



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:24 AM UTC

PDB ID : 4PY8 / pdb\_00004py8  
Title : Crystal structure of Fab 3.1 in complex with the 1918 influenza virus hemagglutinin  
Authors : Dreyfus, C.  
Deposited on : 2014-03-26  
Resolution : 2.91 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

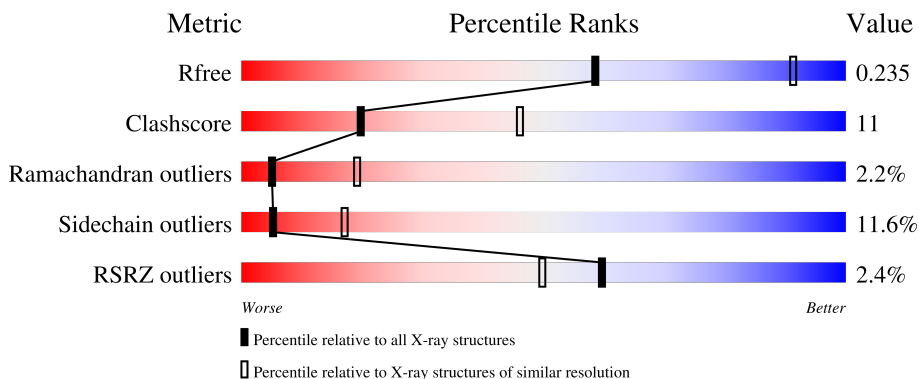
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	331	 2% 73% 24% ..
2	B	179	 3% 83% 9% ...
3	I	219	 2% 62% 28% 8% .
4	J	214	 % 65% 27% 7% .
5	C	2	 50% 50%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7222 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	2528	1595	433	489	11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q9WFX3
A	8	ASP	-	expression tag	UNP Q9WFX3
A	9	PRO	-	expression tag	UNP Q9WFX3
A	10	GLY	-	expression tag	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	171	1376	857	237	276	6	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	expression tag	UNP Q9WFX3
B	178	GLY	-	expression tag	UNP Q9WFX3
B	179	ARG	-	expression tag	UNP Q9WFX3

- Molecule 3 is a protein called antibody 3.1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	219	1644	1038	281	317	8	0	0	0

- Molecule 4 is a protein called antibody 3.1 light chain.

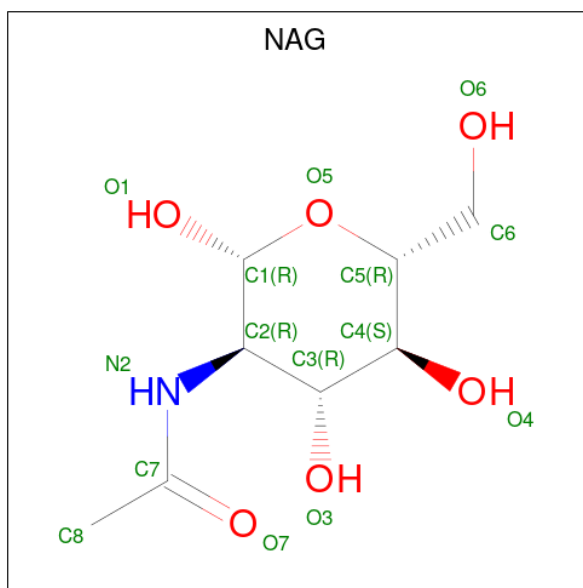
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	J	212	1604	1005	270	324	5	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



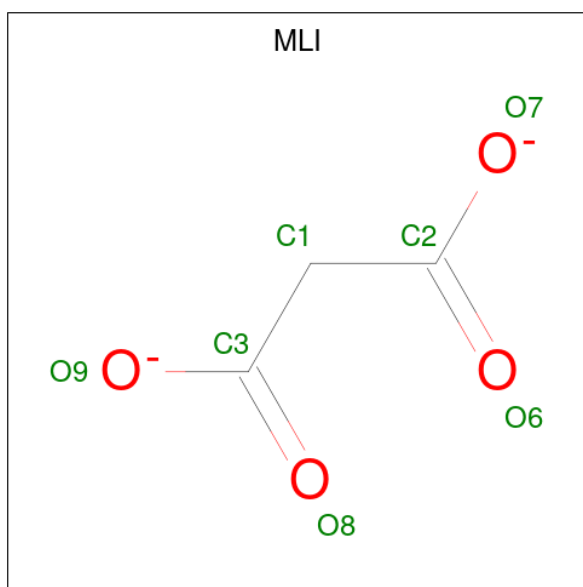
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	2	28	16	2	10		0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	14	8	1	5		0	0
6	A	1	14	8	1	5		0	0

- Molecule 7 is MALONATE ION (CCD ID: MLI) (formula:  $C_3H_2O_4$ ).

