



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:50 PM UTC

PDB ID : 4RWG / pdb_00004rwg
Title : Crystal structure of the CLR:RAMP1 extracellular domain heterodimer with bound high affinity CGRP analog
Authors : Booe, J.; Pioszak, A.
Deposited on : 2014-12-03
Resolution : 2.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

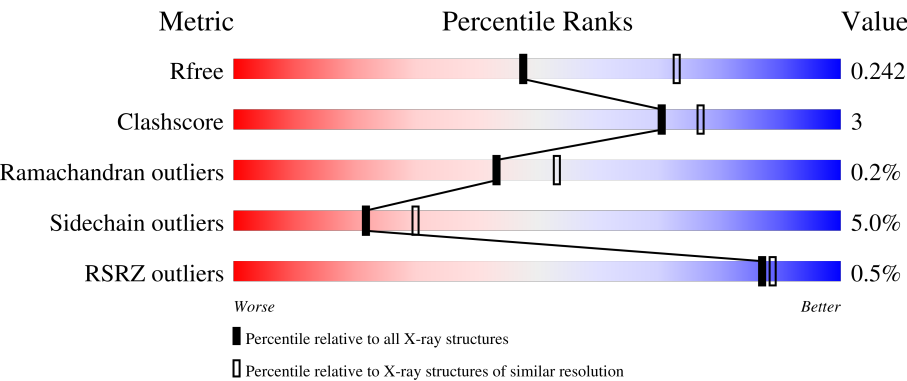
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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.



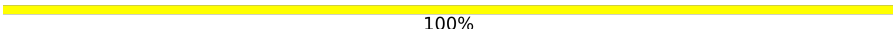
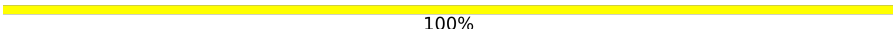
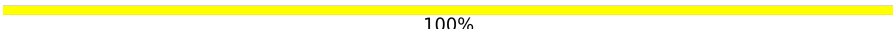
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	593	82%9%6%
1	B	593	% 85%9%
1	C	593	% 82%8%8%
2	D	12	92%8%
2	E	12	75%17%8%

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Mol	Chain	Length	Quality of chain
2	F	12	 92%8%
3	G	2	 100%
3	H	2	 100%
3	I	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13593 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 Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcitonin gene-related peptide type 1 receptor fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4395	2805	732	835	23			
1	B	569	Total	C	N	O	S	0	0	0
			4503	2876	757	847	23			
1	C	546	Total	C	N	O	S	0	0	0
			4308	2753	716	816	23			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0AEX9
A	1109	ARG	-	linker	UNP Q16602
A	1110	ALA	-	linker	UNP Q16602
A	2019	VAL	-	expression tag	UNP Q16602
A	2020	GLY	-	expression tag	UNP Q16602
A	2021	SER	-	expression tag	UNP Q16602
A	2022	ALA	-	expression tag	UNP Q16602
A	2023	GLY	-	expression tag	UNP Q16602
A	2024	SER	-	expression tag	UNP Q16602
A	2025	ALA	-	expression tag	UNP Q16602
A	2026	GLY	-	expression tag	UNP Q16602
A	2027	SER	-	expression tag	UNP Q16602
A	2028	ALA	-	expression tag	UNP Q16602
A	2029	GLU	-	expression tag	UNP Q16602
A	2030	ASP	-	expression tag	UNP Q16602
B	1	MET	-	initiating methionine	UNP P0AEX9
B	1109	ARG	-	linker	UNP Q16602
B	1110	ALA	-	linker	UNP Q16602
B	2019	VAL	-	expression tag	UNP Q16602
B	2020	GLY	-	expression tag	UNP Q16602
B	2021	SER	-	expression tag	UNP Q16602
B	2022	ALA	-	expression tag	UNP Q16602

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2023	GLY	-	expression tag	UNP Q16602
B	2024	SER	-	expression tag	UNP Q16602
B	2025	ALA	-	expression tag	UNP Q16602
B	2026	GLY	-	expression tag	UNP Q16602
B	2027	SER	-	expression tag	UNP Q16602
B	2028	ALA	-	expression tag	UNP Q16602
B	2029	GLU	-	expression tag	UNP Q16602
B	2030	ASP	-	expression tag	UNP Q16602
C	1	MET	-	initiating methionine	UNP P0AEX9
C	1109	ARG	-	linker	UNP Q16602
C	1110	ALA	-	linker	UNP Q16602
C	2019	VAL	-	expression tag	UNP Q16602
C	2020	GLY	-	expression tag	UNP Q16602
C	2021	SER	-	expression tag	UNP Q16602
C	2022	ALA	-	expression tag	UNP Q16602
C	2023	GLY	-	expression tag	UNP Q16602
C	2024	SER	-	expression tag	UNP Q16602
C	2025	ALA	-	expression tag	UNP Q16602
C	2026	GLY	-	expression tag	UNP Q16602
C	2027	SER	-	expression tag	UNP Q16602
C	2028	ALA	-	expression tag	UNP Q16602
C	2029	GLU	-	expression tag	UNP Q16602
C	2030	ASP	-	expression tag	UNP Q16602

- Molecule 2 is a protein called CGRP analog.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	0	0	1
			86	60	12	14			
2	E	12	Total	C	N	O	0	0	1
			86	60	12	14			
2	F	11	Total	C	N	O	0	0	1
			75	51	11	13			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	G	2	Total	C	O	0	0	0
			23	12	11			
3	H	2	Total	C	O	0	0	0
			23	12	11			
3	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

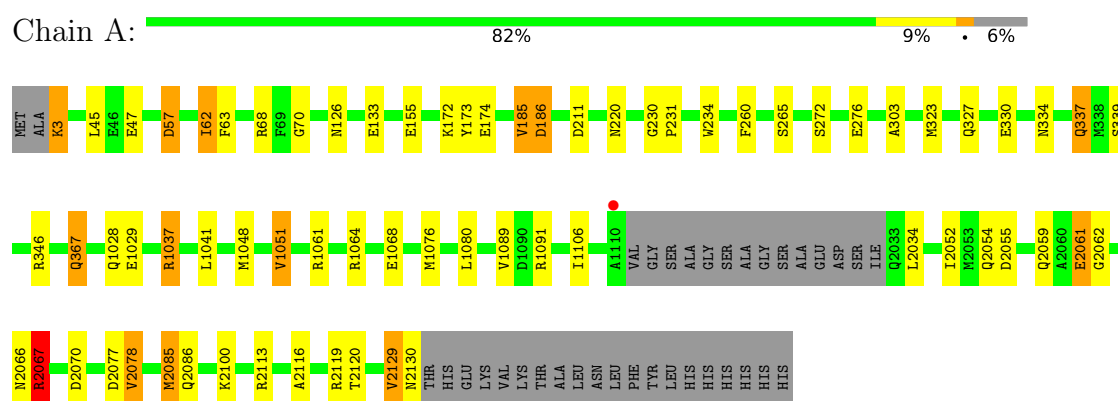
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	23	Total	O	0	0
			23	23		
5	C	6	Total	O	0	0
			6	6		
5	D	1	Total	O	0	0
			1	1		
5	E	1	Total	O	0	0
			1	1		

