



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 09:08 AM EDT

PDB ID : 6JLA  
Title : Crystal structure of a mouse ependymin related protein  
Authors : Park, S.  
Deposited on : 2019-03-04  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

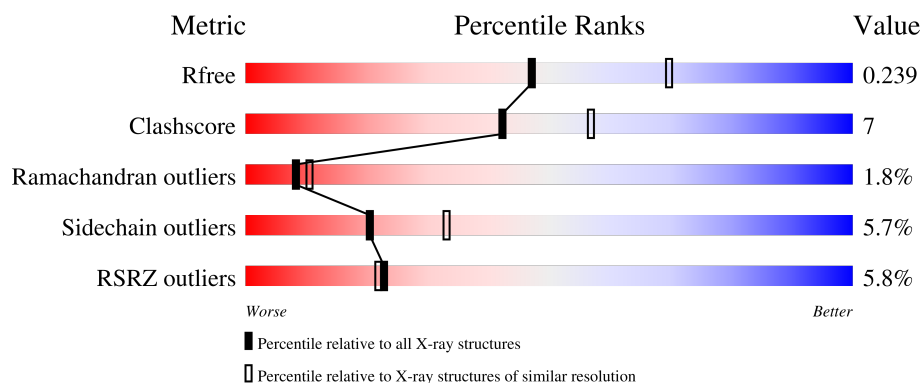
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	198	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>• • 7%</div> </div> </div>
1	B	198	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>• • 8%</div> </div> </div>
1	C	198	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>• 7%</div> </div> </div>
1	D	198	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 5%</div> </div> </div>
2	E	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6201 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 Mammalian ependymin-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1493	944	256	284	9			
1	B	182	Total	C	N	O	S	0	1	0
			1486	941	254	283	8			
1	D	188	Total	C	N	O	S	0	0	0
			1526	963	264	290	9			
1	C	184	Total	C	N	O	S	0	0	0
			1493	944	256	284	9			

There are 44 discrepancies between the modelled and reference sequences:

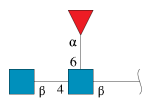
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP Q99M71
A	28	ASP	-	expression tag	UNP Q99M71
A	29	PRO	-	expression tag	UNP Q99M71
A	30	HIS	-	expression tag	UNP Q99M71
A	31	HIS	-	expression tag	UNP Q99M71
A	32	HIS	-	expression tag	UNP Q99M71
A	33	HIS	-	expression tag	UNP Q99M71
A	34	HIS	-	expression tag	UNP Q99M71
A	35	HIS	-	expression tag	UNP Q99M71
A	36	HIS	-	expression tag	UNP Q99M71
A	37	HIS	-	expression tag	UNP Q99M71
B	27	ALA	-	expression tag	UNP Q99M71
B	28	ASP	-	expression tag	UNP Q99M71
B	29	PRO	-	expression tag	UNP Q99M71
B	30	HIS	-	expression tag	UNP Q99M71
B	31	HIS	-	expression tag	UNP Q99M71
B	32	HIS	-	expression tag	UNP Q99M71
B	33	HIS	-	expression tag	UNP Q99M71
B	34	HIS	-	expression tag	UNP Q99M71
B	35	HIS	-	expression tag	UNP Q99M71
B	36	HIS	-	expression tag	UNP Q99M71

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Chain	Residue	Modelled	Actual	Comment	Reference
B	37	HIS	-	expression tag	UNP Q99M71
D	27	ALA	-	expression tag	UNP Q99M71
D	28	ASP	-	expression tag	UNP Q99M71
D	29	PRO	-	expression tag	UNP Q99M71
D	30	HIS	-	expression tag	UNP Q99M71
D	31	HIS	-	expression tag	UNP Q99M71
D	32	HIS	-	expression tag	UNP Q99M71
D	33	HIS	-	expression tag	UNP Q99M71
D	34	HIS	-	expression tag	UNP Q99M71
D	35	HIS	-	expression tag	UNP Q99M71
D	36	HIS	-	expression tag	UNP Q99M71
D	37	HIS	-	expression tag	UNP Q99M71
C	27	ALA	-	expression tag	UNP Q99M71
C	28	ASP	-	expression tag	UNP Q99M71
C	29	PRO	-	expression tag	UNP Q99M71
C	30	HIS	-	expression tag	UNP Q99M71
C	31	HIS	-	expression tag	UNP Q99M71
C	32	HIS	-	expression tag	UNP Q99M71
C	33	HIS	-	expression tag	UNP Q99M71
C	34	HIS	-	expression tag	UNP Q99M71
C	35	HIS	-	expression tag	UNP Q99M71
C	36	HIS	-	expression tag	UNP Q99M71
C	37	HIS	-	expression tag	UNP Q99M71

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		


- Molecule 4 is water.

