



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 01:21 PM EDT

PDB ID : 6MI2  
Title : Structure of the human 4-1BB / Utomilumab Fab complex  
Authors : Kimberlin, C.R.; Chin, S.M.; Roe-Zurz, Z.; Xu, A.; Yang, Y.  
Deposited on : 2018-09-19  
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](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>.

---

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

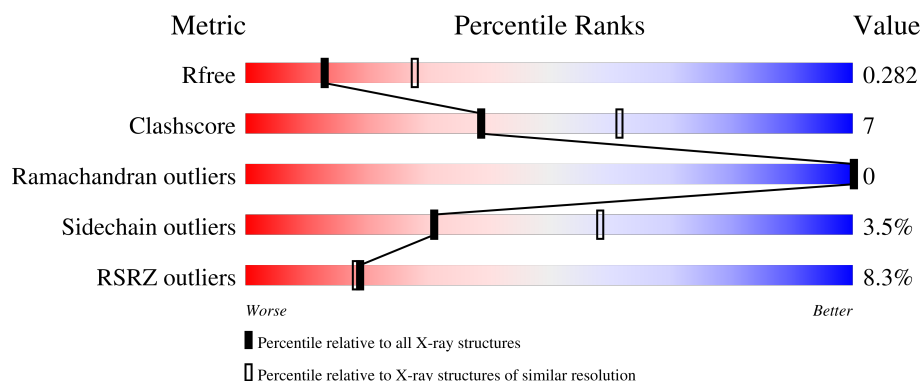
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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  $\geq 3$ , 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	230	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>9%</div> </div> </div>
1	D	230	<div> <div>10%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>9%</div> </div> </div>
2	B	214	<div> <div>8%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>•</div> </div> </div>
2	E	214	<div> <div>11%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>••</div> </div> </div>
3	C	145	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>•</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	145	<div><div></div><div>7%</div><div>65%</div><div>26%</div><div>8%</div></div>
4	G	2	<div><div></div><div>50%</div><div>50%</div></div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8119 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 Utomilumab Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1488	955	244	282	7			
1	D	210	Total	C	N	O	S	0	0	0
			1498	955	244	292	7			

- Molecule 2 is a protein called Utomilumab Fab lambda chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1478	933	244	296	5			
2	E	210	Total	C	N	O	S	0	0	0
			1475	925	246	299	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	133	Total	C	N	O	S	0	0	0
			916	538	166	190	22			
3	C	143	Total	C	N	O	S	0	0	0
			1026	611	183	210	22			

There are 14 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
F	169	GLY	-	expression tag	UNP Q07011
C	163	GLU	-	expression tag	UNP Q07011

*Continued on next page...*

Continued from previous page...

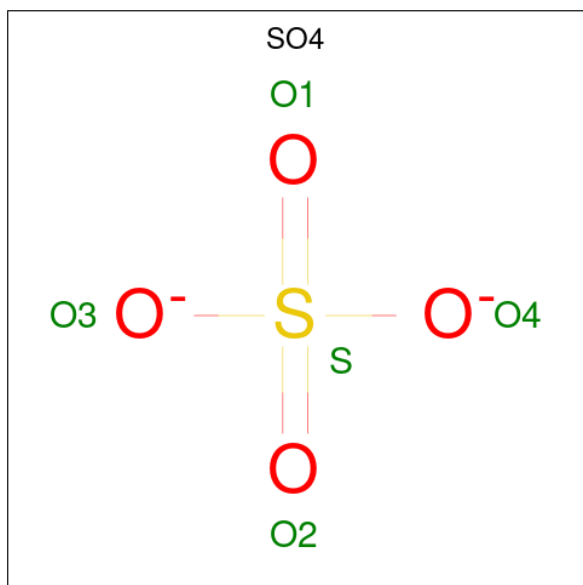
Chain	Residue	Modelled	Actual	Comment	Reference
C	164	ASN	-	expression tag	UNP Q07011
C	165	LEU	-	expression tag	UNP Q07011
C	166	TYR	-	expression tag	UNP Q07011
C	167	PHE	-	expression tag	UNP Q07011
C	168	GLN	-	expression tag	UNP Q07011
C	169	GLY	-	expression tag	UNP Q07011

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

*Continued from previous page...*

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

- 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	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is water.

