



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 11:09 pm GMT

PDB ID : 8OG4  
Title : Exostosin-like 3 UDP complex  
Authors : Sammon, D.; Hohenester, E.  
Deposited on : 2023-03-18  
Resolution : 2.10 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
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) : 2.36

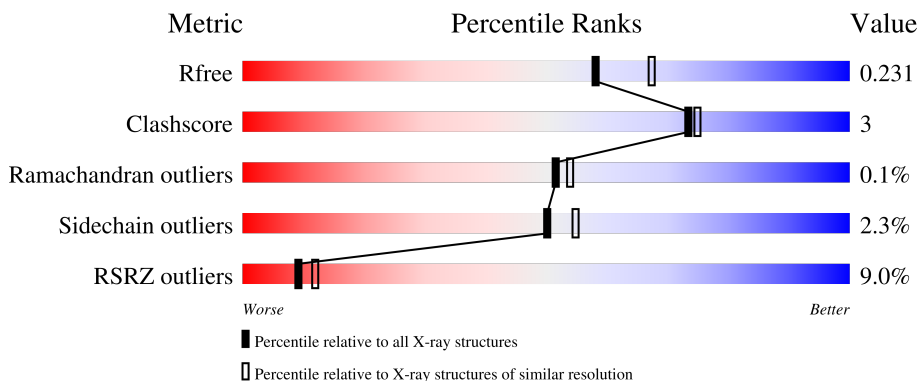
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.



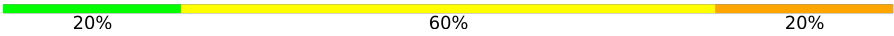
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	891	 7% 72% 7% 20%
1	B	891	 7% 72% 7% 20%
2	C	2	 50% 50%
2	E	2	 50% 50%
3	D	5	 20% 60% 20%

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Mol	Chain	Length	Quality of chain
3	F	5	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 23044 atoms, of which 11305 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 Exostosin-like 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	710	11298	3697	5580	970	1021	30	0	6	0
1	B	710	11292	3696	5575	970	1021	30	0	5	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ALA	-	expression tag	UNP O43909
A	30	PRO	-	expression tag	UNP O43909
A	31	LEU	-	expression tag	UNP O43909
A	32	VAL	-	expression tag	UNP O43909
A	33	HIS	-	expression tag	UNP O43909
A	34	HIS	-	expression tag	UNP O43909
A	35	HIS	-	expression tag	UNP O43909
A	36	HIS	-	expression tag	UNP O43909
A	37	HIS	-	expression tag	UNP O43909
A	38	HIS	-	expression tag	UNP O43909
A	39	ALA	-	expression tag	UNP O43909
A	40	LEU	-	expression tag	UNP O43909
A	41	ASP	-	expression tag	UNP O43909
A	42	GLU	-	expression tag	UNP O43909
A	43	ASN	-	expression tag	UNP O43909
A	44	LEU	-	expression tag	UNP O43909
A	45	TYR	-	expression tag	UNP O43909
A	46	PHE	-	expression tag	UNP O43909
A	47	GLN	-	expression tag	UNP O43909
A	48	GLY	-	expression tag	UNP O43909
A	49	ALA	-	expression tag	UNP O43909
A	50	LEU	-	expression tag	UNP O43909
A	51	ALA	-	expression tag	UNP O43909
B	29	ALA	-	expression tag	UNP O43909
B	30	PRO	-	expression tag	UNP O43909

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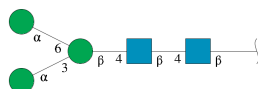
Chain	Residue	Modelled	Actual	Comment	Reference
B	31	LEU	-	expression tag	UNP O43909
B	32	VAL	-	expression tag	UNP O43909
B	33	HIS	-	expression tag	UNP O43909
B	34	HIS	-	expression tag	UNP O43909
B	35	HIS	-	expression tag	UNP O43909
B	36	HIS	-	expression tag	UNP O43909
B	37	HIS	-	expression tag	UNP O43909
B	38	HIS	-	expression tag	UNP O43909
B	39	ALA	-	expression tag	UNP O43909
B	40	LEU	-	expression tag	UNP O43909
B	41	ASP	-	expression tag	UNP O43909
B	42	GLU	-	expression tag	UNP O43909
B	43	ASN	-	expression tag	UNP O43909
B	44	LEU	-	expression tag	UNP O43909
B	45	TYR	-	expression tag	UNP O43909
B	46	PHE	-	expression tag	UNP O43909
B	47	GLN	-	expression tag	UNP O43909
B	48	GLY	-	expression tag	UNP O43909
B	49	ALA	-	expression tag	UNP O43909
B	50	LEU	-	expression tag	UNP O43909
B	51	ALA	-	expression tag	UNP O43909

- Molecule 2 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	H	N	O			
2	C	2	52	16	24	2	10	0	0	0
2	E	2	52	16	24	2	10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

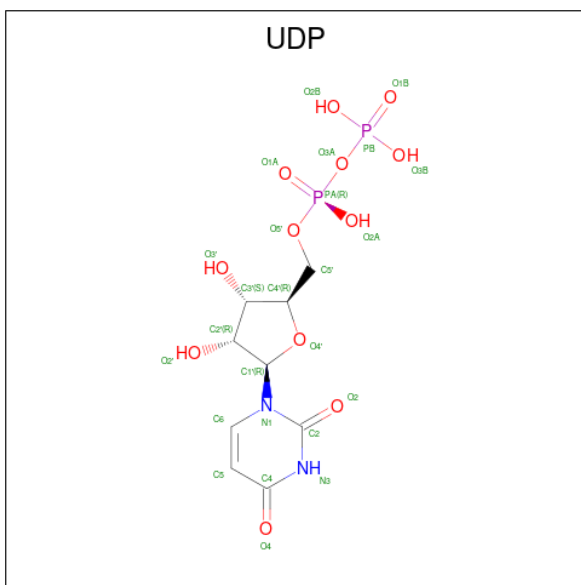


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	D	5	Total	C	H	N	O	0	0	0
			112	34	51	2	25			
3	F	5	Total	C	H	N	O	0	0	0
			112	34	51	2	25			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
5	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	33	Total	O	0	0
			33	33		

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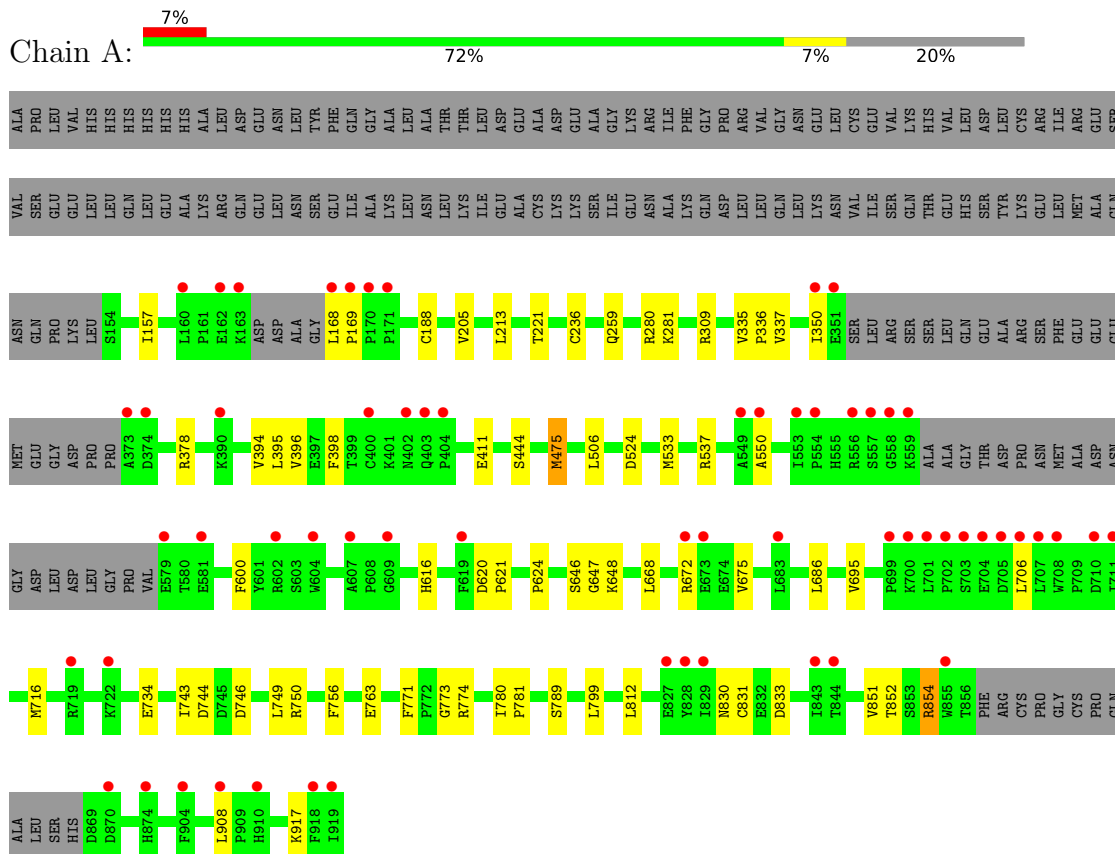
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	B	41	Total	O	0	0
			41	41		

