



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:04 PM UTC

PDB ID : 8OG4 / pdb_00008og4
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

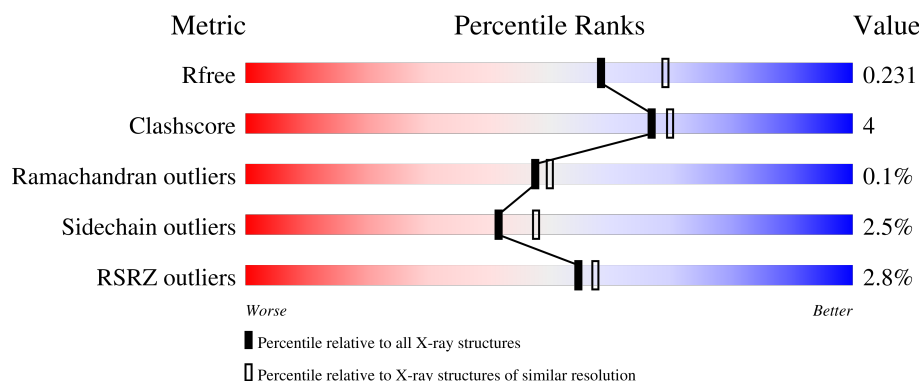
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 ≥ 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	2% 72% 8% 20%
1	B	891	2% 71% 8% 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	20% 60% 20%

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
1	A	710	Total	C	H	N	O	S	0	6	0
			11298	3697	5580	970	1021	30			
1	B	710	Total	C	H	N	O	S	0	5	0
			11292	3696	5575	970	1021	30			

There are 46 discrepancies between the modelled and reference sequences:

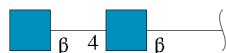
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ALA	-	expression tag	UNP O43909
A	30	PRO	-	expression tag	UNP O43909
A	31	LEU	-	expression tag	UNP O43909
A	32	VAL	-	expression tag	UNP O43909
A	33	HIS	-	expression tag	UNP O43909
A	34	HIS	-	expression tag	UNP O43909
A	35	HIS	-	expression tag	UNP O43909
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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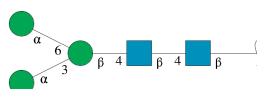
Chain	Residue	Modelled	Actual	Comment	Reference
B	31	LEU	-	expression tag	UNP O43909
B	32	VAL	-	expression tag	UNP O43909
B	33	HIS	-	expression tag	UNP O43909
B	34	HIS	-	expression tag	UNP O43909
B	35	HIS	-	expression tag	UNP O43909
B	36	HIS	-	expression tag	UNP O43909
B	37	HIS	-	expression tag	UNP O43909
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
2	C	2	Total	C	H	N	O	0	0	0
			52	16	24	2	10			
2	E	2	Total	C	H	N	O	0	0	0
			52	16	24	2	10			

- 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.

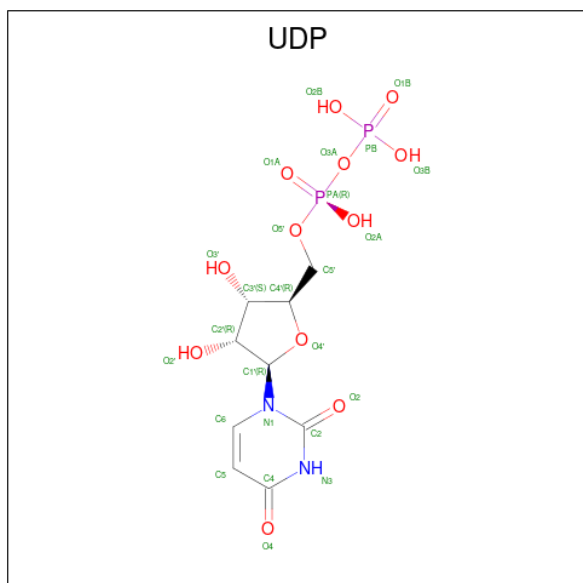


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	5	Total	C	H	N	O	0	0	0
			112	34	51	2	25			
3	F	5	Total	C	H	N	O	0	0	0
			112	34	51	2	25			

- Molecule 4 is MANGANESE (II) ION (CCD ID: 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		

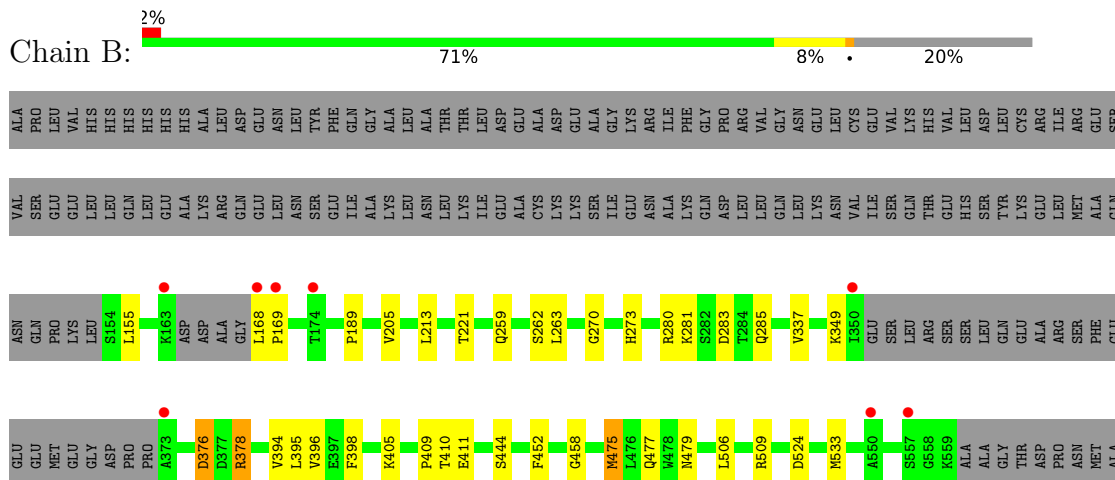
- Molecule 5 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: C₉H₁₄N₂O₁₂P₂).

