



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 10:10 AM BST

PDB ID : 5VQF  
Title : Crystal Structure of pro-TGF-beta 1  
Authors : Zhao, B.; Xu, S.; Dong, X.; Lu, C.; Springer, T.A.  
Deposited on : 2017-05-08  
Resolution : 2.90 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.

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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 : 2.13.1  
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) : 2.13.1

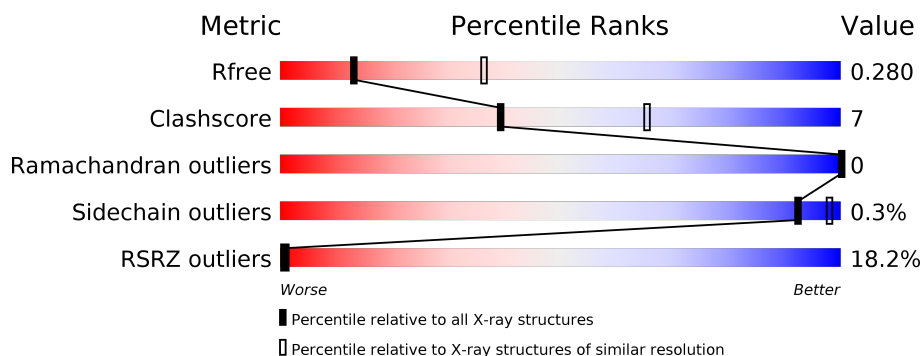
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	363	<div> <div>25%</div> <div> <div>71%</div> <div>22%</div> <div>8%</div> </div> </div>
1	B	363	<div> <div>17%</div> <div> <div>70%</div> <div>18%</div> <div>12%</div> </div> </div>
1	C	363	<div> <div>13%</div> <div> <div>79%</div> <div>15%</div> <div>6%</div> </div> </div>
1	D	363	<div> <div>12%</div> <div> <div>78%</div> <div>14%</div> <div>8%</div> </div> </div>
2	E	3	<div> <div>67%</div> <div>33%</div> </div>
3	F	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	 100%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10753 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 Transforming growth factor beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2684	1706	469	492	17			
1	B	320	Total	C	N	O	S	0	0	0
			2556	1620	452	467	17			
1	C	340	Total	C	N	O	S	0	0	0
			2728	1732	481	498	17			
1	D	335	Total	C	N	O	S	0	0	0
			2690	1711	473	489	17			

There are 20 discrepancies between the modelled and reference sequences:

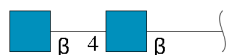
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P07200
A	0	PRO	-	expression tag	UNP P07200
A	4	SER	CYS	engineered mutation	UNP P07200
A	85	VAL	LEU	variant	UNP P07200
A	147	GLN	ASN	engineered mutation	UNP P07200
B	-1	GLY	-	expression tag	UNP P07200
B	0	PRO	-	expression tag	UNP P07200
B	4	SER	CYS	engineered mutation	UNP P07200
B	85	VAL	LEU	variant	UNP P07200
B	147	GLN	ASN	engineered mutation	UNP P07200
C	-1	GLY	-	expression tag	UNP P07200
C	0	PRO	-	expression tag	UNP P07200
C	4	SER	CYS	engineered mutation	UNP P07200
C	85	VAL	LEU	variant	UNP P07200
C	147	GLN	ASN	engineered mutation	UNP P07200
D	-1	GLY	-	expression tag	UNP P07200
D	0	PRO	-	expression tag	UNP P07200
D	4	SER	CYS	engineered mutation	UNP P07200
D	85	VAL	LEU	variant	UNP P07200
D	147	GLN	ASN	engineered mutation	UNP P07200

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

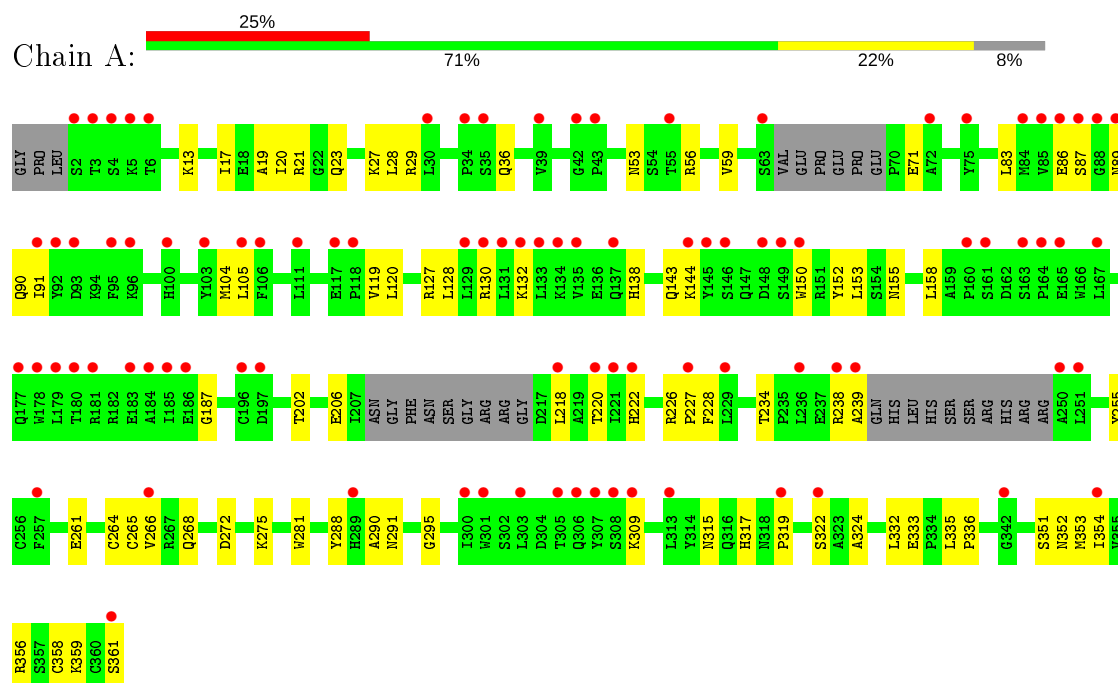


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

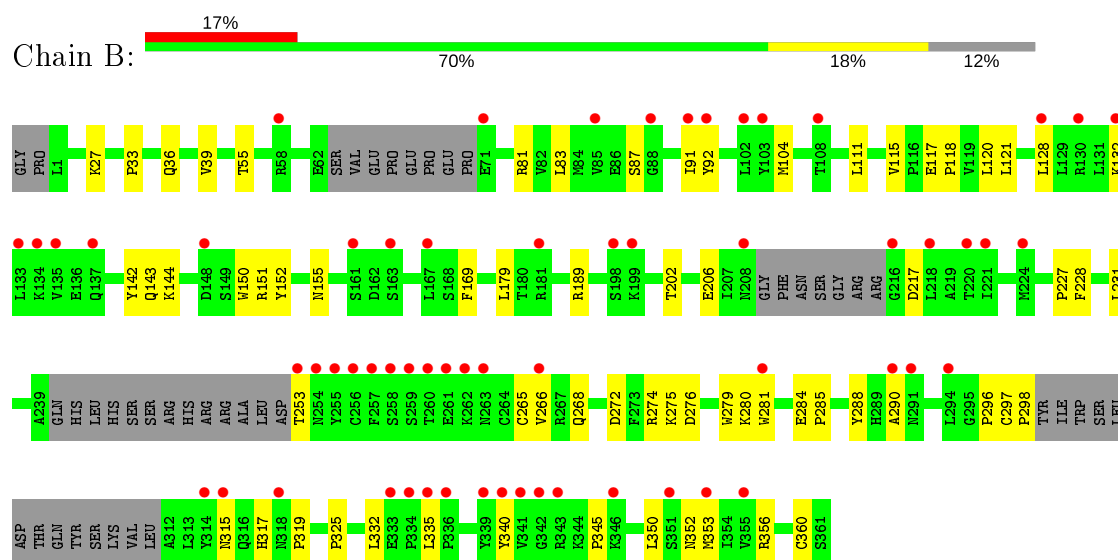
### 3 Residue-property plots [i](#)

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.

