



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:49 PM UTC

PDB ID : 9GFG / pdb\_00009gfg  
Title : BCR Fab from the subset 1 chronic lymphocytic leukaemia case P3129  
Authors : Minici, C.; Degano, M.  
Deposited on : 2024-08-09  
Resolution : 2.30 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](mailto: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>.

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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

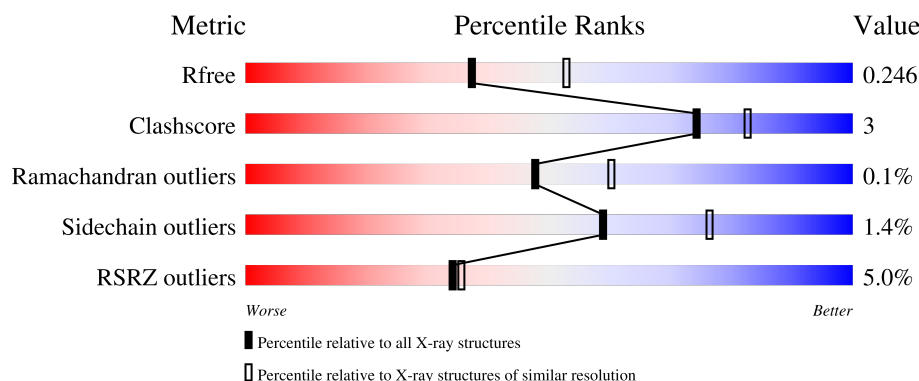
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	225	
1	C	225	
1	E	225	
1	H	225	
2	B	215	

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Mol	Chain	Length	Quality of chain
2	D	215	<div><div>%</div><div><div></div><div>91%</div><div>9%</div></div></div>
2	F	215	<div><div>3%</div><div><div></div><div>91%</div><div>8%</div></div><div></div></div>
2	L	215	<div><div>%</div><div><div></div><div>88%</div><div>11%</div></div></div>
3	G	2	<div><div></div><div><div></div><div>100%</div><div></div></div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 26219 atoms, of which 12876 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 BCR P3129 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	217	Total	C	H	N	O	S	0	1	0
			3303	1054	1630	289	320	10			
1	A	217	Total	C	H	N	O	S	0	1	0
			3301	1053	1629	289	321	9			
1	C	205	Total	C	H	N	O	S	0	0	0
			3107	994	1534	272	299	8			
1	E	200	Total	C	H	N	O	S	0	0	0
			3057	979	1514	267	290	7			

- Molecule 2 is a protein called BCR P3129 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	214	Total	C	H	N	O	S	0	1	0
			3255	1036	1605	273	337	4			
2	B	215	Total	C	H	N	O	S	0	3	0
			3283	1041	1623	274	340	5			
2	D	214	Total	C	H	N	O	S	0	0	0
			3238	1028	1596	273	337	4			
2	F	212	Total	C	H	N	O	S	0	0	0
			3216	1021	1587	271	333	4			

- Molecule 3 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
3	G	2	Total	C	H	N	O		0	0	0
			53	16	25	2	10				

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	H	O	0	0
			14	3	8	3		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		
4	L	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			13	3	7	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			12	3	6	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			13	3	7	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	H	O	0	0
			13	3	7	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	41	Total	O	0	0
			41	41		
6	L	23	Total	O	0	0
			23	23		
6	A	14	Total	O	0	0
			14	14		
6	B	29	Total	O	0	0
			29	29		
6	C	5	Total	O	0	0
			5	5		
6	D	27	Total	O	0	0
			27	27		

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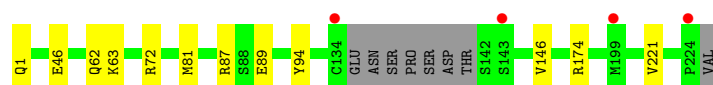
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	11	Total	O	0	0
			11	11		
6	F	11	Total	O	0	0
			11	11		

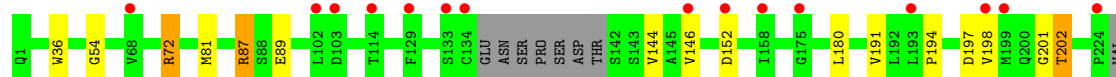
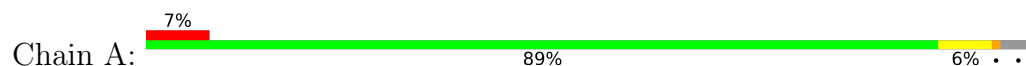
### 3 Residue-property plots [i](#)

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.

