WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 10, 2021 – 08:25 am BST

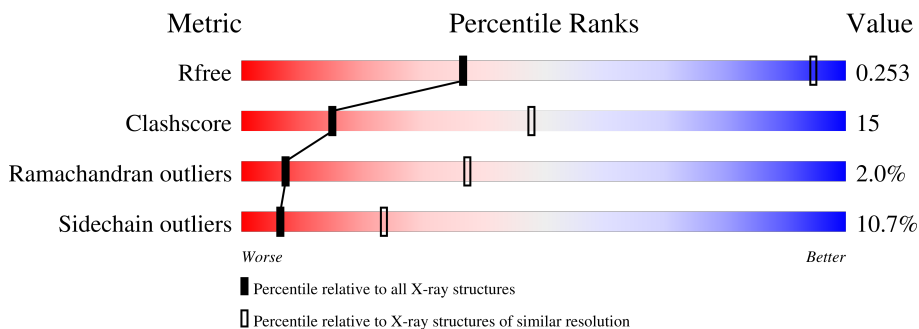|		
PDB ID	:	6TS2
Title	:	Truncated version of Chaetomium thermophilum UDP-Glucose Glucosyl Transferase (UGGT) lacking domain TRXL2 (417-650).
Authors	:	Roversi, P.; Zitzmann, N.
Deposited on	:	2019-12-19
Resolution	:	5.74 Å(reported)

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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 5.74 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.
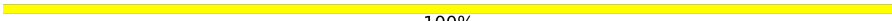
Metric	Percentile Ranks	Value
Rfree		0.253
Clashscore		15
Ramachandran outliers		2.0%
Sidechain outliers		10.7%

■ 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	1006 (7.60-3.86)
Clashscore	141614	1031 (7.58-3.90)
Ramachandran outliers	138981	1002 (7.60-3.86)
Sidechain outliers	138945	1004 (7.60-3.82)

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%

Mol	Chain	Length	Quality of chain
1	A	1260	62% 24% • 12%
1	B	1260	52% 31% 5% 11%
1	C	1260	58% 26% • 12%
1	D	1260	58% 28% • 11%
2	E	5	60% 40%
3	F	3	33% 67%
3	H	3	33% 67%

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Mol	Chain	Length	Quality of chain
4	G	4	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 36079 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 UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1111	Total	C	N	O	S	0	0	0
			8882	5671	1509	1675	27			
1	B	1120	Total	C	N	O	S	0	0	0
			8955	5718	1522	1688	27			
1	C	1113	Total	C	N	O	S	0	0	0
			8898	5680	1512	1678	28			
1	D	1123	Total	C	N	O	S	0	0	0
			8983	5735	1529	1691	28			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
A	1510	HIS	-	expression tag	UNP G0SB58
A	1511	HIS	-	expression tag	UNP G0SB58
A	1512	HIS	-	expression tag	UNP G0SB58
A	1513	HIS	-	expression tag	UNP G0SB58
A	1514	HIS	-	expression tag	UNP G0SB58
B	21	GLU	-	expression tag	UNP G0SB58
B	22	THR	-	expression tag	UNP G0SB58
B	23	GLY	-	expression tag	UNP G0SB58
B	1506	GLY	-	expression tag	UNP G0SB58
B	1507	THR	-	expression tag	UNP G0SB58
B	1508	LYS	-	expression tag	UNP G0SB58
B	1509	HIS	-	expression tag	UNP G0SB58
B	1510	HIS	-	expression tag	UNP G0SB58

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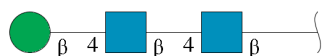| Chain	Residue	Modelled	Actual	Comment	Reference
B	1511	HIS	-	expression tag	UNP G0SB58
B	1512	HIS	-	expression tag	UNP G0SB58
B	1513	HIS	-	expression tag	UNP G0SB58
B	1514	HIS	-	expression tag	UNP G0SB58
C	21	GLU	-	expression tag	UNP G0SB58
C	22	THR	-	expression tag	UNP G0SB58
C	23	GLY	-	expression tag	UNP G0SB58
C	1506	GLY	-	expression tag	UNP G0SB58
C	1507	THR	-	expression tag	UNP G0SB58
C	1508	LYS	-	expression tag	UNP G0SB58
C	1509	HIS	-	expression tag	UNP G0SB58
C	1510	HIS	-	expression tag	UNP G0SB58
C	1511	HIS	-	expression tag	UNP G0SB58
C	1512	HIS	-	expression tag	UNP G0SB58
C	1513	HIS	-	expression tag	UNP G0SB58
C	1514	HIS	-	expression tag	UNP G0SB58
D	21	GLU	-	expression tag	UNP G0SB58
D	22	THR	-	expression tag	UNP G0SB58
D	23	GLY	-	expression tag	UNP G0SB58
D	1506	GLY	-	expression tag	UNP G0SB58
D	1507	THR	-	expression tag	UNP G0SB58
D	1508	LYS	-	expression tag	UNP G0SB58
D	1509	HIS	-	expression tag	UNP G0SB58
D	1510	HIS	-	expression tag	UNP G0SB58
D	1511	HIS	-	expression tag	UNP G0SB58
D	1512	HIS	-	expression tag	UNP G0SB58
D	1513	HIS	-	expression tag	UNP G0SB58
D	1514	HIS	-	expression tag	UNP G0SB58

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.
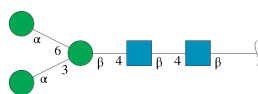
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	5	61	34	2	25	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

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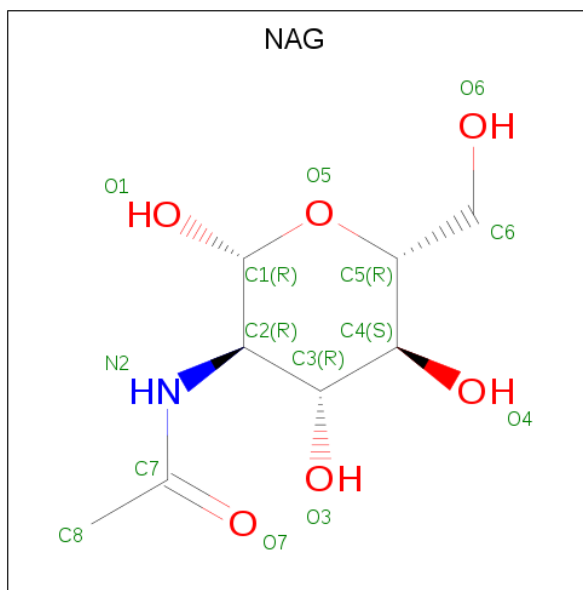
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		

