



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 11, 2025 – 02:01 pm BST

PDB ID : 9GFH / pdb_00009gfh
Title : BCR Fab from the subset 1 chronic lymphocytic leukaemia case P1173
Authors : Cocomazzi, P.G.; Degano, M.
Deposited on : 2024-08-09
Resolution : 2.72 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

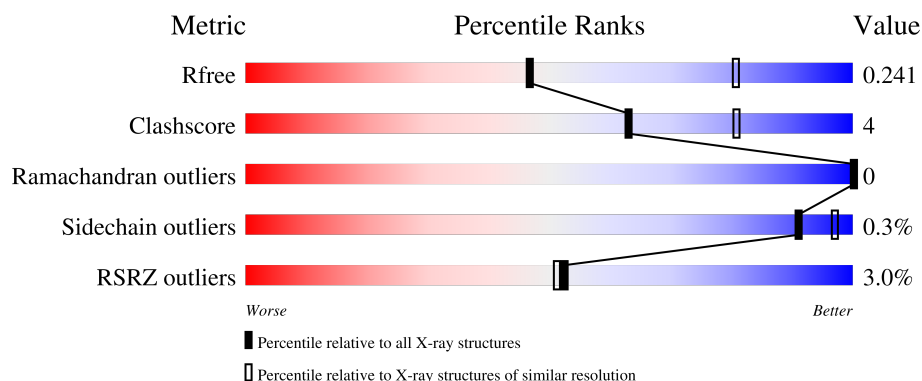
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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}	164625	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	B	215	<div> <div>3%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	D	215	<div> <div>%</div> <div>90%</div> <div>9%</div> </div>
1	F	215	<div> <div>%</div> <div>90%</div> <div>10%</div> </div>
1	L	215	<div> <div>2%</div> <div>89%</div> <div>11%</div> </div>
2	A	225	<div> <div>2%</div> <div>86%</div> <div>5%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	225	<div><div></div><div>4%</div><div>86%</div><div>9%</div><div></div></div>
2	E	225	<div><div></div><div>6%</div><div>88%</div><div>6%</div><div>5%</div></div>
2	H	225	<div><div></div><div>3%</div><div>86%</div><div>10%</div><div></div></div>
3	G	3	<div><div></div><div>67%</div><div>33%</div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 26000 atoms, of which 12792 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.

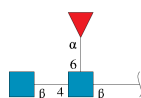
- Molecule 1 is a protein called BCR P1173 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	214	Total	C	H	N	O	S	0	0	0
			3229	1023	1590	275	336	5			
1	B	211	Total	C	H	N	O	S	0	0	0
			3187	1010	1570	272	330	5			
1	D	214	Total	C	H	N	O	S	0	0	0
			3229	1023	1590	275	336	5			
1	F	214	Total	C	H	N	O	S	0	0	0
			3229	1023	1590	275	336	5			

- Molecule 2 is a protein called BCR P1173 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	206	Total	C	H	N	O	S	0	0	0
			3140	1016	1547	265	304	8			
2	H	217	Total	C	H	N	O	S	0	0	0
			3297	1061	1624	280	323	9			
2	C	215	Total	C	H	N	O	S	0	0	0
			3262	1051	1606	277	320	8			
2	E	213	Total	C	H	N	O	S	0	0	0
			3242	1045	1597	275	317	8			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



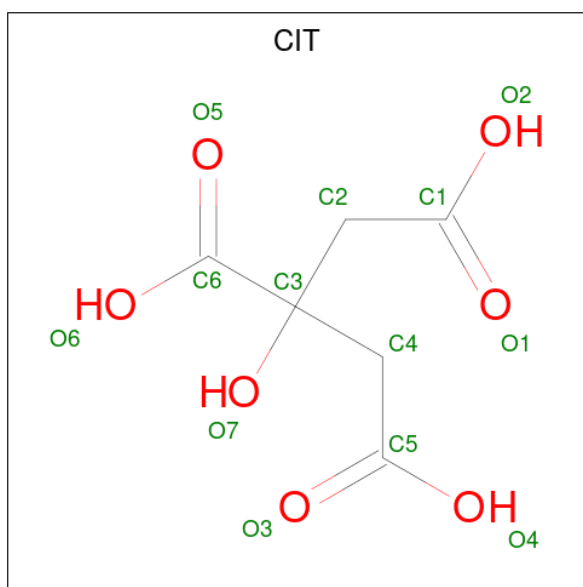
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	H	O	0	0
			18	6	5	7		

