W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2022 – 10:46 AM EST

PDB ID	:	7L74
Title	:	Crystal structure of Beta-hexosyl transferase from Hamamotoa (Sporobolomyces) singularis bound to TRIS
Authors	:	Dagher, S.F.; Edwards, B.F.P.; Meilleur, F.; Bruno-Barcena, J.M.
Deposited on	:	2020-12-25
Resolution	:	2.25 Å(reported)

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

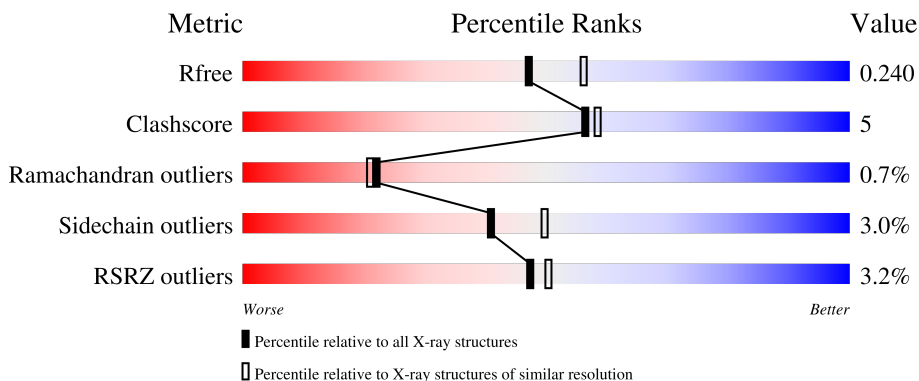|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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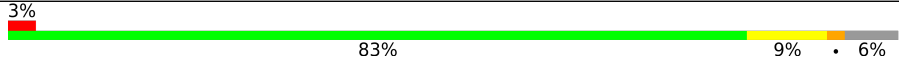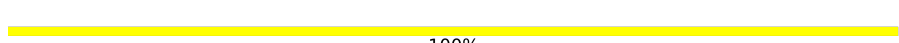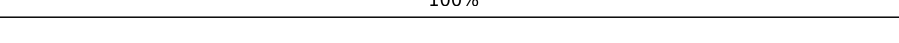*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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		0.240
Clashscore		5
Ramachandran outliers		0.7%
Sidechain outliers		3.0%
RSRZ outliers		3.2%

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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	578	3% / 81% / 12% / · 6%
1	B	578	3% / 83% / 9% / · 6%
2	C	2	100%
2	D	2	100%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	100%
2	G	2	100%
2	H	2	100%
2	I	2	100%
2	J	2	50% 50%

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	NAG	C	2	-	-	-	X
2	NAG	G	2	-	-	-	X
2	NAG	J	2	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 9347 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 Beta-hexosyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	P	S	0	0	0
			4286	2747	707	820	3	9			
1	B	542	Total	C	N	O	P	S	0	0	0
			4297	2753	710	822	3	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	595	HIS	-	expression tag	UNP Q564N5
A	596	HIS	-	expression tag	UNP Q564N5
A	597	HIS	-	expression tag	UNP Q564N5
A	598	HIS	-	expression tag	UNP Q564N5
A	599	HIS	-	expression tag	UNP Q564N5
A	600	HIS	-	expression tag	UNP Q564N5
B	595	HIS	-	expression tag	UNP Q564N5
B	596	HIS	-	expression tag	UNP Q564N5
B	597	HIS	-	expression tag	UNP Q564N5
B	598	HIS	-	expression tag	UNP Q564N5
B	599	HIS	-	expression tag	UNP Q564N5
B	600	HIS	-	expression tag	UNP Q564N5

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).
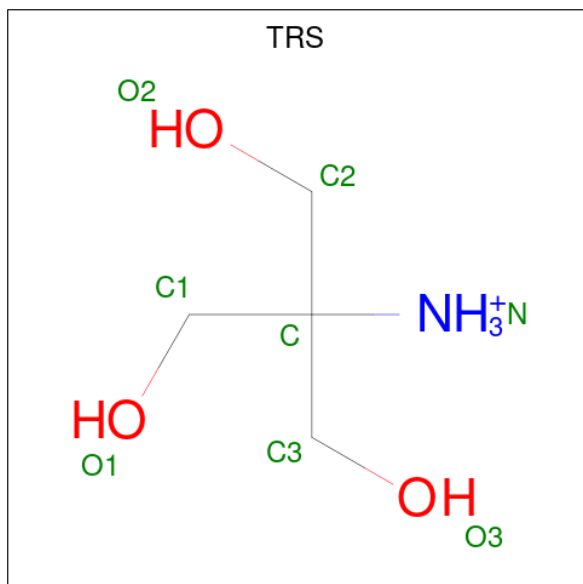
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 8	C 4	N 1	O 3	0	0
4	B	1	Total 8	C 4	N 1	O 3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	258	Total 258	O 258	0	0
5	B	265	Total 265	O 265	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.
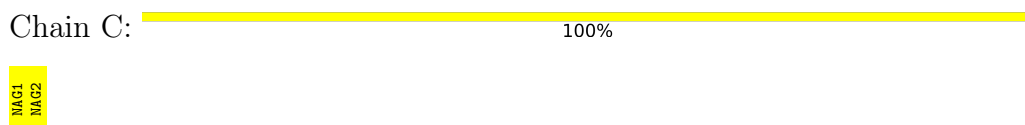
• Molecule 1: Beta-hexosyltransferase
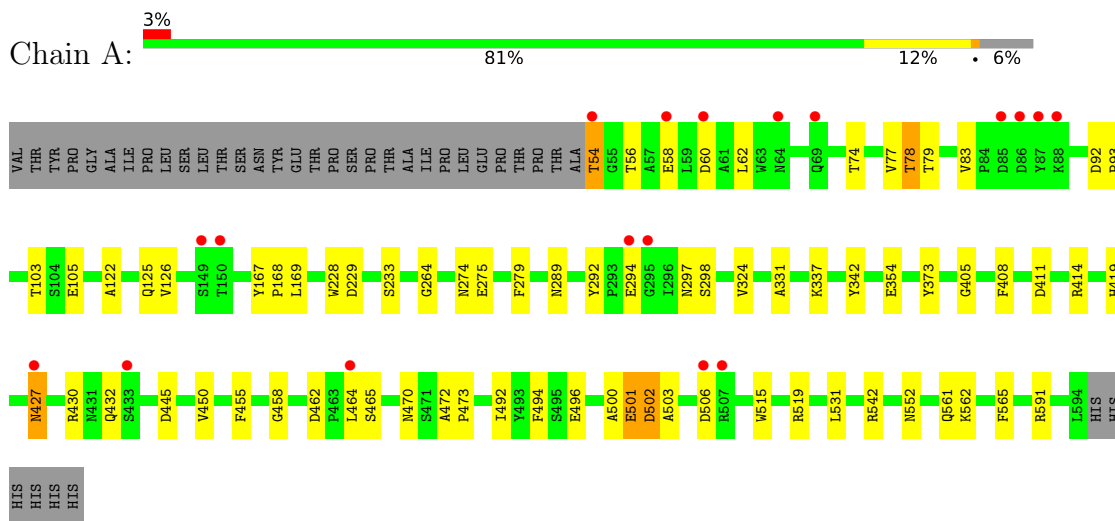
• Molecule 1: Beta-hexosyltransferase
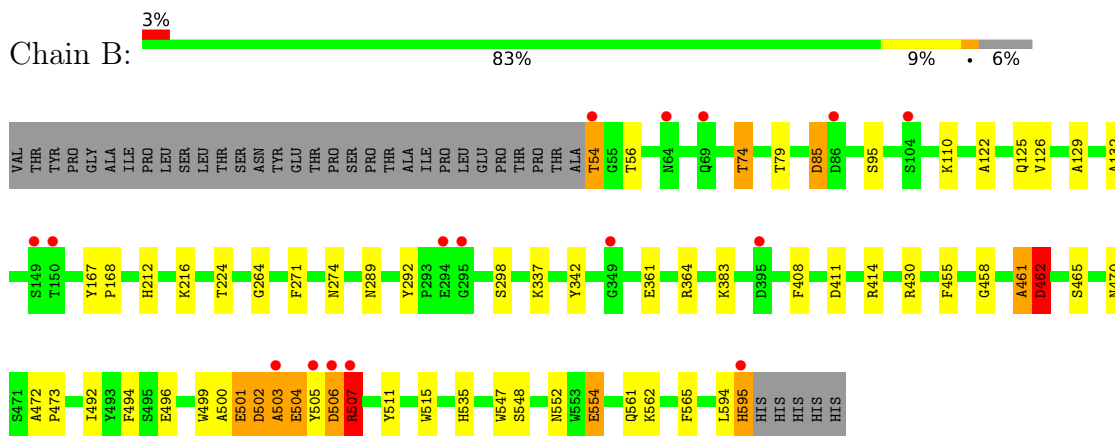
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

