Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2026 – 03:26 pm GMT

PDB ID	:	28UT / pdb_000028ut
Title	:	Crystal structure of the Norovirus GII.4 P domain in complex with Lacto-N-fucopentaose I (LNFP I)
Authors	:	Pisapia, L.; Varrot, A.
Deposited on	:	2026-02-20
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

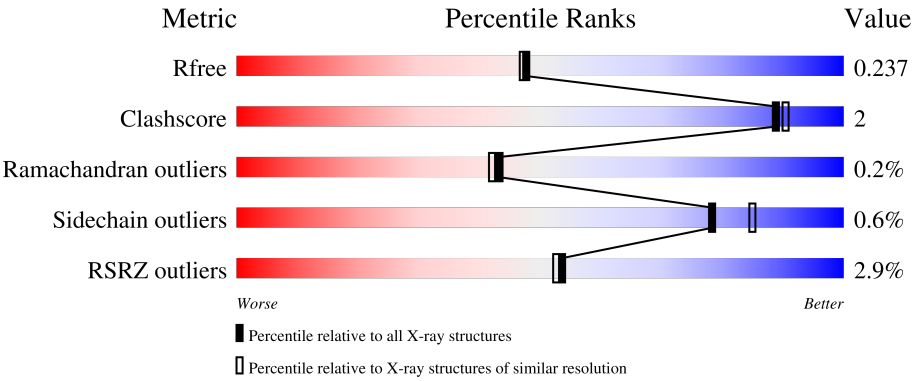
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.00 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.



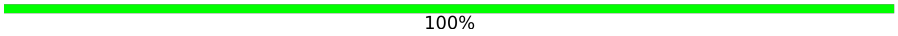
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	310	3% 93% 6% ·
1	B	310	5% 91% 7% ··
1	C	310	2% 92% 5% ·
1	D	310	2% 92% 6% ·
2	E	3	67% 33%

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Mol	Chain	Length	Quality of chain
2	G	3	
3	F	5	

2 Entry composition

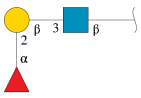
There are 6 unique types of molecules in this entry. The entry contains 10205 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

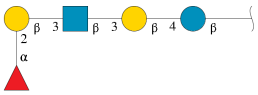
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	3	0
			2408	1522	411	464	11			
1	B	306	Total	C	N	O	S	0	0	0
			2373	1506	403	453	11			
1	C	303	Total	C	N	O	S	0	2	0
			2372	1507	402	452	11			
1	D	307	Total	C	N	O	S	0	0	0
			2391	1517	407	456	11			

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



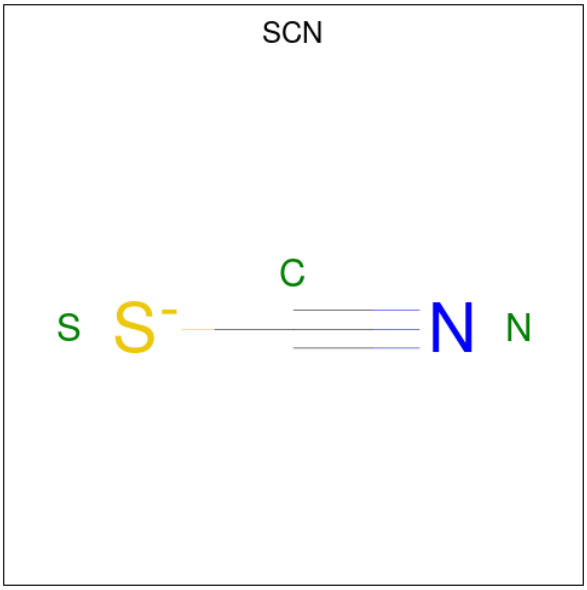
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	G	3	Total	C	N	O	0	0	0
			36	20	1	15			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	5	Total C N O 58 32 1 25	0	0	0

- Molecule 4 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N S 3 1 1 1	0	0
4	D	1	Total C N S 3 1 1 1	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0

- Molecule 6 is water.

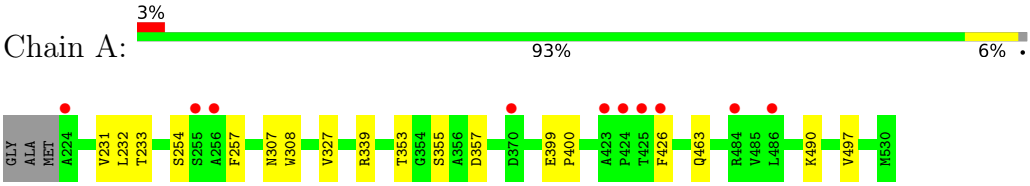
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	132	Total O 133 133	0	1
6	B	117	Total O 117 117	0	0
6	C	120	Total O 121 121	0	1
6	D	150	Total O 150 150	0	0

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.

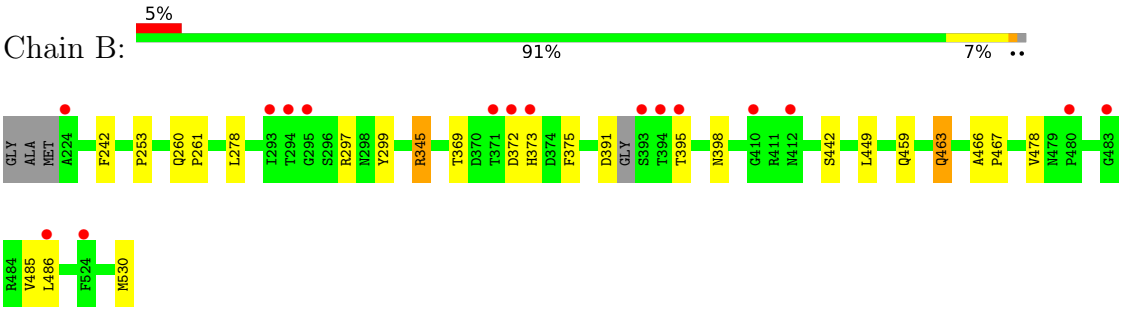
• Molecule 1: VP1

Chain A:



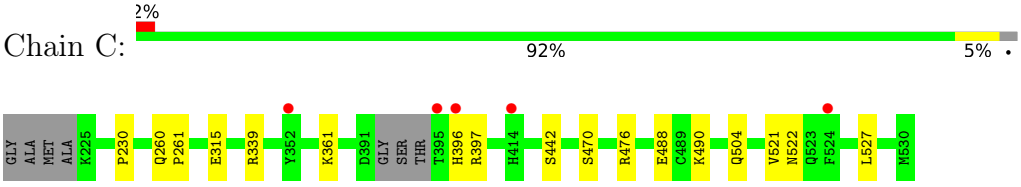
• Molecule 1: VP1

Chain B:



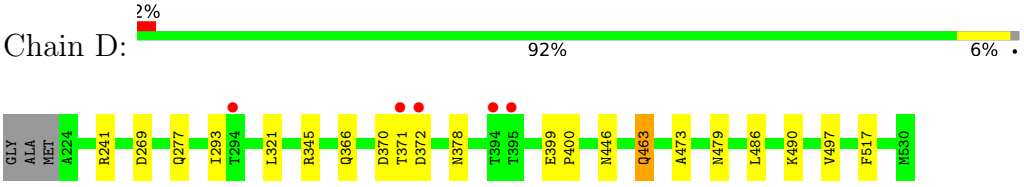
• Molecule 1: VP1

Chain C:



• Molecule 1: VP1

Chain D:



• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:





• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

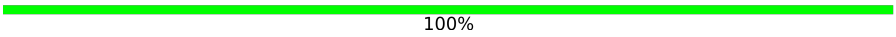
Chain G:





• Molecule 3: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.58Å 128.20Å 102.70Å 90.00° 93.08° 90.00°	Depositor
Resolution (Å)	46.62 – 2.00 46.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.62-2.00) 99.8 (46.62-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.179 , 0.233 0.188 , 0.237	Depositor DCC
R_{free} test set	3857 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10205	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: FUC, BGC, SCN, GAL, NAG, NA

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	0.55	0/2481	1.01	4/3394 (0.1%)
1	B	0.57	0/2442	0.99	3/3341 (0.1%)
1	C	0.56	0/2445	0.95	0/3344
1	D	0.56	0/2462	0.98	2/3367 (0.1%)
All	All	0.56	0/9830	0.98	9/13446 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
1	D	0	2
All	All	0	5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	426	PHE	N-CA-CB	-9.34	99.49	111.35
1	A	463	GLN	CB-CA-C	-8.15	98.02	110.90
1	B	463	GLN	CB-CA-C	-7.75	98.95	110.95
1	D	463	GLN	CB-CA-C	-7.25	98.52	110.85
1	B	345	ARG	CG-CD-NE	-6.02	98.76	112.00
1	D	269	ASP	CA-CB-CG	5.92	118.53	112.60
1	A	233	THR	CA-CB-OG1	-5.88	100.78	109.60
1	B	391	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	426	PHE	CB-CA-C	5.21	117.51	110.37

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	345	ARG	Sidechain
1	C	339	ARG	Sidechain
1	C	476	ARG	Sidechain
1	D	241	ARG	Sidechain
1	D	345	ARG	Sidechain

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	2408	0	2291	10	0
1	B	2373	0	2256	12	0
1	C	2372	0	2251	9	0
1	D	2391	0	2272	10	0
2	E	36	0	33	0	0
2	G	36	0	33	0	0
3	F	58	0	51	0	0
4	A	3	0	0	0	0
4	D	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	133	0	0	0	0
6	B	117	0	0	0	0
6	C	121	0	0	0	0
6	D	150	0	0	0	0
All	All	10205	0	9187	35	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 (35) 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:297:ARG:HA	1:B:372:ASP:CB	2.26	0.65
1:D:293:ILE:HD11	1:D:366:GLN:OE1	1.97	0.64
1:D:479:ASN:HB2	1:D:486:LEU:HD11	1.79	0.64
1:A:339:ARG:NE	1:C:504:GLN:HG3	2.18	0.58
1:B:395:THR:HG22	1:B:398:ASN:HB2	1.86	0.58
1:C:230:PRO:HB3	1:D:463:GLN:OE1	2.11	0.49
1:B:459:GLN:O	1:B:463:GLN:HG3	2.13	0.49
1:A:339:ARG:CZ	1:C:504:GLN:HG3	2.43	0.49
1:B:299:TYR:CE2	1:B:375:PHE:HB2	2.48	0.48
1:C:488:GLU:HG3	1:C:527:LEU:HD22	1.96	0.47
1:D:490:LYS:O	1:D:497:VAL:HA	2.13	0.47
1:A:231:VAL:HG22	1:B:463:GLN:HB3	1.97	0.47
1:D:400:PRO:HD2	1:D:446:ASN:O	2.14	0.46
1:A:490:LYS:O	1:A:497:VAL:HA	2.16	0.45
1:B:478:VAL:HG12	1:B:485:VAL:HG22	1.99	0.45
1:B:260:GLN:N	1:B:261:PRO:CD	2.80	0.44
1:A:232:LEU:HG	1:B:463:GLN:HG2	1.99	0.44
1:C:396:HIS:HB3	1:C:397:ARG:NH1	2.32	0.44
1:A:355:SER:OG	1:A:357:ASP:OD1	2.29	0.44
1:D:399:GLU:HA	1:D:400:PRO:C	2.43	0.44
1:C:470:SER:OG	1:C:521:VAL:O	2.31	0.43
1:A:399:GLU:HA	1:A:400:PRO:C	2.43	0.43
1:D:371:THR:O	1:D:372:ASP:HB2	2.18	0.43
1:B:253:PRO:HB3	1:D:378:ASN:HB3	2.01	0.42
1:B:297:ARG:NH1	1:B:369:THR:O	2.47	0.42
1:D:473:ALA:HB1	1:D:517:PHE:CE1	2.55	0.42
1:A:307:ASN:O	1:A:308:TRP:HB2	2.19	0.42
1:D:277:GLN:HB3	1:D:321:LEU:HB3	2.02	0.42
1:B:466:ALA:HA	1:B:467:PRO:HD3	1.94	0.41
1:A:254:SER:HA	1:A:257:PHE:CE1	2.56	0.41
1:B:242:PHE:HB2	1:B:449:LEU:CD2	2.50	0.41
1:C:490:LYS:HG3	1:C:527:LEU:HD21	2.01	0.41
1:C:315:GLU:O	1:C:361:LYS:NZ	2.54	0.41
1:C:260:GLN:N	1:C:261:PRO:CD	2.83	0.41
1:A:327:VAL:HA	1:A:353:THR:OG1	2.21	0.41

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	308/310 (99%)	298 (97%)	10 (3%)	0	100	100
1	B	302/310 (97%)	288 (95%)	13 (4%)	1 (0%)	36	35
1	C	301/310 (97%)	295 (98%)	5 (2%)	1 (0%)	36	35
1	D	305/310 (98%)	299 (98%)	6 (2%)	0	100	100
All	All	1216/1240 (98%)	1180 (97%)	34 (3%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	373	HIS
1	C	442	SER

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	268/268 (100%)	268 (100%)	0	100	100
1	B	261/268 (97%)	257 (98%)	4 (2%)	57	64
1	C	262/268 (98%)	261 (100%)	1 (0%)	84	89
1	D	263/268 (98%)	262 (100%)	1 (0%)	84	89
All	All	1054/1072 (98%)	1048 (99%)	6 (1%)	78	85

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

Mol	Chain	Res	Type
1	B	278	LEU
1	B	442	SER
1	B	486	LEU
1	B	530	MET
1	C	522	ASN
1	D	370	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	302	ASN
1	C	522	ASN

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)

11 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	2	15,15,15	0.20	0	21,21,21	0.88	1 (4%)
2	GAL	E	2	2	11,11,12	0.50	0	15,15,17	0.52	0
2	FUC	E	3	2	10,10,11	0.40	0	14,14,16	0.66	0
3	BGC	F	1	3	12,12,12	0.50	0	17,17,17	0.71	0
3	GAL	F	2	3	11,11,12	0.59	0	15,15,17	0.82	0
3	NAG	F	3	3	14,14,15	0.47	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GAL	F	4	3	11,11,12	0.59	0	15,15,17	0.47	0
3	FUC	F	5	3	10,10,11	0.51	0	14,14,16	0.74	0
2	NAG	G	1	2	15,15,15	0.17	0	21,21,21	0.53	0
2	GAL	G	2	2	11,11,12	0.56	0	15,15,17	0.63	0
2	FUC	G	3	2	10,10,11	0.29	0	14,14,16	0.77	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2	-	4/6/26/26	0/1/1/1
2	GAL	E	2	2	-	2/2/19/22	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
3	BGC	F	1	3	-	0/2/22/22	0/1/1/1
3	GAL	F	2	3	-	0/2/19/22	0/1/1/1
3	NAG	F	3	3	-	0/6/23/26	0/1/1/1
3	GAL	F	4	3	-	0/2/19/22	0/1/1/1
3	FUC	F	5	3	-	-	0/1/1/1
2	NAG	G	1	2	-	2/6/26/26	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	FUC	G	3	2	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	O3-C3-C2	-2.51	104.59	109.66
2	G	3	FUC	C1-C2-C3	2.37	112.58	109.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

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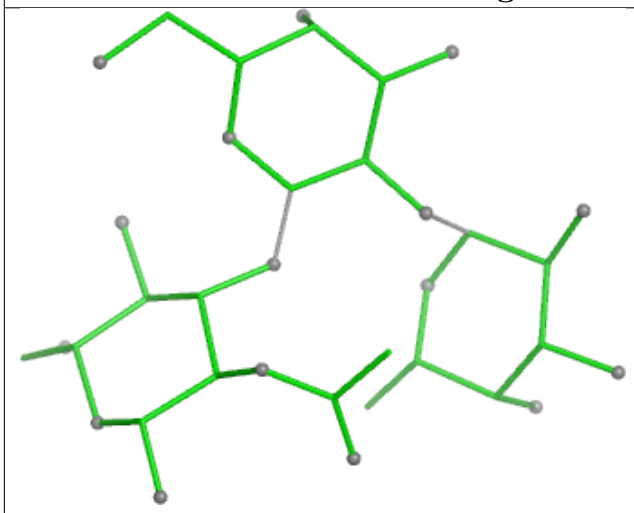
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	E	2	GAL	O5-C5-C6-O6
2	E	2	GAL	C4-C5-C6-O6

There are no ring outliers.