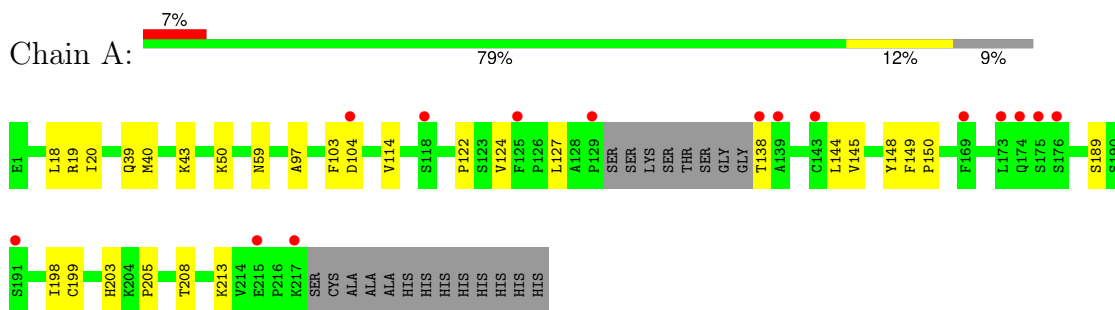
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total	O	0	0
			6	6		
8	B	12	Total	O	0	0
			12	12		
8	D	3	Total	O	0	0
			3	3		
8	E	9	Total	O	0	0
			9	9		
8	F	9	Total	O	0	0
			9	9		
8	C	7	Total	O	0	0
			7	7		



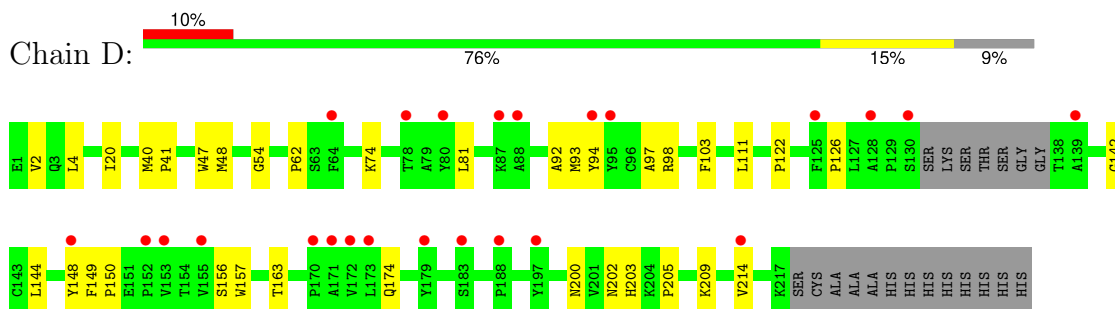
### 3 Residue-property plots [i](#)

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.

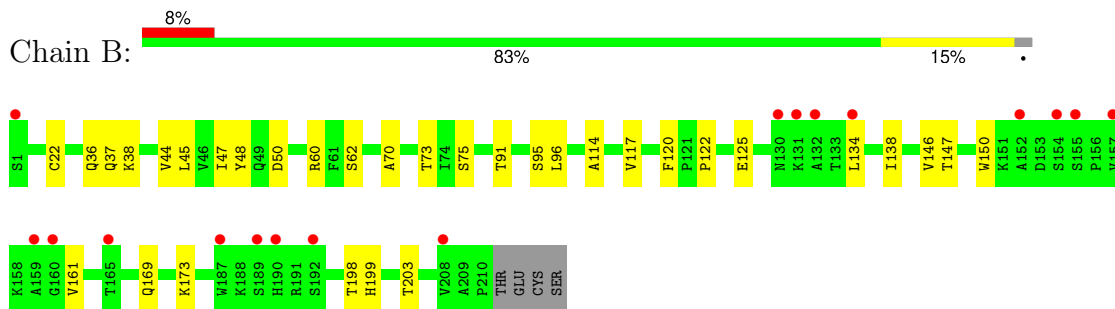
- Molecule 1: Utomilumab Fab heavy chain



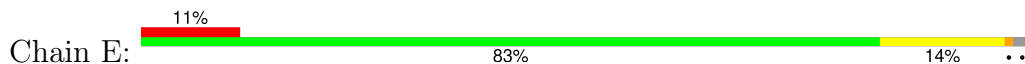
- Molecule 1: Utomilumab Fab heavy chain