Chain D: 100%

NAG1 NAG2

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

Chain E: 100%

NAG1 NAG2

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

Chain F: 100%

NAG1 NAG2

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

Chain G: 100%

NAG1 NAG2

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

Chain H: 100%

NAG1 NAG2

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

Chain I: 100%

NAG1 NAG2

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

Chain J: 50%   50%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.32Å 63.21Å 105.01Å 90.00° 100.42° 90.00°	Depositor
Resolution (Å)	29.96 – 2.25 29.95 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.96-2.25) 98.2 (29.95-2.25)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.189 , 0.235 0.196 , 0.240	Depositor DCC
R_{free} test set	2934 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.7	EDS
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9347	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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: CA, NAG, TPO, TRS

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	0.83	1/4382 (0.0%)	0.97	5/5974 (0.1%)
1	B	0.85	5/4394 (0.1%)	0.95	0/5990
All	All	0.84	6/8776 (0.1%)	0.96	5/11964 (0.0%)

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	A	0	1
1	B	0	3
All	All	0	4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	501	GLU	CD-OE2	9.51	1.36	1.25
1	A	501	GLU	CD-OE1	-6.62	1.18	1.25
1	B	504	GLU	CD-OE2	-5.90	1.19	1.25
1	B	461	ALA	C-O	5.89	1.34	1.23
1	B	554	GLU	CD-OE1	5.64	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	297	ASN	CB-CA-C	-7.49	95.42	110.40
1	A	542	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	519	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	78	THR	CA-CB-CG2	5.43	120.01	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	591	ARG	NE-CZ-NH1	5.30	122.95	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	GLY	Peptide
1	B	264	GLY	Peptide
1	B	503	ALA	Peptide
1	B	507	ARG	Peptide

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	4286	0	4016	43	0
1	B	4297	0	4023	45	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	4	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0
3	A	1	0	0	0	0
4	A	8	0	12	1	0
4	B	8	0	12	0	0
5	A	258	0	0	5	0
5	B	265	0	0	6	0
All	All	9347	0	8263	86	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 5.

The worst 5 of 86 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:501:GLU:OE2	5:A:801:HOH:O	1.77	1.01
1:A:502:ASP:OD1	1:B:503:ALA:HB2	1.62	0.97
1:A:462:ASP:OD1	1:A:502:ASP:HA	1.72	0.89
1:B:462:ASP:OD1	1:B:502:ASP:HA	1.72	0.88
1:B:594:LEU:O	1:B:595:HIS:CG	2.36	0.78

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	536/578 (93%)	517 (96%)	16 (3%)	3 (1%)	25	25
1	B	537/578 (93%)	517 (96%)	16 (3%)	4 (1%)	22	21
All	All	1073/1156 (93%)	1034 (96%)	32 (3%)	7 (1%)	22	21

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	462	ASP
1	B	502	ASP
1	B	505	TYR
1	B	506	ASP
1	A	432	GLN

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	439/472 (93%)	425 (97%)	14 (3%)	39	47
1	B	440/472 (93%)	428 (97%)	12 (3%)	44	54
All	All	879/944 (93%)	853 (97%)	26 (3%)	41	50

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	THR
1	B	342	TYR
1	B	565	PHE
1	B	298	SER
1	B	414	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	227	HIS
1	B	535	HIS
1	B	242	GLN
1	B	561	GLN
1	B	484	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	TPO	B	56	1	8,10,11	1.78	1 (12%)	10,14,16	1.15	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	TPO	A	79	1	8,10,11	1.75	1 (12%)	10,14,16	1.15	1 (10%)
1	TPO	A	74	1	8,10,11	1.54	1 (12%)	10,14,16	0.99	1 (10%)
1	TPO	B	79	1	8,10,11	1.50	1 (12%)	10,14,16	1.11	1 (10%)
1	TPO	B	74	1	8,10,11	1.59	1 (12%)	10,14,16	0.87	1 (10%)
1	TPO	A	56	1	8,10,11	2.44	1 (12%)	10,14,16	1.12	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	B	56	1	-	2/9/11/13	-
1	TPO	A	79	1	-	2/9/11/13	-
1	TPO	A	74	1	-	1/9/11/13	-
1	TPO	B	79	1	-	2/9/11/13	-
1	TPO	B	74	1	-	1/9/11/13	-
1	TPO	A	56	1	-	5/9/11/13	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	TPO	P-OG1	6.54	1.71	1.59
1	B	56	TPO	P-OG1	4.74	1.68	1.59
1	A	79	TPO	P-OG1	4.63	1.68	1.59
1	B	74	TPO	P-OG1	4.26	1.67	1.59
1	A	74	TPO	P-OG1	4.11	1.67	1.59

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	56	TPO	O-C-CA	-2.59	117.98	124.78
1	B	79	TPO	O-C-CA	-2.57	118.03	124.78
1	A	56	TPO	P-OG1-CB	2.42	130.53	123.21
1	A	74	TPO	O-C-CA	-2.23	118.94	124.78
1	A	79	TPO	O3P-P-O2P	2.11	115.71	107.64