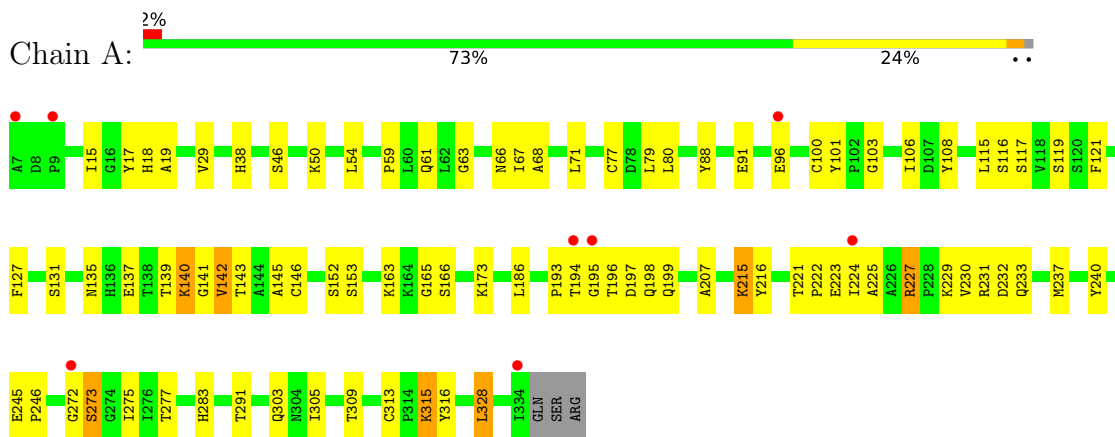


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total C O 7 3 4	0	0
7	J	1	Total C O 7 3 4	0	0

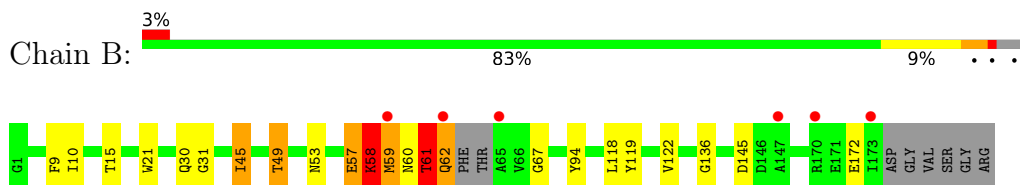
### 3 Residue-property plots [i](#)

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.

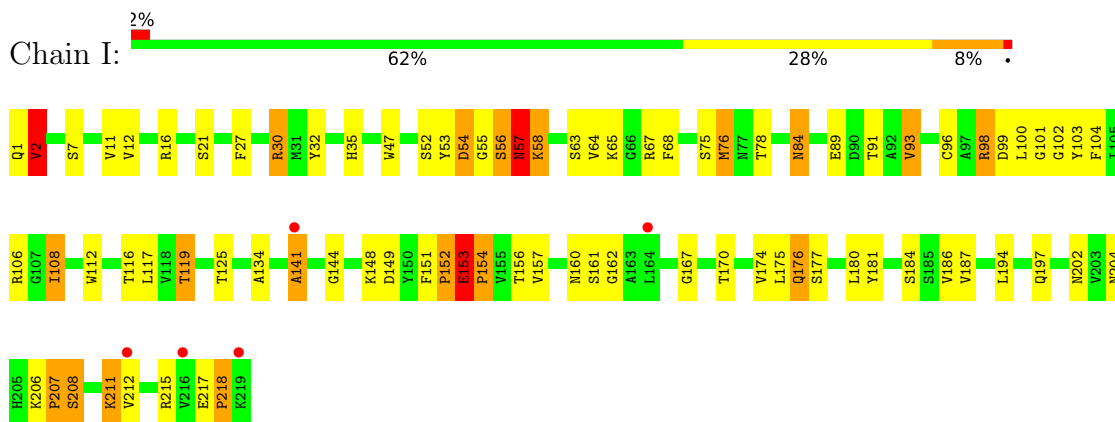
- Molecule 1: Hemagglutinin HA1 chain



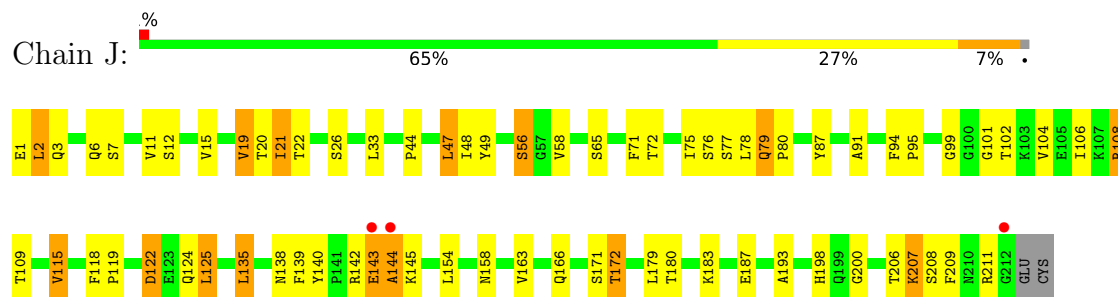
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 3: antibody 3.1 heavy chain



