WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Apr 2, 2024 – 01:37 PM JST

PDB ID : 8K7I

Title : Crystal structure of human lysosomal alpha-galactosidase A in complex with (2R,3S,4R,5R)-2-(hydroxymethyl)-5-((methylamino)methyl)pyrrolidine-3,4-diol

Authors : Li, H.Y.; Huang, K.F.; Ko, T.P.; Cheng, W.C.

Deposited on : 2023-07-26

Resolution : 2.12 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:

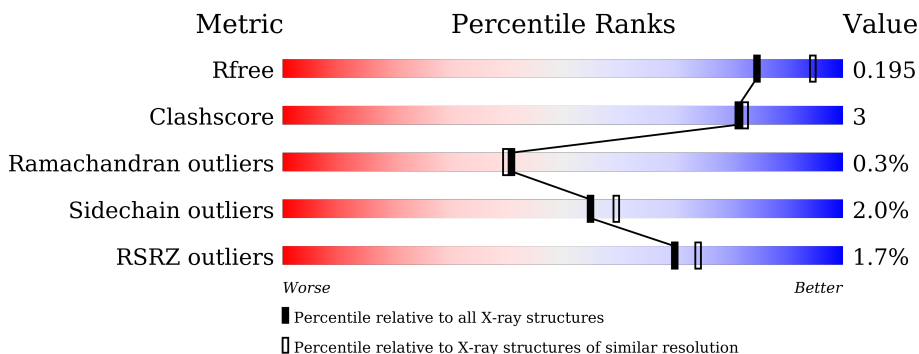|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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		0.195
Clashscore		3
Ramachandran outliers		0.3%
Sidechain outliers		2.0%
RSRZ outliers		1.7%

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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	398	.% 92% 6% •
1	B	398	3% 88% 11% •
2	C	4	100%
2	F	4	50% 50%
3	D	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	E	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BMA	C	3	-	-	-	X
2	MAN	F	4	-	-	-	X
3	NAG	D	2	-	-	-	X
3	NAG	E	2	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7264 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 Alpha-galactosidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total 3128	C 1990	N 537	O 575	S 26	0	2	0
1	B	392	Total 3154	C 2012	N 538	O 577	S 27	0	2	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
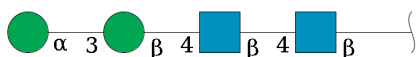
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total 50	C 28	N 2	O 20	0	0	0
2	F	4	Total 50	C 28	N 2	O 20	0	0	0

- Molecule 3 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
3	D	2	Total 28	C 16	N 2	O 10	0	0	0
3	E	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
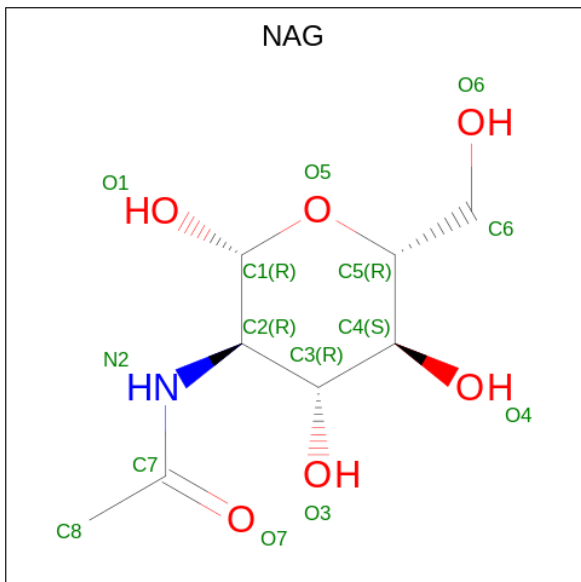
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 5 is (2 {R},3 {S},4 {R},5 {R})-2-(hydroxymethyl)-5-(methylaminomethyl)pyrrolid ine-3,4-diol (three-letter code: VN0) (formula: $C_7H_{16}N_2O_3$) (labeled as "Ligand of Interest" by depositor).
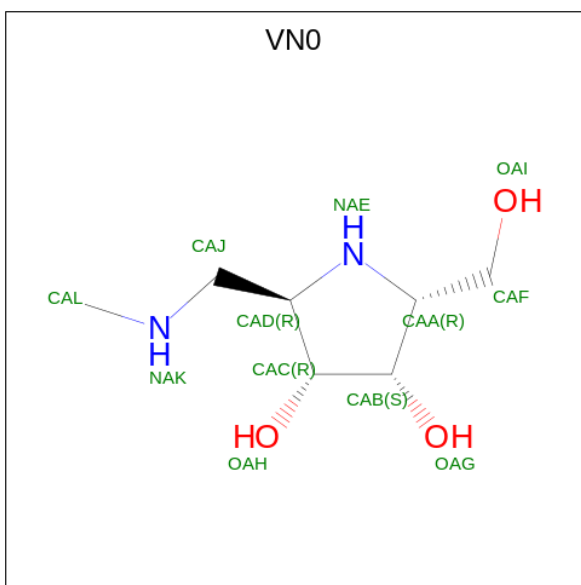
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 12	C 7	N 2	O 3	0	0
5	B	1	Total 12	C 7	N 2	O 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
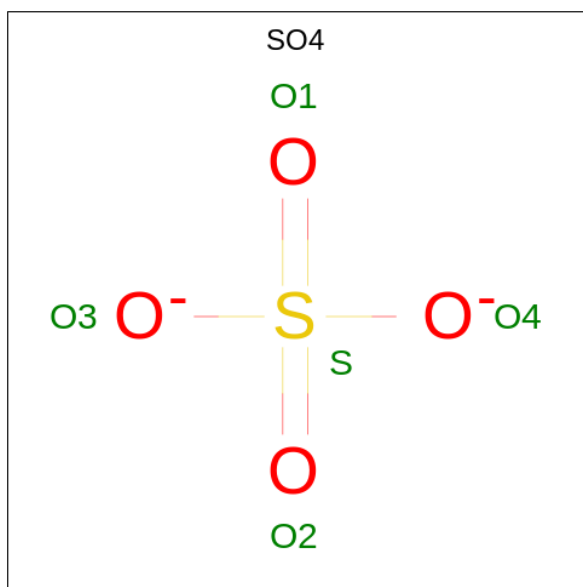
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).

