



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2020 – 04:09 PM JST

PDB ID : 6IK6  
Title : Crystal structure of Tomato beta-galactosidase (TBG) 4 with beta-1,4-galactobiose  
Authors : Matsuyama, K.; Nakae, S.; Igarashi, K.; Tada, T.; Ishimaru, M.  
Deposited on : 2018-10-15  
Resolution : 2.79 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](mailto: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 ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.15.1  
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) : 2.15.1

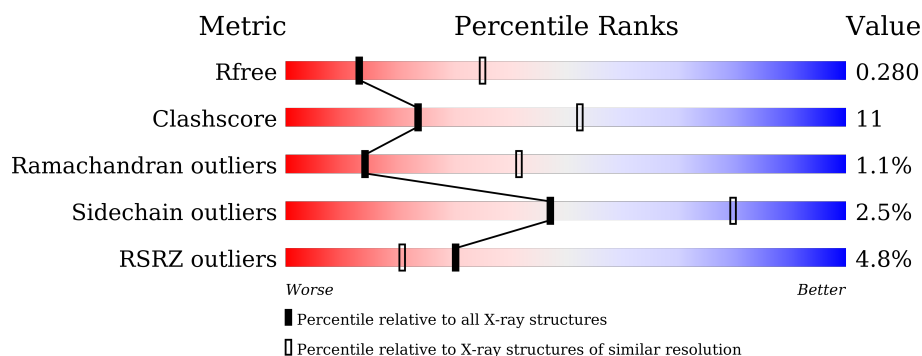
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	718	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>..</div> </div> </div>
1	B	718	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>27%</div> <div>..</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div>100%</div> </div>
3	E	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>
3	F	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>

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
3	GAL	F	1	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11285 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-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	0	0	0
			5527	3533	944	1023	27			
1	B	705	Total	C	N	O	S	0	0	0
			5527	3533	944	1023	27			

There are 36 discrepancies between the modelled and reference sequences:

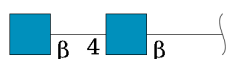
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	-	expression tag	UNP O81100
A	19	ALA	-	expression tag	UNP O81100
A	20	GLU	-	expression tag	UNP O81100
A	21	ALA	-	expression tag	UNP O81100
A	22	GLU	-	expression tag	UNP O81100
A	23	PHE	-	expression tag	UNP O81100
A	181	ALA	GLU	engineered mutation	UNP O81100
A	725	SER	-	expression tag	UNP O81100
A	726	ALA	-	expression tag	UNP O81100
A	727	ALA	-	expression tag	UNP O81100
A	728	ALA	-	expression tag	UNP O81100
A	729	ALA	-	expression tag	UNP O81100
A	730	SER	-	expression tag	UNP O81100
A	731	PHE	-	expression tag	UNP O81100
A	732	LEU	-	expression tag	UNP O81100
A	733	GLU	-	expression tag	UNP O81100
A	734	GLN	-	expression tag	UNP O81100
A	735	LYS	-	expression tag	UNP O81100
B	18	GLU	-	expression tag	UNP O81100
B	19	ALA	-	expression tag	UNP O81100
B	20	GLU	-	expression tag	UNP O81100
B	21	ALA	-	expression tag	UNP O81100
B	22	GLU	-	expression tag	UNP O81100
B	23	PHE	-	expression tag	UNP O81100
B	181	ALA	GLU	engineered mutation	UNP O81100

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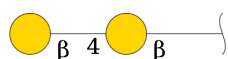
Chain	Residue	Modelled	Actual	Comment	Reference
B	725	SER	-	expression tag	UNP O81100
B	726	ALA	-	expression tag	UNP O81100
B	727	ALA	-	expression tag	UNP O81100
B	728	ALA	-	expression tag	UNP O81100
B	729	ALA	-	expression tag	UNP O81100
B	730	SER	-	expression tag	UNP O81100
B	731	PHE	-	expression tag	UNP O81100
B	732	LEU	-	expression tag	UNP O81100
B	733	GLU	-	expression tag	UNP O81100
B	734	GLN	-	expression tag	UNP O81100
B	735	LYS	-	expression tag	UNP O81100

- 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
			29	16	2	11			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-galactopyranose.

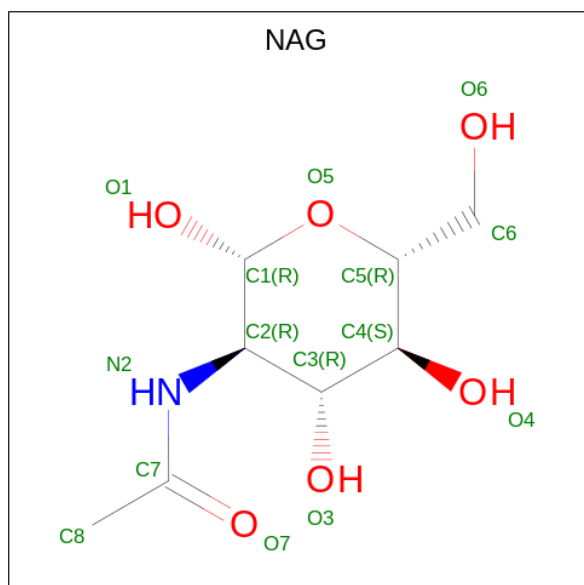


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	0	0	0
			23	12	11			
3	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

