



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2024 – 05:27 PM EDT

PDB ID : 6MHR  
Title : Structure of the human 4-1BB / Urelumab Fab complex  
Authors : Kimberlin, C.R.; Chin, S.M.; Roe-Zurz, Z.; Xu, A.; Yang, Y.  
Deposited on : 2018-09-18  
Resolution : 2.80 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

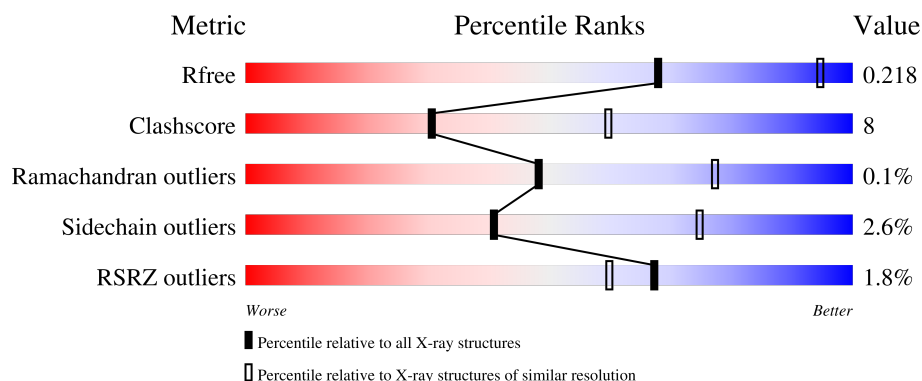
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	235	<div> <div>72%</div> <div>20%</div> <div>7%</div> </div>
1	D	235	<div> <div>74%</div> <div>17%</div> <div>8%</div> </div>
2	B	216	<div> <div>86%</div> <div>13%</div> </div>
2	E	216	<div> <div>85%</div> <div>13%</div> </div>
3	C	144	<div> <div>4%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	144	
4	G	5	
5	H	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	EPE	C	205	-	X	-	-
8	EPE	F	206	-	X	-	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8622 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 Urelumab Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	217	Total	C	N	O	S	0	0	0
			1623	1040	261	318	4			
1	A	219	Total	C	N	O	S	0	0	0
			1624	1040	261	319	4			

- Molecule 2 is a protein called Urelumab Fab kappa chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	215	Total	C	N	O	S	0	0	0
			1624	1018	274	328	4			
2	B	215	Total	C	N	O	S	0	0	0
			1624	1019	275	326	4			

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	140	Total	C	N	O	S	0	0	0
			975	579	176	199	21			
3	C	141	Total	C	N	O	S	0	0	0
			980	583	176	199	22			

There are 12 discrepancies between the modelled and reference sequences:

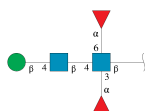
Chain	Residue	Modelled	Actual	Comment	Reference
F	163	GLU	-	expression tag	UNP Q07011
F	164	ASN	-	expression tag	UNP Q07011
F	165	LEU	-	expression tag	UNP Q07011
F	166	TYR	-	expression tag	UNP Q07011
F	167	PHE	-	expression tag	UNP Q07011
F	168	GLN	-	expression tag	UNP Q07011
C	163	GLU	-	expression tag	UNP Q07011
C	164	ASN	-	expression tag	UNP Q07011

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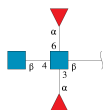
Chain	Residue	Modelled	Actual	Comment	Reference
C	165	LEU	-	expression tag	UNP Q07011
C	166	TYR	-	expression tag	UNP Q07011
C	167	PHE	-	expression tag	UNP Q07011
C	168	GLN	-	expression tag	UNP Q07011

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	5	Total	C	N	O	0	0
			59	34	2	23		0

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



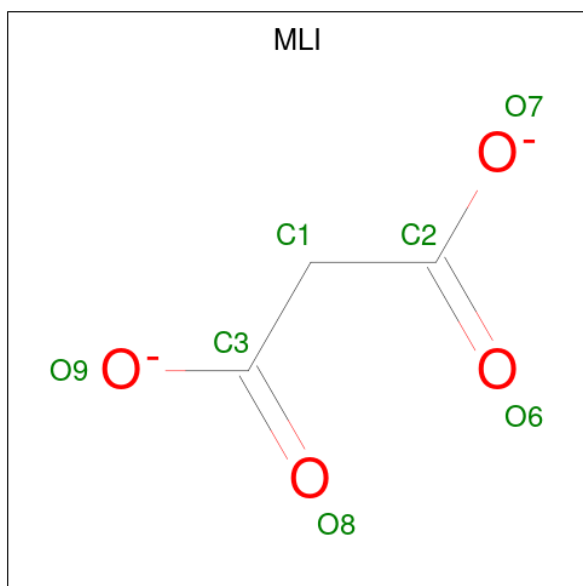
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	H	4	Total	C	N	O	0	0
			48	28	2	18		0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			6	3	3		

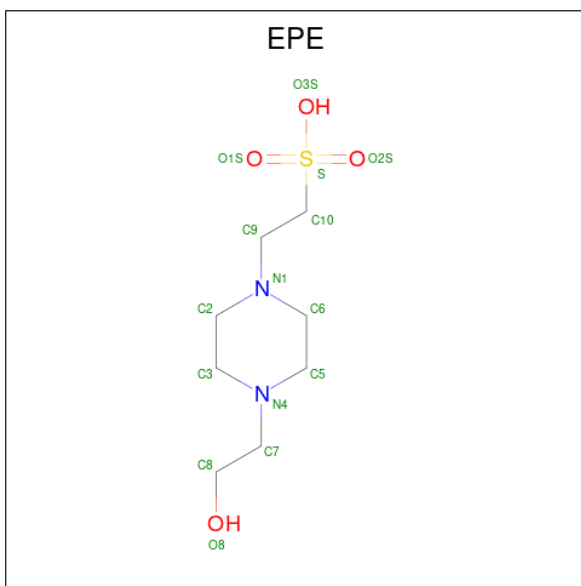
- Molecule 7 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	3	4		
7	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



