



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:30 AM UTC

PDB ID : 2FD6 / pdb\_00002fd6  
Title : Structure of Human Urokinase Plasminogen Activator in Complex with Urokinase Receptor and an anti-upar antibody at 1.9 Å  
Authors : Huang, M.; Huai, Q.; Li, Y.  
Deposited on : 2005-12-13  
Resolution : 1.90 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
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

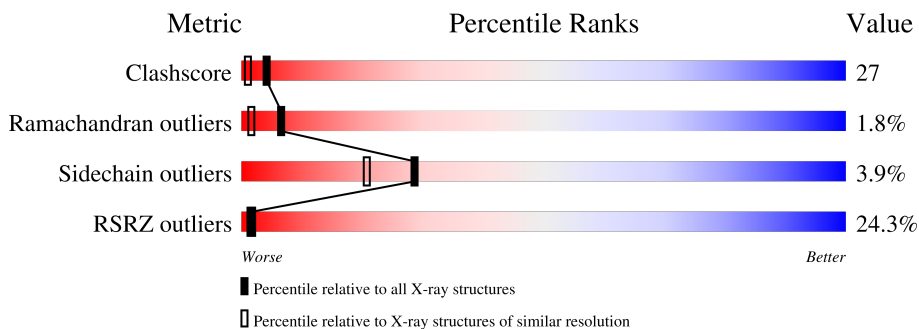
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	122	
2	L	214	
3	H	213	
4	U	276	
5	B	2	
6	C	2	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
12	PG4	U	402	-	-	X	-
5	NAG	B	1	X	-	-	-
5	FUC	B	2	X	-	-	-
6	NAG	C	1	-	-	X	-
6	NAG	C	2	X	-	-	-
8	ETX	L	401	-	-	X	-

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 6600 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 Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	122	967	596	183	174	14	0	0	0

- Molecule 2 is a protein called L chain of Fab of ATN-615 anti-uPAR antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1648	1032	272	337	7	0	0	0

- Molecule 3 is a protein called H chain of Fab of ATN-615 anti-uPAR antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	212	1618	1035	262	315	6	0	0	0

- Molecule 4 is a protein called Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	U	249	1906	1141	349	382	34	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	1A	SER	-	cloning artifact	UNP Q03405

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



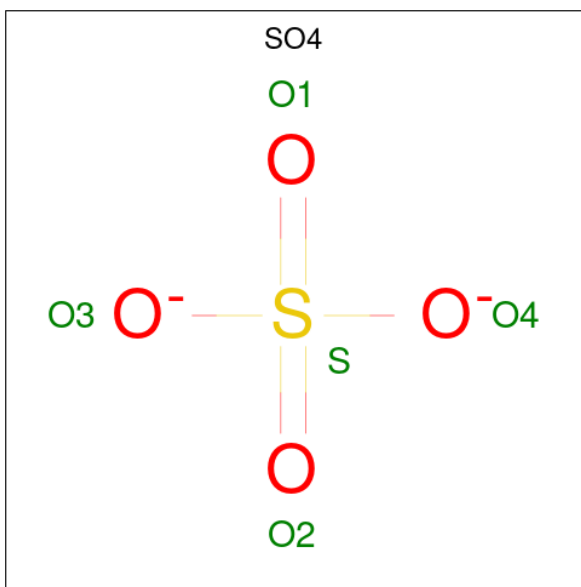
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	B	2	26	14	1	11	0	0	0

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



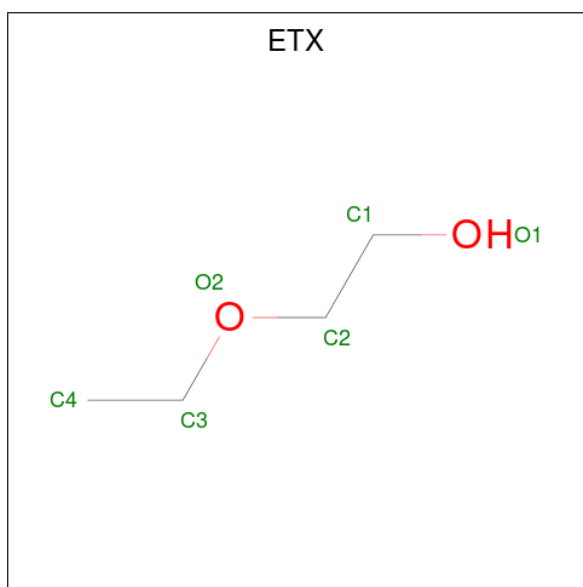
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	C	2	30	16	2	12	0	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



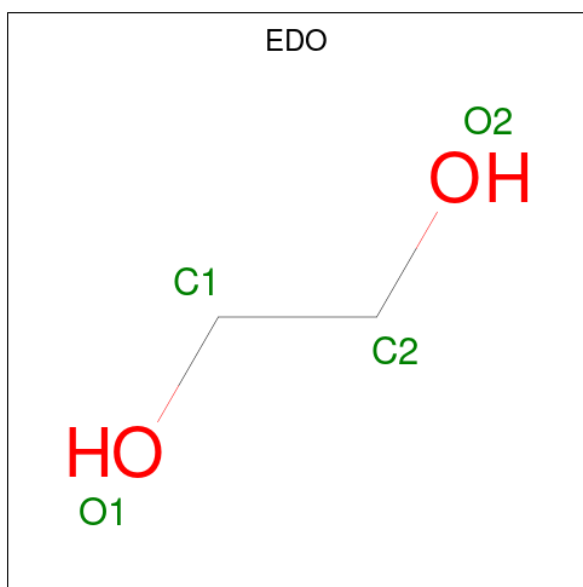
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			O	S		
7	A	1	4	1	0	0

- Molecule 8 is 2-ETHOXYETHANOL (CCD ID: ETX) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			6	4	2		
8	L	1	Total	C	O	0	0
			6	4	2		
8	H	1	Total	C	O	0	0
			6	4	2		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



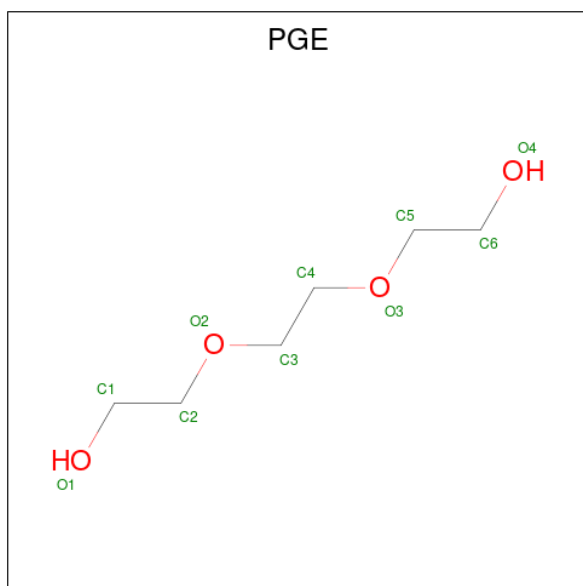
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			4	2	2		

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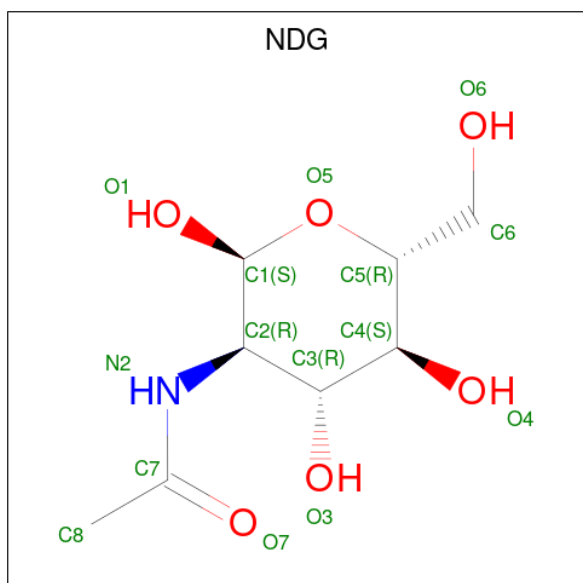
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



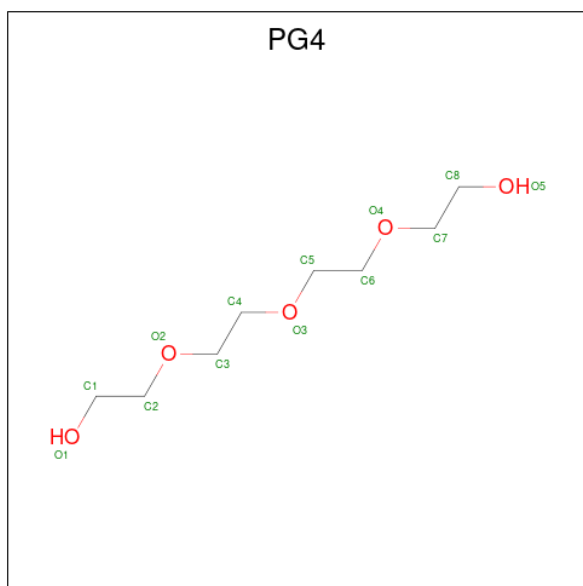
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 11 is 2-acetamido-2-deoxy- $\alpha$ -D-glucopyranose (CCD ID: NDG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	U	1	15	8	1	6	0	0

- Molecule 12 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	U	1	13	8	5	0	0