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	56	TPO	N-CA-CB-CG2
1	A	56	TPO	N-CA-CB-OG1
1	A	56	TPO	C-CA-CB-CG2
1	A	56	TPO	O-C-CA-CB
1	A	56	TPO	CG2-CB-OG1-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	74	TPO	1	0

5.5 Carbohydrates ⓘ

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	2,1	14,14,15	0.62	0	17,19,21	1.32	2 (11%)
2	NAG	C	2	2	14,14,15	0.97	0	17,19,21	2.47	3 (17%)
2	NAG	D	1	2,1	14,14,15	0.47	0	17,19,21	1.72	4 (23%)
2	NAG	D	2	2	14,14,15	1.08	0	17,19,21	1.99	4 (23%)
2	NAG	E	1	2,1	14,14,15	0.94	0	17,19,21	3.31	13 (76%)
2	NAG	E	2	2	14,14,15	1.71	4 (28%)	17,19,21	3.00	9 (52%)
2	NAG	F	1	2,1	14,14,15	1.39	2 (14%)	17,19,21	2.04	6 (35%)
2	NAG	F	2	2	14,14,15	0.73	0	17,19,21	2.51	7 (41%)
2	NAG	G	1	2,1	14,14,15	0.82	0	17,19,21	2.42	6 (35%)
2	NAG	G	2	2	14,14,15	1.60	3 (21%)	17,19,21	2.18	5 (29%)
2	NAG	H	1	2,1	14,14,15	0.70	0	17,19,21	2.11	6 (35%)
2	NAG	H	2	2	14,14,15	0.58	0	17,19,21	1.29	1 (5%)
2	NAG	I	1	2,1	14,14,15	1.13	1 (7%)	17,19,21	1.76	5 (29%)
2	NAG	I	2	2	14,14,15	0.82	0	17,19,21	1.95	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	J	1	2,1	14,14,15	0.89	0	17,19,21	1.93	5 (29%)
2	NAG	J	2	2	14,14,15	0.58	0	17,19,21	3.05	7 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C1-C2	3.73	1.57	1.52
2	G	2	NAG	C2-N2	3.46	1.52	1.46
2	F	1	NAG	O5-C1	-3.20	1.38	1.43
2	I	1	NAG	O5-C1	-2.84	1.39	1.43
2	E	2	NAG	C3-C2	2.67	1.58	1.52

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2	NAG	C4-C3-C2	-8.45	98.63	111.02
2	C	2	NAG	C1-O5-C5	8.40	123.57	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	C4-C3-C2	8.03	122.78	111.02
2	G	2	NAG	O5-C5-C6	5.52	115.86	107.20
2	D	2	NAG	C1-O5-C5	5.42	119.53	112.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C1-C2-N2-C7
2	E	2	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	4	0
2	J	2	NAG	1	0
2	E	1	NAG	4	0

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

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is 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	TRS	B	701	-	7,7,7	0.16	0	9,9,9	0.37	0
4	TRS	A	702	-	7,7,7	0.16	0	9,9,9	0.22	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
4	TRS	B	701	-	-	8/9/9/9	-
4	TRS	A	702	-	-	6/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	TRS	N-C-C1-O1
4	B	701	TRS	C3-C-C1-O1
4	B	701	TRS	N-C-C1-O1
4	B	701	TRS	C1-C-C3-O3
4	B	701	TRS	C2-C-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	TRS	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 TRS B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand TRS A 702