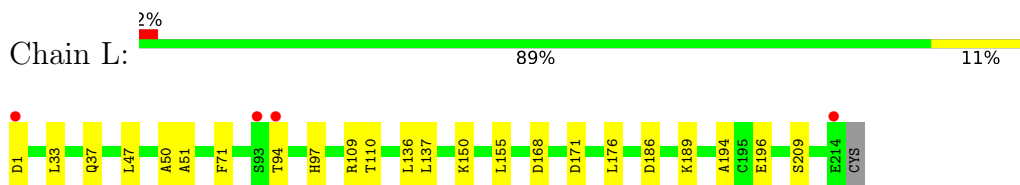
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	3	Total	O	0	0
			3	3		
6	A	1	Total	O	0	0
			1	1		
6	D	2	Total	O	0	0
			2	2		
6	F	1	Total	O	0	0
			1	1		
6	H	4	Total	O	0	0
			4	4		
6	C	2	Total	O	0	0
			2	2		
6	E	1	Total	O	0	0
			1	1		

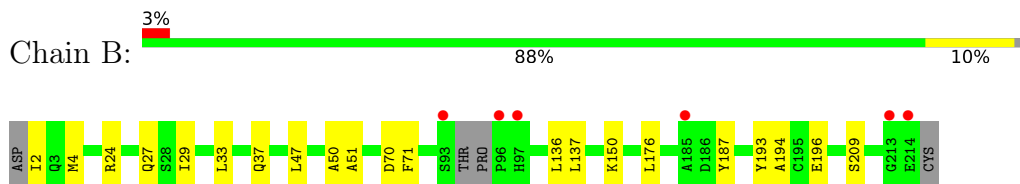
3 Residue-property plots [i](#)

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.

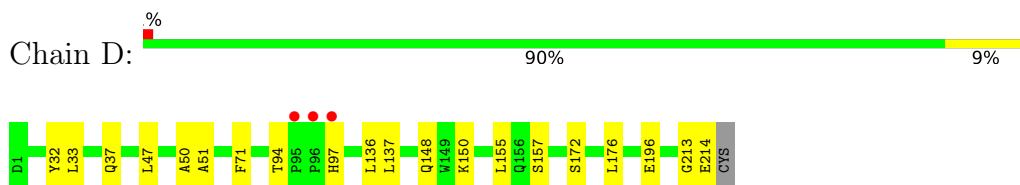
- Molecule 1: BCR P1173 light chain



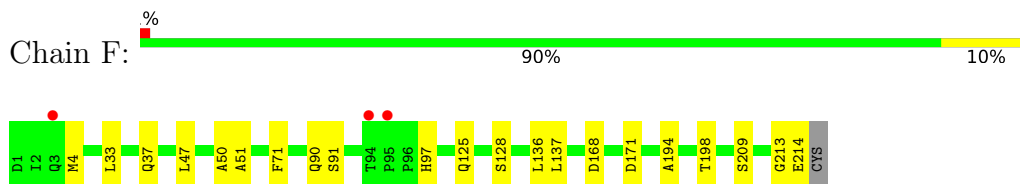
- Molecule 1: BCR P1173 light chain



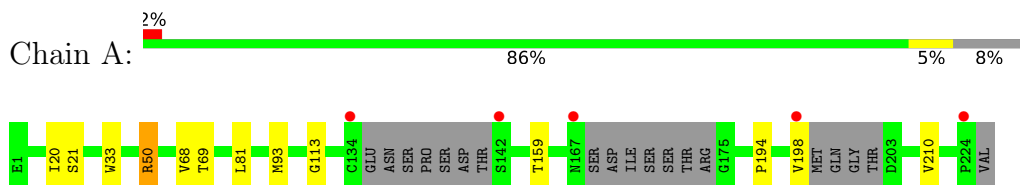
- Molecule 1: BCR P1173 light chain



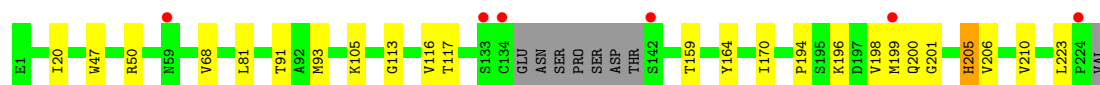
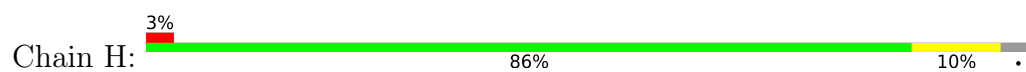
- Molecule 1: BCR P1173 light chain