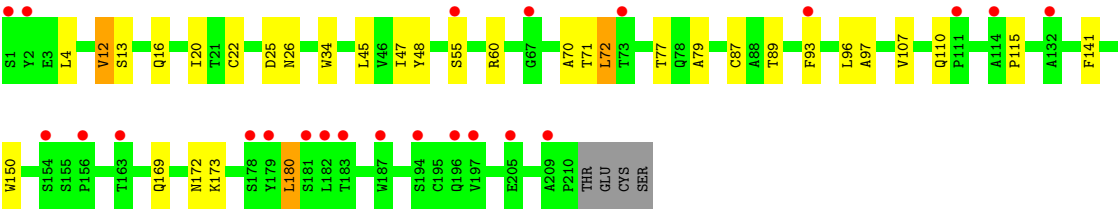


- Molecule 2: Utomilumab Fab lambda chain

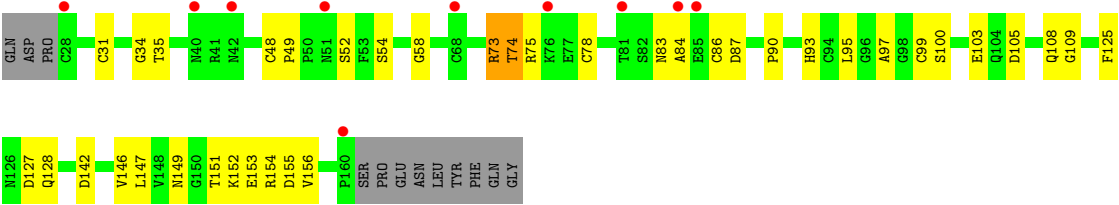


- Molecule 2: Utomilumab Fab lambda chain

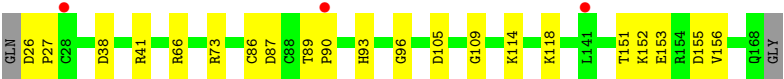
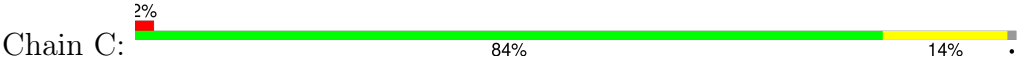




● Molecule 3: Tumor necrosis factor receptor superfamily member 9



● Molecule 3: Tumor necrosis factor receptor superfamily member 9



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.90Å 73.34Å 175.12Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	49.30 – 2.72 49.30 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.30-2.72) 82.6 (49.30-2.72)	Depositor EDS
$R_{merge}$	0.35	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.45 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.238 , 0.278 0.244 , 0.282	Depositor DCC
$R_{free}$ test set	44409 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 82.0	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	0.91	EDS
Total number of atoms	8119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: GOL, SO4, FUC, 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	A	0.25	0/1531	0.45	0/2100
1	D	0.24	0/1541	0.45	0/2117
2	B	0.25	0/1518	0.47	0/2094
2	E	0.25	0/1515	0.47	0/2088
3	C	0.25	0/1045	0.46	0/1414
3	F	0.25	0/931	0.45	0/1262
All	All	0.25	0/8081	0.46	0/11075

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	1488	0	1312	21	0
1	D	1498	0	1318	17	0
2	B	1478	0	1305	19	0
2	E	1475	0	1281	19	0
3	C	1026	0	882	11	0
3	F	916	0	757	20	0
4	G	24	0	22	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	15	0	0	0	0
5	B	25	0	0	1	0
5	C	30	0	0	0	0
5	D	10	0	0	0	0
5	E	10	0	0	0	0
5	F	10	0	0	0	0
6	A	6	0	8	0	0
6	B	18	0	24	1	0
6	C	18	0	24	0	0
6	E	12	0	16	1	0
7	C	14	0	13	0	0
8	A	6	0	0	0	0
8	B	12	0	0	0	0
8	C	7	0	0	0	0
8	D	3	0	0	0	0
8	E	9	0	0	1	0
8	F	9	0	0	1	0
All	All	8119	0	6962	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 7.