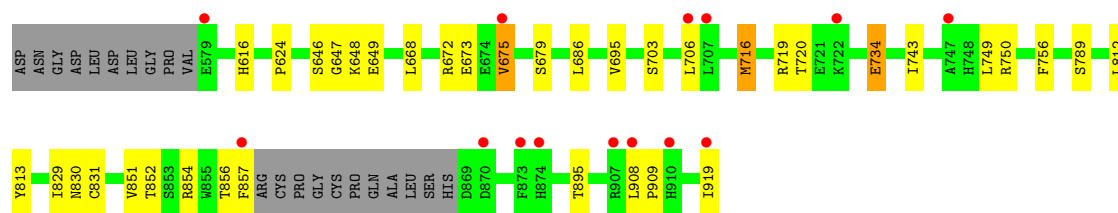


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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	41	Total	O	0	0
			41	41		

- 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%



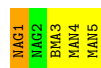
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%



- 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%



- 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%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.62Å 121.62Å 259.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.52 – 2.10 20.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.52-2.10) 93.2 (20.52-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18rc1_3769, PHENIX 1.18rc1_3769	Depositor
R, R_{free}	0.192 , 0.231 0.195 , 0.231	Depositor DCC
R_{free} test set	6562 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23044	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, CSO, MN, MAN, 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	0.59	0/5891	0.74	0/8022
1	B	0.58	0/5887	0.74	0/8016
All	All	0.59	0/11778	0.74	0/16038

There are no bond length outliers.

There are no bond angle outliers.

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	41	0
1	B	5717	5575	5600	48	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	41	0	0	0	0
All	All	11739	11305	11376	84	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 4.

All (84) 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:395:LEU:C	1:B:395:LEU:HD23	2.29	0.57
1:A:329:MET:HE1	1:A:886:VAL:HG22	1.87	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:B:475[A]:MET:HE2	1:B:533:MET:HG2	1.90	0.53
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
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:A:395:LEU:C	1:A:395:LEU:HD23	2.37	0.50
1:A:280:ARG:NH2	1:A:281:LYS:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:409:PRO:C	1:B:410:THR:HG23	2.37	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:A:396:VAL:HG12	1:A:398:PHE:CE2	2.50	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:830:ASN:O	1:B:831:CYS:HB2	2.15	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:B:396:VAL:CG1	1:B:398:PHE:CE2	2.99	0.45
1:A:452:PHE:CD1	1:A:452:PHE:C	2.95	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:813:TYR:C	1:B:813:TYR:CD1	2.95	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: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:B:646:SER:OG	1:B:647:GLY:N	2.44	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:262:SER:O	1:B:263:LEU:C	2.61	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:CD2	1:B:189:PRO:HG3	2.50	0.41
1:B:452:PHE:CD1	1:B:452:PHE:C	2.99	0.41
1:A:813:TYR:CD1	1:A:813:TYR:C	2.99	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:705:ASP:O	1:A:705:ASP:CG	2.63	0.40
1:B:649:GLU:H	1:B:649:GLU:CD	2.29	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%)	48	50
1	B	704/891 (79%)	673 (96%)	30 (4%)	1 (0%)	48	50
All	All	1409/1782 (79%)	1345 (96%)	62 (4%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	771	PHE
1	B	909	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	621/785 (79%)	607 (98%)	14 (2%)	44	51
1	B	621/785 (79%)	602 (97%)	19 (3%)	35	39
All	All	1242/1570 (79%)	1209 (97%)	33 (3%)	42	45

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	LEU
1	A	285	GLN
1	A	305	THR
1	A	350	ILE
1	A	378	ARG
1	A	394	VAL
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	B	213	LEU
1	B	285	GLN
1	B	376	ASP
1	B	378	ARG
1	B	394	VAL
1	B	475[A]	MET
1	B	475[B]	MET
1	B	616	HIS
1	B	648	LYS
1	B	673	GLU
1	B	675	VAL
1	B	679	SER
1	B	686	LEU

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Mol	Chain	Res	Type
1	B	716	MET
1	B	734	GLU
1	B	750	ARG
1	B	812	LEU
1	B	856	THR
1	B	908	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	A	277	ASN
1	A	662	GLN
1	A	684	ASN
1	A	690	ASN
1	B	277	ASN
1	B	393	GLN
1	B	872	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	B	606	1	3,6,7	0.76	0	1,6,8	1.33	0
1	CSO	A	606	1	3,6,7	0.78	0	1,6,8	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	B	606	1	-	0/1/5/7	-
1	CSO	A	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