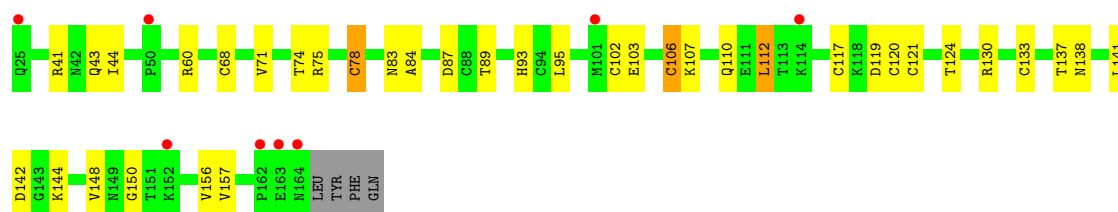
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is water.

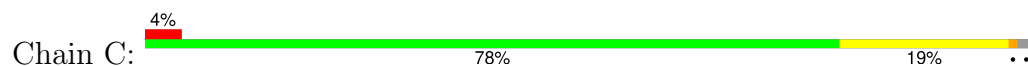
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	O	0	0
			2	2		
9	E	5	Total	O	0	0
			5	5		
9	A	1	Total	O	0	0
			1	1		
9	B	4	Total	O	0	0
			4	4		
9	F	1	Total	O	0	0
			1	1		
9	C	2	Total	O	0	0
			2	2		







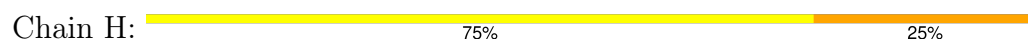
- Molecule 3: Tumor necrosis factor receptor superfamily member 9



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



- Molecule 5: alpha-L-fucopyranose-(1-3)-[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	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.15Å 192.06Å 344.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 2.80 49.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.65-2.80) 93.5 (49.65-2.80)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.83 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.200 , 0.222 0.196 , 0.218	Depositor DCC
$R_{free}$ test set	1995 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.7	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC, BMA, EPE, GOL, MLI

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	0.41	0/1671	0.62	0/2296
1	D	0.49	1/1670 (0.1%)	0.65	0/2292
2	B	0.46	0/1661	0.66	0/2265
2	E	0.51	0/1661	0.66	0/2266
3	C	0.53	2/997 (0.2%)	0.63	0/1353
3	F	0.57	1/992 (0.1%)	0.82	4/1346 (0.3%)
All	All	0.49	4/8652 (0.0%)	0.67	4/11818 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	117	CYS	CB-SG	-8.18	1.68	1.82
1	D	119	VAL	CB-CG2	-5.56	1.41	1.52
3	C	37	CYS	CB-SG	-5.37	1.73	1.81
3	C	31	CYS	CB-SG	-5.24	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	117	CYS	CA-CB-SG	12.02	135.63	114.00
3	F	102	CYS	CA-CB-SG	-5.46	104.17	114.00
3	F	106	CYS	CA-CB-SG	-5.43	104.22	114.00
3	F	133	CYS	CA-CB-SG	5.07	123.12	114.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	1624	0	1510	30	0
1	D	1623	0	1528	34	0
2	B	1624	0	1553	17	0
2	E	1624	0	1546	21	1
3	C	980	0	817	17	0
3	F	975	0	822	25	0
4	G	59	0	52	0	0
5	H	48	0	43	2	0
6	D	6	0	8	0	0
7	A	7	0	2	0	0
7	B	7	0	2	0	0
8	C	15	0	18	5	0
8	F	15	0	18	1	0
9	A	1	0	0	0	0
9	B	4	0	0	0	0
9	C	2	0	0	0	0
9	D	2	0	0	0	0
9	E	5	0	0	0	0
9	F	1	0	0	0	0
All	All	8622	0	7919	136	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 8.