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)
2:B:36:GLN:HE22	6:B:308:GOL:H12	1.54	0.72
3:F:149:ASN:HB2	4:G:1:NAG:N2	2.05	0.70
3:F:75:ARG:H	3:F:86:CYS:HA	1.56	0.69
1:A:59:ASN:ND2	2:B:95:SER:O	2.27	0.67
2:E:4:LEU:HD11	2:E:89:THR:HG22	1.77	0.65
1:A:124:VAL:HG22	1:A:145:VAL:HG12	1.80	0.63
3:C:73:ARG:NH2	3:C:87:ASP:OD2	2.30	0.62
1:A:122:PRO:HB3	1:A:148:TYR:HB3	1.83	0.60
2:E:60:ARG:NH1	8:E:401:HOH:O	2.35	0.60
3:C:66:ARG:NE	3:C:86:CYS:SG	2.74	0.60
1:A:138:THR:N	1:A:189:SER:HG	1.99	0.58
3:F:48:CYS:SG	3:F:54:SER:OG	2.61	0.58
4:G:1:NAG:H83	4:G:1:NAG:H3	1.85	0.58
2:E:12:VAL:HG22	2:E:16:GLN:HG3	1.84	0.58
3:F:78:CYS:HB3	3:F:84:ALA:HB2	1.86	0.57
2:B:147:THR:HG1	2:B:198:THR:HG1	1.51	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD11	1:A:20:ILE:HG23	1.88	0.55
2:E:22:CYS:N	2:E:70:ALA:O	2.39	0.55
1:A:203:HIS:HB3	1:A:208:THR:HB	1.89	0.54
2:B:45:LEU:HD21	2:B:48:TYR:HB3	1.89	0.54
1:A:122:PRO:HD3	1:A:203:HIS:CD2	2.44	0.53
2:E:12:VAL:HG11	2:E:77:THR:HG21	1.90	0.53
3:F:151:THR:HG22	3:F:154:ARG:HG2	1.89	0.53
2:E:45:LEU:HD21	2:E:48:TYR:HB3	1.89	0.53
1:D:62:PRO:HD3	2:E:96:LEU:HD11	1.91	0.53
1:A:127:LEU:HD21	1:A:144:LEU:HB2	1.91	0.52
3:F:151:THR:HG23	3:F:153:GLU:H	1.75	0.52
2:E:79:ALA:HA	2:E:107:VAL:HG21	1.92	0.51
3:F:125:PHE:CZ	3:F:155:ASP:HB2	2.45	0.51
1:A:50:LYS:HZ3	1:A:59:ASN:HD22	1.59	0.51
2:B:22:CYS:N	2:B:70:ALA:O	2.42	0.51
1:D:20:ILE:HD11	1:D:81:LEU:HD23	1.91	0.51
1:A:39:GLN:HE22	2:B:37:GLN:HE22	1.59	0.51
3:F:128:GLN:NE2	8:F:302:HOH:O	2.39	0.50
1:A:198:ILE:HA	1:A:213:LYS:HA	1.94	0.49
1:A:97:ALA:HB1	1:A:103:PHE:HB3	1.94	0.49
1:D:142:GLY:HA2	1:D:157:TRP:CZ2	2.47	0.49
2:E:34:TRP:CE3	2:E:72:LEU:HD22	2.48	0.49
3:F:34:GLY:H	3:F:54:SER:HB2	1.77	0.49
3:F:83:ASN:OD1	3:F:84:ALA:N	2.44	0.48
1:D:142:GLY:HA2	1:D:157:TRP:HZ2	1.79	0.48
1:D:156:SER:OG	1:D:200:ASN:HB2	2.14	0.48
3:F:108:GLN:NE2	3:F:127:ASP:O	2.47	0.48
3:C:38:ASP:HB3	3:C:41:ARG:HD2	1.95	0.48
2:E:110:GLN:NE2	2:E:172:ASN:O	2.45	0.47
3:C:26:ASP:HB3	3:C:27:PRO:HD3	1.96	0.47
2:B:169:GLN:HE21	2:B:173:LYS:HB2	1.79	0.47
1:D:54:GLY:O	1:D:74:LYS:NZ	2.37	0.47
1:D:41:PRO:HD3	1:D:92:ALA:HA	1.96	0.47
1:D:97:ALA:HB1	1:D:103:PHE:HB3	1.96	0.47
2:E:34:TRP:CZ3	2:E:87:CYS:HB3	2.50	0.46
2:E:150:TRP:CE3	2:E:180:LEU:HD12	2.50	0.46
1:D:93:MET:HG3	1:D:111:LEU:HA	1.97	0.46
3:C:93:HIS:ND1	3:C:105:ASP:OD1	2.40	0.46
2:B:122:PRO:HD3	2:B:134:LEU:HD23	1.97	0.46
1:D:4:LEU:HD11	1:D:98:ARG:HB2	1.98	0.46
1:D:203:HIS:CD2	1:D:205:PRO:HD2	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:115:PRO:HB3	2:E:141:PHE:HB3	1.97	0.46
1:A:127:LEU:HB3	2:B:120:PHE:CD1	2.51	0.46
3:F:97:ALA:O	3:F:100:SER:OG	2.34	0.45
2:B:125:GLU:OE2	2:B:125:GLU:N	2.38	0.45
1:A:39:GLN:HE22	2:B:37:GLN:NE2	2.14	0.45
2:B:50:ASP:OD2	3:C:114:LYS:NZ	2.43	0.45
2:E:169:GLN:HG2	2:E:173:LYS:O	2.17	0.45
2:B:150:TRP:CD1	2:B:161:VAL:HG21	2.52	0.45
1:D:48:MET:HE1	1:D:94:TYR:HD1	1.81	0.45
2:E:34:TRP:HB2	2:E:47:ILE:HB	1.98	0.45
1:A:149:PHE:HA	1:A:150:PRO:HA	1.81	0.45
3:F:87:ASP:HA	3:F:99:CYS:SG	2.58	0.44
1:D:126:PRO:HB3	1:D:214:VAL:HG22	2.00	0.44
3:F:109:GLY:HA2	3:F:152:LYS:O	2.17	0.44
3:C:155:ASP:OD1	3:C:156:VAL:N	2.49	0.43
3:F:73:ARG:NH1	3:F:90:PRO:HD3	2.34	0.43
3:F:146:VAL:HG23	3:F:156:VAL:HG13	2.00	0.43
2:B:60:ARG:HB2	2:B:75:SER:O	2.19	0.43
2:E:13:SER:O	2:E:16:GLN:HG2	2.18	0.43
2:B:114:ALA:N	5:B:304:SO4:O3	2.49	0.43
1:D:149:PHE:HA	1:D:150:PRO:HA	1.77	0.43
1:D:202:ASN:HA	1:D:209:LYS:HA	2.01	0.43
3:F:31:CYS:O	3:F:58:GLY:N	2.51	0.43
1:D:122:PRO:HB3	1:D:148:TYR:HB3	2.00	0.43
2:E:55:SER:HB2	6:E:304:GOL:H12	2.00	0.43
2:E:20:ILE:HB	2:E:72:LEU:HD23	2.01	0.43
3:C:151:THR:HG23	3:C:153:GLU:H	1.82	0.43
1:D:47:TRP:CG	2:E:97:ALA:HB3	2.53	0.42
2:B:117:VAL:HG22	2:B:138:ILE:HG23	2.01	0.42
2:B:62:SER:HB3	2:B:73:THR:HB	2.00	0.42
1:A:203:HIS:CE1	1:A:205:PRO:HD2	2.55	0.42
1:A:40:MET:HB2	1:A:43:LYS:HB2	2.02	0.42
2:B:146:VAL:HG12	2:B:199:HIS:HB2	2.01	0.42
3:F:74:THR:HA	3:F:86:CYS:SG	2.60	0.42
3:F:49:PRO:O	3:F:52:SER:OG	2.32	0.41
1:A:50:LYS:NZ	1:A:59:ASN:HD22	2.17	0.41
3:C:109:GLY:HA2	3:C:152:LYS:O	2.20	0.41
2:B:36:GLN:NE2	2:B:38:LYS:HE3	2.36	0.41
1:A:18:LEU:HD22	1:A:19:ARG:H	1.85	0.41
3:C:89:THR:HB	3:C:90:PRO:HD2	2.02	0.40
1:A:104:ASP:HB2	3:C:96:GLY:HA2	2.04	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:93:HIS:NE2	3:F:103:GLU:HB3	2.36	0.40
1:A:203:HIS:N	1:A:208:THR:O	2.48	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	205/230 (89%)	193 (94%)	12 (6%)	0	100	100
1	D	206/230 (90%)	195 (95%)	11 (5%)	0	100	100
2	B	208/214 (97%)	196 (94%)	12 (6%)	0	100	100
2	E	208/214 (97%)	201 (97%)	7 (3%)	0	100	100
3	C	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
3	F	131/145 (90%)	126 (96%)	5 (4%)	0	100	100
All	All	1099/1178 (93%)	1050 (96%)	49 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	138/194 (71%)	136 (99%)	2 (1%)	62	83