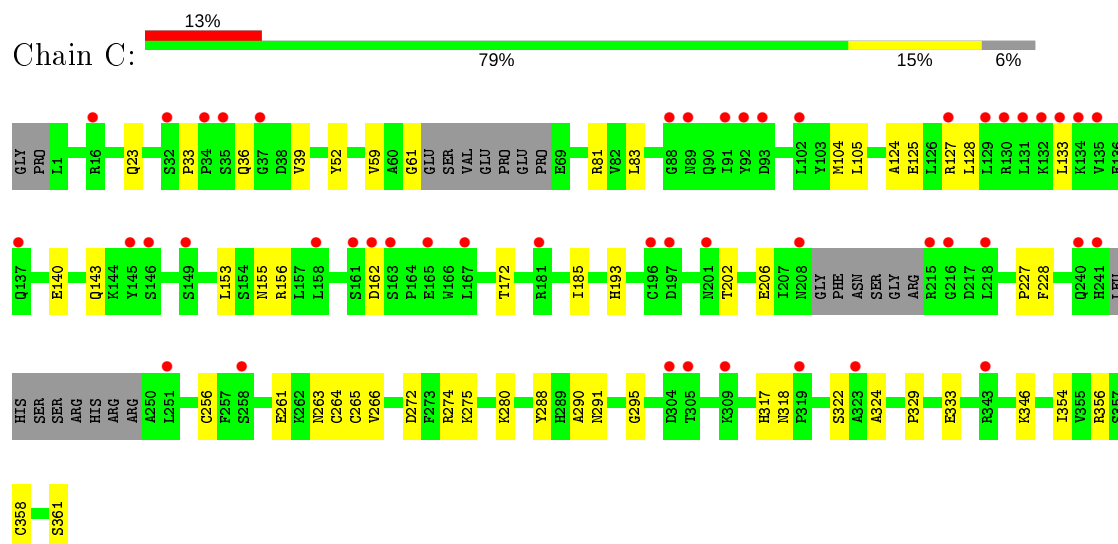
#### • Molecule 1: Transforming growth factor beta-1



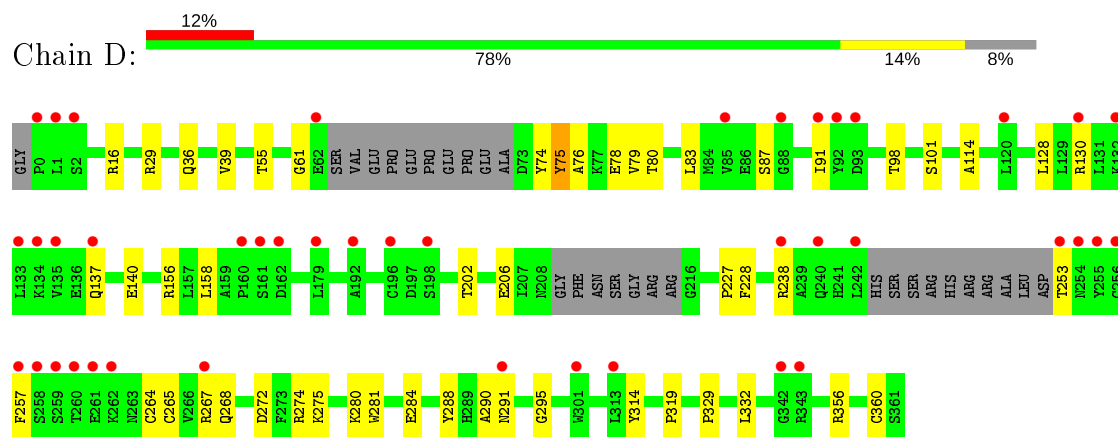
#### • Molecule 1: Transforming growth factor beta-1



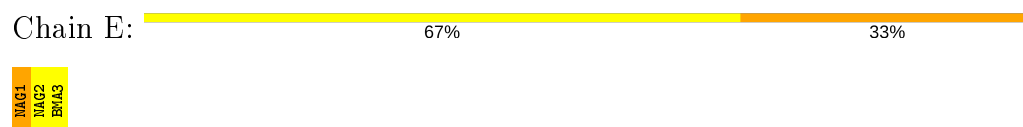
- Molecule 1: Transforming growth factor beta-1



- Molecule 1: Transforming growth factor beta-1



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



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

100%

EMG1  
EMG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.66Å 126.92Å 137.92Å 90.00° 96.70° 90.00°	Depositor
Resolution (Å)	37.14 – 2.90 37.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.2 (37.14-2.90) 96.3 (37.14-2.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.239 , 0.280 0.239 , 0.280	Depositor DCC
$R_{free}$ test set	1354 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	129.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 130.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.25% 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: BMA, 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	0.29	0/2747	0.49	1/3723 (0.0%)
1	B	0.28	0/2613	0.50	1/3537 (0.0%)
1	C	0.29	0/2792	0.50	1/3784 (0.0%)
1	D	0.33	0/2754	0.51	1/3732 (0.0%)
All	All	0.30	0/10906	0.50	4/14776 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	265	CYS	CA-CB-SG	9.06	130.31	114.00
1	A	265	CYS	CA-CB-SG	6.90	126.42	114.00
1	B	265	CYS	CA-CB-SG	6.30	125.34	114.00
1	C	265	CYS	CA-CB-SG	5.35	123.62	114.00