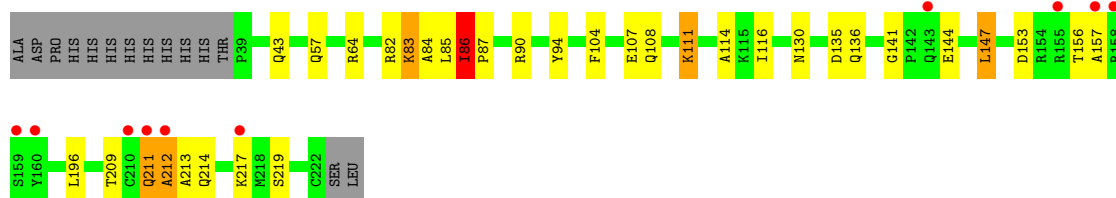
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	30	Total	O	0	0
			30	30		
4	D	14	Total	O	0	0
			14	14		
4	C	50	Total	O	0	0
			50	50		

### 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.

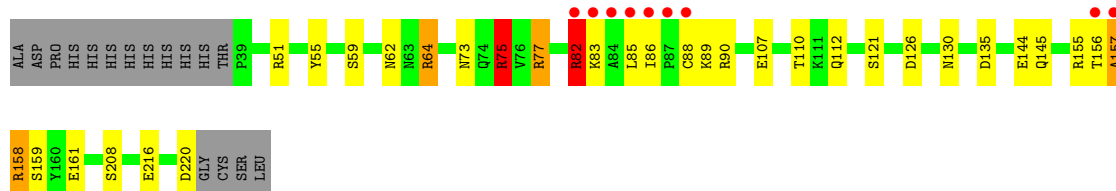
- Molecule 1: Mammalian endymin-related protein 1

Chain A: 




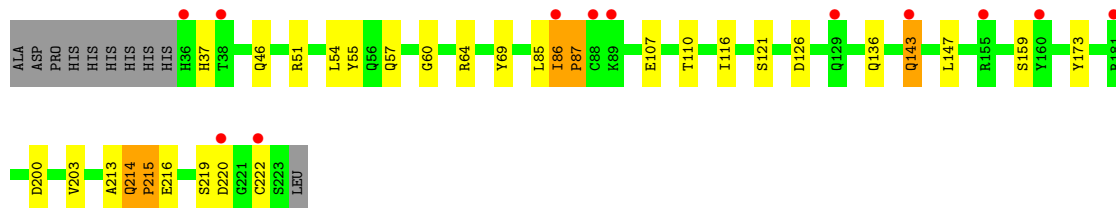
- Molecule 1: Mammalian endymin-related protein 1

Chain B: 




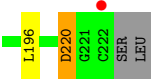
- Molecule 1: Mammalian endymin-related protein 1

Chain D: 

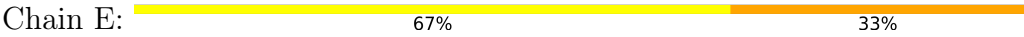


- Molecule 1: Mammalian endymin-related protein 1

Chain C: 