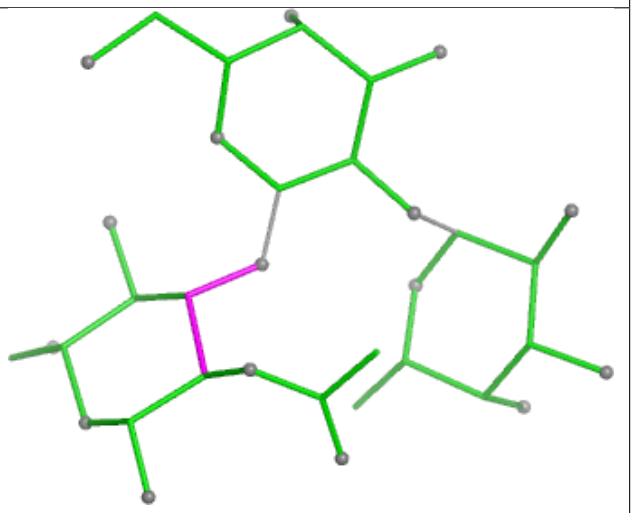
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

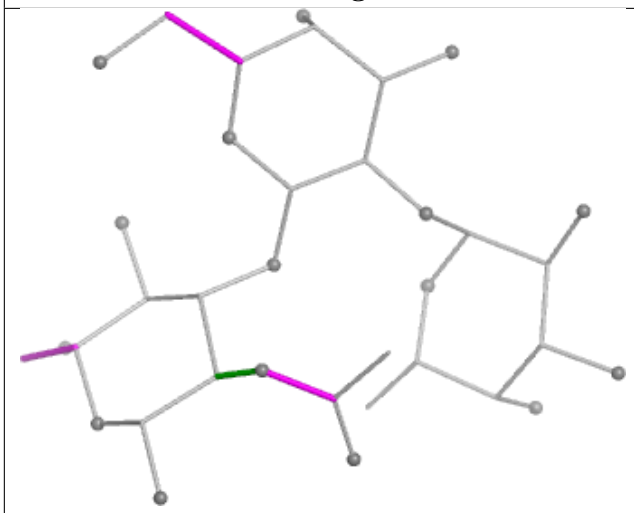
Oligosaccharide Chain E



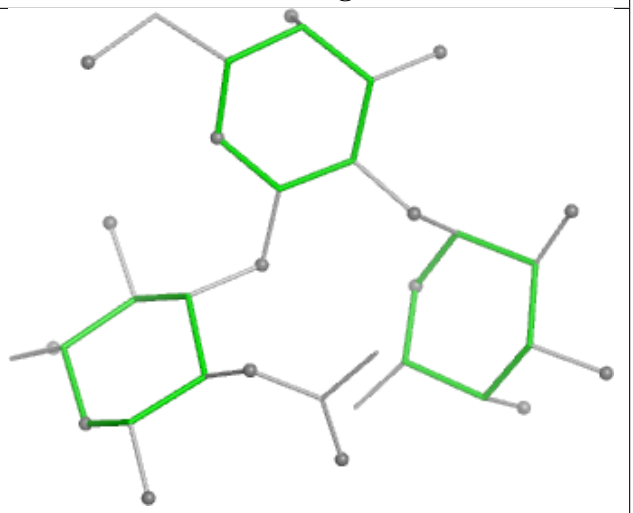
Bond lengths



Bond angles

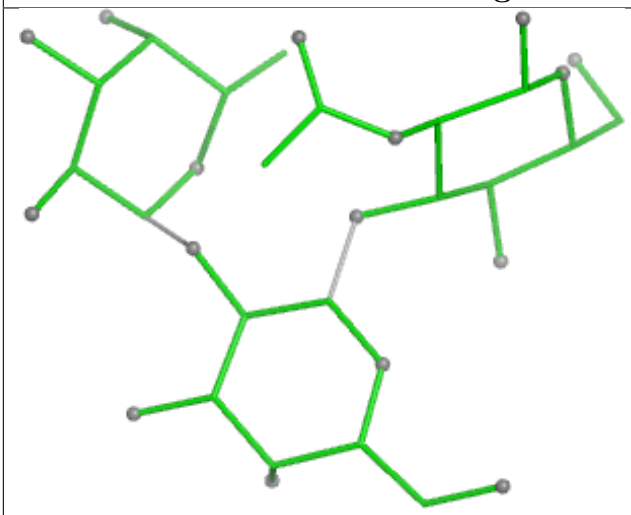


Torsions

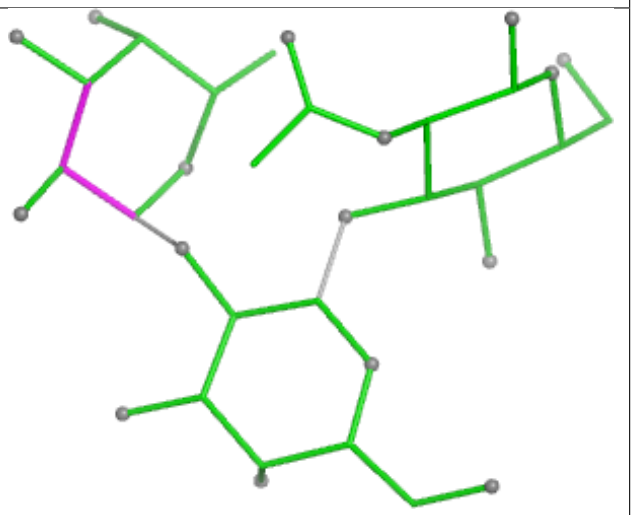


Rings

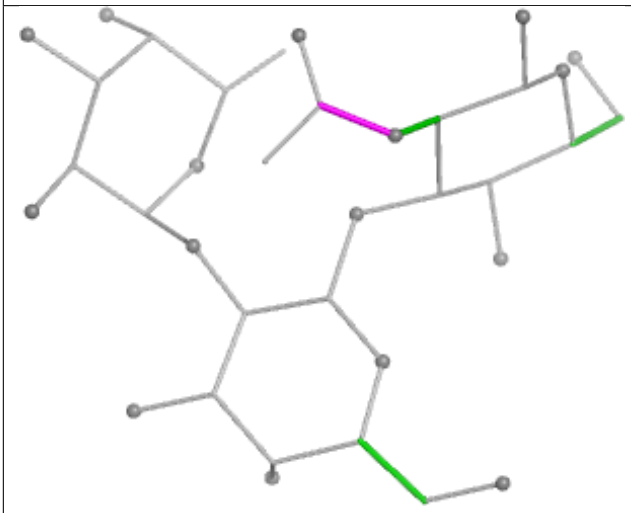
Oligosaccharide Chain G



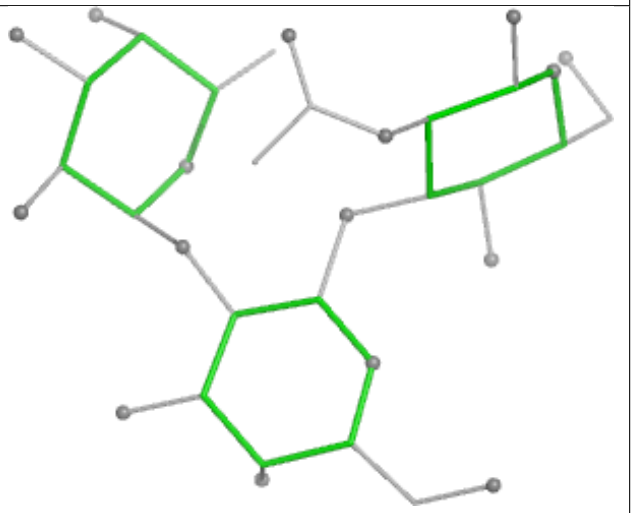
Bond lengths



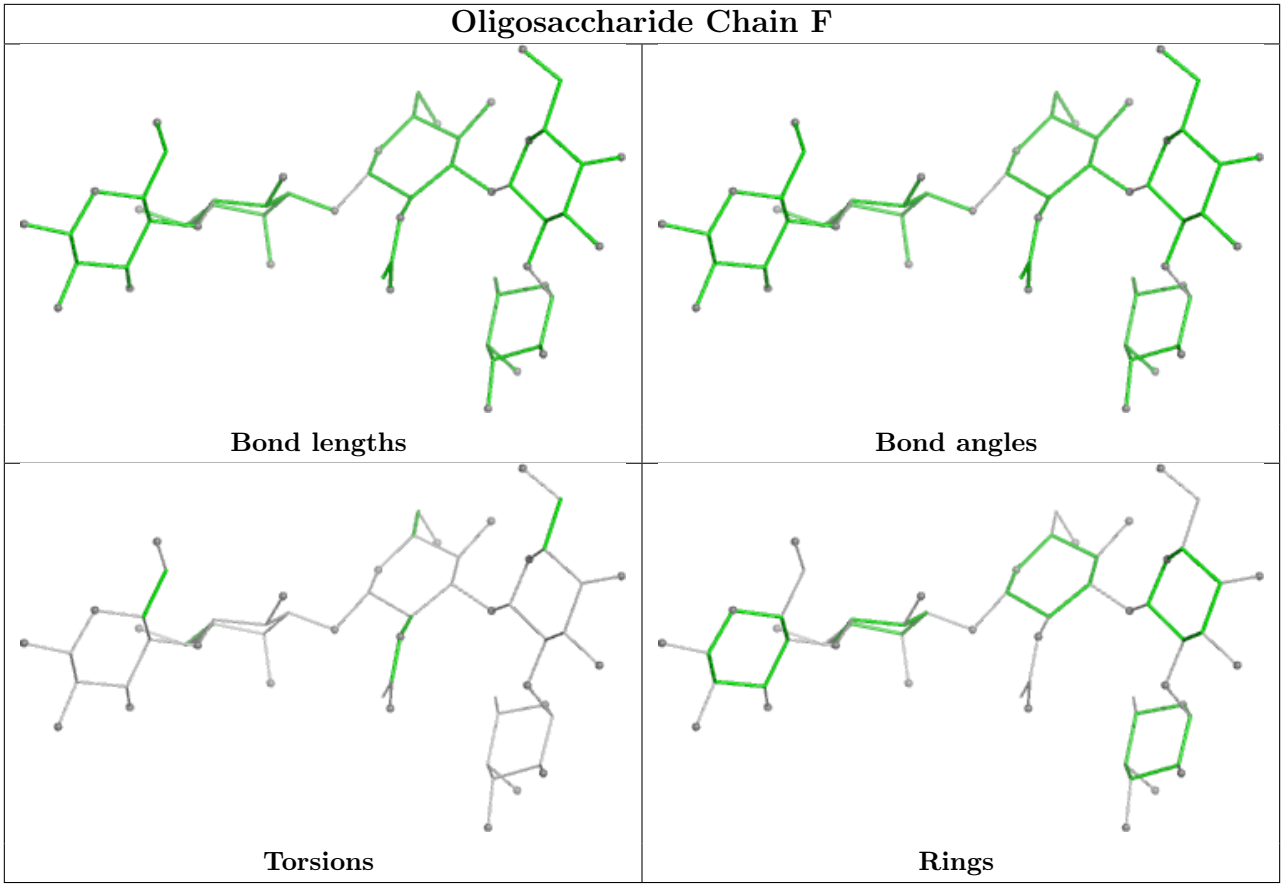
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
4	SCN	D	601	-	1,2,2	0.95	0	0,1,1	-	-
4	SCN	A	601	-	1,2,2	0.25	0	0,1,1	-	-

There are no bond length outliers.

There are no bond angle outliers.

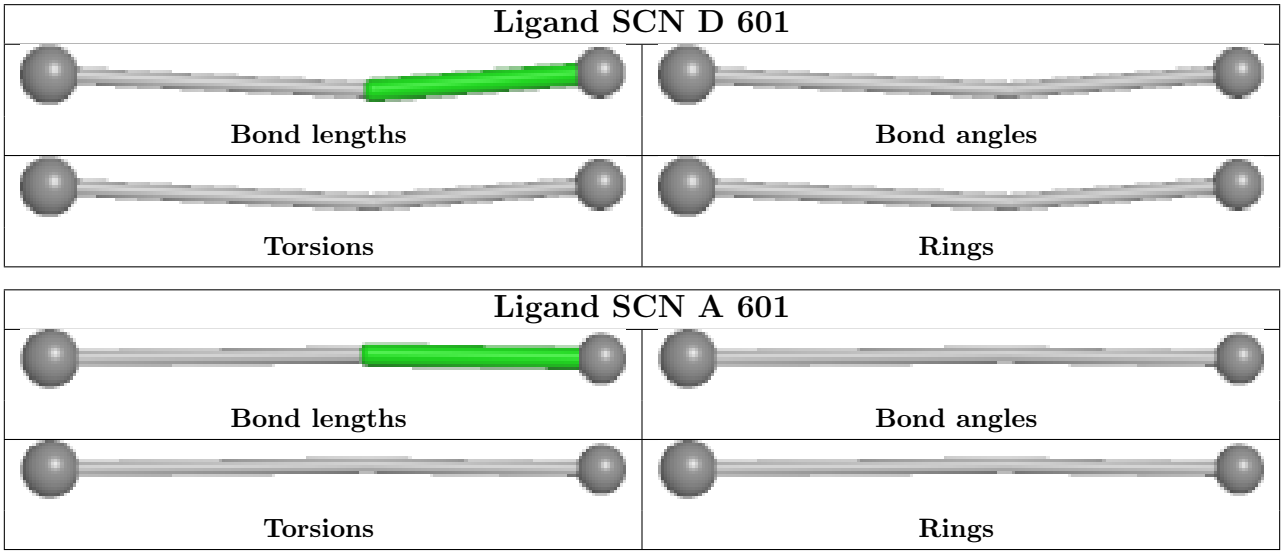
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	307/310 (99%)	0.10	10 (3%)	49	48	15, 29, 48, 62	4 (1%)
1	B	306/310 (98%)	0.21	16 (5%)	33	31	19, 29, 57, 80	1 (0%)