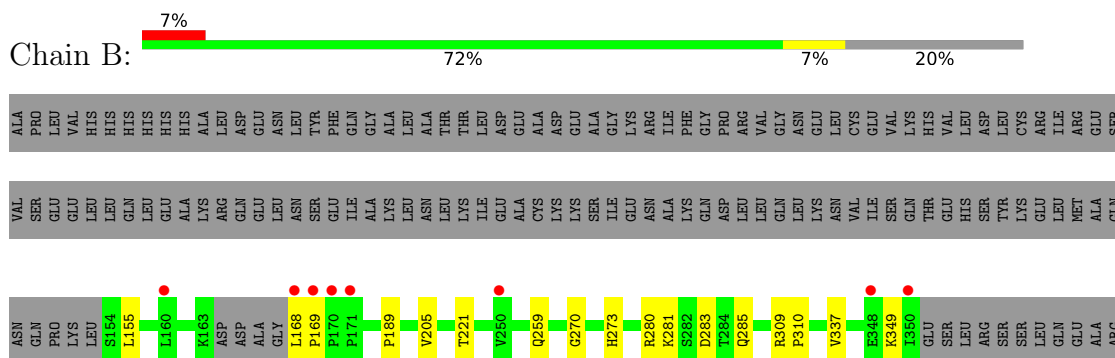
### 3 Residue-property plots [i](#)

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.

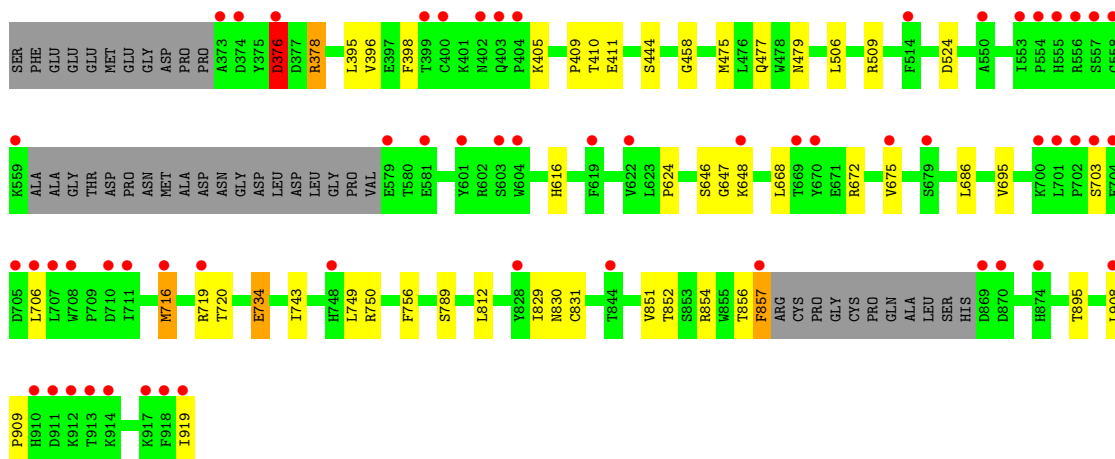
#### • Molecule 1: Exostosin-like 3



#### • Molecule 1: Exostosin-like 3







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

Chain C: 50% 50%

MAG1  
MAG2

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

Chain E: 50% 50%

MAG1  
MAG2

- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 20% 60% 20%

MAG1  
MAG2  
EMA3  
MAIV4  
MAN5

- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 20% 60% 20%

MAG1  
MAG2  
EMA3  
MAIV4  
MAN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.62Å 121.62Å 259.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.52 – 2.10 55.24 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.52-2.10) 93.3 (55.24-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.18rc1_3769, PHENIX 1.18rc1_3769	Depositor
R, $R_{free}$	0.192 , 0.231 0.192 , 0.231	Depositor DCC
$R_{free}$ test set	6107 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23044	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to  $7.4124e-03$ . The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: UDP, NAG, MAN, CSO, MN, BMA

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	0.64	2/5891 (0.0%)	0.75	1/8022 (0.0%)
1	B	0.63	0/5887	0.77	1/8016 (0.0%)
All	All	0.64	2/11778 (0.0%)	0.76	2/16038 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	CYS	CB-SG	-5.20	1.73	1.81
1	A	188	CYS	CB-SG	5.11	1.91	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	854	ARG	NE-CZ-NH2	6.29	123.45	120.30

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	5718	5580	5600	39	0
1	B	5717	5575	5600	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	24	25	0	0
2	E	28	24	25	0	0
3	D	61	51	52	1	0
3	F	61	51	52	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	25	0	11	0	0
5	B	25	0	11	1	0
6	A	33	0	0	1	0
6	B	41	0	0	0	0
All	All	11739	11305	11376	77	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 3.

All (77) 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:851:VAL:HG12	1:B:852:THR:HG23	1.50	0.92
1:A:851:VAL:HG12	1:A:852:THR:HG23	1.54	0.88
1:A:411:GLU:OE1	1:A:444:SER:OG	2.05	0.73
1:B:349:LYS:NZ	1:B:376:ASP:OD2	2.25	0.70
1:B:477:GLN:OE1	1:B:479:ASN:ND2	2.26	0.67
1:A:716:MET:SD	1:A:734:GLU:HG2	2.35	0.66
1:B:854:ARG:HD3	1:B:857:PHE:CE2	2.32	0.65
1:B:411:GLU:OE1	1:B:444:SER:OG	2.05	0.64
1:A:668:LEU:HD12	1:A:695:VAL:HB	1.80	0.62
1:A:221:THR:HG23	1:A:524:ASP:OD1	2.00	0.62
1:B:854:ARG:HG3	1:B:854:ARG:HH21	1.66	0.61
1:A:743:ILE:HD12	1:A:749:LEU:HD12	1.83	0.60
1:B:789:SER:OG	3:F:1:NAG:H81	2.02	0.59
1:A:854:ARG:HH21	1:A:854:ARG:HG3	1.67	0.59
1:A:506:LEU:HD23	1:B:624:PRO:HD2	1.85	0.59
1:A:646:SER:OG	1:A:647:GLY:N	2.36	0.58
1:A:337:VAL:HG22	1:A:506:LEU:HD13	1.84	0.58
1:A:205:VAL:HG21	1:A:259[B]:GLN:HG3	1.85	0.57
1:B:716:MET:SD	1:B:734:GLU:HG2	2.45	0.57
1:B:703:SER:OG	1:B:706:LEU:HD13	2.06	0.56
1:A:537:ARG:NH1	6:A:1101:HOH:O	2.25	0.55
1:A:624:PRO:HD2	1:B:506:LEU:HD23	1.90	0.53
1:B:221:THR:HG23	1:B:524:ASP:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LEU:C	1:B:395:LEU:HD23	2.29	0.53
1:B:280:ARG:NH2	1:B:281:LYS:HD2	2.23	0.52
1:A:763:GLU:OE2	1:B:895:THR:HA	2.09	0.52
1:B:337:VAL:HG22	1:B:506:LEU:HD13	1.90	0.52
1:B:756:PHE:CE2	1:B:851:VAL:HG13	2.45	0.51
1:B:646:SER:OG	1:B:647:GLY:N	2.44	0.50
1:A:280:ARG:NH2	1:A:281:LYS:HD2	2.27	0.49
1:B:672:ARG:HB3	1:B:675:VAL:HG22	1.95	0.49
1:B:168:LEU:N	1:B:169:PRO:HD2	2.29	0.48
1:B:205:VAL:HG21	1:B:259[B]:GLN:HG3	1.96	0.48
1:A:205:VAL:HG22	1:A:259[A]:GLN:HG2	1.95	0.47
1:B:668:LEU:HD12	1:B:695:VAL:HB	1.96	0.47
1:B:830:ASN:O	1:B:831:CYS:HB2	2.15	0.47
1:A:396:VAL:HG12	1:A:398:PHE:CE2	2.50	0.47
1:A:475[A]:MET:HE3	1:A:533:MET:HG2	1.95	0.47
1:A:335:VAL:HG13	1:A:336:PRO:HA	1.97	0.47
1:A:743:ILE:CD1	1:A:749:LEU:HD12	2.44	0.47
1:B:829:ILE:HG22	1:B:829:ILE:O	2.14	0.47
1:A:672:ARG:HB3	1:A:675:VAL:HG22	1.97	0.46
1:B:743:ILE:HD12	1:B:749:LEU:HD12	1.98	0.46
1:B:283:ASP:OD2	1:B:405:LYS:HD3	2.15	0.46
1:B:205:VAL:CG2	1:B:259[B]:GLN:HG3	2.46	0.46
1:A:395:LEU:C	1:A:395:LEU:HD23	2.37	0.45
1:B:396:VAL:CG1	1:B:398:PHE:CE2	2.99	0.45
1:A:550:ALA:HB3	1:A:734:GLU:OE1	2.17	0.45
1:A:168:LEU:N	1:A:169:PRO:HD2	2.32	0.44
1:B:719:ARG:NE	1:B:720:THR:H	2.14	0.44
1:A:780:ILE:HB	1:A:781:PRO:HD3	1.98	0.44
1:B:409:PRO:C	1:B:410:THR:HG23	2.37	0.44
1:B:716:MET:SD	1:B:734:GLU:CG	3.06	0.44
1:A:773:GLY:O	1:A:774:ARG:HD3	2.18	0.43
1:A:756:PHE:CE2	1:A:851:VAL:HG13	2.54	0.43
1:A:620:ASP:OD1	1:A:621:PRO:HD2	2.19	0.43
1:A:799:LEU:HD22	1:A:833:ASP:OD2	2.18	0.43
1:A:205:VAL:CG2	1:A:259[B]:GLN:HG3	2.47	0.43
1:A:789:SER:OG	3:D:1:NAG:H81	2.17	0.43
1:B:706:LEU:HD12	1:B:706:LEU:HA	1.81	0.43
1:A:706:LEU:HD12	1:A:706:LEU:HA	1.90	0.43
1:A:157:ILE:CD1	1:B:378:ARG:HG2	2.49	0.42
1:B:672:ARG:NH2	5:B:1002:UDP:O1A	2.52	0.42
1:A:744:ASP:HB3	1:A:746:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:ASN:OD1	1:A:831:CYS:N	2.52	0.42
1:B:396:VAL:HG12	1:B:398:PHE:CE2	2.55	0.41
1:B:270:GLY:O	1:B:273:HIS:HB2	2.20	0.41
1:B:919:ILE:HD13	1:B:919:ILE:HG21	1.88	0.41
1:B:756:PHE:HE2	1:B:851:VAL:HG13	1.86	0.41
1:B:155:LEU:CD2	1:B:189:PRO:HG3	2.50	0.41
1:A:394:VAL:HG23	1:A:395:LEU:N	2.36	0.41
1:A:475[B]:MET:SD	1:A:600:PHE:CE1	3.14	0.41
1:B:205:VAL:HG22	1:B:259[A]:GLN:HG2	2.03	0.41
1:B:458:GLY:O	1:B:509:ARG:NE	2.43	0.40
1:B:349:LYS:HE3	1:B:410:THR:O	2.21	0.40
1:A:157:ILE:HD11	1:B:378:ARG:HG2	2.04	0.40
1:A:396:VAL:CG1	1:A:398:PHE:CZ	3.05	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	705/891 (79%)	672 (95%)	32 (4%)	1 (0%)	51	54
1	B	704/891 (79%)	673 (96%)	30 (4%)	1 (0%)	51	54
All	All	1409/1782 (79%)	1345 (96%)	62 (4%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	771	PHE
1	B	909	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	621/785 (79%)	608 (98%)	13 (2%)	53	59
1	B	621/785 (79%)	604 (97%)	17 (3%)	44	48
All	All	1242/1570 (79%)	1212 (98%)	30 (2%)	50	53