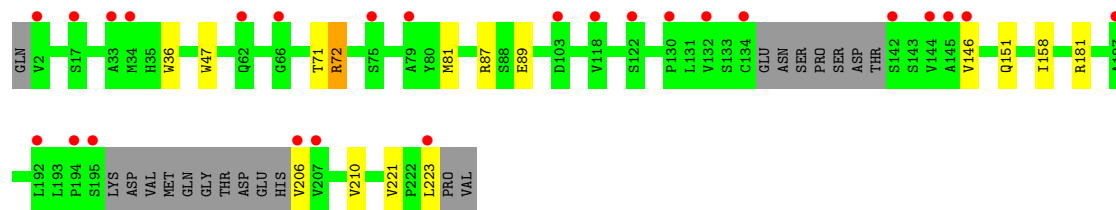
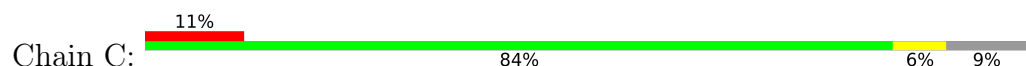
- Molecule 1: BCR P3129 heavy chain



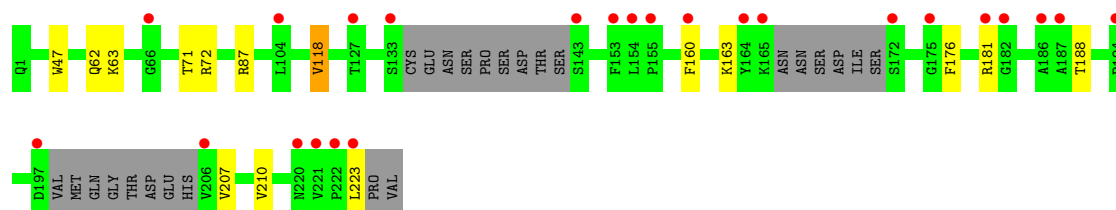
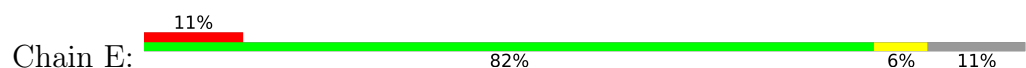
- Molecule 1: BCR P3129 heavy chain



- Molecule 1: BCR P3129 heavy chain

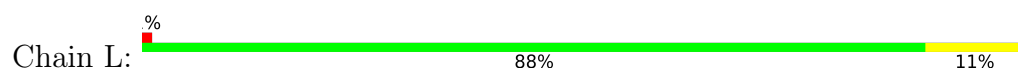


- Molecule 1: BCR P3129 heavy chain

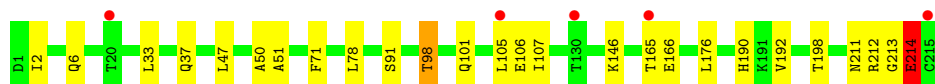
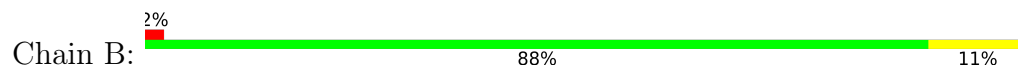


- Molecule 2: BCR P3129 light chain





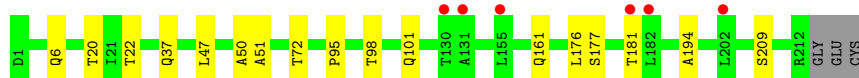
- Molecule 2: BCR P3129 light chain



- Molecule 2: BCR P3129 light chain



- Molecule 2: BCR P3129 light chain



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.70Å 87.89Å 115.53Å 90.00° 94.59° 90.00°	Depositor
Resolution (Å)	80.60 – 2.30 80.60 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (80.60-2.30) 99.9 (80.60-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.220 , 0.246 0.220 , 0.246	Depositor DCC
$R_{free}$ test set	4553 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.2	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26219	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, GOL

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	0.13	0/1715	0.35	0/2329
1	C	0.11	0/1610	0.34	0/2185
1	E	0.12	0/1579	0.34	0/2140
1	H	0.16	0/1716	0.38	0/2329
2	B	0.15	0/1705	0.37	0/2317
2	D	0.14	0/1678	0.38	0/2280
2	F	0.13	0/1665	0.35	0/2263
2	L	0.15	0/1690	0.38	0/2296
All	All	0.14	0/13358	0.36	0/18139

