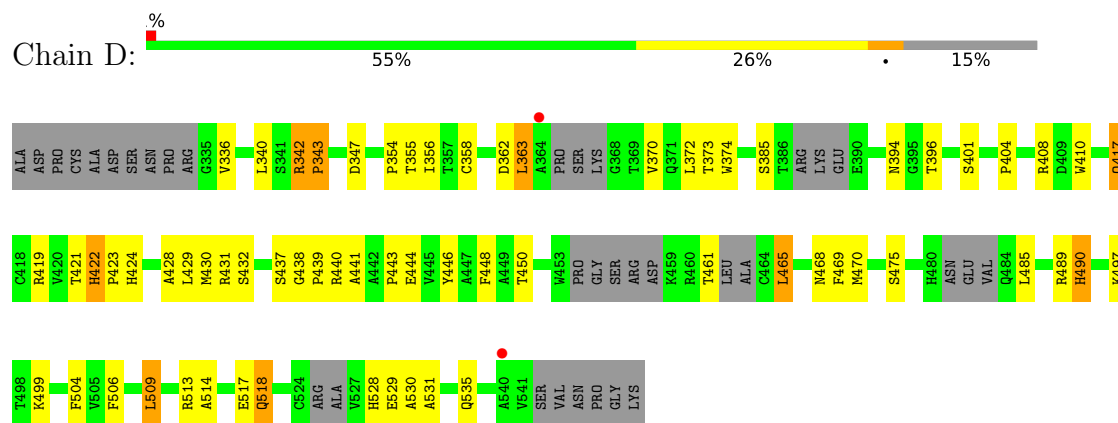
3 Residue-property plots

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.

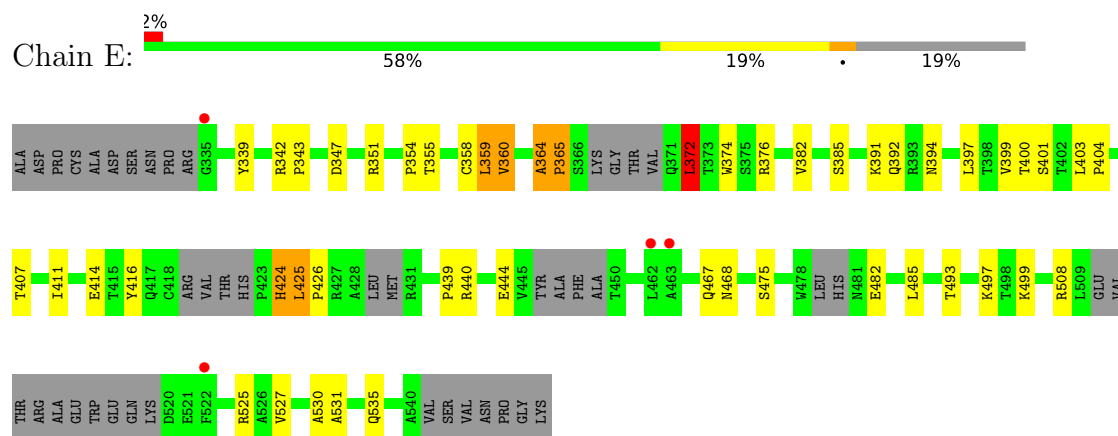
• Molecule 1: Ig epsilon chain C region



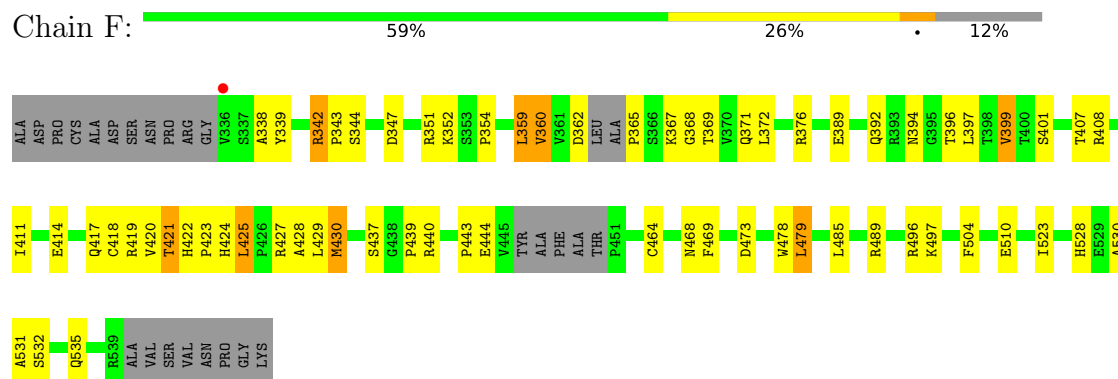
- Molecule 1: Ig epsilon chain C region



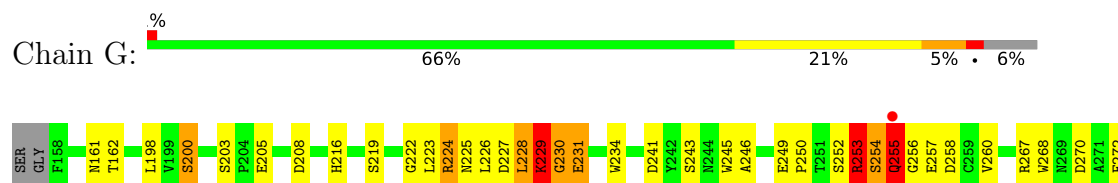
- Molecule 1: Ig epsilon chain C region

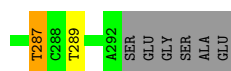


- Molecule 1: Ig epsilon chain C region

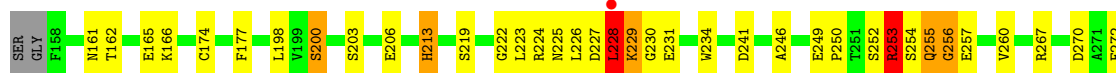


- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor





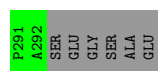
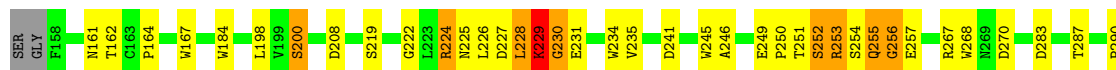
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



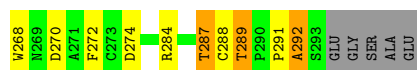
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



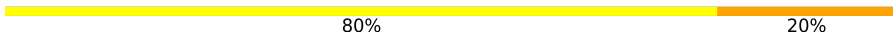
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



● Molecule 3: 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:  80% 20%

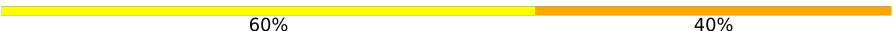


● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  40% 60%

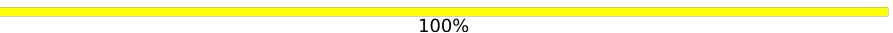


● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  60% 40%

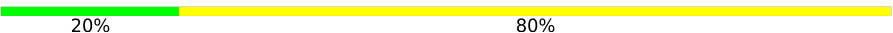


● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

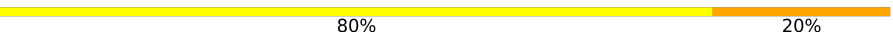


● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  20% 80%



● Molecule 3: 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 R:  80% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.83Å 110.13Å 367.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.50 – 3.30 73.50 – 3.30	Depositor EDS
% Data completeness (in resolution range)	85.1 (73.50-3.30) 85.1 (73.50-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.273 , 0.312 0.271 , 0.314	Depositor DCC
R_{free} test set	1684 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	94.9	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 111.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16217	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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: NAG, CA, MAN, 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	1.33	10/1689 (0.6%)	1.24	3/2300 (0.1%)
1	B	1.14	1/1684 (0.1%)	1.15	3/2290 (0.1%)
1	C	1.41	11/1605 (0.7%)	1.31	9/2182 (0.4%)
1	D	1.32	8/1533 (0.5%)	1.27	8/2079 (0.4%)
1	E	1.04	1/1444 (0.1%)	1.07	2/1955 (0.1%)
1	F	0.99	0/1608	1.07	8/2181 (0.4%)
2	G	1.13	1/1117 (0.1%)	1.20	3/1514 (0.2%)
2	H	1.20	1/1104 (0.1%)	1.15	3/1495 (0.2%)
2	I	1.29	2/1112 (0.2%)	1.33	12/1507 (0.8%)
2	J	1.29	3/1117 (0.3%)	1.27	3/1514 (0.2%)
2	K	0.91	0/1116	0.97	2/1512 (0.1%)
2	L	1.24	3/1123 (0.3%)	1.20	3/1522 (0.2%)
All	All	1.20	41/16252 (0.3%)	1.19	59/22051 (0.3%)