1	C	303/310 (97%)	0.08	5 (1%)	69	68	16, 30, 52, 68	4 (1%)
1	D	307/310 (99%)	-0.09	5 (1%)	70	70	20, 27, 45, 64	2 (0%)
All	All	1223/1240 (98%)	0.07	36 (2%)	53	52	15, 29, 52, 80	11 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	371	THR	5.2
1	B	524	PHE	5.2
1	A	426	PHE	3.9
1	B	412	ASN	3.8
1	C	395	THR	3.8
1	A	484	ARG	3.6
1	A	424	PRO	3.5
1	A	425	THR	3.5
1	B	371	THR	3.2
1	A	256	ALA	3.1
1	A	255	SER	3.1
1	B	294	THR	3.0
1	B	393	SER	2.9
1	C	396	HIS	2.8
1	C	414	HIS	2.7
1	C	352	TYR	2.7
1	B	394	THR	2.6
1	B	486	LEU	2.6
1	D	395	THR	2.6
1	C	524	PHE	2.6
1	D	394	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	293	ILE	2.5
1	B	224	ALA	2.4
1	B	373	HIS	2.4
1	D	372	ASP	2.4
1	A	224	ALA	2.3
1	B	395	THR	2.3
1	A	423	ALA	2.3
1	B	483	GLY	2.3
1	B	480	PRO	2.2
1	D	294	THR	2.2
1	A	370	ASP	2.1
1	B	372	ASP	2.1
1	A	486	LEU	2.0
1	B	295	GLY	2.0
1	B	410	GLY	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