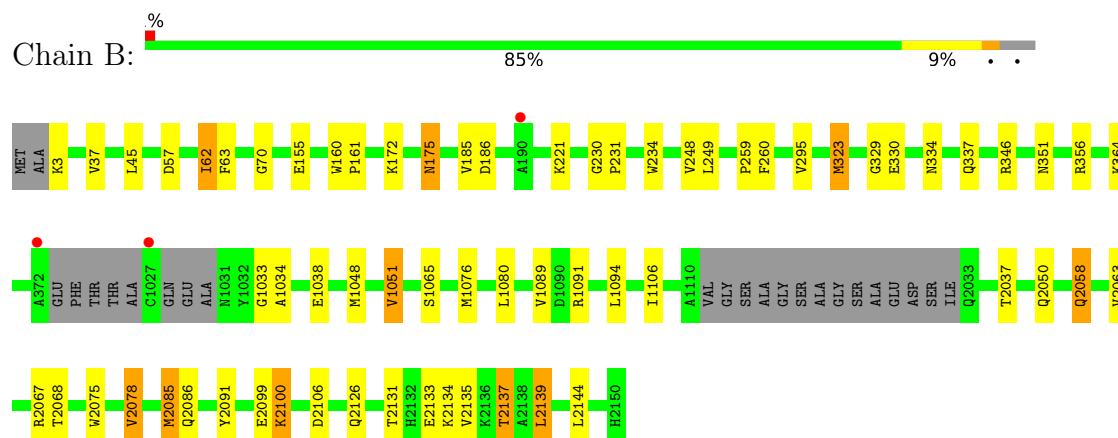
3 Residue-property plots

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.

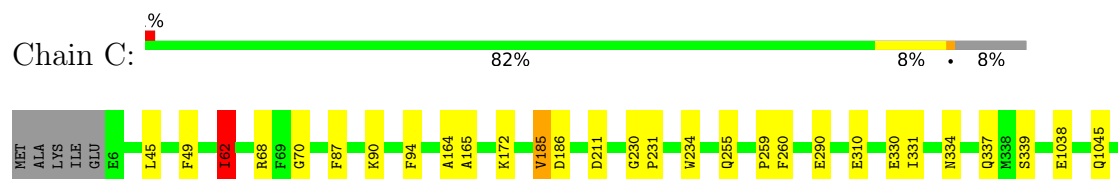
- Molecule 1: Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcitonin gene-related peptide type 1 receptor fusion protein

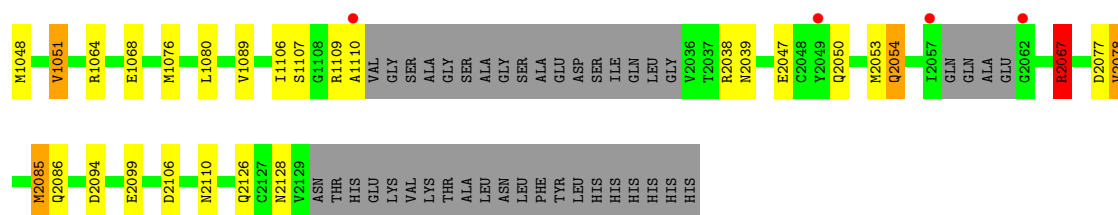


- Molecule 1: Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcitonin gene-related peptide type 1 receptor fusion protein



- Molecule 1: Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcitonin gene-related peptide type 1 receptor fusion protein





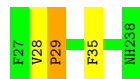
- Molecule 2: CGRP analog

Chain D: 92% 8%



- Molecule 2: CGRP analog

Chain E: 75% 17% 8%



- Molecule 2: CGRP analog

Chain F: 92% 8%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G: 100%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H: 100%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	172.81Å 104.62Å 136.48Å 90.00° 122.43° 90.00°	Depositor
Resolution (Å)	50.00 – 2.44 50.00 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.44) 99.5 (50.00-2.44)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.200 , 0.243 0.203 , 0.242	Depositor DCC
R_{free} test set	3827 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13593	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: GLC, MG, NH2

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	1.00	1/4507 (0.0%)	1.02	13/6122 (0.2%)
1	B	0.88	2/4621 (0.0%)	0.96	4/6273 (0.1%)
1	C	0.74	1/4419 (0.0%)	0.90	7/6003 (0.1%)
2	D	1.14	1/89 (1.1%)	1.21	0/122
2	E	0.92	1/89 (1.1%)	1.11	0/122
2	F	0.92	0/77	0.90	0/106
All	All	0.88	6/13802 (0.0%)	0.96	24/18748 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	VAL	C-O	-6.09	1.17	1.24
1	C	259	PRO	C-O	-5.50	1.17	1.23
2	E	35	PHE	CA-CB	5.16	1.61	1.53
2	D	36	ALA	CA-C	5.13	1.60	1.53
1	A	57	ASP	N-CA	5.10	1.52	1.46
1	B	2058	GLN	CA-C	-5.06	1.46	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2067	ARG	CG-CD-NE	-6.74	97.16	112.00
1	B	2078	VAL	CB-CA-C	-6.51	99.45	110.71
1	B	230	GLY	CA-C-N	6.31	126.79	119.47
1	B	230	GLY	C-N-CA	6.31	126.79	119.47
1	A	2078	VAL	CB-CA-C	-6.19	100.04	111.18
1	A	2055	ASP	CA-C-N	-6.08	114.01	120.03
1	A	2055	ASP	C-N-CA	-6.08	114.01	120.03
1	A	2067	ARG	CB-CG-CD	6.07	125.27	111.30
1	A	185	VAL	N-CA-CB	-5.79	105.84	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1028	GLN	N-CA-C	-5.71	106.21	112.72
1	A	272	SER	CA-C-N	-5.58	114.26	120.45
1	A	272	SER	C-N-CA	-5.58	114.26	120.45
1	C	230	GLY	CA-C-N	5.49	125.58	119.32
1	C	230	GLY	C-N-CA	5.49	125.58	119.32
1	A	230	GLY	CA-C-N	5.48	125.57	119.32
1	A	230	GLY	C-N-CA	5.48	125.57	119.32
1	C	2078	VAL	CB-CA-C	-5.45	101.27	110.71
1	B	2139	LEU	CB-CA-C	-5.36	102.24	110.81
1	A	2100	LYS	N-CA-C	5.21	118.06	109.72
1	A	2062	GLY	N-CA-C	5.17	121.17	112.85
1	C	185	VAL	N-CA-CB	-5.10	106.60	112.21
1	C	2039	ASN	N-CA-C	5.10	117.73	111.82
1	C	2067	ARG	CG-CD-NE	-5.07	100.85	112.00
1	C	62	ILE	CB-CA-C	-5.04	103.16	110.63