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	G	0	1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	ARG	CZ-NH2	9.64	1.46	1.33
1	C	465	LEU	C-O	-8.02	1.14	1.24
1	C	525	ARG	N-CA	6.95	1.54	1.46
1	A	532	SER	C-O	6.63	1.30	1.24
1	C	392	GLN	CA-C	-6.58	1.43	1.53

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	226	LEU	CB-CA-C	-12.10	93.52	111.91
2	I	226	LEU	CA-CB-CG	10.47	152.95	116.30
2	J	230	GLY	N-CA-C	-9.33	91.07	113.18
2	G	229	LYS	N-CA-C	-8.95	91.75	110.80
1	C	438	GLY	CA-C-N	8.75	128.79	119.78

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	255	GLN	Peptide

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	1647	0	1625	54	0
1	B	1642	0	1629	34	0
1	C	1565	0	1548	78	0
1	D	1499	0	1475	82	0
1	E	1414	0	1394	37	0
1	F	1570	0	1557	50	0
2	G	1083	0	995	52	0
2	H	1071	0	983	35	1
2	I	1078	0	991	34	1
2	J	1083	0	996	44	1
2	K	1082	0	993	37	0
2	L	1089	0	1000	49	1
3	M	61	0	52	5	0
3	N	61	0	52	4	0
3	O	61	0	52	17	0
3	P	61	0	51	2	0
3	Q	61	0	52	7	0
3	R	61	0	52	5	0
4	C	22	0	20	7	0
5	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
All	All	16217	0	15517	541	2

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 17.

The worst 5 of 541 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:I:226:LEU:O	2:I:228:LEU:N	1.65	1.28
4:C:607:MAN:C1	3:O:5:MAN:O6	1.80	1.26
1:D:417:GLN:CG	1:D:430:MET:SD	2.30	1.20
1:D:417:GLN:HG2	1:D:430:MET:CE	1.72	1.18
1:D:417:GLN:HG2	1:D:430:MET:SD	1.88	1.13

All (2) 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)
2:I:287:THR:OG1	2:L:287:THR:OG1[4_445]	1.85	0.35
2:H:287:THR:OG1	2:J:287:THR:OG1[3_345]	2.19	0.01

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	205/223 (92%)	189 (92%)	14 (7%)	2 (1%)	12 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	203/223 (91%)	187 (92%)	14 (7%)	2 (1%)	12	40
1	C	192/223 (86%)	172 (90%)	19 (10%)	1 (0%)	24	55
1	D	175/223 (78%)	165 (94%)	10 (6%)	0	100	100
1	E	166/223 (74%)	155 (93%)	9 (5%)	2 (1%)	10	37
1	F	191/223 (86%)	175 (92%)	15 (8%)	1 (0%)	24	55
2	G	133/143 (93%)	113 (85%)	17 (13%)	3 (2%)	5	25
2	H	131/143 (92%)	112 (86%)	16 (12%)	3 (2%)	5	25
2	I	132/143 (92%)	113 (86%)	15 (11%)	4 (3%)	3	20
2	J	133/143 (93%)	115 (86%)	16 (12%)	2 (2%)	8	32
2	K	133/143 (93%)	114 (86%)	17 (13%)	2 (2%)	8	32
2	L	134/143 (94%)	118 (88%)	13 (10%)	3 (2%)	5	26
All	All	1928/2196 (88%)	1728 (90%)	175 (9%)	25 (1%)	9	35

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	227	ASP
2	L	292	ALA
2	I	170	PHE
2	I	228	LEU
2	K	228	LEU

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	184/195 (94%)	167 (91%)	17 (9%)	8	30
1	B	184/195 (94%)	174 (95%)	10 (5%)	20	49
1	C	176/195 (90%)	157 (89%)	19 (11%)	6	23
1	D	167/195 (86%)	160 (96%)	7 (4%)	26	55
1	E	159/195 (82%)	149 (94%)	10 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	177/195 (91%)	164 (93%)	13 (7%)	13	39
2	G	115/120 (96%)	102 (89%)	13 (11%)	5	21
2	H	114/120 (95%)	103 (90%)	11 (10%)	8	29
2	I	115/120 (96%)	105 (91%)	10 (9%)	9	32
2	J	115/120 (96%)	104 (90%)	11 (10%)	8	29
2	K	115/120 (96%)	106 (92%)	9 (8%)	11	36
2	L	116/120 (97%)	102 (88%)	14 (12%)	5	20
All	All	1737/1890 (92%)	1593 (92%)	144 (8%)	10	34

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	228	LEU
2	L	289	THR
2	J	253	ARG
2	L	158	PHE
1	D	417	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	392	GLN
2	G	213	HIS
2	L	197	GLN
1	F	394	ASN
1	F	468	ASN

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 ⓘ

30 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	M	1	3	14,14,15	0.56	0	17,19,21	0.62	0
3	NAG	M	2	3	14,14,15	0.55	0	17,19,21	1.98	5 (29%)
3	BMA	M	3	3	11,11,12	0.83	0	15,15,17	1.81	6 (40%)
3	MAN	M	4	3	11,11,12	0.77	0	15,15,17	1.52	3 (20%)
3	MAN	M	5	3	11,11,12	0.81	0	15,15,17	1.38	3 (20%)
3	NAG	N	1	3	14,14,15	0.55	0	17,19,21	0.61	0
3	NAG	N	2	3	14,14,15	0.59	0	17,19,21	1.16	2 (11%)
3	BMA	N	3	3	11,11,12	0.31	0	15,15,17	1.33	2 (13%)
3	MAN	N	4	3	11,11,12	0.59	0	15,15,17	1.48	3 (20%)
3	MAN	N	5	3	11,11,12	0.69	0	15,15,17	1.34	3 (20%)
3	NAG	O	1	3	14,14,15	0.55	0	17,19,21	0.61	0
3	NAG	O	2	3	14,14,15	0.57	0	17,19,21	1.08	1 (5%)
3	BMA	O	3	3	11,11,12	0.60	0	15,15,17	2.14	5 (33%)
3	MAN	O	4	3	11,11,12	0.82	0	15,15,17	1.62	3 (20%)
3	MAN	O	5	3	11,11,12	1.56	2 (18%)	15,15,17	3.38	8 (53%)
3	NAG	P	1	3	14,14,15	0.56	0	17,19,21	0.62	0
3	NAG	P	2	3	14,14,15	0.86	0	17,19,21	1.76	6 (35%)
3	BMA	P	3	3	11,11,12	0.58	0	15,15,17	2.06	5 (33%)
3	MAN	P	4	3	11,11,12	1.36	1 (9%)	15,15,17	2.12	5 (33%)
3	MAN	P	5	3	11,11,12	0.48	0	15,15,17	1.42	2 (13%)
3	NAG	Q	1	3	14,14,15	0.54	0	17,19,21	0.61	0
3	NAG	Q	2	3	14,14,15	0.51	0	17,19,21	1.18	0
3	BMA	Q	3	3	11,11,12	1.00	1 (9%)	15,15,17	1.75	4 (26%)
3	MAN	Q	4	3	11,11,12	0.83	0	15,15,17	1.15	1 (6%)
3	MAN	Q	5	3	11,11,12	0.58	0	15,15,17	1.59	3 (20%)
3	NAG	R	1	3	14,14,15	0.55	0	17,19,21	0.62	0
3	NAG	R	2	3	14,14,15	0.55	0	17,19,21	1.24	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	R	3	3	11,11,12	0.88	0	15,15,17	1.70	3 (20%)
3	MAN	R	4	3	11,11,12	0.80	0	15,15,17	1.33	3 (20%)
3	MAN	R	5	3	11,11,12	0.62	0	15,15,17	1.47	4 (26%)