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	2684	0	2676	60	0
1	B	2556	0	2552	51	0
1	C	2728	0	2720	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2690	0	2687	30	0
2	E	39	0	34	2	0
3	F	28	0	25	3	0
3	G	28	0	25	1	0
All	All	10753	0	10719	158	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 (158) 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:83:LEU:HD13	1:B:228:PHE:HB3	1.54	0.88
1:A:83:LEU:HD13	1:A:228:PHE:HB3	1.58	0.84
1:A:86:GLU:OE2	1:A:222:HIS:ND1	2.11	0.82
1:A:36:GLN:NE2	1:B:281:TRP:HB3	1.96	0.80
1:A:155:ASN:ND2	1:B:152:TYR:OH	2.16	0.79
1:D:83:LEU:HD13	1:D:228:PHE:HB3	1.64	0.78
1:B:298:PRO:HG2	1:B:317:HIS:HE1	1.51	0.75
1:D:288:TYR:CE2	1:D:290:ALA:HB2	2.23	0.74
1:D:29:ARG:HH11	1:D:75:TYR:HE1	1.36	0.72
1:C:288:TYR:CE2	1:C:290:ALA:HB2	2.24	0.72
1:B:132:LYS:NZ	1:B:217:ASP:O	2.24	0.71
1:B:143:GLN:OE1	1:B:151:ARG:NH2	2.25	0.69
1:B:298:PRO:HG2	1:B:317:HIS:CE1	2.28	0.68
1:A:255:TYR:CE2	1:A:261:GLU:OE2	2.49	0.65
1:C:83:LEU:HD13	1:C:228:PHE:HB3	1.78	0.64
1:A:288:TYR:CE2	1:A:290:ALA:HB2	2.32	0.64
1:A:272:ASP:HB3	1:A:275:LYS:HB3	1.79	0.64
1:A:23:GLN:HG2	1:A:27:LYS:NZ	2.13	0.63
1:C:128:LEU:HD23	1:C:227:PRO:HG3	1.82	0.62
1:A:36:GLN:HE21	1:B:281:TRP:HB3	1.65	0.61
1:D:264:CYS:HA	1:D:295:GLY:HA3	1.81	0.61
1:B:288:TYR:CE2	1:B:290:ALA:HB2	2.36	0.61
1:B:117:GLU:HB2	1:B:120:LEU:HD23	1.82	0.61
1:D:76:ALA:HB3	1:D:238:ARG:HH12	1.67	0.60
1:A:143:GLN:HB2	1:A:153:LEU:HD11	1.84	0.60
1:C:52:TYR:CE2	1:D:284:GLU:HB3	2.37	0.59
1:B:87:SER:HA	1:B:91:ILE:HD11	1.85	0.59
2:E:1:NAG:H83	2:E:1:NAG:O3	2.02	0.59
1:C:105:LEU:HB3	1:C:185:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:GLU:HG2	1:C:202:THR:HG22	1.84	0.58
1:D:253:THR:HG23	1:D:356:ARG:HD3	1.83	0.58
1:D:87:SER:HA	1:D:91:ILE:HD11	1.83	0.58
1:A:29:ARG:HD3	1:A:238:ARG:HB3	1.86	0.58
1:A:53:ASN:HD22	1:A:56:ARG:HH21	1.51	0.58
1:A:53:ASN:HD22	1:A:56:ARG:NH2	2.01	0.57
1:C:291:ASN:O	1:D:16:ARG:NH2	2.38	0.56
1:B:128:LEU:HD23	1:B:227:PRO:HG3	1.87	0.56
1:D:74:TYR:HD2	1:D:75:TYR:CD2	2.25	0.55
1:C:317:HIS:ND1	1:C:361:SER:O	2.38	0.55
1:A:23:GLN:HG2	1:A:27:LYS:HZ3	1.73	0.54
1:D:128:LEU:HD23	1:D:227:PRO:HG3	1.90	0.54
3:F:1:NAG:H83	3:F:1:NAG:O3	2.08	0.54
1:B:115:VAL:HG11	1:B:121:LEU:HB2	1.90	0.53
1:D:130:ARG:HH11	1:D:158:LEU:HB3	1.72	0.53
1:B:272:ASP:HB3	1:B:275:LYS:HB3	1.90	0.53
1:C:264:CYS:HA	1:C:295:GLY:HA3	1.90	0.53
3:F:1:NAG:O3	3:F:2:NAG:O5	2.24	0.53
1:C:333:GLU:HB2	1:C:354:ILE:HB	1.90	0.52
1:A:19:ALA:HB1	1:A:319:PRO:HB2	1.91	0.52
1:A:333:GLU:OE2	1:A:356:ARG:NE	2.41	0.52
1:A:315:ASN:O	1:B:352:ASN:ND2	2.42	0.52
1:C:59:VAL:HG11	1:C:127:ARG:NH1	2.25	0.51
1:C:125:GLU:OE1	1:C:127:ARG:NH2	2.43	0.51
1:A:13:LYS:NZ	1:B:268:GLN:O	2.44	0.51
1:B:315:ASN:O	1:B:319:PRO:HG3	2.11	0.51
1:A:119:VAL:HG13	1:A:120:LEU:HD22	1.92	0.50
1:A:130:ARG:HG3	1:A:218:LEU:HD11	1.94	0.50
1:A:120:LEU:HD11	1:A:239:ALA:HB2	1.92	0.50
1:B:128:LEU:HD12	1:B:169:PHE:HE2	1.76	0.50
1:A:264:CYS:HA	1:A:295:GLY:HA3	1.94	0.50
1:A:17:ILE:HD13	1:B:276:ASP:HB3	1.94	0.50
1:D:274:ARG:HH12	1:D:280:LYS:HD3	1.77	0.50
1:B:274:ARG:HH12	1:B:280:LYS:HE2	1.77	0.50
1:D:329:PRO:HB2	1:D:332:LEU:HD21	1.93	0.50
1:A:105:LEU:HG	1:A:187:GLY:HA3	1.94	0.49
1:A:120:LEU:HD12	1:A:234:THR:HB	1.93	0.49
1:A:351:SER:O	1:B:27:LYS:HE2	2.12	0.49
2:E:1:NAG:O3	2:E:2:NAG:O5	2.27	0.49
1:A:144:LYS:HB2	1:A:150:TRP:CZ3	2.48	0.49
1:A:206:GLU:HG2	1:D:202:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLU:HB2	1:A:354:ILE:HB	1.95	0.49
1:B:297:CYS:O	1:B:325:PRO:HG2	2.13	0.48
1:B:202:THR:HG22	1:C:206:GLU:HG2	1.95	0.48
1:B:83:LEU:HA	1:B:228:PHE:HB3	1.95	0.48
1:C:143:GLN:HB2	1:C:153:LEU:HD11	1.94	0.48
1:A:255:TYR:OH	1:A:309:LYS:HD3	2.14	0.48
1:A:104:MET:SD	1:A:128:LEU:HD21	2.54	0.48
1:B:296:PRO:HB2	1:B:298:PRO:HD3	1.95	0.47
1:B:332:LEU:HD13	1:B:352:ASN:HB3	1.96	0.47
1:D:319:PRO:HD2	1:D:360:CYS:O	2.15	0.47
1:B:335:LEU:HB3	1:B:353:MET:HG3	1.96	0.47
1:B:144:LYS:HB2	1:B:150:TRP:CZ3	2.50	0.47
1:B:36:GLN:OE1	1:B:39:VAL:HG21	2.15	0.47
