WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 5, 2023 – 11:09 pm GMT

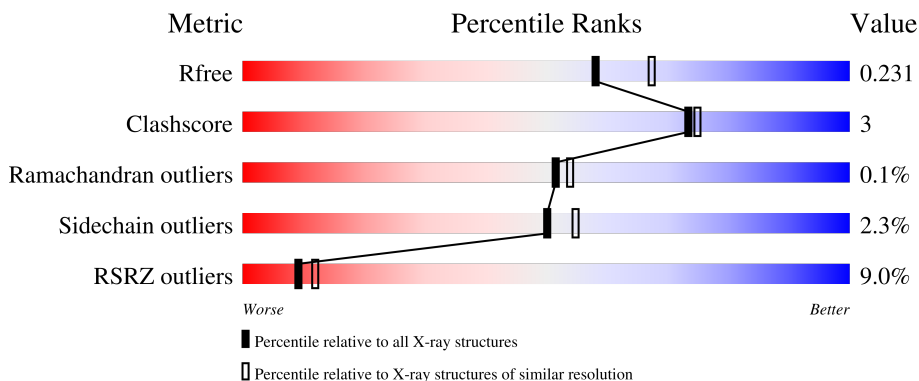|		
PDB ID	:	8OG4
Title	:	Exostosin-like 3 UDP complex
Authors	:	Sammon, D.; Hohenester, E.
Deposited on	:	2023-03-18
Resolution	:	2.10 Å(reported)

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.
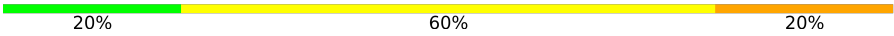
Metric	Percentile Ranks	Value
Rfree		0.231
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		2.3%
RSRZ outliers		9.0%

Worse ... *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 >=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 <=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	

20%   60%   20%

2 Entry composition ⓘ

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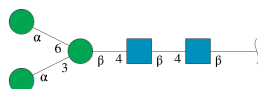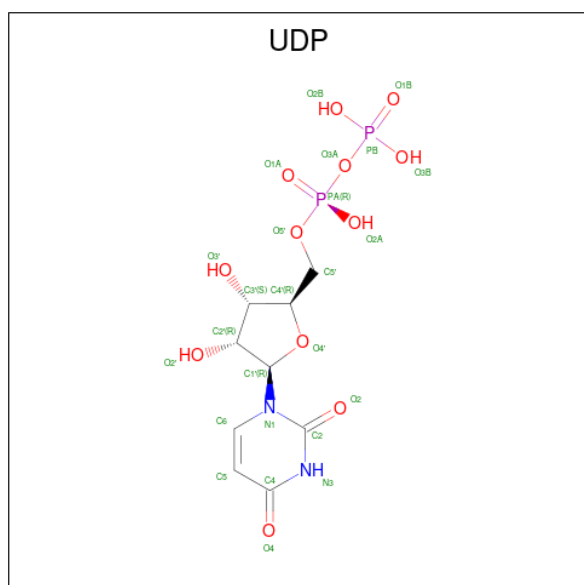
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	5	Total 112	C 34	H 51	N 2	O 25	0	0	0
3	F	5	Total 112	C 34	H 51	N 2	O 25	0	0	0

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

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

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).

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

- Molecule 6 is water.

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

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

3 Residue-property plots ⓘ

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

Chain A:

• Molecule 1: Exostosin-like 3

Chain B:

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

Chain C:

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

Chain E:

• 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:

• 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:

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 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
$< I/\sigma(I) >$ [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 0.192 , 0.231	Depositor DCC
R_{free} test set	6107 reflections (5.04%)	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)	0.41 , 53.1	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5　Model quality ⓘ

5.1　Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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 ⓘ

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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	705/891 (79%)	672 (95%)	32 (4%)	1 (0%)	51	54
1	B	704/891 (79%)	673 (96%)	30 (4%)	1 (0%)	51	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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 ⓘ

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

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	309	ARG
1	B	856	THR
1	B	378	ARG
1	B	908	LEU
1	B	734	GLU

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

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	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 ⓘ

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
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

The worst 5 of 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

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 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