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	4395	0	4235	36	0
1	B	4503	0	4326	31	0
1	C	4308	0	4149	27	0
2	D	86	0	77	0	0
2	E	86	0	77	1	0
2	F	75	0	68	0	0
3	G	23	0	21	0	0
3	H	23	0	21	0	0
3	I	23	0	21	0	0
4	B	1	0	0	0	0
5	A	39	0	0	3	0
5	B	23	0	0	2	0
5	C	6	0	0	0	0
5	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1	0	0	0	0
All	All	13593	0	12995	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (91) 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)
1:B:323:MET:HA	1:B:323:MET:HE2	1.49	0.95
1:B:2137:THR:HG21	1:C:310:GLU:OE2	1.82	0.79
1:A:47:GLU:HG2	5:A:2315:HOH:O	1.83	0.78
1:A:1076:MET:O	1:A:1080:LEU:HD12	1.85	0.76
1:C:1076:MET:O	1:C:1080:LEU:HD12	1.87	0.75
1:A:2129:VAL:HG12	1:A:2129:VAL:O	1.90	0.72
1:B:1076:MET:O	1:B:1080:LEU:HD12	1.97	0.65
1:B:2134:LYS:O	5:B:2308:HOH:O	2.15	0.64
1:B:2135:VAL:O	1:B:2135:VAL:HG12	1.98	0.64
1:B:2137:THR:CG2	1:C:310:GLU:OE2	2.46	0.63
1:B:2144:LEU:HB3	1:C:94:PHE:CE2	2.35	0.61
1:C:49:PHE:CE1	1:C:62:ILE:HG12	2.36	0.60
1:A:2052:ILE:HG12	1:A:2067:ARG:HB2	1.83	0.60
1:B:323:MET:HA	1:B:323:MET:CE	2.29	0.59
1:A:2085:MET:HG2	1:A:2086:GLN:N	2.19	0.57
1:A:173:TYR:O	1:A:174:GLU:HG3	2.04	0.56
1:A:70:GLY:HA3	1:A:334:ASN:O	2.05	0.55
1:A:173:TYR:O	1:A:174:GLU:CG	2.55	0.55
1:C:2106:ASP:OD2	1:C:2110:ASN:HB2	2.07	0.53
1:A:3:LYS:HB2	1:A:57:ASP:OD1	2.08	0.53
1:A:2120:THR:HG22	5:A:2318:HOH:O	2.09	0.53
1:A:186:ASP:OD1	1:A:367:GLN:OE1	2.27	0.52
1:B:1106:ILE:HA	1:B:2050:GLN:HB3	1.90	0.52
1:C:94:PHE:CZ	1:C:331:ILE:HD12	2.46	0.51
1:C:2050:GLN:O	1:C:2053:MET:HB3	2.10	0.50
1:B:351:ASN:OD1	1:B:356:ARG:NH1	2.45	0.49
1:B:295:VAL:HG12	5:B:2315:HOH:O	2.13	0.49
1:C:231:PRO:HA	1:C:234:TRP:CE2	2.48	0.49
1:B:221:LYS:HE3	1:C:290:GLU:HG3	1.93	0.49
1:B:259:PRO:O	1:B:329:GLY:HA3	2.13	0.48
1:A:2061:GLU:HB2	5:A:2306:HOH:O	2.12	0.48
1:C:1107:SER:HA	1:C:2047:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1064:ARG:NH1	1:C:1068:GLU:OE2	2.45	0.48
1:B:1033:GLY:O	1:B:1034:ALA:C	2.57	0.48
1:A:337:GLN:H	1:A:337:GLN:HE21	1.61	0.48
1:B:62:ILE:HG13	1:B:63:PHE:N	2.29	0.48
1:C:2067:ARG:HG2	1:C:2077:ASP:OD1	2.13	0.48
1:B:2085:MET:HG2	1:B:2086:GLN:N	2.29	0.48
1:A:68:ARG:NH1	1:A:339:SER:HB2	2.29	0.47
1:C:1109:ARG:O	1:C:1110:ALA:C	2.57	0.47
1:B:2067:ARG:HG3	1:B:2075:TRP:O	2.14	0.47
1:C:1106:ILE:HD11	1:C:2054:GLN:HG2	1.97	0.47
1:A:1037:ARG:O	1:A:1041:LEU:HB3	2.15	0.47
1:B:231:PRO:HA	1:B:234:TRP:CE2	2.48	0.47
1:B:2135:VAL:O	1:B:2135:VAL:CG1	2.62	0.47
1:A:303:ALA:HB2	1:A:323:MET:HE3	1.96	0.47
1:B:2037:THR:HG23	1:B:2091:TYR:HB3	1.97	0.47
1:A:231:PRO:HA	1:A:234:TRP:CE2	2.50	0.46
1:B:2099:GLU:HG2	1:B:2126:GLN:O	2.15	0.46
1:C:70:GLY:HA3	1:C:334:ASN:O	2.15	0.46
1:C:1107:SER:HA	1:C:2047:GLU:CD	2.40	0.46
1:A:2130:ASN:OD1	1:A:2130:ASN:C	2.58	0.46
1:A:1048:MET:HA	1:A:1051:VAL:HG12	1.98	0.46
1:A:3:LYS:CB	1:A:57:ASP:OD1	2.63	0.46
1:A:62:ILE:HG13	1:A:63:PHE:N	2.30	0.46
1:A:339:SER:OG	1:A:2116:ALA:HB2	2.16	0.46
1:C:2085:MET:HG2	1:C:2086:GLN:N	2.31	0.46
1:C:2094:ASP:O	1:C:2128:ASN:HB3	2.16	0.45
1:B:70:GLY:HA3	1:B:334:ASN:O	2.16	0.45
1:B:2100:LYS:O	1:B:2100:LYS:HG3	2.14	0.45
1:A:337:GLN:H	1:A:337:GLN:NE2	2.15	0.44
2:E:28:VAL:O	2:E:29:PRO:C	2.60	0.44
1:A:2129:VAL:O	1:A:2129:VAL:CG1	2.63	0.44
1:C:2099:GLU:HG2	1:C:2126:GLN:O	2.17	0.44
1:C:1048:MET:HA	1:C:1051:VAL:HG12	1.98	0.44
1:B:2106:ASP:OD1	1:B:2106:ASP:C	2.61	0.44
1:A:155:GLU:OE1	1:A:346:ARG:NH2	2.51	0.43
1:A:2066:ASN:O	1:A:2067:ARG:C	2.62	0.43
1:A:2070:ASP:OD1	1:A:2070:ASP:C	2.62	0.43
1:B:1094:LEU:HD23	1:B:1094:LEU:HA	1.70	0.42
1:B:155:GLU:OE1	1:B:346:ARG:NH2	2.52	0.42
1:A:2067:ARG:HG2	1:A:2077:ASP:OD1	2.20	0.42
1:A:276:GLU:OE1	1:A:276:GLU:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:ARG:NH1	1:A:1068:GLU:HG3	2.35	0.42
1:B:1048:MET:HA	1:B:1051:VAL:HG12	2.02	0.42
1:C:211:ASP:OD1	1:C:211:ASP:C	2.63	0.42
1:A:1106:ILE:HD11	1:A:2054:GLN:HG3	2.02	0.42
1:C:68:ARG:NH1	1:C:339:SER:HB2	2.36	0.41
1:C:164:ALA:O	1:C:165:ALA:C	2.63	0.41
1:C:94:PHE:CE2	1:C:331:ILE:HD12	2.55	0.41
1:A:63:PHE:HA	1:A:265:SER:O	2.21	0.41
1:B:2067:ARG:HG2	1:B:2068:THR:N	2.35	0.41
1:C:1048:MET:HA	1:C:1051:VAL:CG1	2.51	0.41
1:A:220:ASN:N	1:A:220:ASN:HD22	2.19	0.41
1:A:211:ASP:OD1	1:A:211:ASP:C	2.64	0.41
1:A:2113:ARG:HA	1:A:2119:ARG:O	2.21	0.41
1:B:248:VAL:HG12	1:B:249:LEU:O	2.21	0.41
1:A:1048:MET:HA	1:A:1051:VAL:CG1	2.51	0.40
1:B:160:TRP:N	1:B:161:PRO:CD	2.85	0.40
1:B:2099:GLU:CG	1:B:2126:GLN:O	2.70	0.40
1:C:87:PHE:HA	1:C:90:LYS:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/593 (93%)	541 (98%)	11 (2%)	1 (0%)	43	53
1	B	562/593 (95%)	553 (98%)	8 (1%)	1 (0%)	43	53
1	C	540/593 (91%)	525 (97%)	15 (3%)	0	100	100
2	D	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
2	E	10/12 (83%)	8 (80%)	1 (10%)	1 (10%)	0	0
2	F	9/12 (75%)	9 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1684/1815 (93%)	1645 (98%)	36 (2%)	3 (0%)	43	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	ASN
2	E	29	PRO
1	A	2129	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	456/484 (94%)	431 (94%)	25 (6%)	19	26
1	B	467/484 (96%)	440 (94%)	27 (6%)	18	25
1	C	447/484 (92%)	429 (96%)	18 (4%)	28	39
2	D	9/9 (100%)	9 (100%)	0	100	100
2	E	9/9 (100%)	9 (100%)	0	100	100
2	F	8/9 (89%)	8 (100%)	0	100	100
All	All	1396/1479 (94%)	1326 (95%)	70 (5%)	22	30