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	144/194 (74%)	139 (96%)	5 (4%)	31	58
2	B	141/179 (79%)	136 (96%)	5 (4%)	31	58
2	E	139/179 (78%)	132 (95%)	7 (5%)	20	44
3	C	113/126 (90%)	112 (99%)	1 (1%)	75	89
3	F	98/126 (78%)	91 (93%)	7 (7%)	12	29
All	All	773/998 (78%)	746 (96%)	27 (4%)	31	58

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	VAL
1	A	199	CYS
2	B	44	VAL
2	B	47	ILE
2	B	91	THR
2	B	96	LEU
2	B	203	THR
1	D	2	VAL
1	D	40	MET
1	D	144	LEU
1	D	163	THR
1	D	174	GLN
2	E	12	VAL
2	E	25	ASP
2	E	26	ASN
2	E	71	THR
2	E	72	LEU
2	E	93	PHE
2	E	180	LEU
3	F	35	THR
3	F	73	ARG
3	F	74	THR
3	F	95	LEU
3	F	105	ASP
3	F	142	ASP
3	F	147	LEU
3	C	118	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	203	HIS
2	B	36	GLN
2	B	37	GLN
2	B	49	GLN
2	B	169	GLN
1	D	3	GLN
1	D	59	ASN
2	E	26	ASN
2	E	41	GLN
2	E	78	GLN
3	F	104	GLN
3	F	128	GLN
3	C	128	GLN
3	C	168	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	$\# Z  > 2$
4	NAG	G	1	4,3	14,14,15	1.12	1 (7%)	17,19,21	1.50	3 (17%)
4	FUC	G	2	4	10,10,11	0.95	0	14,14,16	1.04	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
4	NAG	G	1	4,3	-	6/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	C1-C2	3.53	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C2-N2-C7	4.54	128.99	122.90
4	G	1	NAG	C1-C2-N2	2.76	114.79	110.43
4	G	1	NAG	C1-O5-C5	2.52	115.56	112.19
4	G	2	FUC	C1-O5-C5	2.06	117.83	112.97

There are no chirality outliers.

All (6) torsion outliers are listed below:

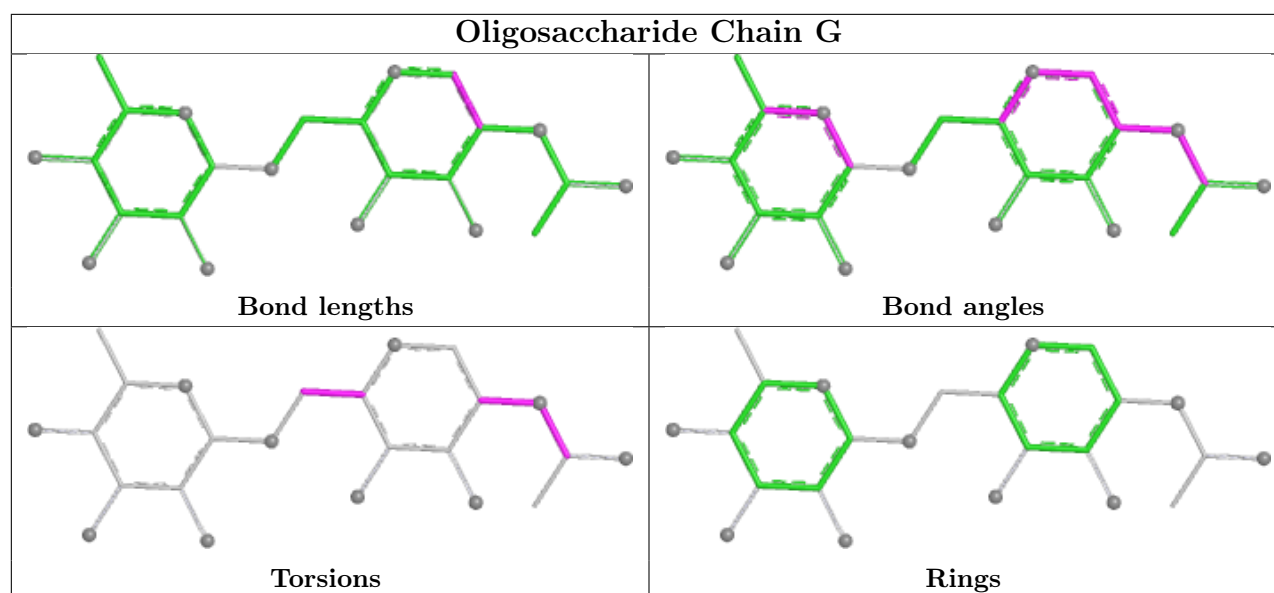
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	1	NAG	C1-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	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](#)