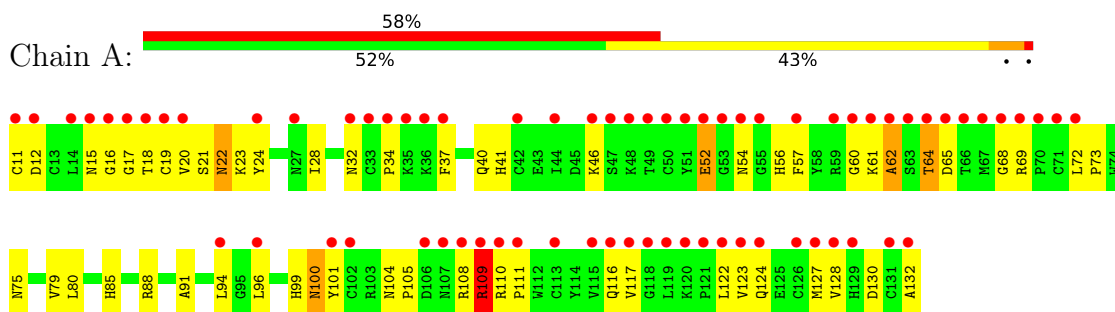
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	22	Total	O	0	0
			22	22		
13	L	121	Total	O	0	0
			121	121		
13	H	121	Total	O	0	0
			121	121		
13	U	72	Total	O	0	0
			72	72		

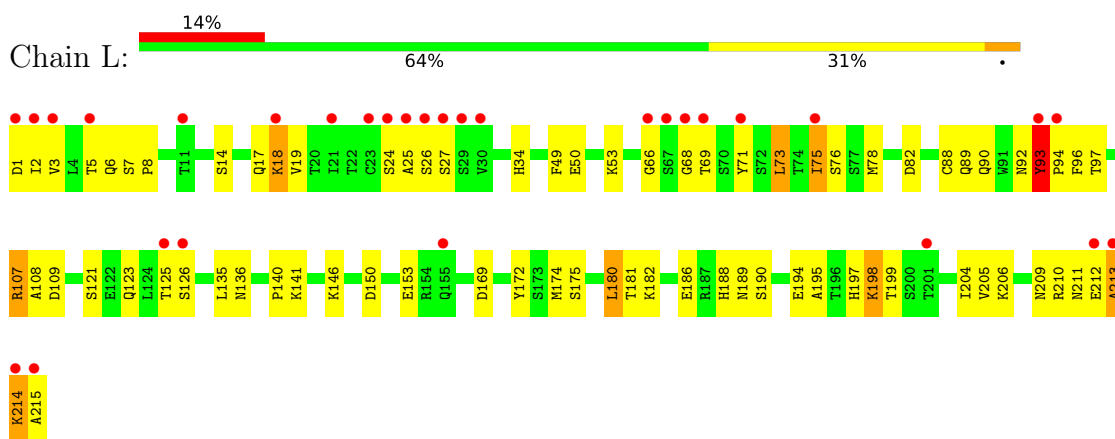
### 3 Residue-property plots [i](#)

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.

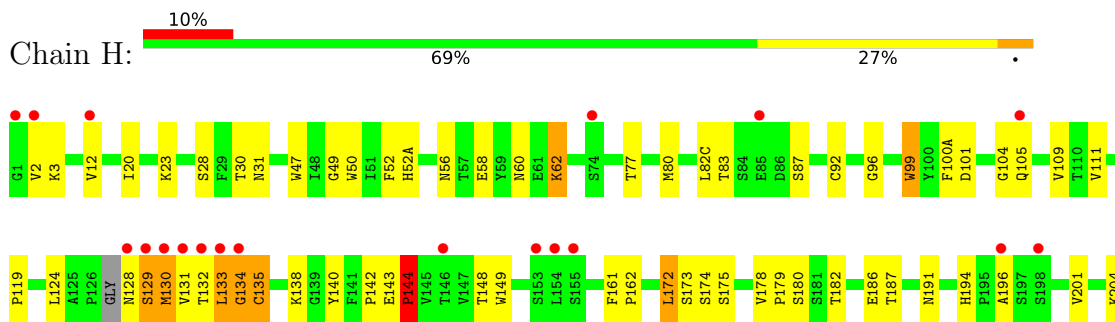
- Molecule 1: Urokinase-type plasminogen activator



- Molecule 2: L chain of Fab of ATN-615 anti-uPAR antibody

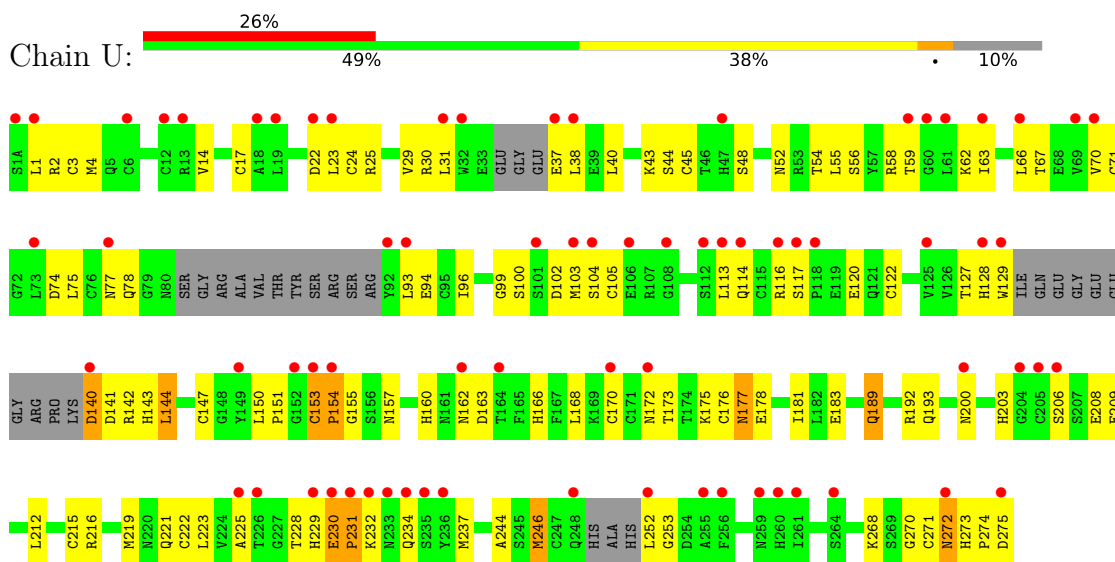


- Molecule 3: H chain of Fab of ATN-615 anti-uPAR antibody





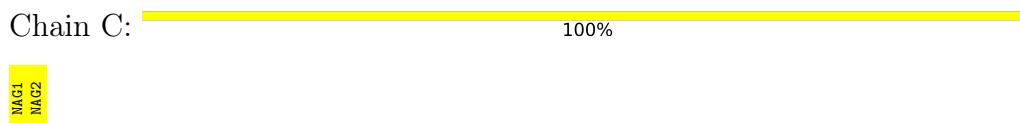
- Molecule 4: Urokinase plasminogen activator surface receptor



- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.79Å 86.81Å 124.69Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	41.36 – 1.90 41.36 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.8 (41.36-1.90) 95.8 (41.36-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 1.86Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.276 0.241 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtrriage
Anisotropy	0.350	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4, ETX, FUC, PG4, EDO, PGE, NDG

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	0.37	0/994	0.90	3/1342 (0.2%)
2	L	0.46	0/1688	1.06	8/2292 (0.3%)
3	H	0.61	3/1668 (0.2%)	1.04	13/2282 (0.6%)
4	U	0.44	0/1933	0.90	3/2599 (0.1%)
All	All	0.49	3/6283 (0.0%)	0.98	27/8515 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	134	GLY	C-N	-13.79	1.14	1.33
3	H	134	GLY	N-CA	-5.57	1.37	1.45
3	H	133	LEU	C-N	-5.55	1.25	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	93	TYR	CA-C-N	-14.10	105.32	119.56
2	L	93	TYR	C-N-CA	-14.10	105.32	119.56
3	H	134	GLY	O-C-N	8.00	133.11	122.70
3	H	133	LEU	CA-C-N	-7.31	107.08	121.41
3	H	133	LEU	C-N-CA	-7.31	107.08	121.41
2	L	93	TYR	N-CA-C	7.14	125.59	109.81
4	U	78	GLN	N-CA-C	6.90	118.80	111.28
3	H	99	TRP	N-CA-C	6.64	120.70	111.74
2	L	92	ASN	N-CA-C	6.58	119.82	110.14
3	H	96	GLY	CA-C-N	6.47	127.93	119.84
3	H	96	GLY	C-N-CA	6.47	127.93	119.84
3	H	96	GLY	N-CA-C	6.06	119.56	112.23
2	L	136	ASN	N-CA-C	5.65	119.18	110.42
1	A	64	THR	N-CA-C	5.64	119.29	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	73	LEU	N-CA-C	-5.64	100.52	109.59
3	H	138	LYS	N-CA-C	5.62	118.64	109.59
3	H	60	ASN	N-CA-C	-5.50	101.71	109.96
3	H	104	GLY	N-CA-C	-5.42	104.12	112.85
1	A	15	ASN	CB-CA-C	-5.38	110.39	116.63
2	L	169	ASP	N-CA-C	5.37	119.80	112.88
2	L	204	ILE	N-CA-C	-5.27	100.16	108.23
3	H	101	ASP	N-CA-C	5.26	118.86	112.23
3	H	129	SER	N-CA-C	-5.20	107.07	113.41
4	U	253	GLY	N-CA-C	5.20	120.64	113.99
4	U	45	CYS	N-CA-C	-5.05	103.86	110.53
3	H	92	CYS	N-CA-C	-5.03	101.49	109.59
1	A	17	GLY	N-CA-C	5.01	118.38	110.71

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	967	0	902	65	0
2	L	1648	0	1577	71	0
3	H	1618	0	1557	64	0
4	U	1906	0	1773	132	0
5	B	26	0	24	6	0
6	C	30	0	27	9	0
7	A	5	0	0	0	0
8	H	6	0	10	3	0
8	L	12	0	20	9	0
9	H	4	0	6	0	0
9	L	4	0	6	0	0
10	H	10	0	14	1	0
11	U	15	0	12	2	0
12	U	13	0	18	11	0
13	A	22	0	0	2	0
13	H	121	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	121	0	0	6	0
13	U	72	0	0	14	0
All	All	6600	0	5946	333	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 27.