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	45	LEU
1	A	62	ILE
1	A	126	ASN
1	A	133	GLU
1	A	172	LYS
1	A	185	VAL
1	A	186	ASP
1	A	260	PHE

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Mol	Chain	Res	Type
1	A	327	GLN
1	A	330	GLU
1	A	337	GLN
1	A	367	GLN
1	A	1029	GLU
1	A	1037	ARG
1	A	1051	VAL
1	A	1061	ARG
1	A	1089	VAL
1	A	1091	ARG
1	A	2034	LEU
1	A	2059	GLN
1	A	2061	GLU
1	A	2067	ARG
1	A	2078	VAL
1	A	2085	MET
1	B	3	LYS
1	B	45	LEU
1	B	57	ASP
1	B	62	ILE
1	B	172	LYS
1	B	175	ASN
1	B	185	VAL
1	B	186	ASP
1	B	260	PHE
1	B	323	MET
1	B	330	GLU
1	B	337	GLN
1	B	364	LYS
1	B	1038	GLU
1	B	1051	VAL
1	B	1065	SER
1	B	1089	VAL
1	B	1091	ARG
1	B	2058	GLN
1	B	2063	VAL
1	B	2078	VAL
1	B	2085	MET
1	B	2100	LYS
1	B	2131	THR
1	B	2133	GLU
1	B	2137	THR

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Mol	Chain	Res	Type
1	B	2139	LEU
1	C	45	LEU
1	C	62	ILE
1	C	172	LYS
1	C	185	VAL
1	C	186	ASP
1	C	255	GLN
1	C	260	PHE
1	C	330	GLU
1	C	337	GLN
1	C	1038	GLU
1	C	1045	GLN
1	C	1051	VAL
1	C	1089	VAL
1	C	2038	ARG
1	C	2054	GLN
1	C	2067	ARG
1	C	2078	VAL
1	C	2085	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	102	ASN
1	A	220	ASN
1	A	337	GLN
1	A	2045	GLN
1	A	2086	GLN
1	A	2126	GLN
1	B	102	ASN
1	B	175	ASN
1	B	220	ASN
1	B	1043	GLN
1	B	1045	GLN
1	B	2086	GLN
1	B	2146	HIS
1	C	20	ASN
1	C	51	GLN
1	C	102	ASN
1	C	220	ASN
1	C	337	GLN

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Mol	Chain	Res	Type
1	C	351	ASN
1	C	357	GLN
1	C	1045	GLN
1	C	2045	GLN
1	C	2086	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 ⓘ