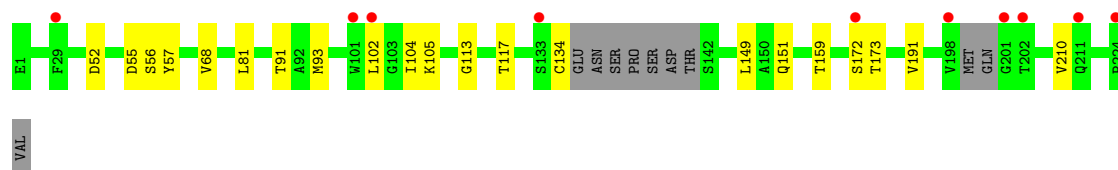
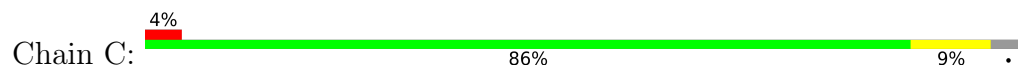
- Molecule 2: BCR P1173 heavy chain



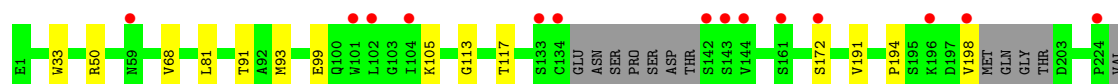
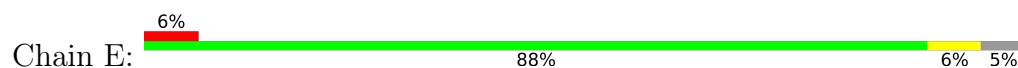
- Molecule 2: BCR P1173 heavy chain



- Molecule 2: BCR P1173 heavy chain



- Molecule 2: BCR P1173 heavy chain



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.42Å 128.51Å 134.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.77 – 2.72 91.77 – 2.72	Depositor EDS
% Data completeness (in resolution range)	70.6 (91.77-2.72) 70.8 (91.77-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.214 , 0.244 0.212 , 0.241	Depositor DCC
R_{free} test set	1997 reflections (3.37%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	26000	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: FUC, CIT, NAG

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	B	0.12	0/1651	0.37	0/2238
1	D	0.13	0/1675	0.37	0/2275
1	F	0.13	0/1675	0.35	0/2275
1	L	0.12	0/1675	0.35	0/2275
2	A	0.13	0/1635	0.34	0/2219
2	C	0.12	0/1699	0.33	0/2307
2	E	0.12	0/1688	0.35	0/2292
2	H	0.14	0/1717	0.36	0/2332
All	All	0.13	0/13415	0.35	0/18213

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	B	1617	1570	1569	12	0
1	D	1639	1590	1590	18	0
1	F	1639	1590	1590	15	0
1	L	1639	1590	1590	15	0
2	A	1593	1547	1544	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1656	1606	1605	15	0
2	E	1645	1597	1595	9	0
2	H	1673	1624	1623	19	0
3	G	38	34	34	2	0
4	A	14	13	13	0	0
4	C	14	13	13	0	0
4	E	14	13	13	0	0
5	H	13	5	5	1	0
6	A	1	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	1	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	H	4	0	0	0	0
6	L	3	0	0	0	0
All	All	13208	12792	12784	100	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 4.