30 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	SO4	C	202	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	B	303	-	4,4,4	0.24	0	6,6,6	0.08	0
6	GOL	E	303	-	5,5,5	0.94	0	5,5,5	1.07	0
5	SO4	E	302	-	4,4,4	0.24	0	6,6,6	0.08	0
6	GOL	C	209	-	5,5,5	0.93	0	5,5,5	1.08	0
5	SO4	C	204	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	B	301	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	B	305	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	F	203	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	A	301	-	4,4,4	0.24	0	6,6,6	0.08	0
7	NAG	C	201	3	14,14,15	0.38	0	17,19,21	0.55	0
5	SO4	B	302	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	C	203	-	4,4,4	0.23	0	6,6,6	0.09	0
6	GOL	B	307	-	5,5,5	0.93	0	5,5,5	1.10	0
5	SO4	E	301	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	C	207	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	D	302	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	C	205	-	4,4,4	0.23	0	6,6,6	0.08	0
6	GOL	B	306	-	5,5,5	0.92	0	5,5,5	1.11	0
5	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	C	206	-	4,4,4	0.23	0	6,6,6	0.07	0
6	GOL	C	208	-	5,5,5	0.91	0	5,5,5	1.13	1 (20%)
5	SO4	B	304	-	4,4,4	0.24	0	6,6,6	0.07	0
6	GOL	B	308	-	5,5,5	0.94	0	5,5,5	1.04	0
6	GOL	A	304	-	5,5,5	0.94	0	5,5,5	1.07	0
5	SO4	A	302	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	D	301	-	4,4,4	0.23	0	6,6,6	0.09	0
6	GOL	C	210	-	5,5,5	0.93	0	5,5,5	1.12	1 (20%)
6	GOL	E	304	-	5,5,5	0.91	0	5,5,5	1.10	0
5	SO4	F	204	-	4,4,4	0.24	0	6,6,6	0.08	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
6	GOL	B	308	-	-	2/4/4/4	-
6	GOL	A	304	-	-	1/4/4/4	-
7	NAG	C	201	3	-	0/6/23/26	0/1/1/1
6	GOL	B	306	-	-	0/4/4/4	-
6	GOL	E	303	-	-	3/4/4/4	-
6	GOL	B	307	-	-	1/4/4/4	-
6	GOL	C	210	-	-	0/4/4/4	-
6	GOL	C	208	-	-	3/4/4/4	-
6	GOL	C	209	-	-	1/4/4/4	-
6	GOL	E	304	-	-	1/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	208	GOL	C3-C2-C1	-2.01	104.41	111.80
6	C	210	GOL	C3-C2-C1	-2.01	104.43	111.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	308	GOL	O1-C1-C2-C3
6	E	303	GOL	C1-C2-C3-O3
6	C	208	GOL	O1-C1-C2-C3
6	B	308	GOL	O1-C1-C2-O2
6	E	304	GOL	O1-C1-C2-O2
6	C	208	GOL	O1-C1-C2-O2
6	E	303	GOL	O1-C1-C2-O2
6	C	209	GOL	O2-C2-C3-O3
6	A	304	GOL	C1-C2-C3-O3
6	E	303	GOL	O2-C2-C3-O3
6	C	208	GOL	O2-C2-C3-O3
6	B	307	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	304	SO4	1	0
6	B	308	GOL	1	0
6	E	304	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	209/230 (90%)	0.67	15 (7%) 23 22	38, 83, 143, 163	0
1	D	210/230 (91%)	0.86	24 (11%) 11 11	46, 99, 147, 160	0
2	B	210/214 (98%)	0.62	17 (8%) 19 19	32, 69, 146, 174	0
2	E	210/214 (98%)	0.83	23 (10%) 12 12	47, 91, 149, 190	0
3	C	143/145 (98%)	0.38	3 (2%) 63 63	33, 68, 94, 118	0
3	F	133/145 (91%)	0.76	10 (7%) 22 21	62, 87, 130, 144	0
All	All	1115/1178 (94%)	0.70	92 (8%) 19 18	32, 81, 143, 190	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	130	SER	5.1
2	B	154	SER	3.8
1	D	172	VAL	3.7
3	C	90	PRO	3.5
2	E	181	SER	3.4
2	E	178	SER	3.4
2	E	194	SER	3.4
1	D	173	LEU	3.3
3	F	42	ASN	3.3
2	B	159	ALA	3.2
1	D	170	PRO	3.2
1	A	173	LEU	3.1
1	A	175	SER	3.1
2	E	2	TYR	3.1
2	B	157	VAL	3.1
1	A	138	THR	3.0
2	E	187	TRP	3.0
1	A	139	ALA	3.0
1	D	128	ALA	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	F	68	CYS	2.9
1	D	87	LYS	2.9
2	B	189	SER	2.8
3	F	51	ASN	2.8
1	A	118	SER	2.8
2	E	163	THR	2.8
2	E	93	PHE	2.8
1	D	155	VAL	2.7
2	B	1	SER	2.7
1	D	152	PRO	2.7
3	F	84	ALA	2.7
2	E	205	GLU	2.7
2	E	197	VAL	2.7
1	D	171	ALA	2.7
2	E	154	SER	2.7
1	A	191	SER	2.6
1	D	188	PRO	2.6
2	B	160	GLY	2.5
3	F	81	THR	2.5
2	E	182	LEU	2.5
3	F	28	CYS	2.5
1	A	174	GLN	2.5
1	D	139	ALA	2.5
2	B	165	THR	2.5
2	E	209	ALA	2.4
1	A	215	GLU	2.4
2	B	155	SER	2.4
2	E	1	SER	2.4
1	A	217	LYS	2.4
2	B	187	TRP	2.4
1	A	176	SER	2.4
2	B	131	LYS	2.4
1	D	80	TYR	2.4
1	D	148	TYR	2.4
3	C	28	CYS	2.4
2	E	183	THR	2.3
1	D	64	PHE	2.3
2	E	132	ALA	2.3
1	D	78	THR	2.3
1	D	125	PHE	2.3
2	B	134	LEU	2.3
2	B	192	SER	2.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	125	PHE	2.3
3	F	85	GLU	2.2
1	A	129	PRO	2.2
3	F	160	PRO	2.2
2	E	73	THR	2.2
2	E	179	TYR	2.2
1	A	104	ASP	2.2
2	B	132	ALA	2.2
2	E	67	GLY	2.2
1	A	143	CYS	2.2
1	D	88	ALA	2.2
2	E	111	PRO	2.1
1	A	169	PHE	2.1
1	D	153	VAL	2.1
2	E	114	ALA	2.1
3	F	40	ASN	2.1
1	D	197	TYR	2.1
2	B	190	HIS	2.1
3	F	76	LYS	2.1
1	D	183	SER	2.1
2	E	55	SER	2.1
2	E	196	GLN	2.1
3	C	141	LEU	2.1
1	D	179	TYR	2.1
2	E	156	PRO	2.0
2	B	130	ASN	2.0
1	D	214	VAL	2.0
2	B	208	VAL	2.0
1	D	94	TYR	2.0
1	D	95	TYR	2.0
2	B	152	ALA	2.0