All (333) 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)
4:U:230:GLU:HB3	4:U:231:PRO:HD2	1.36	1.06
6:C:1:NAG:H61	6:C:2:NAG:H82	1.37	1.05
13:U:530:HOH:O	5:B:1:NAG:H83	1.57	1.02
4:U:221:GLN:HE21	12:U:402:PG4:H32	1.25	1.01
6:C:1:NAG:C6	6:C:2:NAG:H82	1.91	1.00
4:U:172:ASN:ND2	6:C:1:NAG:C7	2.25	0.99
3:H:134:GLY:O	3:H:149:TRP:HH2	1.45	0.98
4:U:244:ALA:HB2	12:U:402:PG4:H31	1.46	0.96
4:U:232:LYS:HB2	4:U:234:GLN:HE22	1.28	0.96
3:H:132:THR:O	3:H:133:LEU:HD23	1.67	0.94
4:U:4:MET:HE1	4:U:14:VAL:HG22	1.50	0.94
4:U:172:ASN:ND2	6:C:1:NAG:O7	2.01	0.93
4:U:23:LEU:HD13	4:U:70:VAL:HG11	1.49	0.93
4:U:189:GLN:H	4:U:189:GLN:HE21	1.07	0.92
3:H:56:ASN:HD22	12:U:402:PG4:H11	1.33	0.92
4:U:52:ASN:ND2	5:B:1:NAG:O1	2.00	0.92
3:H:134:GLY:O	3:H:149:TRP:CH2	2.22	0.92
1:A:99:HIS:HD2	1:A:101:TYR:H	1.21	0.88
4:U:99:GLY:H	4:U:104:SER:HB3	1.38	0.86
4:U:96:ILE:H	4:U:177:ASN:HD21	1.23	0.85
6:C:1:NAG:H61	6:C:2:NAG:C8	2.05	0.85
3:H:132:THR:O	3:H:133:LEU:CD2	2.25	0.84
3:H:128:ASN:O	3:H:180:SER:OG	1.95	0.84
4:U:94:GLU:OE2	4:U:175:LYS:HE2	1.78	0.83
4:U:232:LYS:HB2	4:U:234:GLN:NE2	1.95	0.81
1:A:54:ASN:ND2	1:A:56:HIS:HB2	1.96	0.81
1:A:110:ARG:HD3	1:A:111:PRO:HD2	1.62	0.81
3:H:23:LYS:HD2	8:H:403:ETX:H12	1.62	0.81
3:H:119:PRO:HB3	3:H:140:TYR:HB3	1.63	0.81
1:A:23:LYS:HZ1	4:U:166:HIS:HD2	1.26	0.80
3:H:12:VAL:HG21	3:H:82(C):LEU:CD1	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:221:GLN:HE21	12:U:402:PG4:C3	1.96	0.78
2:L:25:ALA:O	2:L:69:THR:HG23	1.85	0.77
3:H:182:THR:O	3:H:186:GLU:HB2	1.85	0.76
2:L:107:ARG:HG2	2:L:108:ALA:N	2.00	0.75
2:L:19:VAL:HB	2:L:75:ILE:CG2	2.17	0.75
3:H:130:MET:HE2	3:H:178:VAL:C	2.10	0.75
4:U:230:GLU:HB3	4:U:231:PRO:CD	2.14	0.74
2:L:3:VAL:H	2:L:26:SER:CB	2.00	0.74
1:A:22:ASN:HD22	1:A:24:TYR:H	1.36	0.74
1:A:23:LYS:NZ	4:U:166:HIS:HD2	1.86	0.74
4:U:229:HIS:CD2	4:U:230:GLU:H	2.06	0.74
1:A:99:HIS:CD2	1:A:101:TYR:H	2.06	0.73
4:U:153:CYS:O	4:U:170:CYS:HB3	1.87	0.73
4:U:4:MET:CE	4:U:75:LEU:HD22	2.18	0.73
2:L:194:GLU:HG3	2:L:205:VAL:HG22	1.69	0.73
3:H:56:ASN:HD22	12:U:402:PG4:C1	2.03	0.72
1:A:34:PRO:HG2	1:A:37:PHE:HD2	1.54	0.72
4:U:229:HIS:CG	4:U:230:GLU:H	2.07	0.72
4:U:59:THR:HG22	13:U:481:HOH:O	1.90	0.71
1:A:122:LEU:HD12	1:A:123:VAL:H	1.55	0.71
4:U:221:GLN:NE2	12:U:402:PG4:H32	2.03	0.71
4:U:206:SER:HB3	4:U:209:GLU:HG3	1.73	0.70
4:U:128:HIS:NE2	13:U:545:HOH:O	1.96	0.70
4:U:273:HIS:O	4:U:275:ASP:N	2.23	0.70
4:U:52:ASN:HD22	5:B:1:NAG:C1	2.00	0.69
3:H:12:VAL:HG21	3:H:82(C):LEU:HD12	1.73	0.69
4:U:3:CYS:HB3	4:U:77:ASN:HD22	1.56	0.69
4:U:30:ARG:C	4:U:31:LEU:HD12	2.17	0.69
3:H:132:THR:HG22	3:H:133:LEU:H	1.58	0.68
4:U:4:MET:HE3	4:U:75:LEU:HD22	1.76	0.68
12:U:402:PG4:H62	13:U:475:HOH:O	1.93	0.68
2:L:3:VAL:H	2:L:26:SER:HB3	1.59	0.67
1:A:54:ASN:HD22	1:A:56:HIS:HB2	1.58	0.67
1:A:108:ARG:O	1:A:110:ARG:N	2.28	0.66
2:L:1:ASP:HA	8:L:401:ETX:H12	1.78	0.66
4:U:22:ASP:OD1	4:U:48:SER:HB3	1.96	0.66
3:H:132:THR:O	3:H:133:LEU:CG	2.43	0.66
1:A:108:ARG:C	1:A:110:ARG:H	2.04	0.65
4:U:189:GLN:HE21	4:U:189:GLN:N	1.88	0.64
1:A:65:ASP:OD1	1:A:124:GLN:HB3	1.97	0.64
4:U:183:GLU:OE1	13:U:545:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:31:LEU:HD12	4:U:31:LEU:N	2.13	0.64
4:U:52:ASN:ND2	5:B:1:NAG:C2	2.60	0.64
4:U:102:ASP:OD1	4:U:104:SER:HB2	1.97	0.64
4:U:117:SER:HB2	4:U:120:GLU:HG3	1.78	0.64
6:C:1:NAG:H62	6:C:2:NAG:H82	1.77	0.63
4:U:56:SER:HB2	13:U:544:HOH:O	1.99	0.63
2:L:2:ILE:H	8:L:401:ETX:H12	1.62	0.63
3:H:187:THR:HG23	3:H:204:LYS:HG3	1.79	0.63
1:A:60:GLY:O	1:A:101:TYR:HB3	1.98	0.63
1:A:52:GLU:OE2	1:A:57:PHE:HB2	1.99	0.62
3:H:124:LEU:HB2	3:H:134:GLY:H	1.61	0.62
2:L:107:ARG:HG2	2:L:108:ALA:H	1.63	0.62
4:U:58:ARG:HB2	13:U:532:HOH:O	1.98	0.62
3:H:132:THR:O	3:H:133:LEU:HG	1.99	0.62
13:U:530:HOH:O	5:B:1:NAG:C8	2.30	0.62
1:A:22:ASN:ND2	1:A:24:TYR:H	1.96	0.62
4:U:232:LYS:CB	4:U:234:GLN:HE22	2.10	0.62
3:H:56:ASN:ND2	12:U:402:PG4:H11	2.11	0.61
3:H:142:PRO:HD2	3:H:196:ALA:CB	2.30	0.61
2:L:2:ILE:HG13	8:L:401:ETX:H21	1.82	0.61
2:L:49:PHE:HD1	2:L:50:GLU:HG3	1.66	0.61
4:U:215:CYS:HB3	4:U:219:MET:O	2.01	0.61
2:L:34:HIS:HD2	2:L:50:GLU:H	1.49	0.60
2:L:213:ALA:O	2:L:214:LYS:HG2	2.01	0.60
4:U:160:HIS:HE1	4:U:216:ARG:H	1.50	0.60
2:L:188:HIS:O	2:L:210:ARG:NH1	2.34	0.60
4:U:29:VAL:HG12	4:U:31:LEU:HD11	1.84	0.60
1:A:11:CYS:SG	1:A:19:CYS:HB2	2.42	0.59
2:L:94:PRO:HG2	8:L:401:ETX:H11	1.83	0.59
1:A:46:LYS:O	1:A:46:LYS:HG2	2.01	0.59
2:L:94:PRO:HG2	8:L:401:ETX:C1	2.33	0.59
4:U:274:PRO:O	4:U:275:ASP:O	2.20	0.59
2:L:34:HIS:CD2	2:L:50:GLU:H	2.21	0.59
3:H:58:GLU:OE2	4:U:192:ARG:NH1	2.36	0.59
3:H:132:THR:HG22	3:H:133:LEU:N	2.18	0.58
1:A:12:ASP:CG	13:A:523:HOH:O	2.46	0.58
4:U:246:MET:HE2	4:U:246:MET:HA	1.85	0.58
4:U:160:HIS:HD2	13:U:495:HOH:O	1.86	0.57
2:L:75:ILE:CD1	2:L:78:MET:HA	2.34	0.56
1:A:34:PRO:CG	1:A:37:PHE:HD2	2.17	0.56
1:A:100:ASN:H	1:A:100:ASN:HD22	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:121:SER:O	2:L:125:THR:HG23	2.05	0.56
4:U:172:ASN:OD1	6:C:1:NAG:O5	2.24	0.56
3:H:77:THR:OG1	8:H:403:ETX:H21	2.05	0.56