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	1,2	14,14,15	0.52	0	17,19,21	0.63	0
2	NAG	C	2	2	14,14,15	0.82	1 (7%)	17,19,21	0.92	0
3	NAG	D	1	3,1	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
3	NAG	D	2	3	14,14,15	0.42	0	17,19,21	0.71	0
3	BMA	D	3	3	11,11,12	1.55	2 (18%)	15,15,17	1.31	2 (13%)
3	MAN	D	4	3	11,11,12	1.50	2 (18%)	15,15,17	1.75	4 (26%)
3	MAN	D	5	3	11,11,12	2.11	4 (36%)	15,15,17	1.66	3 (20%)
2	NAG	E	1	1,2	14,14,15	0.54	0	17,19,21	0.69	0
2	NAG	E	2	2	14,14,15	0.75	1 (7%)	17,19,21	0.90	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.50	0	17,19,21	0.83	1 (5%)
3	NAG	F	2	3	14,14,15	0.44	0	17,19,21	0.74	0
3	BMA	F	3	3	11,11,12	1.62	3 (27%)	15,15,17	1.25	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	F	4	3	11,11,12	1.97	5 (45%)	15,15,17	1.64	2 (13%)
3	MAN	F	5	3	11,11,12	2.34	6 (54%)	15,15,17	1.61	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	1,2	-	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	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
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	1,2	-	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	3,1	-	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	4.21	1.62	1.52
3	F	5	MAN	C2-C3	3.83	1.58	1.52
3	D	5	MAN	C1-C2	3.52	1.60	1.52
3	D	5	MAN	C2-C3	3.44	1.57	1.52
3	F	4	MAN	O6-C6	3.25	1.56	1.42
3	D	3	BMA	O5-C1	-3.17	1.38	1.43
3	D	5	MAN	O5-C5	3.00	1.49	1.43
3	F	4	MAN	O3-C3	2.83	1.50	1.43
3	F	5	MAN	O5-C5	2.78	1.48	1.43
3	D	4	MAN	C4-C5	2.74	1.58	1.53
2	C	2	NAG	O5-C1	-2.70	1.39	1.43
3	F	5	MAN	C4-C5	2.67	1.58	1.53
3	F	4	MAN	O5-C5	2.64	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	BMA	C4-C3	2.49	1.58	1.52
3	D	4	MAN	C4-C3	2.48	1.58	1.52
3	F	5	MAN	O3-C3	2.45	1.49	1.43
2	E	2	NAG	O5-C1	-2.43	1.39	1.43
3	F	4	MAN	O2-C2	2.35	1.48	1.43
3	D	3	BMA	O5-C5	2.28	1.47	1.43
3	F	4	MAN	C4-C3	2.26	1.58	1.52
3	F	3	BMA	O5-C5	2.20	1.47	1.43
3	D	5	MAN	O3-C3	2.11	1.48	1.43
3	F	5	MAN	C4-C3	2.06	1.57	1.52
3	F	3	BMA	O5-C1	-2.04	1.40	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	MAN	C1-O5-C5	4.10	117.69	112.19
3	D	4	MAN	O2-C2-C1	3.77	117.86	109.22
3	F	4	MAN	O2-C2-C3	-3.53	102.85	110.15
3	F	5	MAN	C1-O5-C5	3.43	116.78	112.19
3	F	4	MAN	O2-C2-C1	3.26	116.68	109.22
3	D	4	MAN	O2-C2-C3	-3.13	103.67	110.15
3	D	5	MAN	C1-C2-C3	2.99	113.99	109.64
2	E	2	NAG	C1-O5-C5	2.66	115.75	112.19
3	F	5	MAN	C1-C2-C3	2.60	113.43	109.64
3	F	1	NAG	C1-O5-C5	2.58	115.64	112.19
3	F	5	MAN	O2-C2-C3	-2.54	104.89	110.15
3	D	3	BMA	C6-C5-C4	2.51	119.18	113.02
3	F	5	MAN	O3-C3-C2	2.47	115.09	110.05
3	D	5	MAN	O2-C2-C3	-2.39	105.20	110.15
3	F	3	BMA	C2-C3-C4	-2.35	106.73	110.86
3	D	4	MAN	C3-C4-C5	2.32	114.44	110.23
3	D	1	NAG	C1-O5-C5	2.06	114.95	112.19
3	D	4	MAN	O4-C4-C3	-2.05	105.55	110.38
3	D	3	BMA	O3-C3-C2	2.04	114.21	110.05
3	F	3	BMA	O2-C2-C3	-2.00	106.00	110.15

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

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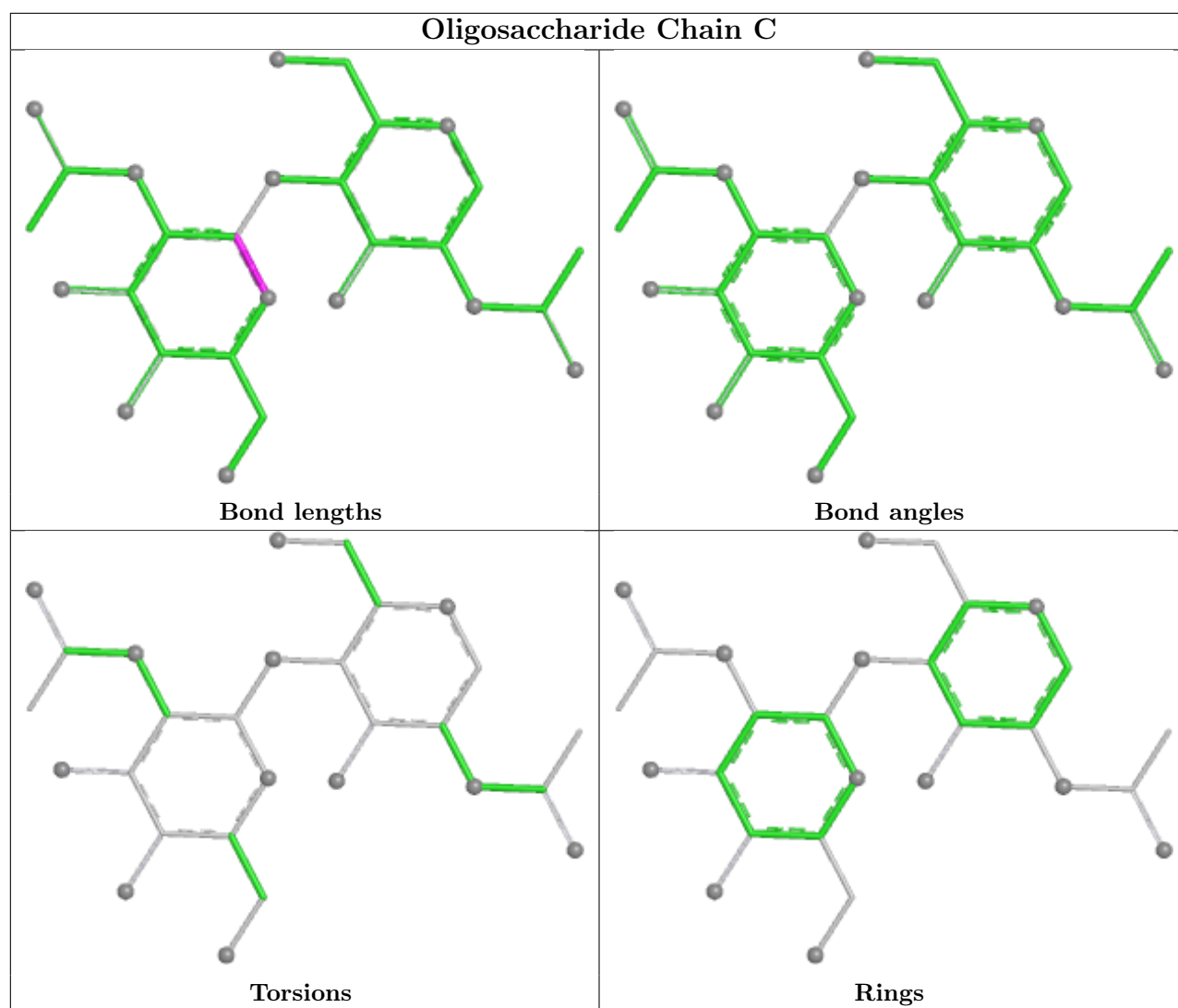
Mol	Chain	Res	Type	Atoms
3	D	4	MAN	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