- Molecule 4: antibody 3.1 light chain



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.06Å 135.06Å 230.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.84 – 2.91 42.84 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.84-2.91) 99.6 (42.84-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.90Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.193 , 0.242 0.188 , 0.235	Depositor DCC
$R_{free}$ test set	1734 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.6	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7222	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: MLI, 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	0.75	0/2593	0.97	3/3536 (0.1%)
2	B	0.72	0/1404	0.94	2/1889 (0.1%)
3	I	0.66	0/1684	1.03	9/2298 (0.4%)
4	J	0.67	0/1639	0.96	2/2227 (0.1%)
All	All	0.71	0/7320	0.98	16/9950 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	153	GLU	CA-C-N	-7.32	110.69	119.84
3	I	153	GLU	C-N-CA	-7.32	110.69	119.84
4	J	56	SER	N-CA-C	6.41	119.08	111.33
3	I	141	ALA	N-CA-C	6.06	118.15	110.33
3	I	134	ALA	CA-C-N	5.96	125.87	119.85
3	I	134	ALA	C-N-CA	5.96	125.87	119.85
2	B	31	GLY	N-CA-C	5.95	117.90	110.29
2	B	61	THR	N-CA-C	5.85	123.26	110.80
3	I	57	ASN	CA-C-N	5.82	132.17	121.70
3	I	57	ASN	C-N-CA	5.82	132.17	121.70
4	J	21	ILE	CB-CA-C	-5.75	102.63	111.31
3	I	53	TYR	N-CA-C	5.58	118.89	111.75
1	A	221	THR	CA-C-N	-5.42	114.34	119.76
1	A	221	THR	C-N-CA	-5.42	114.34	119.76
1	A	275	ILE	N-CA-C	5.13	115.30	108.11
3	I	55	GLY	N-CA-C	-5.04	108.16	115.27

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	2528	0	2433	63	0
2	B	1376	0	1284	19	0
3	I	1644	0	1592	51	0
4	J	1604	0	1558	38	0
5	C	28	0	25	2	0
6	A	28	0	26	0	0
7	I	7	0	2	0	0
7	J	7	0	2	1	0
All	All	7222	0	6922	162	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 11.