6 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	GLC	G	1	3	12,12,12	1.06	1 (8%)	17,17,17	1.75	4 (23%)
3	GLC	G	2	3	11,11,12	1.00	1 (9%)	15,15,17	1.60	3 (20%)
3	GLC	H	1	3	12,12,12	0.59	0	17,17,17	1.93	4 (23%)
3	GLC	H	2	3	11,11,12	0.50	0	15,15,17	1.13	1 (6%)
3	GLC	I	1	3	12,12,12	0.77	0	17,17,17	1.23	1 (5%)
3	GLC	I	2	3	11,11,12	0.62	0	15,15,17	1.27	2 (13%)

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	GLC	G	1	3	-	0/2/22/22	0/1/1/1
3	GLC	G	2	3	-	2/2/19/22	0/1/1/1
3	GLC	H	1	3	-	2/2/22/22	0/1/1/1
3	GLC	H	2	3	-	1/2/19/22	0/1/1/1
3	GLC	I	1	3	-	2/2/22/22	0/1/1/1
3	GLC	I	2	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	GLC	O5-C5	-2.34	1.38	1.44
3	G	2	GLC	O5-C1	-2.12	1.40	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	GLC	O5-C1-C2	4.49	118.19	110.30
3	G	1	GLC	C1-O5-C5	4.15	121.68	113.65
3	H	2	GLC	C2-C3-C4	-3.27	105.11	110.86
3	H	1	GLC	C1-O5-C5	3.22	119.88	113.65
3	G	1	GLC	C6-C5-C4	-2.93	105.83	113.02
3	G	2	GLC	C1-O5-C5	2.85	116.00	112.19
3	G	1	GLC	O5-C1-C2	2.56	114.81	110.30
3	G	1	GLC	C1-C2-C3	2.55	115.55	110.36
3	I	2	GLC	O2-C2-C3	-2.43	105.12	110.15
3	I	2	GLC	O4-C4-C3	-2.42	104.68	110.38
3	G	2	GLC	C2-C3-C4	-2.33	106.76	110.86
3	G	2	GLC	O5-C5-C6	-2.33	103.13	107.66
3	H	1	GLC	O4-C4-C3	-2.31	104.92	110.38
3	I	1	GLC	O5-C1-C2	2.28	114.30	110.30
3	H	1	GLC	O5-C5-C4	2.04	113.37	109.70

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	GLC	C4-C5-C6-O6
3	I	1	GLC	O5-C5-C6-O6
3	G	2	GLC	O5-C5-C6-O6
3	H	2	GLC	C4-C5-C6-O6
3	G	2	GLC	C4-C5-C6-O6

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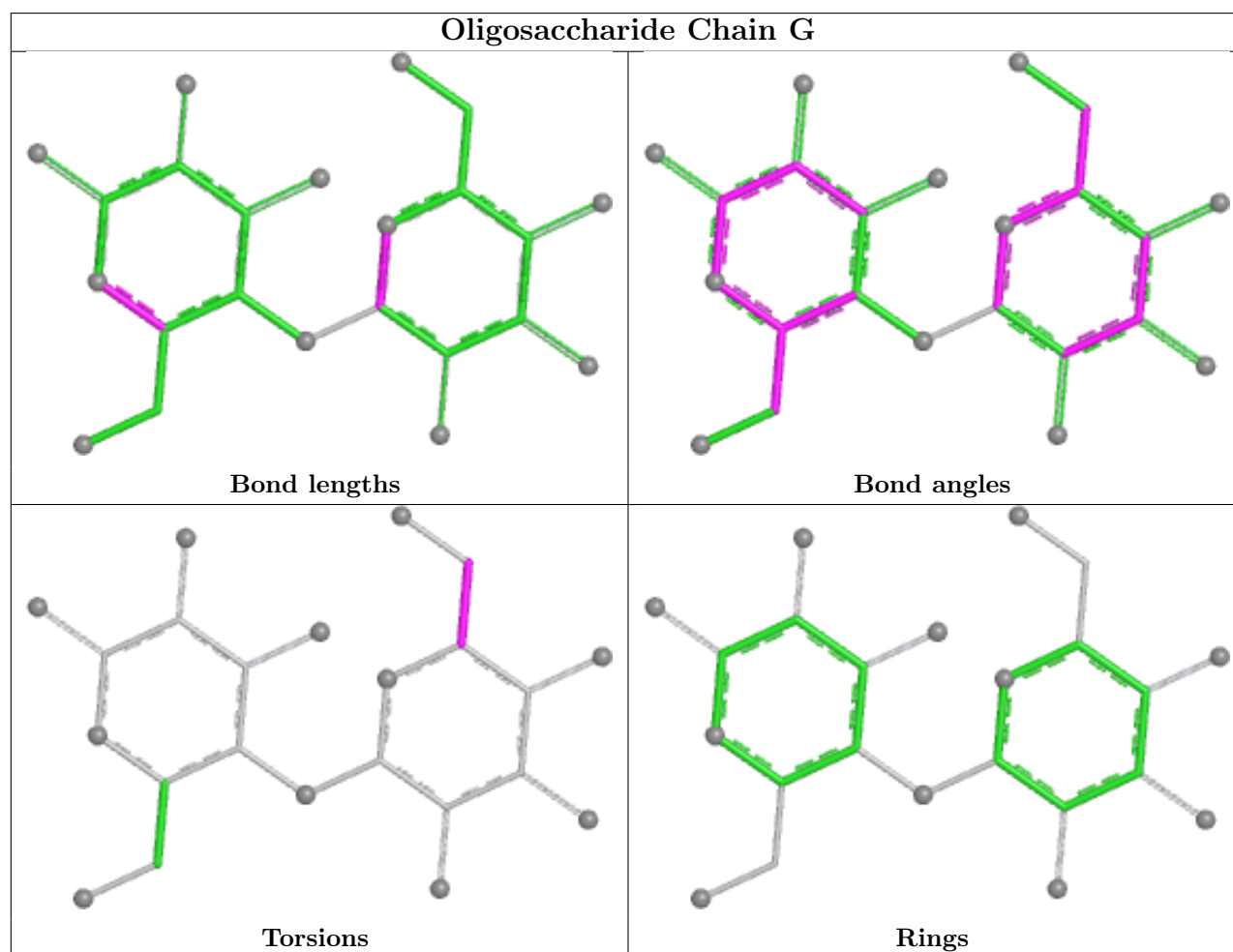
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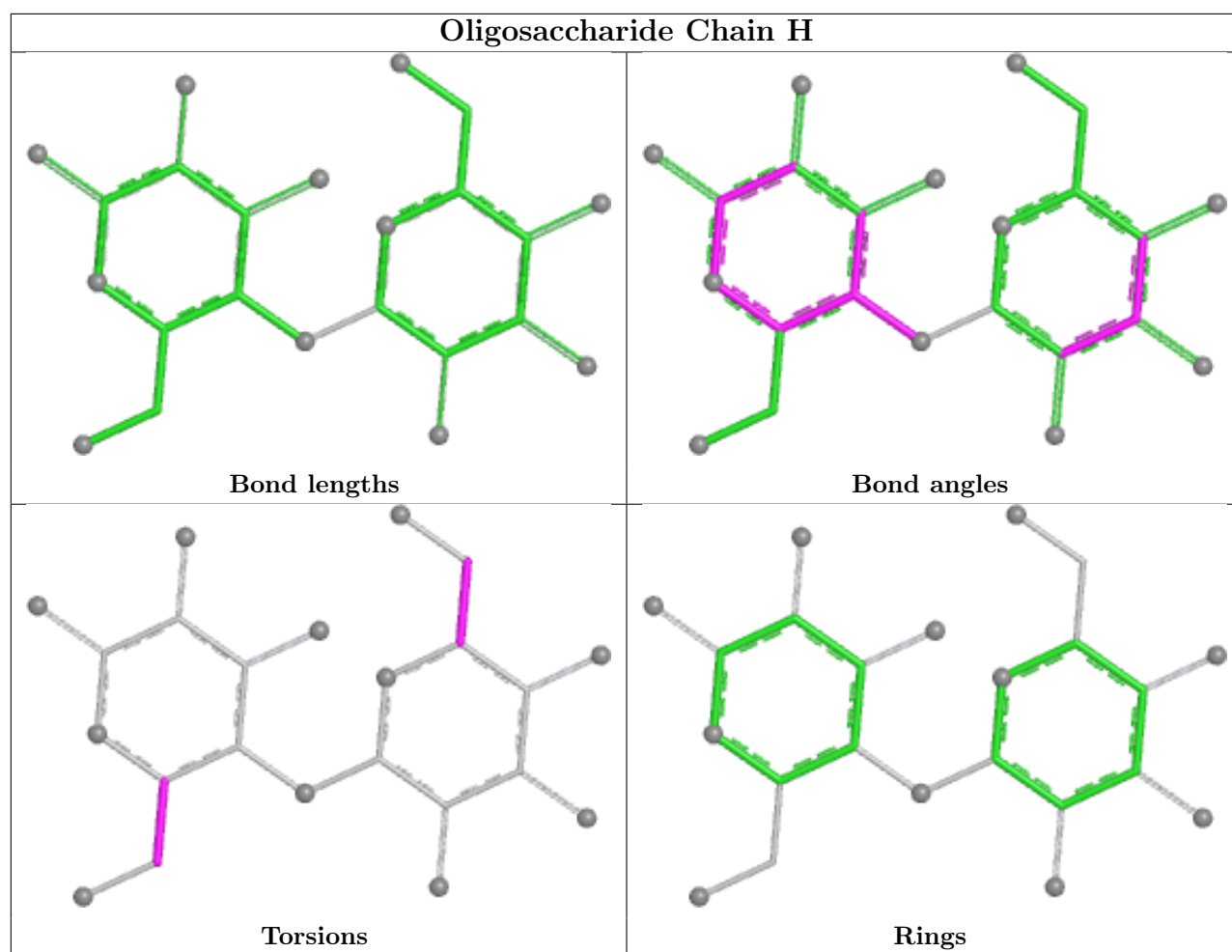
Mol	Chain	Res	Type	Atoms
3	H	1	GLC	C4-C5-C6-O6
3	H	1	GLC	O5-C5-C6-O6