- 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 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0

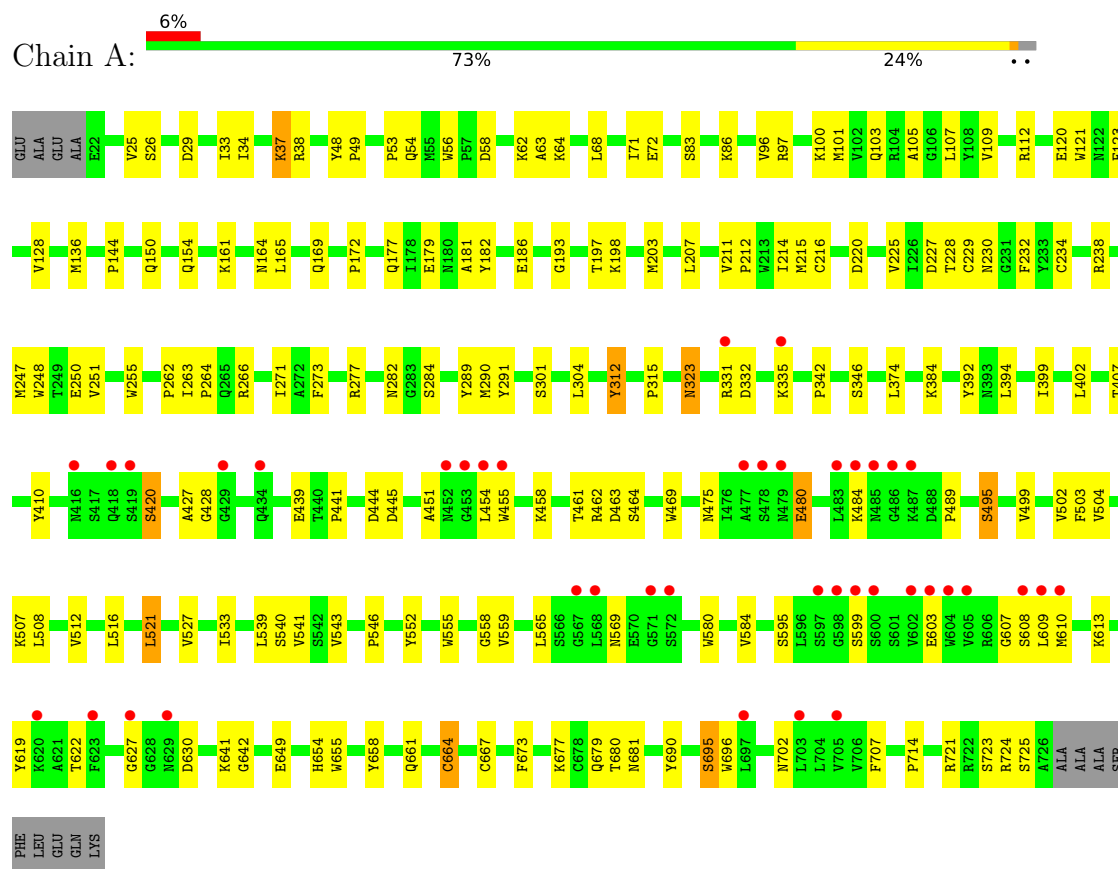
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	64	Total O 64 64	0	0
6	B	34	Total O 34 34	0	0