P6G
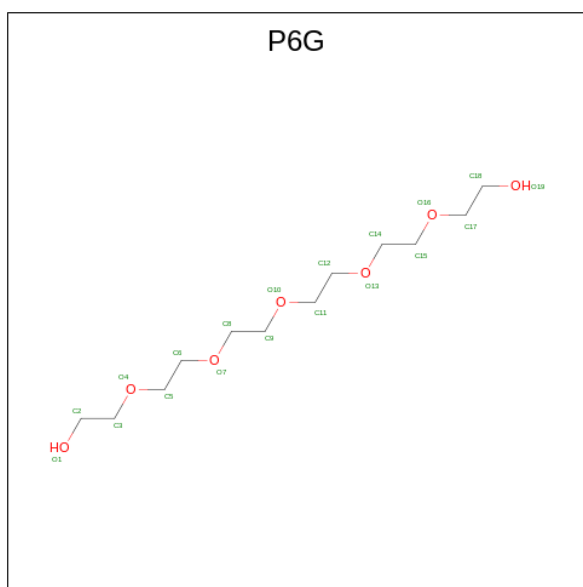
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 13	C 8	O 5	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
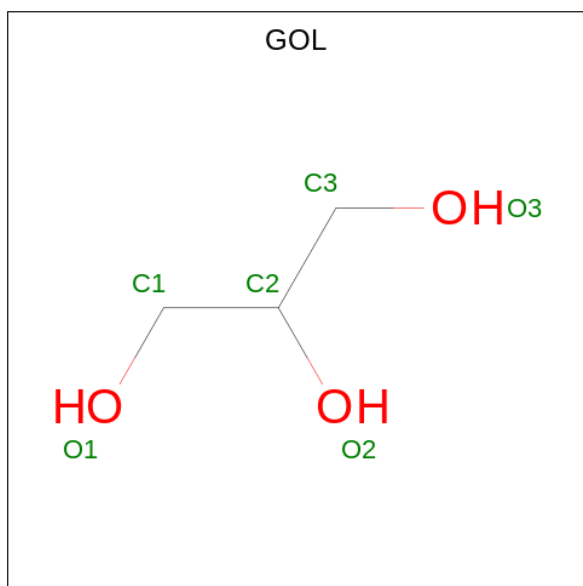
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 6	C 3	O 3	0	0
8	B	1	Total 6	C 3	O 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	391	Total 391	O 391	0	0
9	B	333	Total 333	O 333	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: Alpha-galactosidase A
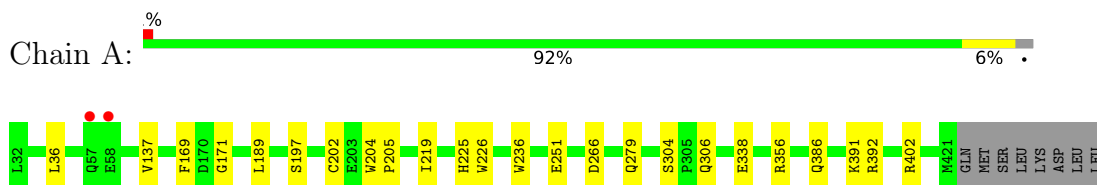
Chain A:

• Molecule 1: Alpha-galactosidase A
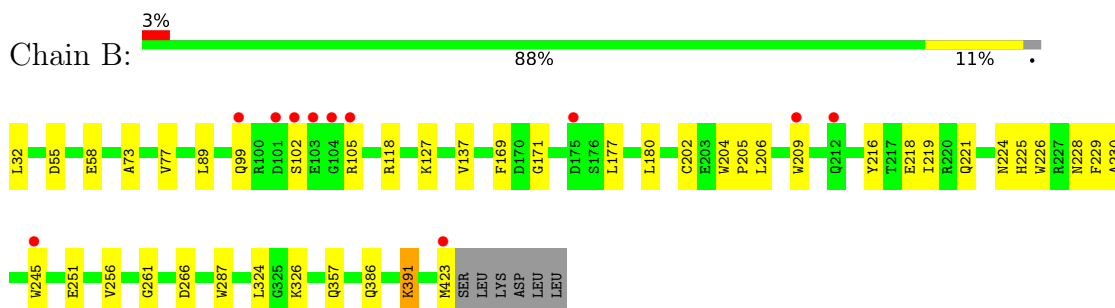
Chain B:

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

Chain C:

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

Chain F:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:
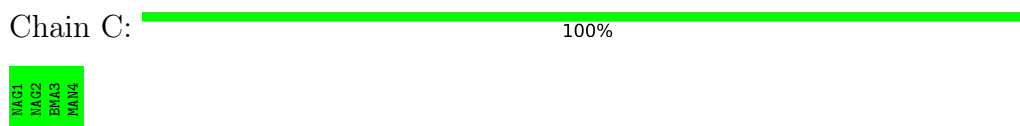
NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

100%

NAG1 NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	90.15Å 90.15Å 215.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.51 – 2.12 29.51 – 2.12	Depositor EDS
% Data completeness (in resolution range)	93.1 (29.51-2.12) 89.4 (29.51-2.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.02 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.160 , 0.195 0.160 , 0.195	Depositor DCC
R_{free} test set	1989 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 66.9	EDS
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7264	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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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: BMA, VN0, NAG, MAN, SO4, GOL, P6G

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	0.31	0/3226	0.56	0/4380
1	B	0.30	0/3254	0.55	0/4419
All	All	0.30	0/6480	0.55	0/8799

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 ⓘ

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	3128	0	2987	12	0
1	B	3154	0	3009	21	0
2	C	50	0	43	0	0
2	F	50	0	43	0	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	12	0	0	0	0
5	B	12	0	0	0	0
6	A	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	15	0	0	1	0
7	A	13	0	17	0	0
8	A	6	0	8	1	0
8	B	6	0	8	0	0
9	A	391	0	0	1	1
9	B	333	0	0	2	0
All	All	7264	0	6191	33	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (33) 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:A:251:GLU:OE1	9:A:601:HOH:O	2.06	0.74
1:B:216:TYR:HB3	1:B:256:VAL:HG11	1.72	0.71
1:B:205:PRO:HG3	1:B:219:ILE:HD13	1.73	0.69
1:A:205:PRO:HG3	1:A:219:ILE:HD13	1.76	0.67
1:A:189:LEU:HD23	8:A:506:GOL:H32	1.82	0.61
1:B:32:LEU:N	6:B:504:SO4:O4	2.35	0.60
1:B:228:ASN:HB3	1:B:245[A]:TRP:CH2	2.37	0.59
1:B:206:LEU:HA	1:B:209:TRP:HD1	1.67	0.58
1:A:402:ARG:NH1	6:A:503:SO4:O1	2.35	0.56
1:B:357:GLN:NE2	9:B:603:HOH:O	2.28	0.55
1:A:36:LEU:HD11	1:A:197:SER:HB3	1.88	0.53
1:B:324:LEU:HG	1:B:326:LYS:HG3	1.90	0.53
1:B:386:GLN:O	1:B:391:LYS:HA	2.09	0.52
1:B:137:VAL:HG12	1:B:171:GLY:HA2	1.94	0.50
1:A:338:GLU:OE2	1:A:356:ARG:NH1	2.44	0.48
1:B:204:TRP:HB3	1:B:205:PRO:HD3	1.94	0.48
1:B:77:VAL:HG21	1:B:127:LYS:HB3	1.96	0.47
1:A:202:CYS:O	1:A:226:TRP:HA	2.16	0.46
1:A:304:SER:OG	1:A:306:GLN:HG2	2.16	0.45
1:B:224:ASN:O	1:B:261:GLY:HA2	2.18	0.43
1:B:202:CYS:O	1:B:226:TRP:HA	2.20	0.42
1:A:204:TRP:HB3	1:A:205:PRO:HD3	2.02	0.41
1:B:218:GLU:O	1:B:221:GLN:HB2	2.20	0.41
1:B:73:ALA:HB2	1:B:89:LEU:HD22	2.02	0.41
1:B:55:ASP:OD2	1:B:58:GLU:HB2	2.20	0.41
1:B:118:ARG:NH1	9:B:616:HOH:O	2.54	0.41
1:A:137:VAL:HG12	1:A:171:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229[A]:PHE:CG	1:B:230:ALA:N	2.89	0.40
1:A:236:TRP:CE3	1:A:279:GLN:HG2	2.56	0.40
1:B:137:VAL:HG11	1:B:180:LEU:HD12	2.04	0.40
1:A:386:GLN:O	1:A:391:LYS:HA	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:611:HOH:O	9:A:856:HOH:O[4_545]	2.10	0.10