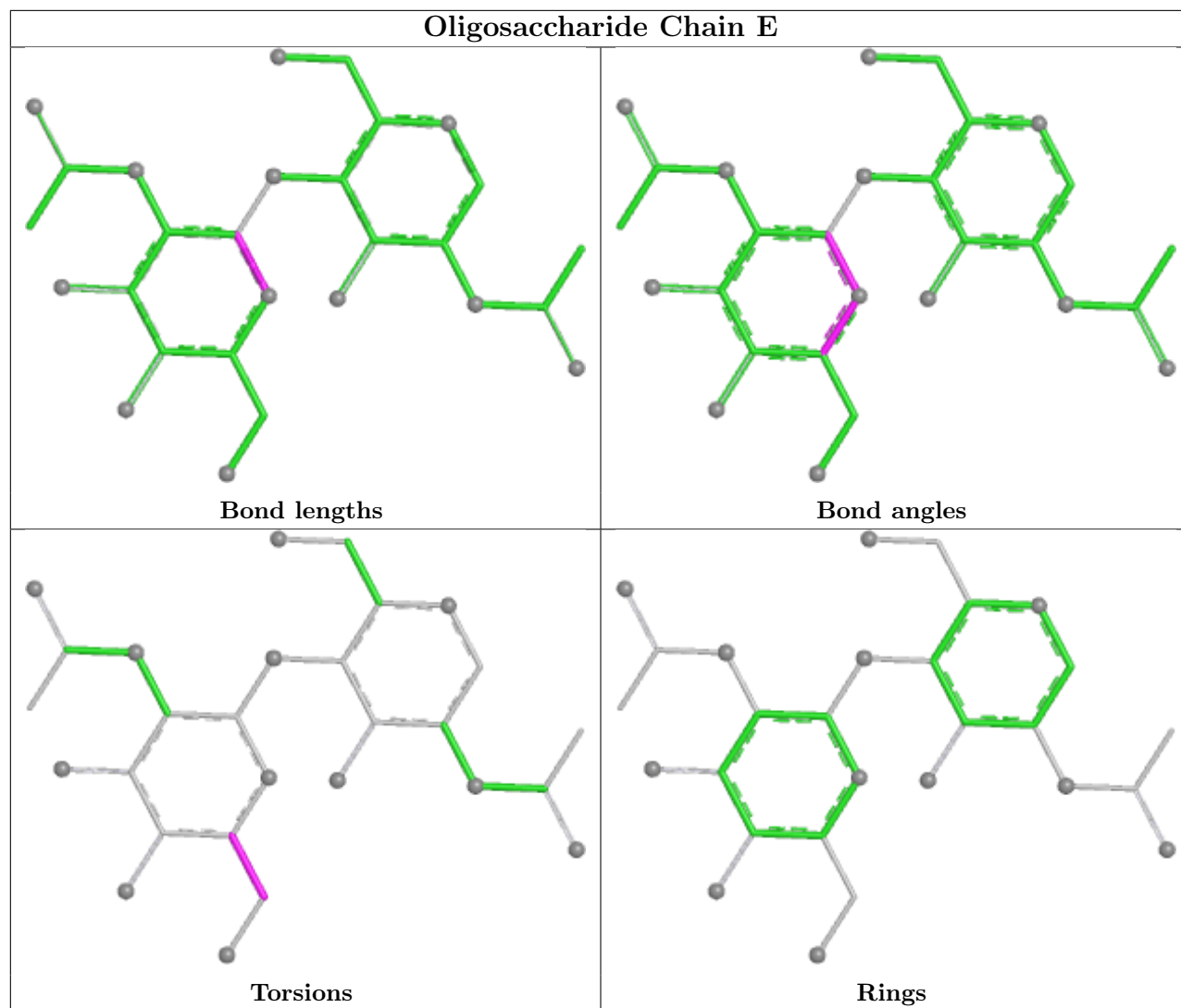
There are no ring outliers.

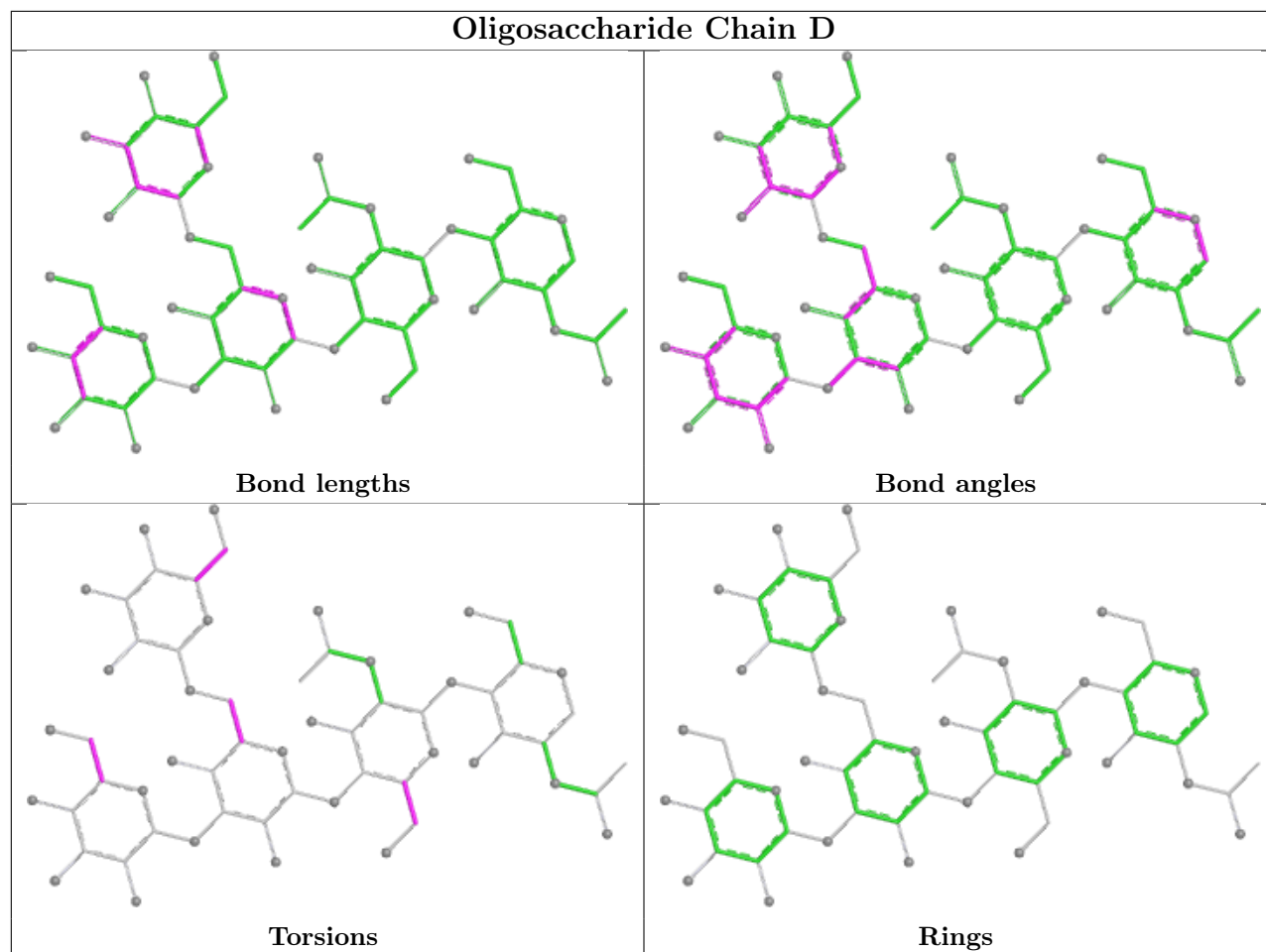
2 monomers are involved in 2 short contacts:

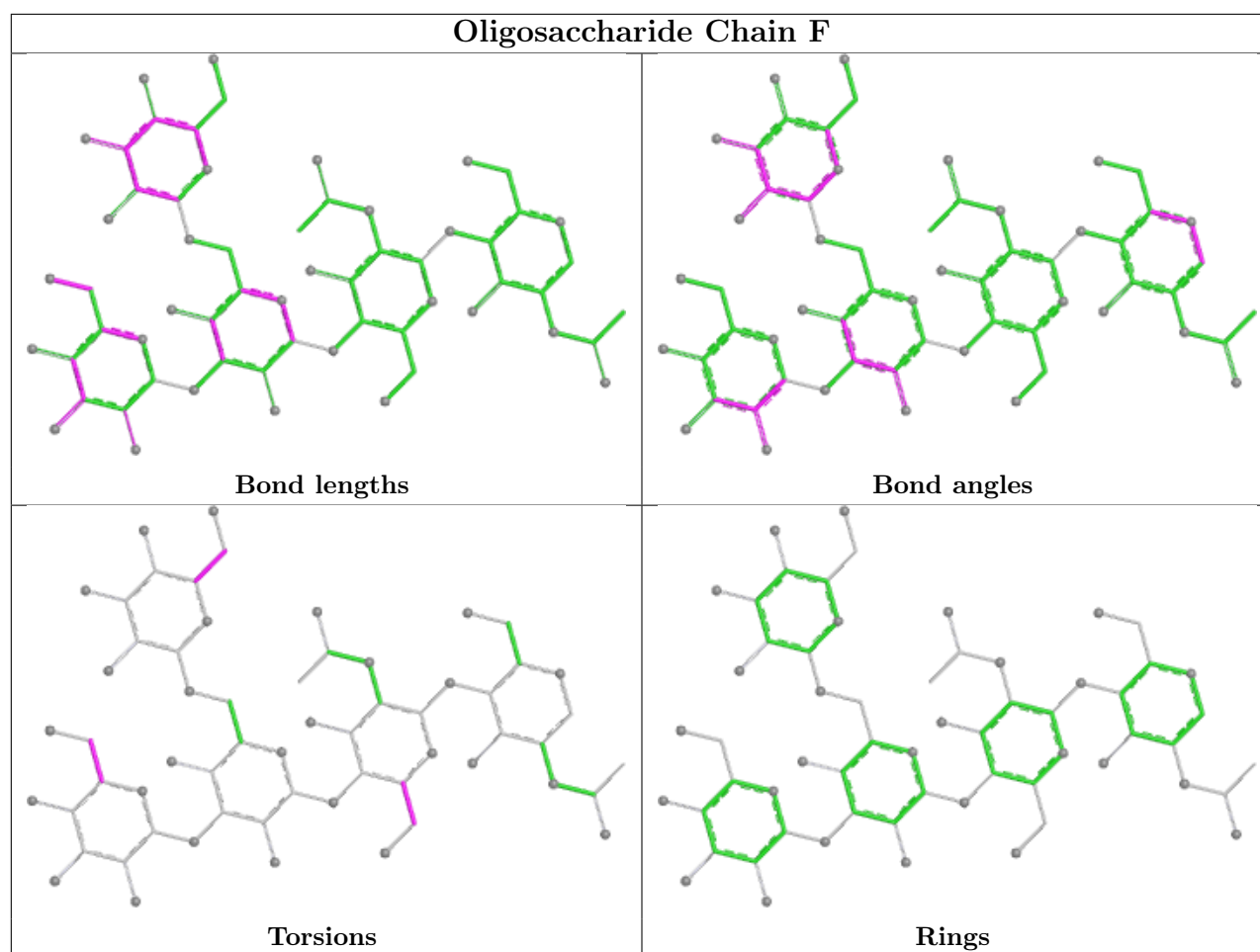
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
3	D	1	NAG	1	0

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	25,26,26	0.73	1 (4%)	38,40,40	0.79	1 (2%)
5	UDP	A	1002	4	25,26,26	0.52	0	38,40,40	0.53	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1002	UDP	PA-O3A	-2.37	1.56	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1002	UDP	O3B-PB-O3A	2.16	111.87	104.64

There are no chirality outliers.