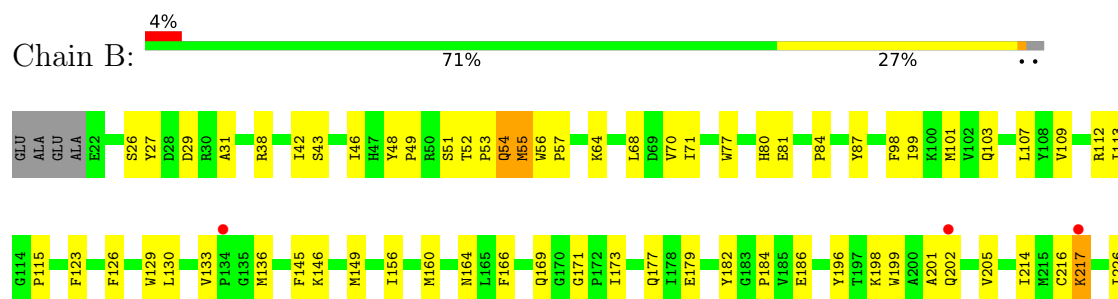
### 3 Residue-property plots

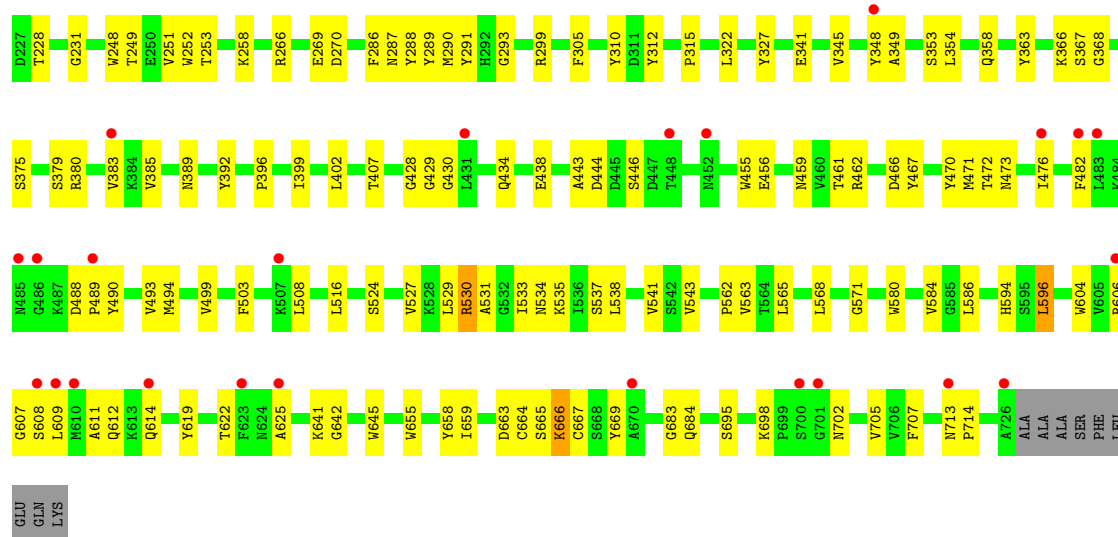
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-galactosidase



#### • Molecule 1: Beta-galactosidase





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

Chain C:  100%



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

Chain D:  100%



- Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain E:  50%



- Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain F:  50%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.03Å 110.73Å 162.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.57 – 2.79 48.57 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.57-2.79) 99.2 (48.57-2.79)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.196 , 0.280 0.196 , 0.280	Depositor DCC
$R_{free}$ test set	2149 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11285	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, NAG, CL

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	0.47	2/5690 (0.0%)	0.60	0/7734
1	B	0.47	0/5690	0.61	1/7734 (0.0%)
All	All	0.47	2/11380 (0.0%)	0.61	1/15468 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	664	CYS	CB-SG	-5.47	1.72	1.81
1	A	323	ASN	C-N	5.11	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	LYS	CD-CE-NZ	-5.09	99.98	111.70

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	5527	0	5352	116	0
1	B	5527	0	5347	129	0
2	C	29	0	27	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	25	0	0
3	E	23	0	21	2	0
3	F	23	0	19	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	14	0	13	0	0
5	B	14	0	13	6	0
6	A	64	0	0	1	0
6	B	34	0	0	2	0
All	All	11285	0	10817	246	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 11.