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	M	1	3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	BMA	M	3	3	-	2/2/19/22	0/1/1/1
3	MAN	M	4	3	-	1/2/19/22	0/1/1/1
3	MAN	M	5	3	-	2/2/19/22	0/1/1/1
3	NAG	N	1	3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	BMA	N	3	3	-	2/2/19/22	0/1/1/1
3	MAN	N	4	3	-	1/2/19/22	0/1/1/1
3	MAN	N	5	3	-	2/2/19/22	0/1/1/1
3	NAG	O	1	3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
3	MAN	O	4	3	-	1/2/19/22	0/1/1/1
3	MAN	O	5	3	-	2/2/19/22	0/1/1/1
3	NAG	P	1	3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	1/6/23/26	0/1/1/1
3	BMA	P	3	3	-	2/2/19/22	0/1/1/1
3	MAN	P	4	3	-	1/2/19/22	0/1/1/1
3	MAN	P	5	3	-	2/2/19/22	0/1/1/1
3	NAG	Q	1	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	1/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	1/2/19/22	0/1/1/1
3	MAN	Q	5	3	-	2/2/19/22	0/1/1/1
3	NAG	R	1	3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	1/6/23/26	0/1/1/1
3	BMA	R	3	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	R	4	3	-	0/2/19/22	0/1/1/1
3	MAN	R	5	3	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	5	MAN	O3-C3	3.92	1.52	1.43
3	P	4	MAN	C2-C3	3.05	1.57	1.52
3	Q	3	BMA	O5-C1	2.51	1.47	1.43
3	O	5	MAN	O6-C6	2.18	1.51	1.42

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	5	MAN	C1-C2-C3	6.63	119.30	109.64
3	O	5	MAN	O2-C2-C3	-6.44	96.82	110.15
3	P	3	BMA	O5-C5-C6	5.21	117.81	107.66
3	O	5	MAN	O3-C3-C2	-4.78	100.29	110.05
3	P	4	MAN	C2-C3-C4	-4.51	102.93	110.86

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	5	MAN	O5-C5-C6-O6
3	R	5	MAN	O5-C5-C6-O6
3	Q	5	MAN	O5-C5-C6-O6
3	N	5	MAN	O5-C5-C6-O6
3	N	3	BMA	O5-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 40 short contacts:

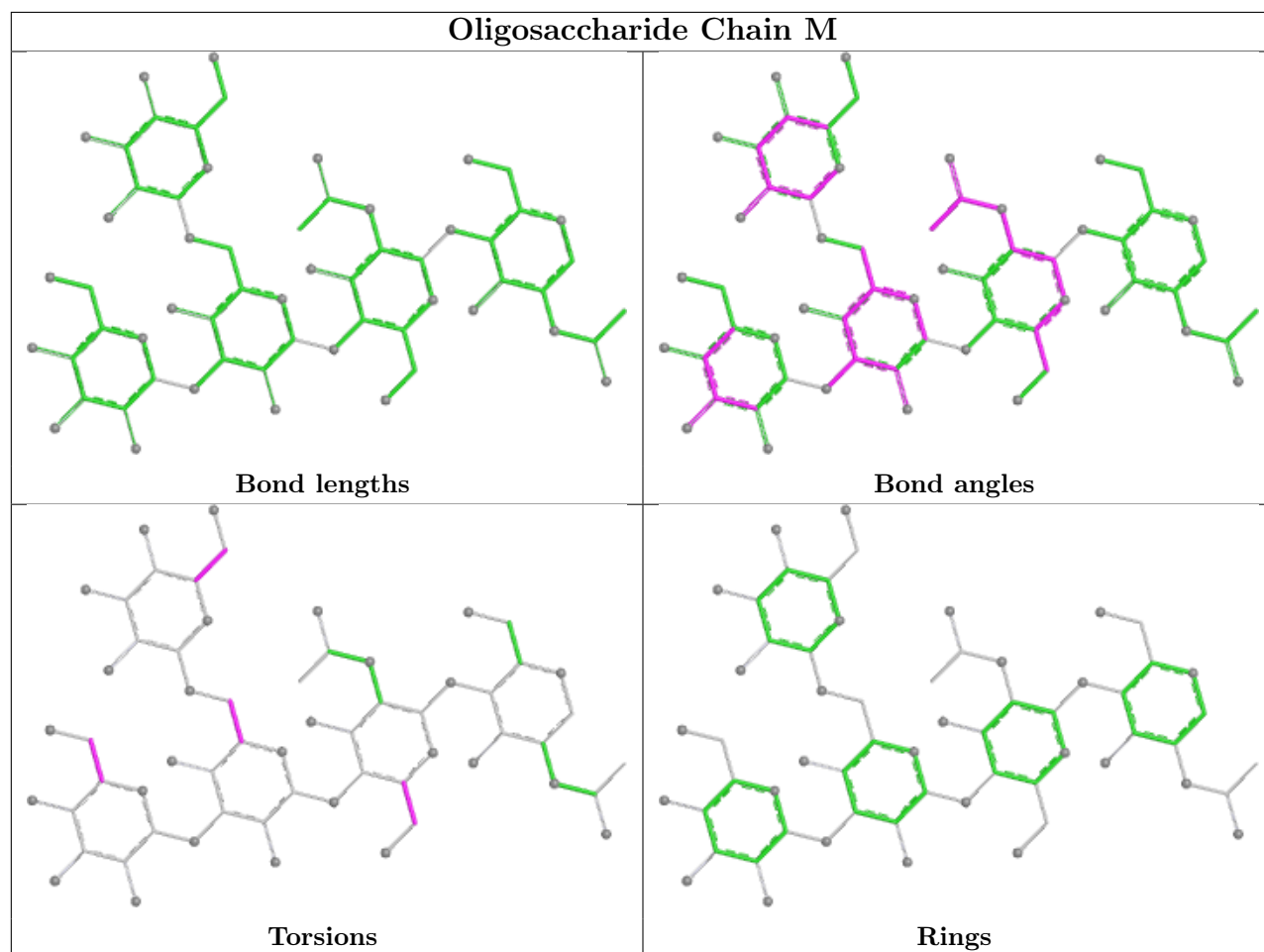
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	5	MAN	8	0
3	Q	1	NAG	7	0
3	M	1	NAG	4	0
3	R	3	BMA	2	0
3	O	1	NAG	9	0
3	N	3	BMA	1	0
3	N	2	NAG	1	0