All (136) 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)
3:C:148:VAL:HG12	3:C:157:VAL:HG22	1.52	0.91
2:E:29:VAL:HG11	2:E:90:GLN:HG3	1.64	0.77
1:D:205:ASN:ND2	1:D:216:ASP:OD1	2.18	0.76
2:B:39:LYS:HD3	2:B:84:ALA:HB2	1.68	0.76
3:F:95:LEU:HD12	3:F:103:GLU:HB2	1.66	0.76
1:D:203:ILE:HD12	1:D:217:LYS:O	1.86	0.75
1:D:146:LEU:HD13	1:D:219:VAL:HG21	1.70	0.74
8:C:205:EPE:O1S	5:H:4:FUC:O4	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HD13	1:A:219:VAL:HG21	1.70	0.74
3:F:93:HIS:HB2	3:F:130:ARG:HH21	1.53	0.74
3:C:78:CYS:HB3	3:C:84:ALA:HB2	1.70	0.73
3:C:96:GLY:HA3	3:C:100:SER:HB3	1.70	0.72
1:A:90:THR:HG23	1:A:118:THR:HA	1.72	0.71
3:F:138:ASN:HB3	3:F:141:LEU:HD23	1.73	0.69
1:A:72:ASP:OD1	1:A:74:SER:OG	2.14	0.66
2:E:122:PRO:HB2	2:E:127:LEU:HD11	1.78	0.65
1:D:160:VAL:HG22	1:D:206:VAL:HG22	1.80	0.64
3:F:107:LYS:CB	3:F:110:GLN:HE21	2.11	0.63
3:F:78:CYS:HB3	3:F:84:ALA:HB2	1.81	0.62
2:E:197:GLU:HG2	2:E:208:THR:HG23	1.82	0.61
3:C:95:LEU:HD22	3:C:103:GLU:HB2	1.81	0.61
3:C:113:THR:HG22	3:C:116:GLY:O	2.00	0.61
3:C:124:THR:HG22	3:C:135:PRO:HA	1.82	0.61
2:E:148:VAL:HG22	2:E:198:VAL:HG22	1.83	0.60
1:D:203:ILE:HD12	1:D:217:LYS:C	2.21	0.60
1:D:86:THR:O	1:D:119:VAL:HG21	2.02	0.59
1:D:106:TRP:CG	2:E:91:ARG:HD3	2.38	0.59
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.38	0.59
2:B:11:LEU:HD13	2:B:13:LEU:HD11	1.85	0.59
3:F:106:CYS:SG	3:F:112:LEU:HB2	2.44	0.58
1:A:47:TRP:CD2	2:B:98:LEU:HD23	2.40	0.57
3:C:139:CYS:SG	3:C:146:VAL:HG22	2.45	0.57
3:C:148:VAL:HG12	3:C:157:VAL:CG2	2.31	0.57
1:A:11:LEU:C	1:A:12:LEU:HD23	2.25	0.57
1:D:203:ILE:CD1	1:D:217:LYS:C	2.75	0.55
1:A:18:LEU:HD12	1:A:117:VAL:HG11	1.89	0.54
1:D:63:LEU:O	1:D:67:VAL:HG23	2.07	0.54
3:C:138:ASN:HD21	8:C:205:EPE:H22	1.73	0.54
1:A:195:SER:OG	1:A:196:SER:N	2.41	0.53
3:C:87:ASP:HA	3:C:94:CYS:SG	2.49	0.53
3:C:66:ARG:NE	3:C:86:CYS:SG	2.82	0.52
3:F:121:CYS:O	3:F:124:THR:OG1	2.19	0.52
3:F:75:ARG:HD3	3:F:87:ASP:OD1	2.09	0.52
2:E:29:VAL:CG1	2:E:90:GLN:HG3	2.38	0.52
1:A:14:PRO:HG2	1:A:121:SER:OG	2.09	0.52
3:C:28:CYS:SG	3:C:43:GLN:HG3	2.50	0.52
3:F:150:GLY:H	3:F:156:VAL:HG12	1.75	0.52
2:E:4:LEU:HD11	2:E:90:GLN:HB3	1.92	0.51
2:B:48:ILE:HD13	2:B:54:ARG:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:107:LYS:HB3	3:F:110:GLN:HE21	1.74	0.51
2:E:90:GLN:HG2	2:E:91:ARG:N	2.27	0.50
1:D:87:ALA:HA	1:D:119:VAL:CG2	2.41	0.50
1:D:150:VAL:CG2	1:D:186:LEU:HG	2.42	0.49
3:C:146:VAL:HG21	8:C:205:EPE:O1S	2.12	0.49
1:A:34:TRP:CZ3	1:A:97:ARG:HB2	2.48	0.48
3:F:138:ASN:HB3	3:F:141:LEU:CD2	2.42	0.48
1:D:147:GLY:HA2	1:D:162:TRP:CH2	2.48	0.48
1:D:196:SER:HA	1:D:199:THR:OG1	2.13	0.48
1:D:205:ASN:HD22	1:D:216:ASP:CG	2.17	0.48
2:B:33:LEU:HD22	2:B:71:PHE:CD1	2.49	0.48
2:E:63:SER:O	2:E:73:LEU:HD12	2.13	0.47
1:A:147:GLY:HA2	1:A:162:TRP:CH2	2.49	0.47
1:A:160:VAL:HG22	1:A:206:VAL:HG22	1.96	0.47
8:C:205:EPE:H102	5:H:4:FUC:O3	2.14	0.47
1:D:199:THR:OG1	1:D:200:GLN:N	2.48	0.47
1:D:107:TYR:CD2	2:E:49:TYR:HB2	2.49	0.47
3:F:138:ASN:OD1	8:F:206:EPE:H92	2.15	0.47
3:F:41:ARG:O	3:F:44:ILE:HG23	2.15	0.46
8:C:205:EPE:H82	8:C:205:EPE:H51	1.72	0.46
1:A:146:LEU:HD13	1:A:219:VAL:CG2	2.44	0.46
2:B:39:LYS:HD3	2:B:84:ALA:CB	2.42	0.46
2:B:94:TRP:HA	2:B:95:PRO:HA	1.81	0.46
1:A:36:TRP:CD1	1:A:80:LEU:HB2	2.51	0.45
1:A:178:LEU:HB2	1:A:184:TYR:CE1	2.51	0.45
2:B:90:GLN:HG2	2:B:91:ARG:N	2.30	0.45
3:F:83:ASN:OD1	3:F:84:ALA:N	2.47	0.45
3:C:132:ILE:H	3:C:132:ILE:HD12	1.81	0.45
1:D:12:LEU:O	1:D:119:VAL:HA	2.17	0.45
3:F:107:LYS:HB2	3:F:110:GLN:HE21	1.80	0.45
1:A:199:THR:OG1	1:A:200:GLN:N	2.50	0.45
3:F:137:THR:O	3:F:156:VAL:HG21	2.16	0.45
1:D:142:GLY:O	1:D:194:SER:OG	2.23	0.45
1:A:107:TYR:CE2	2:B:49:TYR:HB2	2.51	0.45
3:F:141:LEU:HD22	3:F:141:LEU:N	2.31	0.45
1:D:203:ILE:HD12	1:D:218:LYS:HA	1.98	0.45
1:D:132:LEU:HB3	2:E:120:PHE:CD1	2.51	0.45
1:D:150:VAL:HG22	1:D:186:LEU:HG	1.99	0.45
3:F:68:CYS:HB2	3:F:74:THR:HG23	1.99	0.45
1:D:47:TRP:HB2	2:E:98:LEU:HD22	1.99	0.44
1:A:200:GLN:OE1	1:A:201:THR:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:PRO:HD3	1:A:146:LEU:HB3	1.98	0.44
2:B:61:ARG:NH1	2:B:82:ASP:OD1	2.50	0.44
1:D:87:ALA:HA	1:D:119:VAL:HG23	2.00	0.44
1:A:11:LEU:HD22	1:A:155:PRO:HG3	2.00	0.44
1:A:18:LEU:HD21	1:A:20:LEU:HD12	1.99	0.44
2:B:165:VAL:HG22	2:B:177:LEU:HD12	1.99	0.44
3:C:113:THR:HG23	3:C:115:LYS:H	1.81	0.44
3:F:120:CYS:HB3	3:F:124:THR:OG1	2.18	0.44
1:D:106:TRP:CD1	2:E:91:ARG:HD3	2.53	0.44
2:B:136:CYS:HB2	2:B:150:TRP:CZ2	2.52	0.44
1:A:66:ARG:NH2	1:A:89:ASP:OD2	2.50	0.43
1:D:63:LEU:HB3	1:D:67:VAL:CG2	2.48	0.43
3:F:43:GLN:OE1	3:F:60:ARG:NH2	2.52	0.43
3:F:142:ASP:HB2	3:F:144:LYS:HD2	2.00	0.43
1:D:125:LYS:HG2	1:D:126:GLY:N	2.33	0.43
2:B:92:SER:O	2:B:96:PRO:HA	2.18	0.43
1:A:158:VAL:HG12	1:A:208:HIS:CD2	2.54	0.42
1:D:18:LEU:HB3	1:D:82:LEU:HB3	2.01	0.42
1:D:203:ILE:CD1	1:D:218:LYS:HA	2.49	0.42
1:A:132:LEU:HB3	2:B:120:PHE:CG	2.54	0.42
2:E:21:LEU:N	2:E:21:LEU:HD12	2.35	0.42
1:A:30:SER:HA	1:A:53:HIS:HB2	2.01	0.42
3:F:148:VAL:HB	3:F:157:VAL:CG1	2.49	0.42
1:D:127:PRO:HD2	1:D:213:THR:HG21	2.01	0.42
2:E:203:LEU:HD13	2:E:207:VAL:HG13	2.01	0.42
1:A:12:LEU:HD11	1:A:18:LEU:HA	2.02	0.42
1:D:197:LEU:HD12	1:D:197:LEU:HA	1.76	0.42
2:E:117:VAL:HA	2:E:137:LEU:O	2.20	0.42
3:F:138:ASN:CG	3:F:141:LEU:CD2	2.88	0.42
3:C:150:GLY:N	3:C:156:VAL:HG12	2.34	0.42
1:D:158:VAL:HG23	1:D:208:HIS:HB2	2.00	0.41
2:B:160:ASN:O	2:B:181:LEU:HD12	2.19	0.41
1:A:131:PRO:HB3	1:A:219:VAL:HG12	2.02	0.41
3:F:148:VAL:HB	3:F:157:VAL:HG12	2.01	0.41
1:D:47:TRP:CB	2:E:98:LEU:HD22	2.50	0.41
1:D:163:ASN:HB3	1:D:166:ALA:HB3	2.02	0.41
2:E:94:TRP:HA	2:E:95:PRO:HA	1.86	0.41
1:D:131:PRO:HD2	2:E:123:SER:CB	2.51	0.41
1:A:212:ASN:HD22	1:A:212:ASN:HA	1.64	0.41
3:F:71:VAL:O	3:F:89:THR:HG22	2.21	0.41
2:E:108:ILE:HD12	2:E:168:GLN:OE1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:LYS:HB3	2:B:199:THR:HB	2.03	0.40
1:A:100:GLY:HA3	1:A:104:TYR:O	2.20	0.40
1:A:103:ASN:OD1	3:C:43:GLN:NE2	2.55	0.40
1:A:162:TRP:CH2	1:A:204:CYS:HB3	2.57	0.40
2:E:191:HIS:O	2:E:213:ARG:HD3	2.21	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)
2:E:49:TYR:OH	2:E:49:TYR:OH[3_554]	1.66	0.54