All (246) 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)
2:C:1:NAG:O3	2:C:2:NAG:N2	1.96	0.98
1:B:611:ALA:HB1	1:B:614:GLN:HG3	1.53	0.90
1:A:64:LYS:NZ	1:A:105:ALA:O	2.04	0.90
1:B:184:PRO:HD3	1:B:217:LYS:HE2	1.54	0.89
1:B:594:HIS:HA	1:B:705:VAL:HG21	1.60	0.83
1:A:54:GLN:HE21	1:A:695:SER:HB3	1.45	0.82
1:A:282:ASN:OD1	2:C:1:NAG:O1	1.98	0.82
1:B:664:CYS:SG	6:B:908:HOH:O	2.37	0.80
1:A:495:SER:HB2	1:A:559:VAL:HG12	1.64	0.78
1:B:459:ASN:HD22	5:B:801:NAG:H83	1.49	0.77
1:A:25:VAL:HG23	1:A:212:PRO:HD3	1.65	0.77
1:B:473:ASN:HB3	1:B:533:ILE:HD11	1.67	0.75
1:B:493:VAL:HG22	1:B:563:VAL:HG23	1.69	0.74
1:A:83:SER:HB2	1:A:86:LYS:HB3	1.73	0.71
1:B:112:ARG:HA	1:B:177:GLN:HB3	1.71	0.71
1:B:455:TRP:CD1	5:B:801:NAG:H82	2.25	0.70
1:B:456:GLU:H	5:B:801:NAG:H81	1.57	0.70
1:A:29:ASP:OD2	2:C:1:NAG:H81	1.92	0.69
1:B:666:LYS:NZ	6:B:901:HOH:O	2.27	0.67
1:A:161:LYS:NZ	1:A:207:LEU:O	2.29	0.66
1:B:149:MET:HE1	1:B:196:TYR:HE1	1.60	0.66
1:B:565:LEU:HG	1:B:568:LEU:HD11	1.77	0.66
1:A:228:THR:HG22	1:A:247:MET:HB2	1.78	0.65
1:B:470:TYR:HB2	1:B:538:LEU:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ILE:HD11	1:B:529:LEU:HD23	1.77	0.64
1:B:612:GLN:NE2	1:B:713:ASN:OD1	2.30	0.64
1:B:201:ALA:O	1:B:205:VAL:HG23	1.98	0.64
1:B:160:MET:HE2	1:B:173:ILE:HD11	1.80	0.63
1:B:467:TYR:CD2	1:B:586:LEU:HD11	2.33	0.62
1:A:619:TYR:CE1	1:A:714:PRO:HG3	2.34	0.62
1:B:248:TRP:CE2	1:B:251:VAL:HG22	2.34	0.62
1:B:299:ARG:NH1	1:B:466:ASP:OD1	2.34	0.61
1:A:504:VAL:O	1:A:507:LYS:HB3	2.01	0.60
1:A:58:ASP:OD2	1:A:62:LYS:HE3	2.02	0.60
1:A:120:GLU:OE1	3:E:2:GAL:H61	2.02	0.59
1:A:248:TRP:CD2	1:A:251:VAL:HG22	2.37	0.59
1:A:48:TYR:CD2	1:A:49:PRO:HD3	2.38	0.58
1:B:366:LYS:HD2	1:B:366:LYS:O	2.03	0.58
1:B:379:SER:OG	1:B:380:ARG:NH1	2.36	0.58
1:A:282:ASN:CG	2:C:1:NAG:O1	2.41	0.58
1:B:54:GLN:HG3	1:B:695:SER:HB2	1.85	0.58
1:B:29:ASP:OD2	1:B:348:TYR:HE2	1.87	0.57
1:A:54:GLN:NE2	1:A:695:SER:HB3	2.19	0.57
1:B:84:PRO:HG3	1:B:129:TRP:CD2	2.39	0.57
1:A:664:CYS:HB2	1:A:679:GLN:O	2.04	0.57
1:B:434:GLN:HB3	1:B:604:TRP:HB3	1.85	0.57
1:B:149:MET:HE1	1:B:196:TYR:CE1	2.40	0.57
1:B:248:TRP:CD2	1:B:251:VAL:HG22	2.41	0.56
1:A:215:MET:HG3	1:A:225:VAL:HG11	1.88	0.55
1:B:146:LYS:HD2	1:B:199:TRP:CE2	2.40	0.55
1:A:26:SER:O	1:A:33:ILE:N	2.32	0.55
1:B:530:ARG:CG	1:B:531:ALA:H	2.20	0.55
1:B:52:THR:O	1:B:55:MET:HB3	2.07	0.55
1:A:128:VAL:HG21	1:A:463:ASP:HB2	1.89	0.55
1:B:54:GLN:HG3	1:B:695:SER:CB	2.37	0.55
1:A:627:GLY:O	1:A:721:ARG:NH1	2.40	0.54
1:B:202:GLN:O	1:B:202:GLN:HG2	2.07	0.54
1:A:248:TRP:CE2	1:A:251:VAL:HG22	2.42	0.54
1:A:502:VAL:O	1:A:508:LEU:HD12	2.08	0.54
1:B:625:ALA:HB2	1:B:698:LYS:O	2.06	0.54