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	1672	1629	1628	10	0
1	C	1573	1534	1534	10	0
1	E	1543	1514	1514	9	0
1	H	1673	1630	1631	6	0
2	B	1660	1623	1623	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1642	1596	1596	13	0
2	F	1629	1587	1587	12	0
2	L	1650	1605	1605	13	0
3	G	28	25	25	0	0
4	A	12	16	16	0	0
4	B	12	15	16	0	0
4	D	18	22	24	0	0
4	E	6	8	8	0	0
4	F	12	14	16	1	0
4	H	18	24	24	0	0
4	L	6	8	8	0	0
5	A	14	13	13	0	0
5	C	14	13	13	0	0
6	A	14	0	0	0	0
6	B	29	0	0	0	1
6	C	5	0	0	1	0
6	D	27	0	0	0	0
6	E	11	0	0	0	0
6	F	11	0	0	0	0
6	H	41	0	0	0	0
6	L	23	0	0	0	1
All	All	13343	12876	12881	80	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 3.

All (80) 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:L:11:LEU:HD23	2:L:105:LEU:HD13	1.70	0.72
2:L:192:VAL:HG12	2:L:211:ASN:OD1	1.90	0.70
1:H:87:ARG:NH1	1:H:89:GLU:OE2	2.25	0.69
1:A:194:PRO:O	1:A:198:VAL:HG23	1.93	0.68
2:D:20:THR:HB	2:F:72:THR:HG21	1.78	0.66
1:C:87:ARG:NH1	1:C:89:GLU:OE2	2.28	0.65
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.80	0.63
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.81	0.63
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.81	0.62
1:E:188:THR:HG21	2:F:177:SER:OG	1.98	0.62
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.87	0.57
1:A:54:GLY:O	1:A:72:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:22:THR:HG22	2:F:72:THR:HG22	1.88	0.54
2:B:106:GLU:HG2	2:B:107:ILE:N	2.22	0.53
2:B:165[A]:THR:HG22	2:B:166:GLU:N	2.24	0.52
2:D:106:GLU:HG2	2:D:107:ILE:N	2.24	0.52
1:E:188:THR:HG22	4:F:302:GOL:O1	2.11	0.51
1:E:87:ARG:O	1:E:118:VAL:HG11	2.12	0.50
2:B:190:HIS:O	2:B:212:ARG:NH1	2.45	0.50
1:C:206:VAL:HG23	1:C:223:LEU:HD11	1.93	0.50
2:B:78:LEU:HD11	2:B:105[A]:LEU:HD21	1.93	0.50
1:C:181:ARG:NH2	2:D:181:THR:HG21	2.27	0.50
1:H:46:GLU:OE2	1:H:63:LYS:NZ	2.36	0.49
2:D:12:SER:OG	2:D:106:GLU:OE1	2.28	0.49
1:H:174:ARG:NH2	2:L:175:SER:OG	2.46	0.48
2:D:20:THR:HG21	2:F:20:THR:HG21	1.95	0.48
1:A:201:GLY:C	1:A:202:THR:HG23	2.39	0.47
2:L:190:HIS:O	2:L:212:ARG:NH1	2.44	0.47
2:L:106:GLU:HG2	2:L:107:ILE:N	2.29	0.47
2:B:6:GLN:O	2:B:101:GLN:NE2	2.45	0.47
2:B:50:ALA:O	2:B:51:ALA:HB3	2.14	0.46
1:C:146:VAL:CG1	1:C:221:VAL:HG11	2.45	0.46
1:H:1:GLN:OE1	1:H:1:GLN:N	2.38	0.46
1:C:71:THR:HG22	1:C:72:ARG:H	1.80	0.46
2:F:6:GLN:O	2:F:101:GLN:NE2	2.46	0.46
2:D:6:GLN:O	2:D:101:GLN:NE2	2.46	0.46
2:D:50:ALA:O	2:D:51:ALA:HB3	2.16	0.45
1:C:158:ILE:HD11	1:C:210:VAL:HG11	1.97	0.45
1:C:146:VAL:HG13	1:C:221:VAL:HG11	1.99	0.45
2:D:2:ILE:O	2:D:98:THR:HG21	2.17	0.45
2:B:213:GLY:O	2:B:214:GLU:CB	2.66	0.44
2:F:181:THR:O	2:F:181:THR:HG23	2.17	0.44
2:D:22:THR:HG22	2:D:72:THR:HG22	1.98	0.44
1:E:176:PHE:CD1	1:E:188:THR:HG23	2.52	0.44
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.53	0.44
2:L:214:GLU:OE1	2:L:214:GLU:N	2.43	0.43
2:D:176:LEU:C	2:D:176:LEU:HD23	2.44	0.43
2:L:50:ALA:O	2:L:51:ALA:HB3	2.17	0.43
2:L:176:LEU:C	2:L:176:LEU:HD23	2.43	0.43
2:B:192:VAL:HG22	2:B:211:ASN:OD1	2.18	0.43
1:E:181:ARG:NH1	2:F:161:GLN:OE1	2.52	0.43
2:F:50:ALA:O	2:F:51:ALA:HB3	2.17	0.43
2:L:181:THR:C	2:L:182:LEU:HD12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:141:TYR:CG	2:L:142:PRO:HA	2.54	0.42
2:D:106:GLU:OE2	2:D:174:TYR:OH	2.24	0.42
1:E:47:TRP:CZ3	2:F:95:PRO:HB3	2.55	0.42
1:E:160:PHE:CD1	1:E:210:VAL:HG12	2.55	0.42
2:B:2:ILE:O	2:B:98:THR:HG21	2.19	0.42
1:H:81[B]:MET:HE1	1:H:94:TYR:CD2	2.54	0.42
2:L:152:ASP:HA	2:L:192:VAL:CG2	2.50	0.42
1:E:163:LYS:O	1:E:207:VAL:HG22	2.20	0.42
1:C:47:TRP:CZ3	2:D:95:PRO:HB3	2.55	0.42
2:B:213:GLY:O	2:B:214:GLU:HB2	2.20	0.42
1:A:36:TRP:CE2	1:A:81:MET:HB2	2.55	0.41
1:A:152:ASP:O	1:A:152:ASP:OD1	2.37	0.41
1:C:151:GLN:NE2	6:C:402:HOH:O	2.46	0.41
1:A:146:VAL:HG23	1:A:191:VAL:CG2	2.50	0.41
2:B:33:LEU:HD22	2:B:71:PHE:CB	2.50	0.41
2:F:176:LEU:HD23	2:F:176:LEU:C	2.45	0.41
2:B:176:LEU:HD23	2:B:176:LEU:C	2.45	0.41
1:E:223:LEU:N	1:E:223:LEU:HD12	2.35	0.41
1:A:144:VAL:CG1	1:A:198:VAL:HG21	2.51	0.41
2:B:146:LYS:HB3	2:B:198:THR:HB	2.02	0.41
2:F:194:ALA:HB2	2:F:209:SER:HB3	2.03	0.41
1:A:144:VAL:HG11	1:A:198:VAL:HG21	2.02	0.41
1:A:180:LEU:HD23	1:A:180:LEU:C	2.46	0.41
1:A:87:ARG:NH1	1:A:89:GLU:OE1	2.55	0.40
1:H:146:VAL:CG1	1:H:221:VAL:HG11	2.51	0.40
1:C:36:TRP:CE2	1:C:81:MET:HB2	2.57	0.40