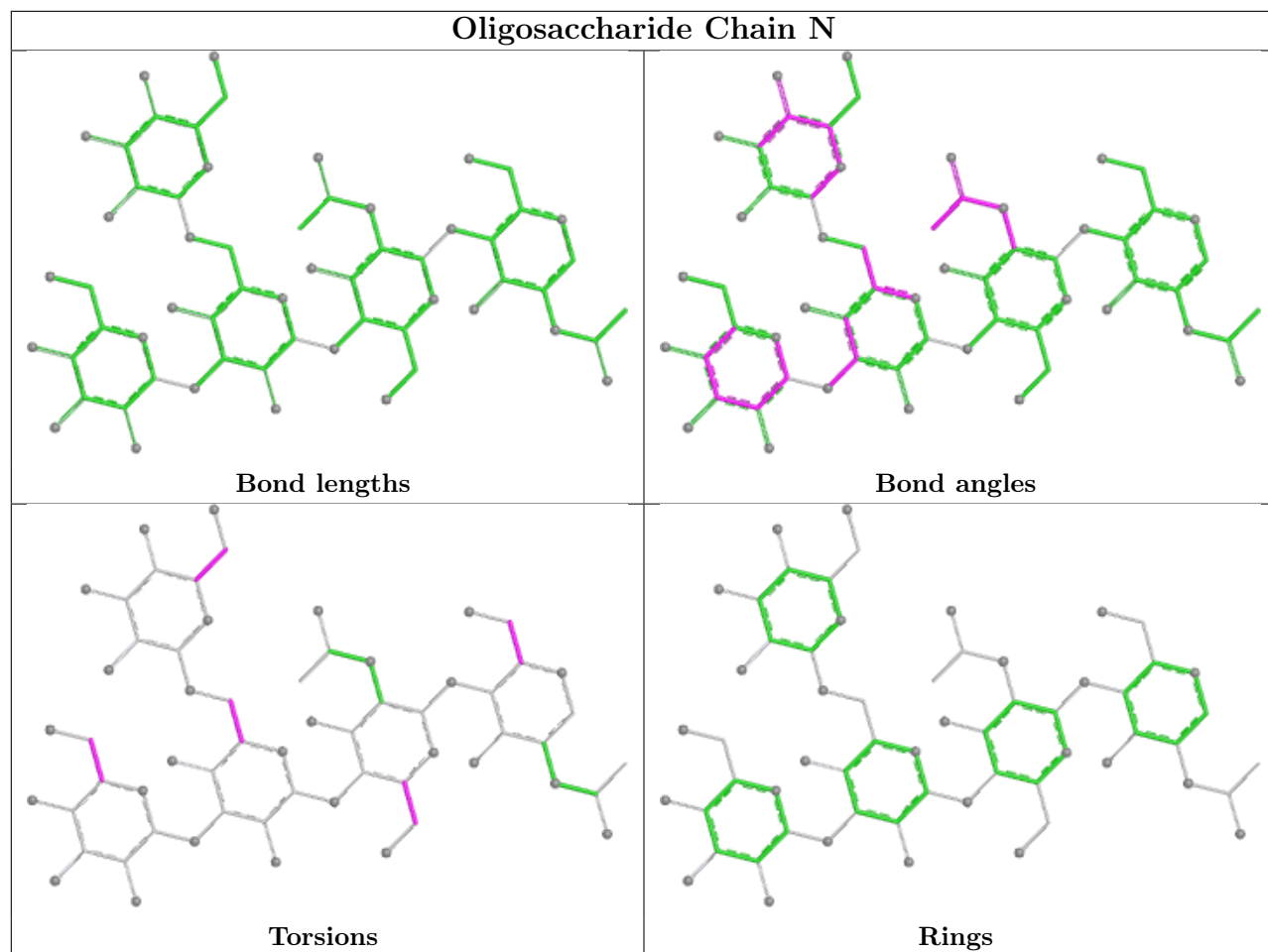
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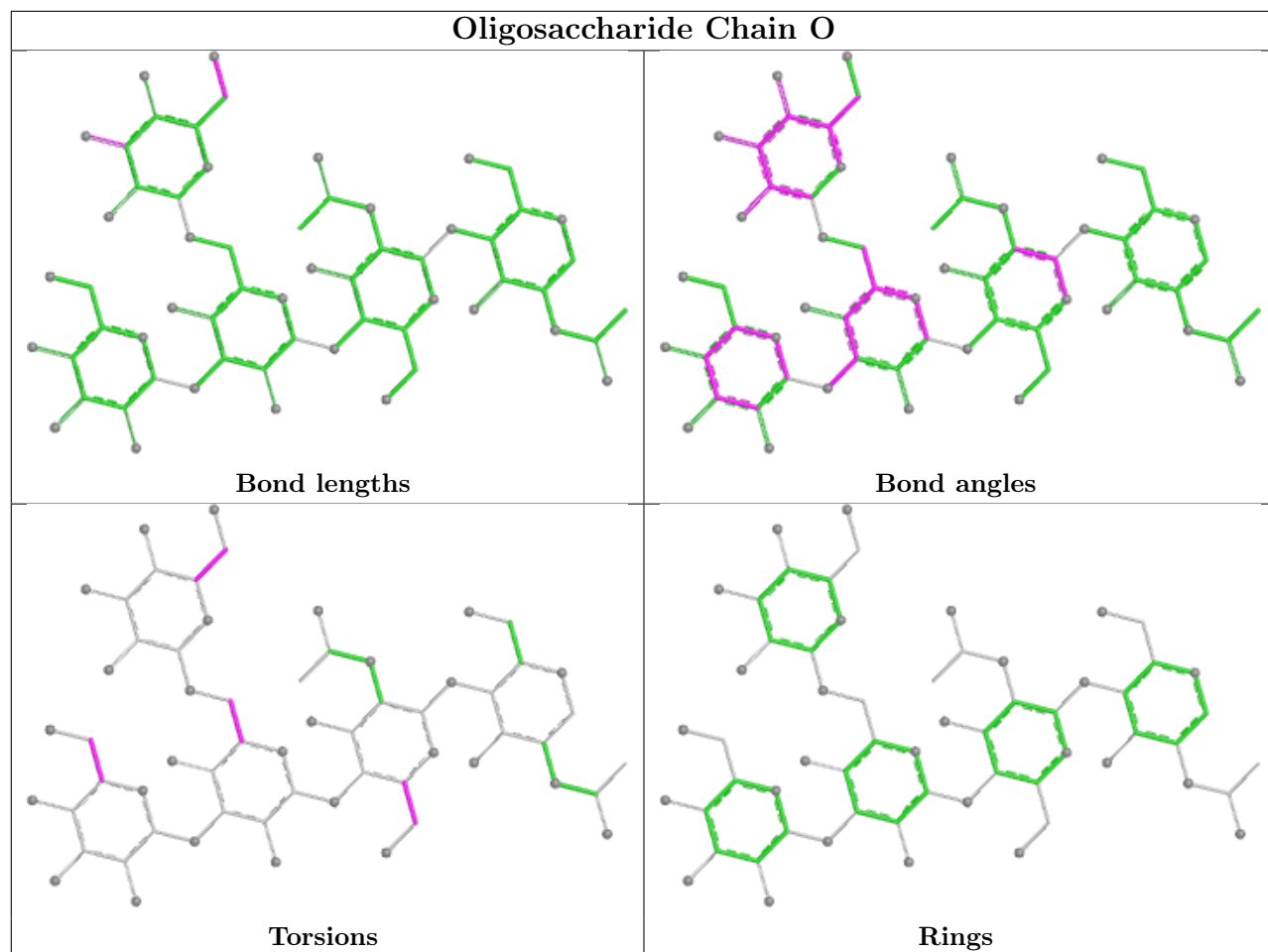
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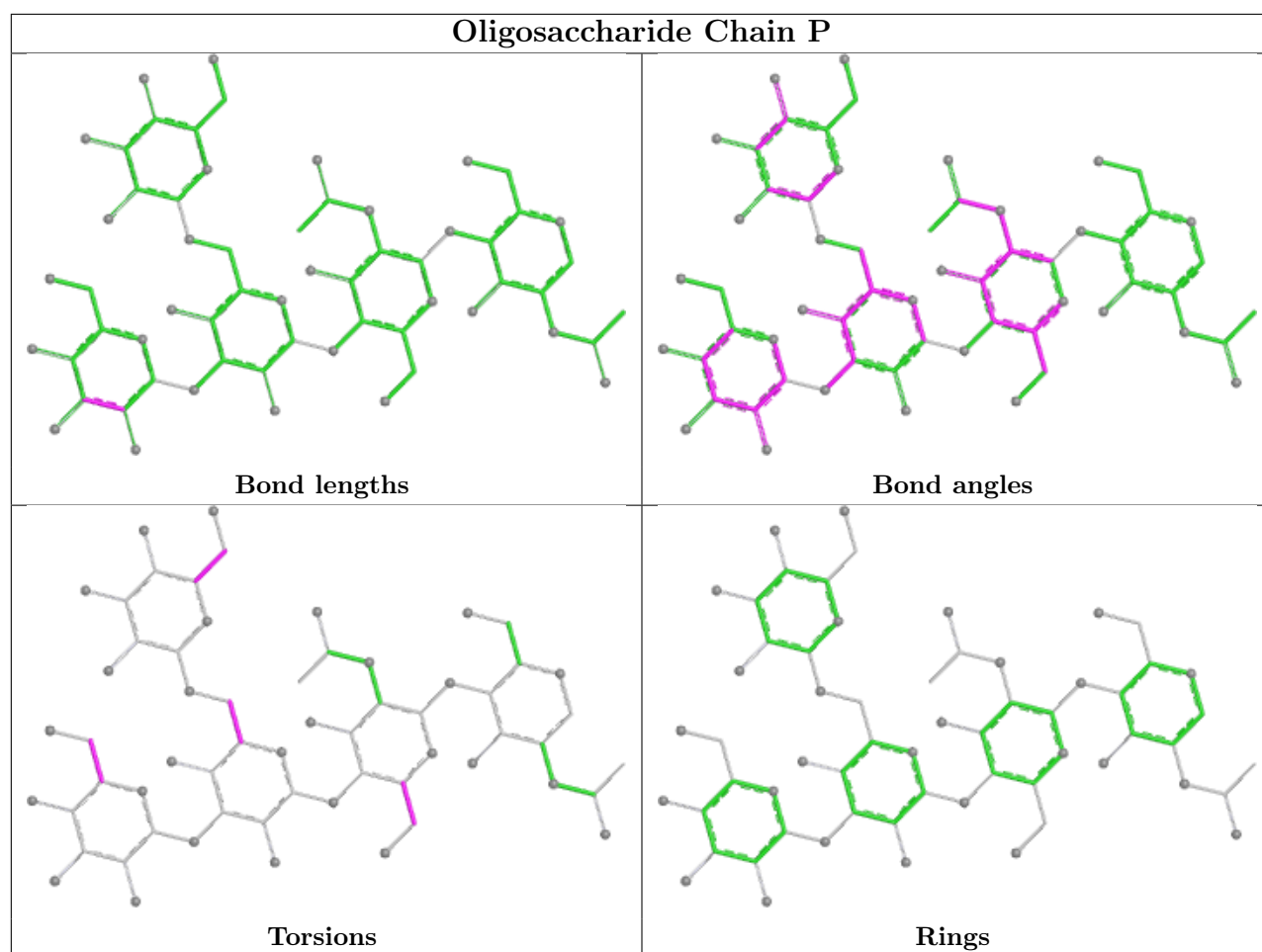
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	NAG	1	0
3	P	1	NAG	2	0
3	N	1	NAG	2	0
3	R	1	NAG	3	0
3	O	3	BMA	1	0
3	N	5	MAN	1	0