1:B:641:LYS:HB2	1:B:655:TRP:CD1	2.43	0.53
1:A:499:VAL:HB	1:A:541:VAL:HB	1.90	0.53
1:A:53:PRO:HA	1:A:56:TRP:CD2	2.43	0.53
1:B:530:ARG:CD	1:B:531:ALA:H	2.22	0.53
1:B:103:GLN:NE2	1:B:171:GLY:HA2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:MET:HE2	1:B:562:PRO:HD2	1.90	0.53
1:B:145:PHE:CE2	1:B:149:MET:HE2	2.44	0.52
1:B:645:TRP:HB2	1:B:705:VAL:HG23	1.89	0.52
1:A:63:ALA:HB1	1:A:68:LEU:HD22	1.91	0.52
1:B:596:LEU:HD12	1:B:596:LEU:H	1.75	0.52
1:A:229:CYS:SG	1:A:234:CYS:CB	2.97	0.52
1:A:342:PRO:O	1:A:346:SER:OG	2.27	0.52
1:B:81:GLU:HG3	1:B:87:TYR:CE1	2.44	0.52
1:A:619:TYR:CD1	1:A:714:PRO:HG3	2.44	0.52
1:A:182:TYR:CE2	1:A:186:GLU:HB2	2.45	0.52
1:A:469:TRP:CE2	1:A:539:LEU:HD13	2.44	0.52
1:A:262:PRO:HD3	1:A:661:GLN:O	2.10	0.52
1:B:455:TRP:CZ2	5:B:801:NAG:H4	2.45	0.52
1:B:77:TRP:O	1:B:80:HIS:N	2.43	0.52
1:B:253:THR:HG21	1:B:288:TYR:HB3	1.91	0.51
1:B:530:ARG:HD3	1:B:531:ALA:H	1.76	0.51
1:B:53:PRO:HA	1:B:56:TRP:CD2	2.45	0.51
1:B:216:CYS:O	1:B:217:LYS:HB3	2.11	0.51
1:A:112:ARG:HA	1:A:177:GLN:HB3	1.93	0.50
1:A:607:GLY:O	1:A:610:MET:HG2	2.10	0.50
1:B:252:TRP:HA	1:B:289:TYR:O	2.10	0.50
1:B:607:GLY:O	1:B:609:LEU:N	2.45	0.50
1:A:165:LEU:O	1:A:172:PRO:HD2	2.12	0.50
1:B:305:PHE:HB2	1:B:516:LEU:HD12	1.93	0.50
1:A:277:ARG:HG2	1:A:399:ILE:HD11	1.94	0.50
1:B:113:ILE:O	1:B:115:PRO:HA	2.12	0.50
1:B:619:TYR:CE1	1:B:714:PRO:HG3	2.47	0.50
1:A:150:GLN:O	1:A:154:GLN:HG2	2.12	0.49
1:A:229:CYS:SG	1:A:234:CYS:HB3	2.51	0.49
1:A:193:GLY:O	1:A:197:THR:HG23	2.11	0.49
1:A:230:ASN:HB3	1:A:250:GLU:HB2	1.94	0.49
1:A:480:GLU:HA	1:A:569:ASN:ND2	2.27	0.49
1:B:184:PRO:HG3	3:F:1:GAL:O1	2.11	0.49
1:B:42:ILE:HG12	1:B:286:PHE:CZ	2.47	0.49
1:B:269:GLU:HB2	1:B:669:TYR:HB2	1.94	0.49
1:A:402:LEU:HA	1:A:407:THR:O	2.12	0.48
1:B:366:LYS:C	1:B:368:GLY:H	2.16	0.48
1:A:495:SER:HB3	1:A:521:LEU:HD11	1.95	0.48
1:B:459:ASN:ND2	5:B:801:NAG:H83	2.25	0.48
1:A:461:THR:O	1:A:464:SER:HB3	2.14	0.48
1:B:459:ASN:O	1:B:462:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:HIS:HA	1:A:690:TYR:CE2	2.47	0.48
1:B:482:PHE:CD1	1:B:489:PRO:HD3	2.49	0.48
1:B:146:LYS:HD2	1:B:199:TRP:CD2	2.49	0.48
1:B:146:LYS:HB3	1:B:199:TRP:CZ2	2.49	0.48
1:B:612:GLN:O	1:B:614:GLN:HG2	2.14	0.48
1:B:166:PHE:HA	1:B:173:ILE:HB	1.96	0.47
1:B:27:TYR:CD2	1:B:226:ILE:HD11	2.49	0.47
1:A:475:ASN:HA	1:A:533:ILE:HD12	1.97	0.47
1:A:642:GLY:HA3	1:A:707:PHE:O	2.14	0.47
1:A:182:TYR:CD2	1:A:197:THR:HG22	2.50	0.47
1:A:25:VAL:HA	1:A:33:ILE:O	2.14	0.47
1:A:266:ARG:HD3	1:A:271:ILE:HG12	1.96	0.47
1:B:266:ARG:NH2	1:B:270:ASP:OD2	2.45	0.47
1:B:641:LYS:HD2	1:B:655:TRP:CD2	2.50	0.47
1:A:312:TYR:OH	3:E:2:GAL:H62	2.16	0.46
1:B:354:LEU:HD13	1:B:385:VAL:HG11	1.98	0.46