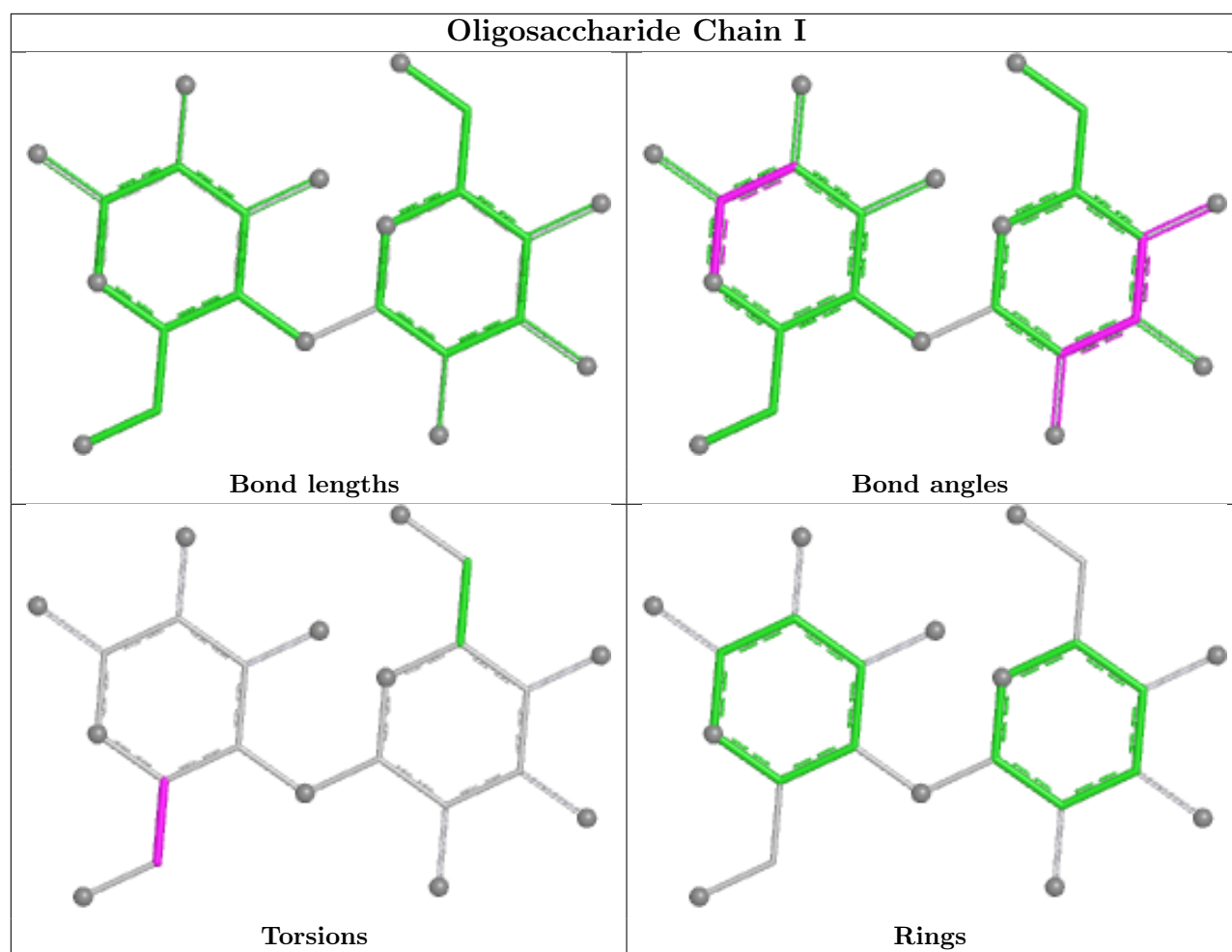
There are no ring outliers.