All (100) 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:150:LYS:NZ	1:B:196:GLU:OE1	2.12	0.82
2:E:172:SER:O	2:E:191:VAL:HG12	1.82	0.80
1:D:94:THR:HG22	1:D:97:HIS:HE1	1.48	0.77
2:C:172:SER:O	2:C:191:VAL:HG12	1.82	0.77
1:B:24:ARG:NE	1:B:70:ASP:OD1	2.24	0.70
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.27	0.69
1:D:150:LYS:NZ	1:D:196:GLU:OE1	2.22	0.68
1:B:37:GLN:HB2	1:B:47:LEU:HD11	1.77	0.67
2:H:93:MET:HE1	2:H:113:GLY:HA3	1.77	0.66
1:D:33:LEU:HD22	1:D:71:PHE:CG	2.30	0.66
1:B:2:ILE:HG22	1:B:4:MET:HE2	1.77	0.66
1:F:97:HIS:NE2	2:E:99:GLU:OE2	2.30	0.64
1:F:4:MET:HE2	1:F:90:GLN:HB2	1.80	0.62
1:F:37:GLN:HB2	1:F:47:LEU:HD11	1.82	0.62
2:E:33:TRP:CE3	2:E:50:ARG:HG2	2.35	0.61
2:H:206:VAL:HG22	2:H:223:LEU:HD21	1.84	0.60
1:D:94:THR:HG22	1:D:97:HIS:CE1	2.34	0.60
1:B:33:LEU:HD22	1:B:71:PHE:CG	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:THR:HG21	2:C:105:LYS:NZ	2.19	0.58
1:L:150:LYS:NZ	1:L:196:GLU:OE1	2.37	0.57
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.87	0.57
1:L:94:THR:HG21	2:H:50:ARG:NH2	2.20	0.57
2:H:91:THR:HG23	2:H:117:THR:HA	1.86	0.57
1:D:148:GLN:NE2	1:D:155:LEU:HD23	2.20	0.56
1:B:187:TYR:O	1:B:193:TYR:OH	2.24	0.56
2:A:68:VAL:HG11	2:A:81:LEU:HD11	1.88	0.56
2:C:93:MET:HE1	2:C:113:GLY:HA3	1.86	0.56
2:E:93:MET:HE1	2:E:113:GLY:HA3	1.87	0.55
1:F:33:LEU:HD22	1:F:71:PHE:CG	2.42	0.54
1:L:155:LEU:HD22	1:D:157:SER:HB2	1.90	0.52
1:F:4:MET:CE	1:F:90:GLN:HB2	2.40	0.51
1:D:37:GLN:HB2	1:D:47:LEU:HD11	1.92	0.51
1:L:50:ALA:O	1:L:51:ALA:HB3	2.09	0.50
2:H:201:GLY:CA	3:G:3:FUC:H62	2.42	0.50
1:B:50:ALA:O	1:B:51:ALA:HB3	2.12	0.50
2:A:93:MET:HE1	2:A:113:GLY:HA3	1.92	0.50
1:F:50:ALA:O	1:F:51:ALA:HB3	2.11	0.49
1:F:213:GLY:O	1:F:214:GLU:HB3	2.13	0.49
1:L:186:ASP:HA	1:L:189:LYS:HD3	1.94	0.49
2:H:194:PRO:O	2:H:198:VAL:HG23	2.13	0.48
1:L:194:ALA:HB2	1:L:209:SER:HB3	1.94	0.48
1:F:136:LEU:C	1:F:137:LEU:HD12	2.38	0.48
1:D:32:TYR:CZ	2:C:104:ILE:HD13	2.48	0.48
1:F:125:GLN:O	1:F:128:SER:OG	2.30	0.47
1:F:194:ALA:HB2	1:F:209:SER:HB3	1.95	0.47
2:A:194:PRO:O	2:A:198:VAL:HG23	2.14	0.47
2:E:194:PRO:O	2:E:198:VAL:HG23	2.15	0.47
1:D:50:ALA:O	1:D:51:ALA:HB3	2.14	0.47
2:C:68:VAL:HG11	2:C:81:LEU:HD11	1.97	0.47
2:C:91:THR:HG23	2:C:117:THR:HA	1.95	0.47
2:H:201:GLY:HA3	3:G:3:FUC:H62	1.97	0.47
2:E:68:VAL:HG11	2:E:81:LEU:HD11	1.96	0.47
1:B:2:ILE:CG2	1:B:4:MET:HE2	2.44	0.46
1:D:136:LEU:C	1:D:137:LEU:HD12	2.40	0.46
2:C:149:LEU:HD21	2:C:151:GLN:NE2	2.30	0.46
2:A:159:THR:O	2:A:210:VAL:HA	2.15	0.46
1:B:136:LEU:C	1:B:137:LEU:HD12	2.41	0.46
1:F:137:LEU:HD12	1:F:137:LEU:N	2.30	0.45
2:H:47:TRP:HZ2	2:H:50:ARG:HG3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:LEU:C	1:L:137:LEU:HD12	2.41	0.45
2:H:68:VAL:HG11	2:H:81:LEU:HD11	1.97	0.45
1:D:32:TYR:CE2	2:C:104:ILE:HD13	2.52	0.45
1:D:213:GLY:O	1:D:214:GLU:HB3	2.17	0.44
2:H:205:HIS:CD2	5:H:301:CIT:O1	2.70	0.44
2:H:164:TYR:CZ	2:H:170:ILE:HG12	2.52	0.44
1:F:168:ASP:HB3	1:F:171:ASP:OD1	2.18	0.44
2:A:33:TRP:CE3	2:A:50:ARG:HD2	2.53	0.44
1:L:109:ARG:NH1	1:L:110:THR:O	2.51	0.43
1:L:94:THR:HG21	2:H:50:ARG:HH22	1.82	0.43
2:C:102:LEU:N	2:C:102:LEU:HD12	2.33	0.43
1:L:97:HIS:CE1	2:H:50:ARG:HH21	2.36	0.43
2:H:50:ARG:NH2	2:H:105:LYS:HE3	2.34	0.43
1:B:27:GLN:O	1:B:29:ILE:HG23	2.19	0.43
1:D:94:THR:HG21	2:C:105:LYS:HZ3	1.82	0.43
2:C:55:ASP:OD2	2:C:57:TYR:HB2	2.19	0.43
1:F:91:SER:HB2	2:E:105:LYS:HB2	2.01	0.42
2:C:172:SER:O	2:C:173:THR:HG23	2.19	0.42
1:L:176:LEU:C	1:L:176:LEU:HD23	2.44	0.42
1:B:194:ALA:HB2	1:B:209:SER:HB3	2.01	0.42
1:D:176:LEU:C	1:D:176:LEU:HD23	2.44	0.42
1:L:168:ASP:HB3	1:L:171:ASP:OD1	2.20	0.42
2:E:33:TRP:HB2	2:E:99:GLU:HB3	2.02	0.42
1:L:137:LEU:HD12	1:L:137:LEU:N	2.35	0.42
2:H:196:LYS:O	2:H:200:GLN:HG2	2.20	0.42
2:E:91:THR:HG23	2:E:117:THR:HA	2.00	0.42
1:F:213:GLY:O	1:F:214:GLU:CB	2.68	0.41
2:H:200:GLN:HG3	2:H:200:GLN:O	2.20	0.41
1:D:214:GLU:HG3	2:C:134:CYS:SG	2.60	0.41
1:F:171:ASP:OD1	1:F:171:ASP:C	2.62	0.41
1:D:33:LEU:HD22	1:D:71:PHE:CB	2.49	0.41
1:D:172:SER:OG	6:D:301:HOH:O	2.22	0.41
2:H:159:THR:O	2:H:210:VAL:HA	2.20	0.41
2:H:199:MET:SD	2:H:199:MET:N	2.93	0.41
2:A:20:ILE:HG22	2:A:21:SER:N	2.35	0.41
2:C:159:THR:O	2:C:210:VAL:HA	2.20	0.41
2:C:52:ASP:O	2:C:56:SER:N	2.49	0.40
2:A:68:VAL:HG12	2:A:69:THR:N	2.36	0.40
1:B:176:LEU:HD23	1:B:176:LEU:C	2.46	0.40
2:H:20:ILE:HD11	2:H:116:VAL:HG21	2.03	0.40
2:A:68:VAL:CG1	2:A:81:LEU:HD11	2.51	0.40