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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
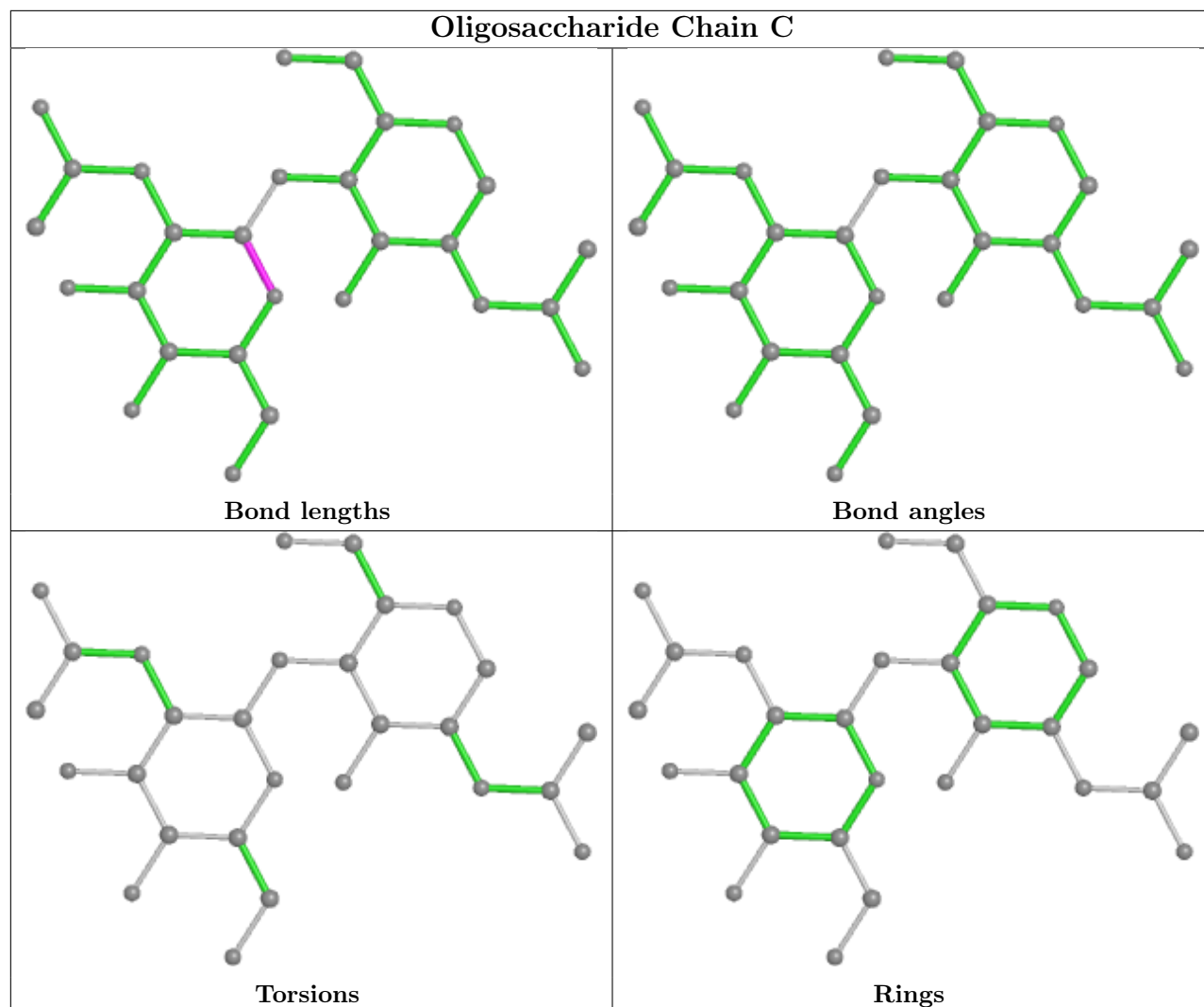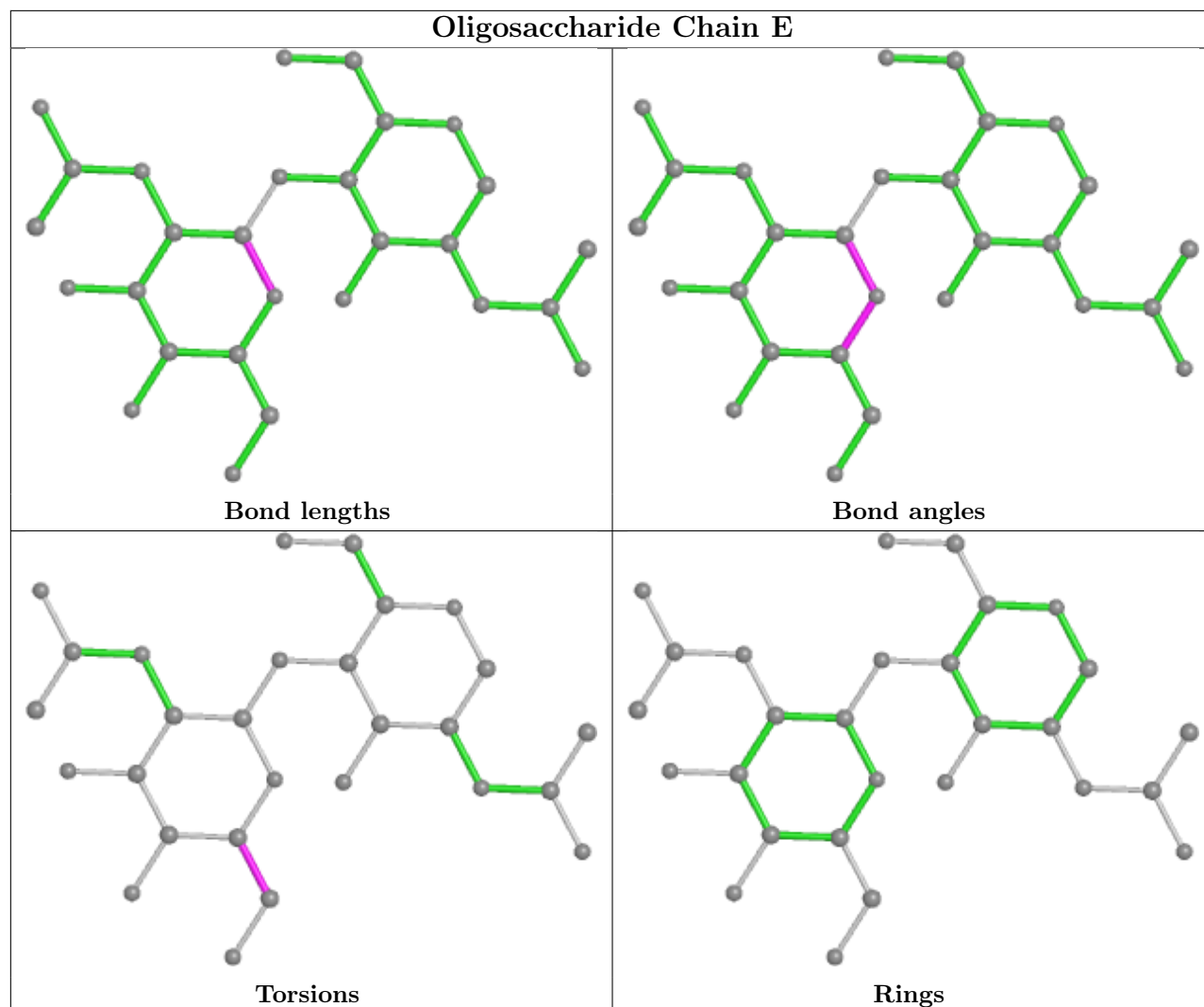