Bond lengths

Bond angles

Torsions

Rings
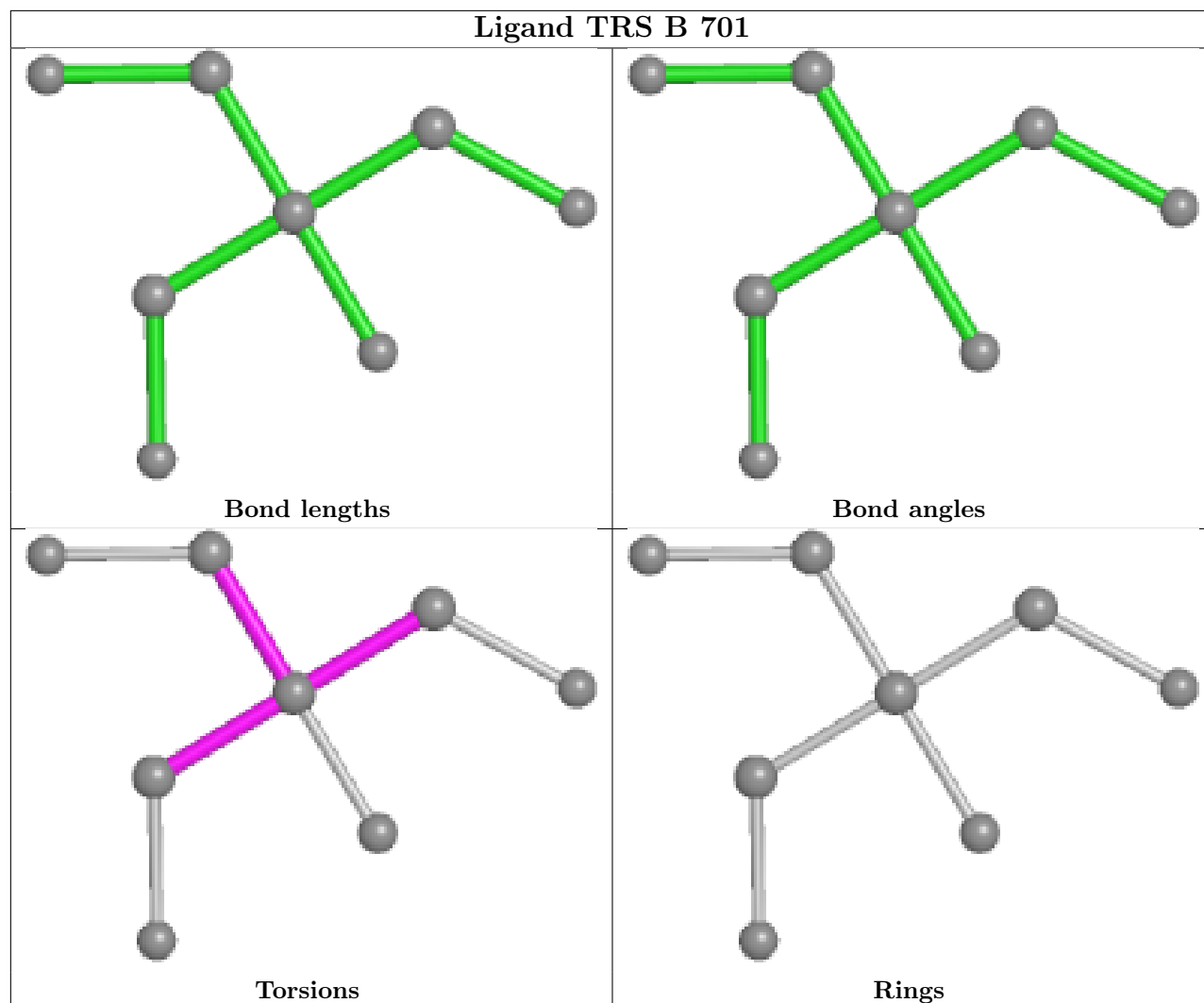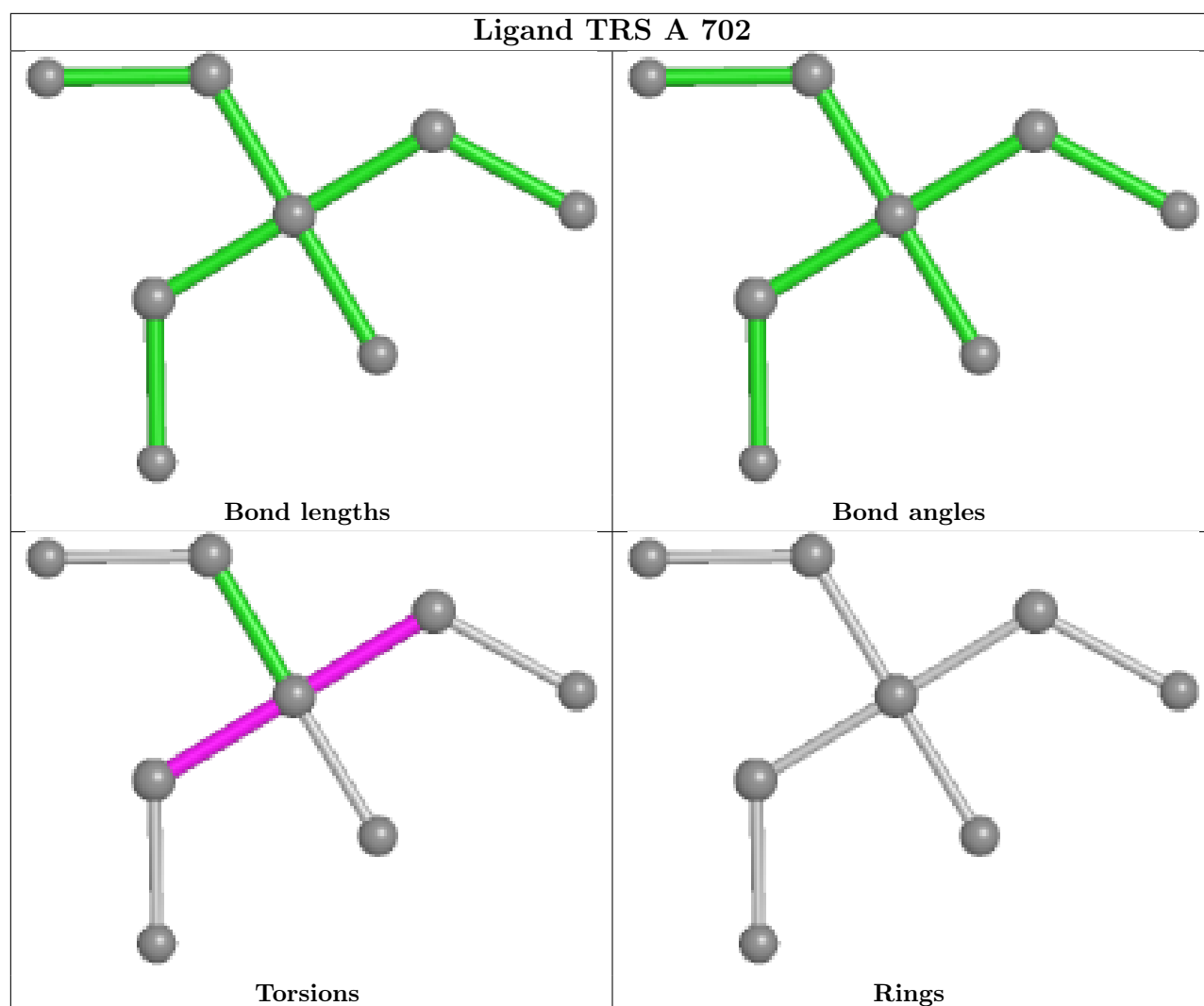
5.7 Other polymers ⓘ

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	538/578 (93%)	0.11	18 (3%)	46	48	17, 28, 47, 77	0
1	B	539/578 (93%)	0.02	16 (2%)	50	53	17, 27, 45, 85	0
All	All	1077/1156 (93%)	0.07	34 (3%)	47	50	17, 28, 46, 85	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	506	ASP	8.8
1	A	506	ASP	5.3
1	A	507	ARG	5.2
1	B	507	ARG	4.7
1	A	433	SER	4.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	A	56	11/12	0.79	0.23	48,56,65,68	4
1	TPO	B	56	11/12	0.83	0.25	47,49,55,56	4
1	TPO	A	74	11/12	0.86	0.21	38,42,55,55	4
1	TPO	B	74	11/12	0.89	0.17	35,44,62,62	4
1	TPO	B	79	11/12	0.91	0.18	32,40,55,56	4
1	TPO	A	79	11/12	0.92	0.12	30,35,40,42	4