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	LEU
1	A	309	ARG
1	A	350	ILE
1	A	378	ARG
1	A	475[A]	MET
1	A	475[B]	MET
1	A	616	HIS
1	A	648	LYS
1	A	686	LEU
1	A	750	ARG
1	A	812	LEU
1	A	908	LEU
1	A	917	LYS
1	B	285	GLN
1	B	309	ARG
1	B	310	PRO
1	B	376	ASP
1	B	378	ARG
1	B	475[A]	MET
1	B	475[B]	MET
1	B	616	HIS
1	B	648	LYS
1	B	686	LEU
1	B	716	MET
1	B	734	GLU
1	B	750	ARG
1	B	812	LEU

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Mol	Chain	Res	Type
1	B	856	THR
1	B	857	PHE
1	B	908	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	CSO	A	606	1	3,6,7	0.75	0	0,6,8	-	-
1	CSO	B	606	1	3,6,7	0.77	0	0,6,8	-	-

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
1	CSO	A	606	1	-	0/1/5/7	-
1	CSO	B	606	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates i

14 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	C	1	2,1	14,14,15	0.53	0	17,19,21	0.62	0
2	NAG	C	2	2	14,14,15	0.85	1 (7%)	17,19,21	0.90	0
3	NAG	D	1	1,3	14,14,15	0.54	0	17,19,21	0.89	1 (5%)
3	NAG	D	2	3	14,14,15	0.43	0	17,19,21	0.70	0
3	BMA	D	3	3	11,11,12	1.58	2 (18%)	15,15,17	1.40	3 (20%)
3	MAN	D	4	3	11,11,12	1.52	2 (18%)	15,15,17	1.90	5 (33%)
3	MAN	D	5	3	11,11,12	2.15	4 (36%)	15,15,17	1.80	4 (26%)
2	NAG	E	1	2,1	14,14,15	0.51	0	17,19,21	0.68	0
2	NAG	E	2	2	14,14,15	0.78	1 (7%)	17,19,21	0.89	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.52	0	17,19,21	0.82	1 (5%)
3	NAG	F	2	3	14,14,15	0.41	0	17,19,21	0.74	0
3	BMA	F	3	3	11,11,12	1.65	3 (27%)	15,15,17	1.31	3 (20%)
3	MAN	F	4	3	11,11,12	1.98	5 (45%)	15,15,17	1.75	2 (13%)
3	MAN	F	5	3	11,11,12	2.40	6 (54%)	15,15,17	1.76	4 (26%)

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	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5	MAN	C1-C2	4.41	1.62	1.52
3	F	5	MAN	C2-C3	3.97	1.58	1.52
3	D	5	MAN	C1-C2	3.69	1.60	1.52
3	D	5	MAN	C2-C3	3.56	1.57	1.52
3	D	3	BMA	O5-C1	-3.35	1.38	1.43
3	F	4	MAN	O6-C6	3.23	1.56	1.42
3	F	4	MAN	O3-C3	2.97	1.50	1.43
3	D	5	MAN	O5-C5	2.88	1.49	1.43
2	C	2	NAG	O5-C1	-2.85	1.39	1.43
3	D	4	MAN	C4-C5	2.77	1.58	1.53
3	F	5	MAN	C4-C5	2.70	1.58	1.53
3	F	5	MAN	O5-C5	2.67	1.48	1.43
3	F	5	MAN	O3-C3	2.57	1.49	1.43
2	E	2	NAG	O5-C1	-2.57	1.39	1.43
3	F	3	BMA	C4-C3	2.55	1.58	1.52
3	D	4	MAN	C4-C3	2.54	1.58	1.52
3	F	4	MAN	O5-C5	2.54	1.48	1.43
3	F	4	MAN	O2-C2	2.32	1.48	1.43
3	F	4	MAN	C4-C3	2.31	1.58	1.52
3	D	5	MAN	O3-C3	2.21	1.48	1.43
3	D	3	BMA	O5-C5	2.19	1.47	1.43
3	F	3	BMA	O5-C1	-2.16	1.40	1.43
3	F	3	BMA	O5-C5	2.11	1.47	1.43
3	F	5	MAN	C4-C3	2.11	1.57	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	O2-C2-C1	4.25	117.86	109.15
3	D	5	MAN	C1-O5-C5	4.05	117.68	112.19
3	F	4	MAN	O2-C2-C1	3.68	116.69	109.15
3	F	4	MAN	O2-C2-C3	-3.64	102.85	110.14
3	D	5	MAN	C1-C2-C3	3.52	113.99	109.67
3	F	5	MAN	C1-O5-C5	3.39	116.78	112.19
3	D	4	MAN	O2-C2-C3	-3.23	103.67	110.14
3	F	5	MAN	C1-C2-C3	3.06	113.43	109.67
3	F	5	MAN	O3-C3-C2	2.66	115.09	109.99
3	D	3	BMA	C6-C5-C4	2.64	119.18	113.00
2	E	2	NAG	C1-O5-C5	2.63	115.75	112.19
3	F	5	MAN	O2-C2-C3	-2.62	104.89	110.14
3	F	1	NAG	C1-O5-C5	2.55	115.64	112.19
3	D	5	MAN	O2-C2-C3	-2.47	105.20	110.14
3	F	3	BMA	C2-C3-C4	-2.40	106.73	110.89
3	D	4	MAN	C3-C4-C5	2.35	114.44	110.24
3	D	5	MAN	O5-C5-C6	2.26	110.74	107.20
3	D	3	BMA	O3-C3-C2	2.20	114.21	109.99
3	D	3	BMA	O5-C5-C6	-2.16	103.82	107.20
3	D	4	MAN	C1-C2-C3	-2.14	107.03	109.67
3	F	3	BMA	O3-C3-C2	2.11	114.04	109.99
3	D	4	MAN	O4-C4-C3	-2.08	105.55	110.35
3	F	3	BMA	O2-C2-C3	-2.07	106.00	110.14
3	D	1	NAG	C1-O5-C5	2.03	114.95	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4	MAN	C4-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