3:H:105:GLN:CD	3:H:105:GLN:H	2.13	0.56
6:C:1:NAG:C6	6:C:2:NAG:C8	2.73	0.56
2:L:5:THR:OG1	2:L:24:SER:HB3	2.05	0.56
2:L:3:VAL:H	2:L:26:SER:HB2	1.70	0.56
3:H:134:GLY:CA	3:H:174:SER:O	2.53	0.56
4:U:54:THR:HG22	4:U:55:LEU:N	2.21	0.56
4:U:275:ASP:HA	13:U:536:HOH:O	2.05	0.56
2:L:146:LYS:HE3	2:L:153:GLU:CD	2.31	0.55
3:H:134:GLY:HA2	3:H:174:SER:O	2.07	0.55
1:A:18:THR:HB	1:A:32:ASN:HB2	1.88	0.55
2:L:19:VAL:HB	2:L:75:ILE:HG22	1.89	0.55
2:L:107:ARG:NH1	2:L:108:ALA:O	2.39	0.55
3:H:130:MET:CE	3:H:179:PRO:N	2.70	0.55
4:U:143:HIS:NE2	13:U:545:HOH:O	1.87	0.55
3:H:52(A):HIS:HB3	12:U:402:PG4:H12	1.89	0.55
3:H:129:SER:O	3:H:179:PRO:HA	2.07	0.55
2:L:14:SER:O	2:L:17:GLN:HB3	2.06	0.55
4:U:140:ASP:N	13:U:502:HOH:O	2.39	0.55
4:U:1:LEU:HD22	4:U:2:ARG:N	2.21	0.55
4:U:100:SER:O	4:U:103:MET:HE2	2.06	0.54
4:U:59:THR:HG23	4:U:59:THR:O	2.06	0.54
1:A:122:LEU:HD12	1:A:123:VAL:N	2.23	0.54
3:H:142:PRO:HD2	3:H:196:ALA:HB1	1.90	0.54
4:U:129:TRP:O	4:U:163:ASP:O	2.24	0.54
1:A:94:LEU:HD23	1:A:105:PRO:HB3	1.88	0.54
4:U:105:CYS:HB3	4:U:181:ILE:HG21	1.89	0.54
4:U:153:CYS:O	4:U:155:GLY:N	2.40	0.54
2:L:69:THR:HG22	2:L:69:THR:O	2.07	0.54
2:L:93:TYR:HA	2:L:96:PHE:CZ	2.43	0.54
2:L:109:ASP:OD2	2:L:198:LYS:HD2	2.09	0.53
1:A:104:ASN:HD21	1:A:108:ARG:H	1.54	0.53
2:L:93:TYR:C	2:L:93:TYR:CD2	2.87	0.53
3:H:130:MET:HE3	3:H:179:PRO:HA	1.91	0.53
4:U:62:LYS:HG2	4:U:63:ILE:N	2.24	0.53
2:L:93:TYR:O	2:L:96:PHE:CD2	2.62	0.53
2:L:180:LEU:N	2:L:180:LEU:HD23	2.23	0.53
4:U:153:CYS:O	4:U:154:PRO:C	2.52	0.52
3:H:56:ASN:OD1	4:U:192:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:268:LYS:O	4:U:271:CYS:SG	2.67	0.52
4:U:150:LEU:HB3	4:U:151:PRO:HD2	1.92	0.52
4:U:177:ASN:H	4:U:177:ASN:HD22	1.58	0.52
1:A:109:ARG:HG3	1:A:109:ARG:HH11	1.75	0.51
4:U:200:ASN:ND2	11:U:400:NDG:C1	2.73	0.51
4:U:113:LEU:HD22	4:U:147:CYS:SG	2.50	0.51
4:U:173:THR:OG1	4:U:176:CYS:HB3	2.10	0.51
1:A:99:HIS:HE1	13:A:503:HOH:O	1.93	0.51
1:A:61:LYS:O	1:A:62:ALA:HB2	2.11	0.51
4:U:43:LYS:HB3	4:U:77:ASN:OD1	2.11	0.51
1:A:108:ARG:HH12	1:A:123:VAL:HG21	1.75	0.51
2:L:146:LYS:HG3	2:L:153:GLU:OE2	2.11	0.51
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.45	0.51
4:U:75:LEU:C	4:U:77:ASN:N	2.67	0.51
4:U:252:LEU:HB2	13:U:494:HOH:O	2.11	0.51
1:A:12:ASP:OD1	1:A:41:HIS:CD2	2.64	0.51
3:H:130:MET:CE	3:H:178:VAL:C	2.81	0.51
4:U:75:LEU:C	4:U:77:ASN:H	2.18	0.51
2:L:93:TYR:CD2	2:L:93:TYR:O	2.64	0.50
4:U:70:VAL:HG12	4:U:71:CYS:N	2.26	0.50
2:L:75:ILE:HD13	2:L:78:MET:HA	1.94	0.50
2:L:7:SER:HA	2:L:8:PRO:C	2.36	0.50
3:H:128:ASN:ND2	13:H:452:HOH:O	2.44	0.50
4:U:1:LEU:HD13	4:U:17:CYS:SG	2.52	0.50
1:A:28:ILE:HD13	4:U:29:VAL:HG23	1.92	0.50
4:U:157:ASN:OD1	4:U:166:HIS:HE1	1.95	0.49
4:U:222:CYS:HB3	4:U:272:ASN:HB2	1.94	0.49
4:U:31:LEU:N	4:U:31:LEU:CD1	2.76	0.49
3:H:143:GLU:OE2	3:H:144:PRO:HA	2.12	0.49
1:A:22:ASN:HD22	1:A:24:TYR:N	2.08	0.49
1:A:110:ARG:NH1	1:A:128:VAL:O	2.45	0.49
2:L:50:GLU:CD	13:H:408:HOH:O	2.55	0.49
8:L:407:ETX:H43	4:U:193:GLN:OE1	2.13	0.49
1:A:64:THR:HG23	1:A:127:MET:HB3	1.93	0.49
1:A:108:ARG:C	1:A:110:ARG:N	2.68	0.49
2:L:214:LYS:HD3	3:H:208:ALA:OXT	2.12	0.49
4:U:4:MET:HE2	4:U:75:LEU:HD22	1.94	0.49
2:L:140:PRO:O	2:L:197:HIS:HE1	1.95	0.49
3:H:50:TRP:CE2	3:H:58:GLU:HB2	2.47	0.49
4:U:52:ASN:CG	5:B:1:NAG:O1	2.56	0.49
4:U:183:GLU:CD	13:U:545:HOH:O	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:N	1:A:109:ARG:NE	2.61	0.49
2:L:180:LEU:HD23	2:L:180:LEU:H	1.78	0.49
4:U:225:ALA:O	4:U:237:MET:HA	2.13	0.49
4:U:128:HIS:O	4:U:129:TRP:C	2.56	0.48
4:U:270:GLY:C	4:U:272:ASN:H	2.21	0.48
4:U:153:CYS:HB3	4:U:154:PRO:HD3	1.95	0.48
1:A:85:HIS:O	1:A:88:ARG:HG2	2.14	0.48
2:L:73:LEU:C	2:L:73:LEU:HD23	2.38	0.48
3:H:134:GLY:O	3:H:135:CYS:HB2	2.12	0.48
4:U:113:LEU:C	4:U:113:LEU:HD23	2.39	0.48
2:L:214:LYS:HG3	2:L:215:ALA:O	2.13	0.48
3:H:12:VAL:HG21	3:H:82(C):LEU:HD13	1.90	0.48
2:L:18:LYS:HD3	2:L:76:SER:HA	1.96	0.48
1:A:117:VAL:HG23	1:A:117:VAL:O	2.14	0.48
1:A:64:THR:HG23	1:A:127:MET:CB	2.43	0.48
2:L:6:GLN:HG3	2:L:88:CYS:SG	2.54	0.47
3:H:172:LEU:HD23	3:H:172:LEU:C	2.38	0.47
4:U:24:CYS:HB3	4:U:77:ASN:ND2	2.28	0.47
3:H:99:TRP:CH2	10:H:406:PGE:H4	2.49	0.47
3:H:130:MET:HE2	3:H:178:VAL:O	2.13	0.47
4:U:29:VAL:HG12	4:U:31:LEU:CD1	2.44	0.47
4:U:200:ASN:HD22	4:U:203:HIS:HB2	1.78	0.47
4:U:127:THR:O	4:U:142:ARG:HA	2.13	0.47
1:A:28:ILE:HD13	4:U:29:VAL:CG2	2.44	0.47
3:H:83:THR:O	3:H:111:VAL:HG21	2.15	0.47
3:H:172:LEU:HD23	3:H:173:SER:N	2.30	0.47
3:H:187:THR:HG23	3:H:204:LYS:HE3	1.96	0.47
2:L:141:LYS:HB2	2:L:172:TYR:CE2	2.50	0.46
4:U:228:THR:HA	4:U:234:GLN:O	2.15	0.46
1:A:94:LEU:HD23	1:A:105:PRO:CB	2.45	0.46
2:L:66:GLY:HA3	2:L:71:TYR:HA	1.97	0.46
4:U:37:GLU:HG2	4:U:38:LEU:N	2.29	0.46
4:U:62:LYS:HG2	4:U:63:ILE:H	1.80	0.46
4:U:177:ASN:HD22	4:U:177:ASN:N	2.11	0.46
3:H:130:MET:CE	3:H:179:PRO:CA	2.93	0.46
4:U:70:VAL:CG1	4:U:71:CYS:N	2.79	0.46
2:L:69:THR:O	2:L:69:THR:CG2	2.64	0.46
4:U:229:HIS:CD2	4:U:230:GLU:N	2.79	0.46
2:L:75:ILE:HD11	2:L:78:MET:HA	1.98	0.46