## 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	215/235 (92%)	198 (92%)	16 (7%)	1 (0%)	25	56
1	D	213/235 (91%)	202 (95%)	11 (5%)	0	100	100
2	B	213/216 (99%)	207 (97%)	6 (3%)	0	100	100
2	E	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
3	C	139/144 (96%)	129 (93%)	10 (7%)	0	100	100
3	F	138/144 (96%)	125 (91%)	13 (9%)	0	100	100
All	All	1131/1190 (95%)	1067 (94%)	63 (6%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	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	172/199 (86%)	167 (97%)	5 (3%)	37	71
1	D	175/199 (88%)	170 (97%)	5 (3%)	37	71
2	B	177/186 (95%)	174 (98%)	3 (2%)	56	84
2	E	177/186 (95%)	171 (97%)	6 (3%)	32	66
3	C	103/126 (82%)	101 (98%)	2 (2%)	52	82
3	F	104/126 (82%)	101 (97%)	3 (3%)	37	71
All	All	908/1022 (89%)	884 (97%)	24 (3%)	41	75

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	28	SER
1	D	35	SER
1	D	204	CYS
1	D	205	ASN
1	D	216	ASP
2	E	33	LEU
2	E	63	SER
2	E	90	GLN
2	E	124	ASP
2	E	144	ARG
2	E	178	SER
1	A	30	SER
1	A	65	SER
1	A	83	SER
1	A	123	SER
1	A	204	CYS
2	B	65	SER
2	B	90	GLN
2	B	178	SER
3	F	78	CYS
3	F	112	LEU
3	F	119	ASP

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Mol	Chain	Res	Type
3	C	78	CYS
3	C	134	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	42	GLN
2	E	201	GLN
1	A	172	HIS
1	A	207	ASN
1	A	212	ASN
2	B	42	GLN
2	B	149	GLN
3	F	67	GLN
3	F	110	GLN
3	C	39	ASN
3	C	51	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 ⓘ