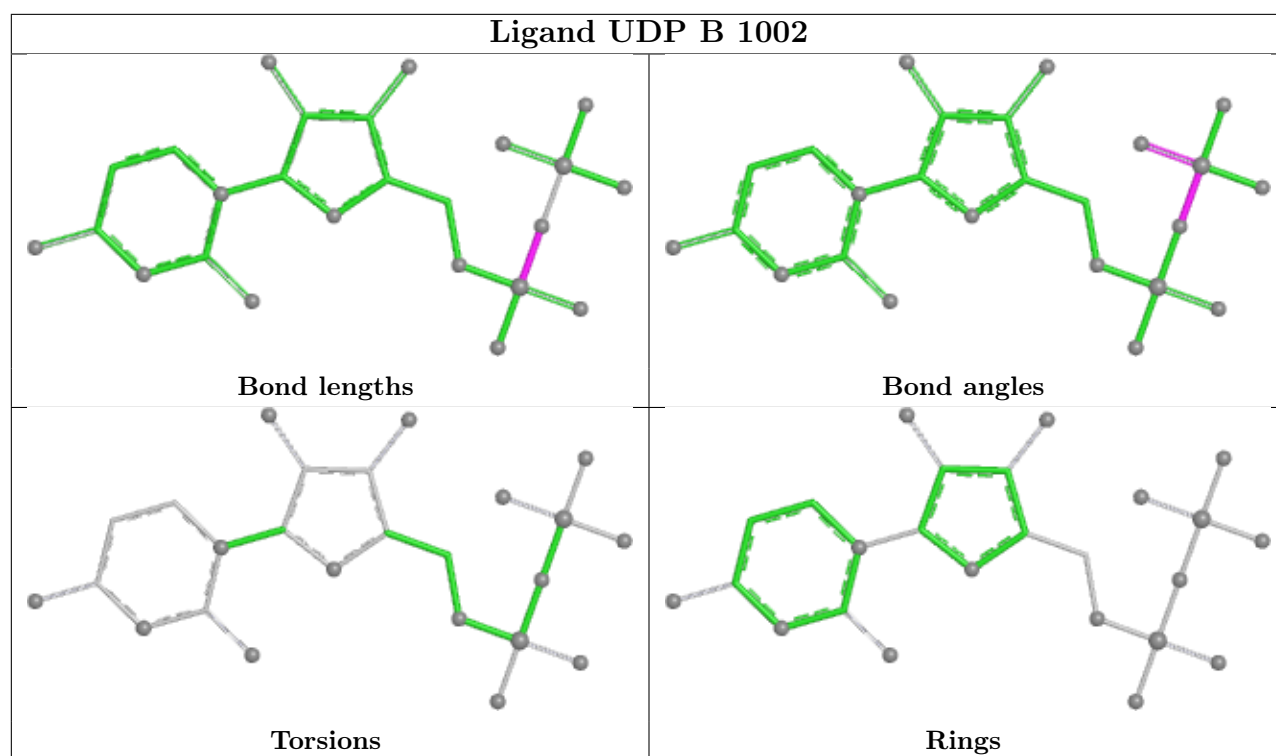
There are no torsion outliers.

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 [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, 95th 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 ²)	Q<0.9
1	A	709/891 (79%)	0.04	17 (2%) 59 62	29, 66, 108, 191	6 (0%)
1	B	709/891 (79%)	0.10	22 (3%) 51 54	31, 67, 111, 168	5 (0%)
All	All	1418/1782 (79%)	0.07	39 (2%) 55 57	29, 66, 109, 191	11 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	LEU	4.1
1	B	168	LEU	4.0
1	A	910	HIS	3.9
1	A	707	LEU	3.7
1	A	373	ALA	3.5
1	A	874	HIS	3.1
1	B	857	PHE	3.1
1	B	910	HIS	3.0
1	B	373	ALA	2.9
1	A	328	PHE	2.9
1	B	706	LEU	2.9
1	A	855	TRP	2.9
1	B	579	GLU	2.8
1	B	350	ILE	2.8
1	A	706	LEU	2.7
1	B	707	LEU	2.7
1	B	919	ILE	2.7
1	B	874	HIS	2.6
1	A	918	PHE	2.5
1	A	558	GLY	2.5
1	A	579	GLU	2.4
1	B	169	PRO	2.4
1	A	619[A]	PHE	2.4
1	A	919	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	907	ARG	2.4
1	B	557	SER	2.4
1	A	722	LYS	2.3
1	B	675	VAL	2.2
1	B	722	LYS	2.2
1	A	351	GLU	2.2
1	B	870	ASP	2.1
1	B	873	PHE	2.1
1	B	550	ALA	2.1
1	A	856	THR	2.0
1	B	174	THR	2.0
1	A	688	TYR	2.0
1	B	163	LYS	2.0
1	B	747	ALA	2.0
1	B	908	LEU	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, 95th 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 ²)	Q<0.9
1	CSO	A	606	7/8	0.95	0.07	37,53,71,86	0
1	CSO	B	606	7/8	0.95	0.07	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, 95th 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.

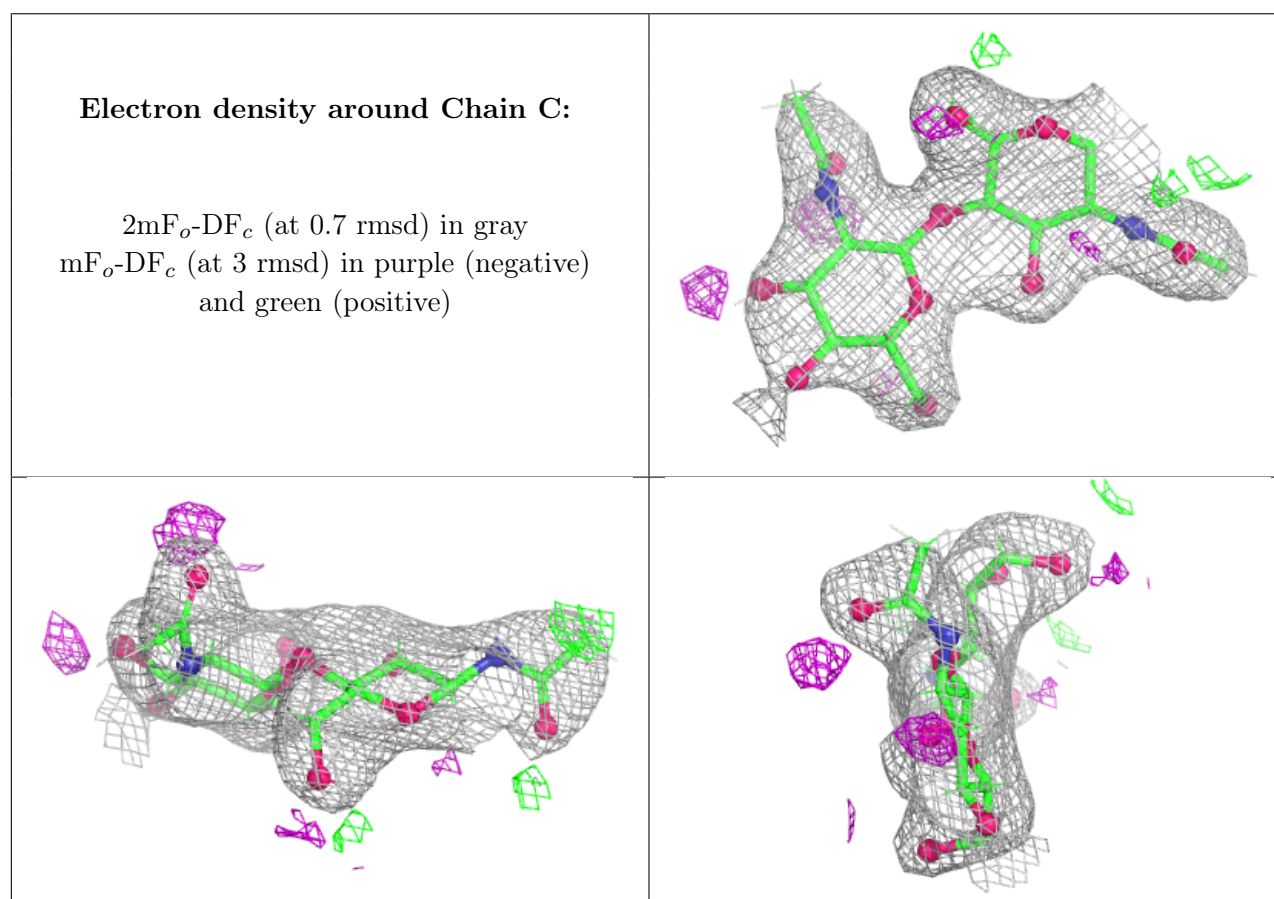
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	D	5	11/12	0.64	0.12	87,119,147,151	0
3	MAN	F	5	11/12	0.76	0.11	82,100,120,129	0
2	NAG	E	2	14/15	0.80	0.11	59,83,104,116	0
3	MAN	D	4	11/12	0.81	0.14	89,104,125,125	0
3	MAN	F	4	11/12	0.84	0.14	66,89,107,107	0
2	NAG	C	2	14/15	0.88	0.10	60,82,102,107	0