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. 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. 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.
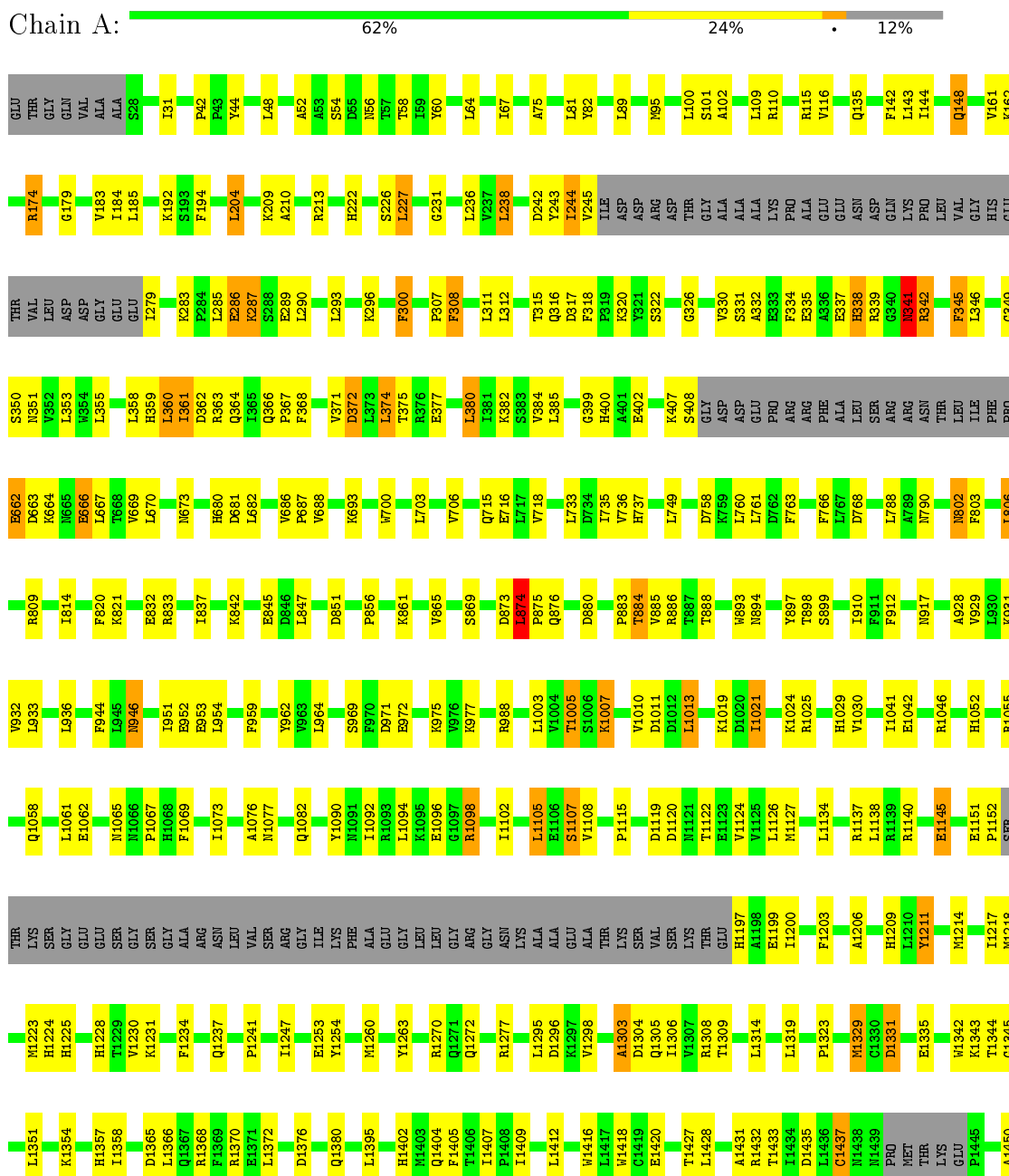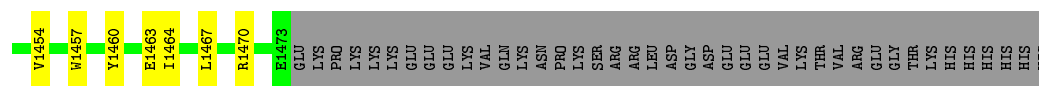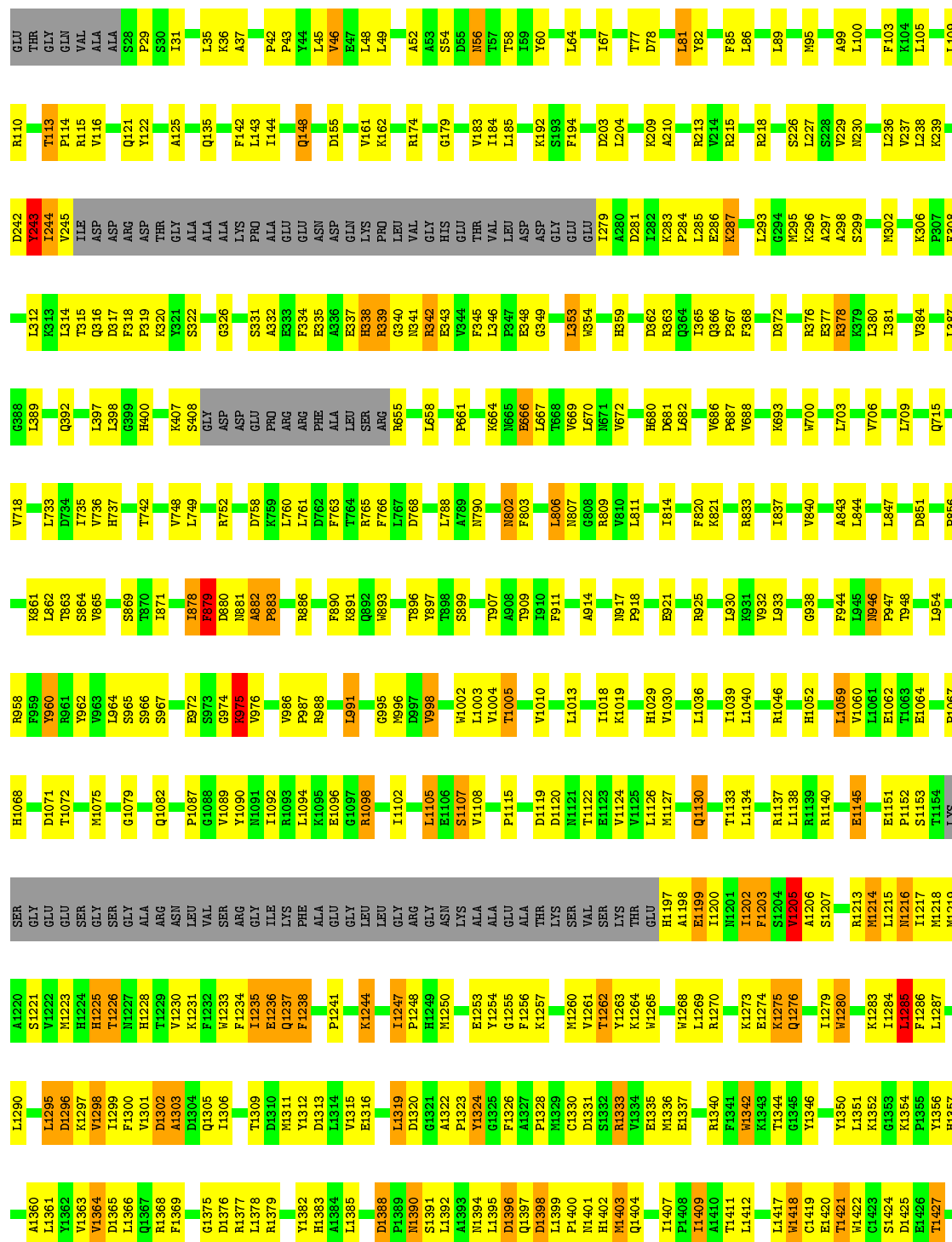
● Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein
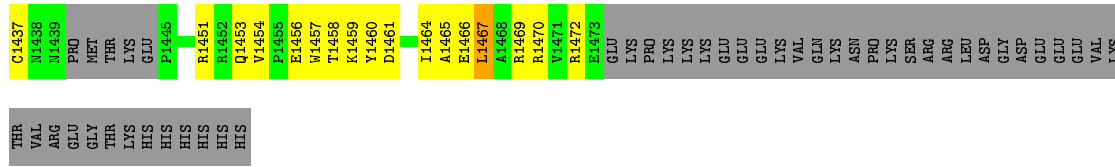
• Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein

