



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:02 PM EDT

PDB ID : 7SJ2
Title : N-acetylglucosamine-1-phosphotransferase (GNPT) alpha and beta subunits (GNPTAB) catalytic domain, from zebrafish, in complex with uridine diphosphate N-acetylglucosamine (UDP-GlcNAc) and magnesium
Authors : Gorelik, A.; Illes, K.; Nagar, B.
Deposited on : 2021-10-15
Resolution : 2.30 Å(reported)

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

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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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

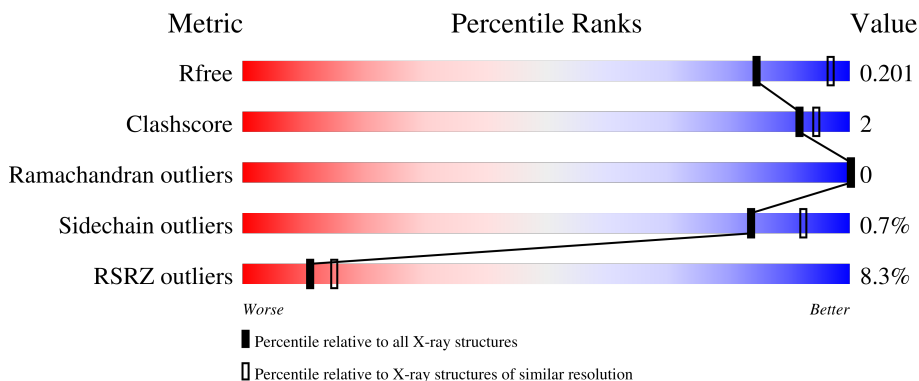
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.




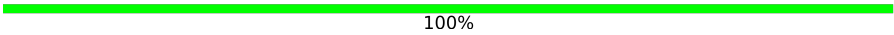

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	495	 5% 82% 14%
1	B	495	 9% 85% 11%
2	C	5	 40% 60%
3	D	3	 67% 33%

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Mol	Chain	Length	Quality of chain
3	G	3	 67% 33%
4	E	2	 100%
5	F	3	 100%

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 15490 atoms, of which 7208 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 N-acetylglucosamine-1-phosphotransferase subunit alpha,N-acetylglucosamine-1-phosphotransferase (GNPT) alpha (GNPTAB) catalytic domain,N-acetylglucosamine-1-phosphotransferase subunit beta.

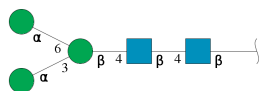
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	428	6987	2253	3451	614	653	16	0	0	0
1	B	439	7194	2319	3556	634	668	17	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ASP	-	expression tag	UNP Q5RGJ8
A	35	ARG	-	expression tag	UNP Q5RGJ8
A	36	HIS	-	expression tag	UNP Q5RGJ8
A	37	HIS	-	expression tag	UNP Q5RGJ8
A	38	HIS	-	expression tag	UNP Q5RGJ8
A	39	HIS	-	expression tag	UNP Q5RGJ8
A	40	HIS	-	expression tag	UNP Q5RGJ8
A	41	HIS	-	expression tag	UNP Q5RGJ8
A	42	GLY	-	expression tag	UNP Q5RGJ8
A	43	SER	-	expression tag	UNP Q5RGJ8
B	34	ASP	-	expression tag	UNP Q5RGJ8
B	35	ARG	-	expression tag	UNP Q5RGJ8
B	36	HIS	-	expression tag	UNP Q5RGJ8
B	37	HIS	-	expression tag	UNP Q5RGJ8
B	38	HIS	-	expression tag	UNP Q5RGJ8
B	39	HIS	-	expression tag	UNP Q5RGJ8
B	40	HIS	-	expression tag	UNP Q5RGJ8
B	41	HIS	-	expression tag	UNP Q5RGJ8
B	42	GLY	-	expression tag	UNP Q5RGJ8
B	43	SER	-	expression tag	UNP Q5RGJ8

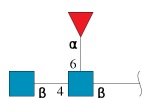
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	5	98	34	37	2	25	0	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	D	3	61	22	23	2	14	0	0	0
3	G	3	61	22	23	2	14	0	0	0

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



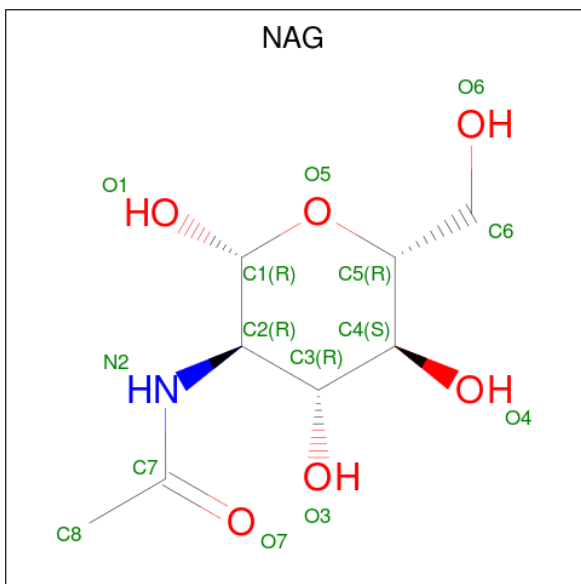
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
4	E	2	39	14	15	1	9	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	F	3	61	22	22	2	15	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			
6	A	1	Total	22	8	8	1	5	0	0
6	A	1	Total	22	8	8	1	5	0	0
6	B	1	Total	22	8	8	1	5	0	0
6	B	1	Total	22	8	8	1	5	0	0

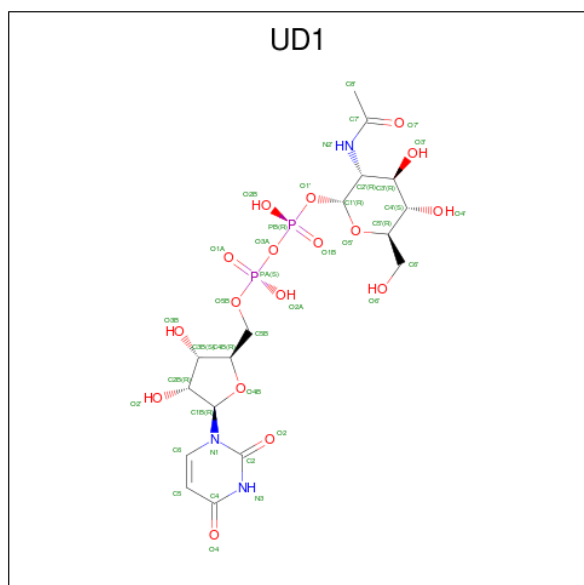
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	Total	1	0	0
7	B	1	Total	1	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Mg 2 2	0	0
8	B	2	Total Mg 2 2	0	0

- Molecule 9 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	A	1	Total	C	H	N	O	P	0	0
			63	17	24	3	17	2		
9	B	1	Total	C	H	N	O	P	0	0
			64	17	25	3	17	2		

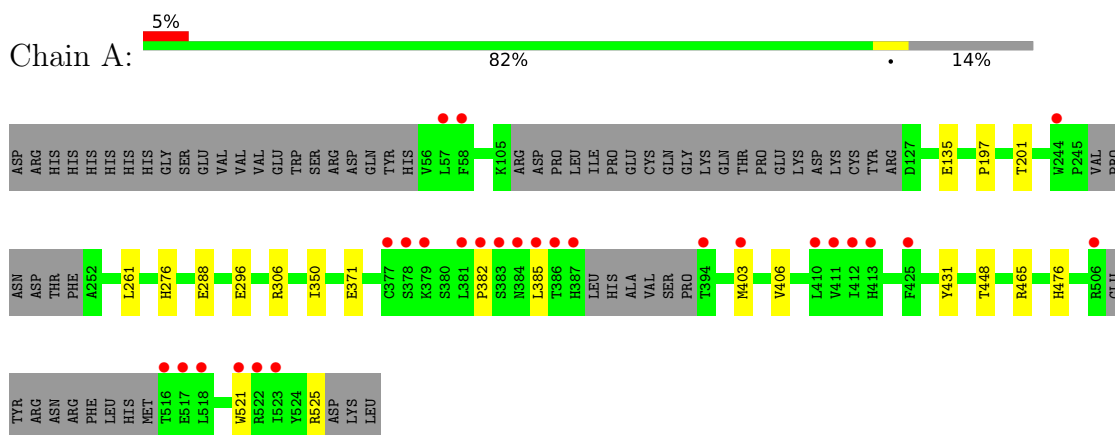
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	465	Total O 465 465	0	0
10	B	303	Total O 303 303	0	0

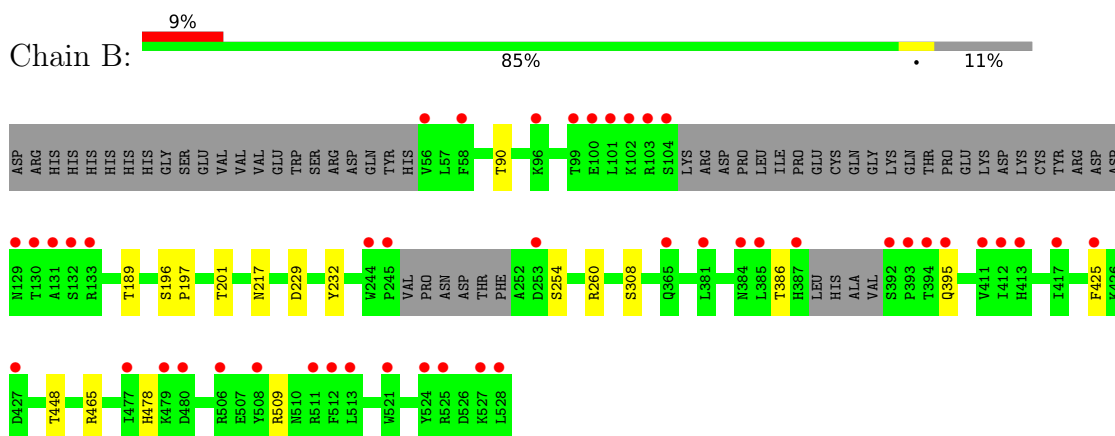
3 Residue-property plots [i](#)