9 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	G	1	4,3	14,14,15	0.96	2 (14%)	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	G	2	4	14,14,15	0.51	0	17,19,21	0.69	0
4	BMA	G	3	4	11,11,12	1.35	3 (27%)	15,15,17	0.99	2 (13%)
4	FUC	G	4	4	10,10,11	1.45	2 (20%)	14,14,16	1.29	2 (14%)
4	FUC	G	5	4	10,10,11	1.15	1 (10%)	14,14,16	1.01	1 (7%)
5	NAG	H	1	3,5	14,14,15	0.83	1 (7%)	17,19,21	0.83	1 (5%)
5	FUC	H	2	5	10,10,11	1.01	1 (10%)	14,14,16	1.30	2 (14%)
5	NAG	H	3	5	14,14,15	0.44	0	17,19,21	0.83	1 (5%)
5	FUC	H	4	5	10,10,11	1.33	1 (10%)	14,14,16	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	NAG	G	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	FUC	G	4	4	-	-	0/1/1/1
4	FUC	G	5	4	-	-	0/1/1/1
5	NAG	H	1	3,5	-	0/6/23/26	0/1/1/1
5	FUC	H	2	5	-	-	0/1/1/1
5	NAG	H	3	5	-	0/6/23/26	0/1/1/1
5	FUC	H	4	5	-	-	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	4	FUC	C2-C3	3.10	1.57	1.52
5	H	1	NAG	O5-C1	-2.98	1.38	1.43
4	G	1	NAG	O5-C1	-2.68	1.39	1.43
4	G	4	FUC	C2-C3	2.54	1.56	1.52
4	G	3	BMA	C1-C2	2.38	1.57	1.52
4	G	3	BMA	C4-C5	2.22	1.57	1.53
4	G	4	FUC	C1-C2	2.20	1.57	1.52
4	G	5	FUC	C4-C3	2.14	1.57	1.52
5	H	2	FUC	O5-C1	2.13	1.47	1.43
4	G	3	BMA	C4-C3	2.10	1.57	1.52
4	G	1	NAG	C1-C2	2.02	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2	FUC	C1-O5-C5	2.84	119.67	112.97
5	H	2	FUC	C1-C2-C3	2.82	113.76	109.64
4	G	4	FUC	C1-C2-C3	2.79	113.71	109.64
4	G	4	FUC	C1-O5-C5	2.66	119.25	112.97
5	H	1	NAG	O3-C3-C2	2.54	114.67	109.40
4	G	5	FUC	C1-C2-C3	2.28	112.96	109.64
5	H	3	NAG	C1-O5-C5	2.12	115.03	112.19
4	G	3	BMA	O2-C2-C3	-2.05	105.90	110.15
4	G	3	BMA	C1-C2-C3	-2.01	106.71	109.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

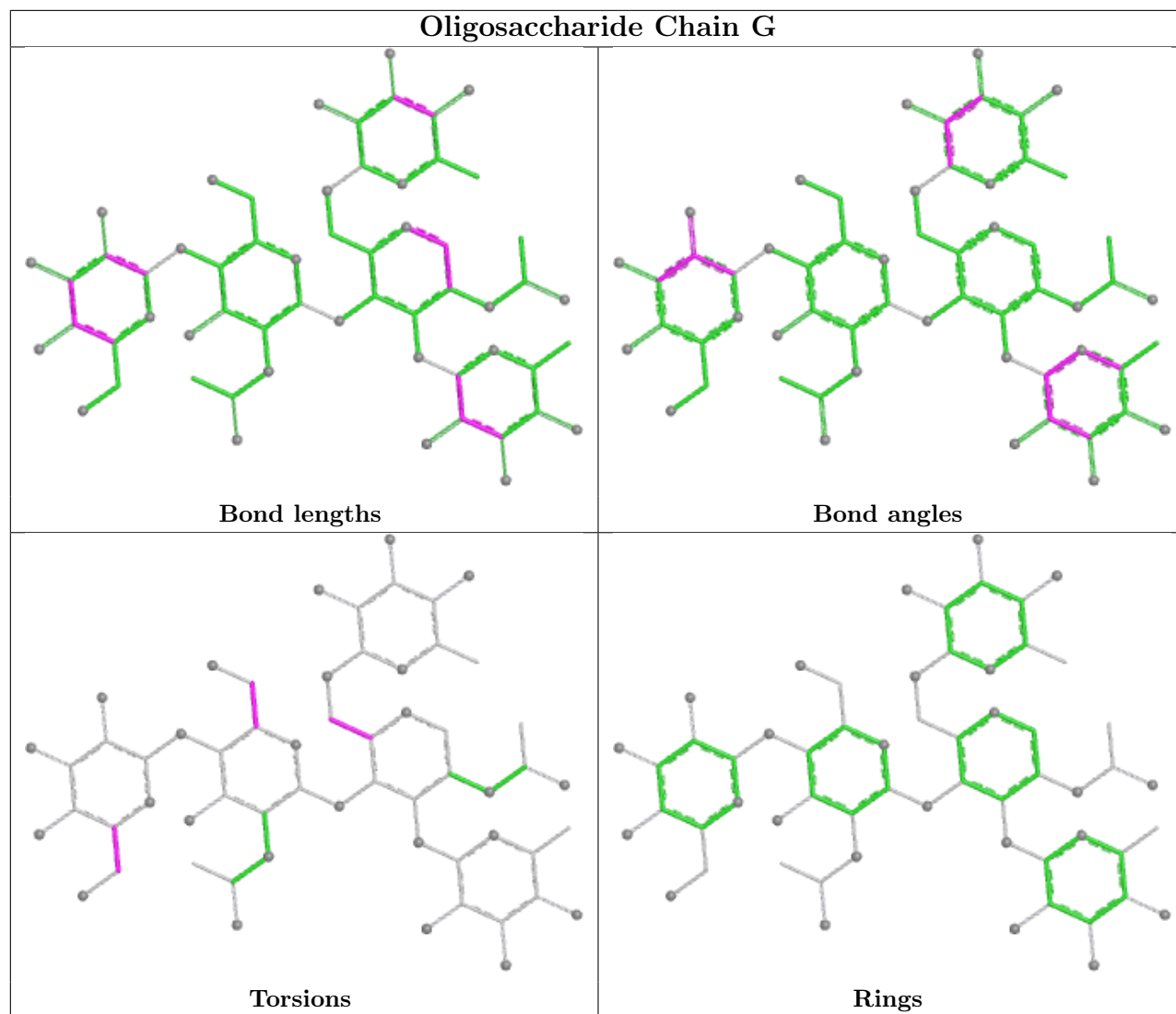
Mol	Chain	Res	Type	Atoms
4	G	3	BMA	O5-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6