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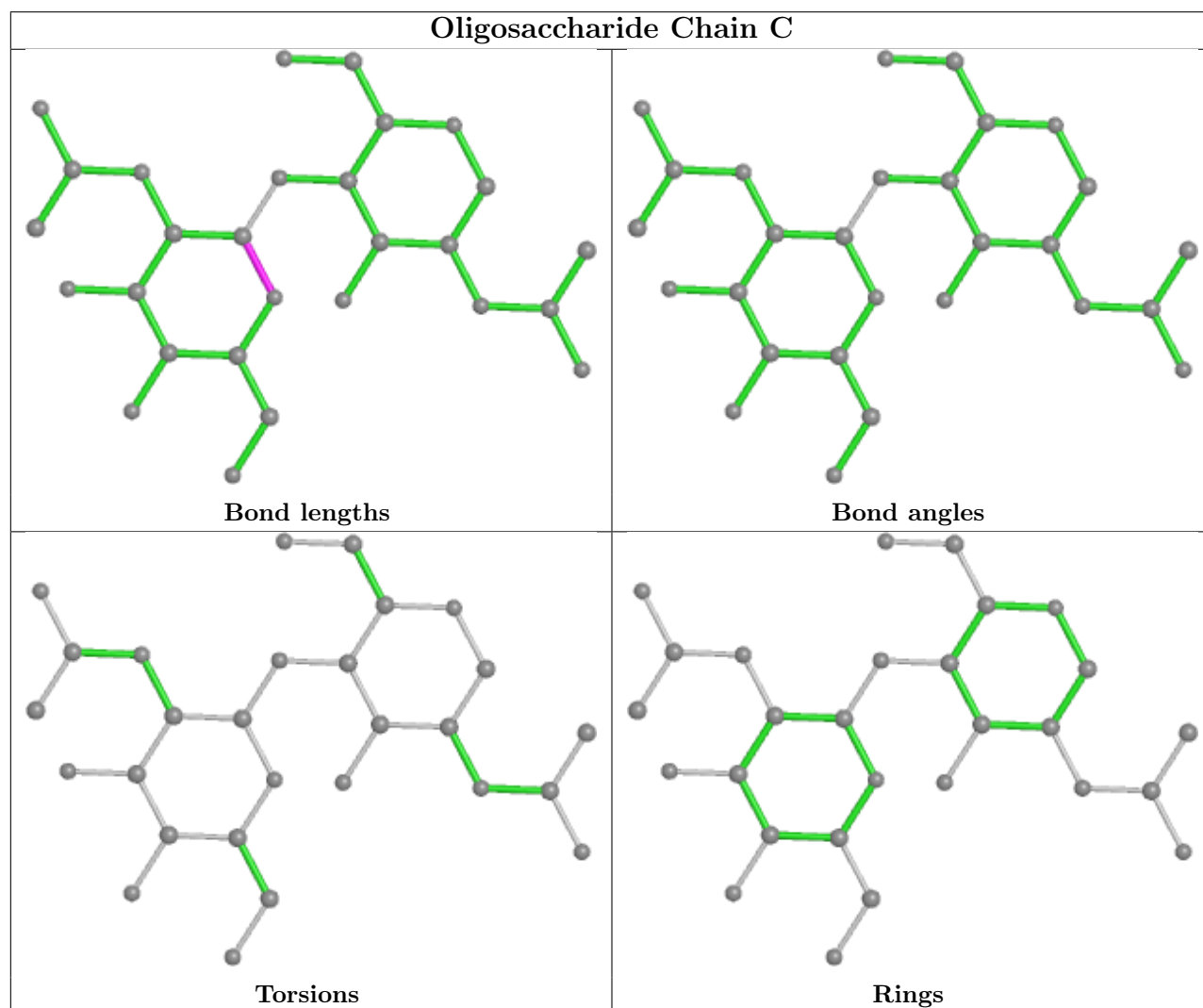
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6

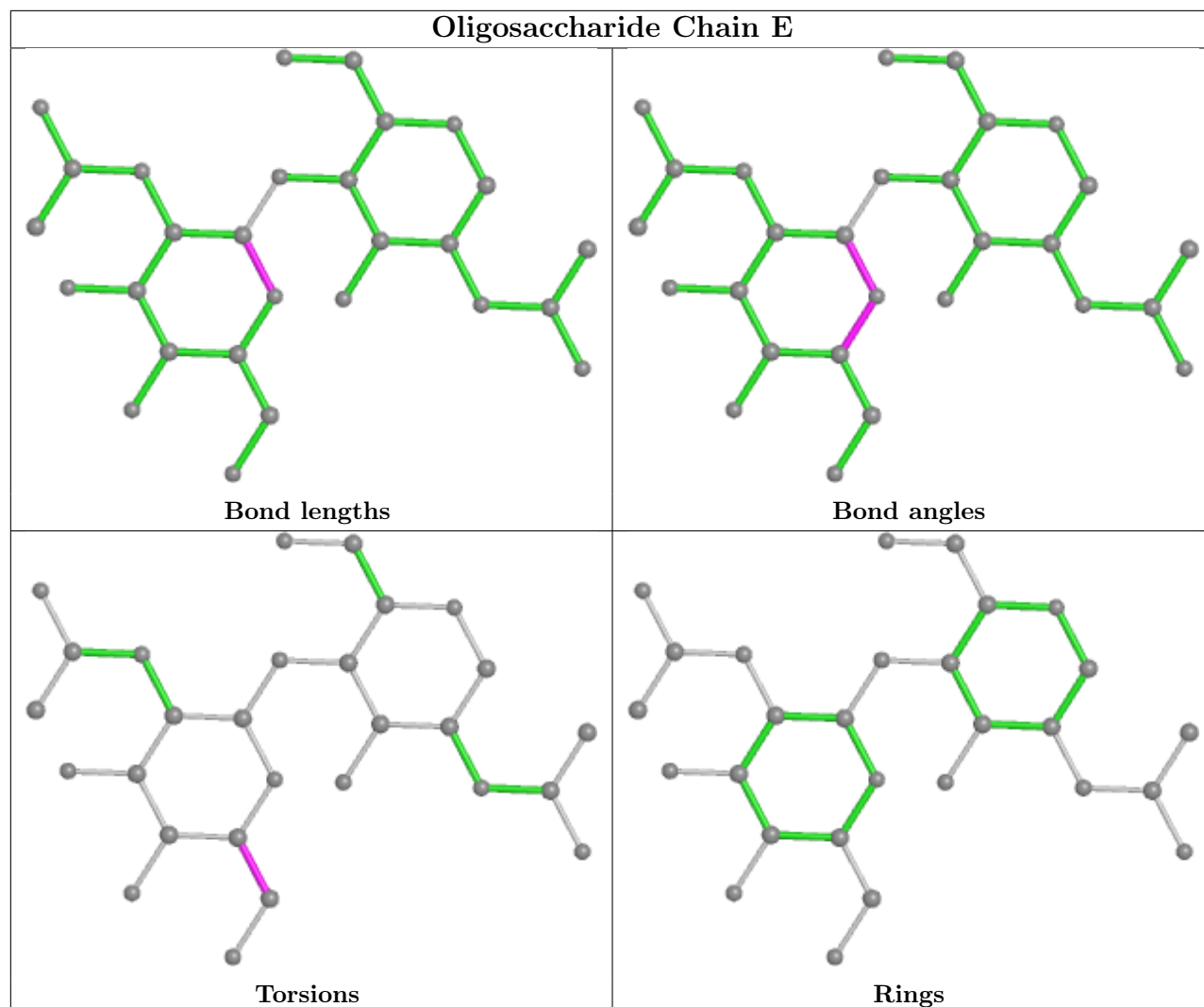
There are no ring outliers.