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: N-acetylglucosamine-1-phosphotransferase subunit alpha,N-acetylglucosamine-1-phosphotransferase (GNPT) alpha (GNPTAB) catalytic domain,N-acetylglucosamine-1-phosphotransferase subunit beta



- Molecule 1: N-acetylglucosamine-1-phosphotransferase subunit alpha,N-acetylglucosamine-1-phosphotransferase (GNPT) alpha (GNPTAB) catalytic domain,N-acetylglucosamine-1-phosphotransferase subunit beta



- Molecule 2: 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





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

Chain D: 67% 33%



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

Chain G: 67% 33%



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

Chain E: 100%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.54Å 87.14Å 108.37Å 90.00° 111.86° 90.00°	Depositor
Resolution (Å)	47.42 – 2.30 47.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.1 (47.42-2.30) 87.7 (47.42-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.160 , 0.202 0.160 , 0.201	Depositor DCC
R_{free} test set	1972 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15490	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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: MG, BMA, UD1, MAN, FUC, NAG, CA

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	0.27	0/3625	0.49	0/4908
1	B	0.25	0/3732	0.48	0/5052
All	All	0.26	0/7357	0.49	0/9960

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	3536	3451	3451	10	0
1	B	3638	3556	3555	10	0
2	C	61	37	52	1	0
3	D	38	23	34	0	0
3	G	38	23	34	1	0
4	E	24	15	22	0	0
5	F	39	22	34	0	0
6	A	28	16	26	0	0
6	B	28	16	26	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	2	0	0	0	0
8	B	2	0	0	0	0
9	A	39	24	25	0	0
9	B	39	25	25	2	0
10	A	465	0	0	2	0
10	B	303	0	0	3	0
All	All	8282	7208	7284	23	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 2.

All (23) 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)
9:B:606:UD1:O1A	10:B:701:HOH:O	2.05	0.72
10:A:1160:HOH:O	2:C:2:NAG:O7	2.12	0.68
9:B:606:UD1:O7'	10:B:702:HOH:O	2.14	0.66
1:A:288:GLU:OE1	1:A:431:TYR:OH	2.14	0.66
1:A:276:HIS:ND1	10:A:704:HOH:O	2.35	0.50
1:B:260:ARG:NH1	10:B:715:HOH:O	2.44	0.49
1:B:395:GLN:N	1:B:395:GLN:OE1	2.47	0.48
1:B:189:THR:HG21	3:G:1:NAG:H62	1.94	0.48
1:A:448:THR:HG22	1:A:448:THR:O	2.14	0.47
1:A:521:TRP:O	1:A:525:ARG:N	2.43	0.46
1:B:197:PRO:O	1:B:201:THR:HG23	2.15	0.46
1:A:197:PRO:O	1:A:201:THR:HG23	2.18	0.43
1:B:229:ASP:HA	1:B:232:TYR:O	2.18	0.43
1:B:196:SER:OG	1:B:197:PRO:HD3	2.19	0.43
1:A:261:LEU:HD11	1:A:296:GLU:HG2	2.01	0.42
1:B:90:THR:O	1:B:90:THR:HG22	2.20	0.42
1:B:254:SER:HA	1:B:308:SER:O	2.19	0.42
1:B:448:THR:HG21	1:B:478:HIS:HB3	2.02	0.42
1:A:350:ILE:HD11	1:A:406:VAL:HG21	2.02	0.42
1:A:371:GLU:HB3	1:A:403:MET:HE1	2.01	0.41
1:B:386:THR:HG22	1:B:386:THR:O	2.20	0.41
1:A:382:PRO:HD2	1:A:385:LEU:HD12	2.03	0.41
1:A:135:GLU:HG2	1:A:476:HIS:CE1	2.57	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	418/495 (84%)	409 (98%)	9 (2%)	0	100	100
1	B	431/495 (87%)	422 (98%)	9 (2%)	0	100	100
All	All	849/990 (86%)	831 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	401/465 (86%)	399 (100%)	2 (0%)	88	95
1	B	412/465 (89%)	408 (99%)	4 (1%)	76	87
All	All	813/930 (87%)	807 (99%)	6 (1%)	84	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	ARG
1	A	465	ARG
1	B	217	ASN
1	B	425	PHE
1	B	465	ARG
1	B	509	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

16 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	0.38	0	17,19,21	0.48	0
2	NAG	C	2	2	14,14,15	0.59	0	17,19,21	0.54	0
2	BMA	C	3	2	11,11,12	0.56	0	15,15,17	0.88	0
2	MAN	C	4	2	11,11,12	0.83	1 (9%)	15,15,17	1.17	2 (13%)
2	MAN	C	5	2	11,11,12	0.77	0	15,15,17	0.94	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.44	0	17,19,21	0.39	0
3	NAG	D	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	FUC	D	3	3	10,10,11	0.82	1 (10%)	14,14,16	1.06	1 (7%)
4	NAG	E	1	1,4	14,14,15	0.33	0	17,19,21	0.59	0
4	FUC	E	2	4	10,10,11	0.70	0	14,14,16	0.80	0
5	NAG	F	1	5,1	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	F	2	5	14,14,15	0.25	0	17,19,21	0.42	0
5	BMA	F	3	5	11,11,12	0.61	0	15,15,17	0.73	0
3	NAG	G	1	3,1	14,14,15	0.23	0	17,19,21	0.39	0
3	NAG	G	2	3	14,14,15	0.25	0	17,19,21	0.44	0
3	FUC	G	3	3	10,10,11	0.66	0	14,14,16	0.87	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	FUC	D	3	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
5	NAG	F	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	FUC	G	3	3	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	MAN	C1-C2	2.21	1.57	1.52
3	D	3	FUC	C1-C2	2.20	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	2.85	116.05	112.19
3	D	3	FUC	C1-C2-C3	2.40	112.62	109.67
2	C	5	MAN	C1-O5-C5	2.28	115.28	112.19
2	C	4	MAN	O2-C2-C3	-2.08	105.96	110.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	O5-C5-C6-O6

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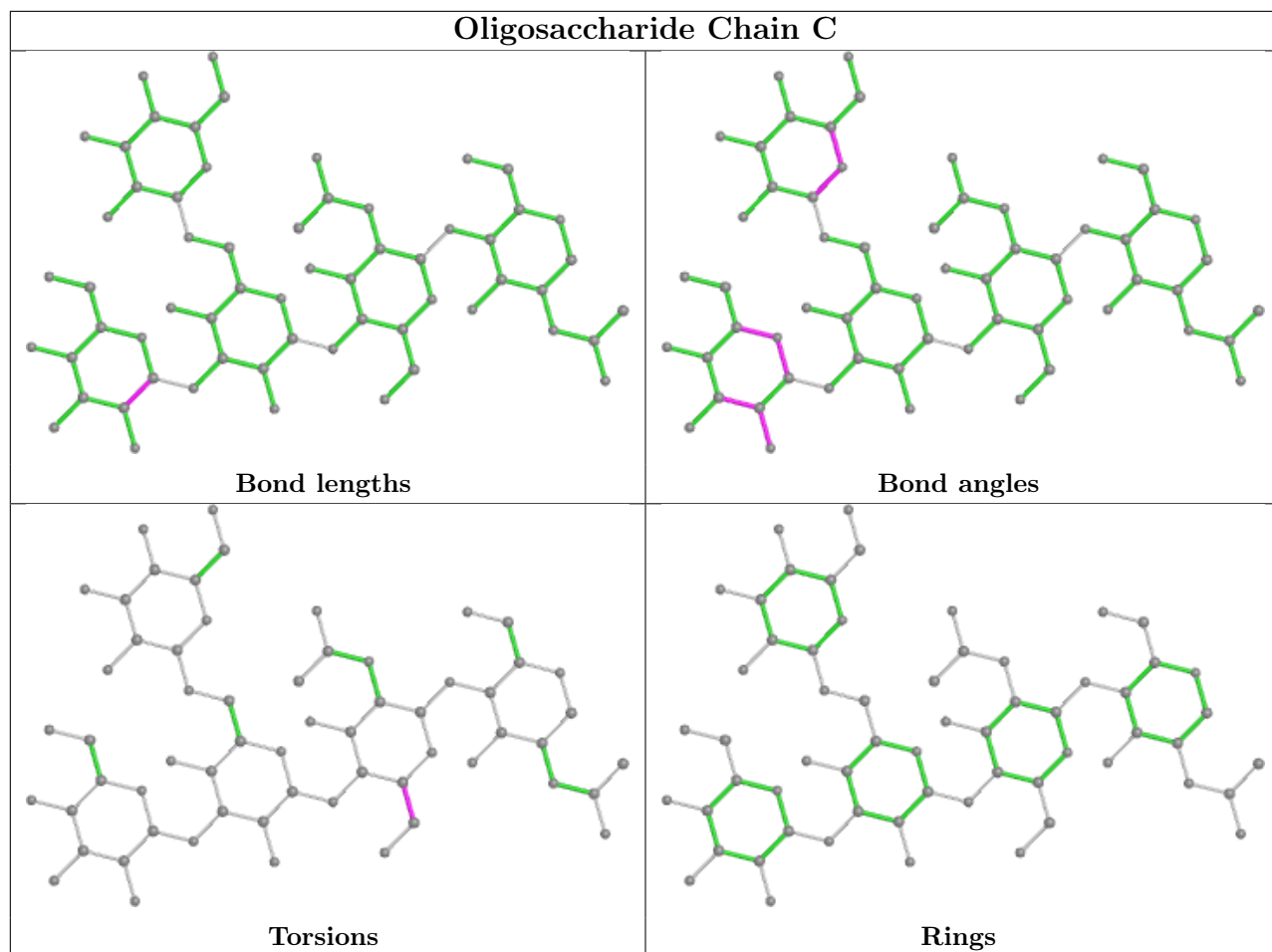
Mol	Chain	Res	Type	Atoms
5	F	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