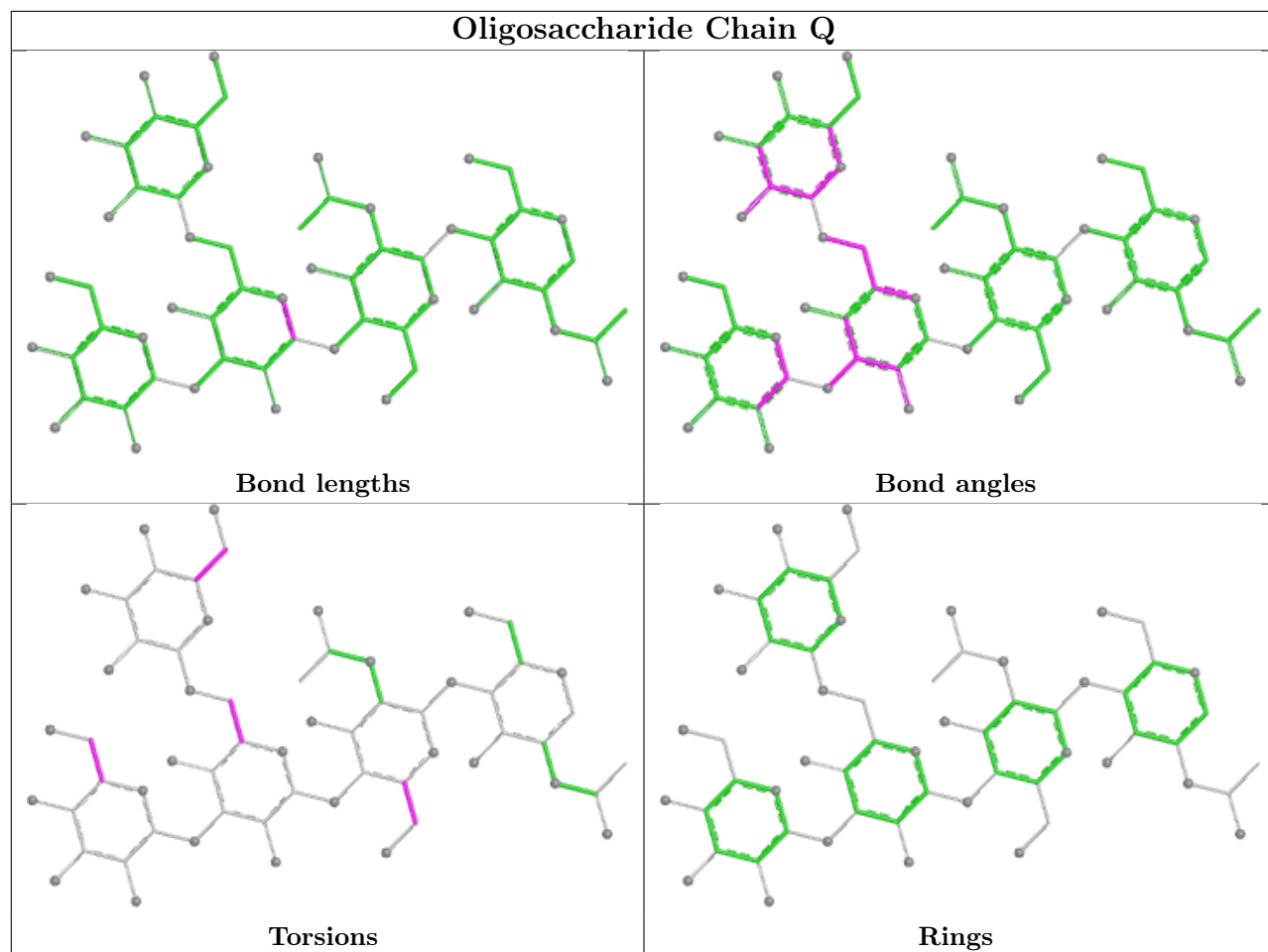
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