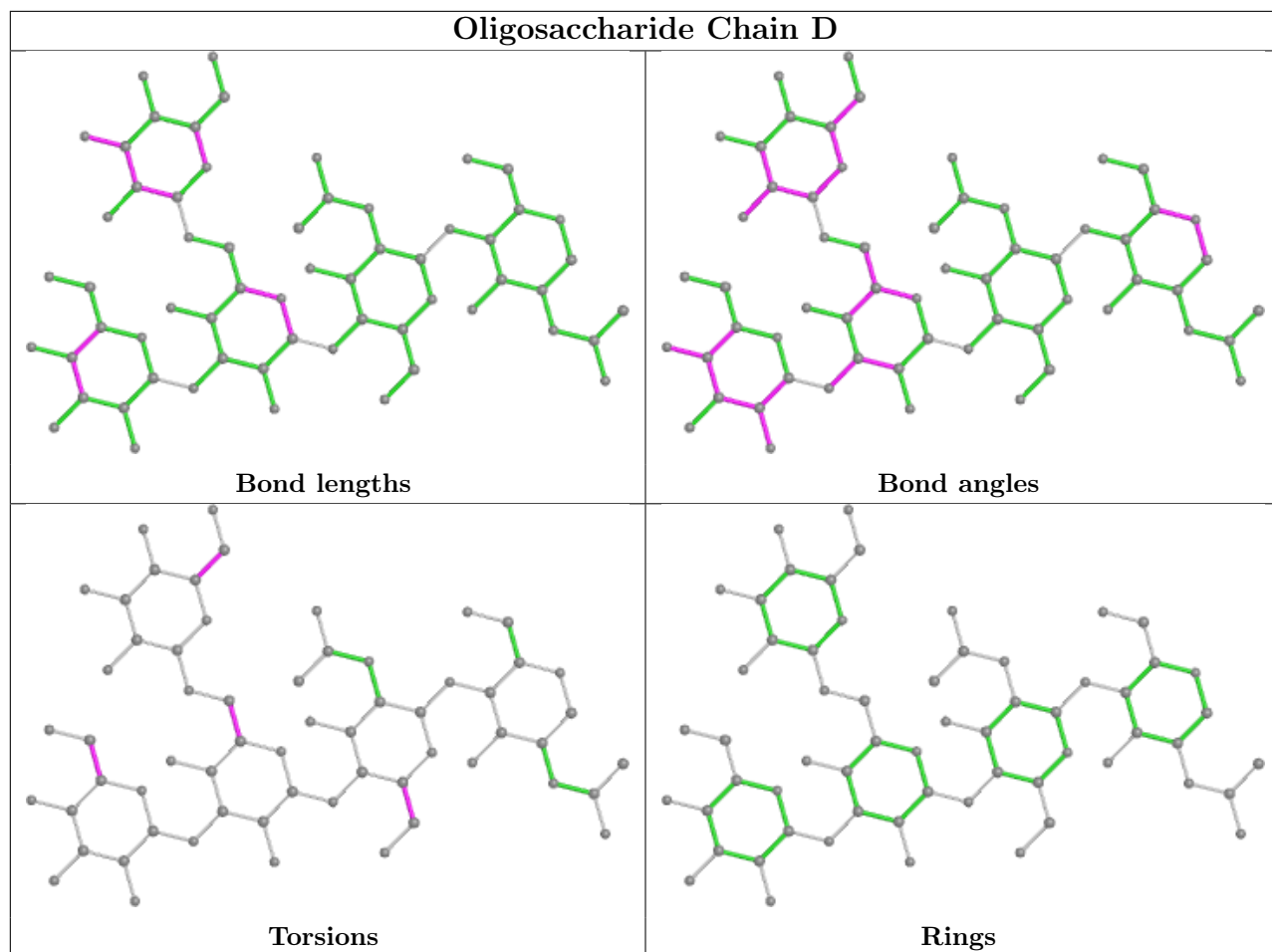
2 monomers are involved in 2 short contacts:

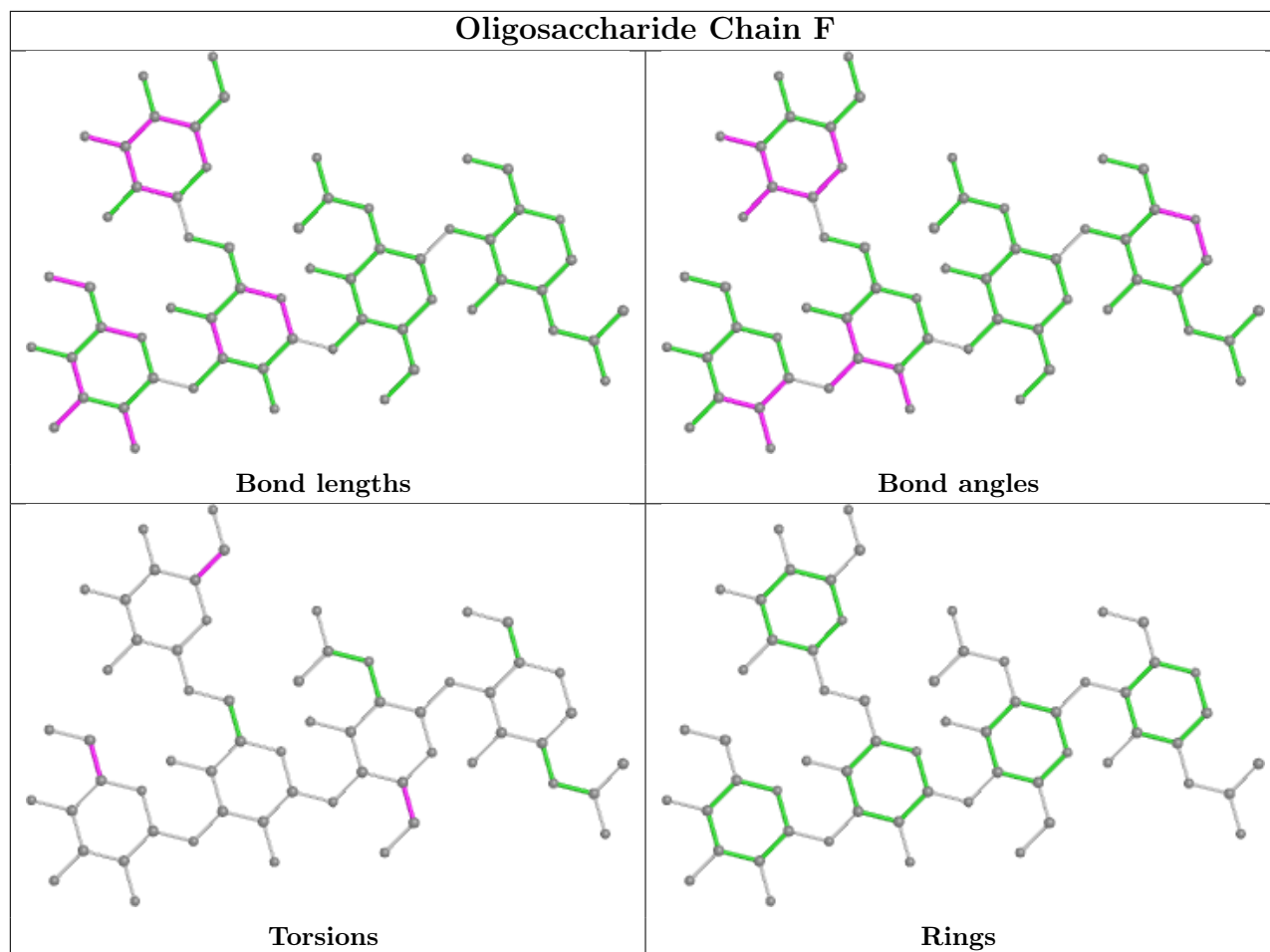
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
3	F	1	NAG	1	0

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 [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	UDP	B	1002	4	24,26,26	0.54	0	37,40,40	0.94	2 (5%)
5	UDP	A	1002	4	24,26,26	0.41	0	37,40,40	0.78	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	UDP	B	1002	4	-	0/16/32/32	0/2/2/2
5	UDP	A	1002	4	-	0/16/32/32	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	B	1002	UDP	PA-O3A-PB	-3.76	119.93	132.83
5	A	1002	UDP	PA-O3A-PB	-3.49	120.84	132.83
5	B	1002	UDP	O3B-PB-O3A	2.16	111.87	104.64

There are no chirality outliers.

There are no torsion outliers.