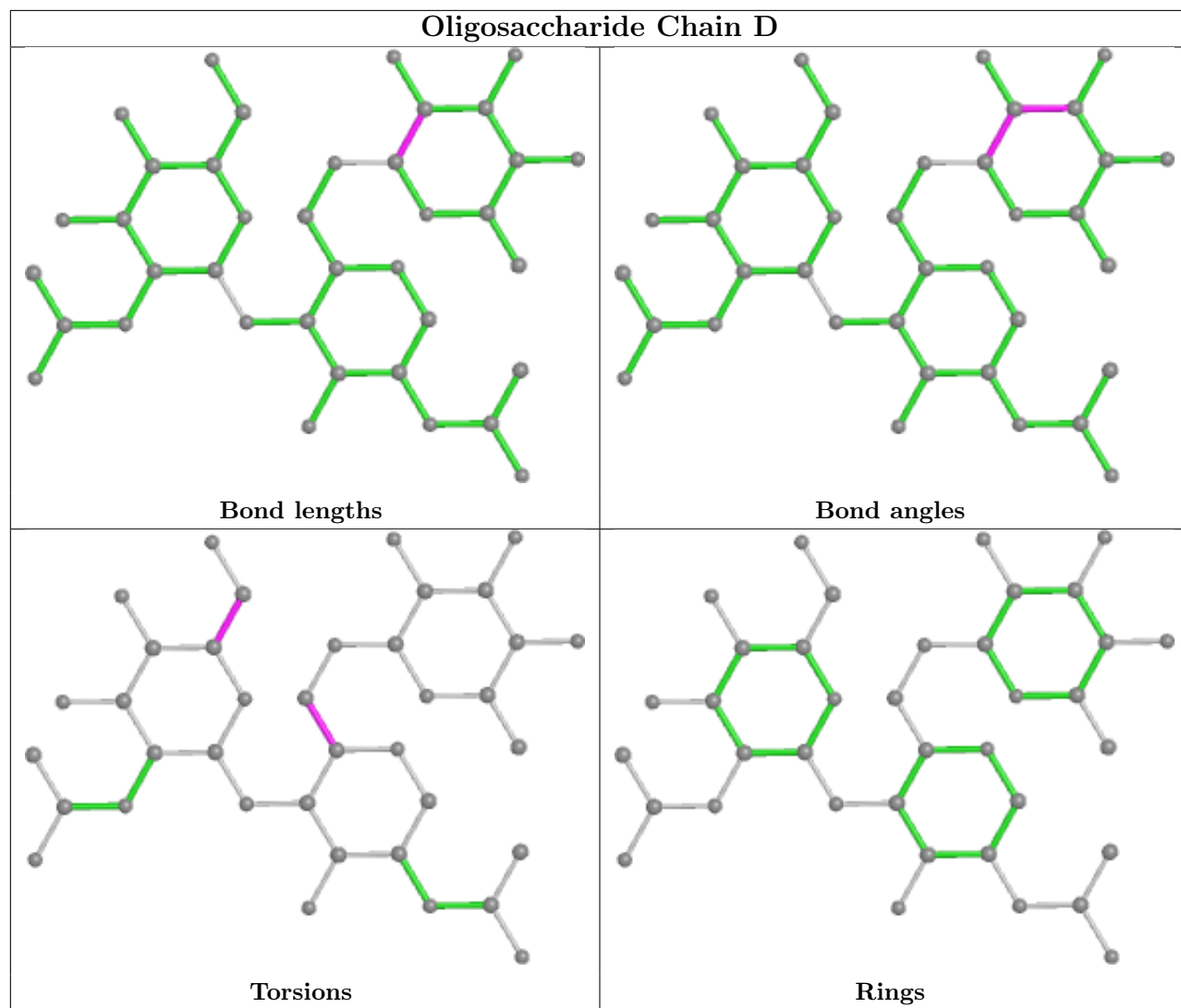
There are no ring outliers.

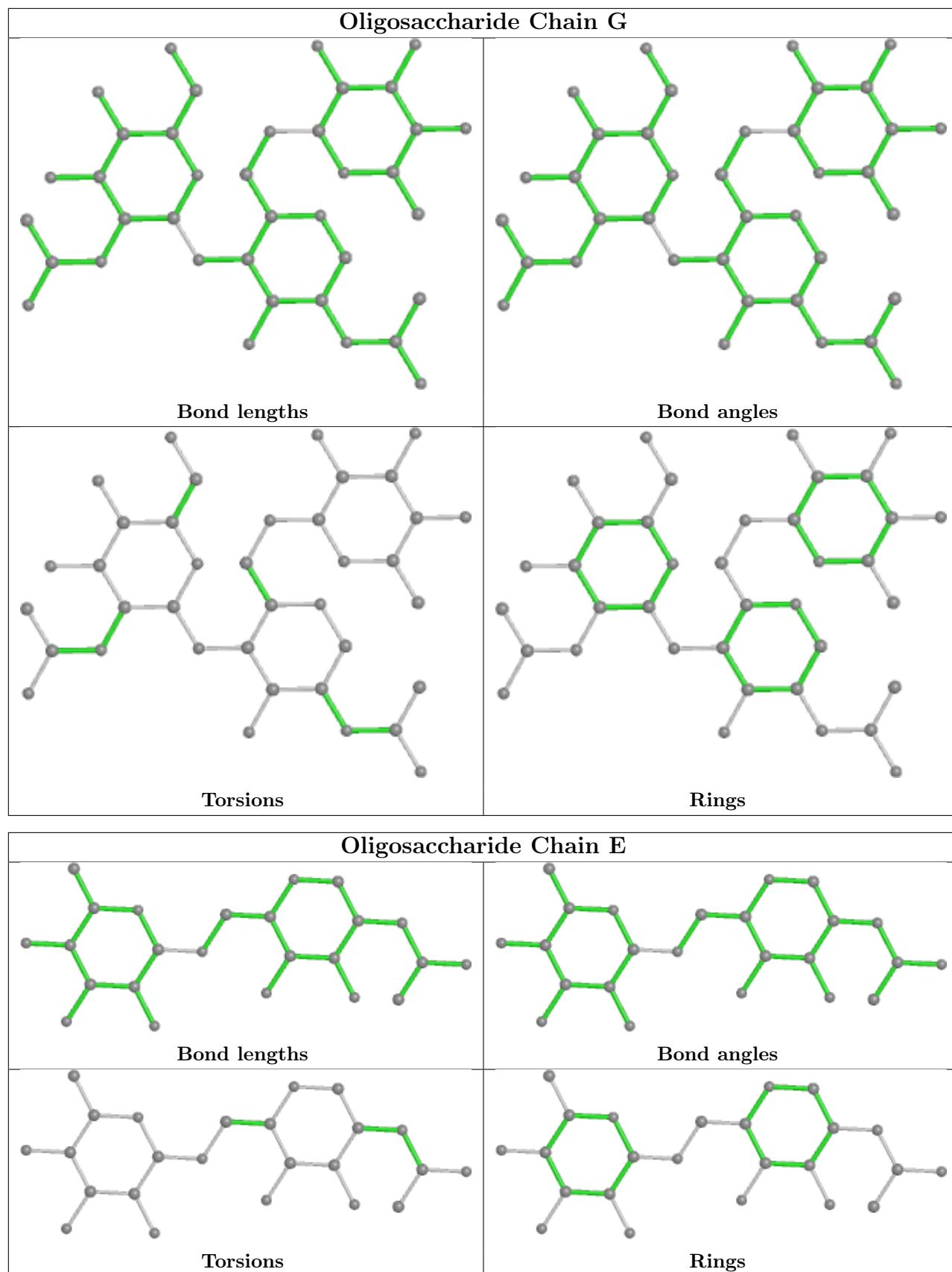
2 monomers are involved in 2 short contacts:

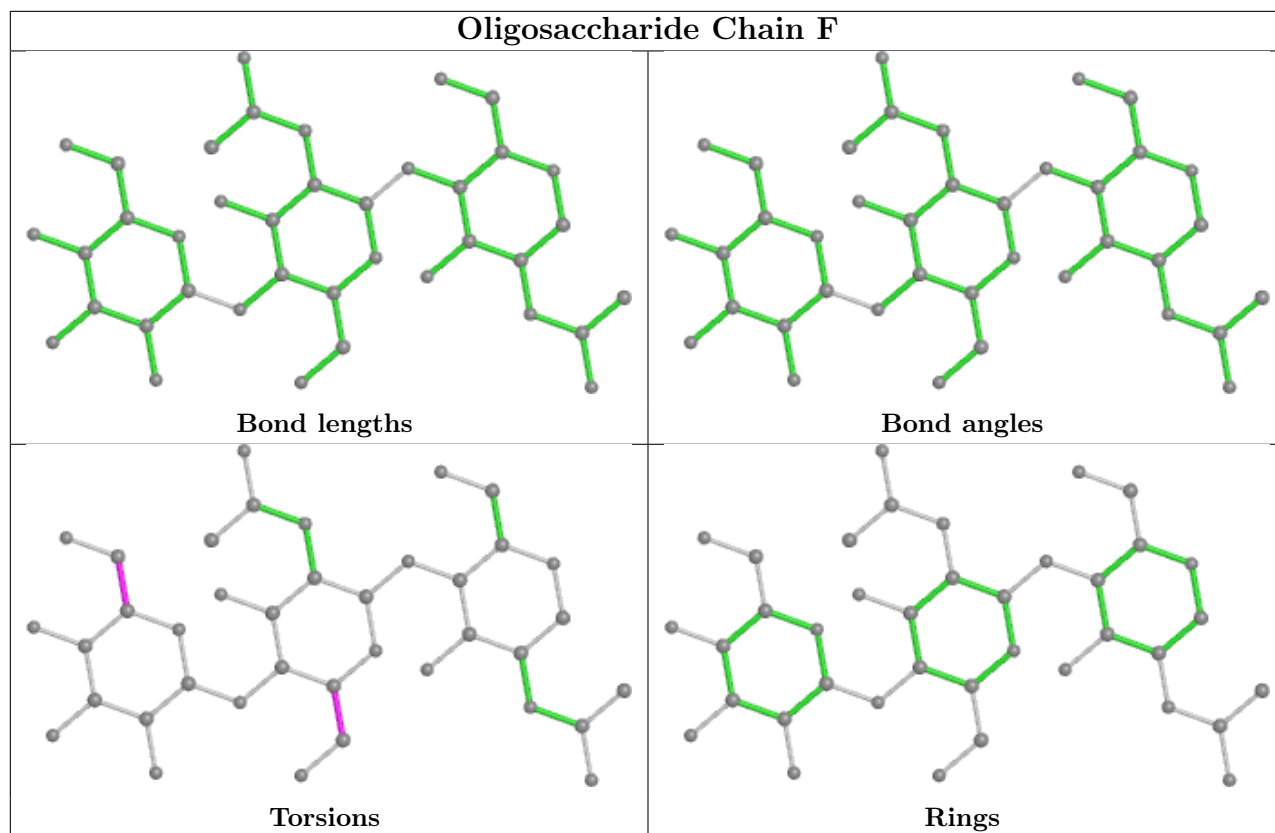
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
3	G	1	NAG	1	0

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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
6	NAG	B	602	1	14,14,15	0.31	0	17,19,21	0.62	1 (5%)
6	NAG	A	601	1	14,14,15	0.32	0	17,19,21	0.60	1 (5%)
6	NAG	B	601	1	14,14,15	0.27	0	17,19,21	0.50	0
9	UD1	B	606	8	38,41,41	0.34	0	57,62,62	1.16	4 (7%)
9	UD1	A	606	8	38,41,41	0.35	0	57,62,62	1.18	3 (5%)
6	NAG	A	602	1	14,14,15	0.30	0	17,19,21	0.55	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
6	NAG	B	602	1	-	0/6/23/26	0/1/1/1
6	NAG	A	601	1	-	0/6/23/26	0/1/1/1
6	NAG	B	601	1	-	0/6/23/26	0/1/1/1
9	UD1	B	606	8	-	3/26/63/63	0/3/3/3
9	UD1	A	606	8	-	5/26/63/63	0/3/3/3
6	NAG	A	602	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	606	UD1	O1'-C1'-C2'	-4.67	99.95	108.40
9	B	606	UD1	O1'-C1'-C2'	-3.84	101.46	108.40
9	B	606	UD1	O3A-PB-O1'	2.53	107.58	102.48
9	B	606	UD1	PB-O1'-C1'	-2.47	110.18	119.74
9	A	606	UD1	O1'-PB-O1B	2.44	118.61	109.47
9	A	606	UD1	C4'-C3'-C2'	-2.29	106.99	110.34
6	B	602	NAG	C1-O5-C5	2.17	115.13	112.19
6	A	601	NAG	C1-O5-C5	2.05	114.96	112.19
9	B	606	UD1	O2'-C2B-C1B	-2.01	103.29	110.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

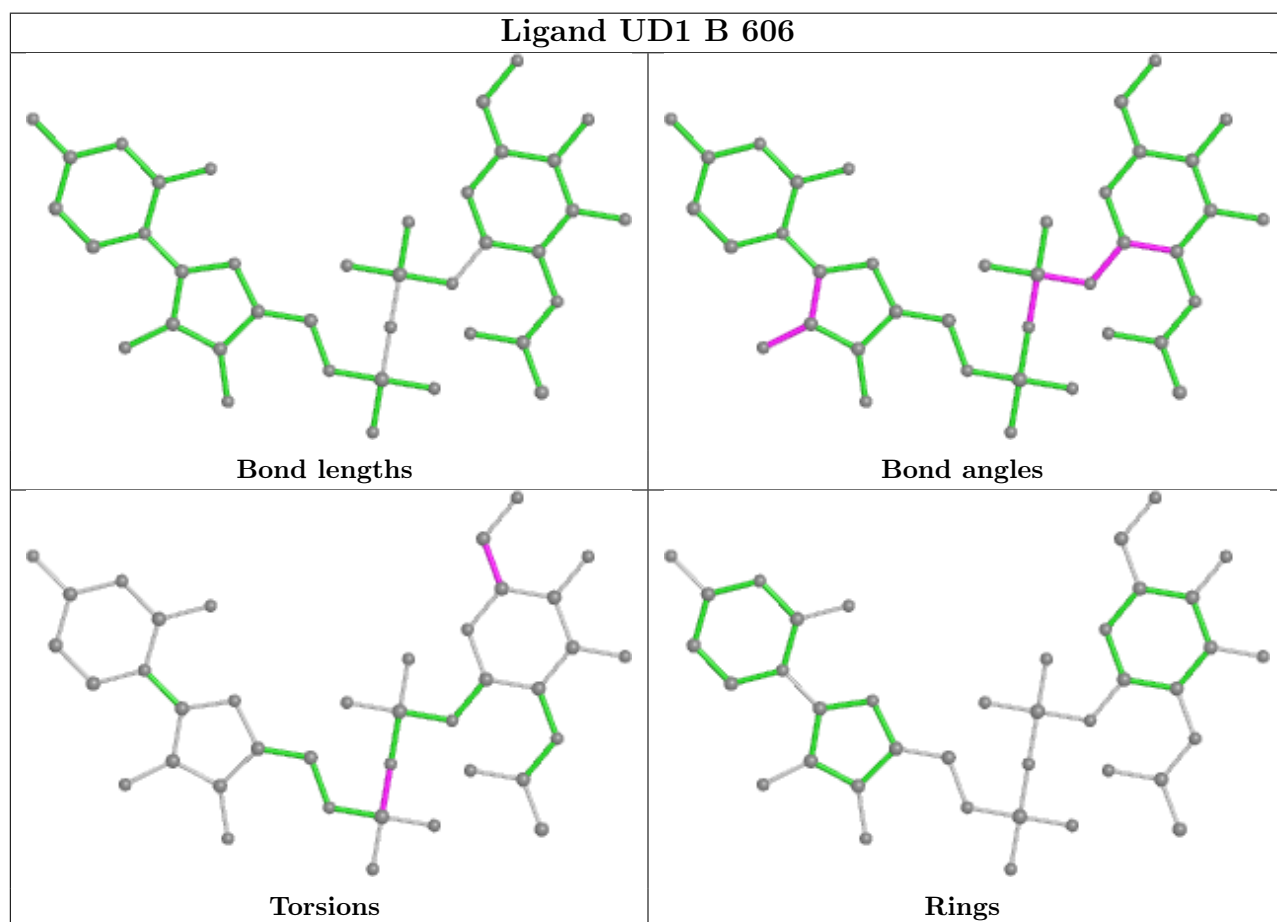
Mol	Chain	Res	Type	Atoms
9	A	606	UD1	C1'-O1'-PB-O3A
6	A	602	NAG	C4-C5-C6-O6
6	A	602	NAG	O5-C5-C6-O6
9	A	606	UD1	C4'-C5'-C6'-O6'
9	A	606	UD1	C1'-O1'-PB-O2B
9	B	606	UD1	C4'-C5'-C6'-O6'
9	B	606	UD1	PB-O3A-PA-O2A
9	A	606	UD1	PA-O3A-PB-O1B
9	A	606	UD1	PA-O3A-PB-O2B
9	B	606	UD1	PB-O3A-PA-O1A