4:U:74:ASP:OD1	4:U:75:LEU:HG	2.16	0.46
4:U:141:ASP:CB	4:U:144:LEU:HD13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HG2	1:A:62:ALA:N	2.31	0.46
1:A:73:PRO:C	1:A:75:ASN:H	2.24	0.46
8:H:403:ETX:H32	13:H:427:HOH:O	2.15	0.46
3:H:134:GLY:O	3:H:149:TRP:CZ2	2.66	0.45
1:A:72:LEU:HD21	1:A:116:GLN:HB2	1.99	0.45
3:H:100(A):PHE:N	3:H:100(A):PHE:CD1	2.85	0.45
1:A:130:ASP:C	1:A:132:ALA:H	2.24	0.45
2:L:206:LYS:HD2	13:L:433:HOH:O	2.16	0.45
4:U:128:HIS:ND1	4:U:142:ARG:NH1	2.65	0.45
1:A:23:LYS:HZ1	4:U:166:HIS:CD2	2.18	0.45
1:A:123:VAL:HG23	1:A:123:VAL:O	2.17	0.45
2:L:182:LYS:O	2:L:186:GLU:HG2	2.16	0.45
1:A:79:VAL:O	1:A:85:HIS:HB3	2.17	0.45
2:L:174:MET:HG2	2:L:175:SER:N	2.32	0.45
4:U:206:SER:HB3	4:U:209:GLU:OE2	2.17	0.45
2:L:75:ILE:HD11	2:L:82:ASP:OD2	2.17	0.44
4:U:96:ILE:HG13	4:U:178:GLU:HB3	1.99	0.44
1:A:109:ARG:HG3	1:A:109:ARG:NH1	2.32	0.44
4:U:29:VAL:HG13	4:U:66:LEU:HD23	1.99	0.44
4:U:229:HIS:CG	4:U:230:GLU:N	2.76	0.44
1:A:91:ALA:HB1	1:A:96:LEU:O	2.17	0.44
1:A:61:LYS:HA	1:A:101:TYR:CD1	2.53	0.44
2:L:49:PHE:CE1	2:L:53:LYS:HD2	2.53	0.44
4:U:113:LEU:HD23	4:U:114:GLN:N	2.32	0.44
2:L:180:LEU:N	2:L:180:LEU:CD2	2.81	0.44
3:H:132:THR:CG2	3:H:133:LEU:H	2.29	0.44
4:U:54:THR:CG2	4:U:55:LEU:N	2.80	0.44
1:A:65:ASP:HB3	1:A:69:ARG:HB3	2.00	0.44
4:U:43:LYS:O	4:U:44:SER:HB3	2.18	0.44
4:U:268:LYS:HB3	4:U:271:CYS:HB3	1.99	0.44
3:H:87:SER:HA	3:H:109:VAL:O	2.18	0.44
3:H:130:MET:HE3	3:H:179:PRO:CA	2.47	0.44
4:U:230:GLU:CB	4:U:231:PRO:HD2	2.25	0.44
2:L:89:GLN:HG2	2:L:90:GLN:O	2.17	0.43
4:U:3:CYS:HB3	4:U:77:ASN:ND2	2.30	0.43
4:U:177:ASN:H	4:U:177:ASN:ND2	2.16	0.43
1:A:40:GLN:HG3	4:U:40:LEU:HD21	2.01	0.43
1:A:100:ASN:C	1:A:100:ASN:ND2	2.76	0.43
8:L:401:ETX:H32	13:L:444:HOH:O	2.18	0.43
3:H:119:PRO:CB	3:H:140:TYR:HB3	2.42	0.43
1:A:128:VAL:O	1:A:128:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2:ILE:HG12	2:L:27:SER:HB2	2.00	0.43
2:L:90:GLN:HE21	2:L:97:THR:HB	1.83	0.43
4:U:116:ARG:HG3	4:U:116:ARG:HH11	1.82	0.43
2:L:123:GLN:O	2:L:126:SER:HB2	2.18	0.43
2:L:150:ASP:HA	2:L:190:SER:HB3	1.99	0.43
1:A:73:PRO:C	1:A:75:ASN:N	2.76	0.43
8:L:407:ETX:H43	4:U:193:GLN:CD	2.44	0.43
1:A:104:ASN:HB2	1:A:111:PRO:HA	2.00	0.43
3:H:148:THR:OG1	3:H:191:ASN:HB2	2.18	0.43
1:A:16:GLY:O	1:A:34:PRO:HD3	2.19	0.43
2:L:135:LEU:N	2:L:135:LEU:HD12	2.34	0.43
1:A:20:VAL:HG22	1:A:21:SER:N	2.34	0.42
2:L:181:THR:HA	13:L:473:HOH:O	2.19	0.42
2:L:188:HIS:CE1	13:L:522:HOH:O	2.72	0.42
3:H:30:THR:HB	3:H:52(A):HIS:CD2	2.54	0.42
3:H:62:LYS:HE3	3:H:62:LYS:HA	2.01	0.42
1:A:23:LYS:NZ	4:U:166:HIS:CD2	2.77	0.42
1:A:80:LEU:HD23	1:A:85:HIS:HB2	2.02	0.42
4:U:160:HIS:CE1	4:U:216:ARG:H	2.31	0.42
4:U:223:LEU:C	4:U:223:LEU:HD23	2.44	0.42
3:H:134:GLY:HA2	3:H:175:SER:HA	2.00	0.42
3:H:194:HIS:CE1	3:H:196:ALA:HB3	2.53	0.42
2:L:2:ILE:N	8:L:401:ETX:H12	2.33	0.42
4:U:200:ASN:HB2	4:U:203:HIS:H	1.85	0.42
2:L:135:LEU:CD2	2:L:195:ALA:HB2	2.50	0.42
4:U:206:SER:CB	4:U:209:GLU:OE2	2.67	0.42
2:L:1:ASP:N	13:L:513:HOH:O	2.51	0.42
2:L:189:ASN:OD1	2:L:211:ASN:ND2	2.53	0.42
4:U:208:GLU:OE1	4:U:208:GLU:N	2.53	0.42
4:U:270:GLY:C	4:U:272:ASN:N	2.78	0.42
3:H:130:MET:CE	3:H:179:PRO:HA	2.50	0.42
3:H:132:THR:C	3:H:133:LEU:HG	2.45	0.42
4:U:273:HIS:CE1	4:U:274:PRO:HD2	2.55	0.42
2:L:146:LYS:HE3	2:L:153:GLU:OE1	2.20	0.41
2:L:93:TYR:O	2:L:96:PHE:CE2	2.73	0.41
2:L:212:GLU:O	2:L:213:ALA:HB2	2.20	0.41
3:H:52:PHE:CE2	12:U:402:PG4:H42	2.55	0.41
2:L:209:ASN:ND2	13:L:475:HOH:O	2.52	0.41
4:U:221:GLN:NE2	12:U:402:PG4:H22	2.35	0.41
4:U:23:LEU:HD13	4:U:70:VAL:CG1	2.35	0.41
1:A:109:ARG:NE	1:A:109:ARG:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:HIS:HA	1:A:104:ASN:HB3	2.02	0.41
2:L:197:HIS:HD2	2:L:199:THR:OG1	2.04	0.41
3:H:20:ILE:HD11	3:H:80:MET:HE2	2.03	0.40
4:U:25:ARG:HD2	4:U:25:ARG:C	2.45	0.40
6:C:1:NAG:C7	6:C:1:NAG:O1	2.48	0.40
3:H:28:SER:HB3	3:H:31:ASN:HD22	1.87	0.40
4:U:122:CYS:HB2	4:U:176:CYS:SG	2.61	0.40
4:U:273:HIS:C	4:U:275:ASP:N	2.80	0.40
1:A:22:ASN:ND2	1:A:24:TYR:HB2	2.36	0.40
1:A:100:ASN:HD22	1:A:100:ASN:N	2.13	0.40
3:H:161:PHE:HA	3:H:162:PRO:HD3	1.94	0.40
2:L:141:LYS:HD2	2:L:172:TYR:CE1	2.57	0.40
4:U:172:ASN:OD1	4:U:172:ASN:N	2.50	0.40
4:U:200:ASN:ND2	11:U:400:NDG:O1	2.54	0.40
4:U:230:GLU:CB	4:U:231:PRO:CD	2.89	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	120/122 (98%)	98 (82%)	18 (15%)	4 (3%)	3	0
2	L	212/214 (99%)	204 (96%)	4 (2%)	4 (2%)	6	1
3	H	208/213 (98%)	199 (96%)	7 (3%)	2 (1%)	12	5
4	U	239/276 (87%)	215 (90%)	20 (8%)	4 (2%)	7	2
All	All	779/825 (94%)	716 (92%)	49 (6%)	14 (2%)	6	1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	62	ALA
1	A	109	ARG
2	L	93	TYR
4	U	230	GLU
2	L	213	ALA
4	U	154	PRO
4	U	162	ASN
1	A	68	GLY
2	L	68	GLY
2	L	214	LYS
3	H	135	CYS
4	U	231	PRO
3	H	144	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	106/106 (100%)	103 (97%)	3 (3%)	38	32
2	L	186/186 (100%)	181 (97%)	5 (3%)	39	34
3	H	182/182 (100%)	174 (96%)	8 (4%)	25	17
4	U	223/244 (91%)	212 (95%)	11 (5%)	22	14
All	All	697/718 (97%)	670 (96%)	27 (4%)	28	21