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.97Å 59.67Å 137.34Å 90.00° 101.29° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 37.57 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.40) 99.7 (37.57-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.15 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.185 , 0.240 0.192 , 0.239	Depositor DCC
$R_{free}$ test set	1787 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6201	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.79	0/1530	0.89	1/2078 (0.0%)
1	B	0.86	0/1526	1.03	7/2073 (0.3%)
1	C	0.90	0/1530	0.94	2/2078 (0.1%)
1	D	0.73	0/1565	0.86	3/2127 (0.1%)
All	All	0.82	0/6151	0.93	13/8356 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	B	75	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	B	51	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	C	51	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	D	51	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	C	51	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	64	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	51	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	77	ARG	NE-CZ-NH2	-6.12	117.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	64	ARG	CG-CD-NE	-5.37	100.53	111.80
1	B	82	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	135	ASP	CB-CG-OD2	-5.05	113.75	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	ILE	Peptide
1	B	158	ARG	Peptide
1	C	89	LYS	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1493	0	1441	30	0
1	B	1486	0	1439	23	0
1	C	1493	0	1445	22	0
1	D	1526	0	1465	18	0
2	E	38	0	34	1	0
3	A	14	0	13	6	0
3	B	14	0	13	4	0
3	D	28	0	26	1	0
4	A	15	0	0	0	0
4	B	30	0	0	0	0
4	C	50	0	0	1	0
4	D	14	0	0	0	0
All	All	6201	0	5876	81	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 (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLU:HG2	1:B:110:THR:HG22	1.38	1.02
1:B:135:ASP:OD2	1:C:64:ARG:NH2	2.07	0.86
1:A:130:ASN:ND2	3:A:300:NAG:O5	2.14	0.79
1:A:111:LYS:O	1:A:209:THR:HG21	1.83	0.78
1:A:86:ILE:HG22	1:A:87:PRO:CD	2.17	0.75
1:A:141:GLY:HA3	1:D:173:TYR:CE2	2.23	0.73
1:A:86:ILE:HG22	1:A:87:PRO:HD2	1.71	0.73
1:B:107:GLU:HG2	1:B:110:THR:CG2	2.18	0.71
1:B:130:ASN:CB	3:B:301:NAG:O5	2.39	0.70
1:B:107:GLU:CG	1:B:110:THR:HG22	2.17	0.70
1:A:153:ASP:OD1	3:A:300:NAG:C8	2.40	0.69
1:B:89:LYS:HG2	1:B:220:ASP:HB3	1.77	0.65
1:B:156:THR:HG23	1:C:85:LEU:HG	1.80	0.64
1:B:64:ARG:HH22	1:C:150:GLU:CD	2.00	0.63
1:D:107:GLU:CG	1:D:110:THR:OG1	2.47	0.62
1:A:43:GLN:CD	1:B:158:ARG:HB3	2.20	0.62
1:A:153:ASP:OD1	3:A:300:NAG:H82	1.99	0.62
1:B:130:ASN:HB3	3:B:301:NAG:O6	2.00	0.61
1:C:110:THR:HB	1:C:112:GLN:H	1.65	0.61
1:C:130:ASN:HD22	1:C:130:ASN:H	1.48	0.60
1:D:54:LEU:C	1:D:54:LEU:HD23	2.22	0.60
3:A:300:NAG:H83	3:A:300:NAG:O3	2.03	0.59