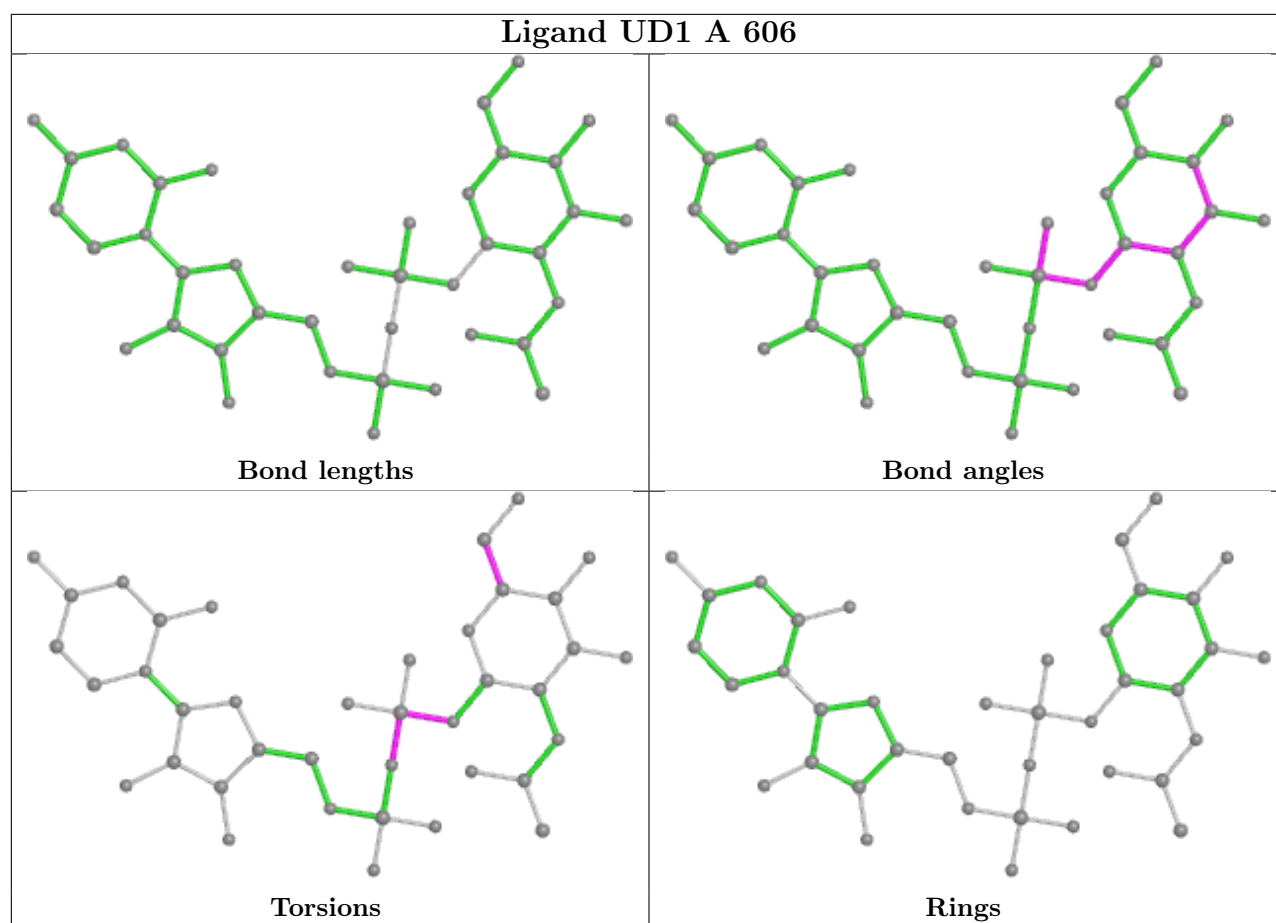
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	606	UD1	2	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	428/495 (86%)	0.19	27 (6%) 20 25	13, 37, 99, 147	0
1	B	439/495 (88%)	0.36	45 (10%) 6 9	22, 49, 108, 147	0
All	All	867/990 (87%)	0.28	72 (8%) 11 15	13, 44, 105, 147	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	LEU	7.8
1	A	518	LEU	7.3
1	B	394	THR	6.7
1	A	386	THR	6.1
1	B	101	LEU	6.0
1	B	393	PRO	5.3
1	A	383	SER	5.1
1	B	392	SER	5.1
1	B	129	ASN	5.0
1	B	103	ARG	4.7
1	B	99	THR	4.3
1	B	387	HIS	4.2
1	A	381	LEU	4.2
1	B	511	ARG	4.2
1	B	244	TRP	4.1
1	A	387	HIS	4.1
1	B	528	LEU	4.1
1	A	384	ASN	4.1
1	B	385	LEU	4.0
1	B	100	GLU	4.0
1	A	58	PHE	3.8
1	B	480	ASP	3.7
1	A	522	ARG	3.6
1	B	131	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	245	PRO	3.3
1	B	130	THR	3.3
1	B	508	TYR	3.3
1	B	521	TRP	3.3
1	B	253	ASP	3.3
1	B	477	ILE	3.3
1	B	395	GLN	3.2
1	A	57	LEU	3.2
1	B	425	PHE	3.1
1	A	410	LEU	3.0
1	B	102	LYS	3.0
1	A	394	THR	3.0
1	B	133	ARG	3.0
1	B	58	PHE	2.9
1	B	412	ILE	2.9
1	B	479	LYS	2.8
1	B	427	ASP	2.8
1	A	377	CYS	2.8
1	B	132	SER	2.8
1	B	104	SER	2.8
1	B	506	ARG	2.7
1	B	384	ASN	2.7
1	A	244	TRP	2.7
1	A	413	HIS	2.7
1	A	403	MET	2.6
1	A	382	PRO	2.6
1	B	381	LEU	2.6
1	B	96	LYS	2.5
1	B	527	LYS	2.5
1	B	365	GLN	2.5
1	A	506	ARG	2.4
1	B	513	LEU	2.4
1	A	425	PHE	2.3
1	A	517	GLU	2.3
1	A	521	TRP	2.2
1	A	516	THR	2.2
1	B	512	PHE	2.2
1	B	411	VAL	2.2
1	A	523	ILE	2.2
1	B	56	VAL	2.2
1	B	417	ILE	2.1
1	A	379	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	411	VAL	2.1
1	B	525	ARG	2.1
1	A	378	SER	2.1
1	A	412	ILE	2.0
1	B	413	HIS	2.0
1	B	524	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

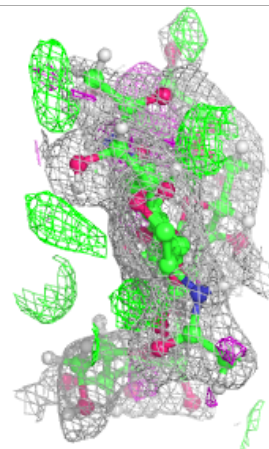
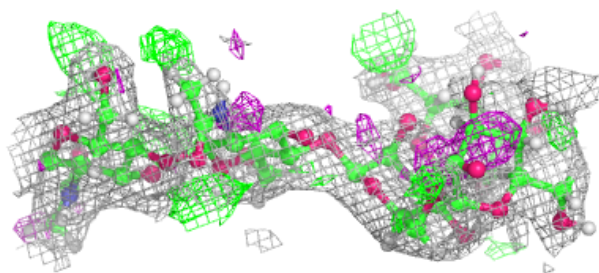
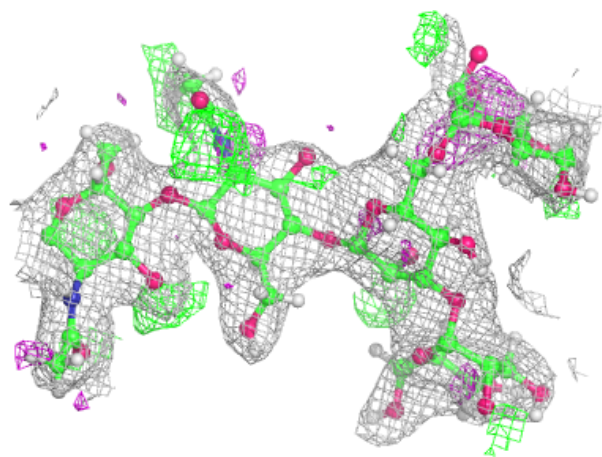
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	C	5	11/12	0.45	0.34	86,110,144,151	0
5	BMA	F	3	11/12	0.54	0.33	104,111,136,143	0
4	NAG	E	1	14/15	0.76	0.21	65,92,118,122	0
3	NAG	D	2	14/15	0.76	0.35	84,101,118,129	0
3	NAG	G	2	14/15	0.79	0.38	90,110,133,147	0
3	NAG	G	1	14/15	0.85	0.26	69,95,112,117	0
5	NAG	F	2	14/15	0.85	0.25	52,87,105,105	0
2	BMA	C	3	11/12	0.85	0.17	62,78,94,101	0
4	FUC	E	2	10/11	0.88	0.28	109,117,136,136	0
2	NAG	C	2	14/15	0.89	0.18	45,59,65,70	0
3	FUC	G	3	10/11	0.89	0.26	82,93,106,110	0
3	NAG	D	1	14/15	0.89	0.18	50,68,83,97	0
2	MAN	C	4	11/12	0.91	0.22	56,70,89,89	0
3	FUC	D	3	10/11	0.93	0.24	66,79,95,99	0
5	NAG	F	1	14/15	0.93	0.11	45,63,76,86	0
2	NAG	C	1	14/15	0.98	0.11	19,32,41,53	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.