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
2	NAG	G	2	14/15	0.59	0.58	73,83,92,95	0
2	NAG	E	2	14/15	0.68	0.38	59,69,72,72	0
2	NAG	D	2	14/15	0.76	0.38	58,61,65,66	14
2	NAG	J	2	14/15	0.76	0.43	38,41,45,45	14
2	NAG	C	2	14/15	0.79	0.49	68,73,78,78	0
2	NAG	J	1	14/15	0.84	0.25	34,37,38,40	14
2	NAG	I	2	14/15	0.84	0.45	57,65,68,70	0
2	NAG	G	1	14/15	0.85	0.26	54,59,60,68	0
2	NAG	H	2	14/15	0.86	0.29	50,58,66,69	0
2	NAG	E	1	14/15	0.87	0.28	55,59,66,66	0
2	NAG	F	2	14/15	0.87	0.45	52,58,62,63	0
2	NAG	D	1	14/15	0.88	0.19	44,49,52,53	14
2	NAG	H	1	14/15	0.88	0.21	45,48,51,53	0
2	NAG	C	1	14/15	0.88	0.34	55,61,64,68	0
2	NAG	F	1	14/15	0.91	0.22	31,37,44,47	0
2	NAG	I	1	14/15	0.93	0.20	32,36,41,49	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)
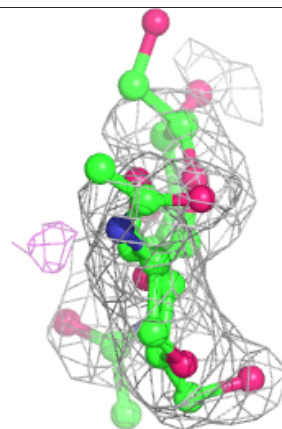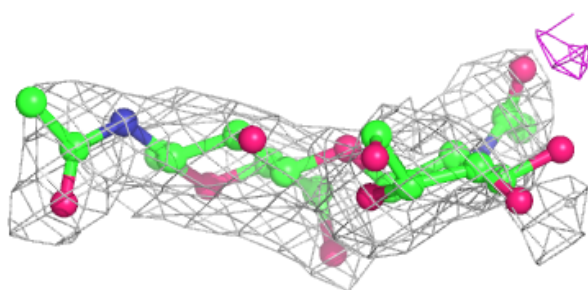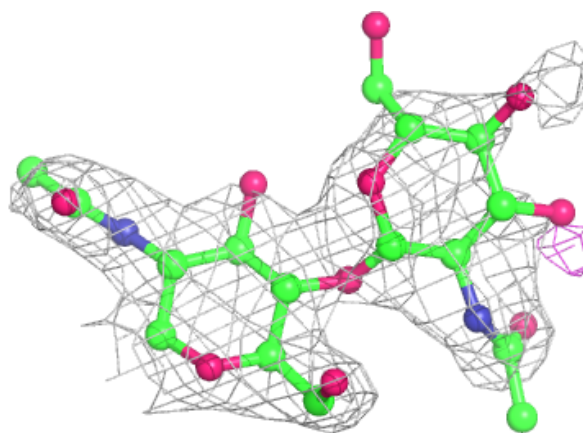
Electron density around Chain D:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
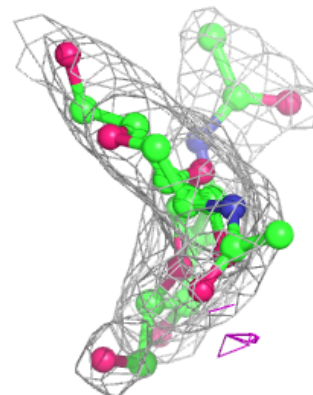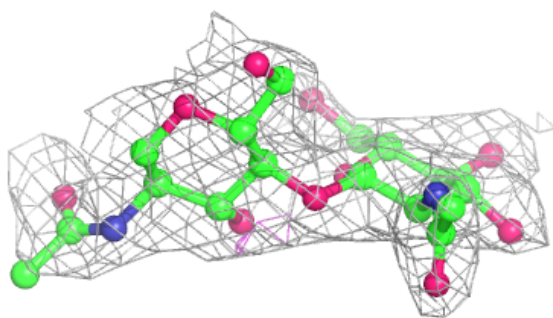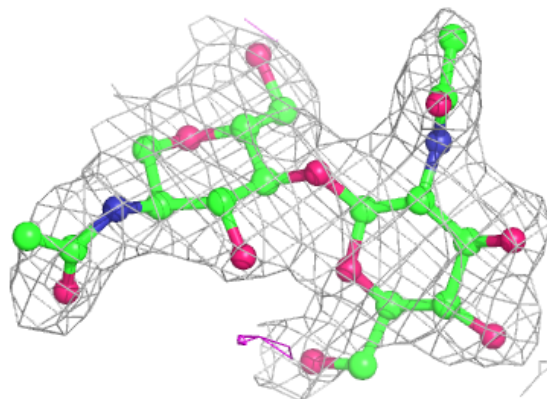and green (positive)
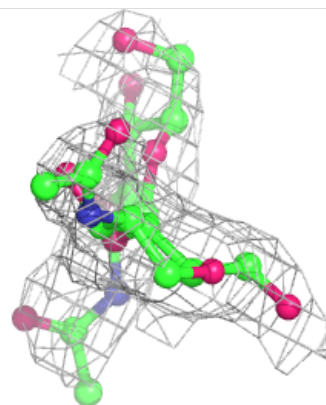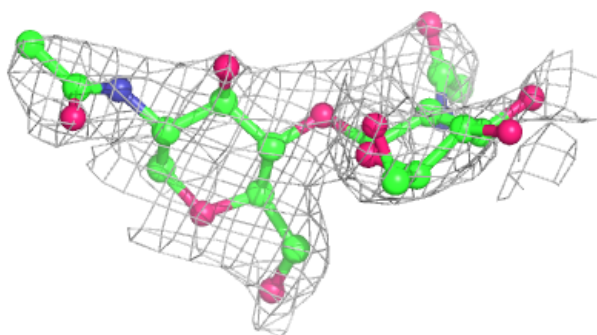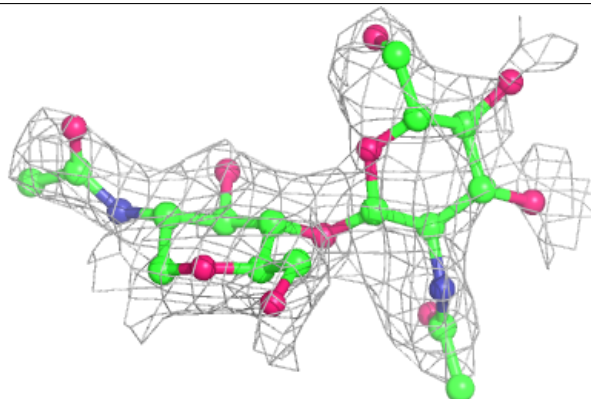
Electron density around Chain E:

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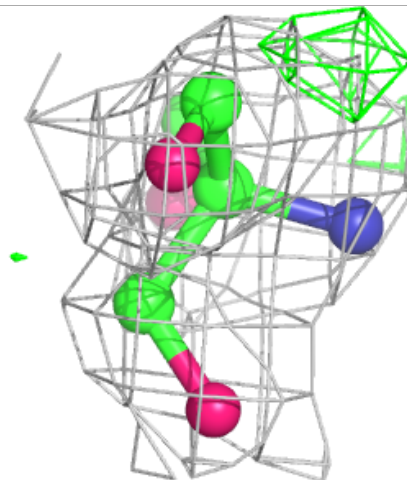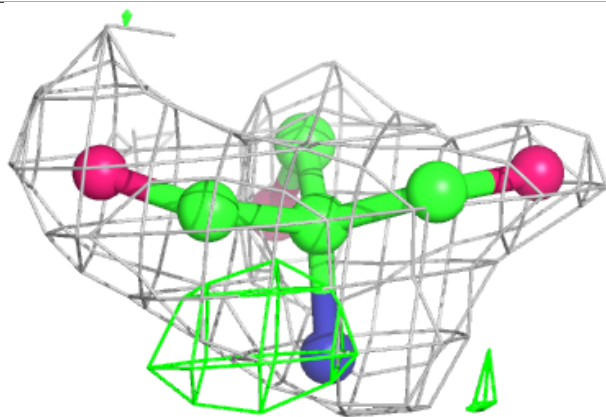mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
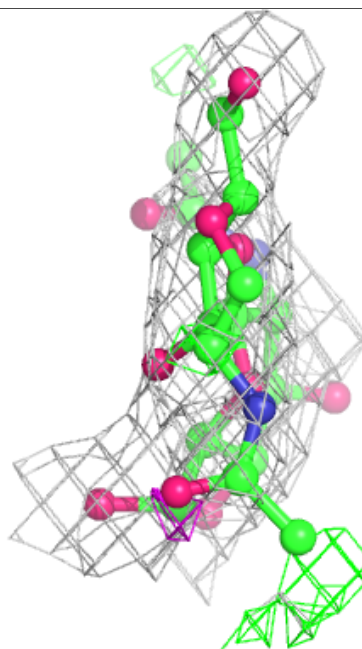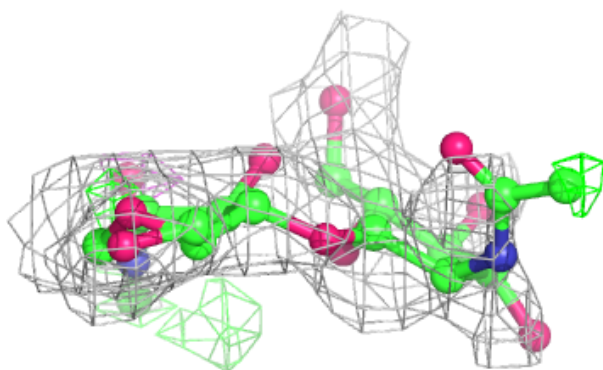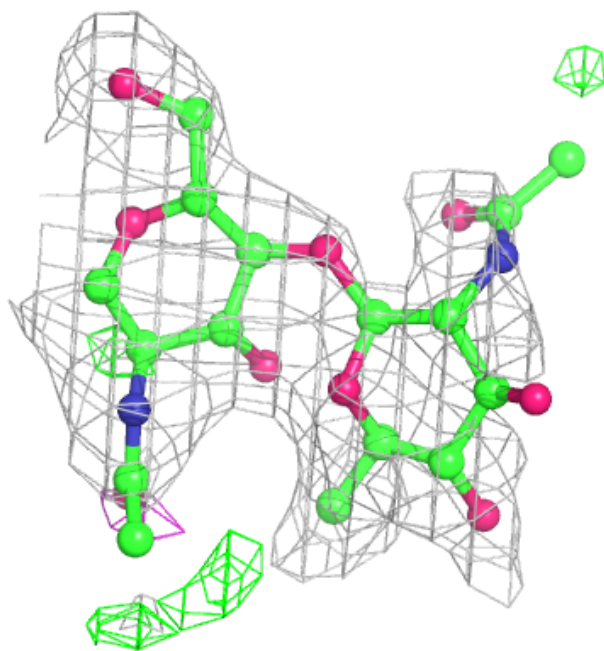
Electron density around Chain F:

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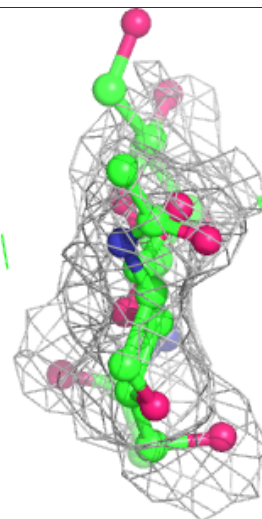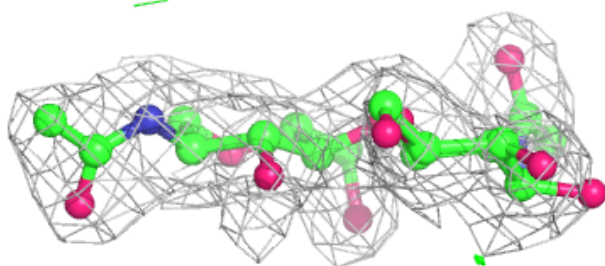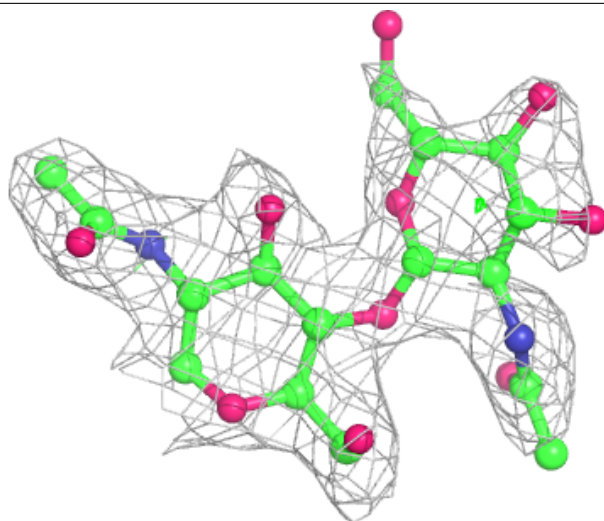
Electron density around Chain G:

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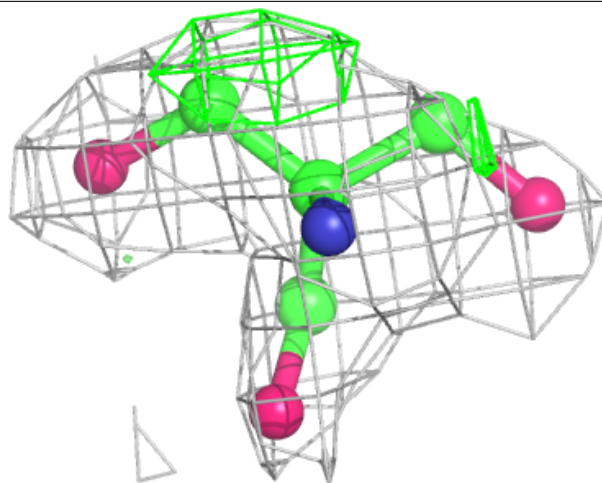mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
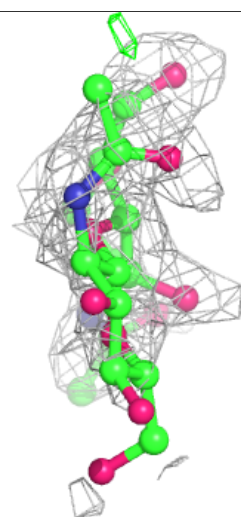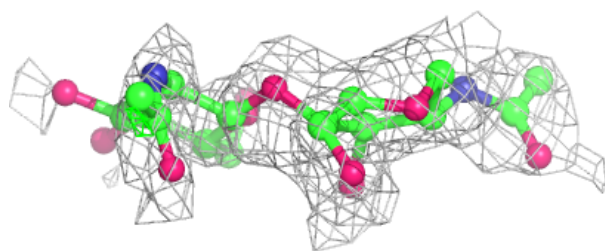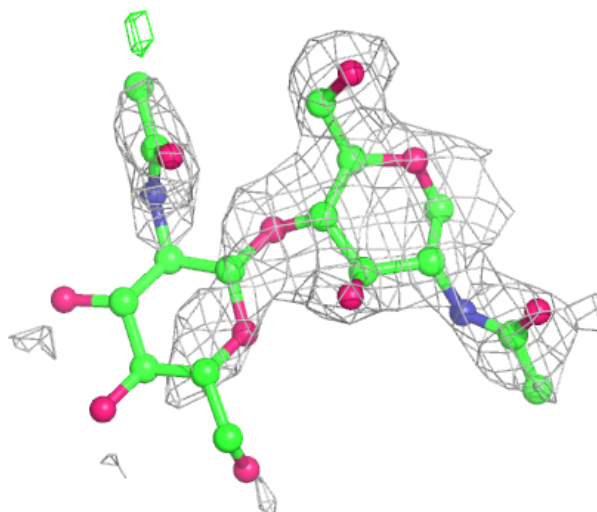
Electron density around Chain H:

$2mF_o$-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 I:

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 J:

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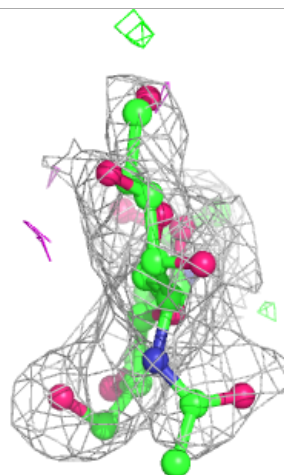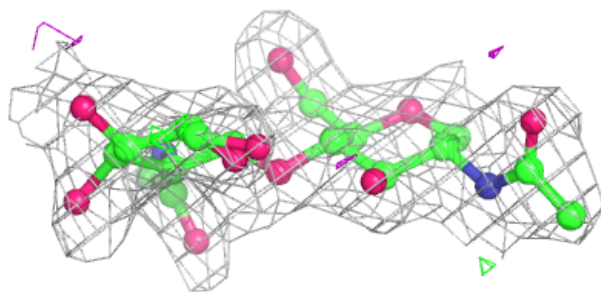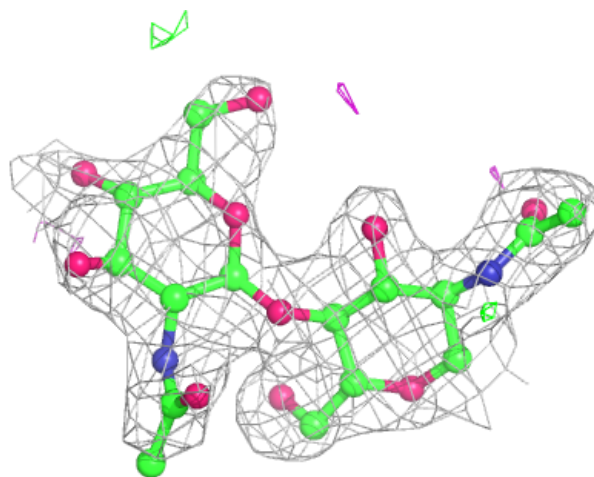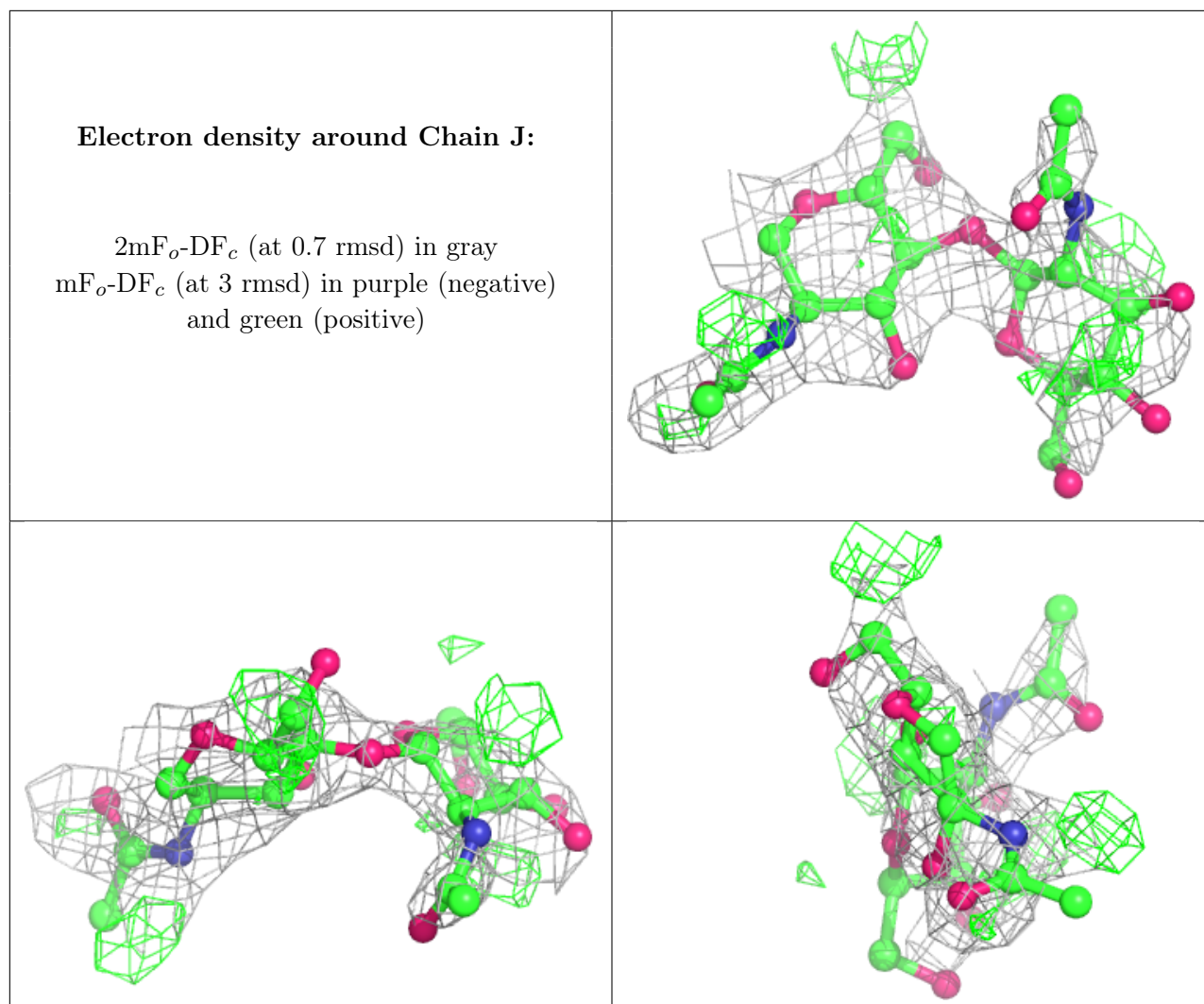
6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TRS	B	701	8/8	0.82	0.27	36,47,51,52	8
4	TRS	A	702	8/8	0.91	0.22	39,43,44,45	0
3	CA	A	701	1/1	0.99	0.06	25,25,25,25	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.
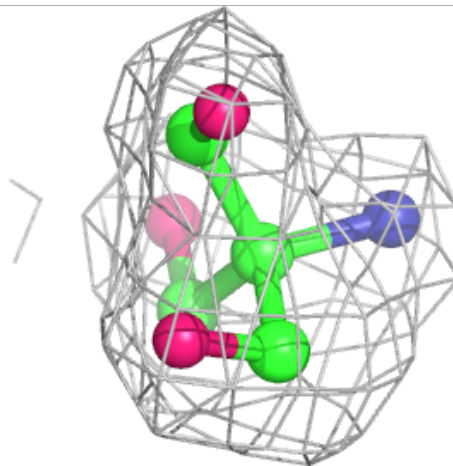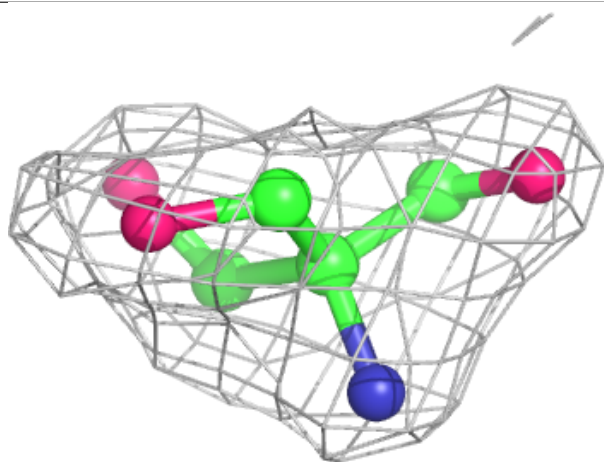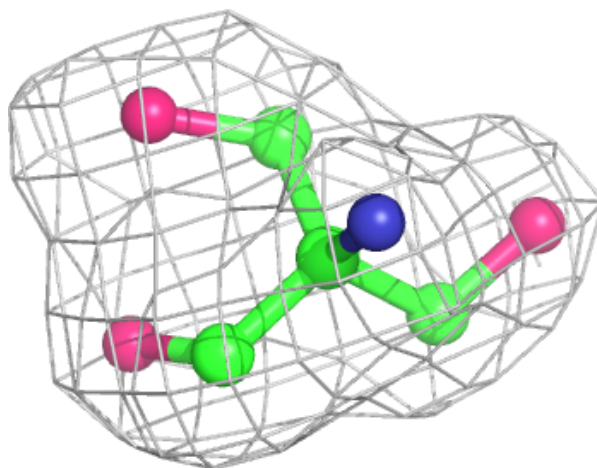
Electron density around TRS B 701:

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

Electron density around TRS A 702:

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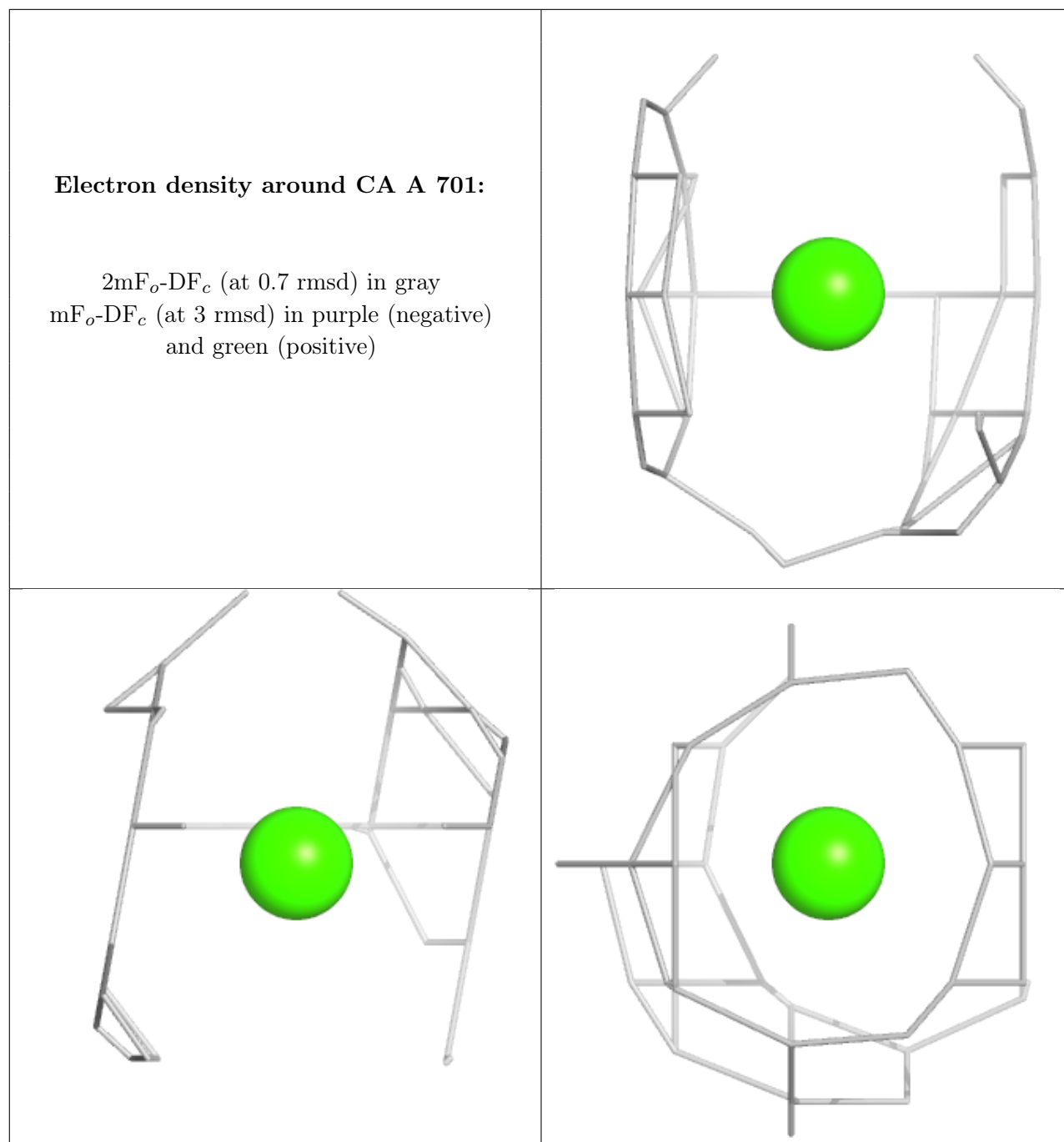and green (positive)

Electron density around CA A 701:

$2mF_o$-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.