1:A:64:ARG:NE	1:A:83:LYS:HG2	2.17	0.59
1:A:153:ASP:OD1	3:A:300:NAG:H81	2.03	0.58
1:A:86:ILE:CG2	1:A:87:PRO:HD2	2.33	0.58
1:D:107:GLU:HG2	1:D:110:THR:OG1	2.04	0.58
1:B:73:ASN:HB2	1:B:75:ARG:HD2	1.87	0.55
1:D:107:GLU:HG3	1:D:110:THR:OG1	2.07	0.54
1:B:144:GLU:HG2	1:C:146:ILE:HG22	1.90	0.54
1:A:211:GLN:HE21	1:A:211:GLN:HA	1.71	0.54
1:A:212:ALA:O	1:A:214:GLN:N	2.41	0.53
1:A:64:ARG:HE	1:A:83:LYS:HG2	1.73	0.53
1:D:200:ASP:O	1:D:203:VAL:HG22	2.08	0.52
1:A:86:ILE:HA	1:D:159:SER:CB	2.39	0.51
1:D:136:GLN:NE2	1:D:147:LEU:HD21	2.25	0.51
1:B:156:THR:HG23	1:C:85:LEU:CG	2.42	0.50
1:B:64:ARG:NH2	1:C:150:GLU:OE2	2.40	0.50
1:D:46:GLN:NE2	1:D:69:TYR:OH	2.40	0.50
1:B:130:ASN:HB3	3:B:301:NAG:O5	2.10	0.49
1:C:156:THR:O	1:C:159:SER:OG	2.31	0.49
1:A:141:GLY:CA	1:D:173:TYR:CE2	2.95	0.48
1:C:90:ARG:HG3	1:C:90:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:GLN:OE1	1:D:143:GLN:N	2.47	0.48
1:A:57:GLN:NE2	1:D:55:TYR:OH	2.48	0.47
3:A:300:NAG:H83	3:A:300:NAG:C3	2.44	0.47
1:A:156:THR:O	1:A:157:ALA:HB3	2.15	0.47
1:B:90:ARG:HB3	1:B:107:GLU:OE1	2.15	0.47
1:C:43:GLN:CD	1:C:43:GLN:H	2.18	0.46
1:C:156:THR:O	1:C:156:THR:HG22	2.16	0.46
1:A:114:ALA:HB1	1:A:116:ILE:HD11	1.98	0.46
1:A:196:LEU:O	2:E:1:NAG:O7	2.33	0.46
1:A:141:GLY:HA3	1:D:173:TYR:CZ	2.50	0.46
1:C:130:ASN:HD22	1:C:130:ASN:N	2.09	0.45
1:A:86:ILE:CG2	1:A:87:PRO:CD	2.93	0.45
1:B:126:ASP:OD1	1:B:126:ASP:C	2.55	0.45
1:B:55:TYR:HB2	1:B:62:ASN:OD1	2.17	0.45
1:A:82:ARG:HG3	1:A:84:ALA:O	2.17	0.44
1:A:64:ARG:HE	1:A:83:LYS:CG	2.29	0.44
1:B:110:THR:OG1	1:B:112:GLN:HG3	2.18	0.44
1:C:45:PRO:HB3	1:C:196:LEU:HD11	1.99	0.43
1:C:64:ARG:HD2	4:C:303:HOH:O	2.18	0.43
1:B:159:SER:OG	1:C:87:PRO:HD3	2.18	0.43
1:D:214:GLN:HB2	1:D:215:PRO:CD	2.48	0.43
1:D:86:ILE:HG13	1:D:87:PRO:CD	2.48	0.43
1:A:90:ARG:NH1	1:A:219:SER:O	2.51	0.43
1:A:136:GLN:CG	1:A:147:LEU:HD21	2.49	0.42
1:B:157:ALA:N	1:B:159:SER:HB3	2.33	0.42
1:A:107:GLU:HG3	1:A:108:GLN:N	2.35	0.42
1:C:55:TYR:HB2	1:C:62:ASN:OD1	2.20	0.42
1:A:116:ILE:HG21	1:A:217:LYS:HE3	2.01	0.42
1:A:57:GLN:HE22	1:D:60:GLY:HA2	1.85	0.41
1:A:94:TYR:HA	1:A:104:PHE:O	2.19	0.41
1:B:130:ASN:CB	3:B:301:NAG:O6	2.67	0.41
1:B:135:ASP:OD2	1:C:51:ARG:NH2	2.51	0.41
1:C:196:LEU:HD12	1:C:196:LEU:HA	1.89	0.41
1:C:55:TYR:CD2	1:C:55:TYR:C	2.94	0.41
1:C:86:ILE:HG22	1:C:87:PRO:HD2	2.02	0.41
3:D:301:NAG:O3	3:D:301:NAG:H82	2.20	0.41
1:D:116:ILE:HD12	1:D:116:ILE:N	2.35	0.41
1:C:82:ARG:O	1:C:83:LYS:C	2.59	0.40
1:D:126:ASP:OD1	1:D:126:ASP:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	182/198 (92%)	170 (93%)	9 (5%)	3 (2%)	9	13
1	B	181/198 (91%)	172 (95%)	6 (3%)	3 (2%)	9	11
1	C	182/198 (92%)	166 (91%)	13 (7%)	3 (2%)	9	13
1	D	186/198 (94%)	172 (92%)	10 (5%)	4 (2%)	6	7
All	All	731/792 (92%)	680 (93%)	38 (5%)	13 (2%)	8	10