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	390/398 (98%)	380 (97%)	9 (2%)	1 (0%)	41	40
1	B	392/398 (98%)	380 (97%)	11 (3%)	1 (0%)	41	40
All	All	782/796 (98%)	760 (97%)	20 (3%)	2 (0%)	41	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ASP
1	B	266	ASP

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	333/339 (98%)	330 (99%)	3 (1%)	78	83
1	B	335/339 (99%)	325 (97%)	10 (3%)	41	43
All	All	668/678 (98%)	655 (98%)	13 (2%)	55	61

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	PHE
1	A	225	HIS
1	A	392	ARG
1	B	99	GLN
1	B	102	SER
1	B	105	ARG
1	B	169	PHE
1	B	177	LEU
1	B	225	HIS
1	B	251	GLU
1	B	287	TRP
1	B	391	LYS
1	B	423	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	330	GLN
1	A	416	GLN
1	B	221	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

12 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	0.34	0	17,19,21	0.43	0
2	NAG	C	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	BMA	C	3	2	11,11,12	0.80	0	15,15,17	1.04	0
2	MAN	C	4	2	11,11,12	0.87	0	15,15,17	0.88	0
3	NAG	D	1	3,1	14,14,15	0.57	0	17,19,21	0.59	0
3	NAG	D	2	3	14,14,15	0.74	1 (7%)	17,19,21	0.71	0
3	NAG	E	1	3,1	14,14,15	0.56	0	17,19,21	0.52	0
3	NAG	E	2	3	14,14,15	0.25	0	17,19,21	0.38	0
2	NAG	F	1	1,2	14,14,15	0.26	0	17,19,21	0.61	0
2	NAG	F	2	2	14,14,15	1.12	1 (7%)	17,19,21	1.61	1 (5%)
2	BMA	F	3	2	11,11,12	0.77	0	15,15,17	0.83	0
2	MAN	F	4	2	11,11,12	0.75	0	15,15,17	1.17	2 (13%)

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	-	2/2/19/22	0/1/1/1
2	MAN	C	4	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	-	4/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	F	3	2	-	1/2/19/22	0/1/1/1
2	MAN	F	4	2	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	O5-C1	4.03	1.50	1.43
3	D	2	NAG	C1-C2	2.16	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C1-O5-C5	6.29	120.71	112.19
2	F	4	MAN	C1-O5-C5	3.11	116.41	112.19
2	F	4	MAN	O2-C2-C3	-2.15	105.83	110.14

There are no chirality outliers.

All (21) torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	F	4	MAN	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	C	3	BMA	O5-C5-C6-O6
2	F	4	MAN	O5-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C1-C2-N2-C7
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C3-C2-N2-C7