C1437 N1438 N1439 PRO MET THR LYS GLU P1445 R1451 R1452 Q1453 V1454 P1455 E1456 W1457 T1458 K1459 Y1460 D1461 I1464 A1465 E1466 L1467 A1468 R1469 R1470 V1471 R1472 E1473 GLU LYS PRO LYS LYS LYS GLU GLU GLU GLU VAL VAL GLN LYS LYS ASN PRO LYS SER ARG ARG LEU ASP GLY ASP GLU GLU GLU VAL LYS

THR VAL ARG GLY THR LYS HIS HIS HIS HIS HIS HIS

• Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein

Chain C:

58%　　　　　　　　　26%　　•　　12%
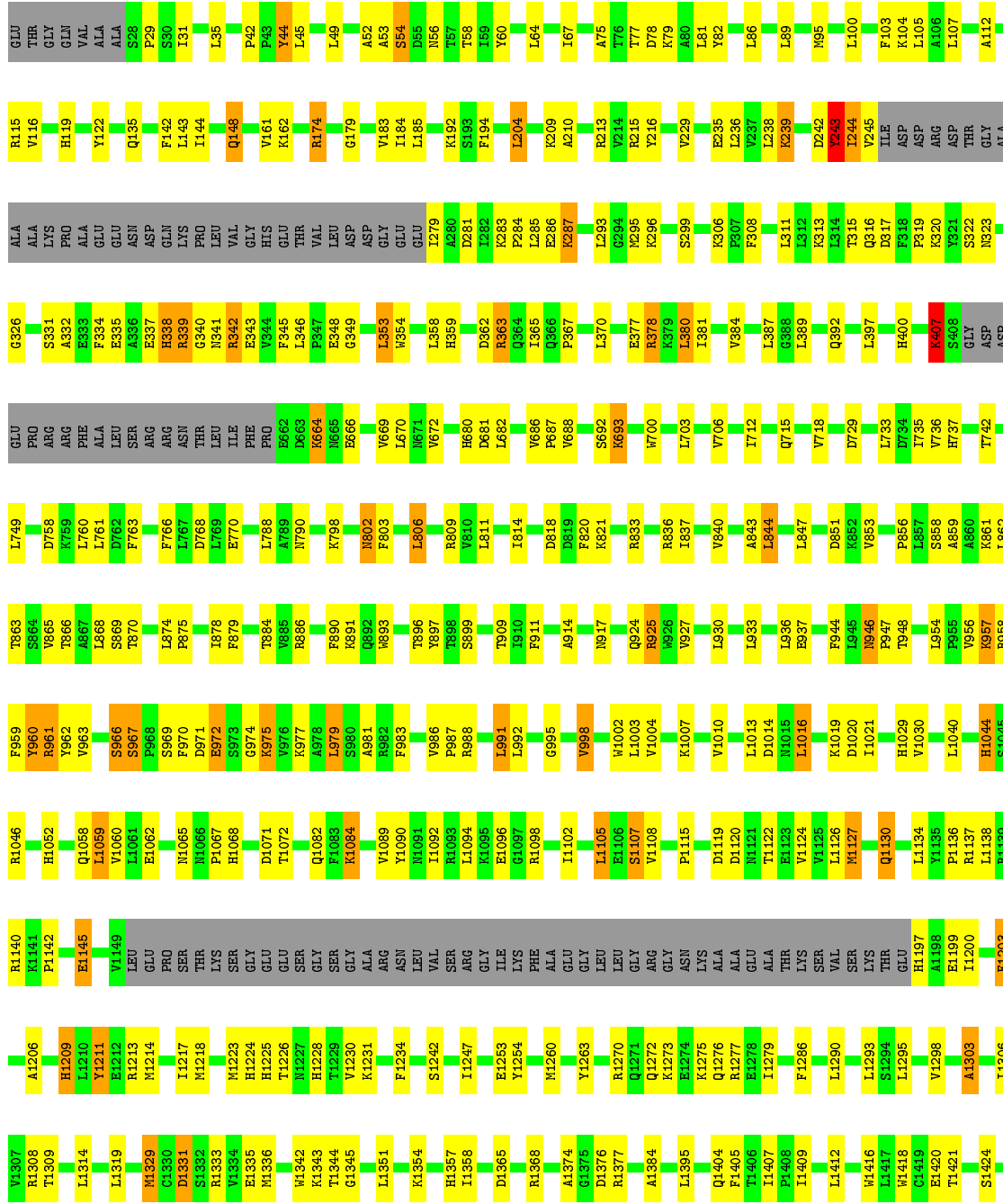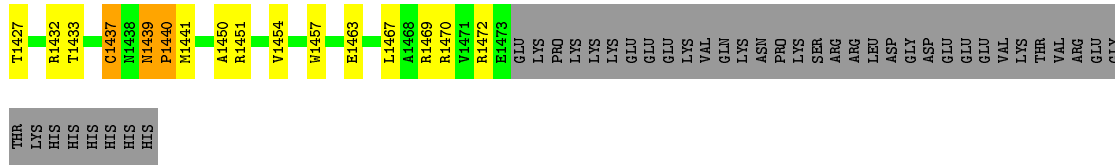
• Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein

Chain D:

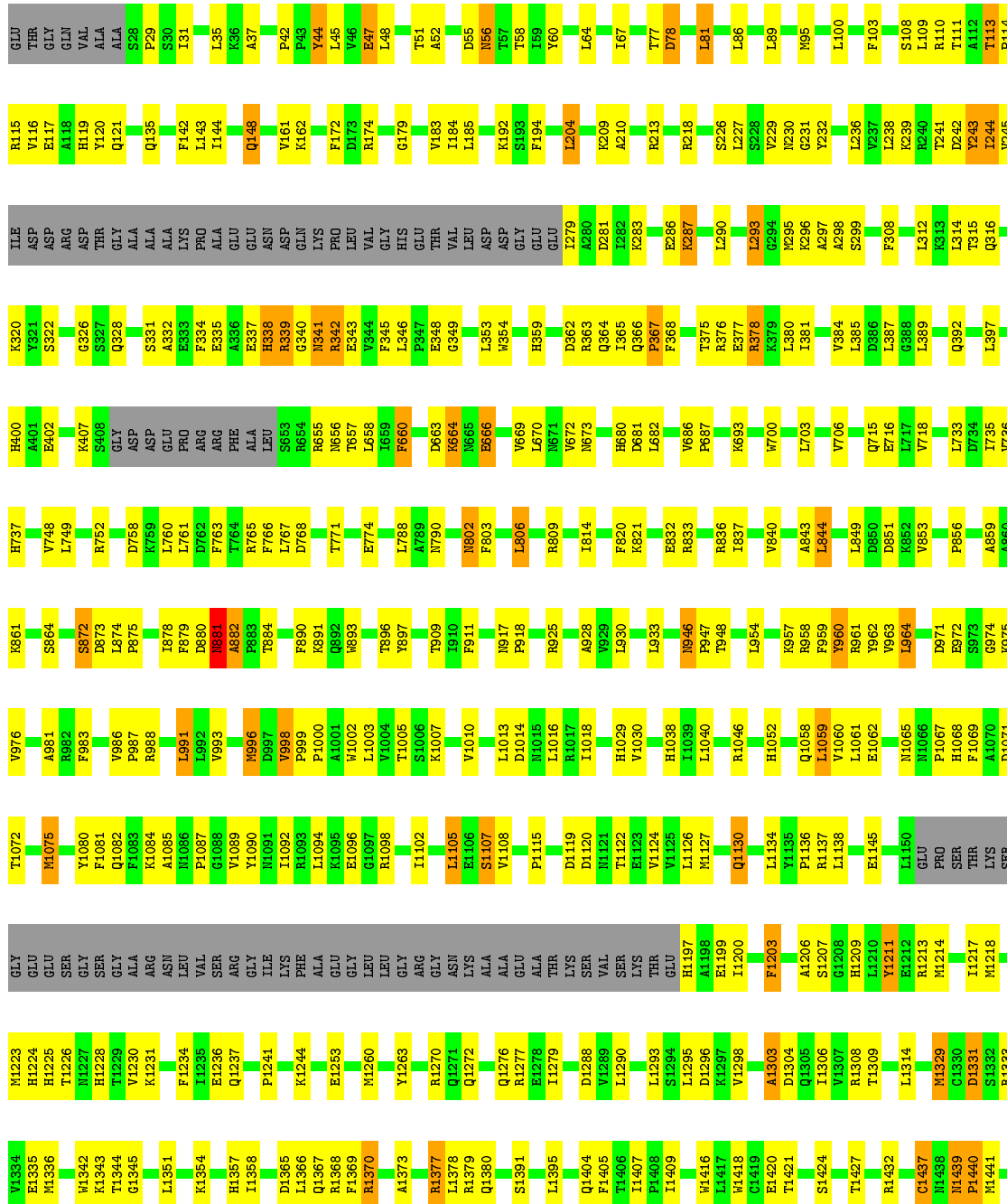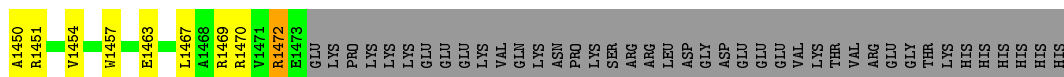A1450 R1451 V1454 W1457 E1463 L1467 A1468 R1469 R1470 V1471 R1472 E1473 GLU LYS PRO LYS LYS LYS GLU GLU GLU LYS VAL GLN LYS ASN PRO LYS SER ARG ARG LEU ASP GLY ASP GLU GLU GLU VAL LYS THR VAL ARG GLU GLY THR LYS HIS HIS HIS HIS HIS HIS

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

Chain E:　　60%　　40%

NAG1 NAG2 BMA3 MAN4 MAN5

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

Chain F:　　33%　　67%

NAG1 NAG2 BMA3

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

Chain H:　　33%　　67%

NAG1 NAG2 BMA3

• Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:　　100%

NAG1 NAG2 BMA3 MAN4

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	151.15Å 191.01Å 158.81Å 90.00° 117.70° 90.00°	Depositor
Resolution (Å)	140.60 – 5.74 140.61 – 5.73	Depositor EDS
% Data completeness (in resolution range)	74.9 (140.60-5.74) 63.9 (140.61-5.73)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.60 (at 5.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.174 , 0.249 0.187 , 0.253	Depositor DCC
R_{free} test set	829 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	290.4	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 185.6	EDS
L-test for twinning[2]	$<\lvert L \rvert> = 0.40, <L^2> = 0.23$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	36079	wwPDB-VP
Average B, all atoms (Å^2)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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 $<\lvert L \rvert>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.45	0/9087	0.66	1/12325 (0.0%)
1	B	0.46	0/9162	0.68	3/12428 (0.0%)
1	C	0.42	0/9104	0.64	2/12349 (0.0%)
1	D	0.43	0/9191	0.65	2/12467 (0.0%)
All	All	0.44	0/36544	0.66	8/49569 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	871	ILE	C-N-CA	5.99	136.68	121.70
1	D	875	PRO	C-N-CA	5.67	135.87	121.70
1	D	243	TYR	C-N-CA	5.33	135.04	121.70
1	B	1274	GLU	C-N-CA	5.23	134.77	121.70
1	A	341	ASN	CA-CB-CG	5.15	124.72	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8882	0	8770	226	0
1	B	8955	0	8846	326	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	8898	0	8788	270	0
1	D	8983	0	8881	287	0
2	E	61	0	52	4	0
3	F	39	0	34	0	0
3	H	39	0	34	0	0
4	G	50	0	43	0	0
5	A	42	0	39	0	0
5	B	42	0	39	0	0
5	C	42	0	39	0	0
5	D	42	0	39	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	36079	0	35604	1080	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 15.