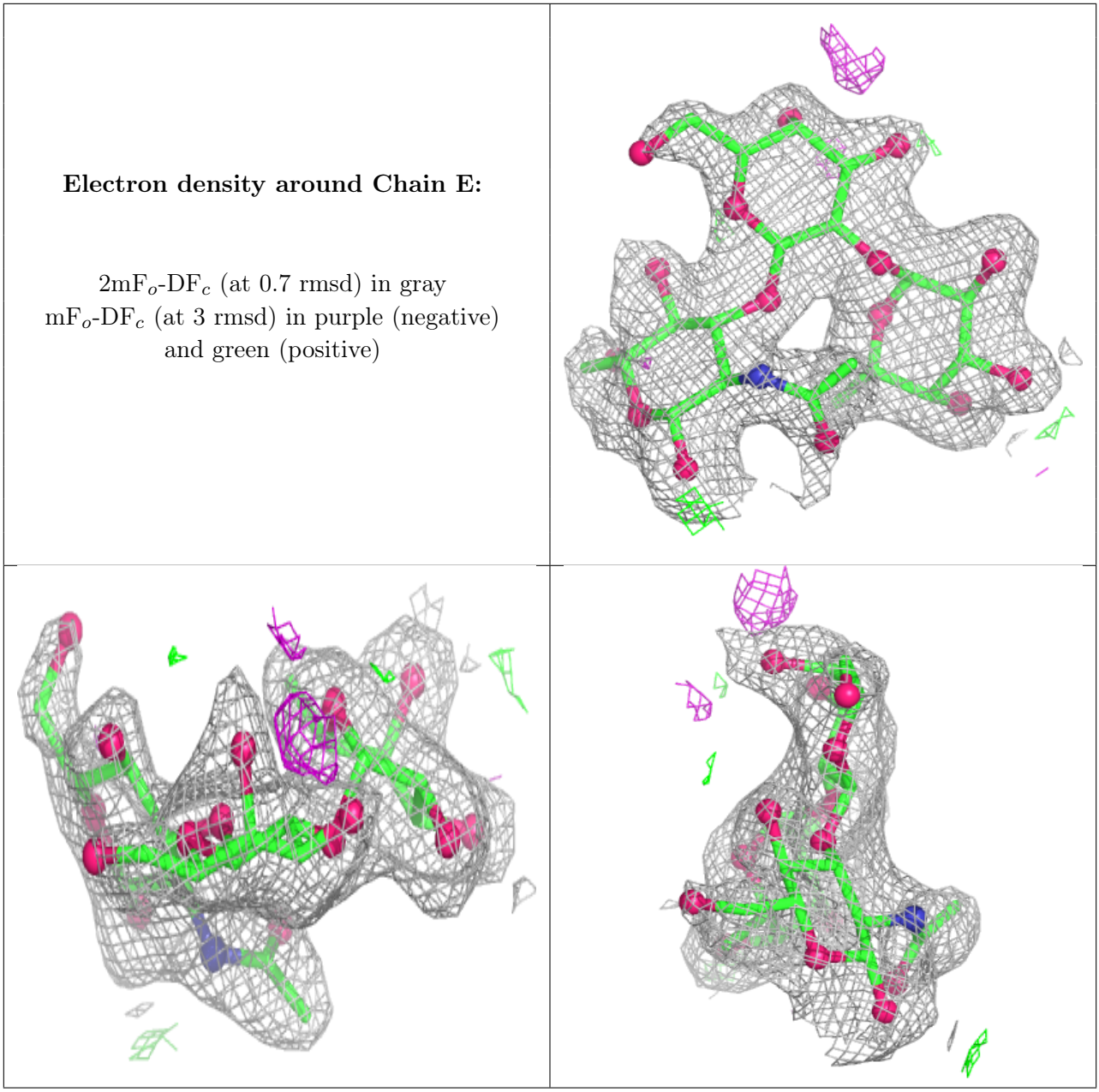
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	G	1	15/15	0.77	0.12	43,51,56,56	0
2	NAG	E	1	15/15	0.80	0.14	43,57,62,63	0
2	GAL	G	2	11/12	0.82	0.11	44,50,52,53	0
2	GAL	E	2	11/12	0.83	0.12	47,52,59,63	0
2	FUC	G	3	10/11	0.91	0.09	28,31,33,33	0
3	GAL	F	4	11/12	0.92	0.08	29,31,35,36	0
3	NAG	F	3	14/15	0.93	0.08	26,33,35,37	0
3	GAL	F	2	11/12	0.94	0.07	30,32,36,41	0
3	FUC	F	5	10/11	0.94	0.07	25,27,29,29	0
2	FUC	E	3	10/11	0.96	0.06	27,30,33,33	0
3	BGC	F	1	12/12	0.97	0.05	21,22,24,24	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

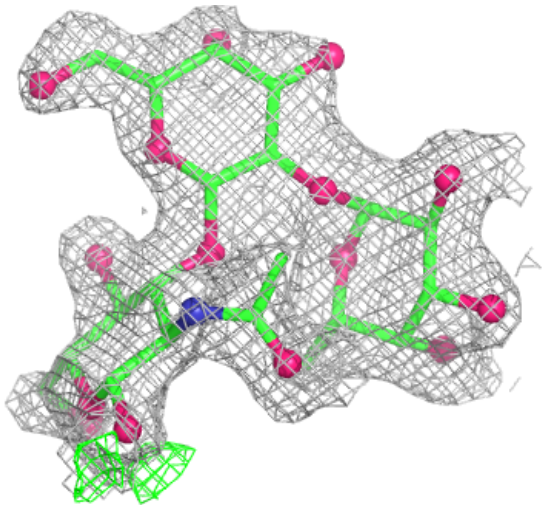
Electron density around Chain E:

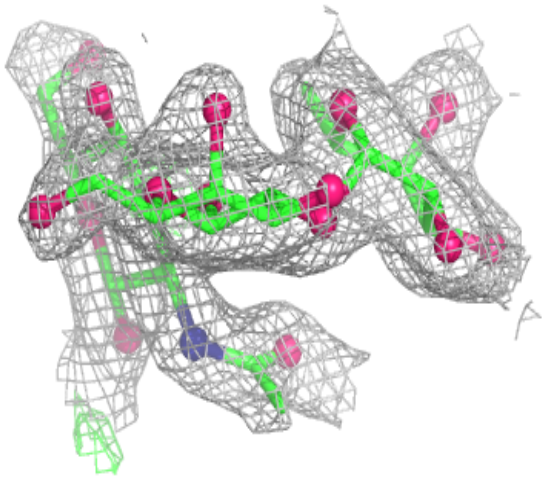
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