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 C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths | Bond angles | Torsions | Rings
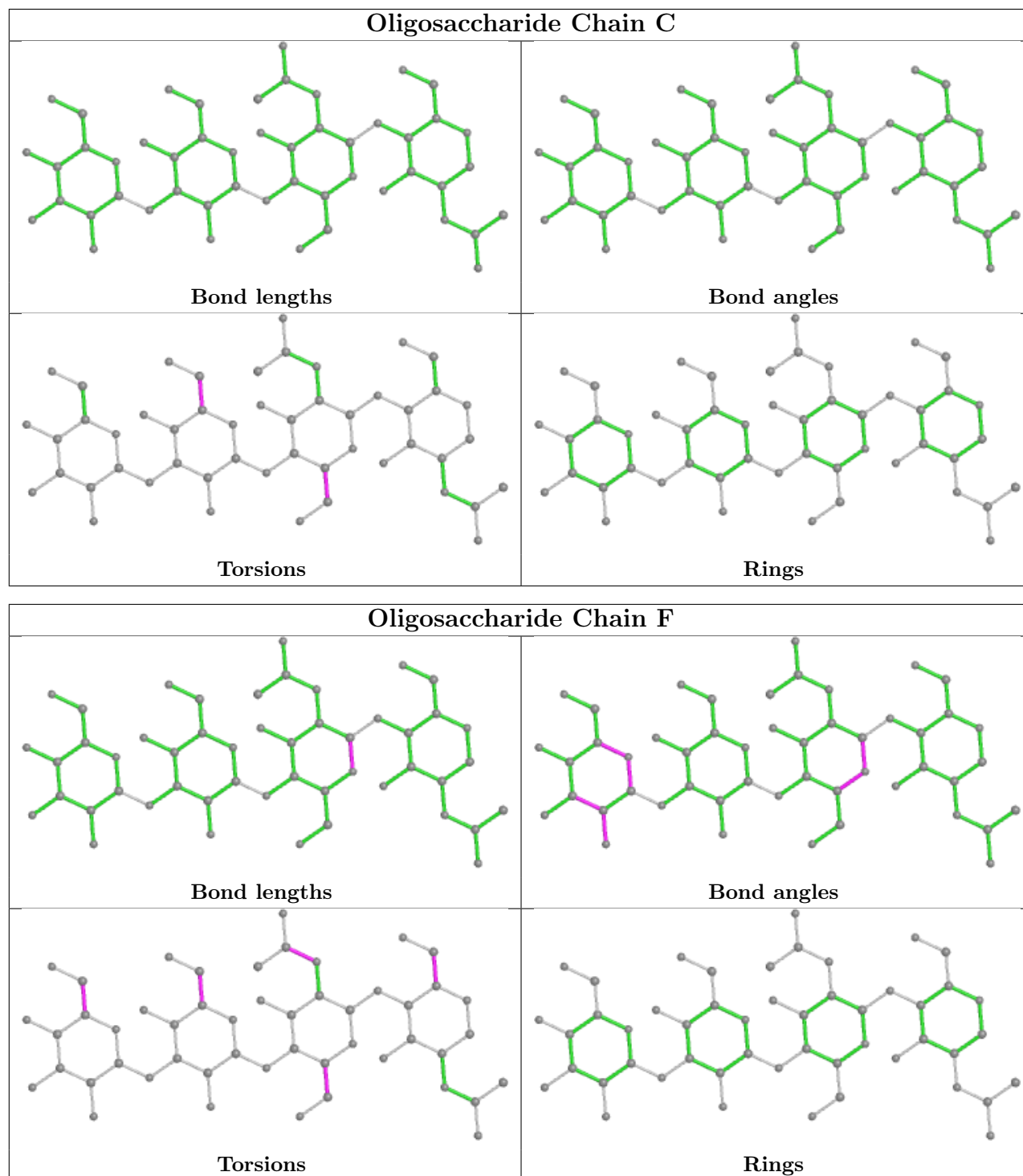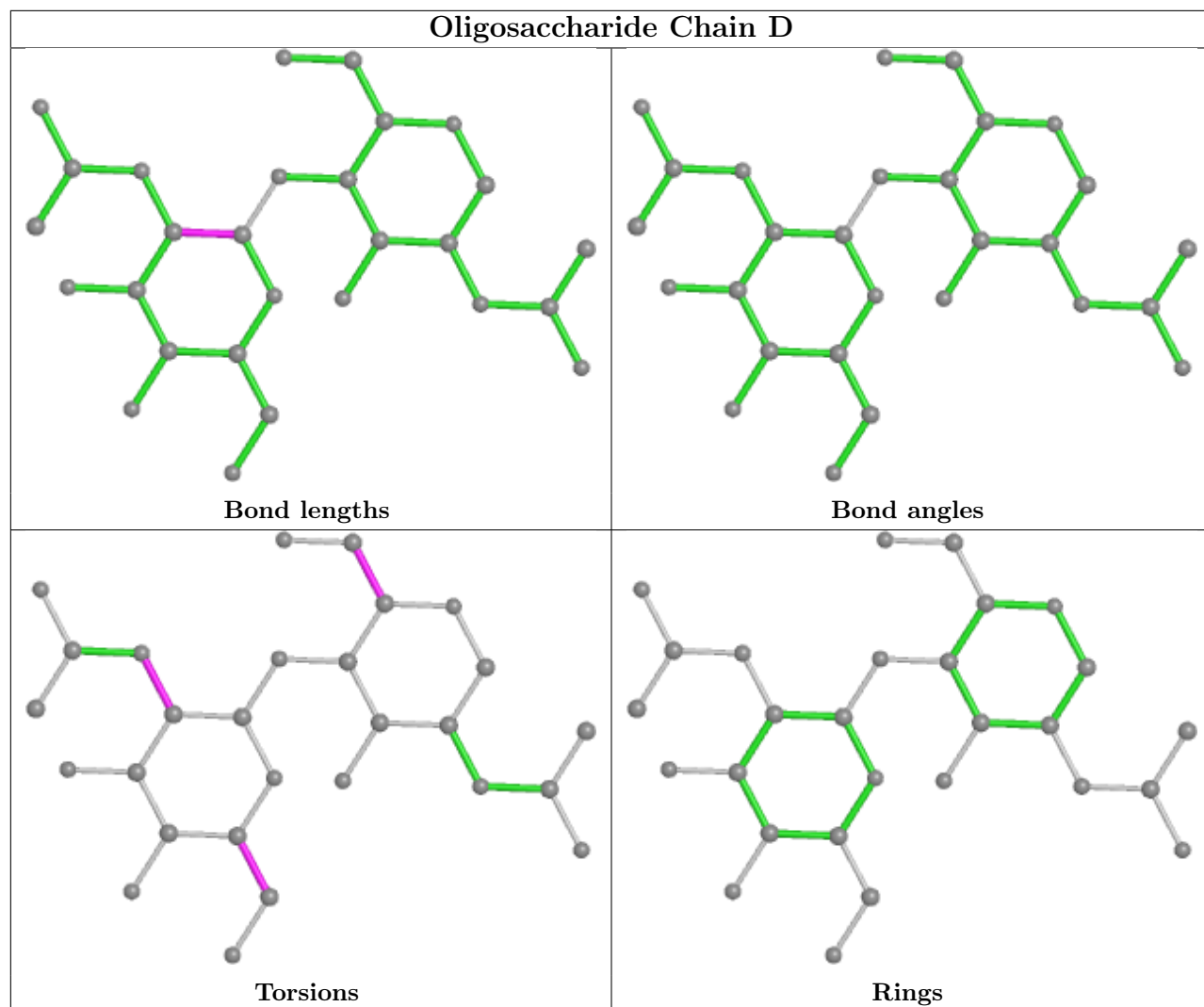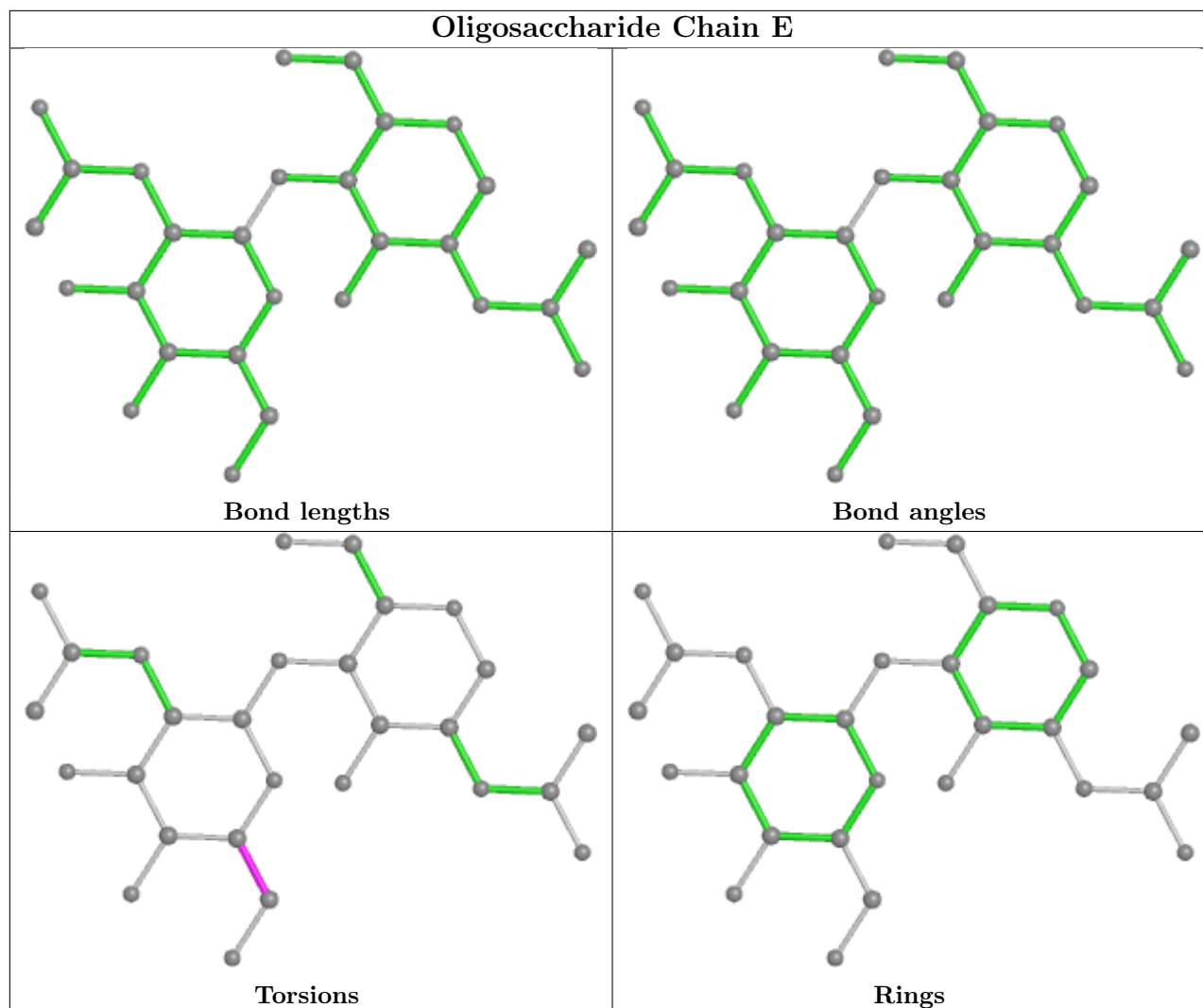
5.6 Ligand geometry ⓘ