The worst 5 of 1080 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:D:78:ASP:HB2	1:D:975:LYS:HA	1.23	1.16
1:B:1376:ASP:HA	1:B:1379:ARG:HD3	1.26	1.15
1:B:1333:ARG:HG3	1:B:1424:SER:HA	1.17	1.13
1:D:1241:PRO:HA	1:D:1244:LYS:HB2	1.32	1.12
1:B:869:SER:HB2	1:B:886:ARG:HE	1.07	1.10

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	1101/1260 (87%)	1009 (92%)	78 (7%)	14 (1%)	12	48
1	B	1110/1260 (88%)	947 (85%)	134 (12%)	29 (3%)	5	31
1	C	1105/1260 (88%)	991 (90%)	98 (9%)	16 (1%)	11	46
1	D	1115/1260 (88%)	987 (88%)	100 (9%)	28 (2%)	5	32
All	All	4431/5040 (88%)	3934 (89%)	410 (9%)	87 (2%)	7	37

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	ALA
1	A	873	ASP
1	A	874	LEU
1	A	876	GLN
1	A	883	PRO

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	965/1088 (89%)	880 (91%)	85 (9%)	10	31
1	B	974/1088 (90%)	844 (87%)	130 (13%)	4	18
1	C	967/1088 (89%)	864 (89%)	103 (11%)	6	23
1	D	977/1088 (90%)	881 (90%)	96 (10%)	8	26
All	All	3883/4352 (89%)	3469 (89%)	414 (11%)	6	23

5 of 414 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	295	MET
1	C	1021	ILE
1	D	1145	GLU
1	C	342	ARG
1	C	820	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	230	ASN
1	C	1197	HIS
1	D	1267	HIS
1	C	338	HIS
1	C	738	ASN

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 ⓘ

15 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	2,1	14,14,15	0.31	0	17,19,21	1.12	2 (11%)
2	NAG	E	2	2	14,14,15	0.46	0	17,19,21	2.46	3 (17%)
2	BMA	E	3	2	11,11,12	0.41	0	15,15,17	1.06	2 (13%)
2	MAN	E	4	2	11,11,12	0.95	1 (9%)	15,15,17	1.95	2 (13%)
2	MAN	E	5	2	11,11,12	0.80	0	15,15,17	1.91	2 (13%)
3	NAG	F	1	1,3	14,14,15	0.30	0	17,19,21	1.19	2 (11%)
3	NAG	F	2	3	14,14,15	0.34	0	17,19,21	1.06	1 (5%)
3	BMA	F	3	3	11,11,12	0.31	0	15,15,17	0.49	0
4	NAG	G	1	1,4	14,14,15	0.29	0	17,19,21	1.06	2 (11%)
4	NAG	G	2	4	14,14,15	0.28	0	17,19,21	1.50	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	BMA	G	3	4	11,11,12	0.36	0	15,15,17	0.91	1 (6%)
4	MAN	G	4	4	11,11,12	0.75	0	15,15,17	1.37	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.29	0	17,19,21	1.04	2 (11%)
3	NAG	H	2	3	14,14,15	0.30	0	17,19,21	1.00	2 (11%)
3	BMA	H	3	3	11,11,12	0.30	0	15,15,17	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	1/1/1/1
2	MAN	E	5	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	MAN	C1-C2	2.02	1.56	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4	MAN	C1-O5-C5	6.09	120.44	112.19
2	E	5	MAN	C1-O5-C5	5.86	120.13	112.19
2	E	2	NAG	O5-C1-C2	-5.82	102.10	111.29
2	E	2	NAG	C1-C2-N2	5.72	120.27	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C1-O5-C5	4.98	118.93	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 4 short contacts:

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

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings
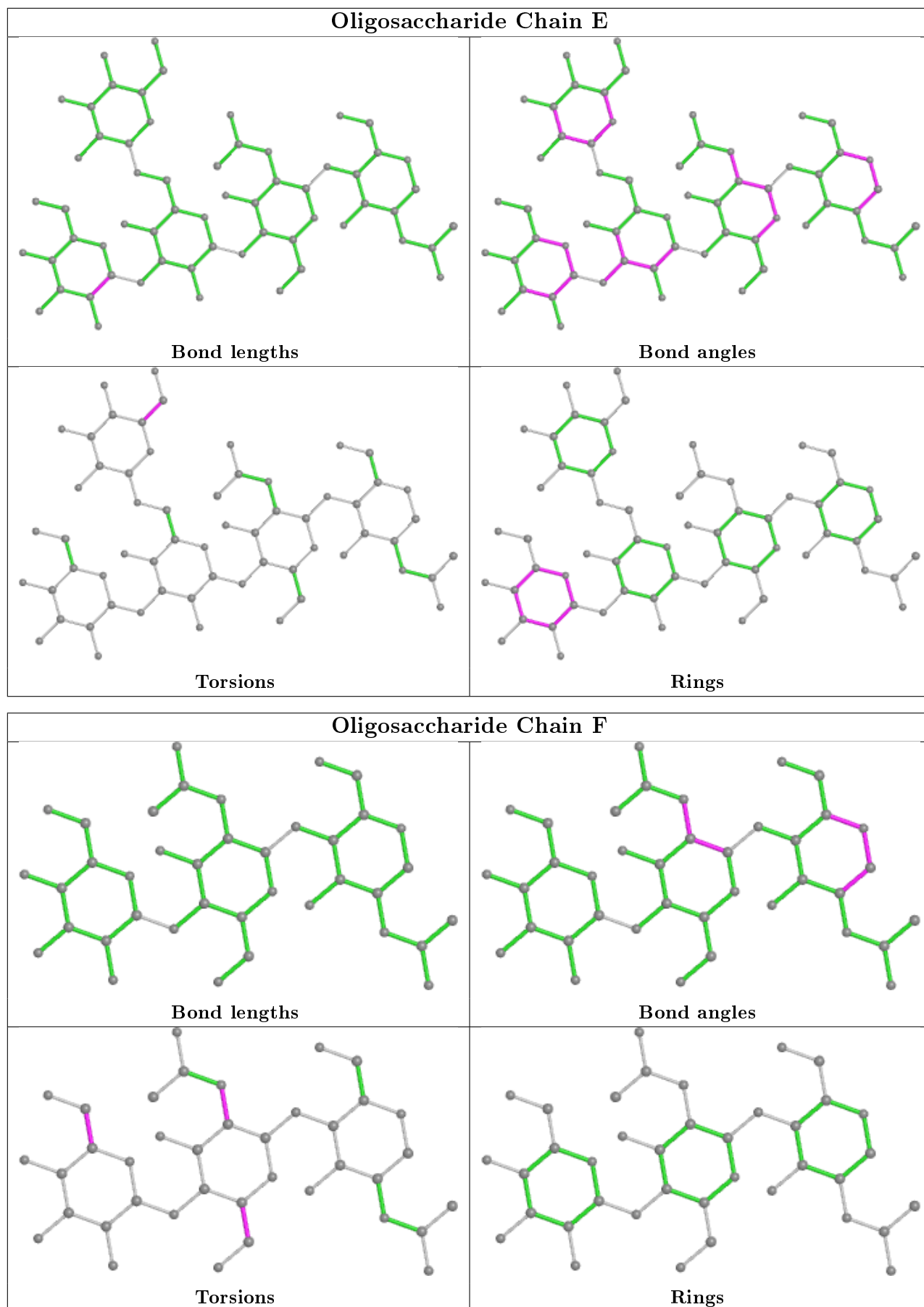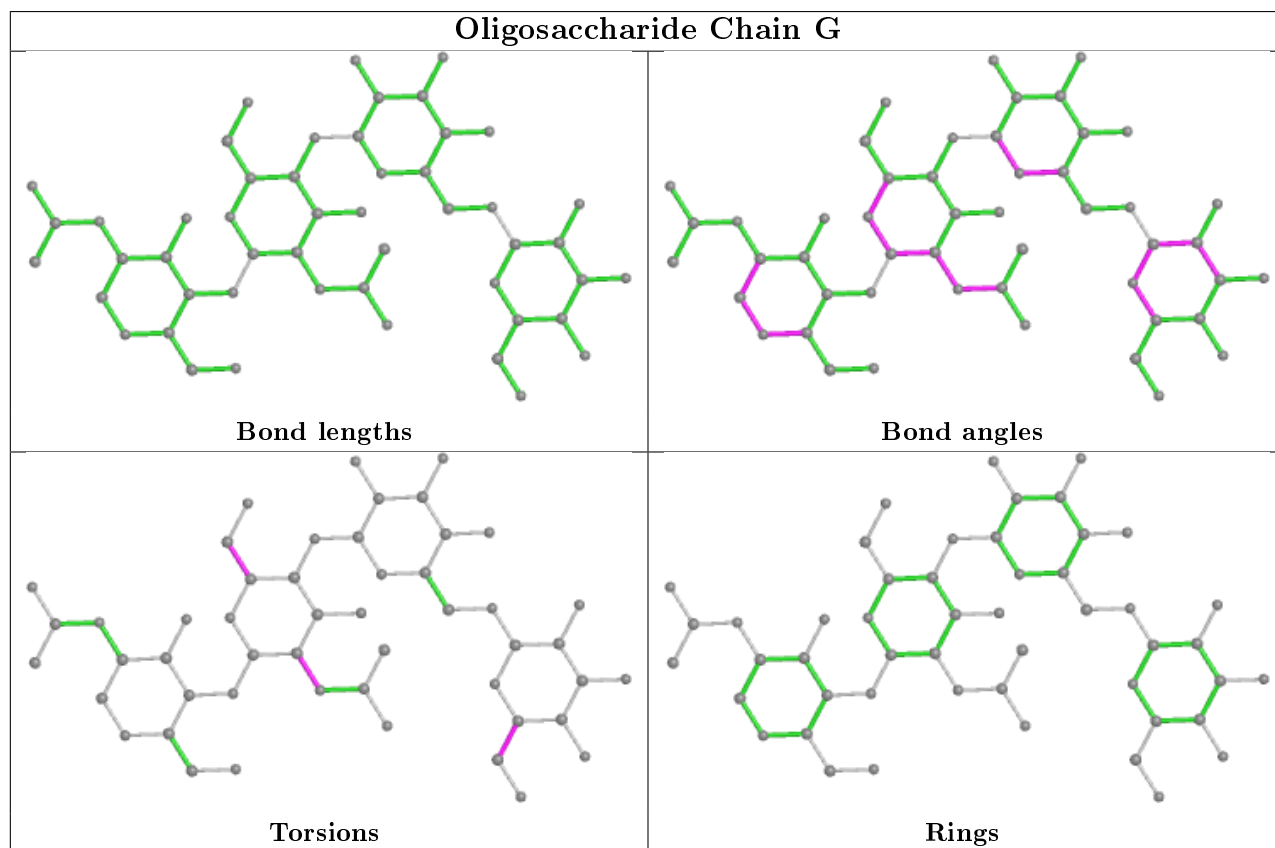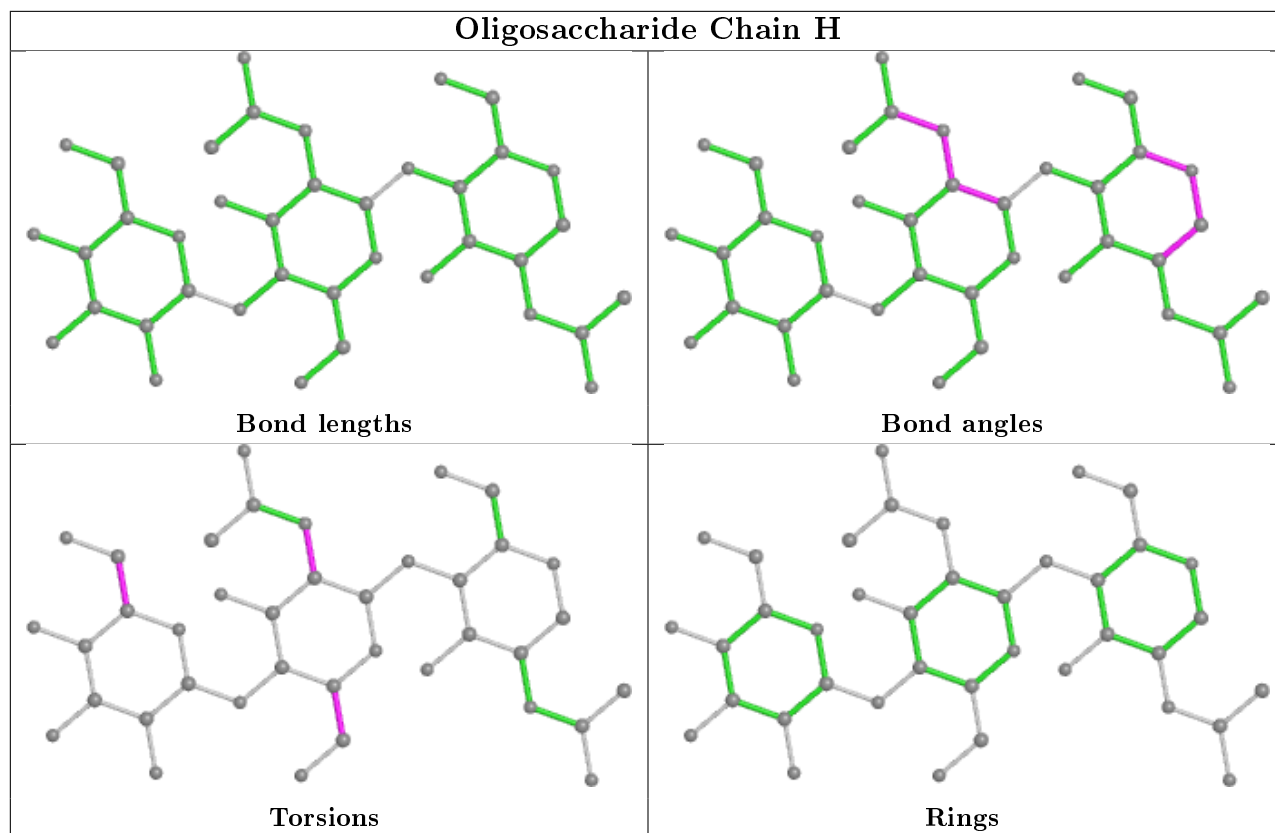
5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	NAG	B	1601	-	14,14,15	0.30	0	17,19,21	0.51	0
5	NAG	D	1605	1	14,14,15	0.35	0	17,19,21	0.70	1 (5%)
5	NAG	C	1607	1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	A	1602	1	14,14,15	0.28	0	17,19,21	0.78	1 (5%)
5	NAG	C	1606	1	14,14,15	0.33	0	17,19,21	0.79	1 (5%)
5	NAG	A	1601	-	14,14,15	0.35	0	17,19,21	0.69	0
5	NAG	C	1601	-	14,14,15	0.51	0	17,19,21	0.81	0
5	NAG	A	1603	1	14,14,15	0.34	0	17,19,21	0.78	1 (5%)
5	NAG	B	1602	1	14,14,15	0.36	0	17,19,21	1.17	1 (5%)
5	NAG	D	1601	-	14,14,15	0.30	0	17,19,21	0.66	0
5	NAG	D	1606	1	14,14,15	0.30	0	17,19,21	0.75	1 (5%)
5	NAG	B	1603	1	14,14,15	0.37	0	17,19,21	0.98	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	D	1605	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1607	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1602	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1606	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	C	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1603	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1602	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	D	1606	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1603	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1602	NAG	C1-O5-C5	4.02	117.64	112.19
5	C	1606	NAG	C1-O5-C5	3.03	116.29	112.19
5	A	1602	NAG	C1-O5-C5	2.94	116.17	112.19
5	B	1603	NAG	C1-O5-C5	2.93	116.17	112.19
5	A	1603	NAG	C1-O5-C5	2.78	115.96	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