1:A:281:TRP:CD1	1:B:33:PRO:HB3	2.50	0.47
1:C:61:GLY:HA2	1:C:156:ARG:NH1	2.30	0.47
3:G:1:NAG:H62	3:G:2:NAG:C1	2.45	0.47
1:A:132:LYS:HZ3	1:A:218:LEU:HA	1.80	0.47
1:A:317:HIS:NE2	1:A:319:PRO:HG3	2.30	0.47
1:D:75:TYR:N	1:D:75:TYR:CD2	2.83	0.47
1:B:319:PRO:HD2	1:B:360:CYS:O	2.14	0.46
1:A:20:ILE:HA	1:A:23:GLN:HB3	1.98	0.46
1:A:202:THR:HG22	1:D:206:GLU:HG2	1.96	0.46
1:A:152:TYR:OH	1:B:155:ASN:ND2	2.47	0.46
1:A:27:LYS:HD2	1:B:350:LEU:HD23	1.98	0.46
1:C:261:GLU:HG3	1:C:263:ASN:H	1.80	0.46
1:A:83:LEU:HD12	1:A:226:ARG:HG2	1.97	0.45
1:D:257:PHE:CE1	1:D:268:GLN:HG3	2.51	0.45
1:A:87:SER:HA	1:A:91:ILE:HD11	1.99	0.45
1:C:256:CYS:SG	1:C:266:VAL:N	2.81	0.45
1:A:27:LYS:HE2	1:B:353:MET:SD	2.56	0.45
1:C:333:GLU:OE2	1:C:356:ARG:NE	2.39	0.45
1:C:124:ALA:HB3	1:C:172:THR:HA	1.98	0.45
1:B:274:ARG:NH1	1:B:280:LYS:HE2	2.32	0.45
1:A:336:PRO:HB3	1:B:55:THR:HG21	1.99	0.44
1:A:20:ILE:HG12	1:A:23:GLN:OE1	2.18	0.44
1:C:36:GLN:HA	1:C:39:VAL:HG23	2.00	0.44
1:A:255:TYR:CZ	1:A:261:GLU:OE2	2.70	0.44
1:A:220:THR:O	1:A:227:PRO:HD3	2.17	0.44
1:D:36:GLN:OE1	1:D:39:VAL:HG21	2.18	0.44
1:D:137:GLN:HG3	1:D:158:LEU:HD12	1.99	0.43
1:D:272:ASP:HB3	1:D:275:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:GLU:HA	1:B:285:PRO:HA	1.78	0.43
1:A:130:ARG:CZ	1:A:158:LEU:HB3	2.48	0.43
1:A:335:LEU:HB3	1:A:353:MET:HG3	2.00	0.43
1:A:128:LEU:HD23	1:A:227:PRO:HG3	2.00	0.43
1:A:322:SER:C	1:A:324:ALA:H	2.20	0.43
1:A:89:ASN:OD1	1:A:90:GLN:HG2	2.19	0.43
1:B:111:LEU:HD22	1:B:231:LEU:HD11	2.00	0.43
1:C:193:HIS:HE1	1:D:140:GLU:OE2	2.01	0.43
1:D:61:GLY:HA2	1:D:156:ARG:NH1	2.33	0.43
1:A:36:GLN:HE22	1:B:281:TRP:HB3	1.79	0.43
1:C:23:GLN:NE2	1:C:318:ASN:OD1	2.49	0.43
1:D:267:ARG:O	1:D:291:ASN:HB3	2.19	0.43
1:B:142:TYR:HB2	1:B:189:ARG:HB3	2.01	0.42
1:C:266:VAL:HG22	1:C:358:CYS:SG	2.59	0.42
1:C:346:LYS:NZ	1:D:78:GLU:OE2	2.51	0.42
1:A:130:ARG:NH1	1:A:158:LEU:HB3	2.34	0.42
1:B:118:PRO:HB3	1:B:179:LEU:HB2	2.01	0.42
1:B:340:TYR:CZ	1:B:345:PRO:HB3	2.55	0.42
1:B:91:ILE:HG13	1:B:92:TYR:CD1	2.55	0.42
1:C:272:ASP:HB3	1:C:275:LYS:HB3	2.02	0.42
1:B:104:MET:SD	1:B:128:LEU:HD21	2.59	0.42
1:B:81:ARG:HD2	1:B:228:PHE:CE2	2.55	0.41
1:D:98:THR:HB	1:D:101:SER:HB3	2.02	0.41
1:A:332:LEU:HD22	1:A:352:ASN:HB3	2.02	0.41
1:C:81:ARG:HD2	1:C:228:PHE:CD2	2.55	0.41
1:C:322:SER:C	1:C:324:ALA:H	2.24	0.41
1:D:55:THR:HG21	1:D:79:VAL:HG11	2.02	0.41
1:B:340:TYR:CE2	1:B:345:PRO:HB3	2.56	0.41
1:A:266:VAL:HG22	1:A:358:CYS:SG	2.61	0.41
1:C:127:ARG:HD2	1:C:228:PHE:CZ	2.55	0.41
1:C:274:ARG:HH12	1:C:280:LYS:HD3	1.85	0.41
1:C:33:PRO:HB3	1:D:281:TRP:CD1	2.55	0.41
1:C:329:PRO:HA	1:C:358:CYS:HA	2.02	0.41
3:F:1:NAG:H83	3:F:1:NAG:C3	2.51	0.41
1:A:359:LYS:HE2	1:A:361:SER:OG	2.21	0.41
1:B:253:THR:HG22	1:B:266:VAL:HG11	2.03	0.41
1:A:59:VAL:HG11	1:A:127:ARG:CZ	2.51	0.41
1:A:132:LYS:NZ	1:A:218:LEU:HA	2.36	0.41
1:B:132:LYS:HA	1:B:132:LYS:HD3	1.88	0.41
1:C:140:GLU:HG2	1:C:155:ASN:HB3	2.03	0.41
1:C:104:MET:SD	1:C:128:LEU:HD21	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD22	1:A:238:ARG:HH22	1.85	0.41
1:A:21:ARG:HG3	1:B:279:TRP:HZ2	1.85	0.40
1:C:133:LEU:HD13	1:C:162:ASP:O	2.22	0.40
1:A:268:GLN:HA	1:A:291:ASN:OD1	2.21	0.40
1:B:253:THR:HG23	1:B:356:ARG:HD3	2.04	0.40
1:D:80:THR:OG1	1:D:114:ALA:HB1	2.22	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	327/363 (90%)	318 (97%)	9 (3%)	0	100	100
1	B	310/363 (85%)	299 (96%)	11 (4%)	0	100	100
1	C	332/363 (92%)	320 (96%)	12 (4%)	0	100	100
1	D	327/363 (90%)	317 (97%)	10 (3%)	0	100	100
All	All	1296/1452 (89%)	1254 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/323 (93%)	297 (99%)	2 (1%)	84	95
1	B	284/323 (88%)	284 (100%)	0	100	100
1	C	303/323 (94%)	303 (100%)	0	100	100
1	D	300/323 (93%)	298 (99%)	2 (1%)	84	95
All	All	1186/1292 (92%)	1182 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	138	HIS
1	D	75	TYR
1	D	314	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	155	ASN
1	B	317	HIS
1	D	263	ASN
1	D	316	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