There are no symmetry-related clashes.

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	B	207/215 (96%)	196 (95%)	11 (5%)	0	100	100
1	D	212/215 (99%)	203 (96%)	9 (4%)	0	100	100
1	F	212/215 (99%)	202 (95%)	10 (5%)	0	100	100
1	L	212/215 (99%)	201 (95%)	11 (5%)	0	100	100
2	A	198/225 (88%)	188 (95%)	10 (5%)	0	100	100
2	C	209/225 (93%)	197 (94%)	12 (6%)	0	100	100
2	E	207/225 (92%)	194 (94%)	13 (6%)	0	100	100
2	H	213/225 (95%)	200 (94%)	13 (6%)	0	100	100
All	All	1670/1760 (95%)	1581 (95%)	89 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	B	186/190 (98%)	186 (100%)	0	100	100
1	D	189/190 (100%)	189 (100%)	0	100	100
1	F	189/190 (100%)	188 (100%)	1 (0%)	86	95
1	L	189/190 (100%)	188 (100%)	1 (0%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	177/195 (91%)	176 (99%)	1 (1%)	84	93
2	C	185/195 (95%)	185 (100%)	0	100	100
2	E	184/195 (94%)	184 (100%)	0	100	100
2	H	187/195 (96%)	186 (100%)	1 (0%)	86	95
All	All	1486/1540 (96%)	1482 (100%)	4 (0%)	91	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
2	A	50	ARG
1	F	198	THR
2	H	205	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	200	GLN
1	L	211	ASN
2	A	220	ASN
1	B	161	GLN
1	D	125	GLN
1	D	211	ASN
1	F	211	ASN
2	H	214	ASN
2	H	220	ASN
2	C	151	GLN
2	C	214	ASN
2	E	211	GLN
2	E	220	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