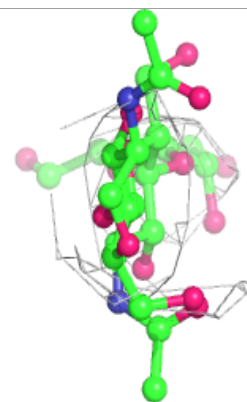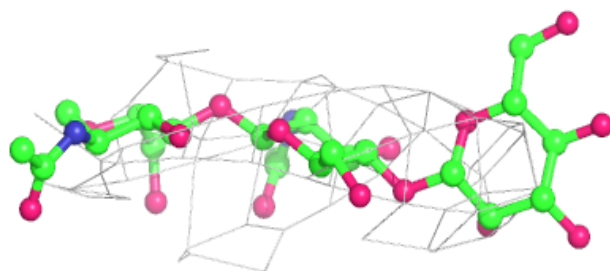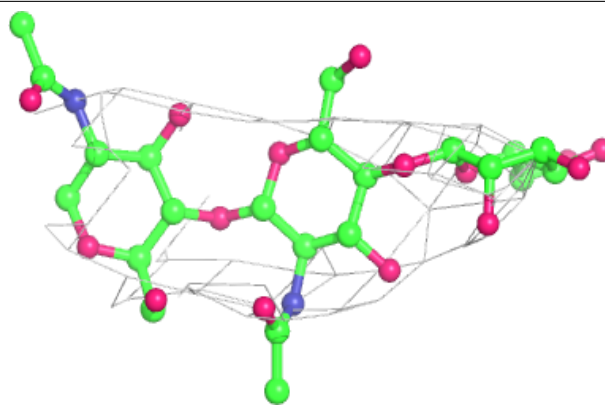Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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 E:

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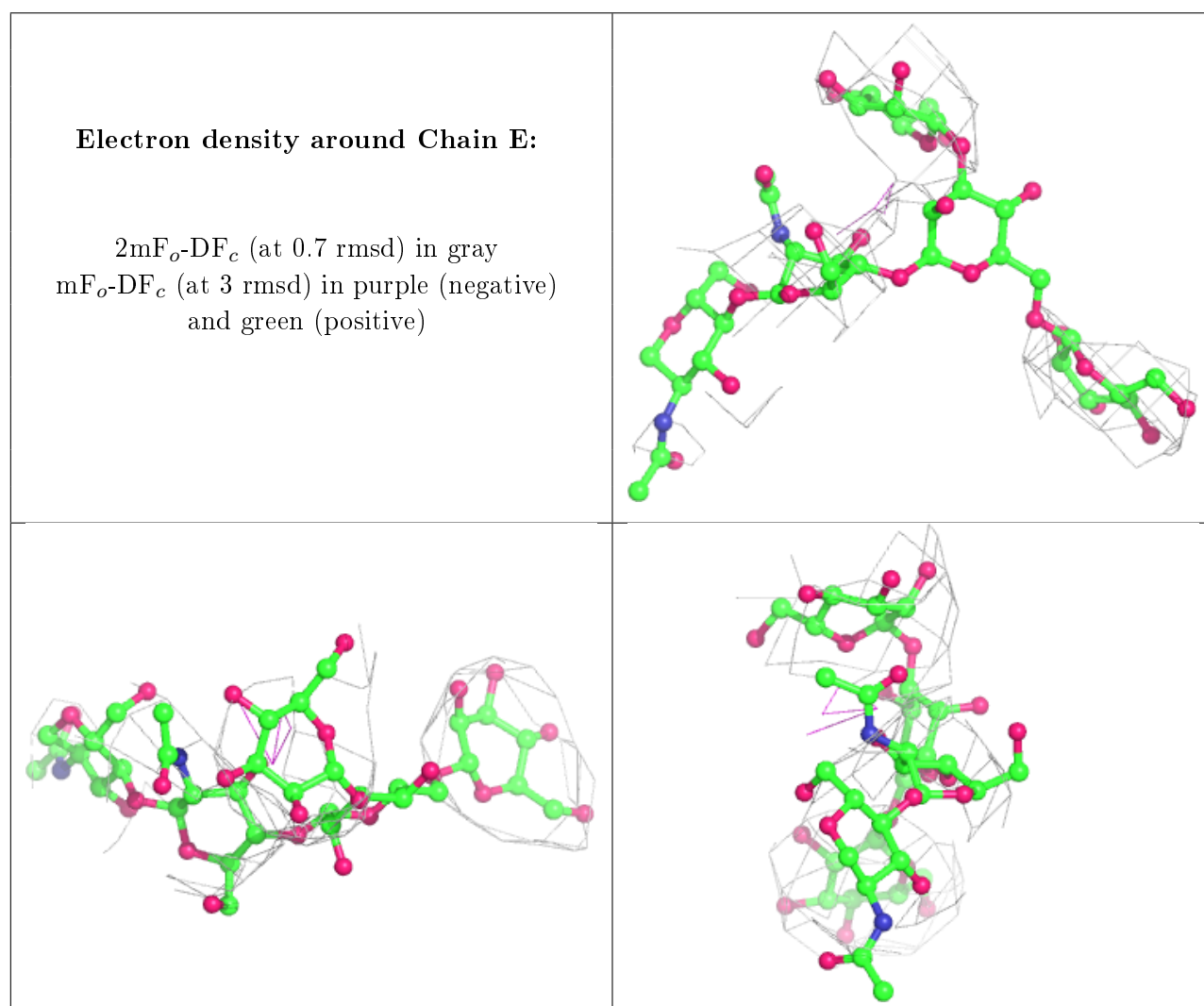
Electron density around Chain F:

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 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 G:

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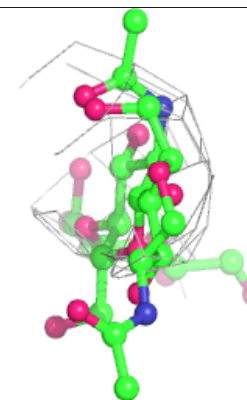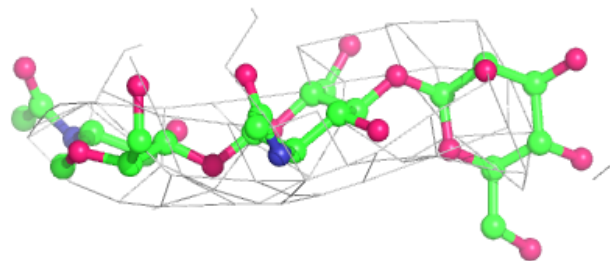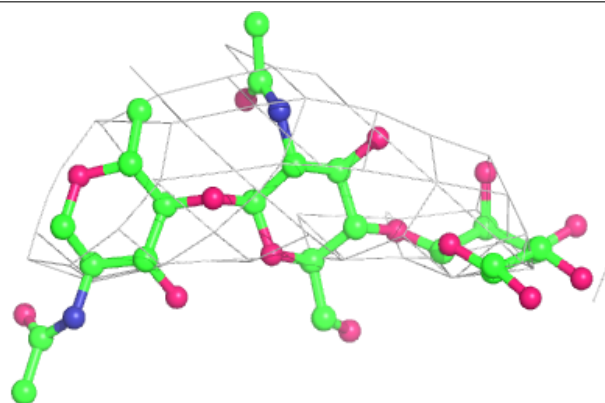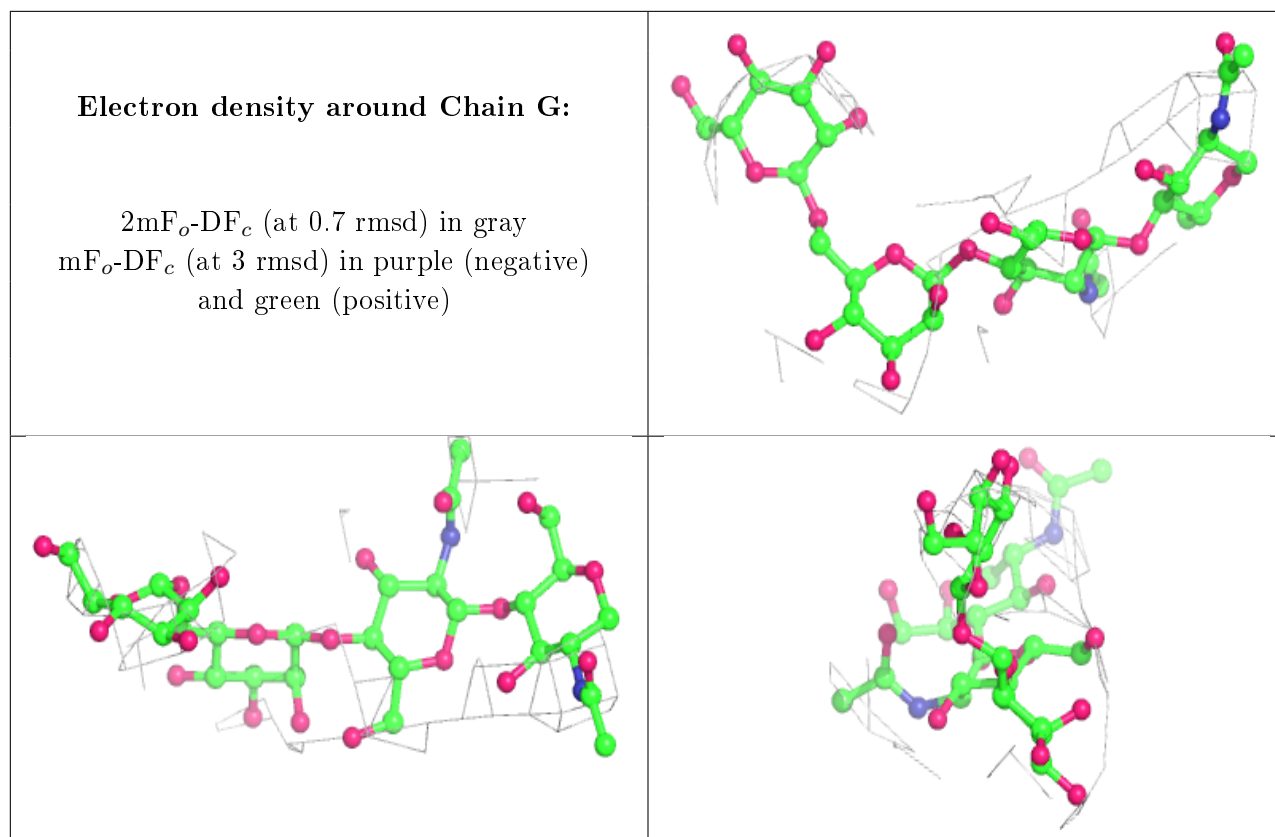
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.