No monomer is involved in short contacts.

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	557/593 (93%)	-0.32	1 (0%) 91 92	35, 67, 106, 132	0
1	B	569/593 (95%)	0.05	3 (0%) 87 89	36, 86, 138, 191	0
1	C	546/593 (92%)	0.11	4 (0%) 84 85	62, 93, 127, 165	0
2	D	11/12 (91%)	-0.01	0 100 100	51, 61, 99, 112	0
2	E	11/12 (91%)	0.30	0 100 100	79, 93, 124, 134	0
2	F	10/12 (83%)	-0.07	0 100 100	67, 81, 94, 101	0
All	All	1704/1815 (93%)	-0.05	8 (0%) 87 89	35, 83, 127, 191	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	372	ALA	4.4
1	B	1027	CYS	3.8
1	A	1110	ALA	2.6
1	C	2057	ILE	2.6
1	C	2062	GLY	2.3
1	B	190	ALA	2.2
1	C	1110	ALA	2.2
1	C	2049	TYR	2.1

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

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

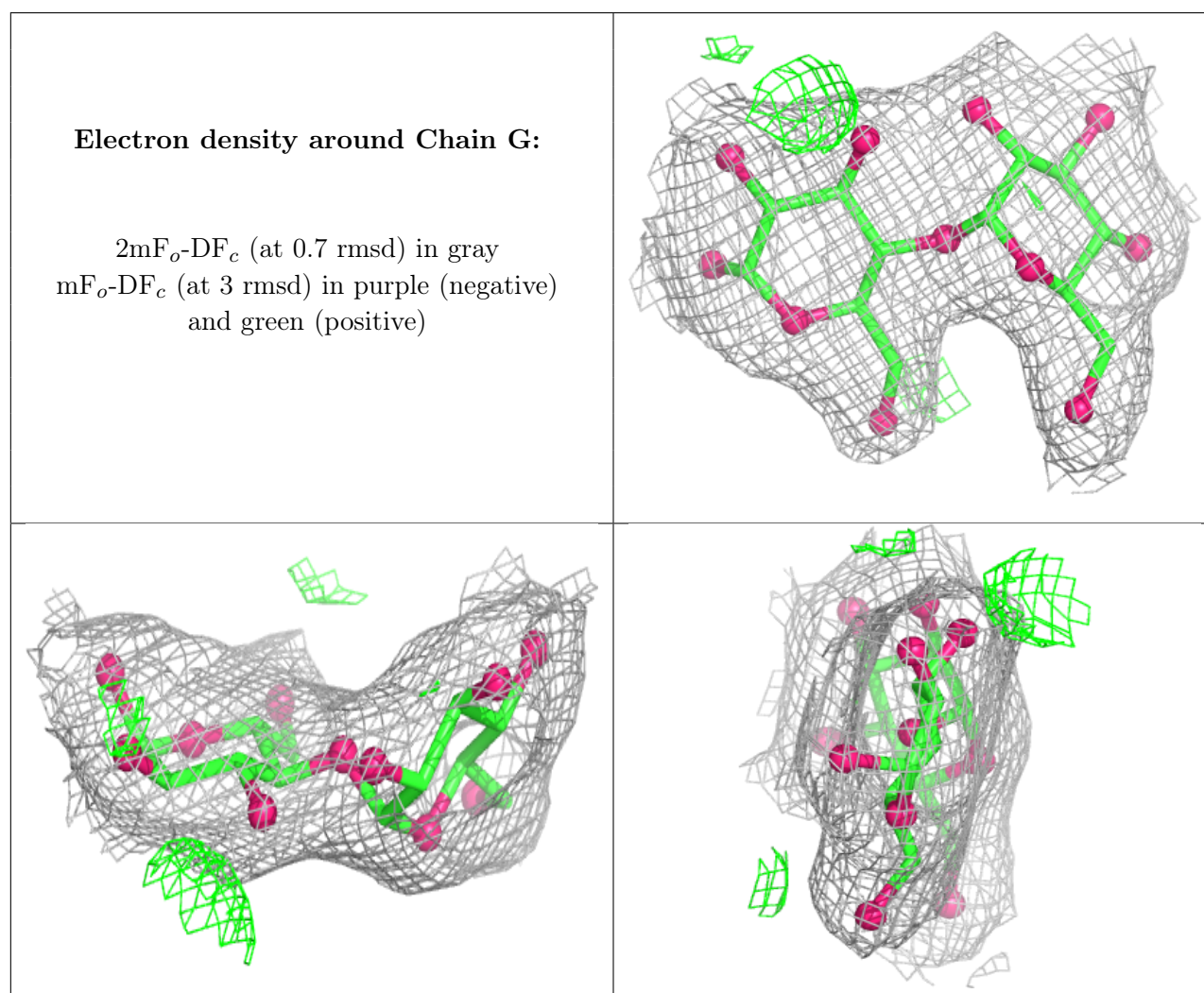
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