All (162) 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:I:153:GLU:HB3	3:I:154:PRO:HD3	1.20	1.14
1:A:117:SER:HA	1:A:273:SER:HB2	1.36	1.02
1:A:141:GLY:HA2	1:A:142:VAL:HB	1.39	0.99
3:I:153:GLU:HB3	3:I:154:PRO:CD	1.96	0.95
3:I:54:ASP:OD2	3:I:56:SER:HB2	1.66	0.94
1:A:225:ALA:HB1	1:A:227:ARG:HH21	1.35	0.91
1:A:231:ARG:NH2	5:C:1:NAG:O3	2.05	0.90
4:J:143:GLU:OE2	4:J:143:GLU:HA	1.73	0.89
2:B:58:LYS:HG3	2:B:59:MET:N	1.87	0.88
1:A:137:GLU:OE2	1:A:139:THR:HG22	1.73	0.88
1:A:141:GLY:CA	1:A:142:VAL:HB	2.06	0.84
3:I:57:ASN:HA	3:I:58:LYS:HB2	1.60	0.84
1:A:116:SER:O	1:A:273:SER:HB2	1.82	0.80
1:A:315:LYS:HD2	2:B:62:GLN:OE1	1.81	0.80
1:A:195:GLY:HA2	1:A:196:THR:HB	1.63	0.79
3:I:144:GLY:HA3	3:I:186:VAL:HG12	1.65	0.78
1:A:224:ILE:O	1:A:224:ILE:HG13	1.84	0.77
1:A:117:SER:HA	1:A:273:SER:CB	2.15	0.76
3:I:102:GLY:HA2	3:I:104:PHE:N	2.00	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLY:HA2	1:A:197:ASP:H	1.50	0.76
1:A:195:GLY:CA	1:A:197:ASP:H	2.03	0.72
2:B:61:THR:O	2:B:62:GLN:HG3	1.90	0.71
3:I:76:MET:CE	3:I:76:MET:HA	2.20	0.71
3:I:64:VAL:HG21	3:I:68:PHE:CG	2.28	0.69
3:I:153:GLU:CB	3:I:154:PRO:HD3	2.12	0.69
1:A:142:VAL:HG13	1:A:152:SER:HB3	1.74	0.68
1:A:225:ALA:CB	1:A:227:ARG:HH21	2.04	0.68
1:A:195:GLY:CA	1:A:197:ASP:N	2.58	0.67
3:I:35:HIS:HD2	3:I:47:TRP:HE1	1.45	0.65
1:A:71:LEU:HD11	1:A:115:LEU:HD11	1.79	0.65
1:A:193:PRO:O	1:A:194:THR:C	2.40	0.65
3:I:57:ASN:HA	3:I:58:LYS:CB	2.27	0.64
1:A:101:TYR:CD2	1:A:237:MET:HB2	2.34	0.62
4:J:108:ARG:HD3	4:J:109:THR:O	1.99	0.62
4:J:122:ASP:HA	4:J:125:LEU:HD23	1.81	0.62
1:A:61:GLN:HE21	1:A:63:GLY:H	1.44	0.62
3:I:217:GLU:HB2	3:I:218:PRO:HD2	1.80	0.62
1:A:50:LYS:HG2	1:A:283:HIS:HD2	1.66	0.61
4:J:144:ALA:HA	4:J:145:LYS:HB3	1.82	0.61
1:A:106:ILE:HG13	1:A:240:TYR:CE2	2.36	0.61
4:J:108:ARG:HD2	4:J:140:TYR:CB	2.31	0.61
1:A:225:ALA:HB1	1:A:227:ARG:NH2	2.13	0.60
1:A:103:GLY:HA3	1:A:237:MET:O	2.02	0.59
3:I:76:MET:HA	3:I:76:MET:HE3	1.83	0.59
4:J:91:ALA:O	7:J:301:MLI:O6	2.20	0.59
3:I:1:GLN:HG2	3:I:2:VAL:H	1.69	0.58
3:I:100:LEU:HD23	3:I:106:ARG:HD3	1.84	0.58
4:J:183:LYS:O	4:J:187:GLU:HG2	2.04	0.58
4:J:138:ASN:C	4:J:172:THR:HG21	2.29	0.57
3:I:1:GLN:NE2	3:I:98:ARG:HH22	2.03	0.57
3:I:67:ARG:O	3:I:84:ASN:ND2	2.37	0.57
1:A:15:ILE:HG23	2:B:118:LEU:HD23	1.85	0.57
3:I:108:ILE:HD12	4:J:49:TYR:HB2	1.86	0.57
1:A:91:GLU:O	1:A:277:THR:HA	2.05	0.56
1:A:116:SER:O	1:A:273:SER:CB	2.52	0.56
3:I:151:PHE:CE2	3:I:152:PRO:HB3	2.40	0.56
1:A:96:GLU:OE1	5:C:1:NAG:H62	2.05	0.56
3:I:64:VAL:HG21	3:I:68:PHE:CD2	2.41	0.55
4:J:6:GLN:HE21	4:J:99:GLY:HA3	1.71	0.55
4:J:198:HIS:CD2	4:J:200:GLY:H	2.24	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:THR:C	2:B:62:GLN:HE21	2.14	0.54
3:I:57:ASN:CA	3:I:58:LYS:HB2	2.31	0.54
1:A:195:GLY:HA2	1:A:196:THR:CB	2.32	0.54
3:I:160:ASN:C	3:I:162:GLY:H	2.16	0.54
1:A:309:THR:HB	1:A:313:CYS:SG	2.49	0.53
3:I:206:LYS:CB	3:I:207:PRO:HD3	2.38	0.53
4:J:6:GLN:NE2	4:J:101:GLY:H	2.07	0.53
3:I:27:PHE:O	3:I:30:ARG:HD2	2.08	0.53
3:I:93:VAL:HG12	3:I:117:LEU:HD13	1.90	0.52
1:A:146:CYS:O	1:A:153:SER:HB3	2.10	0.52
3:I:204:ASN:HD22	3:I:211:LYS:HG3	1.74	0.52
3:I:148:LYS:HG3	3:I:149:ASP:N	2.24	0.52
1:A:38:HIS:CD2	2:B:21:TRP:HE1	2.28	0.52
1:A:291:THR:HG22	1:A:309:THR:HG22	1.92	0.52
3:I:152:PRO:HD2	3:I:207:PRO:HB2	1.91	0.51
4:J:139:PHE:N	4:J:172:THR:HG22	2.25	0.51
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.92	0.51
1:A:195:GLY:HA3	1:A:197:ASP:N	2.25	0.50
3:I:102:GLY:HA2	3:I:103:TYR:C	2.35	0.50
3:I:151:PHE:CD2	3:I:152:PRO:HB3	2.47	0.50
4:J:108:ARG:HD2	4:J:140:TYR:HB2	1.92	0.50
1:A:117:SER:CA	1:A:273:SER:HB2	2.25	0.50
4:J:115:VAL:HG22	4:J:207:LYS:HG3	1.94	0.50
3:I:176:GLN:HE21	3:I:176:GLN:H	1.59	0.50