1:B:48:TYR:HB3	1:B:98:PHE:CG	2.49	0.46
1:A:304:LEU:O	1:A:516:LEU:HD13	2.15	0.46
1:A:72:GLU:CG	1:A:112:ARG:HD2	2.46	0.46
1:A:97:ARG:HH21	1:A:100:LYS:NZ	2.13	0.46
1:B:443:ALA:O	1:B:535:LYS:NZ	2.39	0.46
1:B:123:PHE:CD2	1:B:126:PHE:HB2	2.50	0.46
1:B:182:TYR:CE2	1:B:186:GLU:HB2	2.51	0.46
1:A:121:TRP:HA	1:A:301:SER:O	2.15	0.46
1:A:641:LYS:HG3	1:A:655:TRP:CG	2.51	0.46
1:B:289:TYR:HA	1:B:290:MET:HA	1.77	0.45
1:B:366:LYS:O	1:B:368:GLY:N	2.49	0.45
1:B:594:HIS:HB2	1:B:645:TRP:CG	2.51	0.45
1:A:97:ARG:O	1:A:101:MET:HG3	2.15	0.45
1:B:358:GLN:NE2	1:B:383:VAL:HG21	2.31	0.45
1:A:229:CYS:HG	1:A:234:CYS:CB	2.28	0.45
1:B:291:TYR:HA	1:B:315:PRO:HD2	1.98	0.45
1:A:29:ASP:HB2	2:C:1:NAG:C8	2.46	0.45
1:A:458:LYS:NZ	1:A:555:TRP:O	2.34	0.45
1:B:156:ILE:O	1:B:160:MET:HG2	2.16	0.45
1:A:462:ARG:HD3	1:A:462:ARG:HA	1.78	0.45
1:A:96:VAL:O	1:A:100:LYS:HG3	2.17	0.45
1:B:392:TYR:CE1	1:B:402:LEU:HD21	2.52	0.45
1:B:471:MET:HG2	1:B:537:SER:OG	2.17	0.45
1:A:37:LYS:HD3	1:A:38:ARG:H	1.82	0.44
1:A:64:LYS:HB2	1:A:107:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ASN:HB3	1:B:169:GLN:HB2	1.98	0.44
1:B:472:THR:HB	1:B:580:TRP:CE3	2.52	0.44
1:B:216:CYS:HA	1:B:228:THR:OG1	2.17	0.44
1:A:177:GLN:NE2	1:A:179:GLU:O	2.51	0.44
1:B:214:ILE:HD12	1:B:249:THR:HG21	1.99	0.44
1:B:473:ASN:CB	1:B:533:ILE:HD11	2.42	0.44
1:A:289:TYR:HA	1:A:290:MET:HA	1.78	0.44
1:A:461:THR:HG22	1:A:584:VAL:HG22	1.99	0.44
1:A:332:ASP:HB2	1:A:410:TYR:HE1	1.83	0.44
1:B:217:LYS:O	1:B:217:LYS:HG3	2.17	0.44
1:A:177:GLN:HG3	1:A:214:ILE:HG13	2.00	0.44
1:B:503:PHE:CE1	1:B:508:LEU:HB2	2.53	0.44
1:A:607:GLY:O	1:A:609:LEU:N	2.50	0.44
1:B:499:VAL:HB	1:B:541:VAL:HB	1.99	0.44
1:A:48:TYR:CG	1:A:49:PRO:HD3	2.52	0.43
1:A:489:PRO:HB2	1:A:565:LEU:HD11	2.00	0.43
1:B:349:ALA:HB2	1:B:363:TYR:CZ	2.53	0.43
1:B:455:TRP:CG	5:B:801:NAG:H82	2.53	0.43
1:A:123:PHE:HA	1:A:546:PRO:O	2.19	0.43
1:A:503:PHE:HA	1:A:507:LYS:O	2.19	0.43
1:A:495:SER:CB	1:A:559:VAL:HG12	2.43	0.43
1:B:133:VAL:HG22	1:B:136:MET:HB2	2.00	0.43
1:A:25:VAL:HG12	1:A:34:ILE:HG23	2.01	0.43
1:B:179:GLU:HG3	1:B:182:TYR:HB2	2.00	0.43
1:B:43:SER:O	1:B:287:ASN:HA	2.19	0.43
1:B:402:LEU:HA	1:B:407:THR:O	2.18	0.43
1:A:255:TRP:O	1:A:312:TYR:HA	2.19	0.43
1:B:490:TYR:O	1:B:565:LEU:HD12	2.19	0.43
1:A:58:ASP:O	1:A:62:LYS:HG3	2.19	0.43
1:B:383:VAL:HG12	1:B:385:VAL:HG23	2.01	0.43
1:A:103:GLN:HB2	1:A:172:PRO:HG3	2.01	0.43
1:A:622:THR:HA	1:A:702:ASN:O	2.18	0.43
1:B:438:GLU:OE2	1:B:586:LEU:HB3	2.19	0.43
1:B:476:ILE:HD12	1:B:534:ASN:ND2	2.33	0.43
1:A:331:ARG:HE	1:A:335:LYS:HZ1	1.67	0.42
1:B:29:ASP:OD2	1:B:348:TYR:CE2	2.71	0.42
1:B:43:SER:HB2	1:B:70:VAL:HB	2.01	0.42
1:B:444:ASP:OD2	1:B:446:SER:N	2.52	0.42