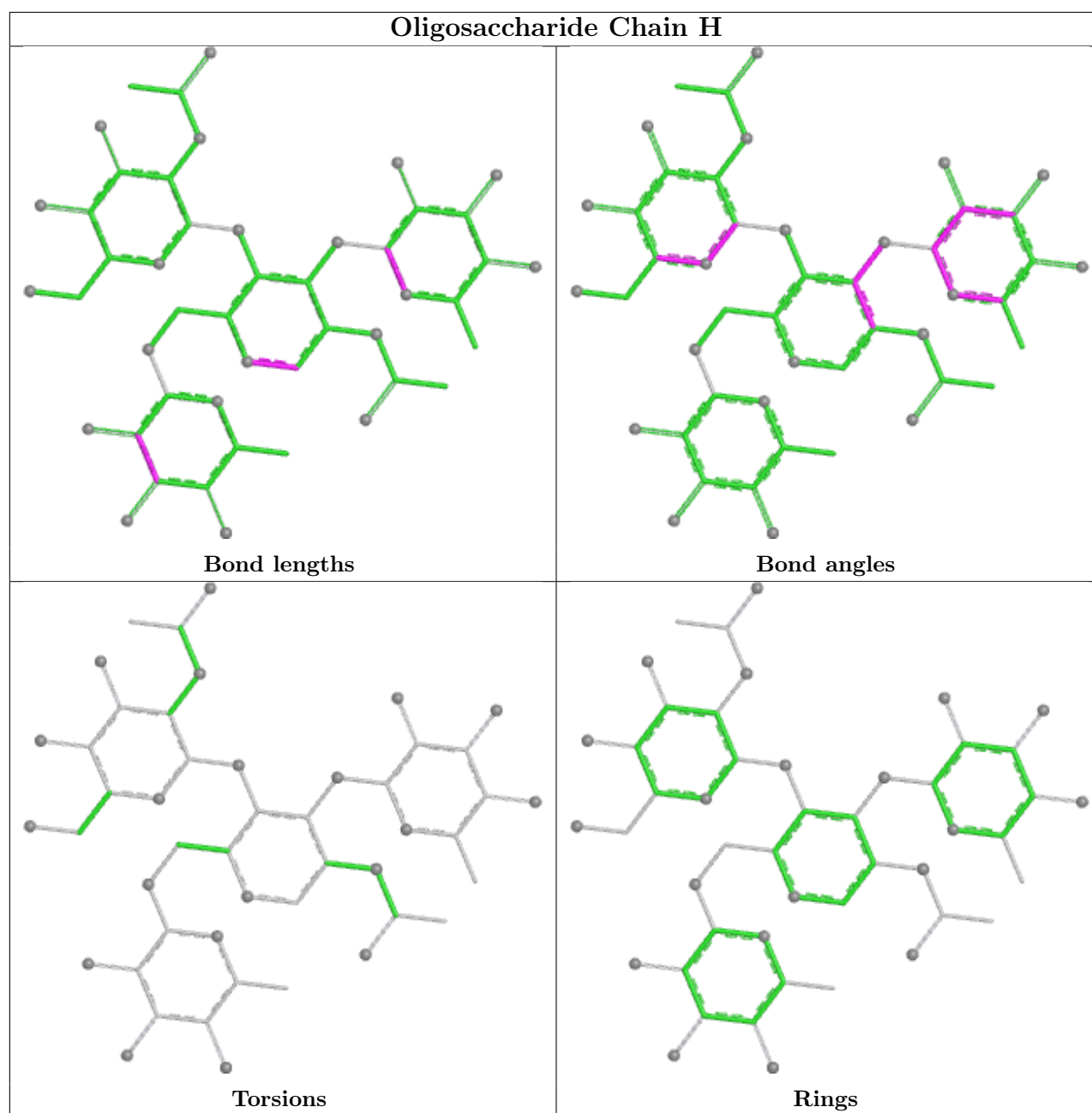
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	4	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 [i](#)

5 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
8	EPE	F	206	-	15,15,15	3.71	14 (93%)	19,20,20	3.17	12 (63%)
7	MLI	B	301	-	6,6,6	1.61	1 (16%)	7,7,7	1.36	1 (14%)
6	GOL	D	301	-	5,5,5	0.77	0	5,5,5	0.91	0
8	EPE	C	205	-	15,15,15	4.41	11 (73%)	19,20,20	3.10	10 (52%)
7	MLI	A	301	-	6,6,6	1.45	0	7,7,7	1.39	1 (14%)