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

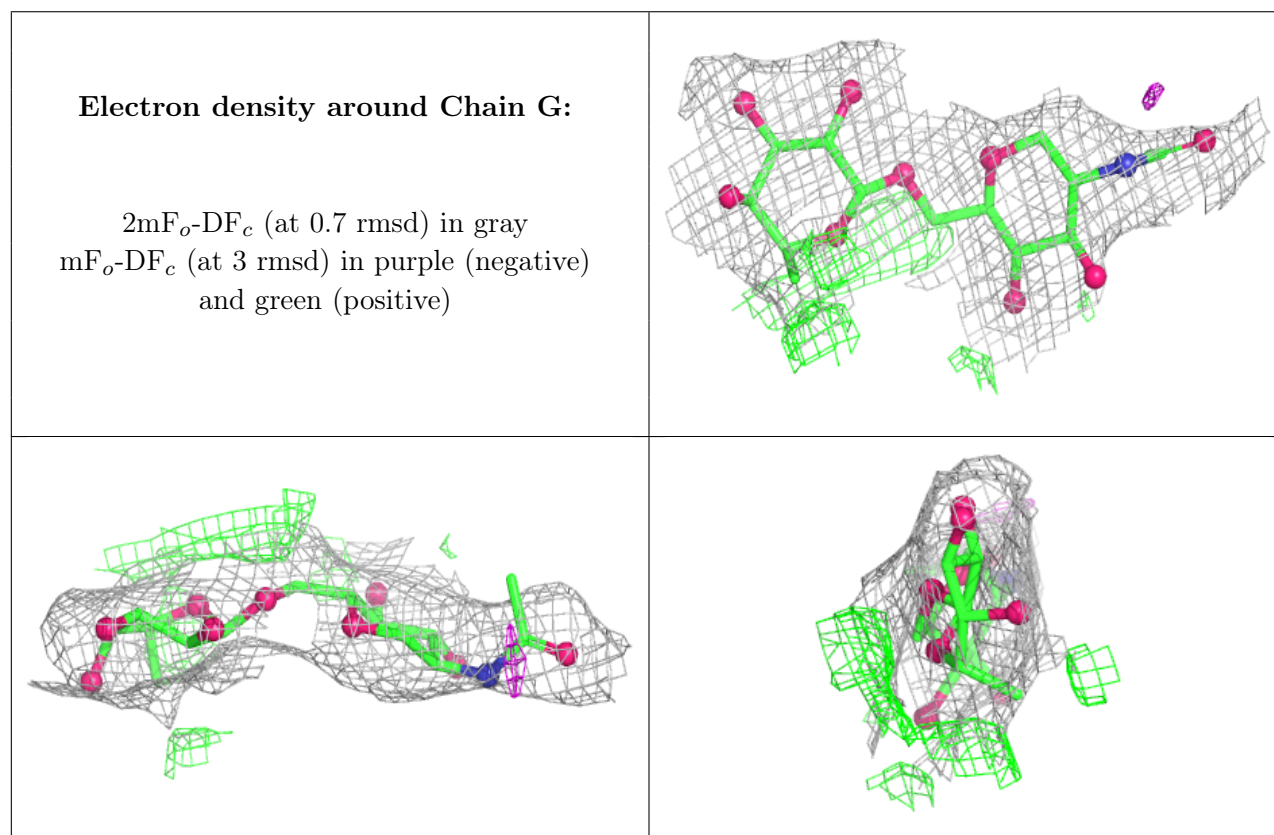
There are no non-standard protein/DNA/RNA residues in this entry.

## 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( $\text{\AA}^2$ )	Q<0.9
4	FUC	G	2	10/11	0.49	0.21	93,111,120,121	0
4	NAG	G	1	14/15	0.70	0.19	95,109,119,120	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 ⓘ

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( $\text{\AA}^2$ )	Q<0.9
5	SO4	B	302	5/5	0.48	0.18	149,151,152,152	0
5	SO4	F	203	5/5	0.50	0.15	148,150,151,152	0
5	SO4	A	303	5/5	0.53	0.14	160,163,166,168	0
5	SO4	B	305	5/5	0.57	0.16	132,133,136,139	0
5	SO4	B	304	5/5	0.58	0.13	167,168,170,171	0
5	SO4	C	206	5/5	0.58	0.16	151,153,156,157	0
5	SO4	C	207	5/5	0.59	0.13	153,158,159,162	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	C	201	14/15	0.59	0.16	89,102,108,115	0
5	SO4	D	302	5/5	0.61	0.13	124,126,130,136	0
5	SO4	A	302	5/5	0.64	0.17	143,147,149,151	0
5	SO4	B	303	5/5	0.68	0.16	137,137,145,150	0
5	SO4	E	302	5/5	0.70	0.14	151,151,152,153	0
5	SO4	F	204	5/5	0.74	0.11	124,127,129,130	0
5	SO4	D	301	5/5	0.76	0.13	113,117,119,120	0
6	GOL	C	208	6/6	0.77	0.18	73,96,97,105	0
5	SO4	C	205	5/5	0.77	0.12	148,149,150,151	0
6	GOL	C	210	6/6	0.78	0.16	77,88,90,90	0
6	GOL	B	308	6/6	0.78	0.21	64,67,68,72	0
6	GOL	E	304	6/6	0.81	0.12	58,70,73,74	0
6	GOL	A	304	6/6	0.82	0.17	67,74,79,80	0
5	SO4	B	301	5/5	0.83	0.15	98,100,104,108	0
6	GOL	C	209	6/6	0.84	0.17	45,62,80,82	0
6	GOL	E	303	6/6	0.85	0.14	90,90,101,103	0
5	SO4	C	202	5/5	0.85	0.16	92,98,101,112	0
5	SO4	C	204	5/5	0.86	0.10	104,111,114,115	0
6	GOL	B	307	6/6	0.86	0.16	83,89,97,102	0
5	SO4	C	203	5/5	0.86	0.18	95,107,107,115	0
5	SO4	A	301	5/5	0.89	0.15	68,74,88,90	0
6	GOL	B	306	6/6	0.89	0.19	94,99,104,105	0
5	SO4	E	301	5/5	0.90	0.10	73,90,91,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.