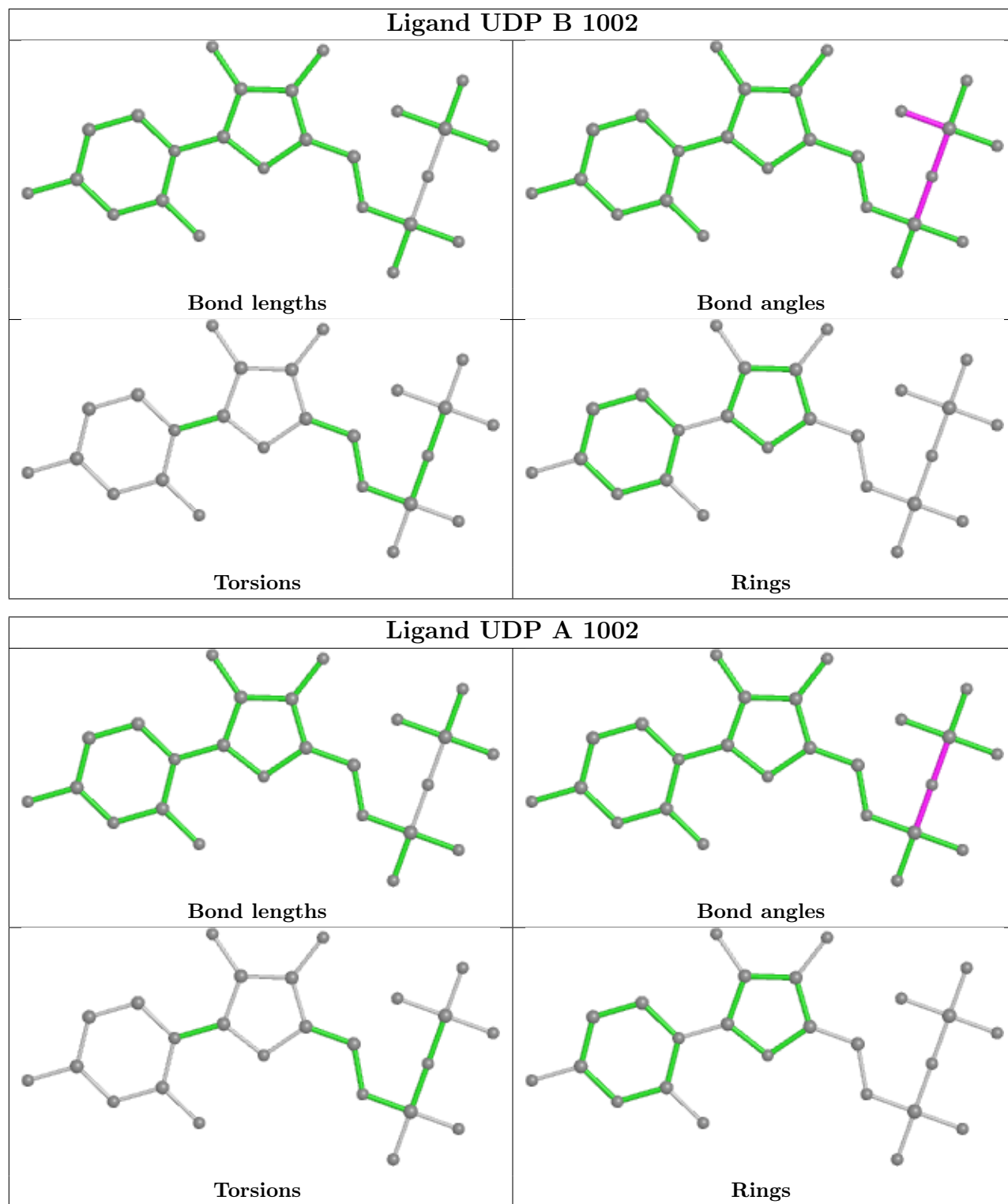
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1002	UDP	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	709/891 (79%)	0.55	61 (8%) <b>10</b>   <b>13</b>	43, 60, 100, 176	0
1	B	709/891 (79%)	0.55	66 (9%) <b>8</b>   <b>11</b>	43, 61, 100, 149	0
All	All	1418/1782 (79%)	0.55	127 (8%) <b>9</b>   <b>12</b>	43, 60, 100, 176	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	707	LEU	10.3
1	B	706	LEU	8.0
1	B	707	LEU	7.7
1	A	706	LEU	7.5
1	A	910	HIS	6.5
1	A	350	ILE	6.4
1	B	557	SER	5.8
1	A	559	LYS	5.7
1	A	619[A]	PHE	5.5
1	A	704	GLU	5.3
1	B	704	GLU	5.3
1	A	558	GLY	5.3
1	B	350	ILE	5.2
1	A	705	ASP	5.1
1	B	169	PRO	5.0
1	B	870	ASP	5.0
1	A	373	ALA	4.9
1	B	374	ASP	4.5
1	B	701	LEU	4.4
1	A	351	GLU	4.3
1	B	558	GLY	4.2
1	A	701	LEU	4.1
1	A	708	TRP	4.1
1	B	703	SER	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	168	LEU	4.0
1	B	908	LEU	3.9
1	B	373	ALA	3.9
1	B	579	GLU	3.9
1	A	403	GLN	3.9
1	A	719	ARG	3.8
1	B	911	ASP	3.8
1	B	553	ILE	3.8
1	B	917	LYS	3.7
1	B	719	ARG	3.6
1	A	919	ILE	3.6
1	B	919	ILE	3.6
1	B	559	LYS	3.5
1	B	400	CYS	3.5
1	B	675	VAL	3.5
1	B	619	PHE	3.4
1	A	711	ILE	3.4
1	B	918	PHE	3.3
1	A	703	SER	3.3
1	A	579	GLU	3.3
1	A	827	GLU	3.2
1	A	404	PRO	3.2
1	A	918	PHE	3.2
1	A	700	LYS	3.1
1	B	869	ASP	3.1
1	A	169	PRO	3.1
1	B	914	LYS	3.1
1	B	160	LEU	3.1
1	A	870	ASP	3.1
1	B	748	HIS	3.0
1	B	556	ARG	3.0
1	B	555	HIS	3.0
1	B	670	TYR	3.0
1	B	376	ASP	3.0
1	A	160	LEU	3.0
1	B	702	PRO	3.0
1	B	910	HIS	3.0
1	A	374	ASP	3.0
1	B	708	TRP	2.9
1	B	912	LYS	2.9
1	B	403	GLN	2.9
1	A	557	SER	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	913	THR	2.9
1	A	168	LEU	2.9
1	A	554	PRO	2.9
1	A	400	CYS	2.9
1	A	702	PRO	2.9
1	A	402	ASN	2.8
1	A	722	LYS	2.8
1	B	170	PRO	2.8
1	A	602	ARG	2.8
1	B	705	ASP	2.7
1	B	550	ALA	2.7
1	A	855	TRP	2.7
1	B	171	PRO	2.6
1	B	679	SER	2.6
1	B	402	ASN	2.6
1	A	829	ILE	2.6
1	A	828	TYR	2.5
1	B	648	LYS	2.5
1	A	710	ASP	2.5
1	B	857	PHE	2.5
1	A	162	GLU	2.5
1	A	607	ALA	2.5
1	A	163	LYS	2.5
1	A	171	PRO	2.4
1	B	710	ASP	2.4
1	A	904	PHE	2.4
1	B	716	MET	2.4
1	A	673	GLU	2.4
1	B	828	TYR	2.4
1	A	556	ARG	2.4
1	B	604	TRP	2.4
1	A	553	ILE	2.3
1	A	672	ARG	2.3
1	B	844	THR	2.3
1	B	348	GLU	2.3
1	B	581	GLU	2.3
1	B	601	TYR	2.3
1	A	844	THR	2.3
1	A	874	HIS	2.3
1	B	874	HIS	2.3
1	A	699	PRO	2.3
1	B	404	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	554	PRO	2.2
1	A	604	TRP	2.2
1	B	250	VAL	2.2
1	B	514	PHE	2.2
1	A	683	LEU	2.2
1	B	622	VAL	2.1
1	A	549	ALA	2.1
1	A	581	GLU	2.1
1	A	908	LEU	2.1
1	A	609	GLY	2.1
1	A	170	PRO	2.1
1	A	550	ALA	2.1
1	A	390	LYS	2.1
1	B	399	THR	2.1
1	B	603	SER	2.1
1	B	700	LYS	2.1
1	A	843	ILE	2.0
1	B	669	THR	2.0
1	B	711	ILE	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(Å <sup>2</sup> )	Q<0.9
1	CSO	A	606	7/8	0.96	0.31	37,53,71,86	0
1	CSO	B	606	7/8	0.96	0.23	39,47,68,81	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.