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ILE
1	B	157	ALA
1	D	213	ALA
1	C	157	ALA
1	A	213	ALA
1	B	82	ARG
1	A	212	ALA
1	D	215	PRO
1	C	220	ASP
1	B	83	LYS
1	D	214	GLN
1	C	84	ALA
1	D	87	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/179 (93%)	159 (96%)	7 (4%)	30	47
1	B	166/179 (93%)	152 (92%)	14 (8%)	11	16
1	C	166/179 (93%)	158 (95%)	8 (5%)	25	41
1	D	170/179 (95%)	160 (94%)	10 (6%)	19	32
All	All	668/716 (93%)	629 (94%)	39 (6%)	20	32

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	85	LEU
1	A	86	ILE
1	A	111	LYS
1	A	144	GLU
1	A	147	LEU
1	A	211	GLN
1	B	59[A]	SER
1	B	59[B]	SER
1	B	75	ARG
1	B	77	ARG
1	B	82	ARG
1	B	85	LEU
1	B	86	ILE
1	B	88	CYS
1	B	121	SER
1	B	145	GLN
1	B	155	ARG
1	B	161	GLU
1	B	208	SER
1	B	216	GLU
1	D	37	HIS
1	D	57	GLN
1	D	85	LEU
1	D	86	ILE
1	D	121	SER
1	D	143	GLN
1	D	216	GLU
1	D	219	SER
1	D	220	ASP
1	D	222	CYS
1	C	43	GLN
1	C	82	ARG

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Mol	Chain	Res	Type
1	C	110	THR
1	C	130	ASN
1	C	155	ARG
1	C	158	ARG
1	C	160	TYR
1	C	220	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	57	GLN
1	A	62	ASN
1	A	108	GLN
1	A	211	GLN
1	A	214	GLN
1	D	46	GLN
1	D	57	GLN
1	D	73	ASN
1	C	73	ASN
1	C	130	ASN
1	C	145	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	300	1	14,14,15	0.85	0	17,19,21	2.91	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	300	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	NAG	O5-C5-C6	7.72	119.30	107.20
3	A	300	NAG	C3-C4-C5	-6.12	99.33	110.24
3	A	300	NAG	C1-O5-C5	4.81	118.71	112.19
3	A	300	NAG	O5-C1-C2	2.73	115.59	111.29
3	A	300	NAG	C4-C3-C2	-2.12	107.92	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300	NAG	C8-C7-N2-C2
3	A	300	NAG	O7-C7-N2-C2
3	A	300	NAG	C1-C2-N2-C7
3	A	300	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	300	NAG	6	0

## 5.5 Carbohydrates [i](#)

3 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAG	E	1	2,1	14,14,15	0.80	0	17,19,21	1.72	4 (23%)
2	NAG	E	2	2	14,14,15	0.67	0	17,19,21	1.47	3 (17%)
2	FUC	E	3	2	10,10,11	0.71	0	14,14,16	2.23	6 (42%)

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	FUC	O2-C2-C3	-4.16	101.80	110.14
2	E	1	NAG	C4-C3-C2	-4.13	104.97	111.02
2	E	3	FUC	C3-C4-C5	3.51	115.24	109.77
2	E	2	NAG	O3-C3-C2	3.38	116.45	109.47
2	E	1	NAG	O5-C1-C2	-3.33	106.03	111.29
2	E	3	FUC	C2-C3-C4	3.18	116.40	110.89
2	E	3	FUC	C1-C2-C3	2.80	113.11	109.67
2	E	3	FUC	O3-C3-C2	-2.70	104.82	109.99
2	E	3	FUC	O5-C5-C4	2.48	113.97	109.52
2	E	1	NAG	O5-C5-C6	2.44	111.03	107.20
2	E	1	NAG	O3-C3-C4	-2.37	104.87	110.35
2	E	2	NAG	C4-C3-C2	2.05	114.03	111.02
2	E	2	NAG	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