7 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	1,2	14,14,15	1.44	1 (7%)	17,19,21	2.88	4 (23%)
2	NAG	E	2	2	14,14,15	0.64	0	17,19,21	0.76	0
2	BMA	E	3	2	11,11,12	0.91	0	15,15,17	0.92	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.51	0	17,19,21	2.73	2 (11%)
3	NAG	F	2	3	14,14,15	0.50	0	17,19,21	0.65	0
3	NAG	G	1	1,3	14,14,15	1.74	1 (7%)	17,19,21	1.08	1 (5%)
3	NAG	G	2	3	14,14,15	1.16	1 (7%)	17,19,21	1.32	2 (11%)

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	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	O5-C1	-6.35	1.33	1.43
2	E	1	NAG	O5-C1	4.49	1.50	1.43
3	G	2	NAG	O5-C1	4.04	1.50	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C2-N2-C7	8.60	135.15	122.90
2	E	1	NAG	C2-N2-C7	8.29	134.71	122.90
3	F	1	NAG	C1-C2-N2	5.83	120.45	110.49
2	E	1	NAG	C1-O5-C5	5.80	120.05	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-C2-N2	3.88	117.12	110.49
3	G	2	NAG	C3-C4-C5	3.25	116.03	110.24
3	G	2	NAG	C1-O5-C5	-2.89	108.27	112.19
3	G	1	NAG	O4-C4-C5	2.49	115.47	109.30
2	E	3	BMA	O2-C2-C3	-2.40	105.33	110.14
2	E	1	NAG	O3-C3-C2	-2.39	104.51	109.47

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C8-C7-N2-C2
2	E	1	NAG	C3-C2-N2-C7
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7
3	F	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C1-C2-N2-C7
3	G	1	NAG	C3-C2-N2-C7
3	G	2	NAG	C3-C2-N2-C7

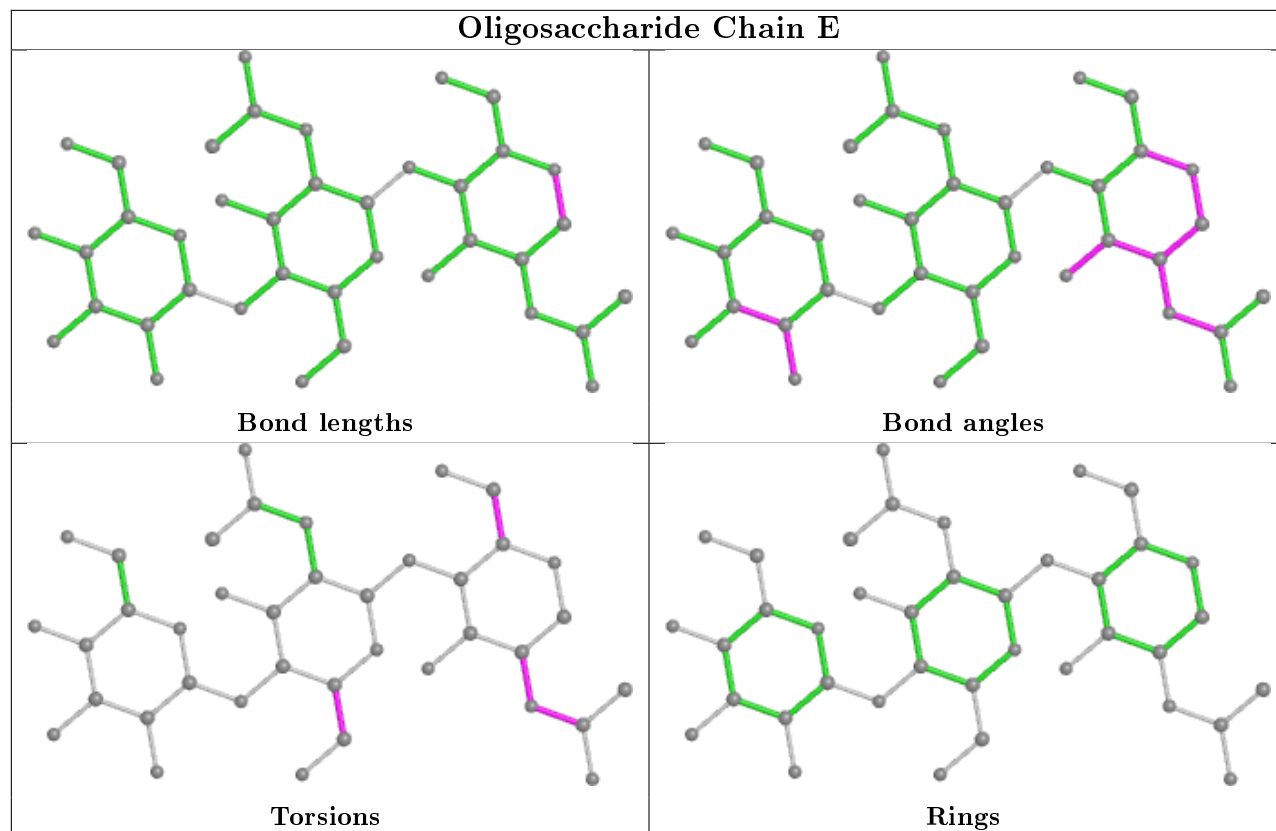
There are no ring outliers.

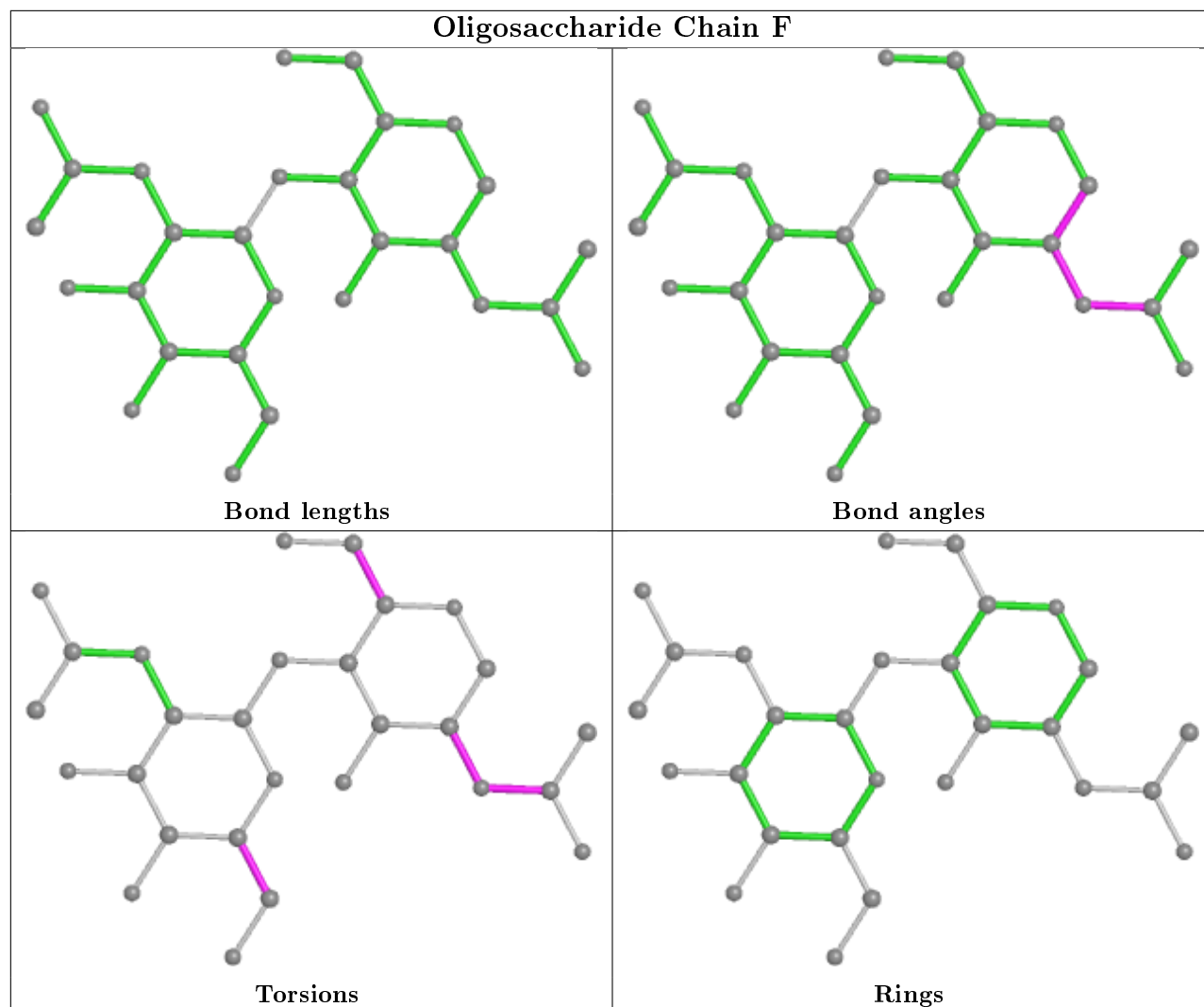
6 monomers are involved in 6 short contacts:

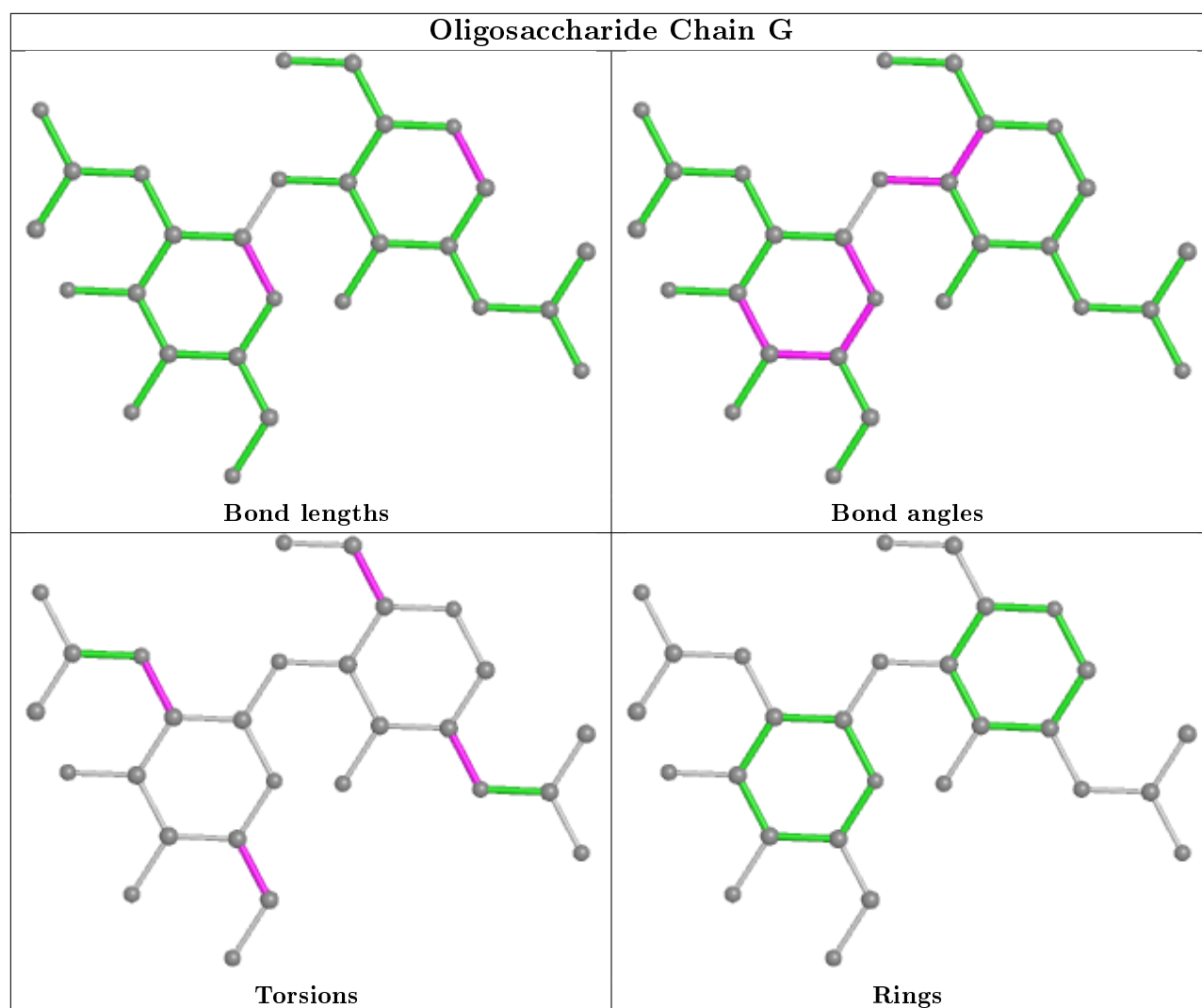
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	1	0
3	G	1	NAG	1	0
3	F	1	NAG	3	0
2	E	1	NAG	2	0
3	G	2	NAG	1	0
2	E	2	NAG	1	0

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 [i](#)

There are no ligands in this entry.