2:B:53:ASN:O	2:B:57:GLU:HB3	2.12	0.50
4:J:209:PHE:C	4:J:209:PHE:CD1	2.90	0.49
3:I:206:LYS:C	3:I:208:SER:H	2.20	0.49
3:I:64:VAL:HG21	3:I:68:PHE:CD1	2.47	0.49
4:J:19:VAL:HG13	4:J:75:ILE:HB	1.94	0.49
4:J:6:GLN:HE21	4:J:99:GLY:CA	2.26	0.48
1:A:145:ALA:O	1:A:231:ARG:NH1	2.45	0.48
1:A:17:TYR:HB2	1:A:328:LEU:HD11	1.95	0.48
3:I:112:TRP:CE3	4:J:44:PRO:HD2	2.49	0.48
1:A:230:VAL:HG12	1:A:231:ARG:HG3	1.96	0.48
4:J:2:LEU:O	4:J:26:SER:OG	2.16	0.48
3:I:167:GLY:O	3:I:187:VAL:HG23	2.13	0.48
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.49	0.47
4:J:144:ALA:HA	4:J:145:LYS:CB	2.44	0.47
1:A:71:LEU:HD11	1:A:115:LEU:CD1	2.43	0.47
2:B:58:LYS:HG3	2:B:59:MET:H	1.71	0.47
4:J:193:ALA:HB2	4:J:208:SER:HB3	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:198:HIS:HD2	4:J:200:GLY:H	1.62	0.47
1:A:315:LYS:CD	2:B:62:GLN:OE1	2.59	0.47
1:A:127:PHE:CE2	1:A:173:LYS:HB3	2.50	0.47
4:J:6:GLN:HE22	4:J:87:TYR:HA	1.79	0.47
4:J:138:ASN:C	4:J:172:THR:CG2	2.87	0.47
3:I:206:LYS:HB2	3:I:207:PRO:HD3	1.97	0.47
4:J:6:GLN:HE21	4:J:99:GLY:C	2.22	0.47
4:J:94:PHE:HA	4:J:95:PRO:C	2.39	0.47
1:A:66:ASN:O	1:A:67:ILE:C	2.55	0.46
1:A:101:TYR:HD2	1:A:237:MET:HB2	1.79	0.46
1:A:195:GLY:HA2	1:A:197:ASP:N	2.22	0.46
1:A:193:PRO:O	1:A:195:GLY:N	2.48	0.46
4:J:19:VAL:CG1	4:J:78:LEU:HG	2.45	0.46
1:A:229:LYS:HA	1:A:233:GLN:O	2.16	0.46
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.51	0.46
4:J:108:ARG:HG2	4:J:171:SER:HB2	1.98	0.46
4:J:33:LEU:HD22	4:J:71:PHE:CG	2.51	0.46
1:A:61:GLN:NE2	1:A:63:GLY:H	2.14	0.46
4:J:22:THR:HG22	4:J:72:THR:HG22	1.96	0.46
3:I:141:ALA:HB3	3:I:194:LEU:HD11	1.98	0.45
3:I:101:GLY:O	3:I:102:GLY:C	2.59	0.45
3:I:176:GLN:NE2	3:I:180:LEU:O	2.49	0.45
3:I:206:LYS:O	3:I:208:SER:N	2.49	0.45
3:I:76:MET:HA	3:I:76:MET:HE2	1.99	0.44
1:A:77:CYS:HB3	1:A:80:LEU:HD12	1.97	0.44
4:J:158:ASN:O	4:J:179:LEU:HD12	2.17	0.44
1:A:195:GLY:HA3	1:A:198:GLN:H	1.81	0.44
3:I:151:PHE:HA	3:I:152:PRO:HA	1.74	0.44
1:A:100:CYS:O	1:A:231:ARG:HD3	2.18	0.44
1:A:207:ALA:O	1:A:222:PRO:HD3	2.17	0.44
2:B:30:GLN:HE22	2:B:145:ASP:HB2	1.83	0.44
3:I:91:THR:HG23	3:I:119:THR:HA	2.00	0.44
4:J:118:PHE:HA	4:J:119:PRO:HD2	1.86	0.43
1:A:245:GLU:HG3	1:A:246:PRO:HD2	2.00	0.43
3:I:56:SER:HB3	3:I:57:ASN:OD1	2.19	0.43
3:I:52:SER:HB3	3:I:57:ASN:O	2.19	0.43
2:B:58:LYS:HE3	2:B:58:LYS:C	2.43	0.43
2:B:45:ILE:O	2:B:49:THR:OG1	2.33	0.43
3:I:7:SER:HB3	3:I:21:SER:HB2	2.00	0.43
1:A:119:SER:HB3	1:A:272:GLY:HA3	2.00	0.42
3:I:35:HIS:HE1	3:I:99:ASP:OD1	2.02	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:21:ILE:HG12	4:J:102:THR:HG21	2.00	0.42
1:A:59:PRO:HB3	1:A:88:TYR:CZ	2.54	0.42
3:I:175:LEU:HD13	3:I:181:TYR:CZ	2.54	0.42
4:J:115:VAL:HA	4:J:135:LEU:O	2.19	0.42
1:A:272:GLY:O	1:A:273:SER:C	2.62	0.42
1:A:68:ALA:HB2	1:A:108:TYR:CE1	2.55	0.42
2:B:59:MET:H	2:B:59:MET:HG2	1.56	0.42
1:A:140:LYS:HA	1:A:141:GLY:HA2	1.69	0.42
1:A:19:ALA:O	2:B:15:THR:HA	2.20	0.42
3:I:1:GLN:HE22	3:I:98:ARG:HH22	1.68	0.42
4:J:79:GLN:HG3	4:J:80:PRO:HD2	2.01	0.41
2:B:60:ASN:CG	2:B:61:THR:HG22	2.45	0.41
3:I:32:TYR:CD1	3:I:98:ARG:HD3	2.55	0.41
1:A:215:LYS:HG2	1:A:216:TYR:N	2.35	0.41
3:I:35:HIS:O	3:I:96:CYS:HA	2.21	0.41
4:J:47:LEU:HA	4:J:58:VAL:HG21	2.03	0.41
1:A:163:LYS:O	1:A:163:LYS:HG3	2.20	0.41
4:J:108:ARG:NH2	4:J:109:THR:O	2.43	0.40
1:A:303:GLN:O	1:A:316:TYR:HA	2.21	0.40
1:A:18:HIS:HB2	2:B:21:TRP:HA	2.04	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	326/331 (98%)	293 (90%)	29 (9%)	4 (1%)	10	32
2	B	168/179 (94%)	158 (94%)	7 (4%)	3 (2%)	6	23
3	I	217/219 (99%)	184 (85%)	23 (11%)	10 (5%)	2	6
4	J	210/214 (98%)	193 (92%)	14 (7%)	3 (1%)	9	29
All	All	921/943 (98%)	828 (90%)	73 (8%)	20 (2%)	5	19