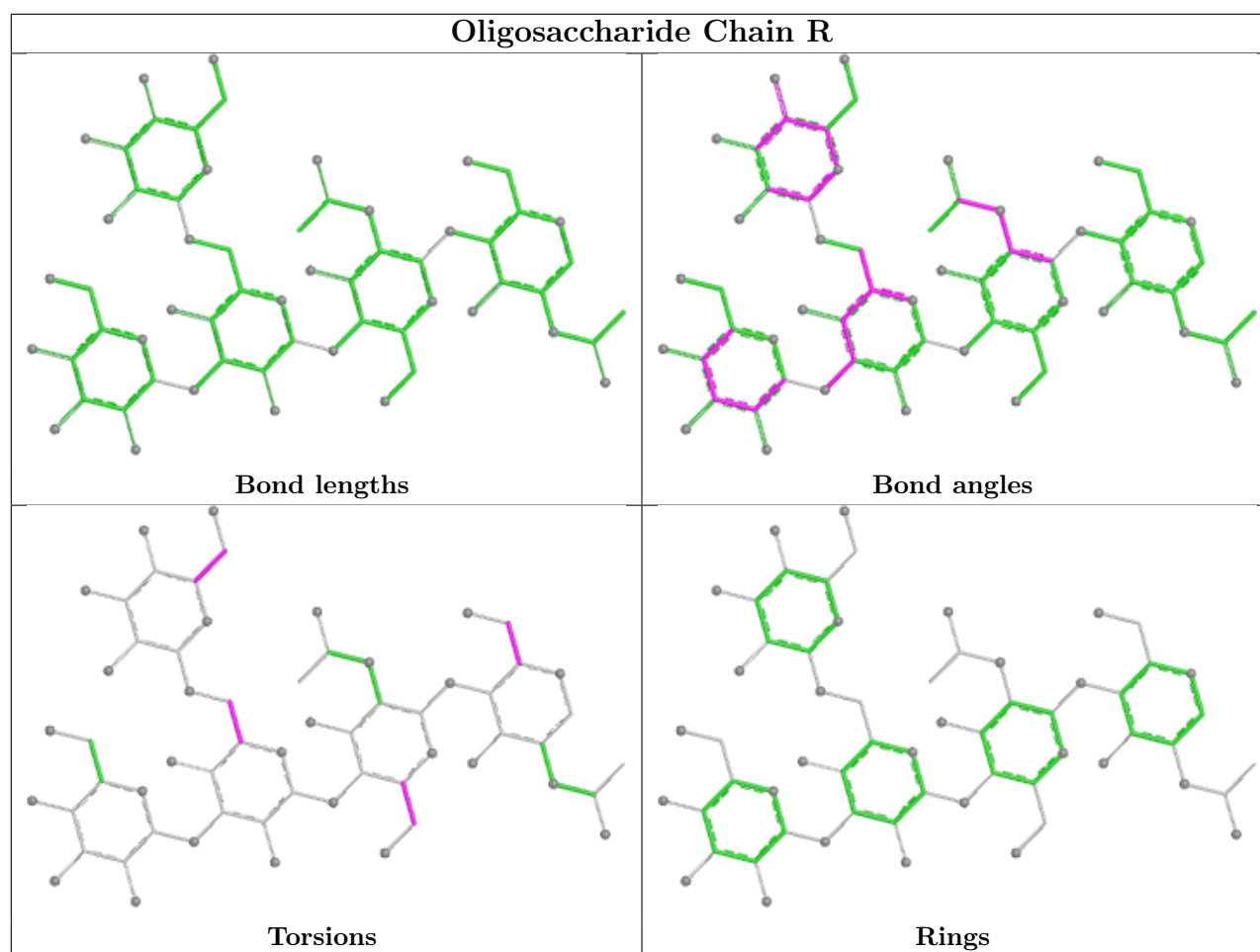












5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z > 2$
4	MAN	C	607	-	11,11,12	1.97	4 (36%)	15,15,17	2.39	6 (40%)
4	MAN	C	606	-	11,11,12	1.95	4 (36%)	15,15,17	5.22	8 (53%)

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	MAN	C	607	-	-	0/2/19/22	1/1/1/1
4	MAN	C	606	-	-	1/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	607	MAN	O5-C5	3.68	1.50	1.43
4	C	606	MAN	C4-C5	3.48	1.60	1.53
4	C	606	MAN	C1-C2	3.37	1.60	1.52
4	C	607	MAN	C4-C5	2.95	1.59	1.53
4	C	607	MAN	O5-C1	2.74	1.48	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	606	MAN	O2-C2-C1	13.59	140.35	109.22
4	C	606	MAN	C1-C2-C3	-11.52	92.88	109.64
4	C	606	MAN	O3-C3-C4	6.27	125.16	110.38
4	C	607	MAN	C1-O5-C5	5.53	119.60	112.19
4	C	606	MAN	C6-C5-C4	4.76	124.70	113.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	606	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	607	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	607	MAN	4	0
4	C	606	MAN	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	209/223 (93%)	-0.42	3 (1%) 73 55	94, 119, 157, 195	0
1	B	207/223 (92%)	-0.40	1 (0%) 87 76	99, 125, 208, 246	0
1	C	197/223 (88%)	-0.22	4 (2%) 65 46	91, 122, 180, 240	1 (0%)
1	D	189/223 (84%)	-0.20	2 (1%) 78 60	99, 142, 228, 268	0
1	E	180/223 (80%)	-0.25	4 (2%) 62 43	140, 176, 225, 256	0
1	F	197/223 (88%)	-0.34	1 (0%) 87 76	120, 154, 222, 232	0
2	G	135/143 (94%)	-0.44	1 (0%) 84 70	124, 156, 195, 239	0
2	H	133/143 (93%)	-0.61	1 (0%) 82 68	105, 128, 152, 182	0
2	I	134/143 (93%)	-0.50	0 100 100	90, 141, 200, 225	0
2	J	135/143 (94%)	-0.50	0 100 100	90, 125, 156, 179	0
2	K	135/143 (94%)	-0.02	0 100 100	175, 231, 352, 467	0
2	L	136/143 (95%)	-0.51	1 (0%) 84 70	104, 126, 159, 196	0
All	All	1987/2196 (90%)	-0.36	18 (0%) 81 65	90, 139, 229, 467	1 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	364	ALA	3.6
1	A	335	GLY	3.4
1	C	538	GLN	3.0
1	E	335	GLY	2.9
1	A	463	ALA	2.7