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
8	EPE	F	206	-	-	1/9/19/19	0/1/1/1
7	MLI	B	301	-	-	0/4/4/4	-
6	GOL	D	301	-	-	2/4/4/4	-
8	EPE	C	205	-	-	4/9/19/19	0/1/1/1
7	MLI	A	301	-	-	2/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	205	EPE	O2S-S	8.18	1.68	1.45
8	C	205	EPE	C10-S	7.59	1.88	1.77
8	C	205	EPE	O1S-S	6.89	1.64	1.45
8	F	206	EPE	O2S-S	6.19	1.62	1.45
8	F	206	EPE	O1S-S	5.82	1.61	1.45
8	C	205	EPE	O3S-S	5.31	1.67	1.47
8	C	205	EPE	C9-N1	5.22	1.59	1.47
8	F	206	EPE	C10-S	4.82	1.84	1.77
8	F	206	EPE	C7-N4	3.96	1.56	1.47
8	F	206	EPE	C2-N1	3.85	1.57	1.46
8	C	205	EPE	C6-N1	3.69	1.56	1.46
8	F	206	EPE	C9-N1	3.60	1.55	1.47
8	F	206	EPE	C6-N1	3.59	1.56	1.46
8	F	206	EPE	O3S-S	3.47	1.60	1.47
8	C	205	EPE	C9-C10	3.46	1.61	1.52
8	F	206	EPE	C7-C8	2.98	1.62	1.51
8	F	206	EPE	C3-N4	2.93	1.54	1.46
8	C	205	EPE	C2-N1	2.92	1.54	1.46
8	C	205	EPE	C3-N4	2.70	1.54	1.46
8	C	205	EPE	C7-C8	2.66	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	206	EPE	C6-C5	2.60	1.61	1.51
8	F	206	EPE	O8-C8	2.59	1.55	1.42
8	F	206	EPE	C5-N4	2.26	1.53	1.46
8	F	206	EPE	C9-C10	2.12	1.57	1.52
7	B	301	MLI	C1-C3	2.12	1.54	1.51
8	C	205	EPE	O8-C8	2.07	1.52	1.42

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	205	EPE	O3S-S-C10	7.33	120.35	106.00
8	C	205	EPE	O2S-S-C10	-5.85	97.89	106.73
8	F	206	EPE	C3-C2-N1	-5.58	99.39	110.65
8	F	206	EPE	O2S-S-C10	-5.06	99.08	106.73
8	F	206	EPE	C6-C5-N4	-4.98	100.61	110.65
8	C	205	EPE	O3S-S-O2S	-4.87	99.22	111.40
8	F	206	EPE	O1S-S-C10	4.83	114.03	106.73
8	F	206	EPE	C7-N4-C5	4.27	122.61	111.24
8	C	205	EPE	C5-N4-C3	3.95	117.36	108.84
8	F	206	EPE	C7-N4-C3	3.73	121.19	111.24
8	C	205	EPE	O3S-S-O1S	3.32	119.71	111.40
8	F	206	EPE	O3S-S-O1S	-3.07	103.72	111.40
8	C	205	EPE	C7-N4-C3	2.97	119.16	111.24
8	F	206	EPE	C9-N1-C2	-2.91	103.48	111.24
8	C	205	EPE	O8-C8-C7	-2.79	99.73	111.22
8	F	206	EPE	C10-C9-N1	-2.75	101.96	112.36
8	C	205	EPE	C3-C2-N1	-2.64	105.32	110.65
8	F	206	EPE	C2-C3-N4	-2.59	105.43	110.65
8	C	205	EPE	C9-N1-C6	-2.46	104.68	111.24
8	F	206	EPE	C9-N1-C6	2.31	117.39	111.24
7	B	301	MLI	O9-C3-C1	2.05	120.88	114.51
7	A	301	MLI	O9-C3-C1	2.04	120.84	114.51
8	F	206	EPE	C6-N1-C2	-2.04	104.44	108.84
8	C	205	EPE	O1S-S-C10	-2.03	103.66	106.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	301	GOL	O1-C1-C2-O2
6	D	301	GOL	O1-C1-C2-C3
8	C	205	EPE	C10-C9-N1-C6

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Mol	Chain	Res	Type	Atoms
8	C	205	EPE	C8-C7-N4-C5
8	F	206	EPE	C8-C7-N4-C5
8	C	205	EPE	N4-C7-C8-O8
7	A	301	MLI	C3-C1-C2-O6
8	C	205	EPE	C10-C9-N1-C2
7	A	301	MLI	C3-C1-C2-O7

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	206	EPE	1	0
8	C	205	EPE	5	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	219/235 (93%)	0.15	3 (1%) 73 66	58, 88, 108, 126	0
1	D	217/235 (92%)	-0.31	3 (1%) 73 66	48, 70, 103, 125	0
2	B	215/216 (99%)	-0.45	0 100 100	51, 68, 90, 108	0
2	E	215/216 (99%)	-0.56	1 (0%) 87 83	46, 64, 93, 126	0
3	C	141/144 (97%)	0.38	6 (4%) 40 32	75, 95, 114, 130	0
3	F	140/144 (97%)	0.52	8 (5%) 30 24	55, 96, 130, 145	0
All	All	1147/1190 (96%)	-0.11	21 (1%) 67 60	46, 78, 110, 145	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	164	ASN	7.4
3	C	165	LEU	6.7
1	A	135	SER	4.7
3	F	162	PRO	4.5
3	F	163	GLU	3.8
3	C	163	GLU	3.6
3	C	164	ASN	3.6
1	D	222	LYS	3.2
1	D	136	SER	3.2
1	A	136	SER	3.2
3	F	101	MET	3.2
3	C	25	GLN	3.1
3	F	25	GLN	2.9
1	D	135	SER	2.5
3	F	152	LYS	2.3
1	A	222	LYS	2.3
3	F	114	LYS	2.3
2	E	124	ASP	2.3
3	C	26	ASP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	F	50	PRO	2.2
3	C	162	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](#)

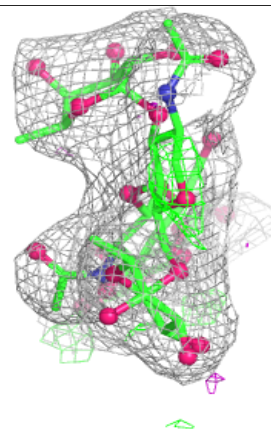
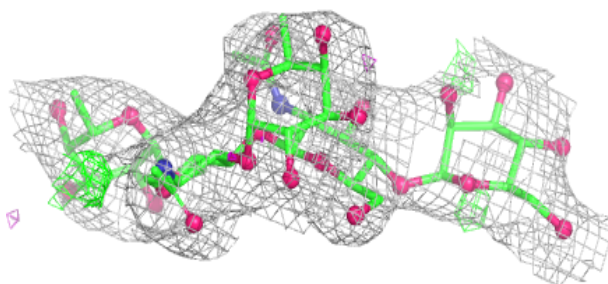
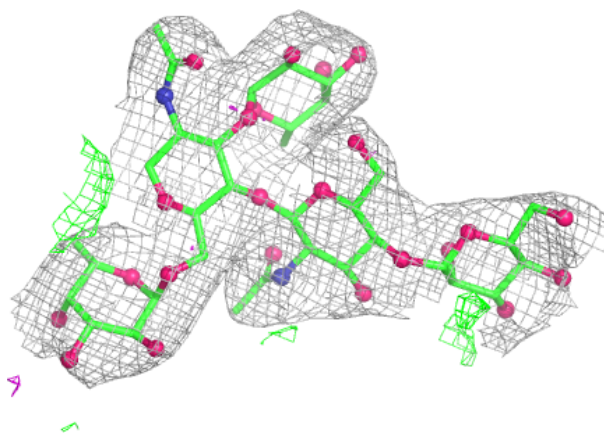
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