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

Mol	Chain	Res	Type
1	A	22	ASN
1	A	100	ASN
1	A	109	ARG
2	L	18	LYS
2	L	75	ILE
2	L	107	ARG
2	L	180	LEU
2	L	198	LYS

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Mol	Chain	Res	Type
3	H	2	VAL
3	H	3	LYS
3	H	62	LYS
3	H	130	MET
3	H	131	VAL
3	H	144	PRO
3	H	172	LEU
3	H	201	VAL
4	U	67	THR
4	U	93	LEU
4	U	140	ASP
4	U	144	LEU
4	U	153	CYS
4	U	168	LEU
4	U	177	ASN
4	U	189	GLN
4	U	212	LEU
4	U	246	MET
4	U	272	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	22	ASN
1	A	32	ASN
1	A	40	GLN
1	A	82	GLN
1	A	85	HIS
1	A	93	GLN
1	A	99	HIS
1	A	100	ASN
2	L	34	HIS
2	L	90	GLN
2	L	197	HIS
2	L	209	ASN
2	L	211	ASN
3	H	31	ASN
3	H	52(A)	HIS
3	H	128	ASN
3	H	159	HIS
3	H	166	GLN

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Mol	Chain	Res	Type
4	U	21	GLN
4	U	78	GLN
4	U	121	GLN
4	U	160	HIS
4	U	166	HIS
4	U	172	ASN
4	U	177	ASN
4	U	189	GLN
4	U	193	GLN
4	U	200	ASN
4	U	203	HIS
4	U	221	GLN
4	U	229	HIS
4	U	248	GLN
4	U	260	HIS
4	U	272	ASN

### 5.3.3 RNA [i](#)

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](#)

4 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	B	1	5,4	15,15,15	0.46	0	21,21,21	0.80	1 (4%)
5	FUC	B	2	5	11,11,11	0.39	0	16,16,16	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	C	1	4,6	15,15,15	0.42	0	21,21,21	0.61	0
6	NAG	C	2	6	15,15,15	0.46	0	21,21,21	0.55	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1	5,4	1/1/6/7	5/6/26/26	0/1/1/1
5	FUC	B	2	5	1/1/5/5	-	0/1/1/1
6	NAG	C	1	4,6	-	5/6/26/26	0/1/1/1
6	NAG	C	2	6	1/1/6/7	4/6/26/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	NAG	O5-C1-C2	2.06	111.58	109.52

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1	NAG	C1
5	B	2	FUC	C1
6	C	2	NAG	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1	NAG	C8-C7-N2-C2
5	B	1	NAG	O7-C7-N2-C2
6	C	1	NAG	C1-C2-N2-C7
6	C	1	NAG	C8-C7-N2-C2
6	C	1	NAG	O7-C7-N2-C2
6	C	2	NAG	C8-C7-N2-C2
6	C	2	NAG	O7-C7-N2-C2
6	C	1	NAG	O5-C5-C6-O6
6	C	1	NAG	C4-C5-C6-O6
5	B	1	NAG	O5-C5-C6-O6
5	B	1	NAG	C4-C5-C6-O6

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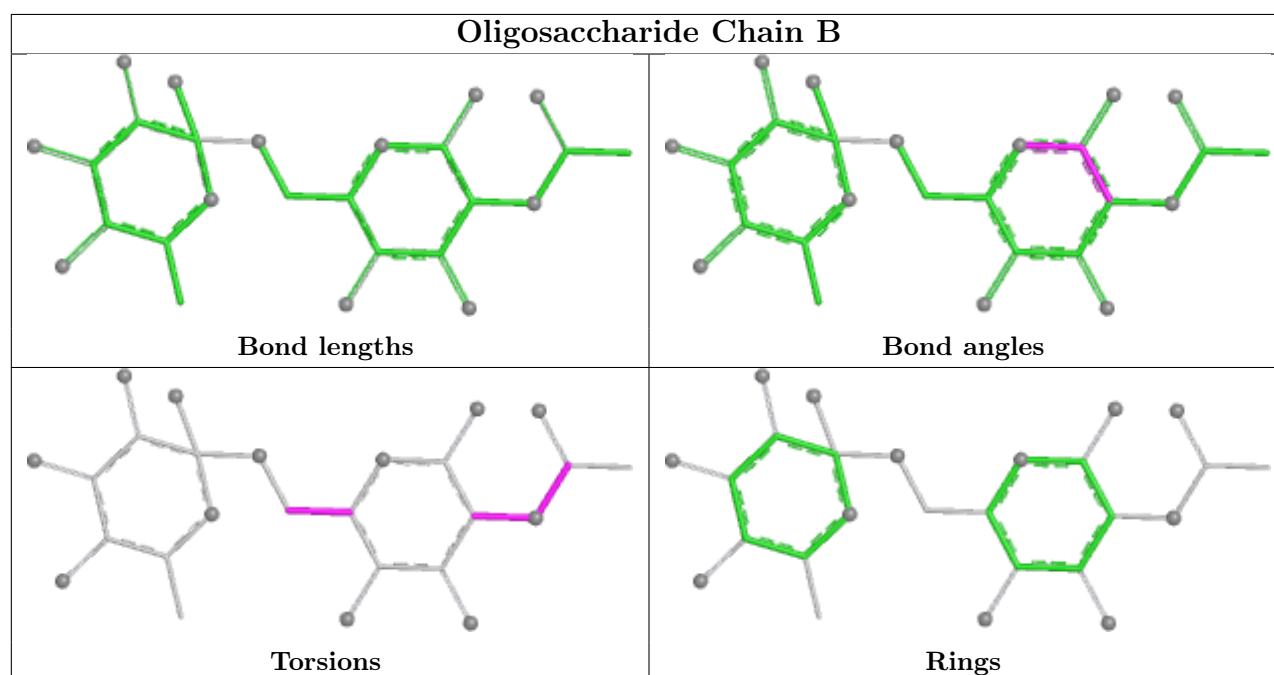
Mol	Chain	Res	Type	Atoms
6	C	2	NAG	O5-C5-C6-O6
6	C	2	NAG	C4-C5-C6-O6
5	B	1	NAG	C1-C2-N2-C7

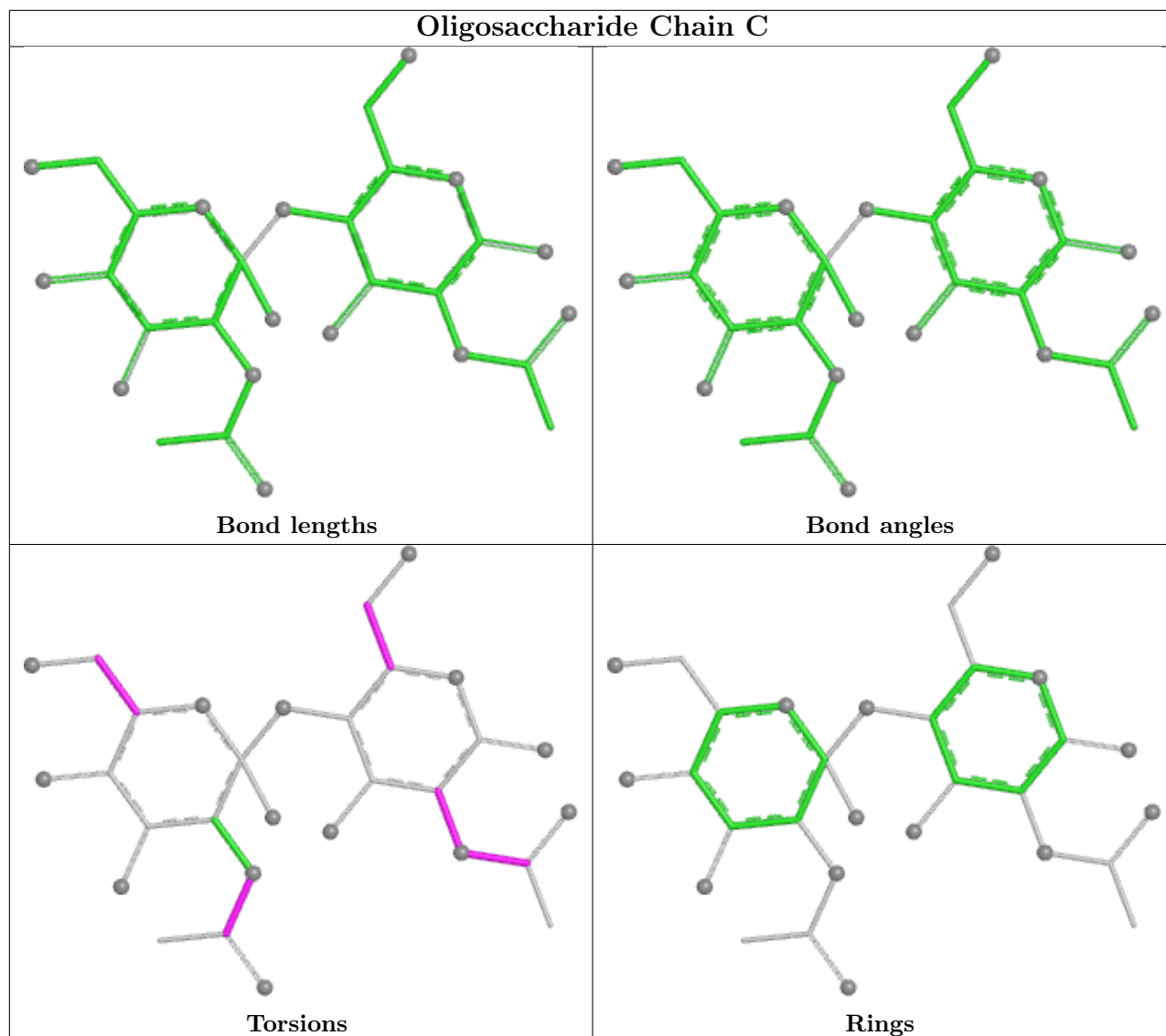
There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2	NAG	5	0
6	C	1	NAG	9	0
5	B	1	NAG	6	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](#)