12 ligands 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	#$\|Z\| > 2$
8	GOL	A	506	-	5,5,5	0.88	0	5,5,5	1.02	0
6	SO4	A	503	-	4,4,4	0.13	0	6,6,6	0.11	0
6	SO4	A	504	-	4,4,4	0.13	0	6,6,6	0.08	0
7	P6G	A	505	-	12,12,18	0.13	0	11,11,17	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
5	VN0	A	502	-	11,12,12	1.19	2 (18%)	10,16,16	1.03	0
6	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.07	0
4	NAG	B	501	1	14,14,15	0.37	0	17,19,21	0.38	0
4	NAG	A	501	1	14,14,15	0.65	0	17,19,21	0.64	1 (5%)
5	VN0	B	502	-	11,12,12	1.13	1 (9%)	10,16,16	0.97	0
8	GOL	B	506	-	5,5,5	0.91	0	5,5,5	0.98	0
6	SO4	B	505	-	4,4,4	0.16	0	6,6,6	0.33	0
6	SO4	B	504	-	4,4,4	0.14	0	6,6,6	0.09	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
8	GOL	A	506	-	-	2/4/4/4	-
7	P6G	A	505	-	-	0/10/10/16	-
5	VN0	A	502	-	-	3/5/21/21	0/1/1/1
4	NAG	B	501	1	-	0/6/23/26	0/1/1/1
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
5	VN0	B	502	-	-	3/5/21/21	0/1/1/1
8	GOL	B	506	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	VN0	CAB-CAA	-3.30	1.50	1.53
5	A	502	VN0	CAB-CAA	-2.90	1.50	1.53
5	A	502	VN0	CAC-CAD	-2.07	1.51	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	NAG	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	VN0	NAE-CAD-CAJ-NAK

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	502	VN0	NAE-CAD-CAJ-NAK
8	A	506	GOL	C1-C2-C3-O3
8	A	506	GOL	O2-C2-C3-O3
5	A	502	VN0	NAE-CAA-CAF-OAI
5	B	502	VN0	NAE-CAA-CAF-OAI
5	A	502	VN0	CAC-CAD-CAJ-NAK
5	B	502	VN0	CAC-CAD-CAJ-NAK

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	506	GOL	1	0
6	A	503	SO4	1	0
6	B	504	SO4	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 VN0 A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand VN0 B 502

Bond lengths

Bond angles

Torsions

Rings
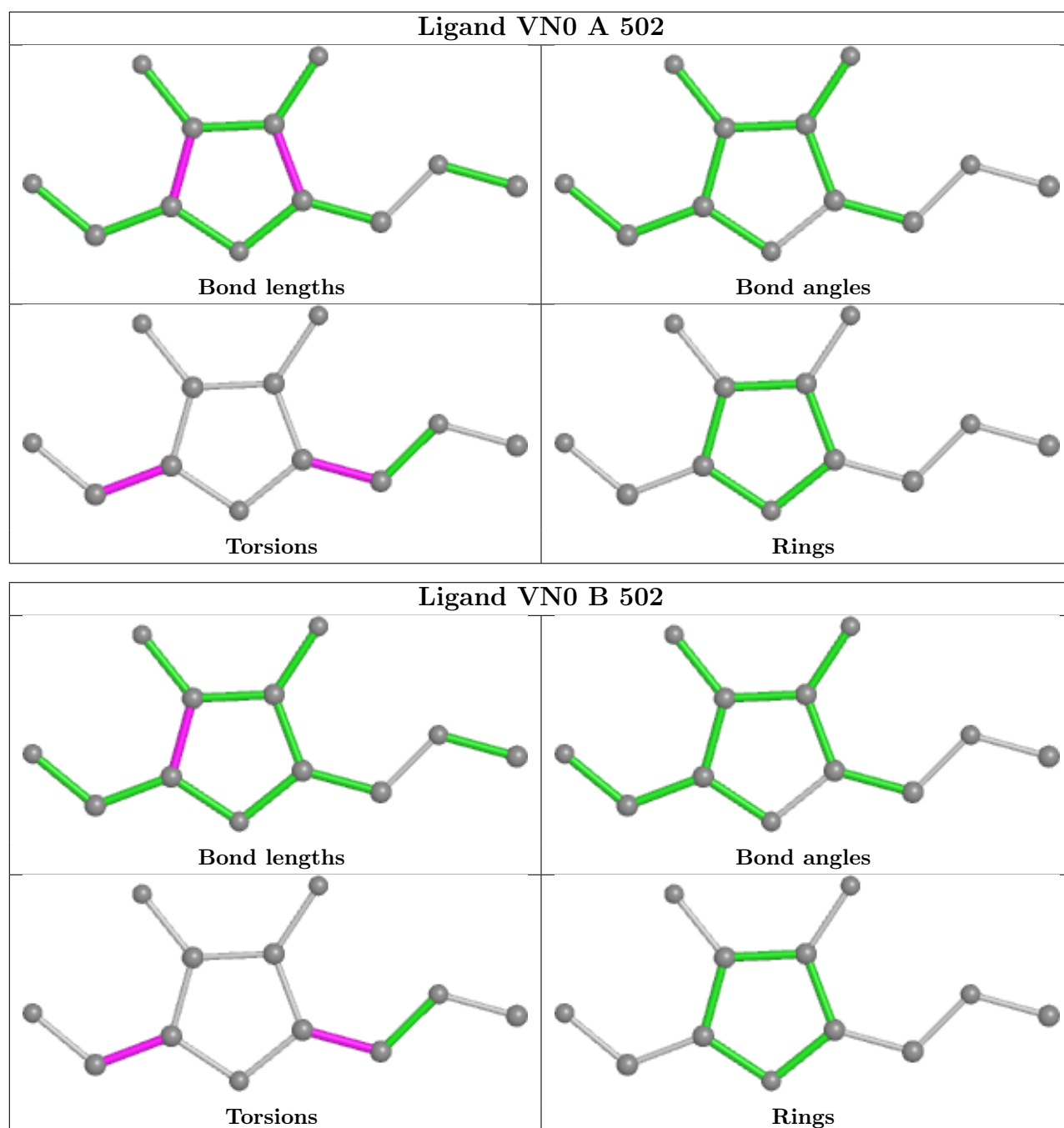
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	390/398 (97%)	-0.55	2 (0%) 91	92	12, 24, 42, 70	0
1	B	392/398 (98%)	-0.20	11 (2%) 53	59	13, 32, 60, 86	0
All	All	782/796 (98%)	-0.37	13 (1%) 70	74	12, 27, 55, 86	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	SER	4.7
1	B	209	TRP	4.0
1	A	57	GLN	3.6
1	B	104	GLY	3.5
1	B	103	GLU	3.2
1	B	101	ASP	2.9
1	B	423	MET	2.7
1	B	105	ARG	2.7
1	B	212	GLN	2.5
1	B	245[A]	TRP	2.4
1	B	175	ASP	2.3
1	A	58	GLU	2.1
1	B	99	GLN	2.1