1:A:444:ASP:OD1	1:A:445:ASP:N	2.52	0.42
1:B:31:ALA:HB3	1:B:38:ARG:HB3	2.00	0.42
1:B:375:SER:HB3	1:B:399:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:TRP:HB3	1:A:264:PRO:HG2	2.01	0.42
1:A:489:PRO:HD2	1:A:527:VAL:O	2.19	0.42
1:A:273:PHE:CZ	1:A:277:ARG:HD2	2.54	0.42
1:A:484:LYS:HD3	1:A:484:LYS:HA	1.89	0.42
1:B:622:THR:HA	1:B:702:ASN:O	2.18	0.42
1:A:136:MET:HE2	1:A:144:PRO:HB2	2.02	0.42
1:A:392:TYR:CE2	1:A:402:LEU:HD21	2.55	0.42
1:A:420:SER:HA	1:A:725:SER:O	2.20	0.42
1:A:512:VAL:HG12	1:A:521:LEU:HB2	2.01	0.42
1:B:130:LEU:O	1:B:136:MET:HG2	2.19	0.42
1:B:396:PRO:O	1:B:669:TYR:OH	2.18	0.42
1:B:42:ILE:HG22	1:B:68:LEU:HD12	2.00	0.42
1:B:322:LEU:HD13	1:B:327:TYR:CD2	2.55	0.42
1:B:488:ASP:HB3	1:B:527:VAL:O	2.20	0.42
1:B:530:ARG:HD3	1:B:531:ALA:N	2.34	0.42
1:A:150:GLN:HG3	1:A:203:MET:SD	2.60	0.41
1:B:461:THR:HG22	1:B:584:VAL:HG13	2.02	0.41
1:B:46:ILE:HD12	1:B:71:ILE:HD12	2.02	0.41
1:A:164:ASN:HA	1:A:169:GLN:OE1	2.19	0.41
1:A:71:ILE:O	1:A:109:VAL:HA	2.20	0.41
1:B:99:ILE:HD13	1:B:160:MET:HE2	2.02	0.41
1:B:529:LEU:O	1:B:530:ARG:HB2	2.19	0.41
1:A:420:SER:OG	1:A:420:SER:O	2.37	0.41
1:A:451:ALA:HB2	1:A:455:TRP:CZ2	2.54	0.41
1:A:495:SER:HB3	1:A:521:LEU:CD1	2.50	0.41
1:A:552:TYR:HA	1:A:555:TRP:CE2	2.55	0.41
1:B:341:GLU:O	1:B:345:VAL:HG22	2.19	0.41
1:B:366:LYS:C	1:B:368:GLY:N	2.73	0.41
1:A:263:ILE:O	1:A:680:THR:HG22	2.21	0.41
1:B:64:LYS:HG3	1:B:107:LEU:HD11	2.02	0.41
1:B:231:GLY:HA2	1:B:252:TRP:CH2	2.55	0.41
1:B:258:LYS:HB2	1:B:258:LYS:HE2	1.67	0.41
1:B:684:GLN:OE1	1:B:684:GLN:HA	2.20	0.41
1:A:198:LYS:HD2	6:A:960:HOH:O	2.19	0.41
1:A:215:MET:O	1:A:227:ASP:HA	2.21	0.41
1:A:97:ARG:HE	1:A:100:LYS:NZ	2.19	0.41
1:B:231:GLY:HA2	1:B:252:TRP:CZ3	2.55	0.41
1:B:48:TYR:CG	1:B:49:PRO:HD3	2.55	0.41
1:A:238:ARG:HG3	1:A:238:ARG:HH11	1.84	0.41
1:A:595:SER:O	1:A:599:SER:HB2	2.21	0.41
1:A:667:CYS:SG	1:A:677:LYS:HG2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLY:HA3	1:B:310:TYR:O	2.20	0.41
1:A:331:ARG:HE	1:A:335:LYS:NZ	2.19	0.41
1:A:374:LEU:HB3	1:A:394:LEU:HD11	2.02	0.41
1:A:181:ALA:HA	1:A:216:CYS:O	2.21	0.41
1:A:454:LEU:HD21	1:A:580:TRP:CE2	2.56	0.41
1:B:71:ILE:O	1:B:109:VAL:HA	2.21	0.40
1:A:323:ASN:HA	1:A:724:ARG:CZ	2.51	0.40
1:B:57:PRO:HG3	1:B:101:MET:SD	2.60	0.40
1:B:543:VAL:O	1:B:543:VAL:HG13	2.22	0.40
1:B:642:GLY:HA3	1:B:707:PHE:O	2.21	0.40
1:B:659:ILE:HD12	1:B:683:GLY:O	2.21	0.40
1:A:25:VAL:HG22	1:A:211:VAL:HG12	2.03	0.40
1:A:540:SER:OG	1:A:558:GLY:HA2	2.21	0.40
1:A:232:PHE:CE1	1:A:673:PHE:HE2	2.40	0.40
1:A:291:TYR:HA	1:A:315:PRO:HD2	2.04	0.40
1:A:441:PRO:HD2	1:A:469:TRP:CZ2	2.57	0.40
1:A:649:GLU:HG3	1:A:696:TRP:CH2	2.56	0.40