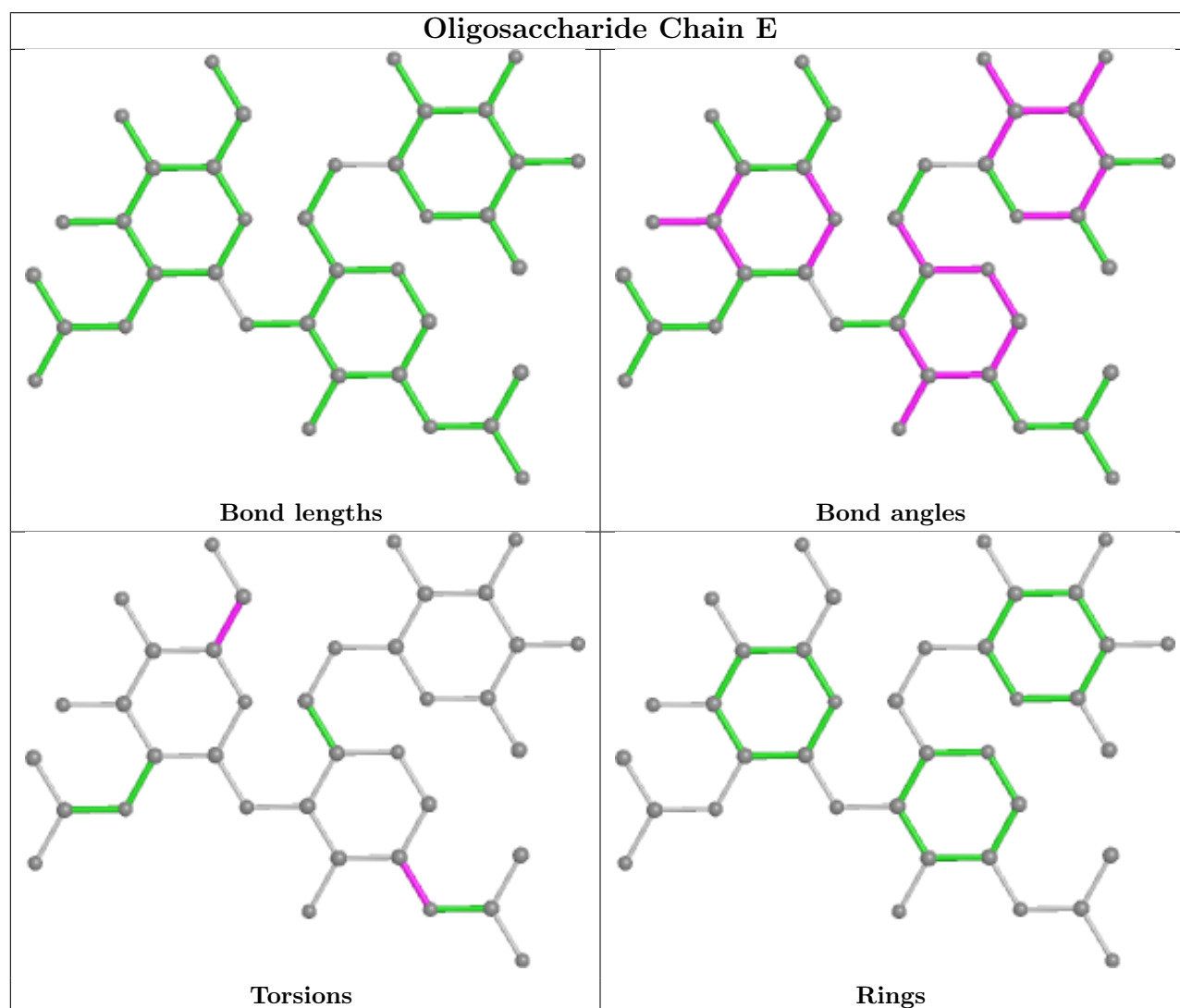
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0