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

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

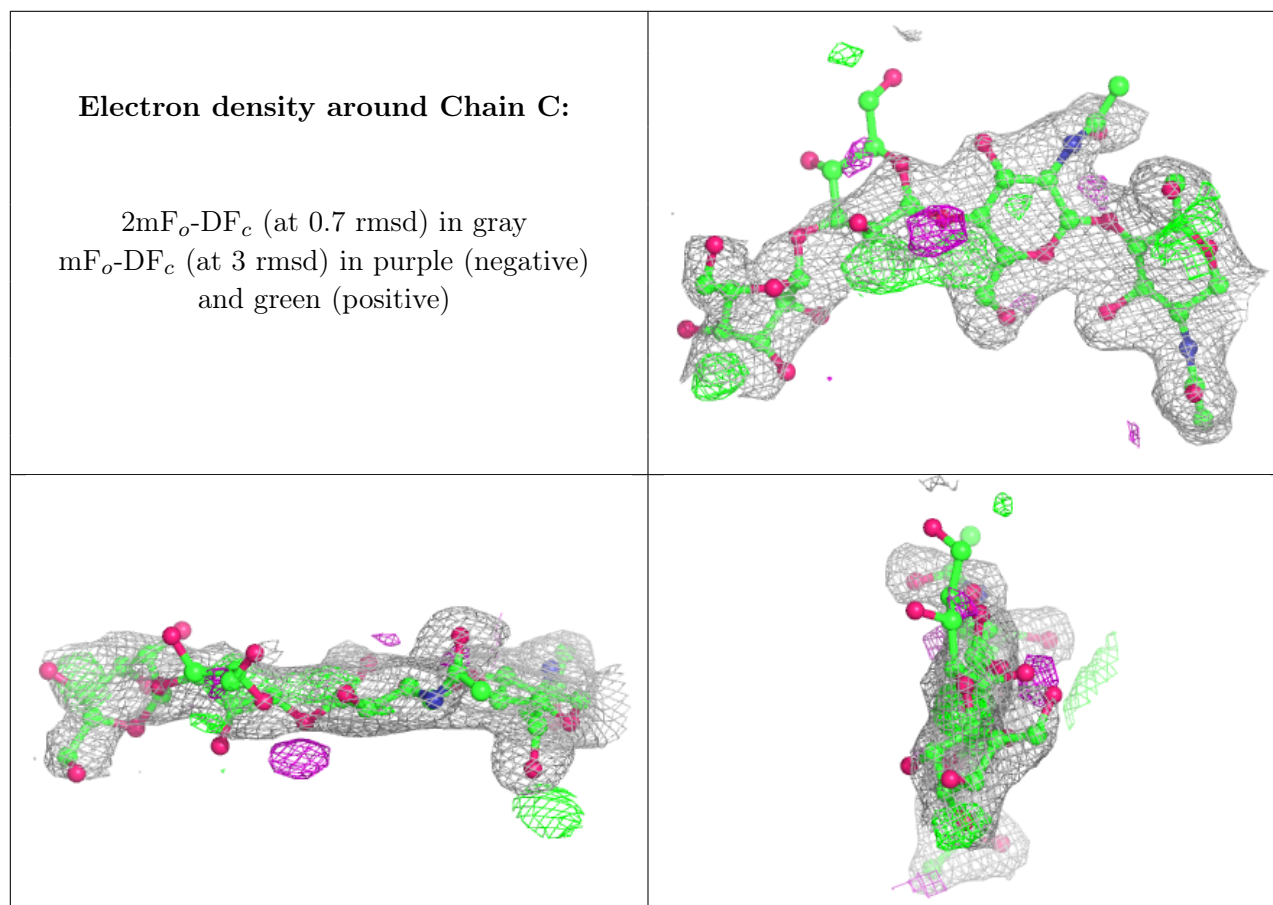## 6.3 Carbohydrates ⓘ

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	1	14/15	0.66	0.36	62,77,85,87	0
2	BMA	C	3	11/12	0.69	0.47	75,95,99,99	0
3	NAG	E	2	14/15	0.72	0.48	76,86,93,93	0
2	MAN	F	4	11/12	0.75	0.42	64,86,91,93	0
3	NAG	D	2	14/15	0.77	0.44	84,89,95,95	0
2	MAN	C	4	11/12	0.78	0.34	89,98,105,108	0
2	BMA	F	3	11/12	0.80	0.35	84,91,101,109	0
2	NAG	F	2	14/15	0.85	0.30	57,67,75,78	0
3	NAG	D	1	14/15	0.87	0.27	52,63,79,80	0
2	NAG	C	2	14/15	0.90	0.20	40,49,66,72	0
2	NAG	F	1	14/15	0.92	0.20	42,49,58,59	0