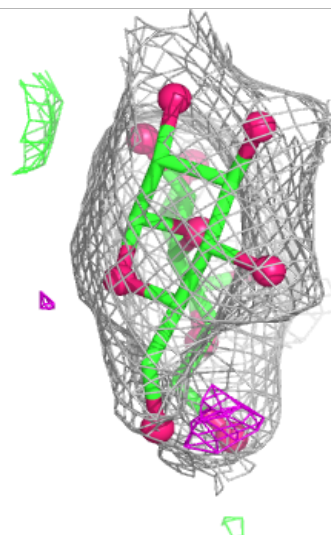
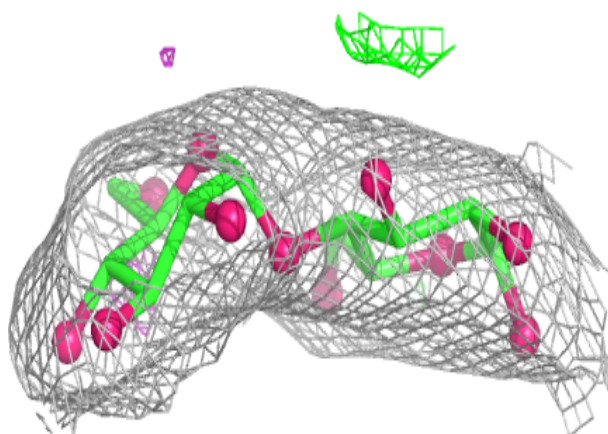
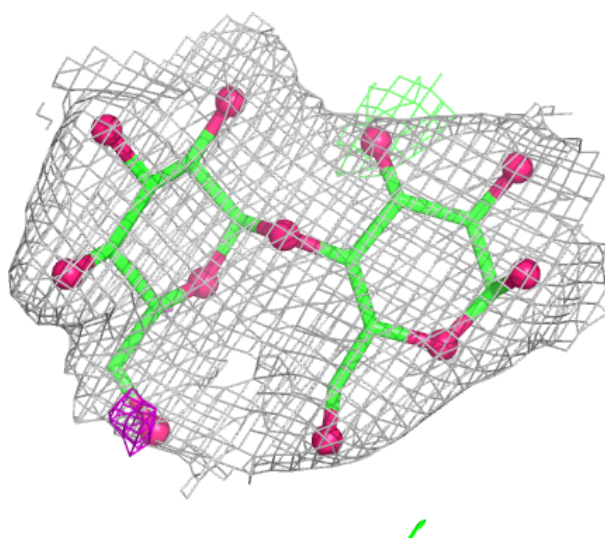
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	I	1	12/12	0.90	0.10	73,80,84,85	0
3	GLC	H	2	11/12	0.95	0.07	59,61,65,67	0
3	GLC	H	1	12/12	0.96	0.06	65,68,69,75	0
3	GLC	G	1	12/12	0.96	0.05	43,46,52,56	0
3	GLC	G	2	11/12	0.96	0.07	42,44,46,48	0
3	GLC	I	2	11/12	0.97	0.06	66,68,74,77	0

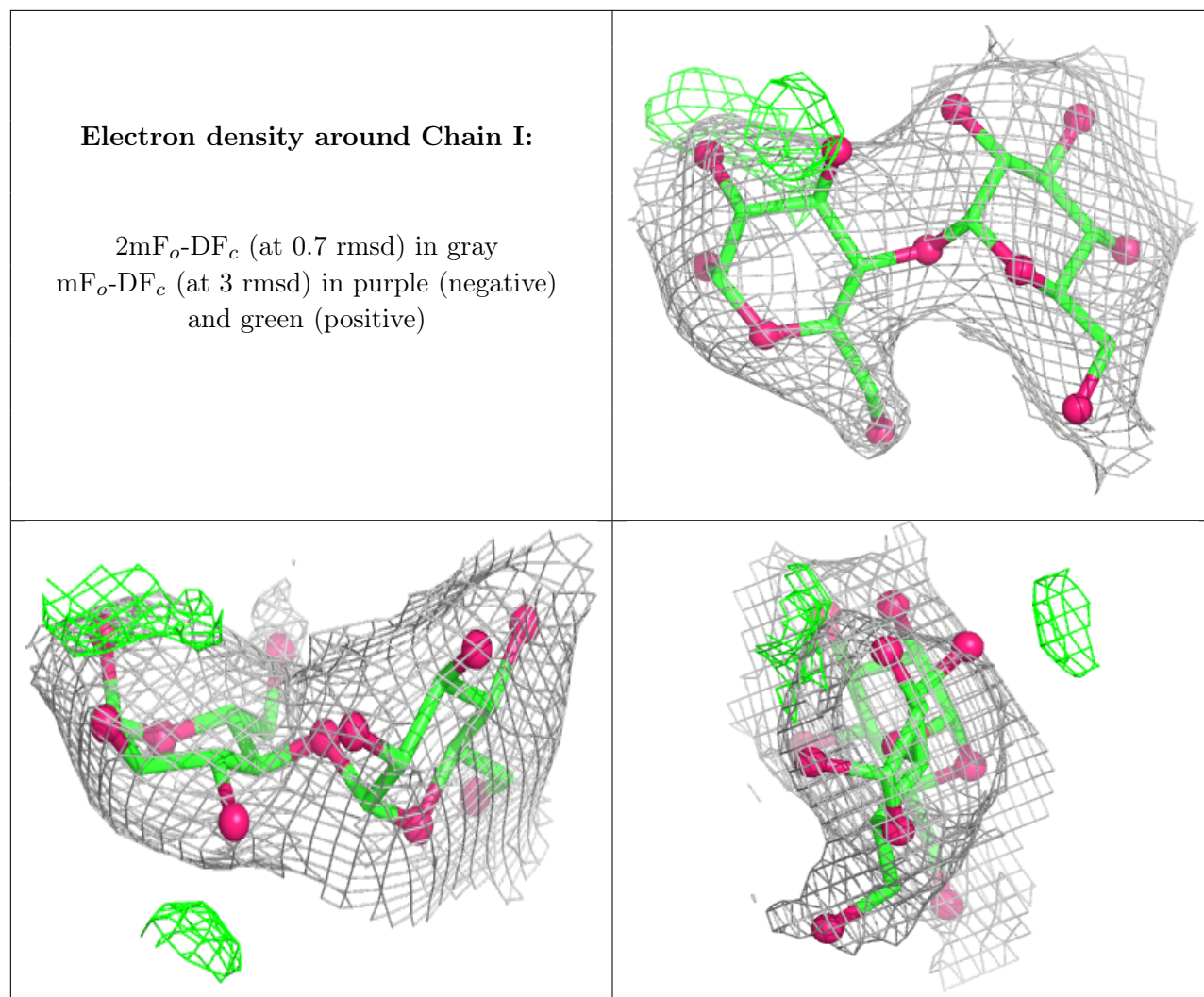
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain H:

$2mF_o-DF_c$ (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	MG	B	2202	1/1	0.99	0.04	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.