3 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	3,2	14,14,15	0.33	0	17,19,21	0.65	0
3	NAG	G	2	3	14,14,15	0.30	0	17,19,21	0.41	0
3	FUC	G	3	3	10,10,11	1.06	1 (10%)	14,14,16	1.21	1 (7%)

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	3,2	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	FUC	G	3	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	FUC	C1-C2	3.11	1.59	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	FUC	C1-C2-C3	3.00	113.35	109.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

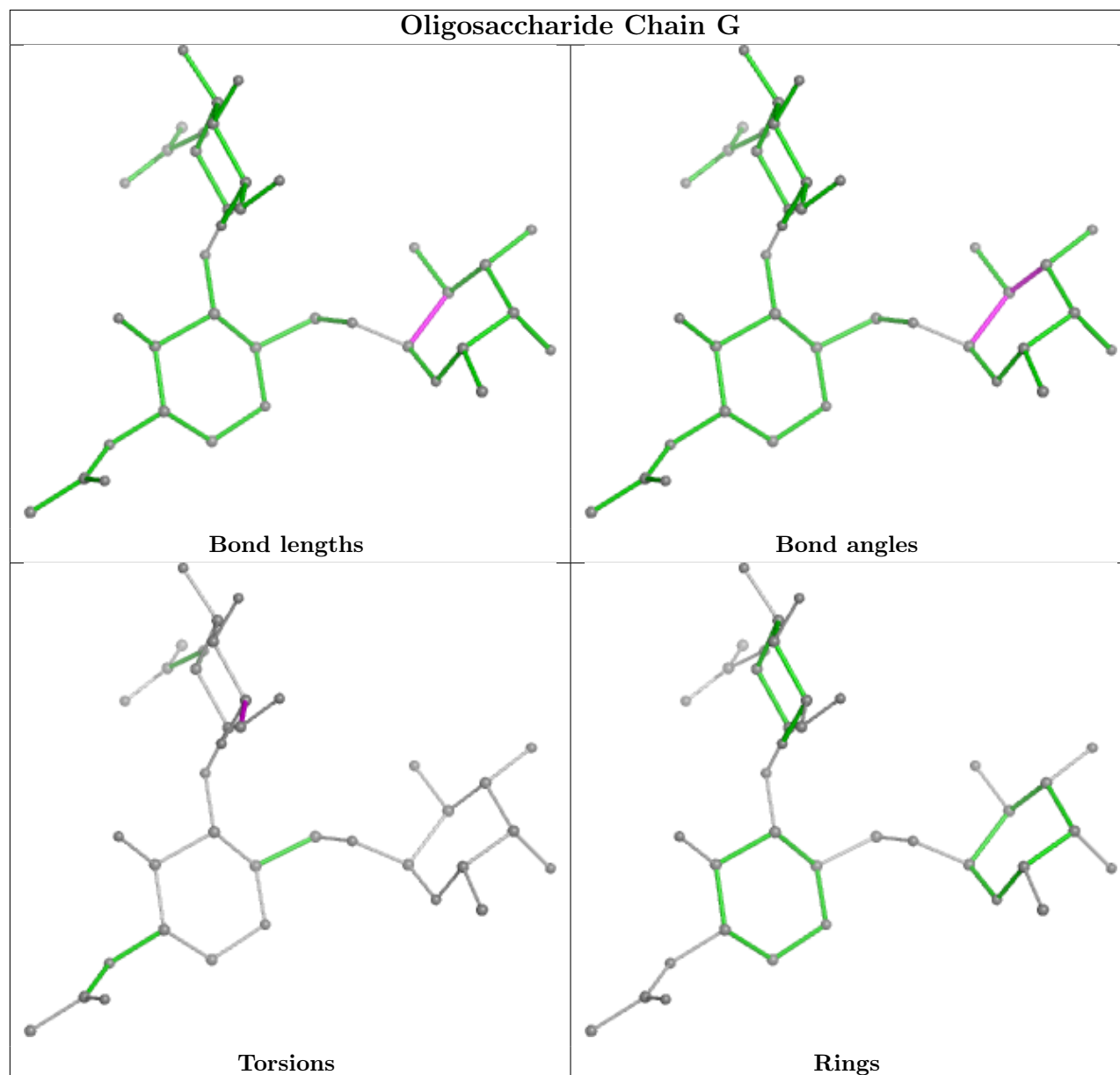
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	3	FUC	2	0