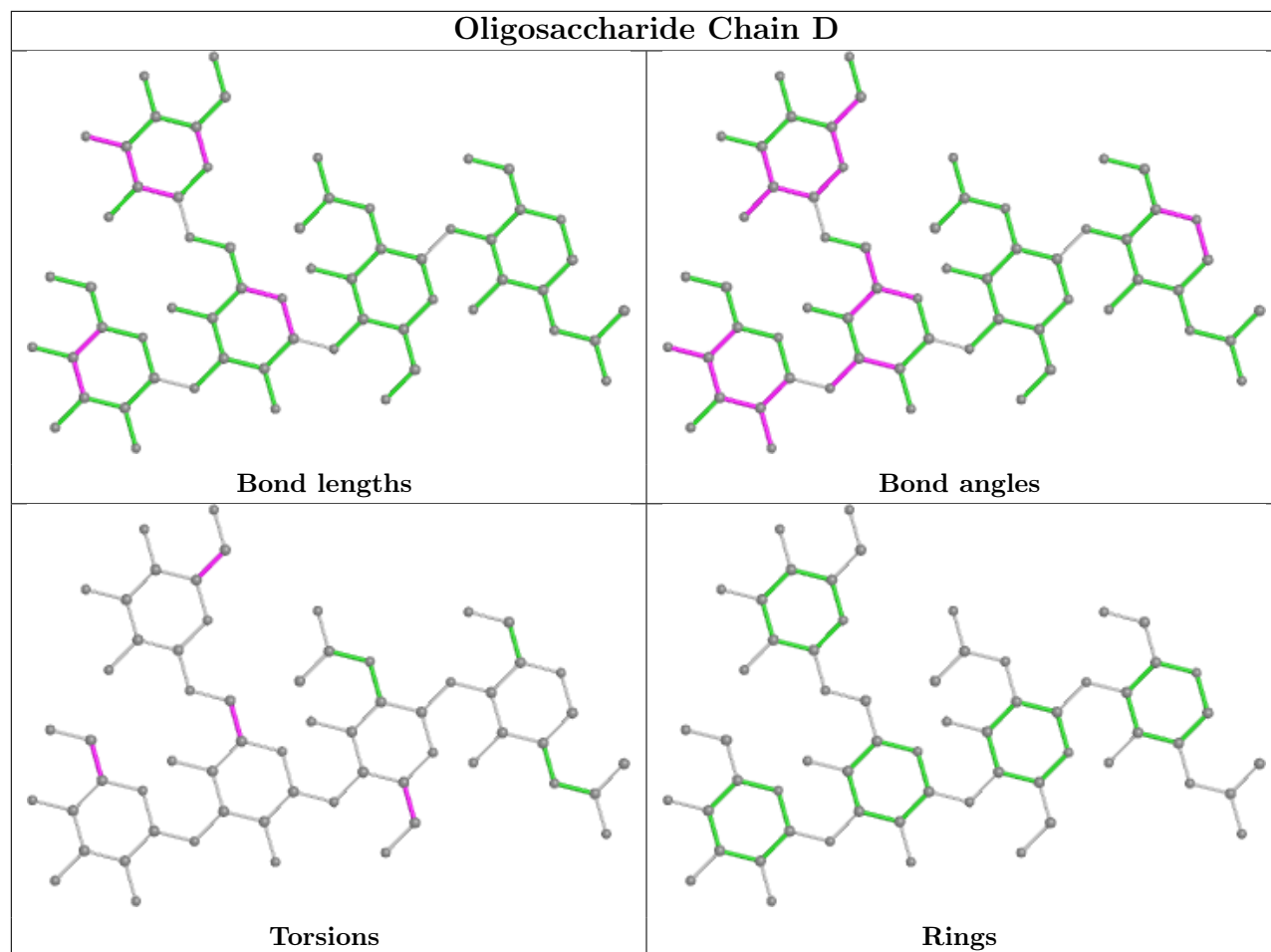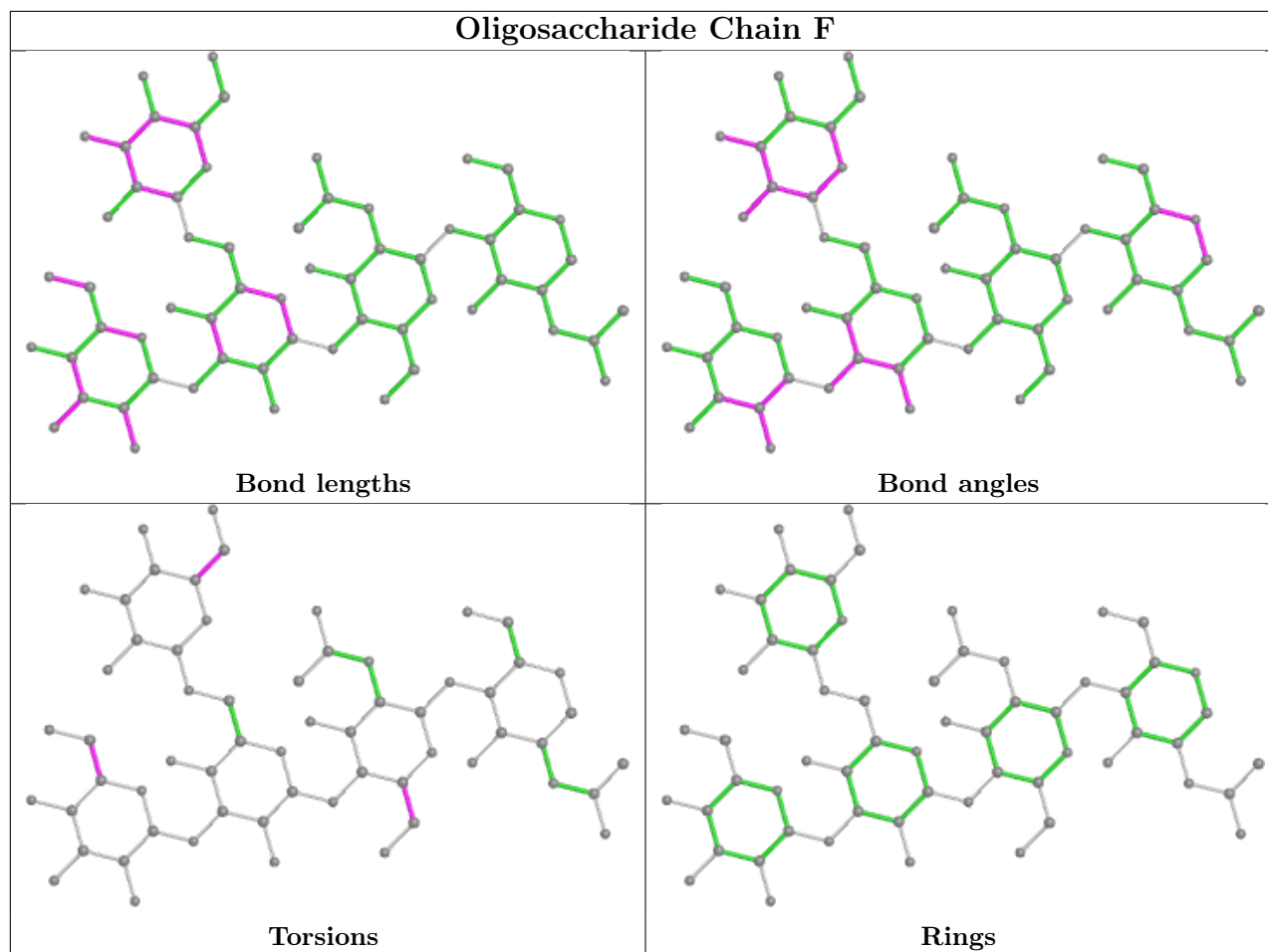
5.6 Ligand geometry ⓘ