9 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$
10	PGE	H	406	-	9,9,9	1.17	1 (11%)	8,8,8	1.90	2 (25%)
8	ETX	L	407	-	5,5,5	1.16	0	4,4,4	2.54	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	ETX	H	403	-	5,5,5	1.16	0	4,4,4	2.61	1 (25%)
9	EDO	L	405	-	3,3,3	0.53	0	2,2,2	0.52	0
9	EDO	H	404	-	3,3,3	0.45	0	2,2,2	0.45	0
8	ETX	L	401	-	5,5,5	1.21	0	4,4,4	2.61	1 (25%)
12	PG4	U	402	-	12,12,12	1.12	1 (8%)	11,11,11	0.81	0
7	SO4	A	501	-	4,4,4	0.31	0	6,6,6	0.12	0
11	NDG	U	400	-	15,15,15	0.43	0	21,21,21	0.64	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
10	PGE	H	406	-	-	4/7/7/7	-
8	ETX	H	403	-	-	1/3/3/3	-
9	EDO	L	405	-	-	1/1/1/1	-
9	EDO	H	404	-	-	1/1/1/1	-
8	ETX	L	401	-	-	2/3/3/3	-
12	PG4	U	402	-	-	7/10/10/10	-
8	ETX	L	407	-	-	1/3/3/3	-
11	NDG	U	400	-	-	5/6/26/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	402	PG4	O2-C3	2.20	1.51	1.42
10	H	406	PGE	C4-C3	2.08	1.59	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	403	ETX	C3-O2-C2	4.90	130.26	113.06
8	L	401	ETX	C3-O2-C2	4.83	130.01	113.06
8	L	407	ETX	C3-O2-C2	4.81	129.94	113.06
10	H	406	PGE	C5-O3-C4	3.95	130.56	113.26
10	H	406	PGE	O2-C2-C1	2.68	121.92	110.11

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	U	400	NDG	C1-C2-N2-C7
11	U	400	NDG	C8-C7-N2-C2
11	U	400	NDG	O7-C7-N2-C2
10	H	406	PGE	O1-C1-C2-O2
11	U	400	NDG	O5-C5-C6-O6
12	U	402	PG4	O2-C3-C4-O3
11	U	400	NDG	C4-C5-C6-O6
8	L	401	ETX	C4-C3-O2-C2
8	L	401	ETX	O1-C1-C2-O2
12	U	402	PG4	O4-C7-C8-O5
12	U	402	PG4	O3-C5-C6-O4
9	L	405	EDO	O1-C1-C2-O2
12	U	402	PG4	C1-C2-O2-C3
12	U	402	PG4	C3-C4-O3-C5
12	U	402	PG4	C8-C7-O4-C6
12	U	402	PG4	C6-C5-O3-C4
10	H	406	PGE	C6-C5-O3-C4
10	H	406	PGE	C3-C4-O3-C5
8	L	407	ETX	C1-C2-O2-C3
9	H	404	EDO	O1-C1-C2-O2
8	H	403	ETX	C4-C3-O2-C2
10	H	406	PGE	O2-C3-C4-O3

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	406	PGE	1	0
8	L	407	ETX	2	0
8	H	403	ETX	3	0
8	L	401	ETX	7	0
12	U	402	PG4	11	0
11	U	400	NDG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	134:GLY	C	135:CYS	N	1.14

## 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	122/122 (100%)	2.43	71 (58%) 0 0	33, 56, 82, 86	0
2	L	214/214 (100%)	0.88	30 (14%) 6 6	21, 33, 54, 91	0
3	H	212/213 (99%)	0.71	21 (9%) 13 13	17, 33, 52, 64	0
4	U	249/276 (90%)	1.49	72 (28%) 1 1	22, 43, 70, 99	0
All	All	797/825 (96%)	1.26	194 (24%) 2 1	17, 39, 72, 99	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	134	GLY	7.8
1	A	53	GLY	7.7
3	H	128	ASN	7.1
2	L	215	ALA	6.4
4	U	129	TRP	6.3
2	L	213	ALA	6.3
1	A	62	ALA	6.0
1	A	122	LEU	5.8
4	U	153	CYS	5.8
1	A	63	SER	5.4
1	A	64	THR	5.2
1	A	36	LYS	5.2
4	U	32	TRP	5.1
1	A	52	GLU	5.0
4	U	252	LEU	4.9
4	U	231	PRO	4.9
1	A	35	LYS	4.9
3	H	208	ALA	4.9
3	H	131	VAL	4.8
2	L	1	ASP	4.7
4	U	92	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
3	H	132	THR	4.6
3	H	133	LEU	4.5
3	H	130	MET	4.5
1	A	60	GLY	4.4
2	L	3	VAL	4.3
1	A	117	VAL	4.2
1	A	119	LEU	4.2
1	A	126	CYS	4.2
1	A	66	THR	4.2
3	H	129	SER	4.2
4	U	229	HIS	4.1
1	A	128	VAL	4.1
1	A	49	THR	4.1
1	A	110	ARG	4.1
4	U	154	PRO	4.1
1	A	16	GLY	4.0
1	A	123	VAL	4.0
2	L	27	SER	3.9
4	U	233	ASN	3.7
1	A	33	CYS	3.7
1	A	68	GLY	3.7
1	A	131	CYS	3.7
1	A	51	TYR	3.6
2	L	68	GLY	3.6
1	A	65	ASP	3.6
1	A	109	ARG	3.6
2	L	214	LYS	3.6
4	U	230	GLU	3.6
1	A	120	LYS	3.6
1	A	12	ASP	3.5
4	U	116	ARG	3.5
4	U	77	ASN	3.5
4	U	200	ASN	3.5
1	A	37	PHE	3.5
4	U	260	HIS	3.5
4	U	47	HIS	3.4
4	U	63	ILE	3.4
1	A	61	LYS	3.4
4	U	235	SER	3.4
1	A	121	PRO	3.4
3	H	196	ALA	3.4
4	U	18	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	26	SER	3.3
2	L	69	THR	3.3
1	A	127	MET	3.3
2	L	93	TYR	3.3
4	U	38	LEU	3.2
4	U	61	LEU	3.2
1	A	14	LEU	3.2
4	U	113	LEU	3.2
1	A	42	CYS	3.2
4	U	232	LYS	3.2
4	U	275	ASP	3.2
1	A	116	GLN	3.1
1	A	118	GLY	3.1
1	A	59	ARG	3.1
1	A	129	HIS	3.1
1	A	50	CYS	3.0
4	U	19	LEU	3.0
1	A	11	CYS	3.0
1	A	111	PRO	2.9
4	U	140	ASP	2.9
4	U	248	GLN	2.9
4	U	22	ASP	2.9
4	U	149	TYR	2.9
1	A	107	ASN	2.9
4	U	93	LEU	2.9
2	L	75	ILE	2.8
4	U	104	SER	2.8
1	A	55	GLY	2.8
1	A	94	LEU	2.8
1	A	108	ARG	2.8
1	A	70	PRO	2.8
1	A	54	ASN	2.8
4	U	272	ASN	2.8
2	L	155	GLN	2.8
1	A	17	GLY	2.8
2	L	2	ILE	2.8
1	A	57	PHE	2.7
1	A	18	THR	2.7
2	L	29	SER	2.7
4	U	13	ARG	2.7
1	A	67	MET	2.7
4	U	59	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	23	CYS	2.7
4	U	1(A)	SER	2.7
4	U	261	ILE	2.7
1	A	71	CYS	2.6
1	A	34	PRO	2.6
4	U	66	LEU	2.6
4	U	205	CYS	2.6
1	A	72	LEU	2.6
1	A	48	LYS	2.6
4	U	172	ASN	2.6
1	A	44	ILE	2.6
3	H	1	GLY	2.6
2	L	25	ALA	2.6
4	U	125	VAL	2.6
1	A	32	ASN	2.6
2	L	94	PRO	2.5
3	H	153	SER	2.5
4	U	204	GLY	2.5
2	L	21	ILE	2.5
4	U	70	VAL	2.5
4	U	114	GLN	2.5
4	U	164	THR	2.5
4	U	234	GLN	2.5
4	U	152	GLY	2.5
1	A	15	ASN	2.5
1	A	132	ALA	2.5
3	H	74	SER	2.4
3	H	198	SER	2.4
1	A	69	ARG	2.4
4	U	206	SER	2.4
4	U	73	LEU	2.4
1	A	101	TYR	2.4
4	U	256	PHE	2.4
2	L	125	THR	2.4
4	U	255	ALA	2.4
3	H	105	GLN	2.4
4	U	118	PRO	2.4
1	A	106	ASP	2.3
3	H	154	LEU	2.3
2	L	5	THR	2.3
3	H	146	THR	2.3
4	U	226	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	115	VAL	2.3
2	L	24	SER	2.3
2	L	126	SER	2.3
1	A	102	CYS	2.3
4	U	31	LEU	2.3
2	L	201	THR	2.3
2	L	66	GLY	2.3
1	A	47	SER	2.3
4	U	264	SER	2.3
4	U	12	CYS	2.3
4	U	170	CYS	2.3
4	U	103	MET	2.3
3	H	2	VAL	2.3
4	U	69	VAL	2.3
4	U	128	HIS	2.3
2	L	67	SER	2.2
1	A	27	ASN	2.2
4	U	23	LEU	2.2
4	U	117	SER	2.2
2	L	30	VAL	2.2
3	H	85	GLU	2.2
3	H	155	SER	2.2
1	A	24	TYR	2.2
2	L	71	TYR	2.2
2	L	212	GLU	2.2
4	U	37	GLU	2.2
4	U	6	CYS	2.2
4	U	162	ASN	2.1
4	U	236	TYR	2.1
4	U	101	SER	2.1
4	U	108	GLY	2.1
3	H	207	ALA	2.1
4	U	112	SER	2.1
3	H	12	VAL	2.1
2	L	18	LYS	2.1
4	U	225	ALA	2.1
1	A	46	LYS	2.1
2	L	11	THR	2.1
4	U	60	GLY	2.1
1	A	124	GLN	2.1
1	A	96	LEU	2.1
1	A	113	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	U	259	ASN	2.0
1	A	19	CYS	2.0
4	U	1	LEU	2.0
4	U	106	GLU	2.0
1	A	20	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](#)