## 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	335/363 (92%)	1.30	92 (27%) <b>0</b> <b>0</b>	122, 208, 301, 367	0
1	B	320/363 (88%)	1.17	61 (19%) <b>1</b> <b>0</b>	130, 195, 272, 364	0
1	C	340/363 (93%)	0.92	47 (13%) <b>2</b> <b>2</b>	92, 161, 257, 344	0
1	D	335/363 (92%)	1.04	42 (12%) <b>3</b> <b>3</b>	106, 160, 258, 308	0
All	All	1330/1452 (91%)	1.11	242 (18%) <b>1</b> <b>1</b>	92, 183, 274, 367	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	242	LEU	16.1
1	A	91	ILE	10.3
1	B	342	GLY	9.9
1	B	260	THR	8.6
1	D	258	SER	8.5
1	D	253	THR	8.3
1	A	305	THR	8.2
1	D	93	ASP	7.3
1	B	92	TYR	7.0
1	D	255	TYR	7.0
1	C	146	SER	6.9
1	D	0	PRO	6.9
1	C	92	TYR	6.8
1	B	91	ILE	6.8
1	D	88	GLY	6.8
1	C	145	TYR	6.5
1	D	240	GLN	6.5
1	D	256	CYS	6.4
1	D	257	PHE	6.2
1	D	254	ASN	6.2
1	B	256	CYS	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	255	TYR	6.0
1	D	161	SER	5.8
1	A	238	ARG	5.7
1	B	258	SER	5.7
1	D	301	TRP	5.7
1	A	179	LEU	5.6
1	A	307	TYR	5.5
1	B	220	THR	5.3
1	B	134	LYS	5.3
1	C	93	ASP	5.3
1	C	218	LEU	5.2
1	D	259	SER	5.1
1	A	129	LEU	5.1
1	A	2	SER	5.1
1	B	133	LEU	4.9
1	A	221	ILE	4.9
1	A	186	GLU	4.8
1	B	132	LYS	4.7
1	D	260	THR	4.7
1	A	306	GLN	4.4
1	C	216	GLY	4.4
1	A	134	LYS	4.4
1	A	105	LEU	4.3
1	A	342	GLY	4.3
1	B	314	TYR	4.3
1	A	117	GLU	4.2
1	A	181	ARG	4.2
1	B	259	SER	4.2
1	B	261	GLU	4.1
1	C	132	LYS	4.1
1	C	208	ASN	4.1
1	D	261	GLU	4.0
1	A	361	SER	4.0
1	A	250	ALA	4.0
1	C	149	SER	4.0
1	A	34	PRO	3.9
1	B	135	VAL	3.9
1	D	91	ILE	3.9
1	C	130	ARG	3.9
1	B	71	GLU	3.9
1	A	222	HIS	3.8
1	C	131	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	135	VAL	3.8
1	A	92	TYR	3.7
1	A	180	THR	3.7
1	A	239	ALA	3.7
1	D	132	LYS	3.7
1	B	340	TYR	3.7
1	B	181	ARG	3.7
1	B	318	ASN	3.7
1	A	184	ALA	3.6
1	A	165	GLU	3.6
1	A	251	LEU	3.6
1	C	240	GLN	3.6
1	C	88	GLY	3.6
1	B	130	ARG	3.6
1	B	161	SER	3.6
1	A	89	ASN	3.6
1	D	92	TYR	3.5
1	A	229	LEU	3.5
1	B	341	VAL	3.4
1	A	106	PHE	3.4
1	B	343	ARG	3.4
1	D	262	LYS	3.4
1	C	135	VAL	3.4
1	A	63	SER	3.3
1	B	334	PRO	3.3
1	D	134	LYS	3.3
1	B	257	PHE	3.3
1	C	162	ASP	3.3
1	C	181	ARG	3.3
1	C	37	GLY	3.2
1	A	39	VAL	3.2
1	A	103	TYR	3.2
1	D	238	ARG	3.2
1	A	88	GLY	3.2
1	A	145	TYR	3.2
1	A	319	PRO	3.2
1	D	1	LEU	3.2
1	B	346	LYS	3.1
1	B	85	VAL	3.1
1	B	355	VAL	3.1
1	A	86	GLU	3.1
1	A	183	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	167	LEU	3.1
1	A	309	LYS	3.1
1	C	161	SER	3.1
1	C	89	ASN	3.1
1	A	177	GLN	3.0
1	C	167	LEU	3.0
1	D	267	ARG	3.0
1	C	309	LYS	3.0
1	D	2	SER	3.0
1	A	354	ILE	3.0
1	B	199	LYS	3.0
1	C	134	LYS	3.0
1	B	262	LYS	2.9
1	C	163	SER	2.9
1	A	236	LEU	2.9
1	A	161	SER	2.9
1	B	148	ASP	2.9
1	A	87	SER	2.9
1	B	163	SER	2.9
1	C	305	THR	2.9
1	A	84	MET	2.9
1	C	323	ALA	2.9
1	B	58	ARG	2.9
1	A	96	LYS	2.9
1	D	342	GLY	2.9
1	A	132	LYS	2.9
1	D	160	PRO	2.8
1	B	291	ASN	2.8
1	B	198	SER	2.8
1	A	42	GLY	2.8
1	B	254	ASN	2.8
1	B	263	ASN	2.8
1	B	266	VAL	2.8
1	D	179	LEU	2.8
1	A	72	ALA	2.8
1	C	215	ARG	2.8
1	A	137	GLN	2.8
1	A	266	VAL	2.7
1	C	133	LEU	2.7
1	D	130	ARG	2.7
1	D	62	GLU	2.7
1	D	162	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	218	LEU	2.7
1	C	102	LEU	2.7
1	B	290	ALA	2.7
1	D	291	ASN	2.6
1	A	300	ILE	2.6
1	A	167	LEU	2.6
1	A	4	SER	2.6
1	C	137	GLN	2.6
1	A	131	LEU	2.6
1	B	294	LEU	2.6
1	B	336	PRO	2.6
1	C	127	ARG	2.6
1	A	85	VAL	2.6
1	A	178	TRP	2.6
1	A	303	LEU	2.6
1	A	322	SER	2.6
1	C	165	GLU	2.6
1	A	308	SER	2.6
1	A	6	THR	2.5
1	C	197	ASP	2.5
1	A	163	SER	2.5
1	C	241	HIS	2.5
1	C	258	SER	2.5
1	A	313	LEU	2.5
1	D	137	GLN	2.5
1	D	313	LEU	2.5
1	B	108	THR	2.5
1	A	3	THR	2.5
1	A	220	THR	2.5
1	D	85	VAL	2.4
1	D	343	ARG	2.4
1	A	75	TYR	2.4
1	A	135	VAL	2.4
1	C	196	CYS	2.4
1	C	343	ARG	2.4
1	B	218	LEU	2.4
1	C	201	ASN	2.4
1	A	196	CYS	2.4
1	B	339	TYR	2.4
1	B	137	GLN	2.4
1	A	197	ASP	2.4
1	B	315	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	221	ILE	2.4
1	A	95	PHE	2.3
1	A	148	ASP	2.3
1	A	133	LEU	2.3
1	B	216	GLY	2.3
1	D	192	ALA	2.3
1	B	335	LEU	2.3
1	C	158	LEU	2.3
1	A	43	PRO	2.3
1	C	304	ASP	2.3
1	A	130	ARG	2.3
1	A	146	SER	2.3
1	D	198	SER	2.3
1	B	103	TYR	2.2
1	A	35	SER	2.2
1	A	149	SER	2.2
1	A	227	PRO	2.2
1	A	289	HIS	2.2
1	A	5	LYS	2.2
1	C	91	ILE	2.2
1	C	35	SER	2.2
1	A	100	HIS	2.2
1	C	16	ARG	2.2
1	B	224	MET	2.2
1	C	129	LEU	2.2
1	A	164	PRO	2.2
1	D	133	LEU	2.1
1	A	118	PRO	2.1
1	A	160	PRO	2.1
1	D	196	CYS	2.1
1	A	30	LEU	2.1
1	C	319	PRO	2.1
1	A	55	THR	2.1
1	A	93	ASP	2.1
1	C	34	PRO	2.1
1	B	128	LEU	2.1
1	C	251	LEU	2.1
1	B	253	THR	2.1
1	B	88	GLY	2.1
1	B	351	SER	2.1
1	C	32	SER	2.1
1	D	120	LEU	2.0

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	301	TRP	2.0
1	B	353	MET	2.0
1	B	208	ASN	2.0
1	B	281	TRP	2.0
1	B	333	GLU	2.0
1	A	144	LYS	2.0
1	A	185	ILE	2.0
1	A	111	LEU	2.0
1	A	150	TRP	2.0
1	A	257	PHE	2.0
1	B	102	LEU	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](#)