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(^{o})	Ideal(^{o})
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 then 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.

Ligand UDP B 1002

Bond lengths

Bond angles

Torsions

Rings

Ligand UDP A 1002

Bond lengths

Bond angles

Torsions

Rings
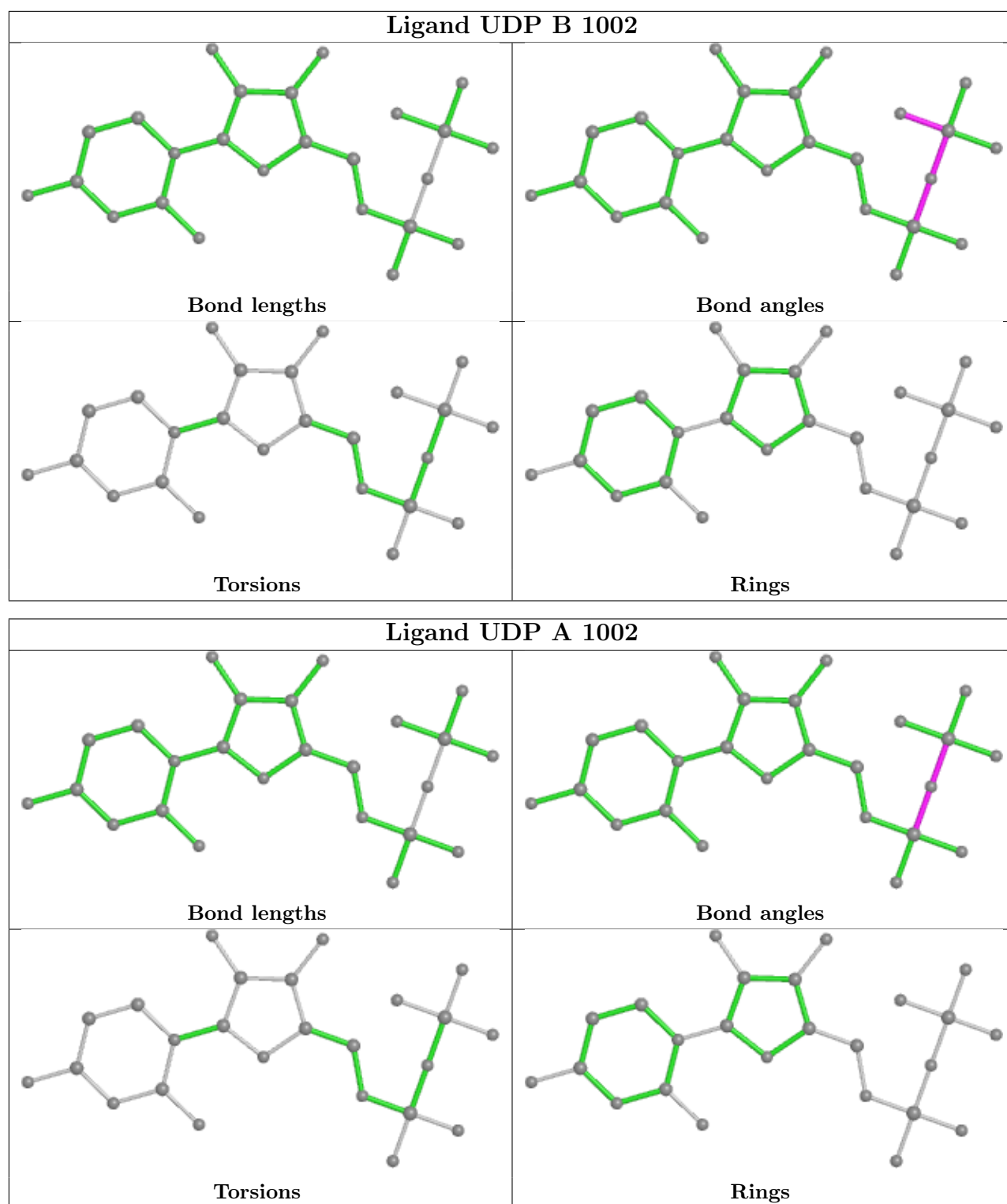
5.7 Other polymers ⓘ

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

The worst 5 of 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

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

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.
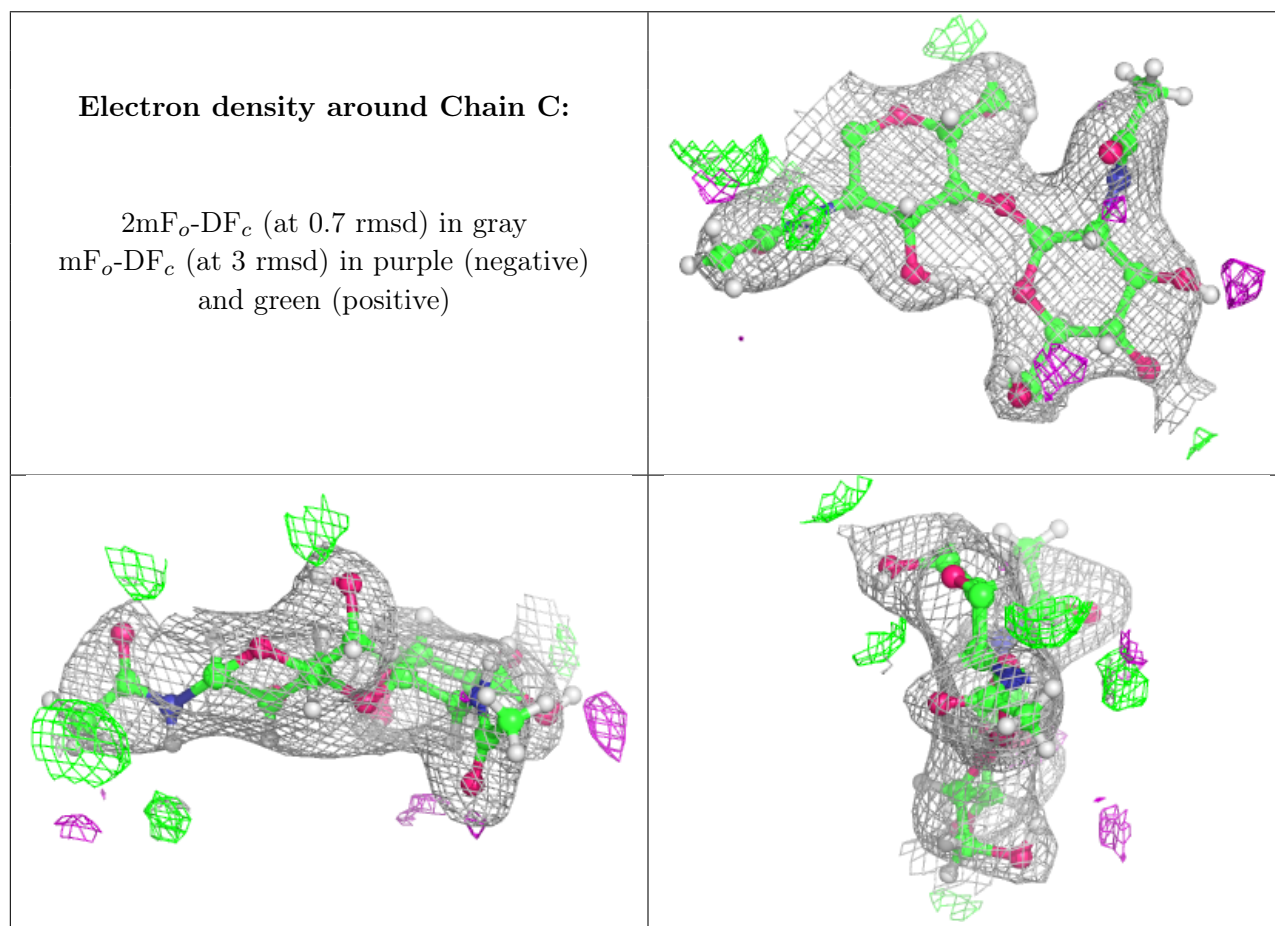
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSO	A	606	7/8	0.96	0.31	37,53,71,86	0
1	CSO	B	606	7/8	0.96	0.23	39,47,68,81	0