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	61	THR
3	I	58	LYS
3	I	152	PRO
3	I	153	GLU
1	A	140	LYS
1	A	142	VAL
1	A	165	GLY
3	I	154	PRO
3	I	161	SER
2	B	58	LYS
2	B	67	GLY
3	I	65	LYS
1	A	166	SER
3	I	208	SER
4	J	3	GLN
4	J	144	ALA
3	I	2	VAL
4	J	211	ARG
3	I	218	PRO
3	I	207	PRO

### 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	278/285 (98%)	260 (94%)	18 (6%)	15	42
2	B	145/152 (95%)	137 (94%)	8 (6%)	19	49
3	I	179/184 (97%)	146 (82%)	33 (18%)	1	5
4	J	181/185 (98%)	149 (82%)	32 (18%)	2	6
All	All	783/806 (97%)	692 (88%)	91 (12%)	5	17

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	46	SER
1	A	54	LEU
1	A	79	LEU
1	A	121	PHE
1	A	131	SER
1	A	135	ASN
1	A	143	THR
1	A	186	LEU
1	A	199	GLN
1	A	215	LYS
1	A	223	GLU
1	A	227	ARG
1	A	232	ASP
1	A	273	SER
1	A	305	ILE
1	A	315	LYS
1	A	328	LEU
2	B	45	ILE
2	B	49	THR
2	B	57	GLU
2	B	58	LYS
2	B	59	MET
2	B	62	GLN
2	B	94	TYR
2	B	172	GLU
3	I	2	VAL
3	I	11	VAL
3	I	12	VAL
3	I	16	ARG
3	I	30	ARG
3	I	54	ASP
3	I	56	SER
3	I	57	ASN
3	I	63	SER
3	I	75	SER
3	I	76	MET
3	I	78	THR
3	I	84	ASN
3	I	89	GLU
3	I	93	VAL
3	I	98	ARG
3	I	108	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	I	116	THR
3	I	119	THR
3	I	125	THR
3	I	153	GLU
3	I	156	THR
3	I	157	VAL
3	I	170	THR
3	I	174	VAL
3	I	176	GLN
3	I	177	SER
3	I	184	SER
3	I	197	GLN
3	I	202	ASN
3	I	211	LYS
3	I	212	VAL
3	I	215	ARG
4	J	1	GLU
4	J	2	LEU
4	J	7	SER
4	J	11	VAL
4	J	12	SER
4	J	15	VAL
4	J	19	VAL
4	J	20	THR
4	J	47	LEU
4	J	48	ILE
4	J	56	SER
4	J	65	SER
4	J	76	SER
4	J	77	SER
4	J	79	GLN
4	J	104	VAL
4	J	106	ILE
4	J	108	ARG
4	J	115	VAL
4	J	122	ASP
4	J	124	GLN
4	J	125	LEU
4	J	135	LEU
4	J	142	ARG
4	J	143	GLU
4	J	154	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	J	163	VAL
4	J	166	GLN
4	J	172	THR
4	J	180	THR
4	J	206	THR
4	J	207	LYS

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

Mol	Chain	Res	Type
1	A	38	HIS
1	A	61	GLN
1	A	94	ASN
1	A	136	HIS
1	A	233	GLN
1	A	283	HIS
2	B	26	HIS
2	B	38	GLN
2	B	125	GLN
3	I	1	GLN
3	I	35	HIS
3	I	84	ASN
3	I	169	HIS
3	I	176	GLN
3	I	197	GLN
3	I	204	ASN
3	I	209	ASN
4	J	6	GLN
4	J	37	GLN
4	J	92	ASN
4	J	137	ASN
4	J	138	ASN
4	J	166	GLN
4	J	198	HIS

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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
5	NAG	C	1	1,5	14,14,15	0.54	0	17,19,21	1.25	2 (11%)
5	NAG	C	2	5	14,14,15	0.83	1 (7%)	17,19,21	1.14	1 (5%)

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	NAG	C	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2	NAG	C1-C2	2.20	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	NAG	C1-O5-C5	3.15	116.41	112.19
5	C	2	NAG	C4-C3-C2	2.97	115.36	111.02
5	C	1	NAG	C4-C3-C2	2.31	114.41	111.02

There are no chirality outliers.