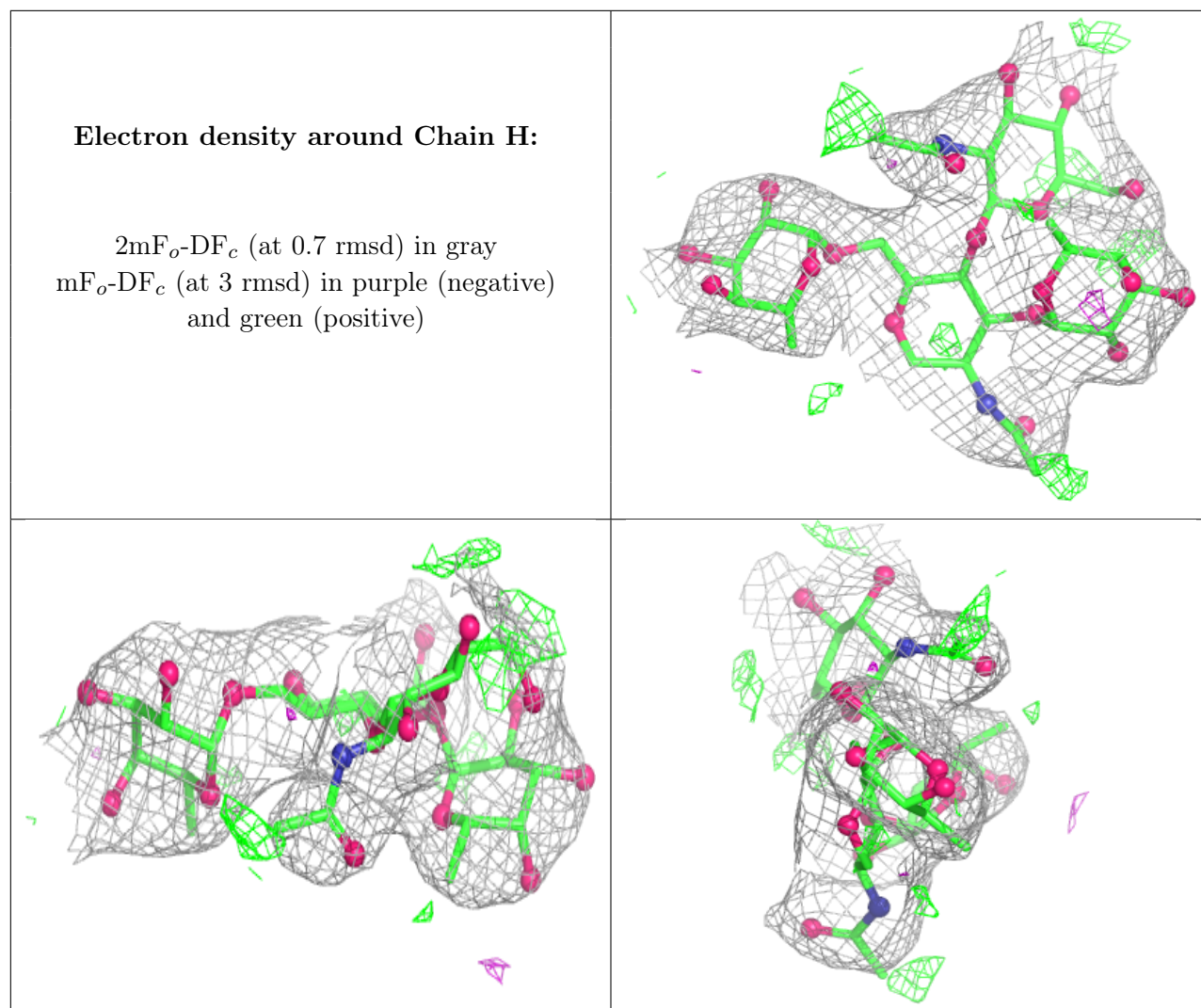
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	G	3	11/12	0.58	0.14	127,132,140,142	0
5	FUC	H	2	10/11	0.75	0.16	126,139,142,144	0
5	NAG	H	3	14/15	0.75	0.16	110,131,138,138	0
5	NAG	H	1	14/15	0.90	0.09	106,112,124,128	0
5	FUC	H	4	10/11	0.92	0.14	91,109,115,118	0
4	NAG	G	2	14/15	0.93	0.09	75,104,113,125	0
4	FUC	G	5	10/11	0.93	0.11	73,85,92,98	0
4	FUC	G	4	10/11	0.94	0.10	93,101,105,105	0
4	NAG	G	1	14/15	0.96	0.07	85,91,102,104	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 G:**

$2mF_o-DF_c$  (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, 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
7	MLI	B	301	7/7	0.73	0.12	103,108,114,124	0
7	MLI	A	301	7/7	0.75	0.12	110,127,129,131	0
6	GOL	D	301	6/6	0.83	0.14	86,92,95,95	0
8	EPE	C	205	15/15	0.88	0.18	92,96,108,114	0
8	EPE	F	206	15/15	0.93	0.15	71,81,99,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.