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



5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
5	CIT	H	301	-	12,12,12	1.82	6 (50%)	17,17,17	2.52	6 (35%)
4	NAG	A	301	2	14,14,15	0.38	0	17,19,21	0.46	0
4	NAG	E	301	2	14,14,15	0.32	0	17,19,21	0.44	0
4	NAG	C	301	2	14,14,15	0.36	0	17,19,21	0.41	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
5	CIT	H	301	-	-	3/16/16/16	-
4	NAG	A	301	2	-	2/6/23/26	0/1/1/1
4	NAG	E	301	2	-	2/6/23/26	0/1/1/1
4	NAG	C	301	2	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	301	CIT	O5-C6	2.73	1.30	1.22
5	H	301	CIT	O3-C5	2.64	1.30	1.22
5	H	301	CIT	O4-C5	-2.63	1.21	1.30
5	H	301	CIT	O2-C1	-2.61	1.21	1.30
5	H	301	CIT	O1-C1	2.61	1.30	1.22
5	H	301	CIT	O6-C6	-2.16	1.22	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	301	CIT	O5-C6-C3	-6.48	113.08	122.25
5	H	301	CIT	O6-C6-C3	5.40	122.43	113.05
5	H	301	CIT	O1-C1-C2	-3.41	112.97	122.94
5	H	301	CIT	O3-C5-C4	-2.86	114.60	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	301	CIT	O2-C1-C2	2.78	123.29	114.35
5	H	301	CIT	O4-C5-C4	2.47	122.28	114.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	301	CIT	C2-C3-C4-C5
5	H	301	CIT	O7-C3-C4-C5
4	A	301	NAG	C4-C5-C6-O6
4	E	301	NAG	C4-C5-C6-O6
4	A	301	NAG	O5-C5-C6-O6
4	C	301	NAG	C4-C5-C6-O6
4	E	301	NAG	O5-C5-C6-O6
4	C	301	NAG	O5-C5-C6-O6
5	H	301	CIT	C6-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	301	CIT	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, 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	B	211/215 (98%)	0.02	6 (2%)	55	54	49, 71, 114, 135	0
1	D	214/215 (99%)	-0.09	3 (1%)	73	73	47, 65, 103, 147	0
1	F	214/215 (99%)	0.07	3 (1%)	73	73	54, 76, 110, 153	0
1	L	214/215 (99%)	-0.12	4 (1%)	66	65	44, 63, 107, 151	0
2	A	206/225 (91%)	-0.01	5 (2%)	59	59	46, 66, 119, 163	0
2	C	215/225 (95%)	0.18	10 (4%)	37	36	51, 71, 110, 162	0
2	E	213/225 (94%)	0.38	14 (6%)	26	24	62, 78, 122, 170	0
2	H	217/225 (96%)	0.07	6 (2%)	55	54	47, 68, 102, 134	0
All	All	1704/1760 (96%)	0.06	51 (2%)	52	51	44, 70, 113, 170	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	PRO	6.0
2	C	201	GLY	5.1
2	E	172	SER	3.7
2	H	133	SER	3.7
2	H	224	PRO	3.6
2	E	101	TRP	3.5
2	E	133	SER	3.3
2	C	172	SER	3.2
2	C	101	TRP	3.2
1	B	93	SER	3.1
2	E	224	PRO	3.1
1	D	97	HIS	3.0
2	E	102	LEU	3.0
1	F	94	THR	2.9
2	A	142	SER	2.9
2	E	198	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	59	ASN	2.9
2	A	224	PRO	2.9
2	E	142	SER	2.8
2	E	134	CYS	2.8
2	A	198	VAL	2.7
2	E	143	SER	2.7
2	C	224	PRO	2.6
1	L	94	THR	2.6
1	D	96	PRO	2.6
1	F	95	PRO	2.6
1	L	93	SER	2.5
2	C	202	THR	2.5
2	C	211	GLN	2.5
2	C	133	SER	2.4
1	F	3	GLN	2.2
2	E	104	ILE	2.2
2	H	199	MET	2.2
1	L	214	GLU	2.2
2	C	198	VAL	2.2
1	L	1	ASP	2.2
2	E	161	SER	2.2
1	B	185	ALA	2.2
2	C	102	LEU	2.1
2	H	134	CYS	2.1
1	B	214	GLU	2.1
1	D	95	PRO	2.1
2	E	196	LYS	2.1
2	E	144	VAL	2.1
2	H	142	SER	2.1
1	B	213	GLY	2.1
2	A	134	CYS	2.1
2	C	29	PHE	2.1
2	A	167	ASN	2.0
2	H	59	ASN	2.0
1	B	97	HIS	2.0