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)
6:L:420:HOH:O	6:B:405:HOH:O[1_554]	2.18	0.02

## 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	214/225 (95%)	205 (96%)	9 (4%)	0	100	100
1	C	199/225 (88%)	193 (97%)	6 (3%)	0	100	100
1	E	192/225 (85%)	188 (98%)	4 (2%)	0	100	100
1	H	214/225 (95%)	207 (97%)	7 (3%)	0	100	100
2	B	216/215 (100%)	210 (97%)	5 (2%)	1 (0%)	24	31
2	D	212/215 (99%)	204 (96%)	8 (4%)	0	100	100
2	F	210/215 (98%)	203 (97%)	7 (3%)	0	100	100
2	L	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
All	All	1670/1760 (95%)	1615 (97%)	54 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	214	GLU

### 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	184/191 (96%)	180 (98%)	4 (2%)	45	65
1	C	172/191 (90%)	171 (99%)	1 (1%)	78	89
1	E	167/191 (87%)	162 (97%)	5 (3%)	36	53
1	H	184/191 (96%)	182 (99%)	2 (1%)	65	81
2	B	193/190 (102%)	189 (98%)	4 (2%)	47	66
2	D	189/190 (100%)	188 (100%)	1 (0%)	81	90
2	F	188/190 (99%)	187 (100%)	1 (0%)	81	90
2	L	190/190 (100%)	187 (98%)	3 (2%)	55	73
All	All	1467/1524 (96%)	1446 (99%)	21 (1%)	59	76