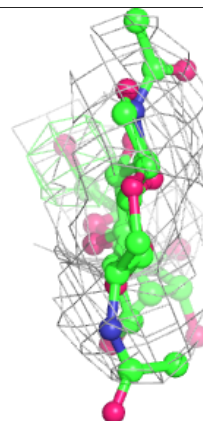
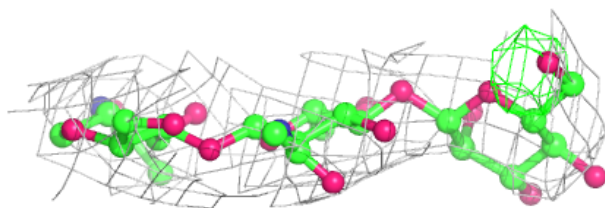
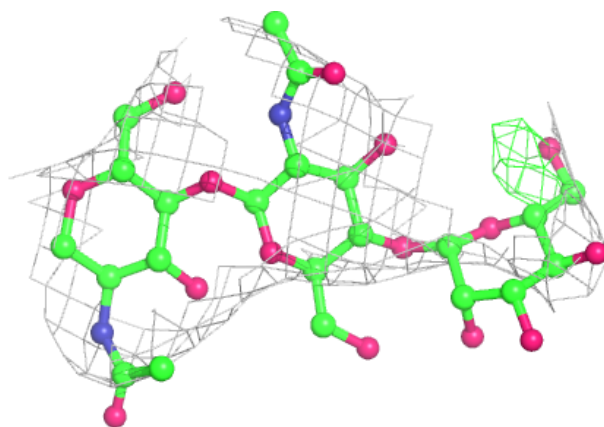
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
2	BMA	E	3	11/12	0.41	0.36	381,388,392,393	0
3	NAG	G	2	14/15	0.71	0.32	245,281,331,396	0
3	NAG	F	2	14/15	0.73	0.33	248,281,331,396	0
3	NAG	G	1	14/15	0.84	0.14	173,207,246,264	0
2	NAG	E	2	14/15	0.85	0.20	241,286,333,396	0
3	NAG	F	1	14/15	0.91	0.15	159,210,239,242	0
2	NAG	E	1	14/15	0.92	0.14	159,212,228,250	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.

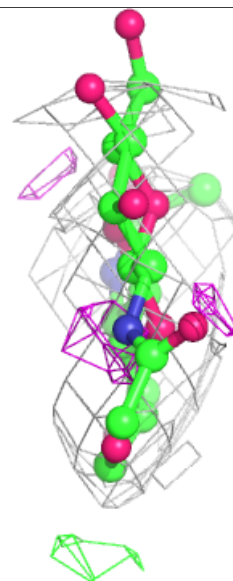
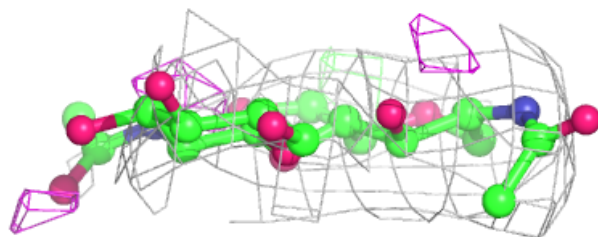
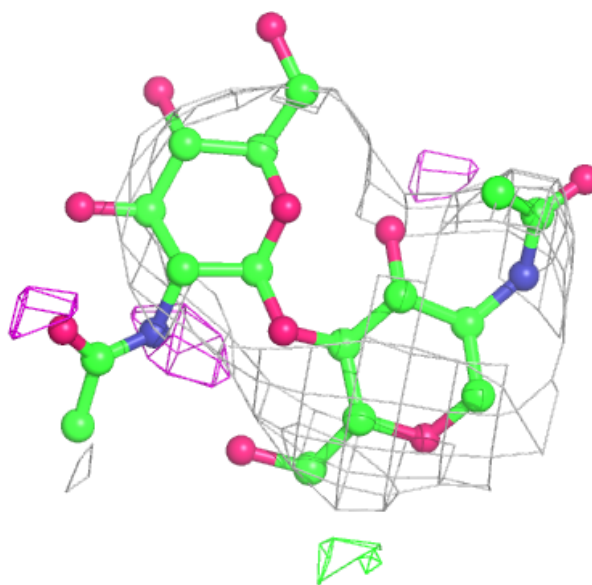
**Electron density around Chain E:**

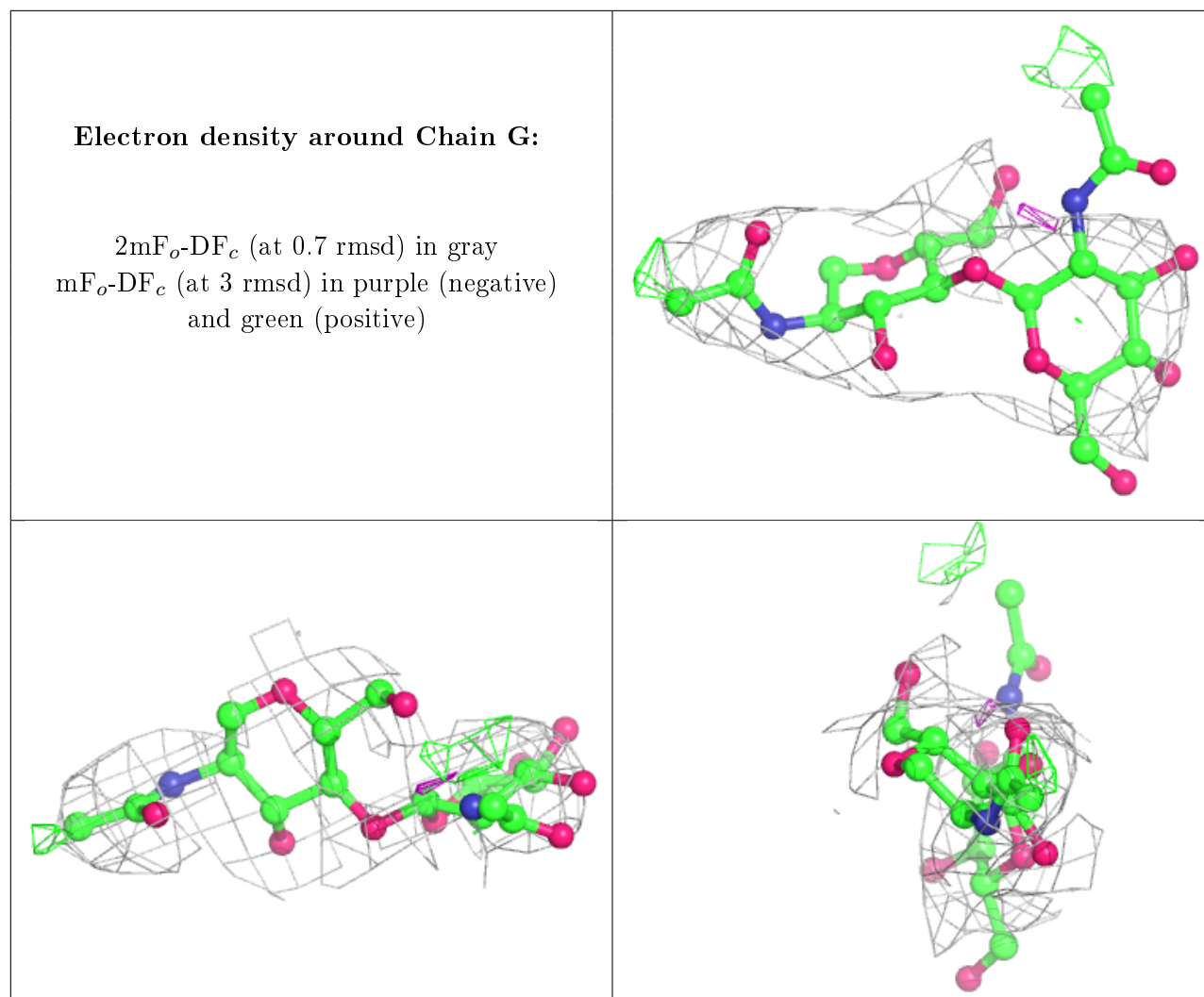
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain F:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.