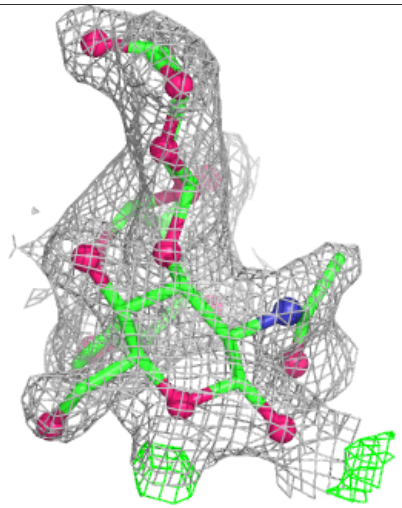


Electron density around Chain G:

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

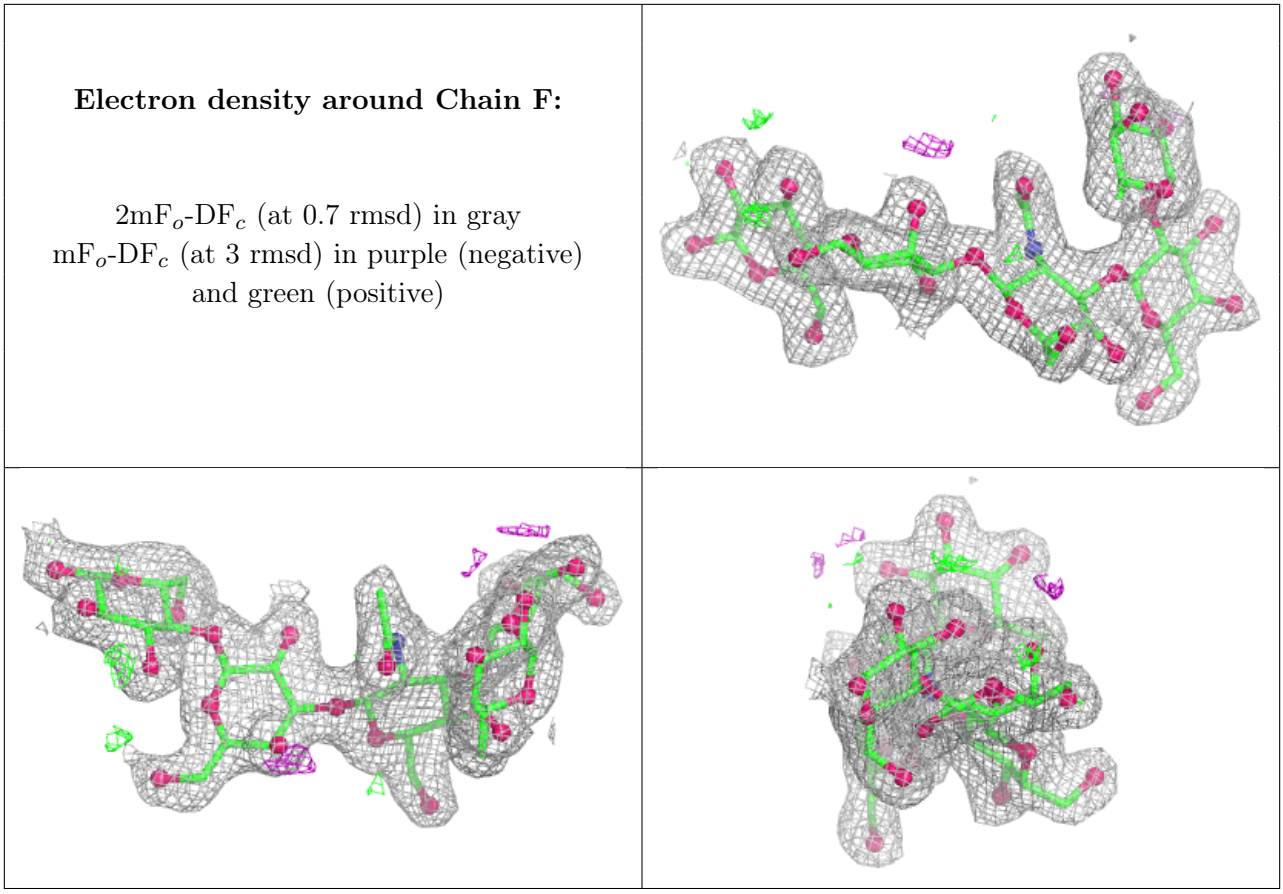






Electron density around Chain F:

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



6.4 Ligands

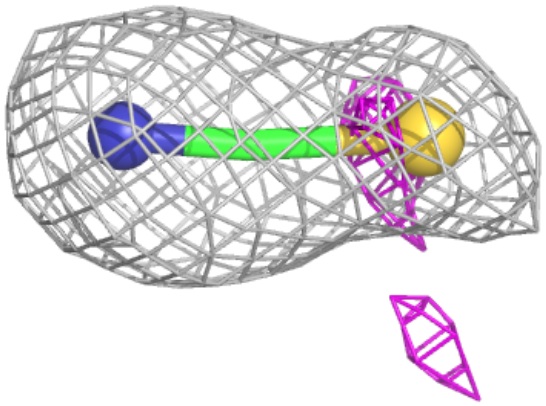
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

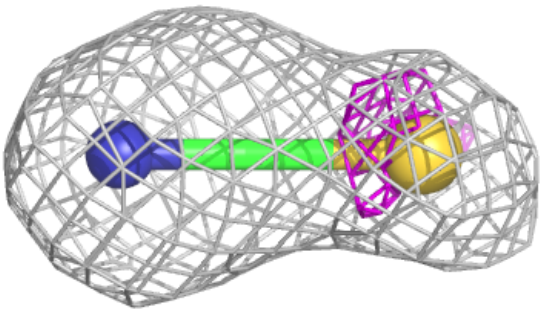
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SCN	D	601	3/3	0.79	0.18	29,29,33,53	0
5	NA	A	602	1/1	0.89	0.08	48,48,48,48	0
5	NA	D	602	1/1	0.94	0.04	27,27,27,27	0
5	NA	B	601	1/1	0.95	0.07	25,25,25,25	0
4	SCN	A	601	3/3	0.95	0.09	38,38,41,43	0
5	NA	C	601	1/1	0.97	0.04	27,27,27,27	0

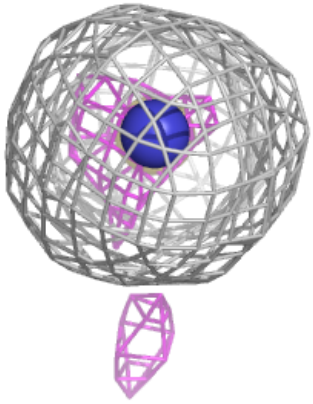
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SCN D 601:

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

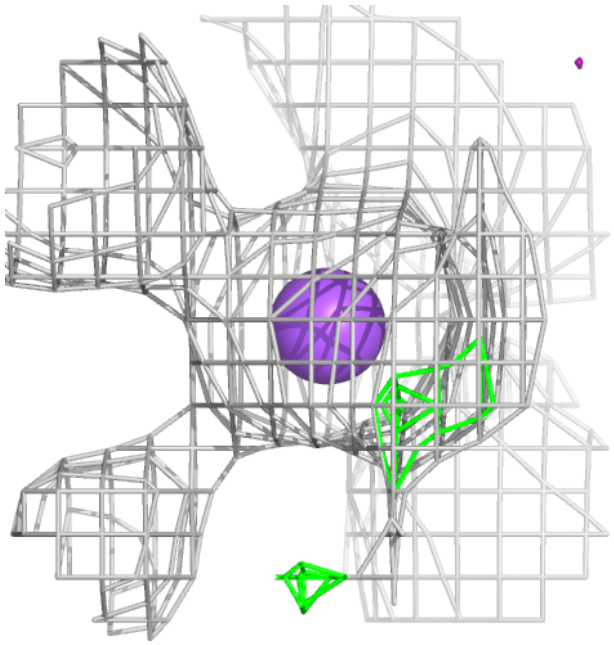




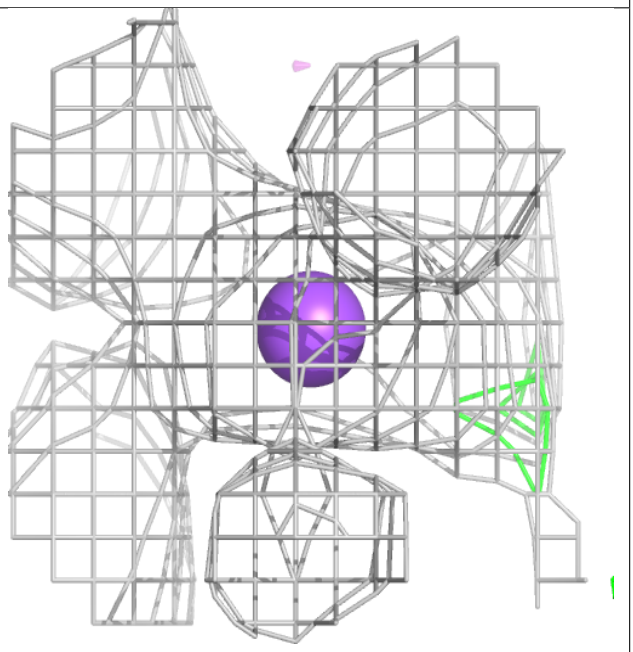


Electron density around NA A 602:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

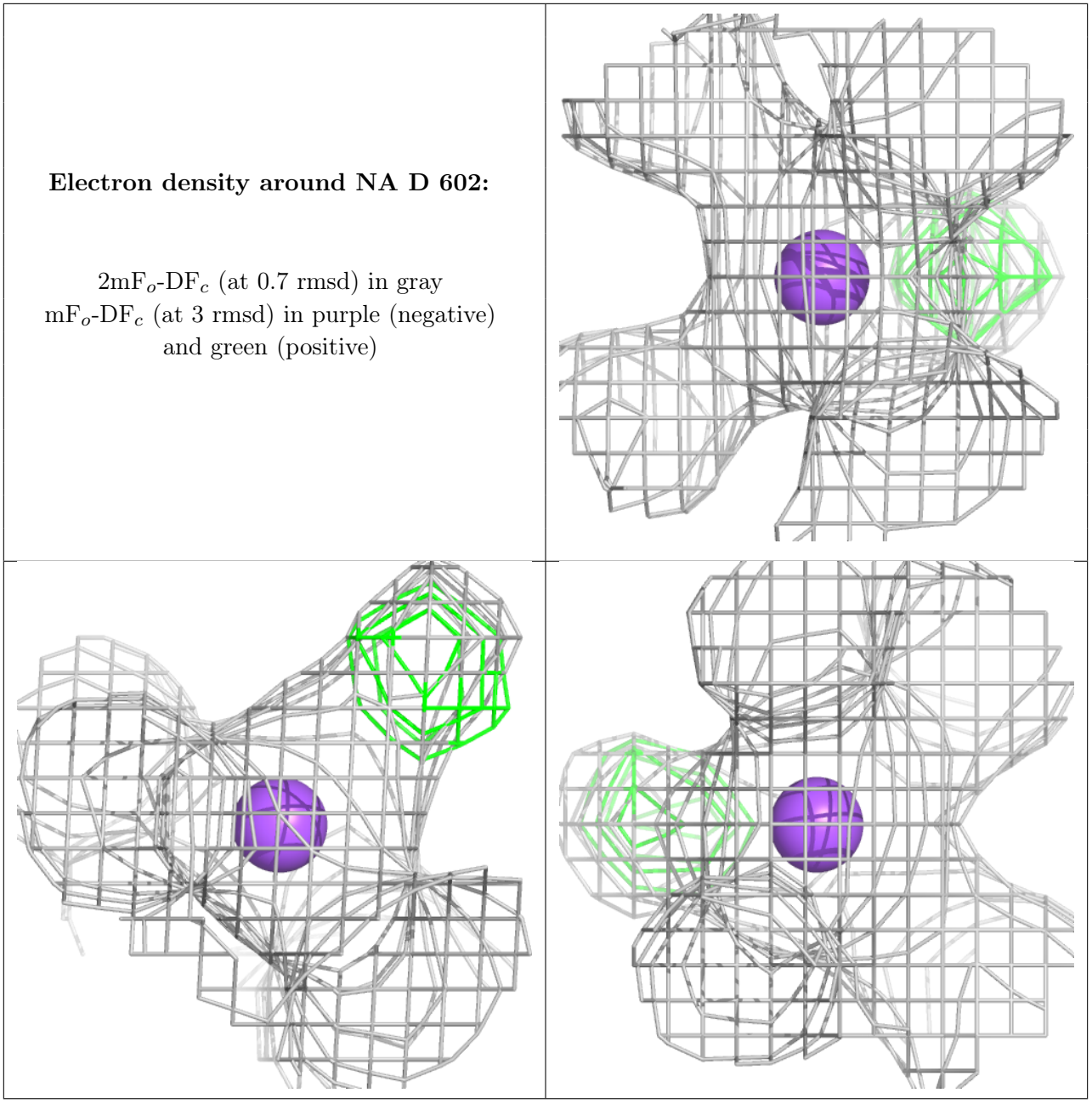






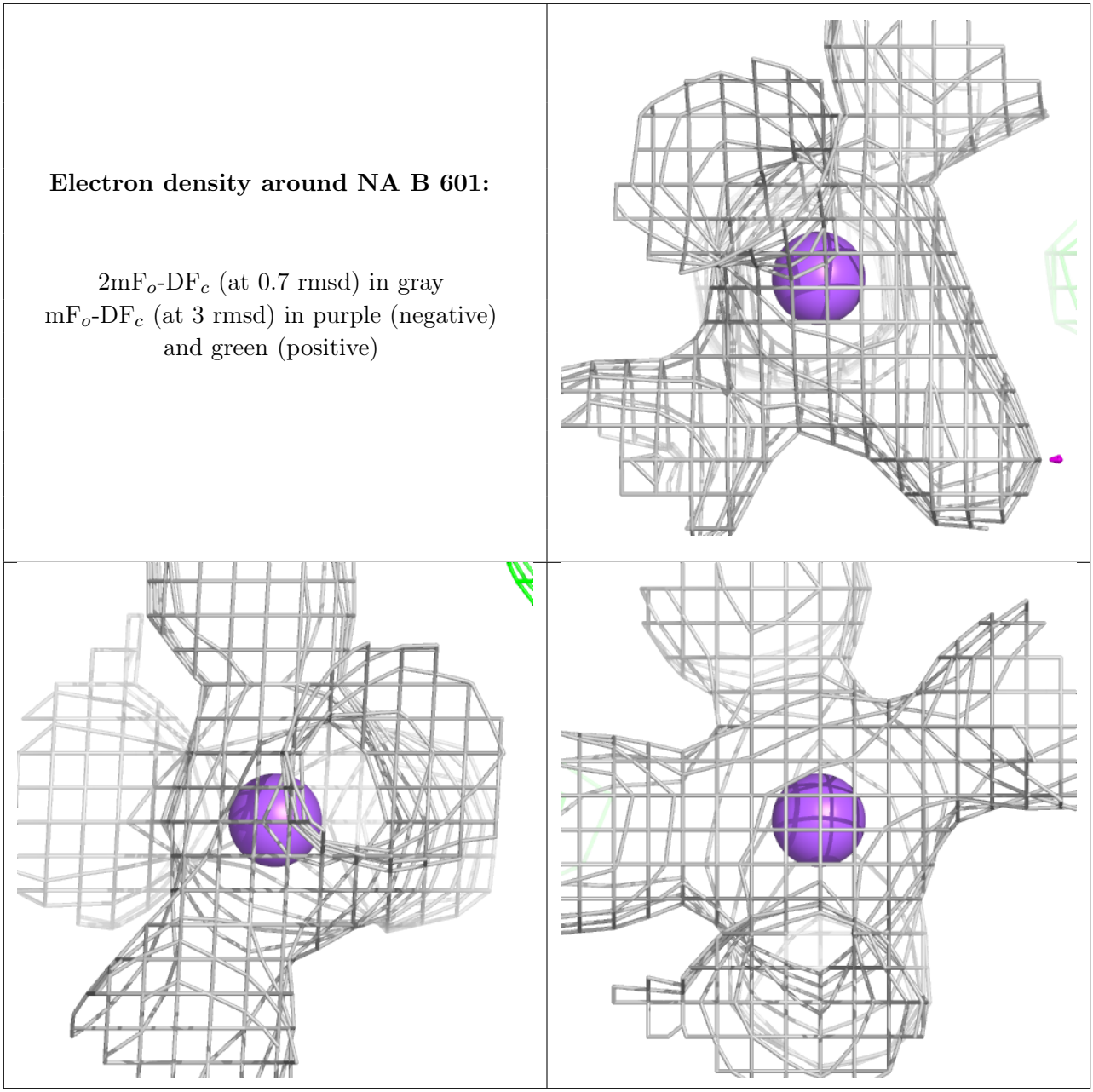
Electron density around NA D 602:

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



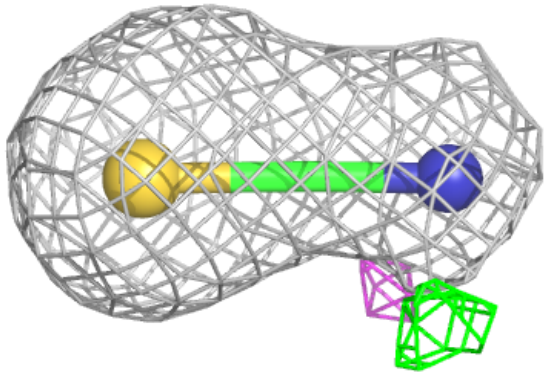
Electron density around NA B 601:

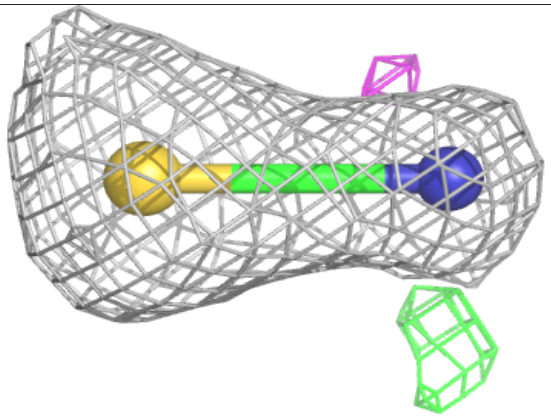
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

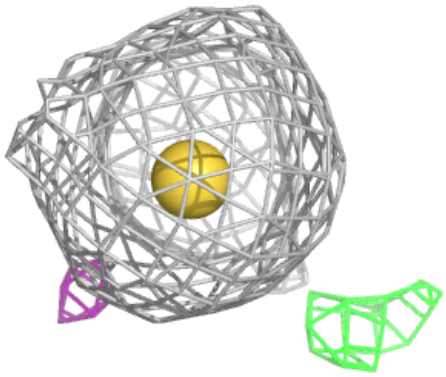


Electron density around SCN A 601:

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

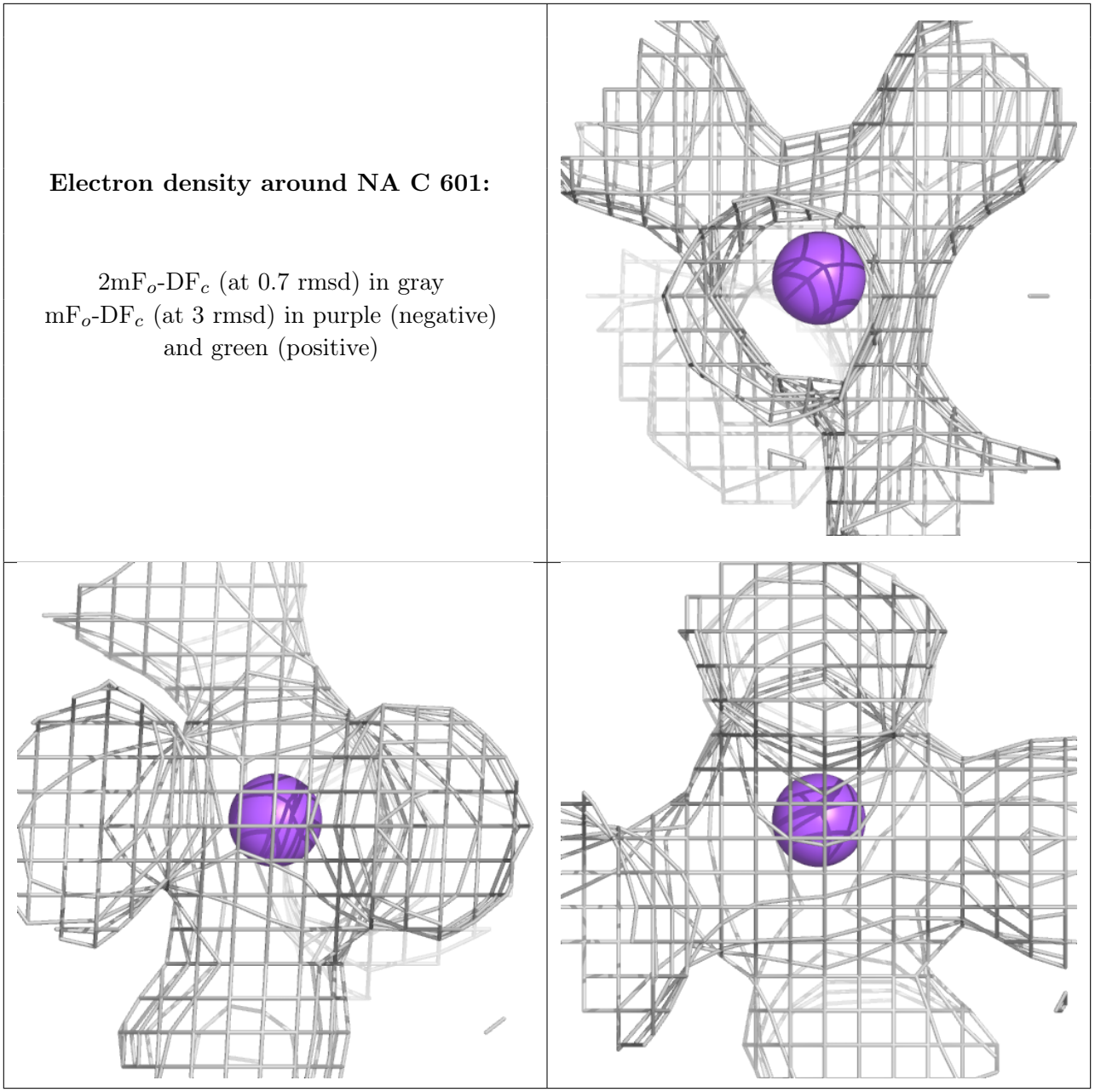






Electron density around NA C 601:

$2mF_o$-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.