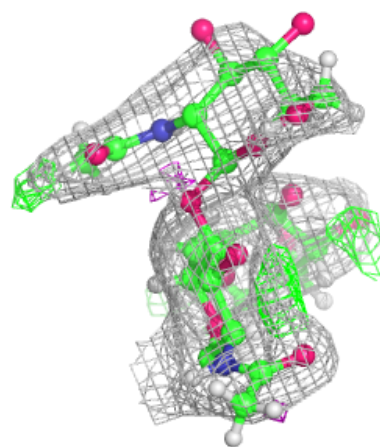
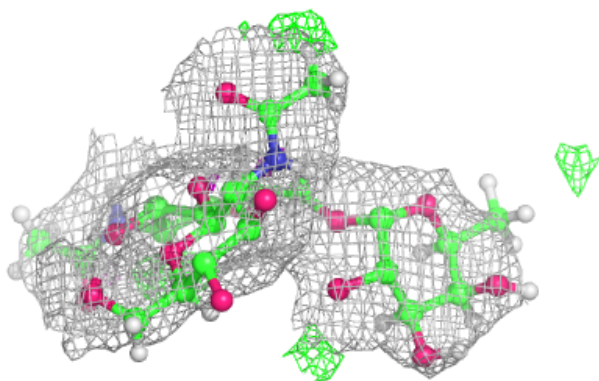
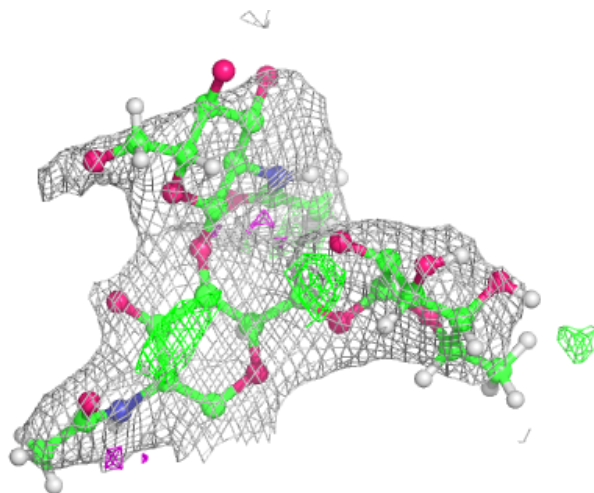
Electron density around Chain C:

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



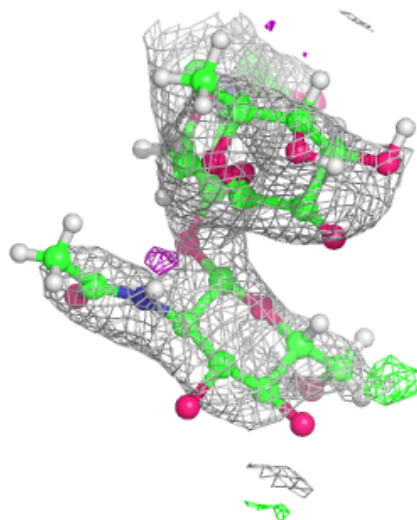
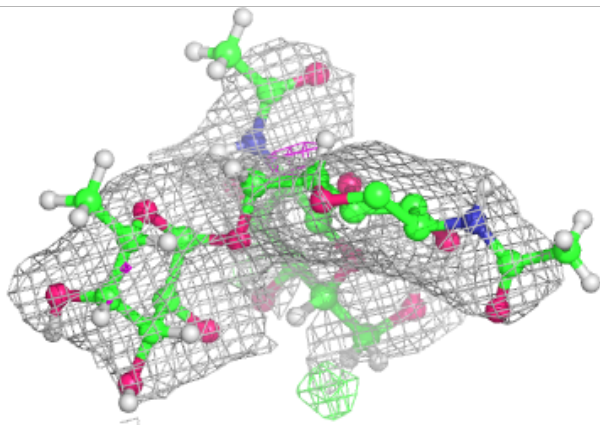
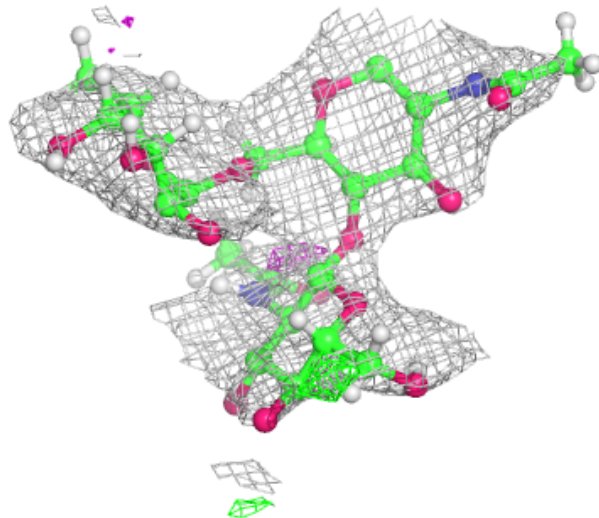
Electron density around Chain D:

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



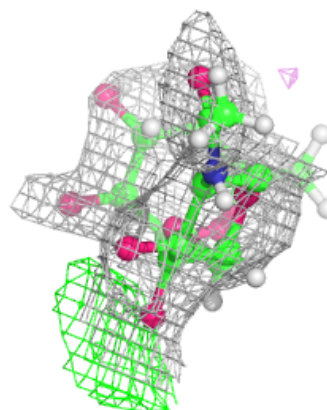
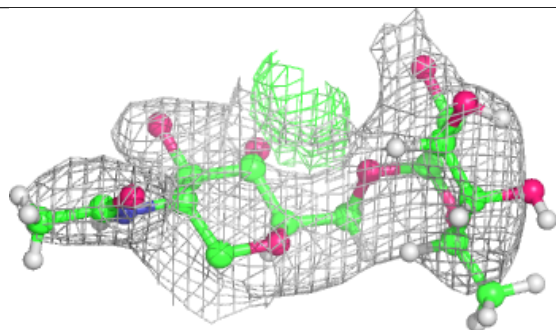
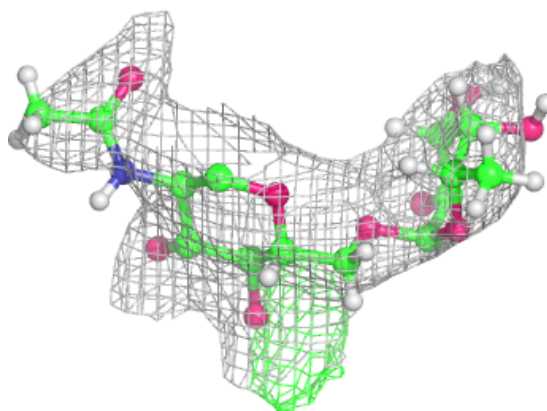
Electron density around Chain G:

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

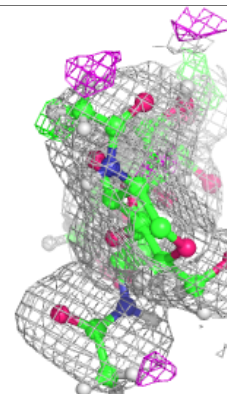
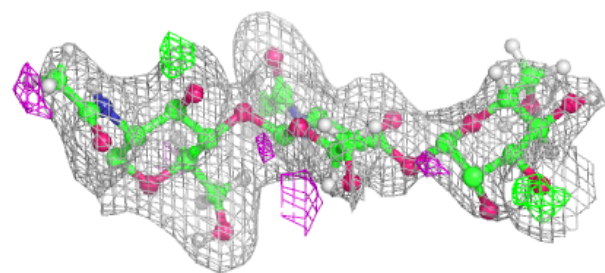
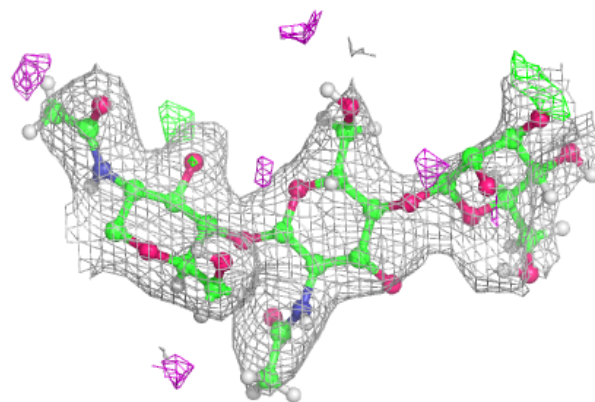


Electron density around Chain E:

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

**Electron density around Chain F:**

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



6.4 Ligands

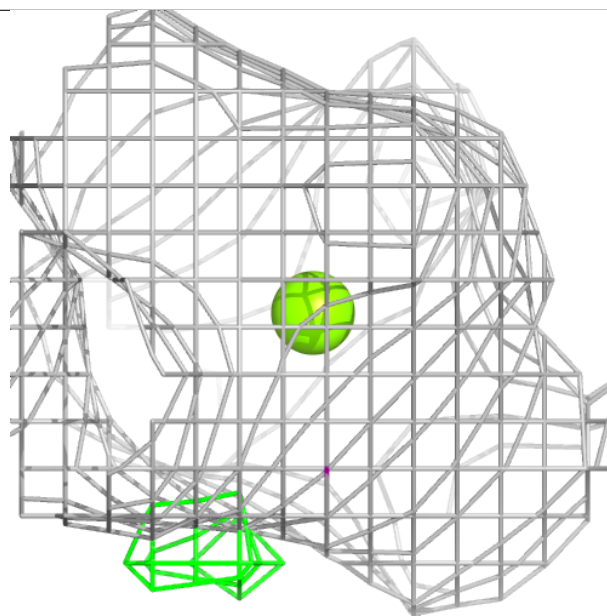
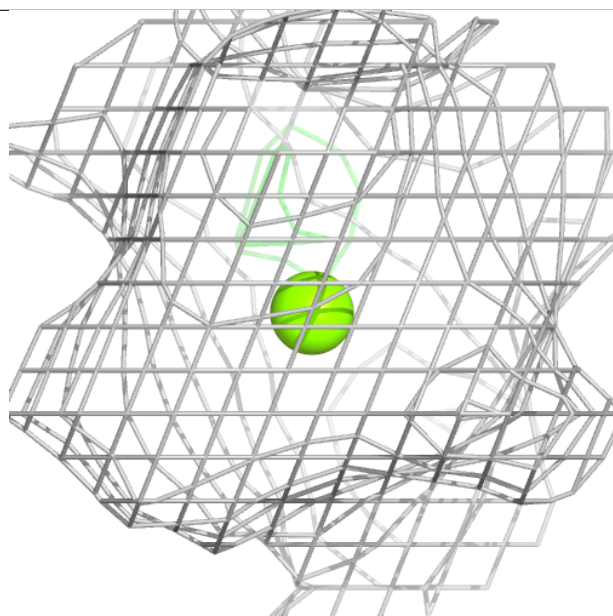
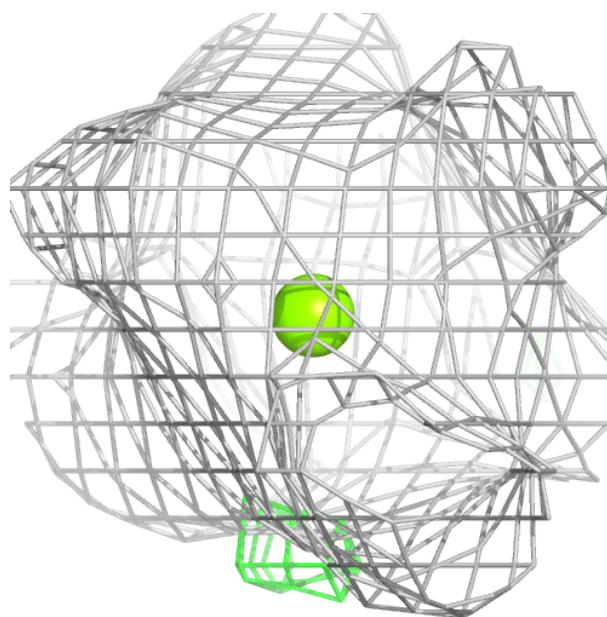
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	B	602	14/15	0.78	0.24	97,109,125,130	0
6	NAG	A	602	14/15	0.79	0.27	62,90,106,114	0
6	NAG	A	601	14/15	0.79	0.39	84,104,125,136	0
6	NAG	B	601	14/15	0.84	0.31	68,88,104,110	0
8	MG	B	605	1/1	0.94	0.12	49,49,49,49	0
8	MG	B	604	1/1	0.96	0.14	43,43,43,43	0
9	UD1	B	606	39/39	0.97	0.12	31,48,67,76	0
8	MG	A	605	1/1	0.98	0.17	19,19,19,19	0
7	CA	B	603	1/1	0.99	0.09	33,33,33,33	0
8	MG	A	604	1/1	0.99	0.15	19,19,19,19	0
9	UD1	A	606	39/39	0.99	0.15	11,18,29,35	0
7	CA	A	603	1/1	0.99	0.09	44,44,44,44	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.

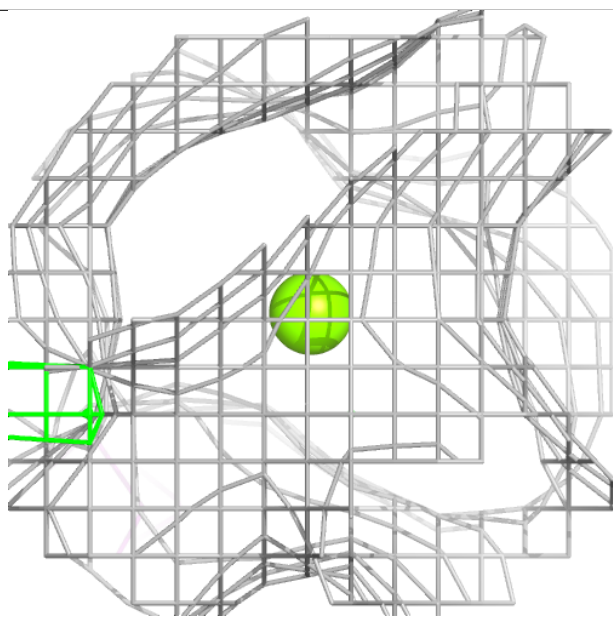
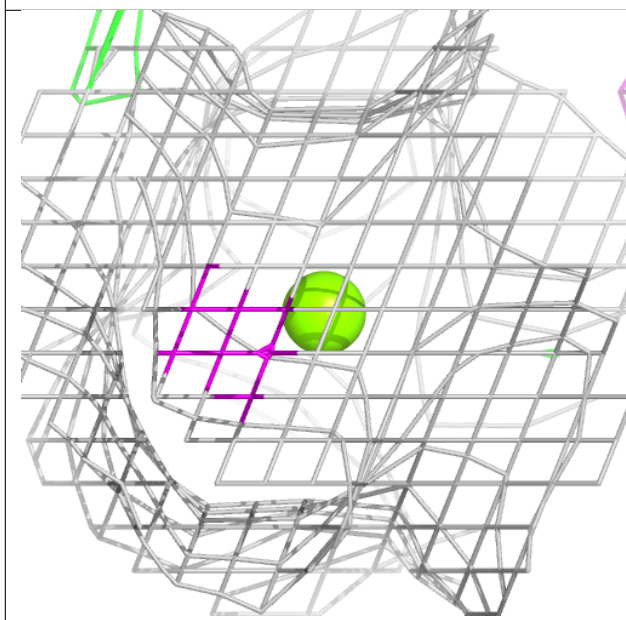
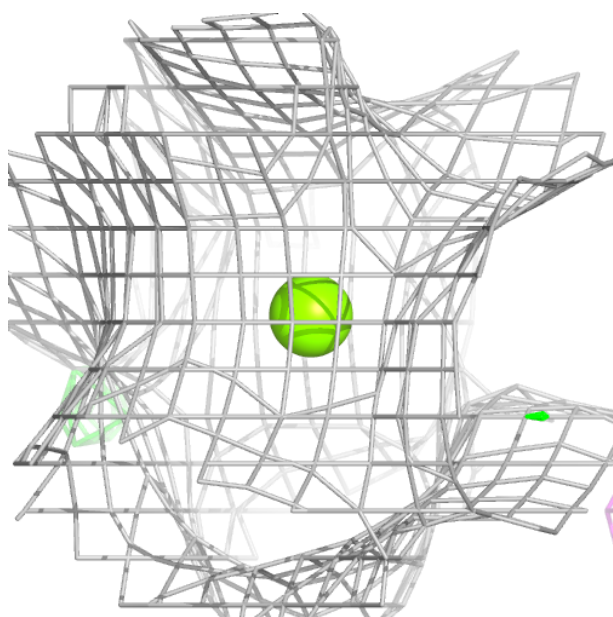
Electron density around MG B 605:

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



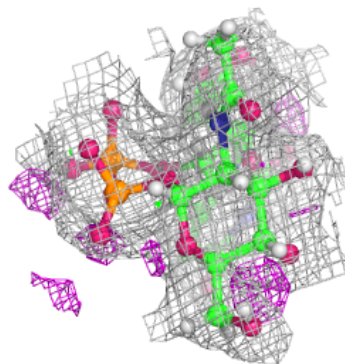
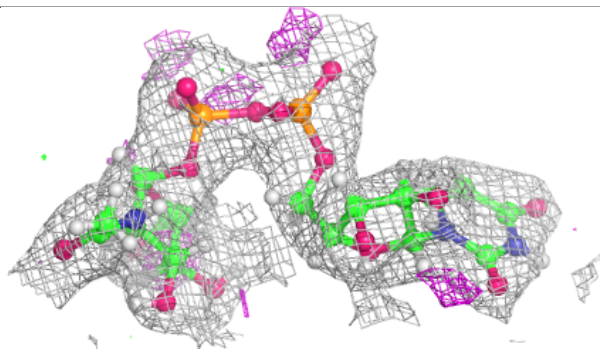
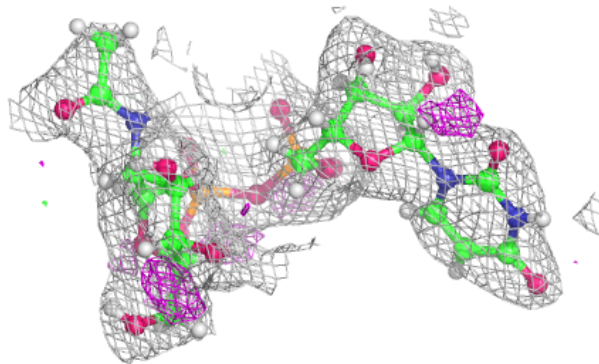
Electron density around MG B 604:

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



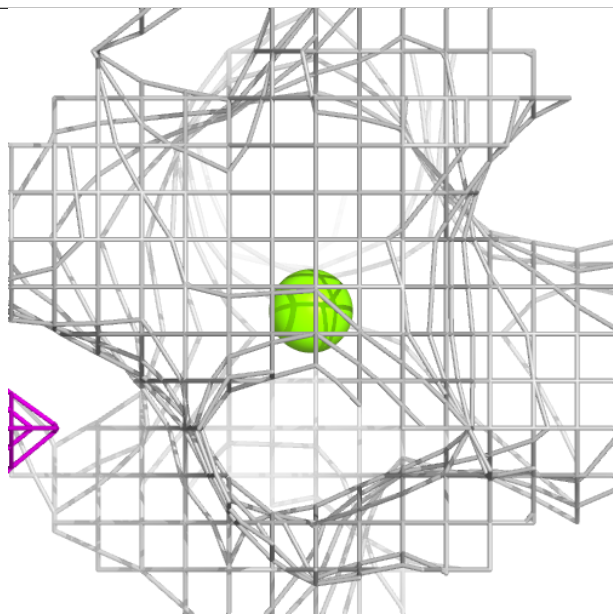
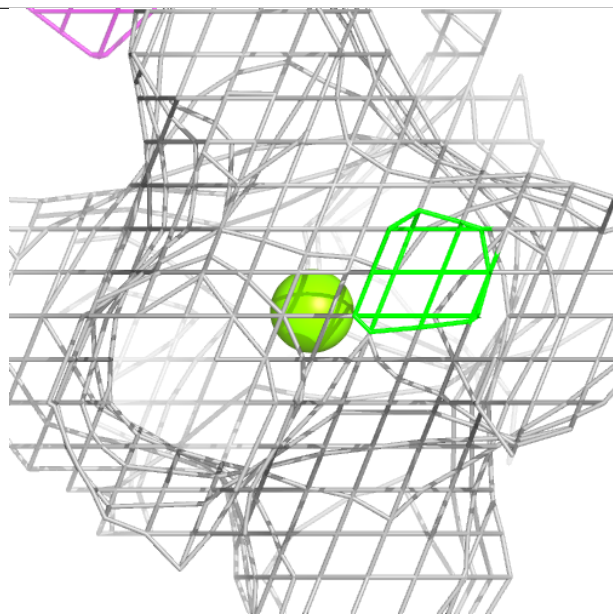
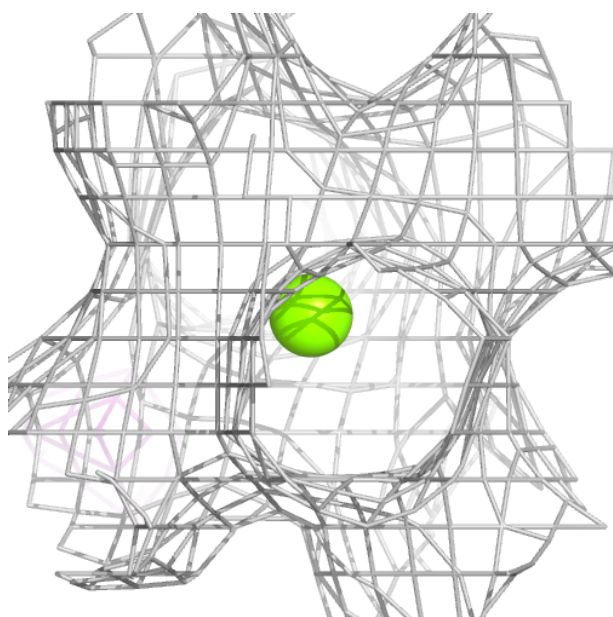
Electron density around UD1 B 606:

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



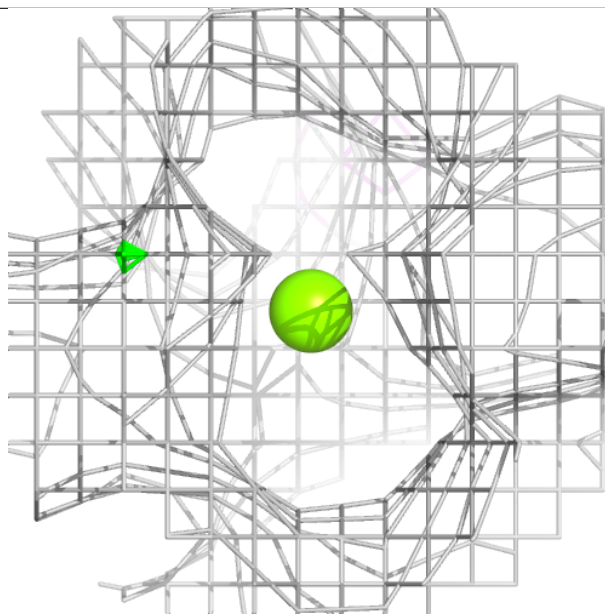
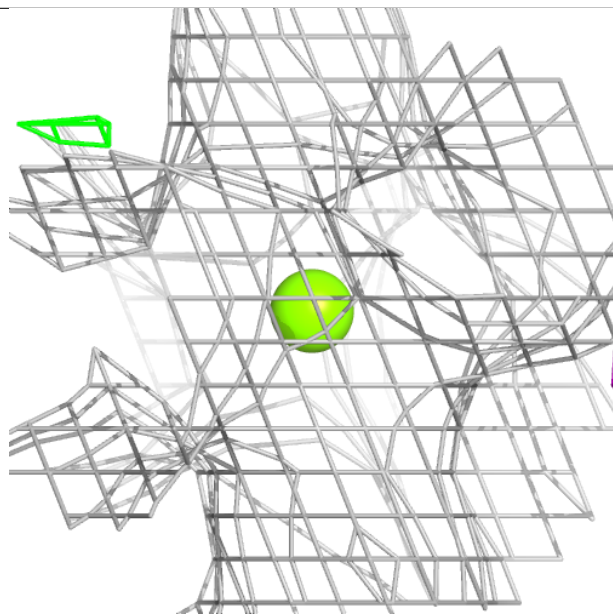
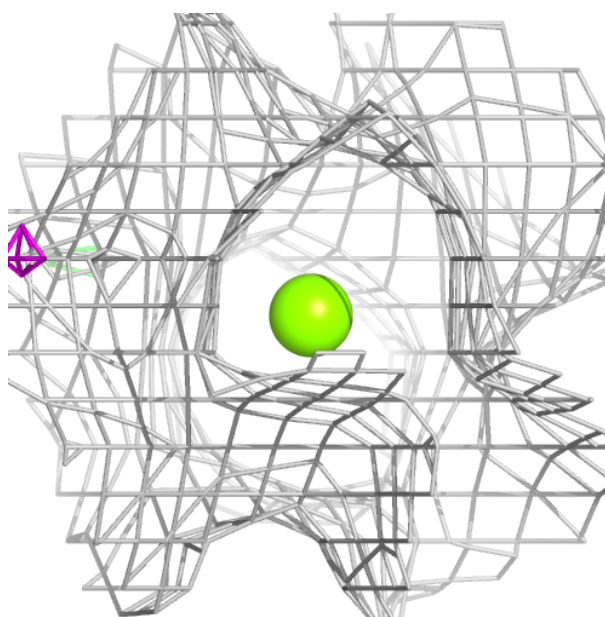
Electron density around MG A 605:

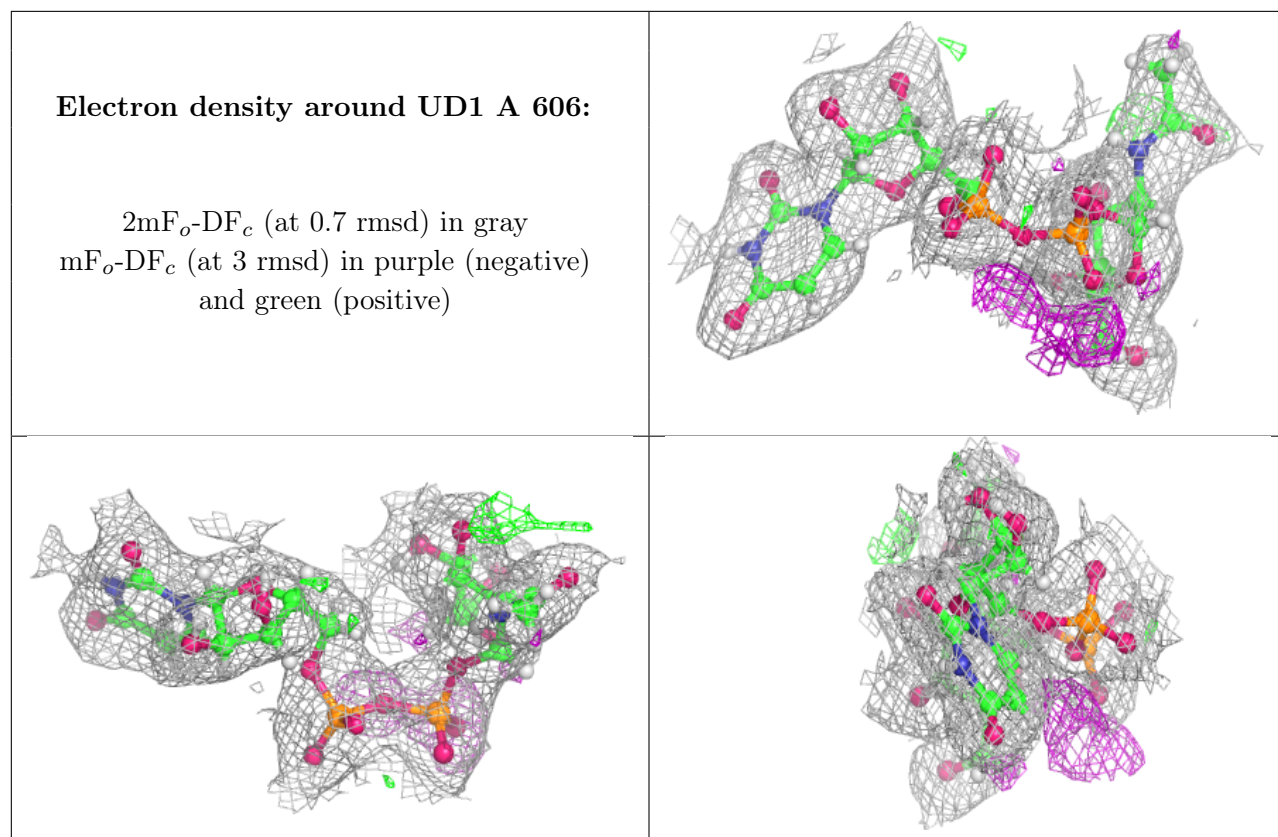
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 604:

$2mF_o-DF_c$ (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.