6.3   Carbohydrates   ⓘ

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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	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
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.
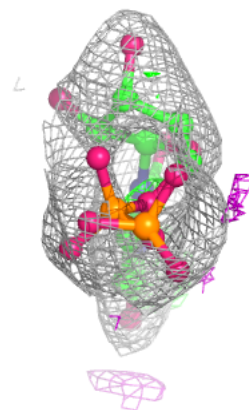

Electron density around Chain C:

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 E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
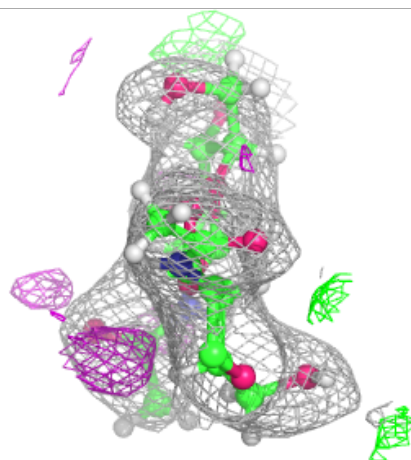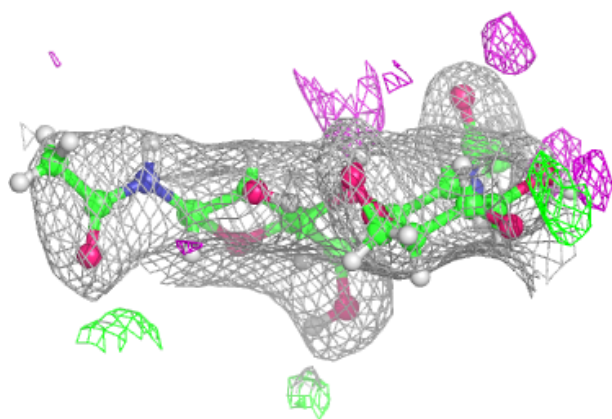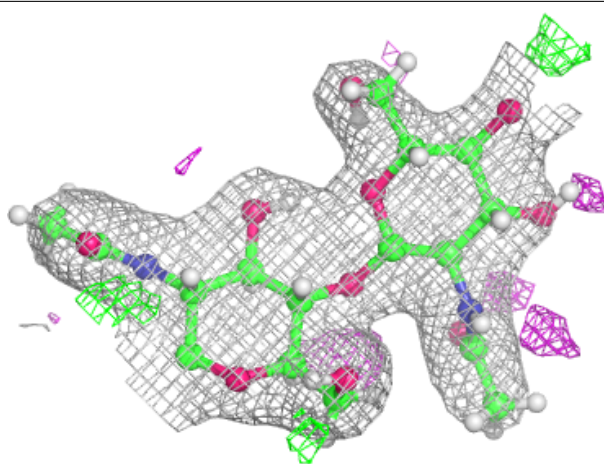
Electron density around Chain D:

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

Electron density around Chain F:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
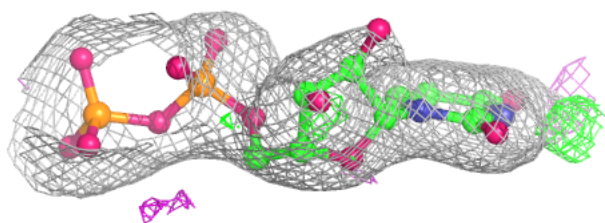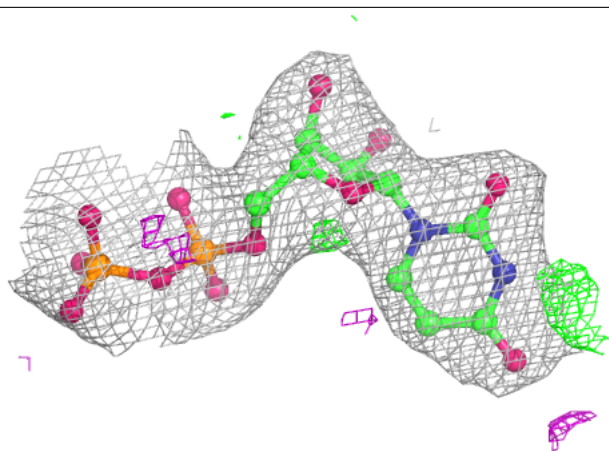and green (positive)
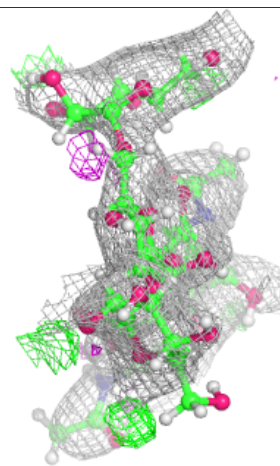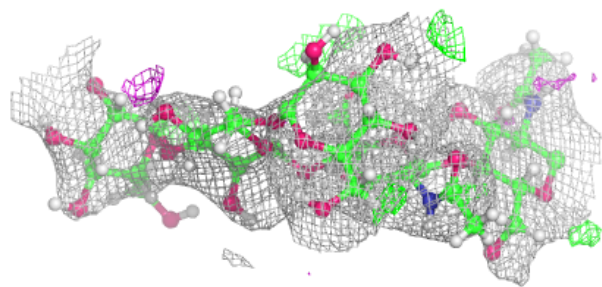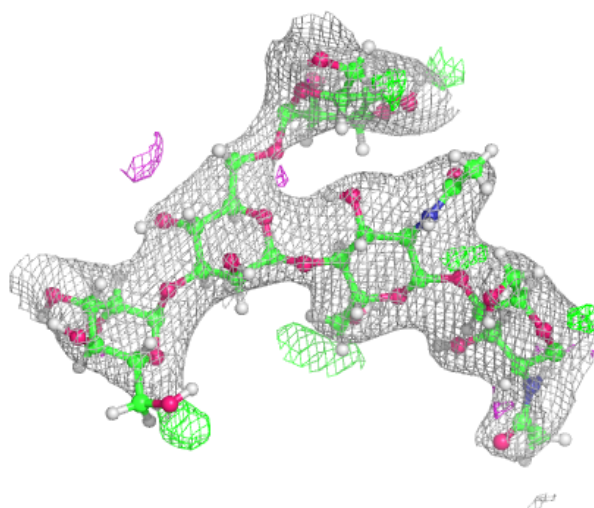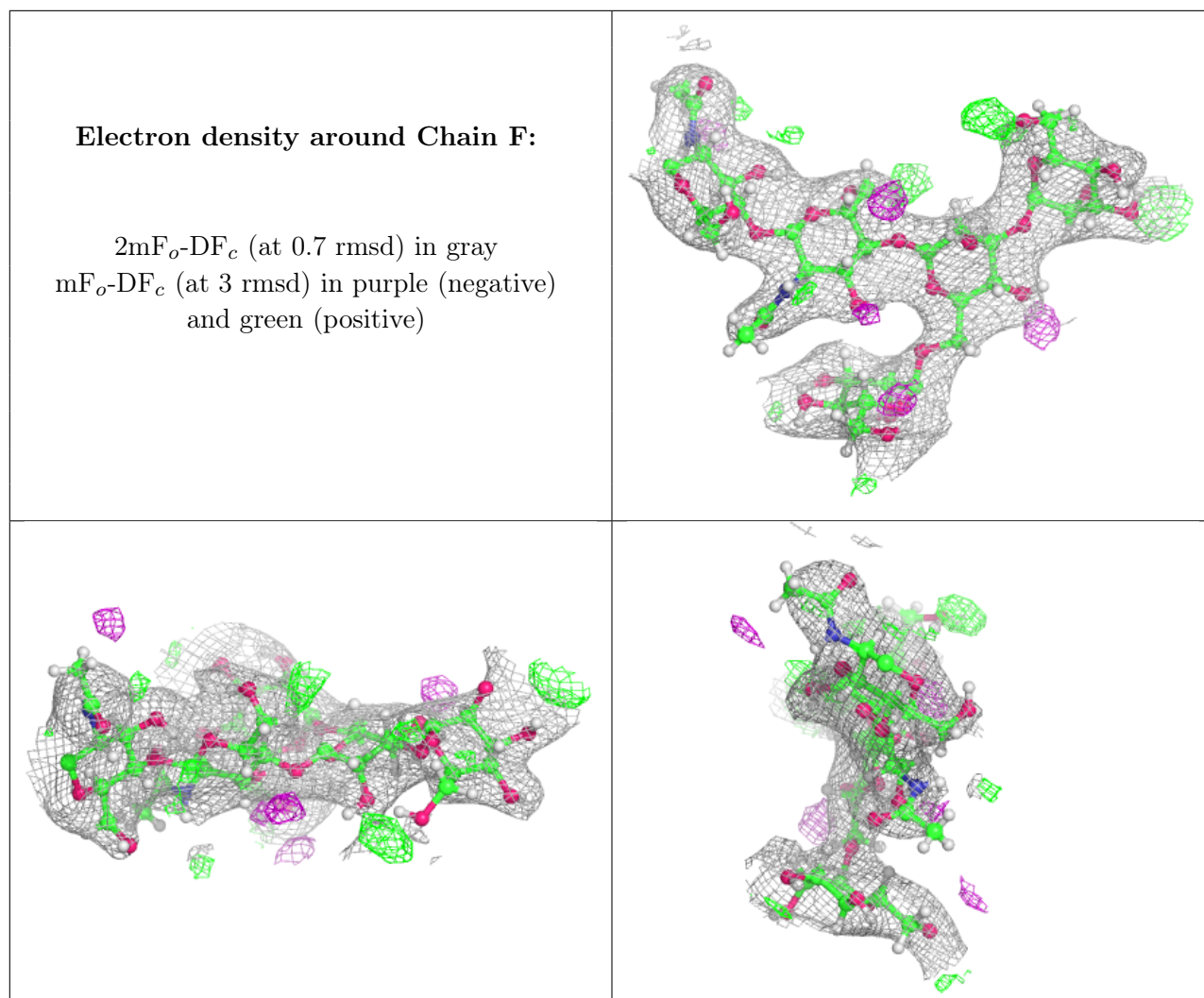
6.4 Ligands (i)