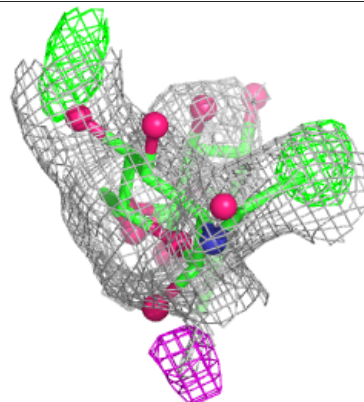
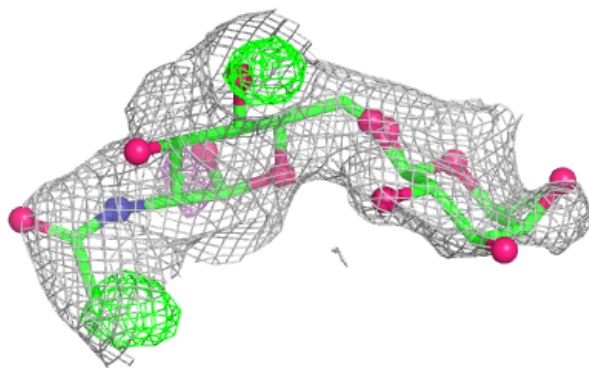
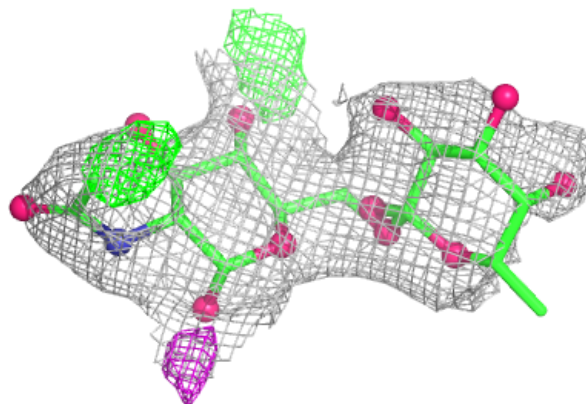
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

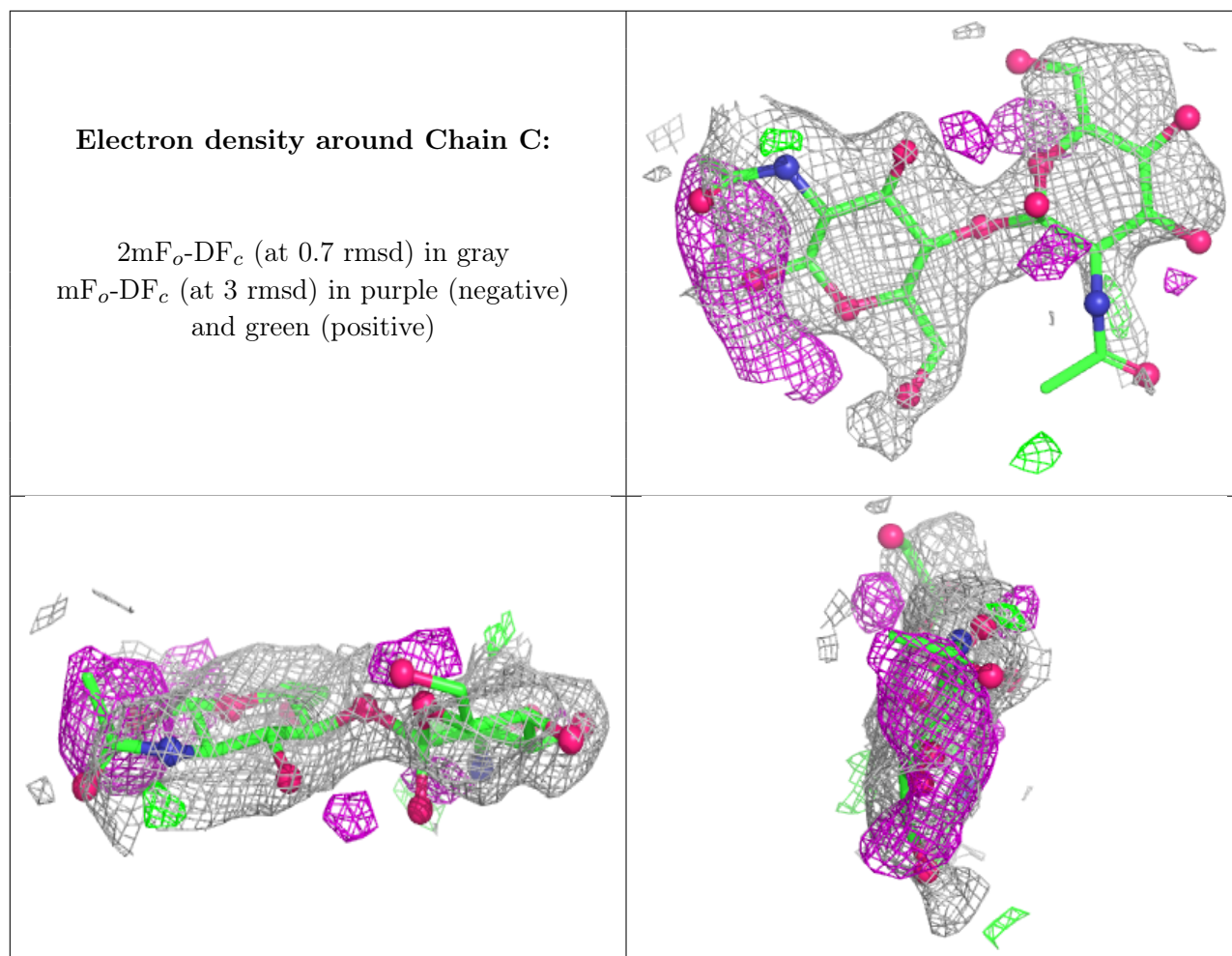
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	1	15/15	-	-	78,81,84,86	0
5	FUC	B	2	11/11	-	-	98,99,101,102	0
6	NAG	C	1	15/15	-	-	71,76,79,80	0
6	NAG	C	2	15/15	-	-	98,102,104,105	0

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 B:**

$2mF_o-DF_c$  (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
8	ETX	L	401	6/6	0.59	0.30	41,48,52,61	0
8	ETX	L	407	6/6	0.60	0.28	52,56,59,59	0
8	ETX	H	403	6/6	0.62	0.28	43,48,49,52	0
11	NDG	U	400	15/15	0.62	0.20	71,81,83,85	0
12	PG4	U	402	13/13	0.74	0.23	44,48,54,58	0
10	PGE	H	406	10/10	0.76	0.24	38,61,63,64	0
9	EDO	H	404	4/4	0.84	0.21	42,46,50,53	0
9	EDO	L	405	4/4	0.84	0.14	47,49,49,50	0
7	SO4	A	501	5/5	0.93	0.12	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.