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



## 5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	D	302	1	14,14,15	0.59	0	17,19,21	1.13	2 (11%)
3	NAG	D	301	1	14,14,15	0.51	0	17,19,21	0.97	1 (5%)
3	NAG	B	301	1	14,14,15	0.67	0	17,19,21	2.15	6 (35%)
3	NAG	A	300	1	14,14,15	0.85	0	17,19,21	2.91	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	302	1	-	2/6/23/26	0/1/1/1
3	NAG	D	301	1	-	4/6/23/26	0/1/1/1
3	NAG	B	301	1	-	1/6/23/26	0/1/1/1
3	NAG	A	300	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	NAG	O5-C5-C6	7.72	119.30	107.20
3	A	300	NAG	C3-C4-C5	-6.12	99.33	110.24
3	B	301	NAG	O5-C1-C2	-5.27	102.97	111.29
3	A	300	NAG	C1-O5-C5	4.81	118.71	112.19
3	B	301	NAG	C4-C3-C2	3.68	116.41	111.02
3	B	301	NAG	C1-C2-N2	2.88	115.41	110.49
3	B	301	NAG	C3-C4-C5	2.81	115.24	110.24
3	A	300	NAG	O5-C1-C2	2.73	115.59	111.29
3	D	301	NAG	C6-C5-C4	-2.50	107.15	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	NAG	O7-C7-C8	-2.50	117.42	122.06
3	D	302	NAG	C1-O5-C5	2.39	115.43	112.19
3	D	302	NAG	O5-C5-C6	2.28	110.79	107.20
3	B	301	NAG	O5-C5-C6	2.18	110.62	107.20
3	A	300	NAG	C4-C3-C2	-2.12	107.92	111.02

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300	NAG	C8-C7-N2-C2
3	A	300	NAG	O7-C7-N2-C2
3	D	301	NAG	C8-C7-N2-C2
3	D	301	NAG	O7-C7-N2-C2
3	D	301	NAG	C4-C5-C6-O6
3	D	301	NAG	O5-C5-C6-O6
3	A	300	NAG	C1-C2-N2-C7
3	A	300	NAG	C3-C2-N2-C7
3	D	302	NAG	C1-C2-N2-C7
3	B	301	NAG	O5-C5-C6-O6
3	D	302	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	NAG	1	0
3	B	301	NAG	4	0
3	A	300	NAG	6	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	184/198 (92%)	0.29	10 (5%) 25 24	32, 52, 93, 125	0
1	B	182/198 (91%)	0.11	9 (4%) 29 28	28, 41, 100, 168	0
1	C	184/198 (92%)	0.23	12 (6%) 18 17	26, 39, 101, 146	0
1	D	188/198 (94%)	0.20	12 (6%) 19 18	31, 53, 99, 126	0
All	All	738/792 (93%)	0.21	43 (5%) 23 22	26, 47, 101, 168	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	ILE	8.3
1	A	160	TYR	6.6
1	A	159	SER	5.5
1	B	88	CYS	5.0
1	D	86	ILE	4.5
1	C	157	ALA	4.4
1	C	87	PRO	4.3
1	C	160	TYR	4.2
1	B	156	THR	4.0
1	B	87	PRO	4.0
1	B	85	LEU	3.7
1	A	211	GLN	3.7
1	C	86	ILE	3.6
1	C	143	GLN	3.6
1	B	84	ALA	3.5
1	A	143	GLN	3.5
1	D	155	ARG	3.5
1	A	158	ARG	3.4
1	B	82	ARG	3.3
1	C	175	VAL	3.2
1	C	85	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	157	ALA	3.1
1	C	158	ARG	3.0
1	A	155	ARG	2.9
1	C	159	SER	2.8
1	A	217	LYS	2.7
1	A	210	CYS	2.7
1	D	36	HIS	2.7
1	D	220	ASP	2.6
1	B	83	LYS	2.6
1	D	160	TYR	2.6
1	C	166	VAL	2.6
1	D	88	CYS	2.3
1	A	212	ALA	2.3
1	B	157	ALA	2.3
1	C	183	TYR	2.2
1	D	89	LYS	2.1
1	D	129	GLN	2.1
1	D	143	GLN	2.1
1	D	222	CYS	2.1
1	D	38	THR	2.1
1	C	222	CYS	2.0
1	D	181	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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.