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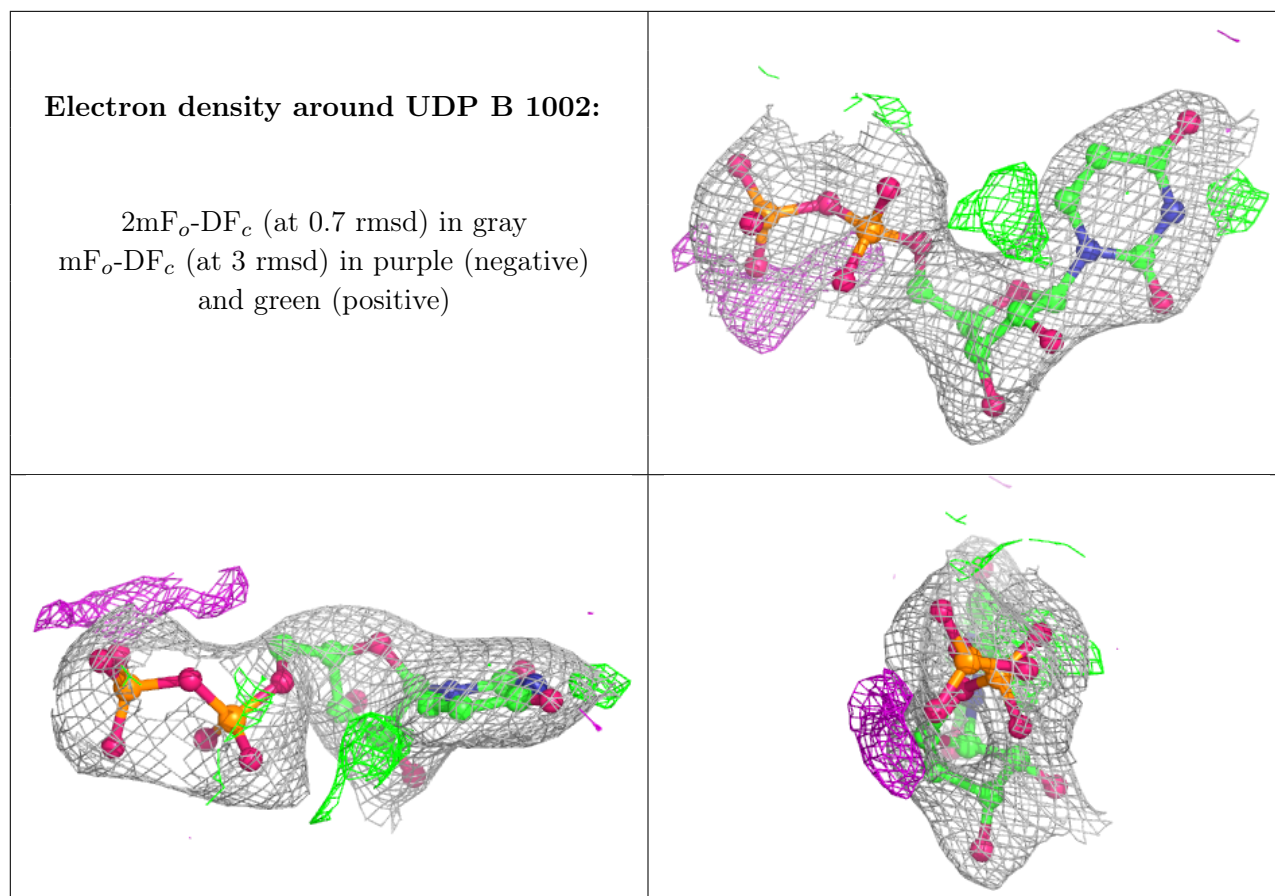
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MN	A	1001	1/1	0.82	0.05	105,105,105,105	0
4	MN	B	1001	1/1	0.95	0.07	94,94,94,94	0
5	UDP	A	1002	25/25	0.95	0.11	57,78,109,120	0
5	UDP	B	1002	25/25	0.95	0.11	58,73,98,103	0

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:

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

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 ⓘ

There are no such residues in this entry.