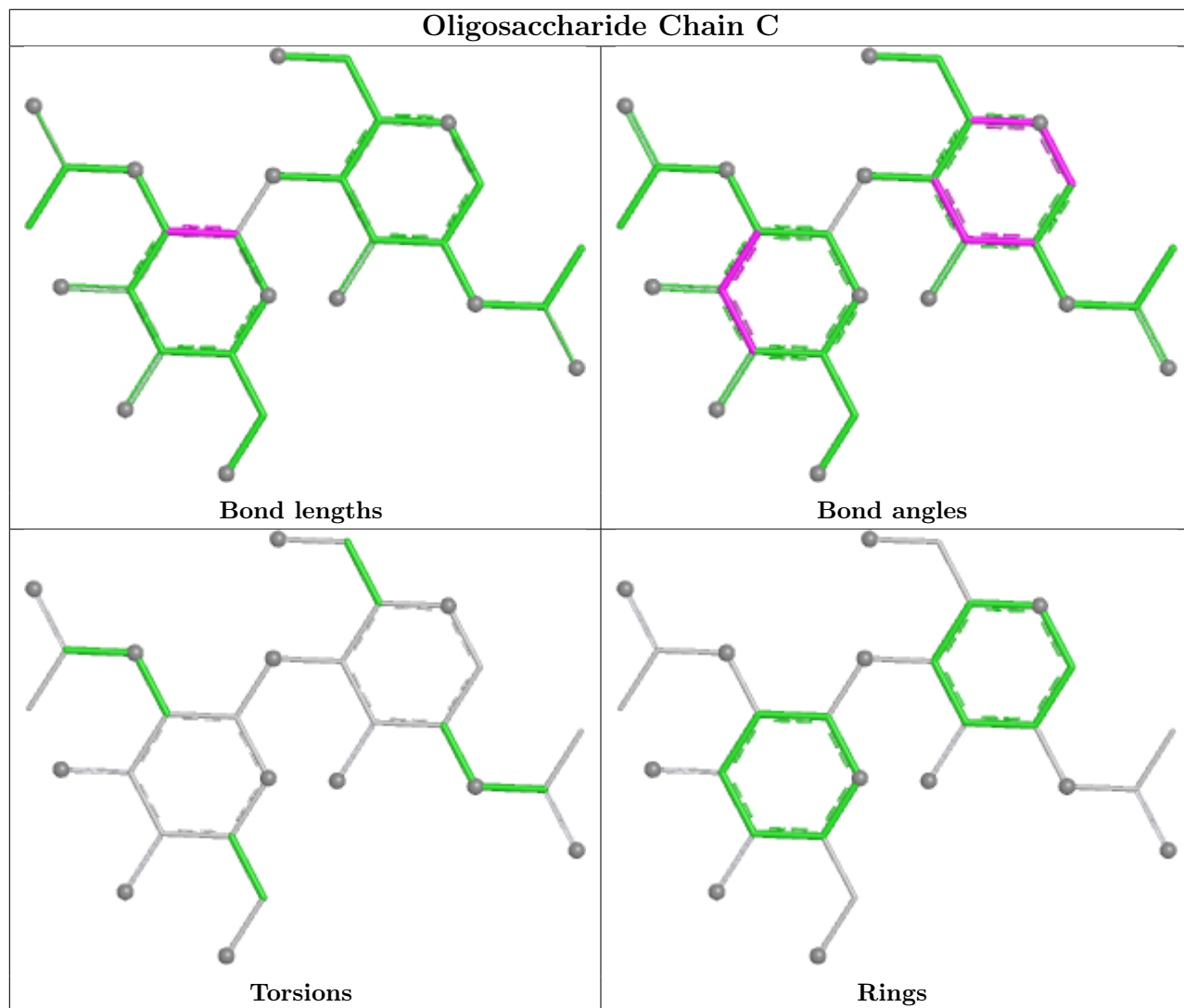
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	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](#)

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
7	MLI	J	301	-	6,6,6	1.29	0	7,7,7	1.43	1 (14%)
6	NAG	A	404	1	14,14,15	0.69	0	17,19,21	1.47	2 (11%)
6	NAG	A	401	1	14,14,15	0.70	0	17,19,21	1.39	2 (11%)
7	MLI	I	301	-	6,6,6	1.16	0	7,7,7	0.94	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
7	MLI	J	301	-	-	2/4/4/4	-
6	NAG	A	404	1	-	1/6/23/26	0/1/1/1
6	NAG	A	401	1	-	1/6/23/26	0/1/1/1
7	MLI	I	301	-	-	0/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	401	NAG	C1-O5-C5	3.27	116.57	112.19
6	A	404	NAG	C1-O5-C5	3.19	116.46	112.19
6	A	404	NAG	C4-C3-C2	-2.88	106.80	111.02
7	J	301	MLI	O7-C2-C1	2.51	122.30	114.51
6	A	401	NAG	C4-C3-C2	2.48	114.65	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	NAG	O5-C5-C6-O6
6	A	404	NAG	O5-C5-C6-O6
7	J	301	MLI	C3-C1-C2-O7
7	J	301	MLI	C3-C1-C2-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	301	MLI	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	328/331 (99%)	-0.25	8 (2%) 59 50	58, 74, 96, 145	0
2	B	171/179 (95%)	-0.06	6 (3%) 47 38	47, 85, 136, 168	1 (0%)
3	I	219/219 (100%)	0.18	5 (2%) 61 51	65, 102, 172, 195	0
4	J	212/214 (99%)	-0.16	3 (1%) 73 65	60, 89, 149, 173	0
All	All	930/943 (98%)	-0.09	22 (2%) 59 50	47, 82, 150, 195	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	THR	4.3
3	I	219	LYS	3.6
2	B	65	ALA	3.3
4	J	144	ALA	3.3
1	A	7	ALA	3.1
1	A	334	ILE	2.8
1	A	9	PRO	2.8
2	B	173	ILE	2.7
3	I	164	LEU	2.6
4	J	212	GLY	2.5
1	A	195	GLY	2.4
2	B	147	ALA	2.4
3	I	212	VAL	2.3
1	A	272	GLY	2.3
4	J	143	GLU	2.3
2	B	62	GLN	2.3
1	A	224	ILE	2.3
3	I	141	ALA	2.3
2	B	59	MET	2.1
2	B	170	ARG	2.0
1	A	96	GLU	2.0
3	I	216	VAL	2.0