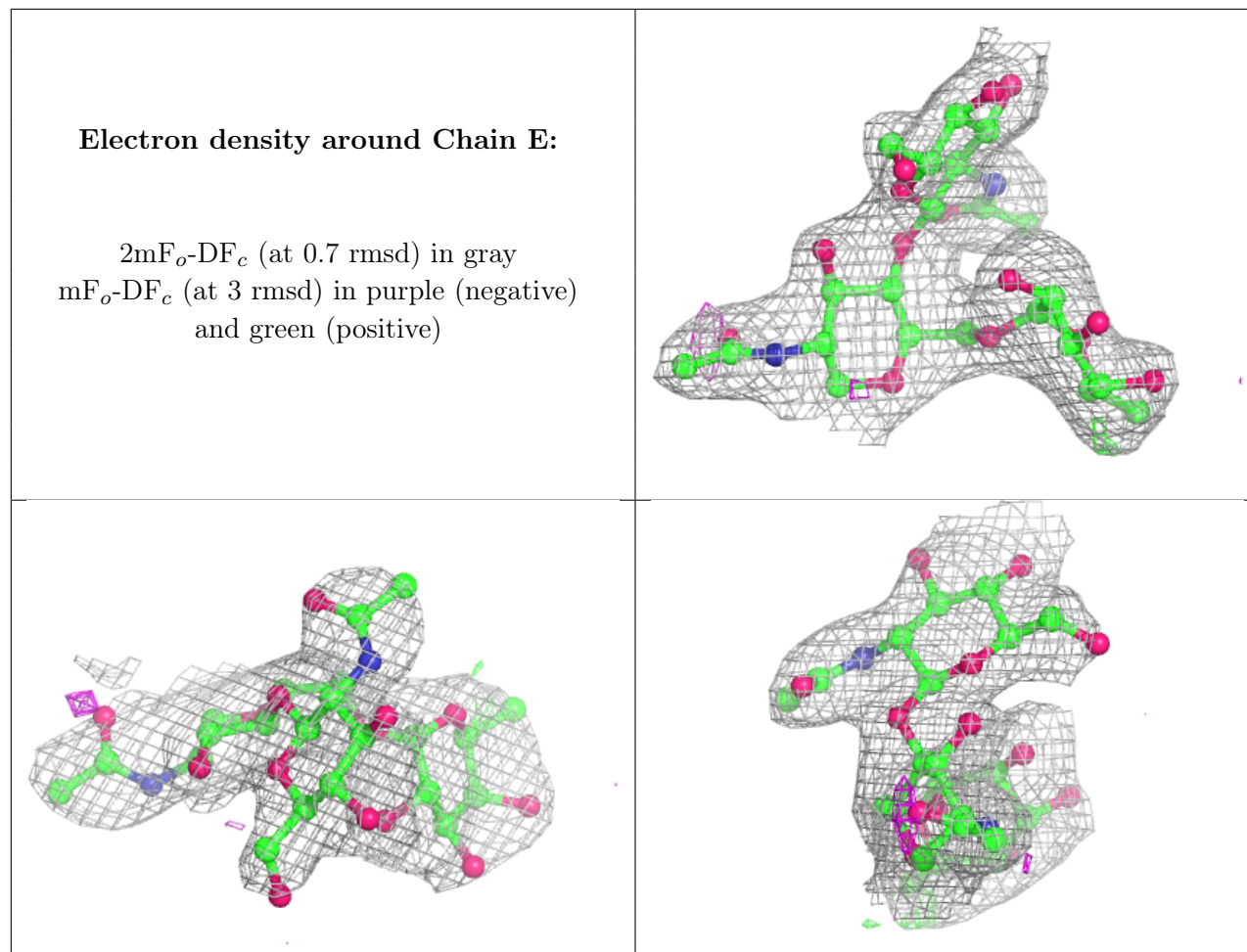
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	300	14/15	0.75	0.39	70,82,95,102	0

## 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
2	NAG	E	2	14/15	0.91	0.31	68,74,82,86	0
2	FUC	E	3	10/11	0.91	0.17	59,65,73,93	0
2	NAG	E	1	14/15	0.95	0.20	44,51,62,65	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
3	NAG	B	301	14/15	0.58	0.38	98,114,117,118	0
3	NAG	D	302	14/15	0.65	0.29	94,110,118,120	0
3	NAG	D	301	14/15	0.67	0.30	90,98,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	300	14/15	0.75	0.39	70,82,95,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.