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	62	GLN
1	H	72	ARG
2	L	20	THR
2	L	28	SER
2	L	98	THR
1	A	72	ARG
1	A	87	ARG
1	A	197	ASP
1	A	202	THR
2	B	91[A]	SER
2	B	91[B]	SER
2	B	98	THR
2	B	214	GLU
1	C	72	ARG
2	D	212	ARG
1	E	62	GLN
1	E	63	LYS
1	E	71	THR
1	E	72	ARG
1	E	118	VAL
2	F	98	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	190	GLN
2	L	3	GLN
2	L	138	ASN
1	A	190	GLN
1	A	200	GLN
2	B	138	ASN
2	B	161	GLN
1	C	190	GLN
2	D	138	ASN
2	D	148	GLN
2	D	161	GLN
2	F	148	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 ⓘ

2 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	G	1	1,3	14,14,15	1.09	1 (7%)	17,19,21	0.92	1 (5%)
3	NAG	G	2	3	14,14,15	0.62	1 (7%)	17,19,21	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	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	NAG	O5-C1	-3.58	1.37	1.43
3	G	2	NAG	O5-C1	-2.21	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C3-C4-C5	2.17	114.16	110.23

There are no chirality outliers.

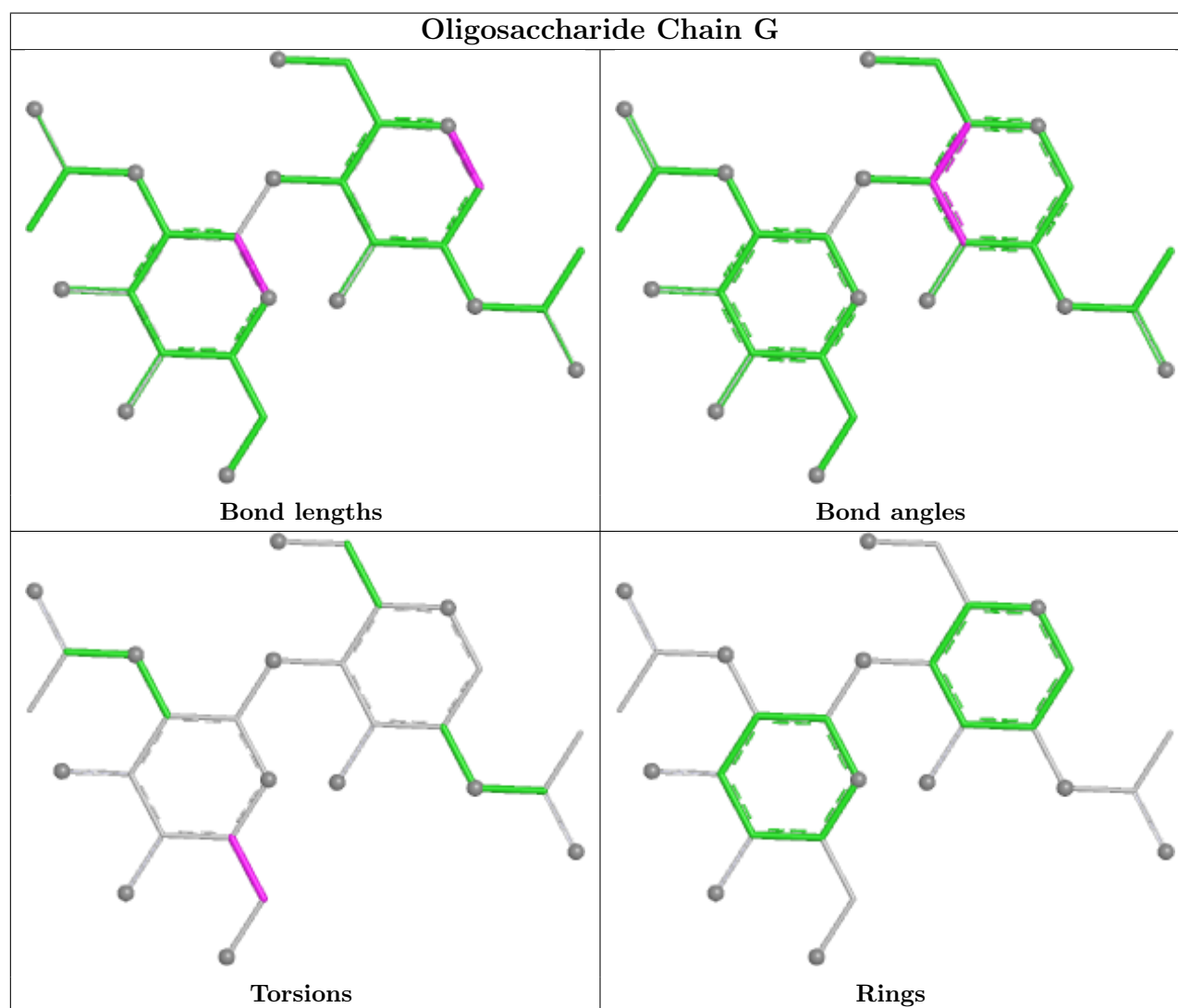
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	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