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

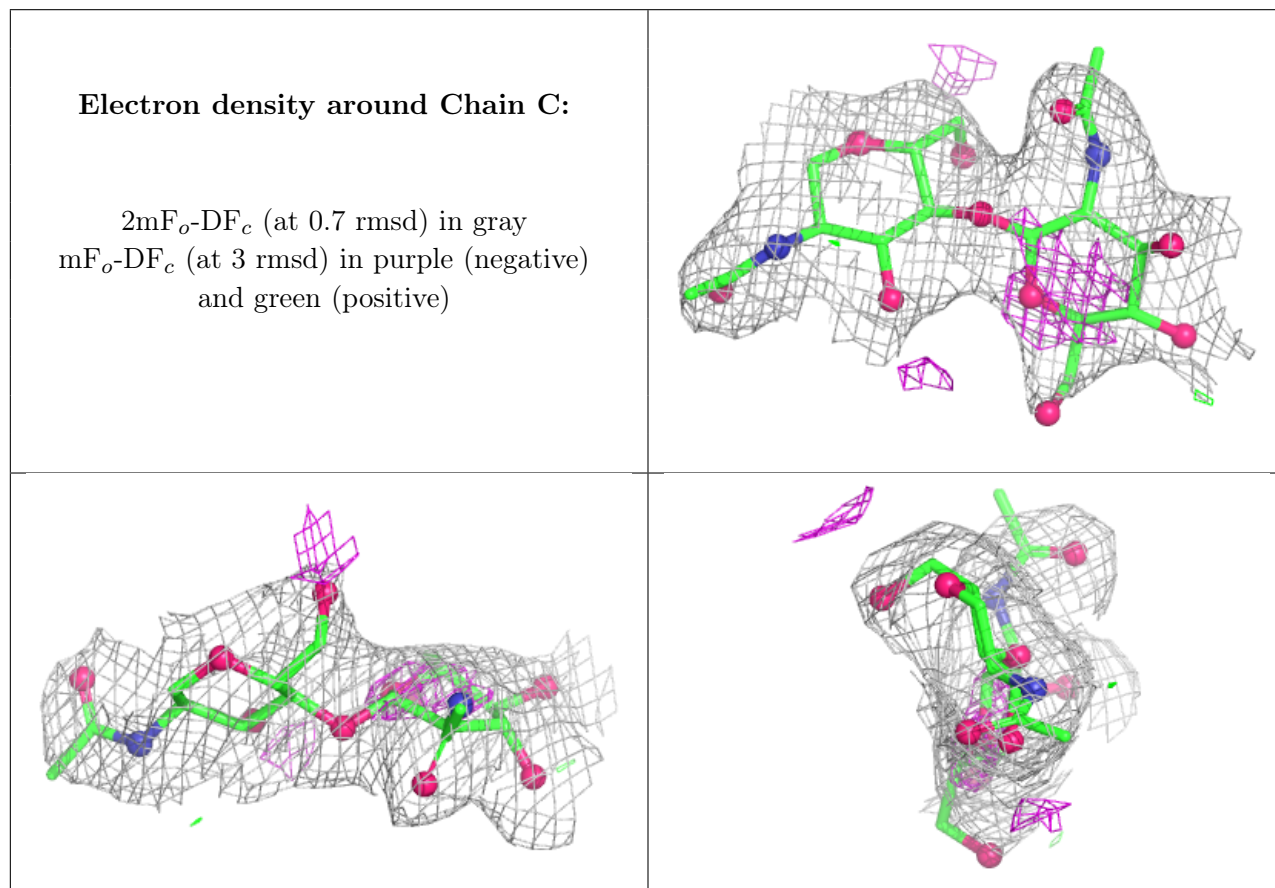
There are no non-standard protein/DNA/RNA residues in this entry.

## 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
5	NAG	C	1	14/15	-	-	80,85,91,96	0
5	NAG	C	2	14/15	-	-	101,103,104,104	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.



## 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
6	NAG	A	404	14/15	0.75	0.13	84,91,97,98	0
6	NAG	A	401	14/15	0.77	0.12	88,97,99,100	0
7	MLI	J	301	7/7	0.92	0.11	95,96,97,97	0
7	MLI	I	301	7/7	0.96	0.10	95,97,97,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.