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

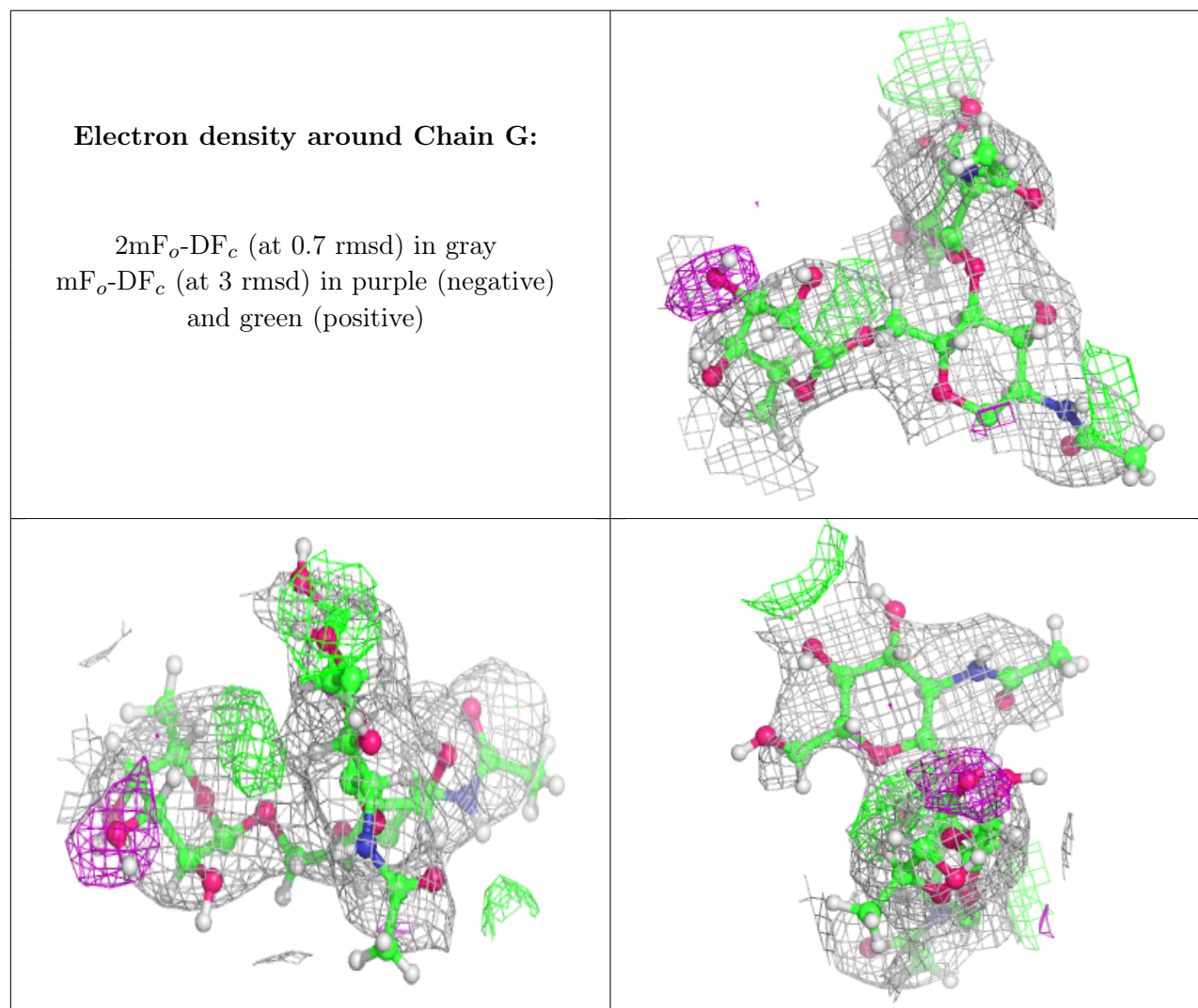
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	G	1	14/15	-	-	62,72,86,90	0
3	NAG	G	2	14/15	-	-	74,81,97,98	0
3	FUC	G	3	10/11	-	-	76,89,103,108	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, 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(\AA^2)	Q<0.9
4	NAG	A	301	14/15	0.57	0.17	99,107,125,128	0
4	NAG	E	301	14/15	0.68	0.18	93,101,125,125	0
5	CIT	H	301	13/13	0.71	0.12	72,76,92,95	0
4	NAG	C	301	14/15	0.82	0.11	72,82,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.