16 ligands 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	GOL	F	301	-	5,5,5	0.91	0	5,5,5	1.05	0
4	GOL	A	303	-	5,5,5	0.91	0	5,5,5	1.03	0
4	GOL	E	301	-	5,5,5	0.87	0	5,5,5	1.10	0
5	NAG	A	301	1	14,14,15	0.29	0	17,19,21	1.00	1 (5%)
4	GOL	A	302	-	5,5,5	0.92	0	5,5,5	1.05	0
4	GOL	H	303	-	5,5,5	0.98	0	5,5,5	0.91	0
4	GOL	H	301	-	5,5,5	0.88	0	5,5,5	0.93	0
4	GOL	H	302	-	5,5,5	0.94	0	5,5,5	1.08	0
4	GOL	B	301	-	5,5,5	0.98	0	5,5,5	1.07	0
4	GOL	B	302	-	5,5,5	0.92	0	5,5,5	1.01	0
4	GOL	F	302	-	5,5,5	0.98	0	5,5,5	1.04	0
5	NAG	C	301	-	14,14,15	0.33	0	17,19,21	0.73	0
4	GOL	D	302	-	5,5,5	1.04	0	5,5,5	0.91	0
4	GOL	D	301	-	5,5,5	0.93	0	5,5,5	1.03	0
4	GOL	D	303	-	5,5,5	1.00	0	5,5,5	0.82	0
4	GOL	L	301	-	5,5,5	1.18	0	5,5,5	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	F	301	-	-	2/4/4/4	-
4	GOL	A	303	-	-	2/4/4/4	-
4	GOL	E	301	-	-	0/4/4/4	-
5	NAG	A	301	1	-	0/6/23/26	0/1/1/1
4	GOL	A	302	-	-	0/4/4/4	-
4	GOL	H	303	-	-	4/4/4/4	-
4	GOL	H	301	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	302	-	-	2/4/4/4	-
4	GOL	B	301	-	-	0/4/4/4	-
4	GOL	B	302	-	-	4/4/4/4	-
4	GOL	F	302	-	-	2/4/4/4	-
5	NAG	C	301	-	-	3/6/23/26	0/1/1/1
4	GOL	D	302	-	-	4/4/4/4	-
4	GOL	D	301	-	-	0/4/4/4	-
4	GOL	D	303	-	-	3/4/4/4	-
4	GOL	L	301	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	301	NAG	C1-O5-C5	3.72	117.18	112.19