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

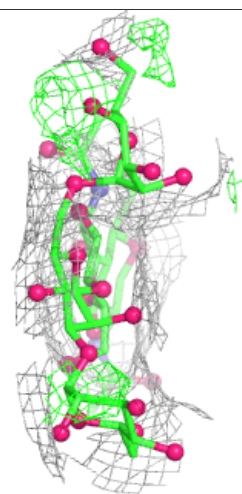
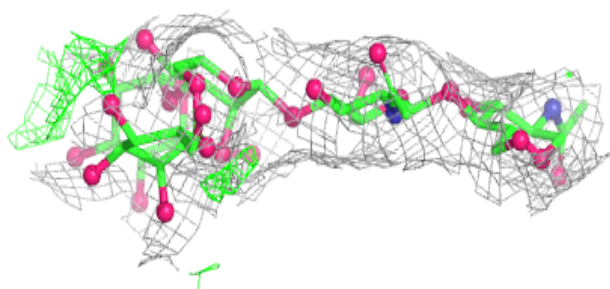
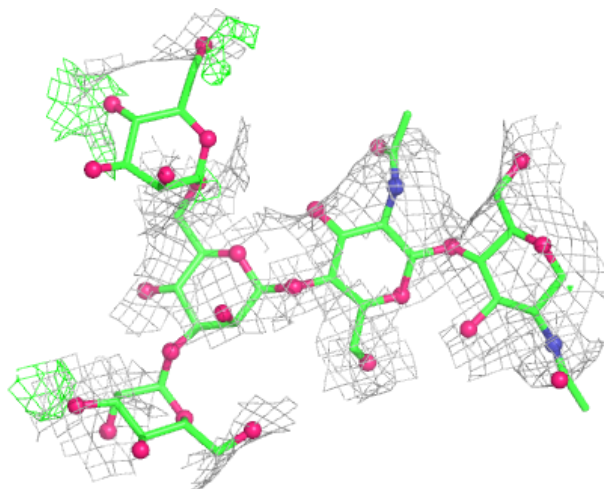
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	MAN	N	5	11/12	0.40	0.11	197,213,228,250	0
3	MAN	M	5	11/12	0.45	0.13	139,148,174,219	0
3	MAN	R	5	11/12	0.60	0.10	148,159,170,180	0
3	MAN	M	4	11/12	0.62	0.09	157,162,166,175	0
3	MAN	N	4	11/12	0.70	0.09	173,186,197,201	0
3	MAN	O	5	11/12	0.72	0.10	123,131,144,153	0
3	MAN	P	4	11/12	0.74	0.10	126,144,170,194	0
3	NAG	O	1	14/15	0.75	0.12	146,152,164,184	0
3	MAN	O	4	11/12	0.77	0.10	161,172,197,198	0
3	NAG	P	1	14/15	0.77	0.14	140,144,149,153	0
3	NAG	R	1	14/15	0.80	0.10	170,179,203,213	0
3	NAG	N	1	14/15	0.82	0.09	197,214,222,233	0
3	MAN	Q	5	11/12	0.82	0.09	156,163,174,181	0
3	NAG	O	2	14/15	0.83	0.10	137,149,162,165	0
3	MAN	Q	4	11/12	0.84	0.07	149,156,165,170	0
3	BMA	O	3	11/12	0.85	0.08	135,141,147,150	0
3	MAN	P	5	11/12	0.85	0.07	127,135,144,145	0
3	NAG	M	1	14/15	0.85	0.13	136,142,158,159	0
3	MAN	R	4	11/12	0.86	0.08	152,164,174,179	0
3	NAG	Q	1	14/15	0.87	0.09	160,163,169,170	0
3	BMA	N	3	11/12	0.87	0.08	167,195,218,224	0
3	NAG	N	2	14/15	0.88	0.07	175,193,202,202	0
3	BMA	M	3	11/12	0.89	0.07	131,140,149,160	0
3	NAG	R	2	14/15	0.89	0.09	164,180,191,195	0
3	BMA	Q	3	11/12	0.90	0.06	150,157,167,175	0
3	BMA	R	3	11/12	0.90	0.06	157,162,168,169	0
3	NAG	Q	2	14/15	0.91	0.07	155,161,177,180	0
3	BMA	P	3	11/12	0.91	0.08	132,135,143,153	0
3	NAG	M	2	14/15	0.91	0.10	140,148,153,155	0
3	NAG	P	2	14/15	0.95	0.09	121,125,131,131	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.

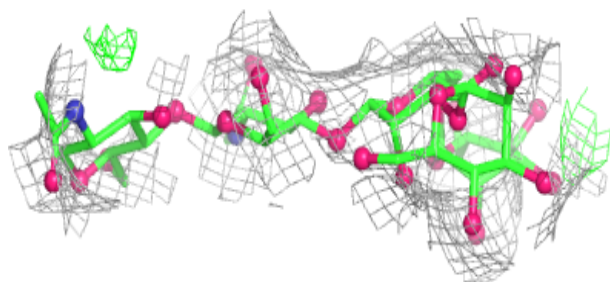
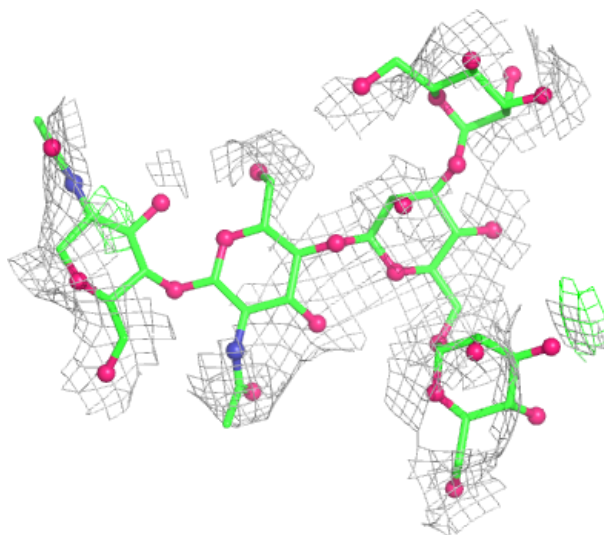
Electron density around Chain M:

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



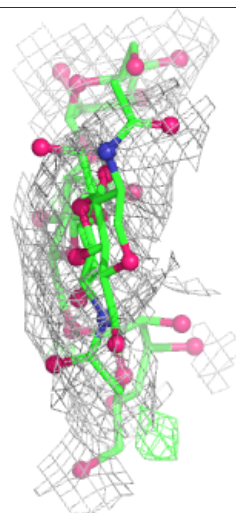
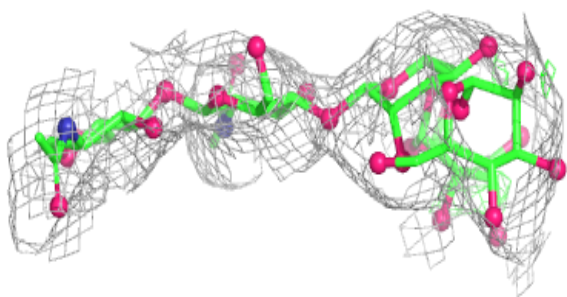
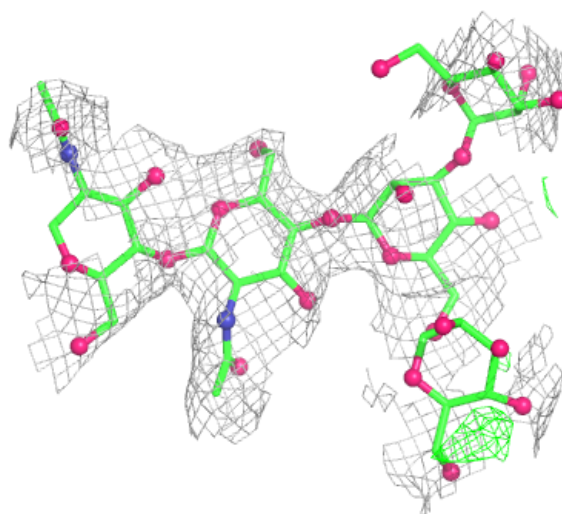
Electron density around Chain N:

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



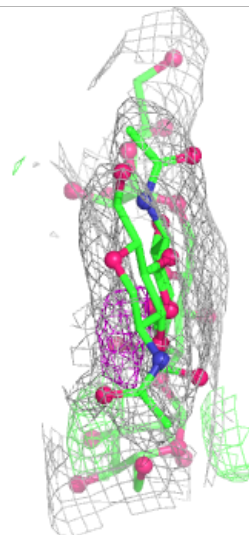
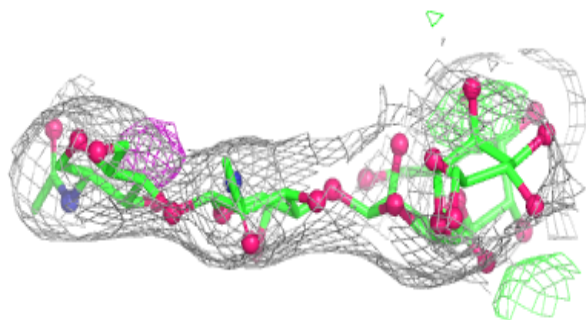
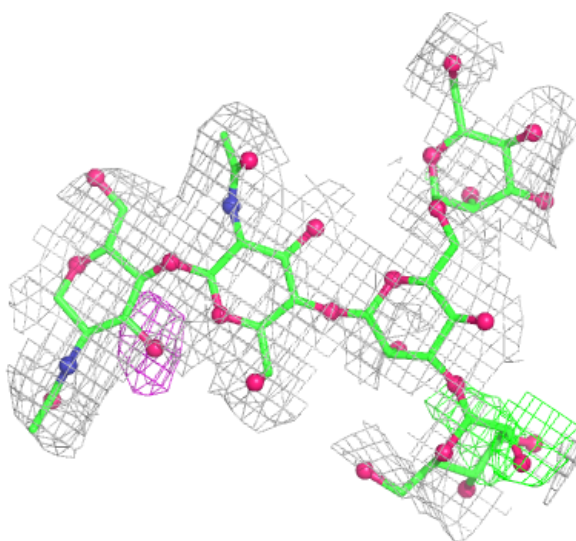
Electron density around Chain O:

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



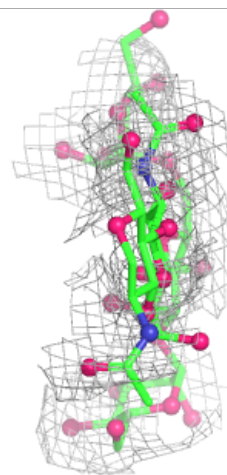
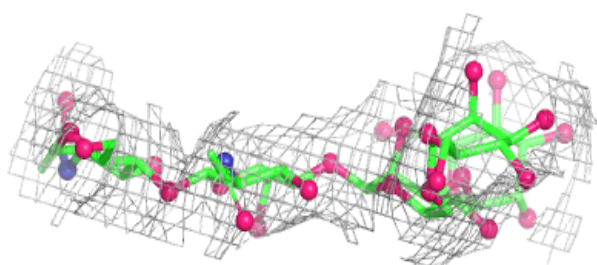
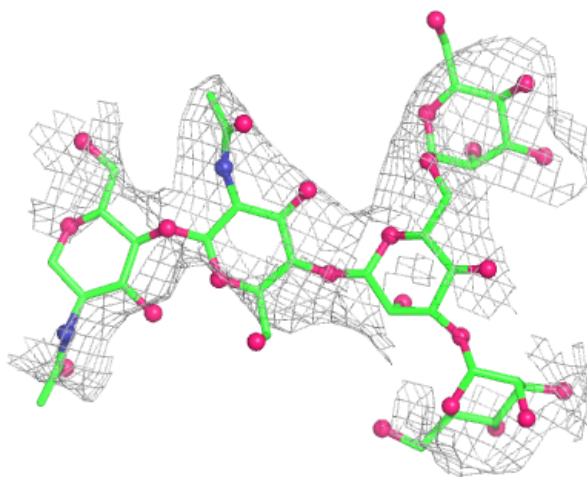
Electron density around Chain P:

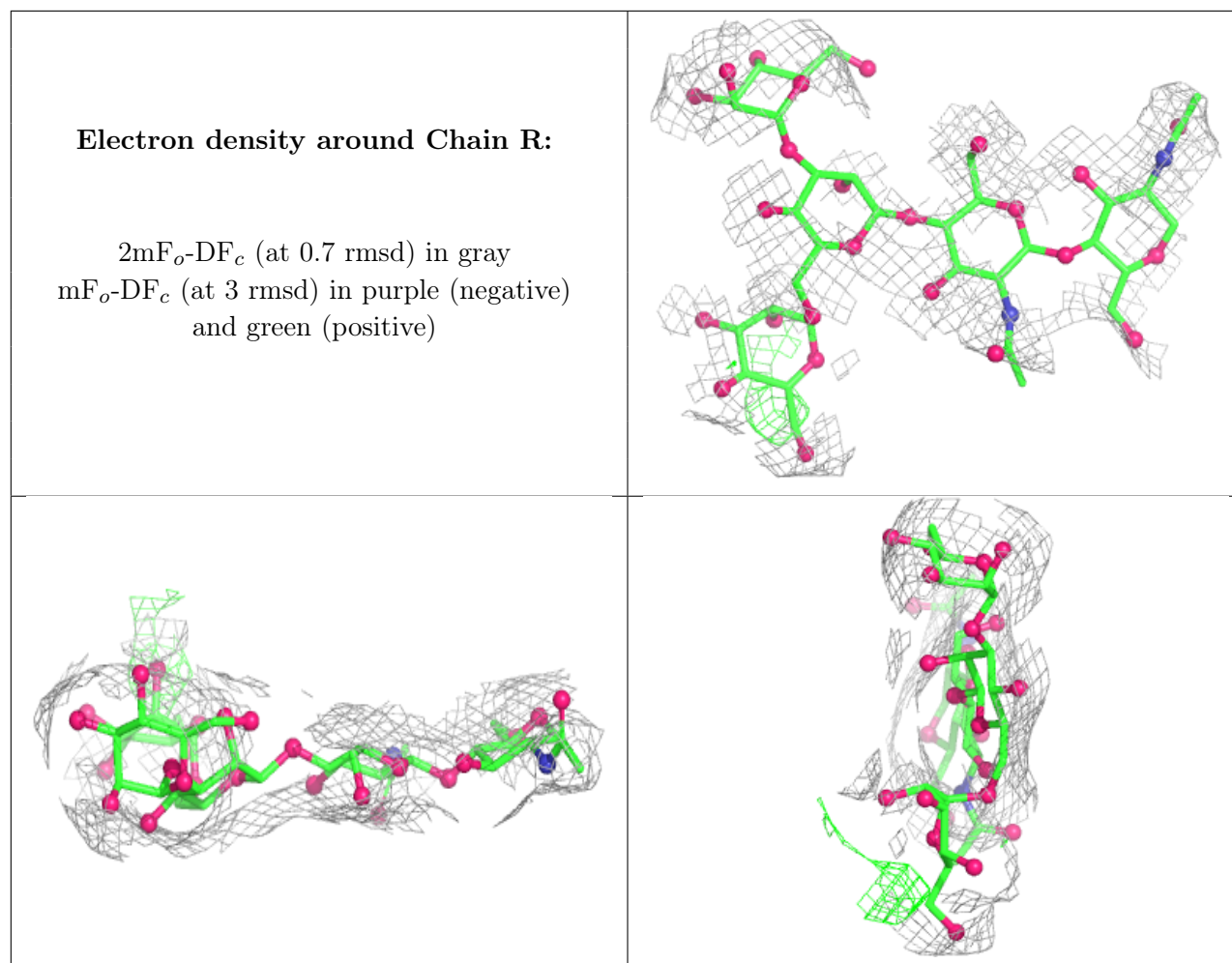
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain Q:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
4	MAN	C	606	11/12	0.56	0.12	155,175,185,193	0
4	MAN	C	607	11/12	0.73	0.10	111,125,127,128	0
5	CA	J	301	1/1	0.82	0.09	222,222,222,222	0
5	CA	L	301	1/1	0.83	0.10	222,222,222,222	0
5	CA	K	301	1/1	0.85	0.06	232,232,232,232	0
5	CA	I	301	1/1	0.87	0.12	242,242,242,242	0
5	CA	G	301	1/1	0.93	0.04	224,224,224,224	0
5	CA	H	301	1/1	0.97	0.06	117,117,117,117	0

6.5 Other polymers [i](#)

There are no such residues in this entry.