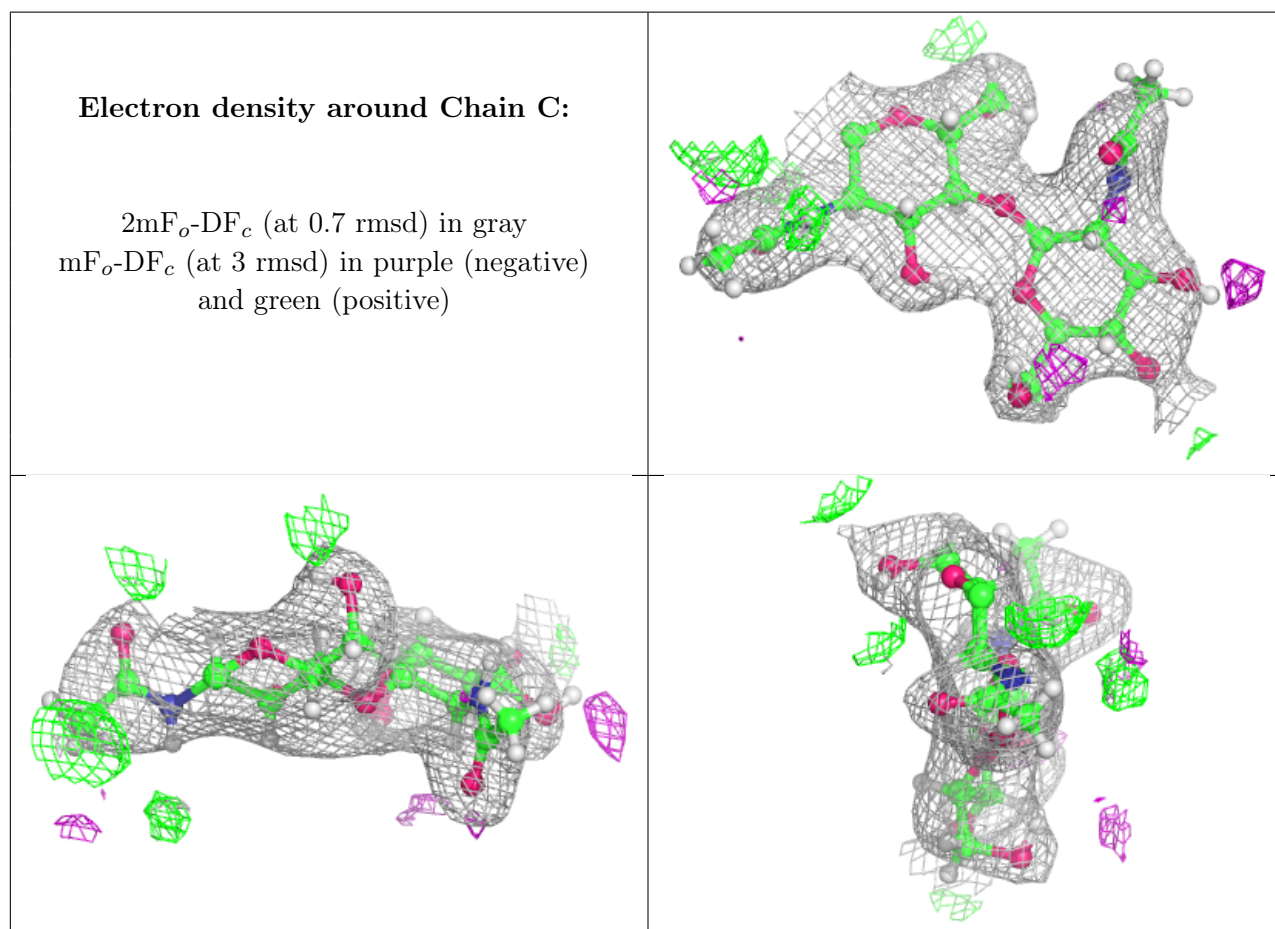
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	D	5	11/12	0.62	0.24	87,119,147,151	0
3	MAN	F	5	11/12	0.78	0.17	82,100,120,129	0

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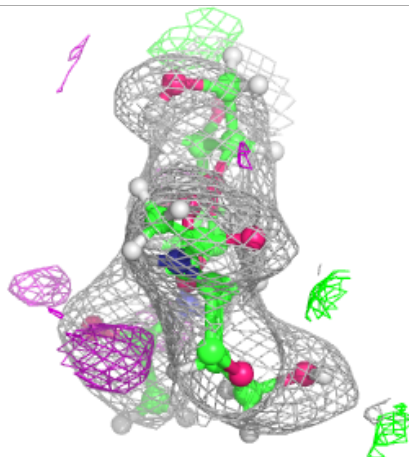
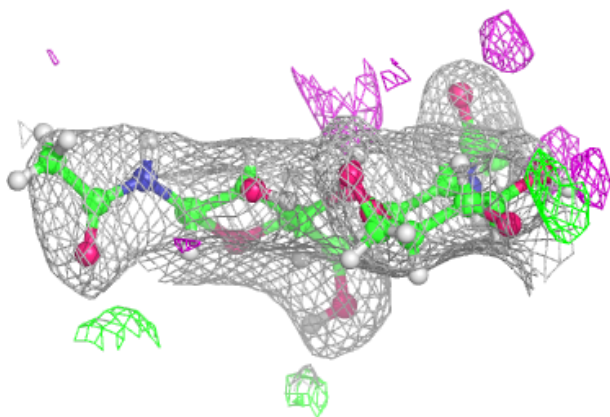
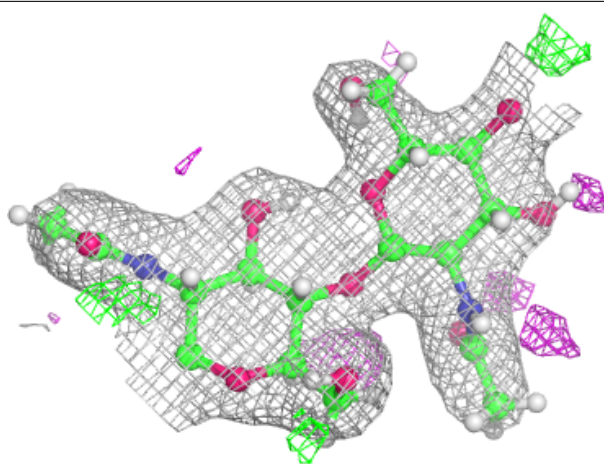
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	E	2	14/15	0.85	0.16	59,83,104,116	0
3	MAN	F	4	11/12	0.89	0.16	66,89,107,107	0
3	BMA	D	3	11/12	0.89	0.20	81,102,122,123	0
3	MAN	D	4	11/12	0.90	0.24	89,104,125,125	0
3	NAG	D	2	14/15	0.94	0.11	65,88,106,110	0
3	NAG	F	2	14/15	0.94	0.13	59,79,95,99	0
2	NAG	C	2	14/15	0.94	0.17	60,82,102,107	0
3	NAG	D	1	14/15	0.94	0.12	61,79,93,107	0
3	BMA	F	3	11/12	0.96	0.11	60,77,104,104	0
3	NAG	F	1	14/15	0.96	0.12	56,70,91,99	0
2	NAG	C	1	14/15	0.96	0.10	51,63,73,77	0
2	NAG	E	1	14/15	0.97	0.09	52,63,74,83	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:**

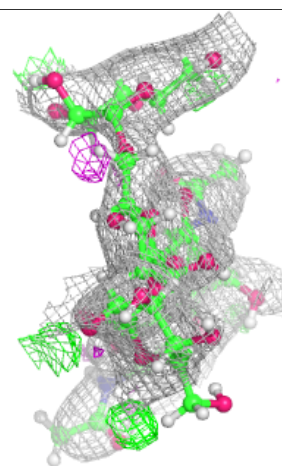
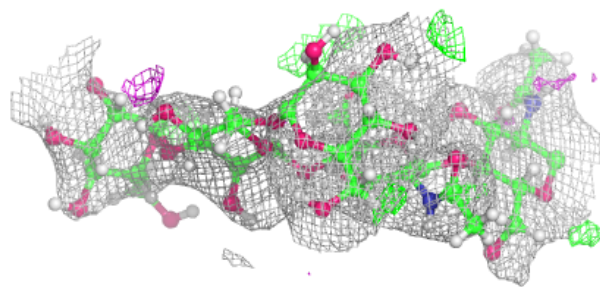
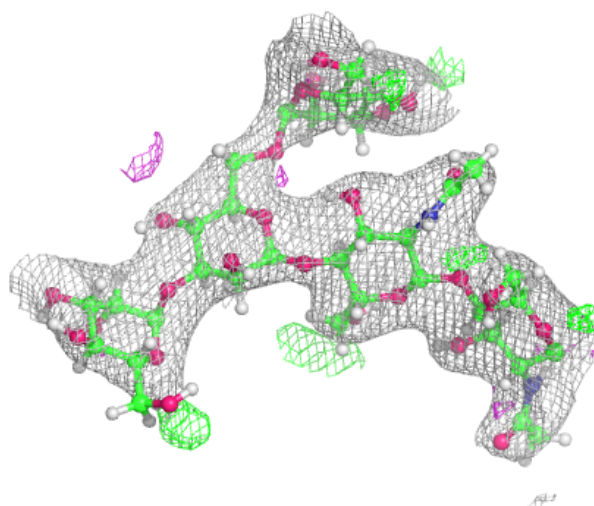
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