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	302	GOL	C1-C2-C3-O3
4	H	302	GOL	O2-C2-C3-O3
4	L	301	GOL	C1-C2-C3-O3
4	L	301	GOL	O2-C2-C3-O3
4	B	302	GOL	O1-C1-C2-C3
4	D	302	GOL	O1-C1-C2-C3
4	D	303	GOL	C1-C2-C3-O3
4	F	301	GOL	C1-C2-C3-O3
4	F	301	GOL	O2-C2-C3-O3
4	F	302	GOL	C1-C2-C3-O3
4	F	302	GOL	O2-C2-C3-O3
5	C	301	NAG	C8-C7-N2-C2
5	C	301	NAG	O7-C7-N2-C2
4	H	301	GOL	C1-C2-C3-O3
4	H	303	GOL	O1-C1-C2-C3
4	H	303	GOL	C1-C2-C3-O3
4	B	302	GOL	C1-C2-C3-O3
4	D	302	GOL	C1-C2-C3-O3
4	B	302	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	302	GOL	O1-C1-C2-O2
4	D	303	GOL	O2-C2-C3-O3
4	H	303	GOL	O2-C2-C3-O3
5	C	301	NAG	O5-C5-C6-O6
4	L	301	GOL	O1-C1-C2-C3
4	H	303	GOL	O1-C1-C2-O2
4	A	303	GOL	O2-C2-C3-O3
4	D	302	GOL	O2-C2-C3-O3
4	A	303	GOL	C1-C2-C3-O3
4	D	303	GOL	O1-C1-C2-C3
4	H	301	GOL	O2-C2-C3-O3
4	B	302	GOL	O2-C2-C3-O3
4	L	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	302	GOL	1	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	217/225 (96%)	0.82	15 (6%)	23 25	50, 91, 147, 172	1 (0%)
1	C	205/225 (91%)	1.12	25 (12%)	8 9	76, 118, 141, 152	0
1	E	200/225 (88%)	1.01	24 (12%)	9 9	71, 110, 159, 187	0
1	H	217/225 (96%)	0.39	4 (1%)	67 69	46, 72, 117, 168	1 (0%)
2	B	215/215 (100%)	0.43	5 (2%)	61 63	44, 78, 119, 130	3 (1%)
2	D	214/215 (99%)	0.64	3 (1%)	73 75	63, 80, 122, 147	0
2	F	212/215 (98%)	0.71	6 (2%)	55 57	63, 90, 163, 179	0
2	L	214/215 (99%)	0.41	2 (0%)	81 82	39, 78, 108, 124	1 (0%)
All	All	1694/1760 (96%)	0.69	84 (4%)	34 35	39, 87, 148, 187	6 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	195	SER	5.2
1	E	165	LYS	5.0
1	C	223	LEU	4.6
1	A	224	PRO	4.6
1	E	223	LEU	4.2
1	C	142	SER	4.0
1	C	206	VAL	3.5
1	E	197	ASP	3.4
2	F	155	LEU	3.3
1	C	194	PRO	3.3
1	A	199	MET	3.2
1	E	127	THR	3.1
1	E	104	LEU	3.1
1	E	153	PHE	3.1
2	F	181	THR	3.0
1	C	144	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	133	SER	3.0
1	A	158	ILE	3.0
1	A	198	VAL	3.0
1	C	134	CYS	2.9
1	H	224	PRO	2.8
2	D	155	LEU	2.8
1	C	2	VAL	2.8
1	A	175	GLY	2.7
1	E	160	PHE	2.7
1	E	206	VAL	2.7
1	H	134	CYS	2.7
1	E	221	VAL	2.7
1	E	172	SER	2.7
1	C	207	VAL	2.7
1	C	145	ALA	2.6
1	C	146	VAL	2.6
2	F	130	THR	2.6
1	C	66	GLY	2.6
1	A	152	ASP	2.6
1	A	134	CYS	2.6
2	D	51	ALA	2.6
1	A	133	SER	2.4
1	E	175	GLY	2.4
1	A	114	THR	2.4
2	B	20	THR	2.4
2	B	215	CYS	2.4
1	E	154	LEU	2.4
2	L	136	LEU	2.4
1	E	220	ASN	2.3
1	E	194	PRO	2.3
2	B	130	THR	2.3
1	E	164	TYR	2.3
1	C	132	VAL	2.3
1	C	103	ASP	2.3
1	C	62	GLN	2.3
1	C	118	VAL	2.3
1	E	66	GLY	2.3
1	E	187	ALA	2.3
2	B	165[A]	THR	2.3
1	C	17	SER	2.3
1	C	79	ALA	2.2
1	E	222	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	182	GLY	2.2
1	C	34	MET	2.2
1	A	193	LEU	2.2
2	F	182	LEU	2.2
1	A	146	VAL	2.1
1	C	33	ALA	2.1
2	L	118	ILE	2.1
1	A	103	ASP	2.1
1	A	68	VAL	2.1
1	A	129	PHE	2.1
1	E	155	PRO	2.1
1	E	186	ALA	2.1
2	B	105[A]	LEU	2.1
1	E	181	ARG	2.1
1	C	75	SER	2.1
1	A	102	LEU	2.1
2	D	191	LYS	2.0
1	H	143	SER	2.0
1	C	122	SER	2.0
1	H	199	MET	2.0
1	C	187	ALA	2.0
2	F	131	ALA	2.0
1	C	192	LEU	2.0
2	F	202	LEU	2.0
1	E	143	SER	2.0
1	C	130	PRO	2.0