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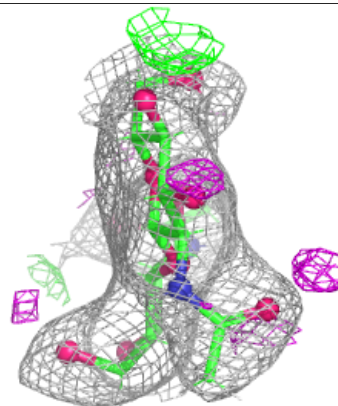
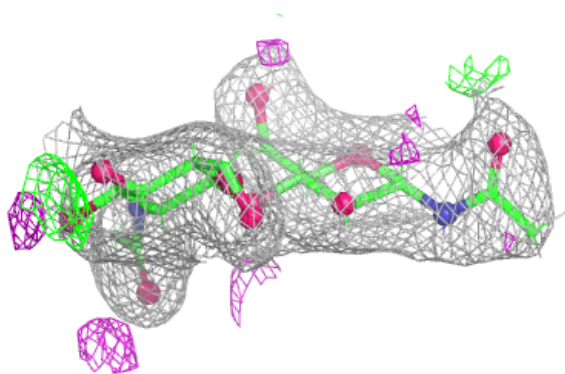
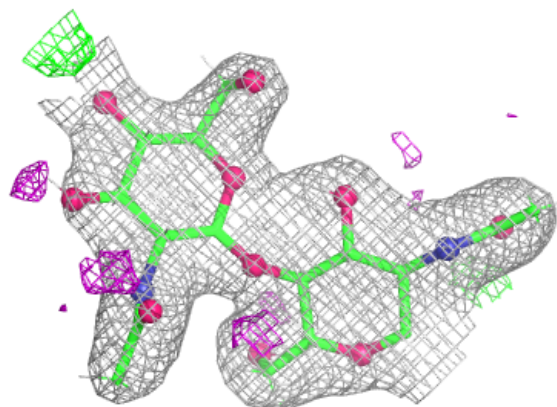
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	D	1	14/15	0.89	0.12	61,79,93,107	0
3	NAG	D	2	14/15	0.89	0.11	65,88,106,110	0
3	BMA	F	3	11/12	0.91	0.09	60,77,104,104	0
3	NAG	F	2	14/15	0.92	0.10	59,79,95,99	0
3	BMA	D	3	11/12	0.92	0.09	81,102,122,123	0
2	NAG	C	1	14/15	0.93	0.08	51,63,73,77	0
3	NAG	F	1	14/15	0.94	0.10	56,70,91,99	0
2	NAG	E	1	14/15	0.96	0.05	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.



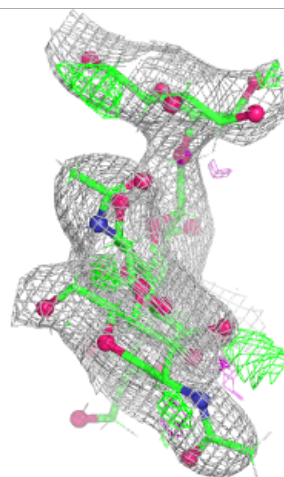
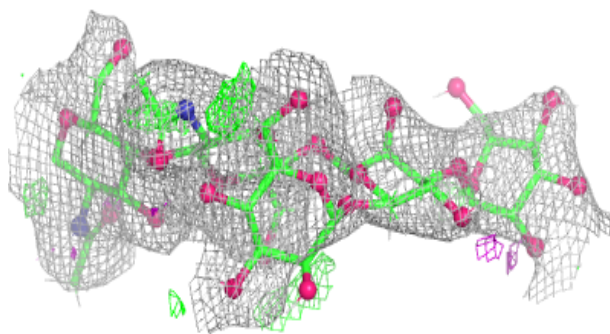
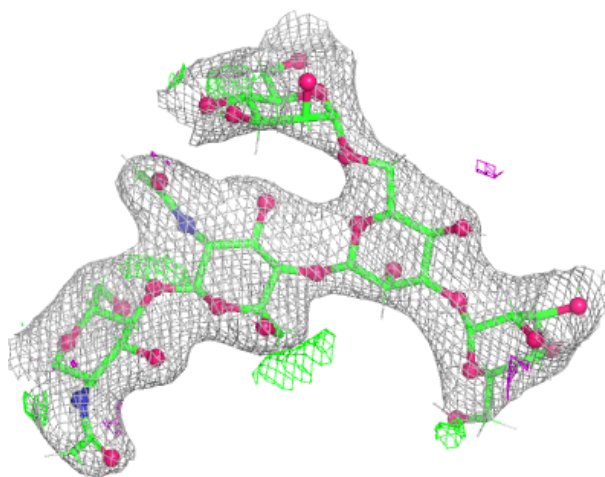
Electron density around Chain E:

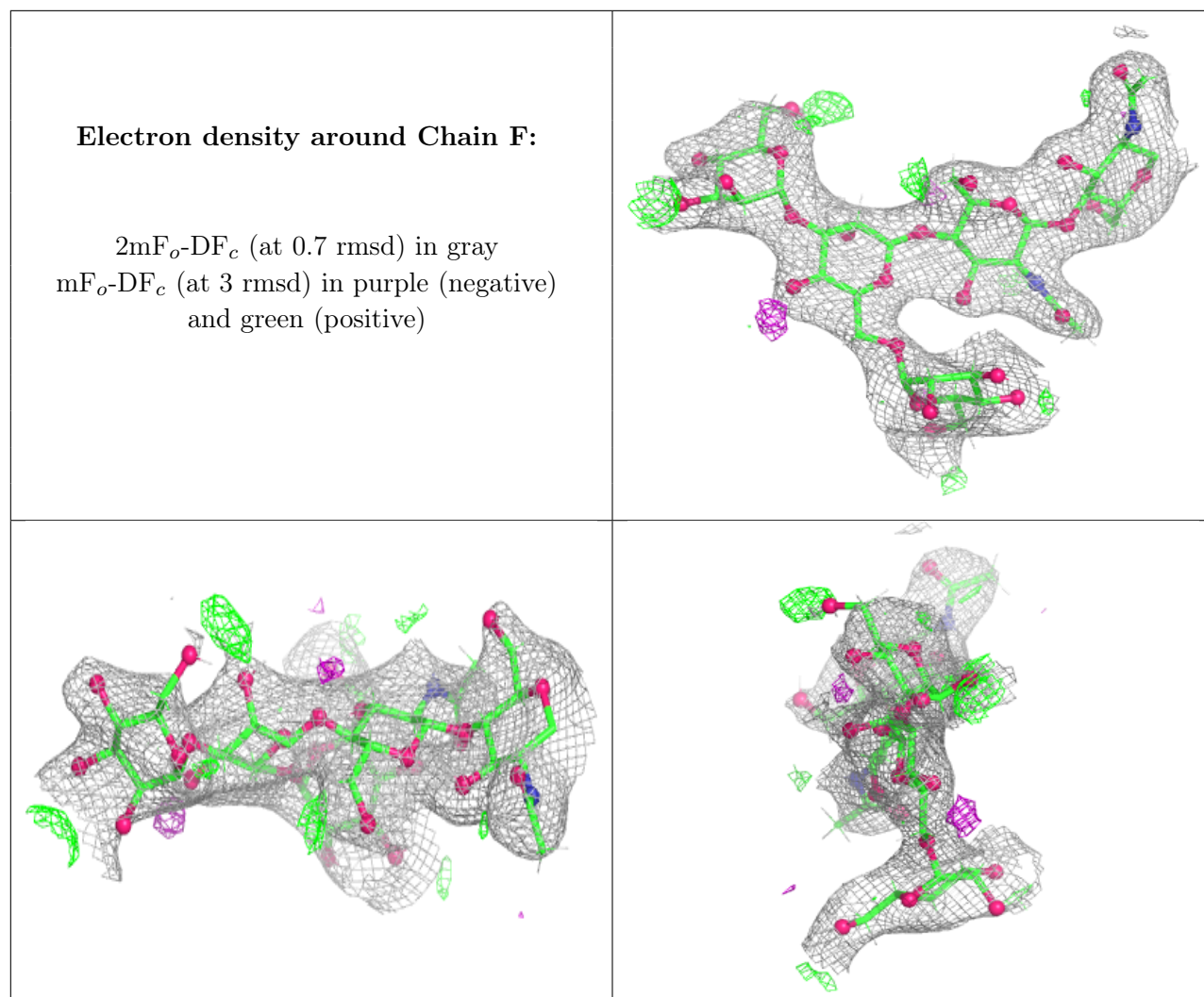
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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](#)

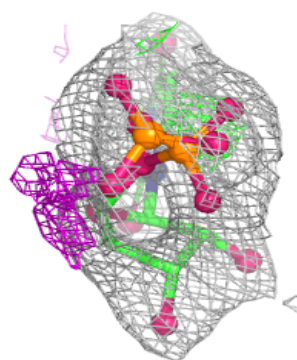
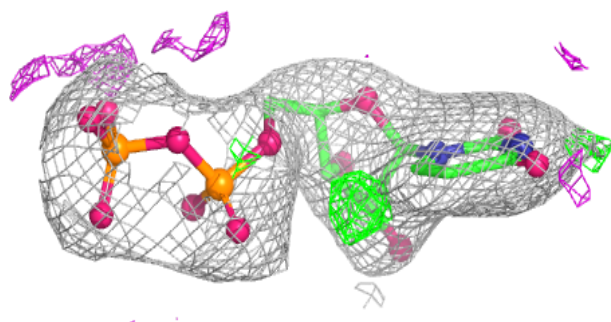
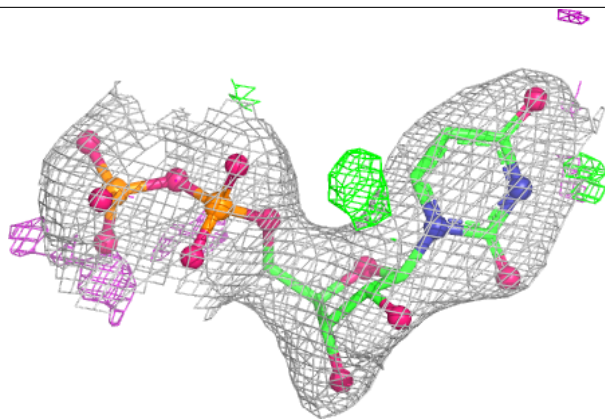
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	UDP	A	1002	25/25	0.89	0.10	57,78,109,120	0
5	UDP	B	1002	25/25	0.91	0.10	58,73,98,103	0
4	MN	B	1001	1/1	0.95	0.06	94,94,94,94	0
4	MN	A	1001	1/1	0.96	0.05	105,105,105,105	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 B 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.