2	NAG	C	1	14/15	0.96	0.07	27,34,41,42	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.
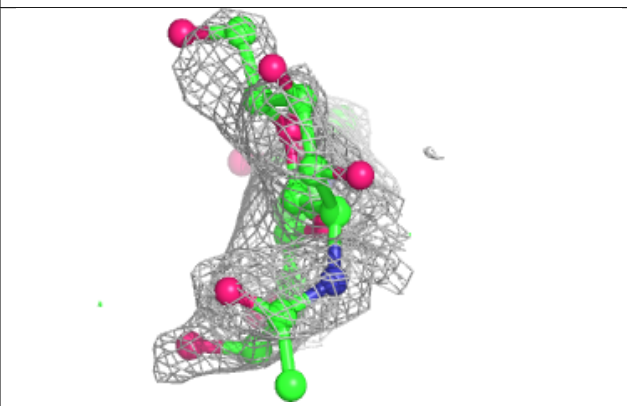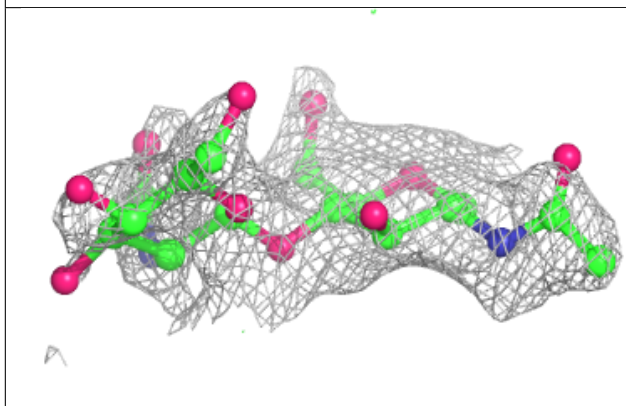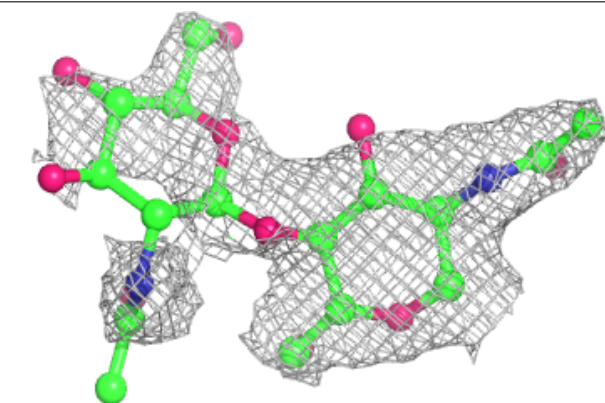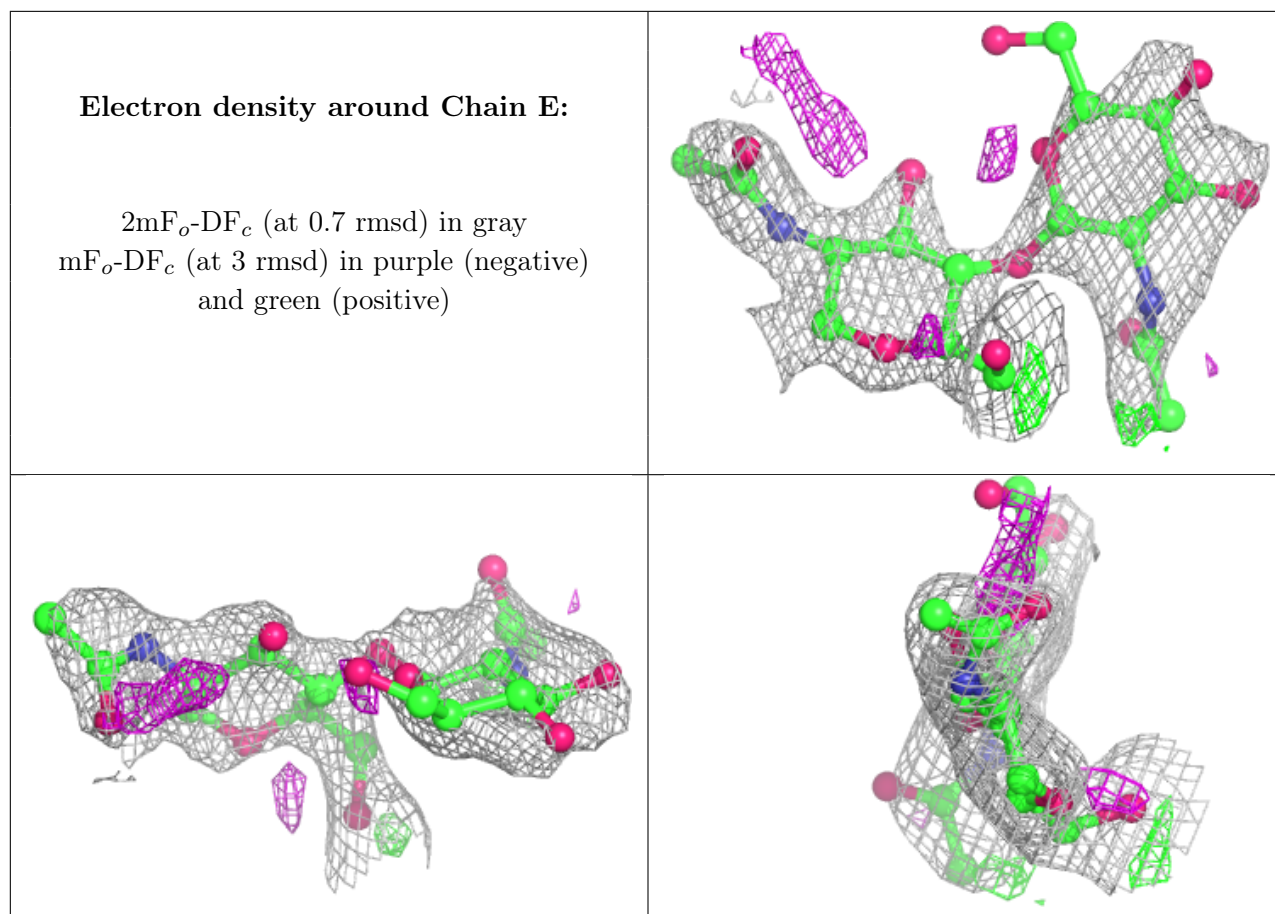

Electron density around Chain C:

$2mF_o$-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 F:

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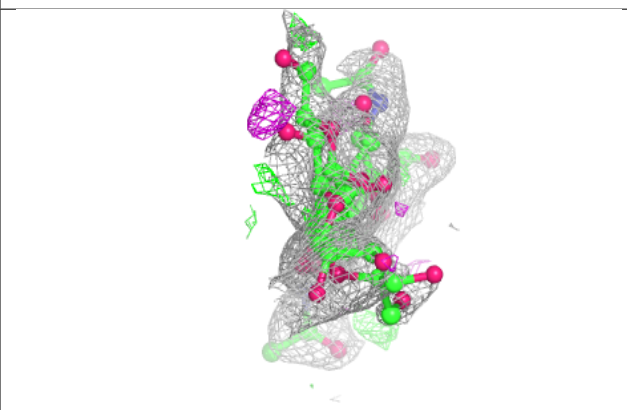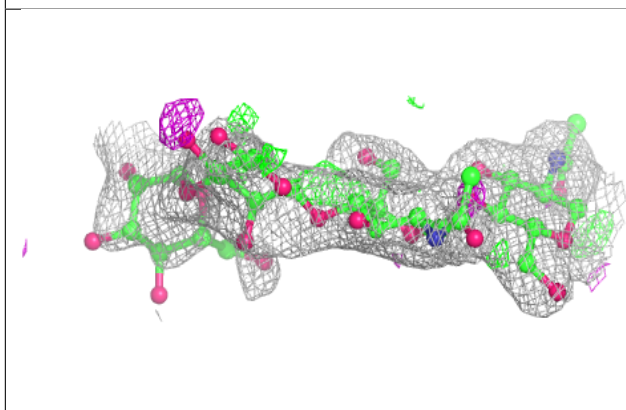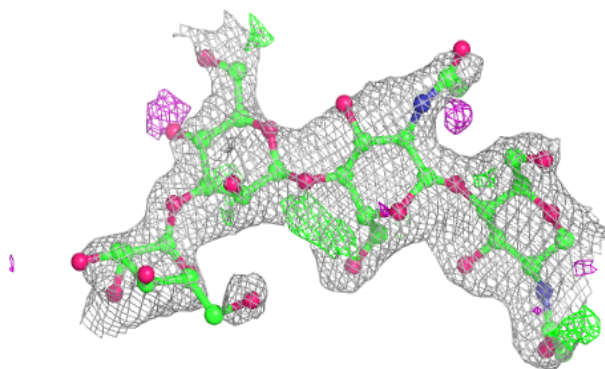
Electron density around Chain D:

$2mF_o$-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 E:

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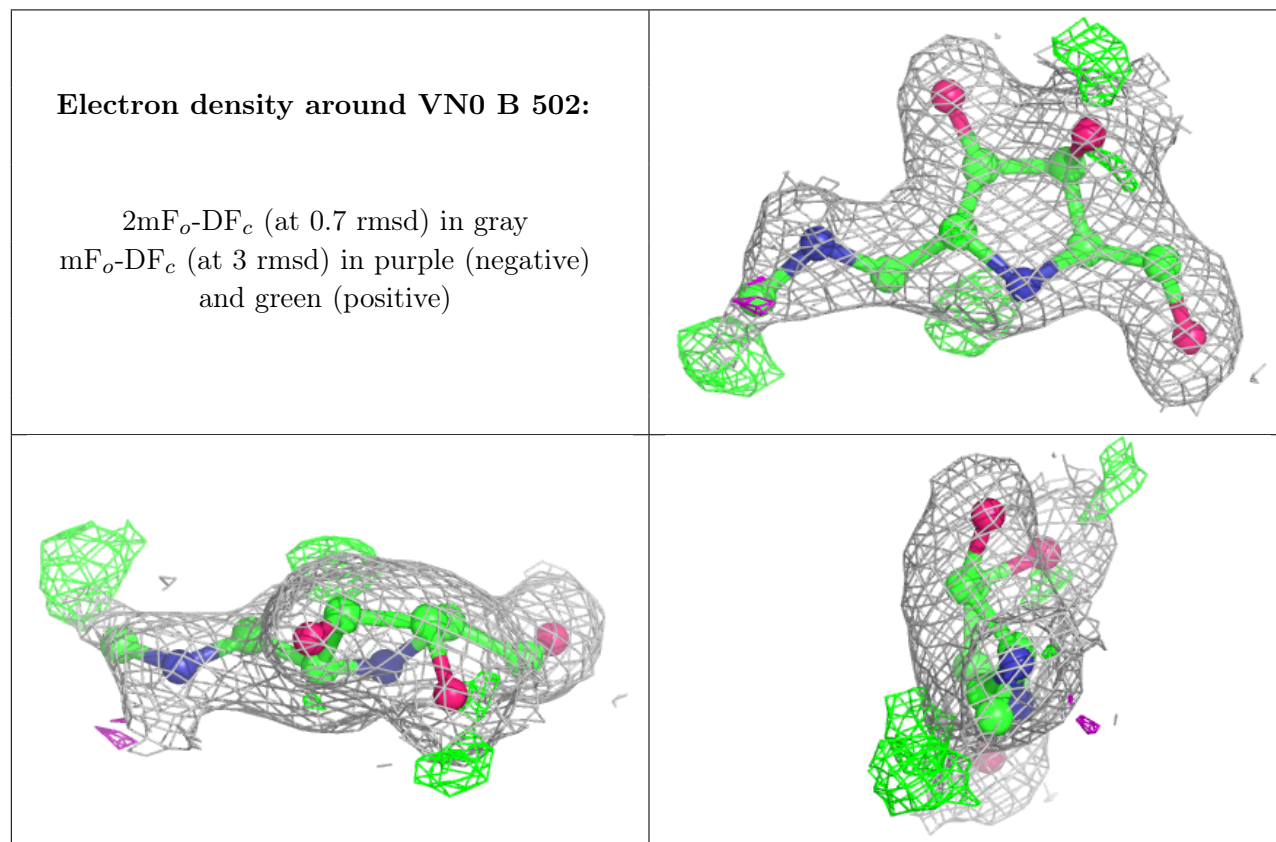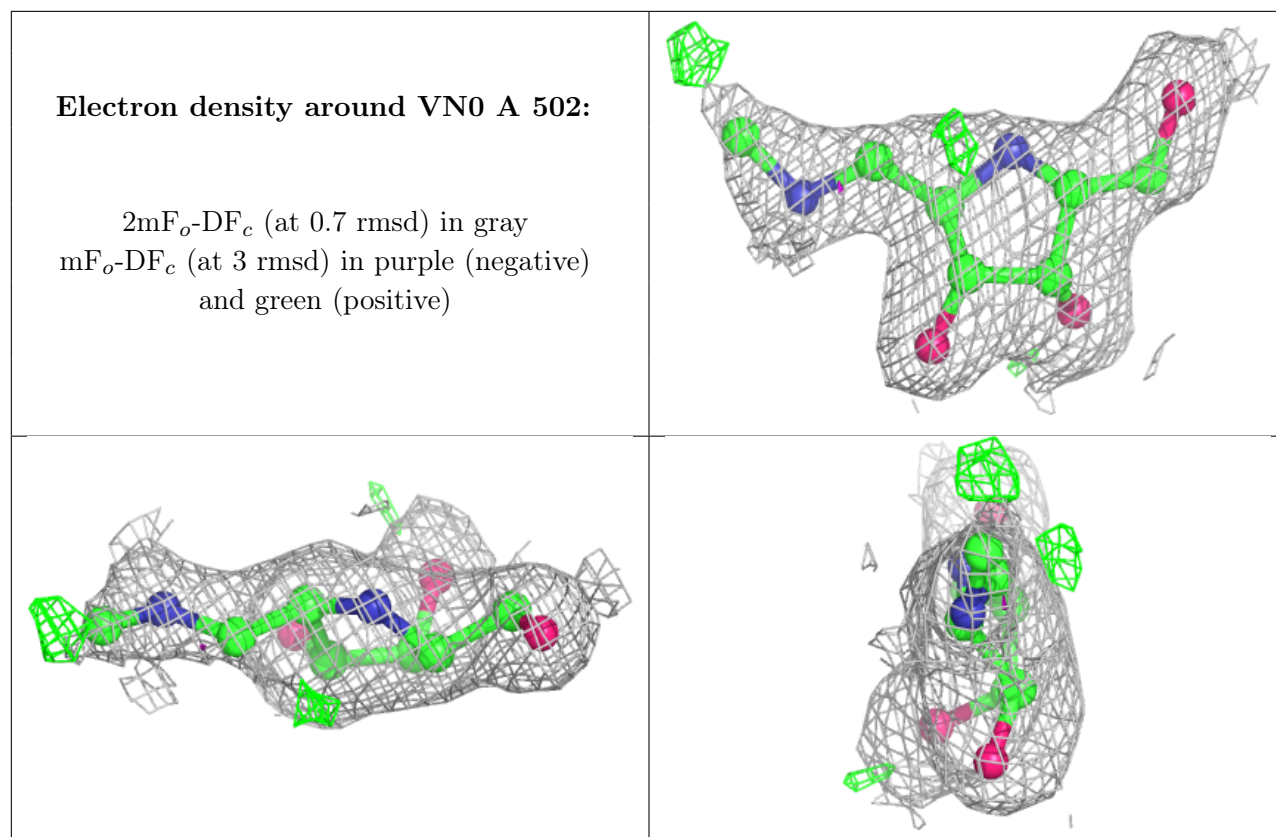mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

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
4	NAG	B	501	14/15	0.72	0.38	75,78,83,87	0
4	NAG	A	501	14/15	0.85	0.18	34,47,52,58	0
6	SO4	B	504	5/5	0.85	0.32	68,70,82,94	0
5	VN0	B	502	12/12	0.87	0.16	30,36,40,40	0
7	P6G	A	505	13/19	0.90	0.15	25,32,47,55	0
5	VN0	A	502	12/12	0.92	0.13	23,28,38,39	0
8	GOL	A	506	6/6	0.92	0.15	36,45,51,60	0
6	SO4	A	504	5/5	0.95	0.24	35,58,71,82	0
6	SO4	A	503	5/5	0.96	0.10	40,45,50,55	0
8	GOL	B	506	6/6	0.96	0.08	34,35,36,39	0
6	SO4	B	505	5/5	0.97	0.13	20,26,40,51	0
6	SO4	B	503	5/5	0.97	0.12	50,55,57,59	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 VN0 B 502:

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

Electron density around VN0 A 502:

$2mF_o$-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.