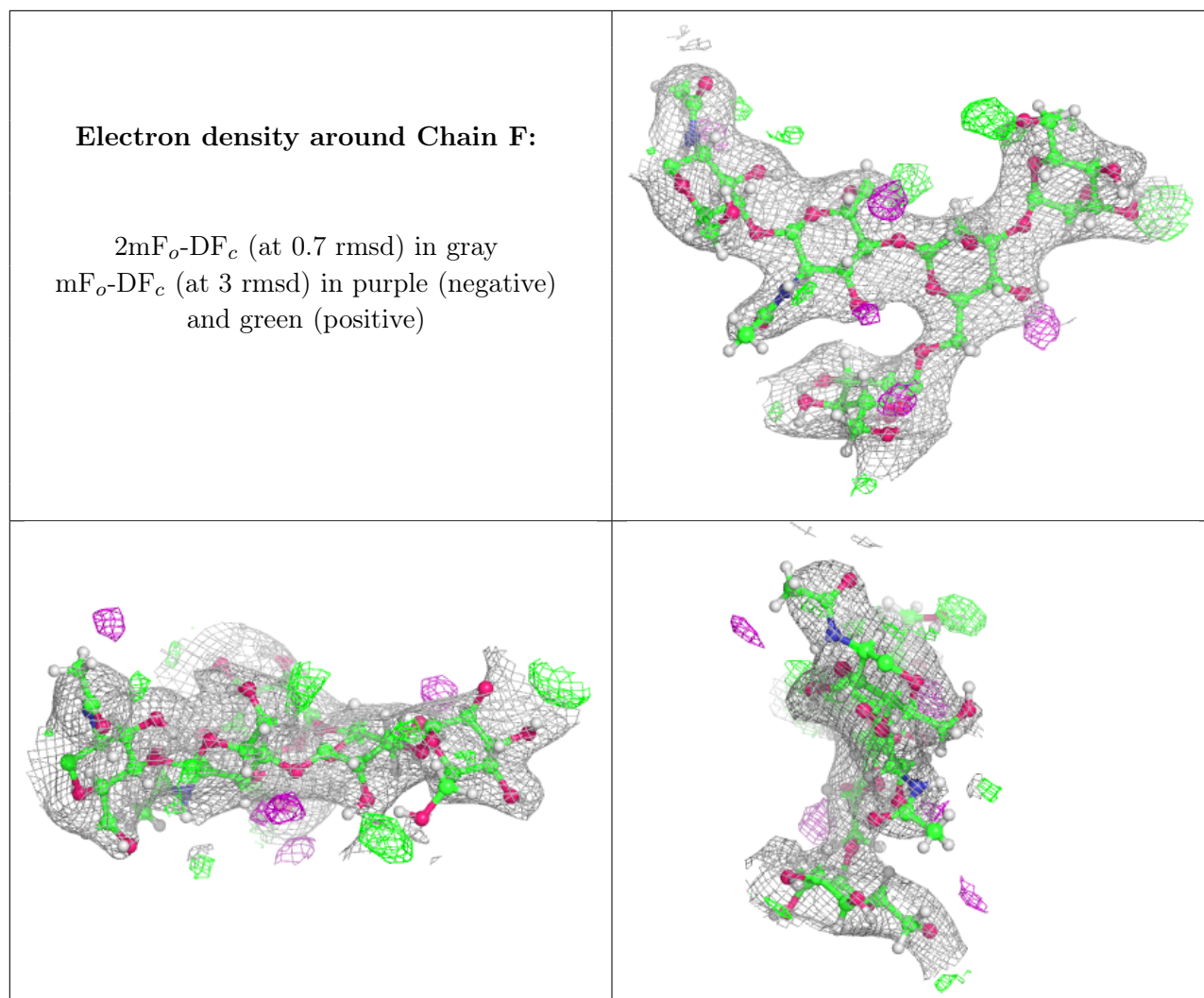




**Electron density around Chain D:**

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





## 6.4 Ligands [i](#)

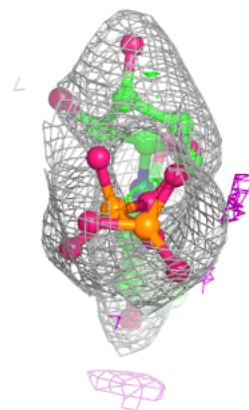
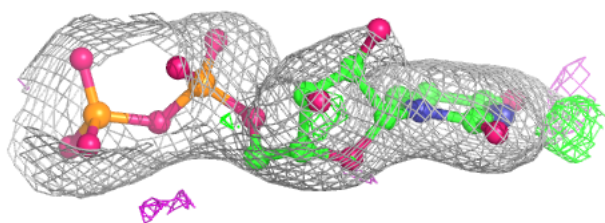
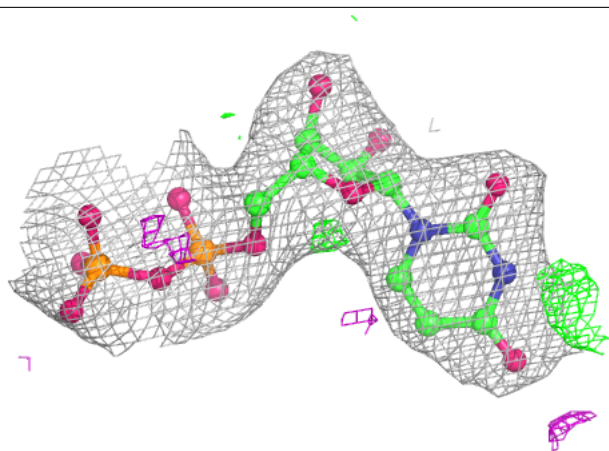
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

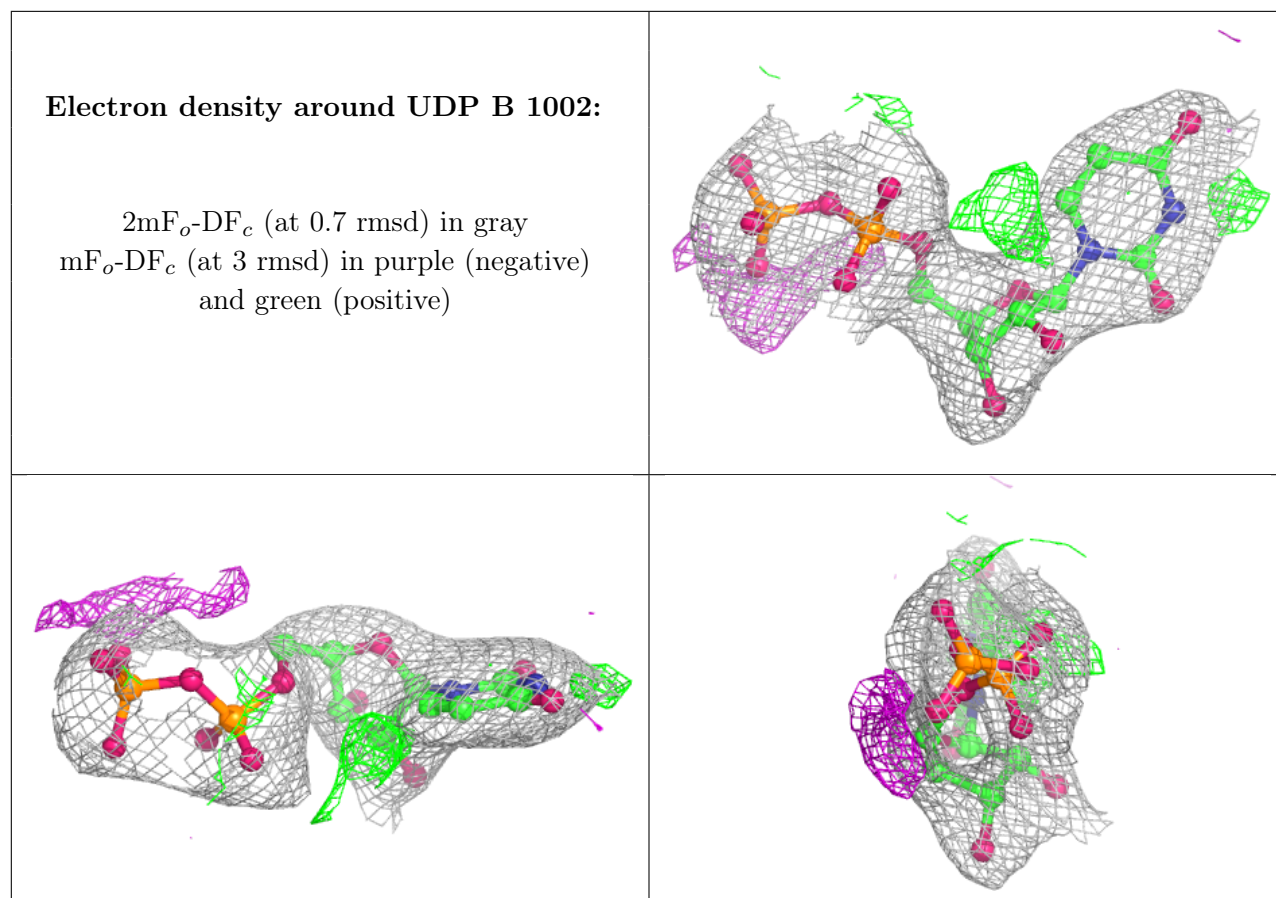
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MN	A	1001	1/1	0.82	0.05	105,105,105,105	0
4	MN	B	1001	1/1	0.95	0.07	94,94,94,94	0
5	UDP	A	1002	25/25	0.95	0.11	57,78,109,120	0
5	UDP	B	1002	25/25	0.95	0.11	58,73,98,103	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around UDP A 1002:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.