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

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

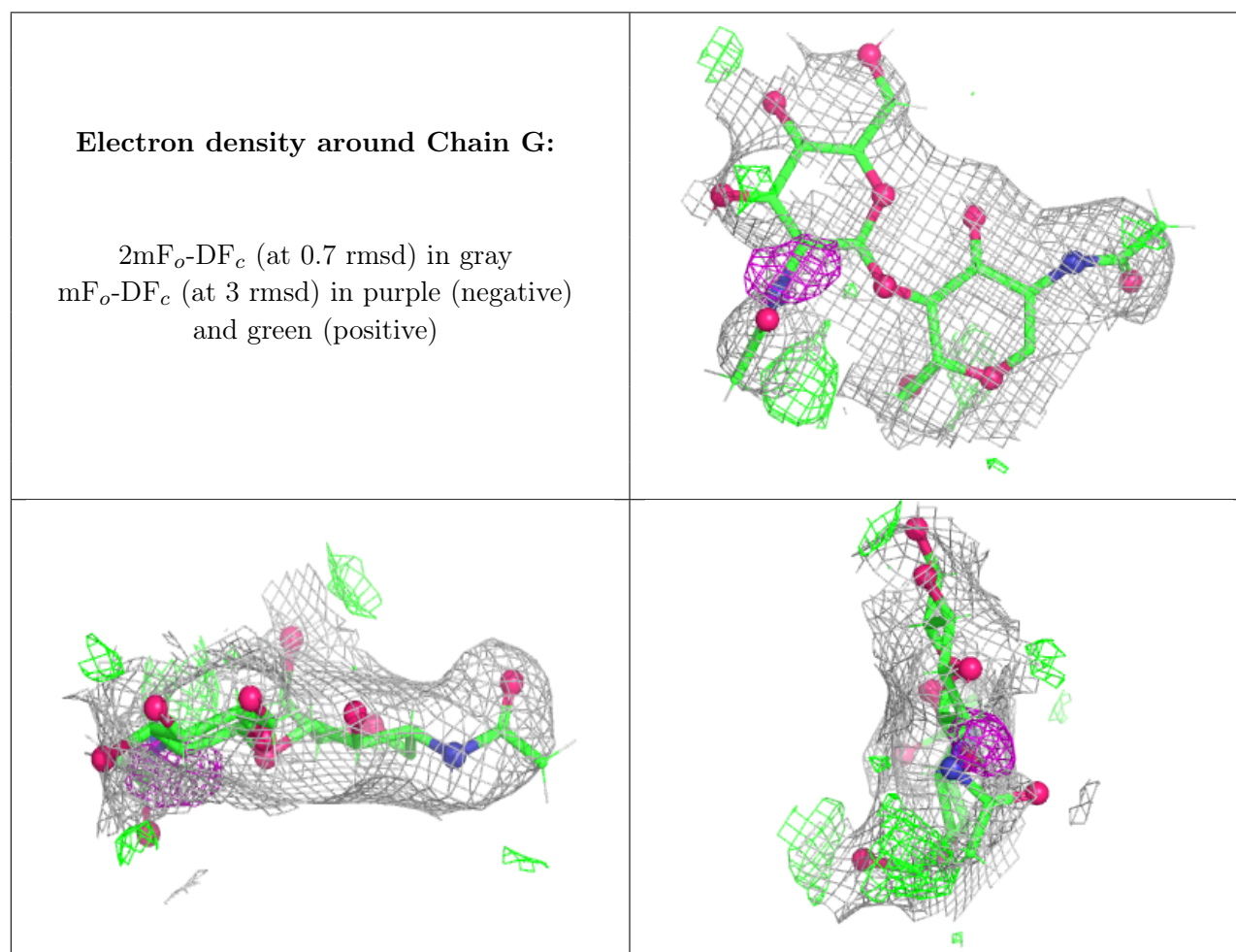
## 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	G	1	14/15	-	-	97,114,144,144	0
3	NAG	G	2	14/15	-	-	100,109,131,132	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.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	C	301	14/15	0.49	0.19	134,140,168,168	0
5	NAG	A	301	14/15	0.68	0.17	130,138,164,165	0
4	GOL	B	302	6/6	0.74	0.16	65,78,91,92	0
4	GOL	D	303	6/6	0.76	0.14	77,96,115,116	0
4	GOL	H	301	6/6	0.80	0.18	66,79,89,89	0
4	GOL	D	302	6/6	0.82	0.17	71,89,108,108	0
4	GOL	H	303	6/6	0.82	0.17	74,93,111,128	0
4	GOL	B	301	6/6	0.83	0.18	54,62,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	303	6/6	0.84	0.16	69,83,91,95	0
4	GOL	L	301	6/6	0.88	0.14	57,70,81,85	0
4	GOL	E	301	6/6	0.88	0.13	74,89,91,94	0
4	GOL	F	301	6/6	0.91	0.10	74,81,91,92	0
4	GOL	F	302	6/6	0.93	0.12	102,110,132,132	0
4	GOL	H	302	6/6	0.94	0.08	57,68,73,73	0
4	GOL	D	301	6/6	0.96	0.07	70,77,91,91	0
4	GOL	A	302	6/6	0.96	0.08	73,88,92,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.