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	703/718 (98%)	653 (93%)	42 (6%)	8 (1%)	14	41
1	B	703/718 (98%)	650 (92%)	46 (6%)	7 (1%)	15	44
All	All	1406/1436 (98%)	1303 (93%)	88 (6%)	15 (1%)	14	41

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	681	ASN

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Mol	Chain	Res	Type
1	A	608	SER
1	B	55	MET
1	B	571	GLY
1	B	608	SER
1	A	220	ASP
1	B	367	SER
1	A	427	ALA
1	A	439	GLU
1	A	613	LYS
1	B	428	GLY
1	A	695	SER
1	B	430	GLY
1	B	429	GLY
1	A	428	GLY

### 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	590/598 (99%)	577 (98%)	13 (2%)	52	83
1	B	590/598 (99%)	574 (97%)	16 (3%)	44	78
All	All	1180/1196 (99%)	1151 (98%)	29 (2%)	47	80

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	284	SER
1	A	312	TYR
1	A	384	LYS
1	A	420	SER
1	A	480	GLU
1	A	495	SER
1	A	521	LEU
1	A	543	VAL

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Mol	Chain	Res	Type
1	A	603	GLU
1	A	630	ASP
1	A	658	TYR
1	A	723	SER
1	B	26	SER
1	B	51	SER
1	B	54	GLN
1	B	198	LYS
1	B	312	TYR
1	B	353	SER
1	B	389	ASN
1	B	524	SER
1	B	530	ARG
1	B	596	LEU
1	B	606	ARG
1	B	658	TYR
1	B	663	ASP
1	B	665	SER
1	B	666	LYS
1	B	667	CYS

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	54	GLN
1	B	103	GLN
1	B	180	ASN
1	B	437	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 ⓘ

8 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	15,15,15	0.99	2 (13%)	21,21,21	2.20	7 (33%)
2	NAG	C	2	2	14,14,15	0.59	0	17,19,21	1.49	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.69	1 (7%)	17,19,21	0.90	1 (5%)
2	NAG	D	2	2	14,14,15	0.54	0	17,19,21	0.84	1 (5%)
3	GAL	E	1	3	12,12,12	1.41	1 (8%)	17,17,17	1.73	4 (23%)
3	GAL	E	2	3	11,11,12	1.94	3 (27%)	15,15,17	2.45	5 (33%)
3	GAL	F	1	1,3	12,12,12	2.77	7 (58%)	17,17,17	3.35	5 (29%)
3	GAL	F	2	3	11,11,12	2.89	4 (36%)	15,15,17	4.40	8 (53%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	GAL	O5-C1	6.84	1.54	1.43
3	F	2	GAL	O5-C5	5.54	1.54	1.43
3	E	2	GAL	O5-C1	4.99	1.51	1.43
3	F	1	GAL	O5-C1	4.79	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	GAL	O3-C3	3.94	1.52	1.43
3	F	1	GAL	O4-C4	3.81	1.51	1.43
3	E	1	GAL	O5-C1	3.41	1.51	1.42
3	F	1	GAL	O2-C2	3.10	1.50	1.43
3	F	1	GAL	C4-C3	3.07	1.60	1.52
3	F	1	GAL	O5-C5	2.84	1.51	1.44
3	F	1	GAL	C3-C2	2.83	1.59	1.52
2	C	1	NAG	O5-C1	-2.65	1.36	1.42
3	E	2	GAL	C2-C3	-2.61	1.48	1.52
3	F	2	GAL	C1-C2	2.55	1.58	1.52
3	F	2	GAL	O3-C3	2.24	1.48	1.43
3	E	2	GAL	O5-C5	2.10	1.47	1.43
2	C	1	NAG	C1-C2	-2.05	1.50	1.52
2	D	1	NAG	C1-C2	2.04	1.55	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	GAL	C1-C2-C3	11.92	124.32	109.67
3	F	1	GAL	C4-C3-C2	10.46	129.08	110.82
3	F	2	GAL	O5-C1-C2	-6.21	101.19	110.77
3	F	2	GAL	O2-C2-C3	-5.79	98.53	110.14
3	E	2	GAL	C1-C2-C3	5.37	116.27	109.67
3	F	1	GAL	O2-C2-C3	5.30	122.60	110.35
3	F	2	GAL	O5-C5-C6	5.26	115.45	107.20
2	C	2	NAG	C1-O5-C5	5.13	119.14	112.19
3	E	2	GAL	O5-C1-C2	4.71	118.05	110.77
2	C	1	NAG	O1-C1-C2	-4.67	99.52	109.22
3	F	1	GAL	O1-C1-O5	-4.50	96.86	110.38
2	C	1	NAG	O4-C4-C5	4.39	120.19	109.30
3	F	2	GAL	C2-C3-C4	3.81	117.49	110.89
2	C	1	NAG	C3-C4-C5	-3.69	103.66	110.24
3	E	2	GAL	C6-C5-C4	-3.63	104.51	113.00
3	E	1	GAL	C1-C2-C3	-3.43	103.20	110.31
2	C	1	NAG	C6-C5-C4	3.35	120.86	113.00
2	C	1	NAG	C1-C2-N2	-3.26	106.95	110.73
3	F	2	GAL	C6-C5-C4	-3.24	105.42	113.00
2	C	1	NAG	O3-C3-C2	-3.20	103.19	109.66
3	E	2	GAL	C1-O5-C5	3.00	116.25	112.19
3	E	2	GAL	O5-C5-C6	2.89	111.73	107.20
3	F	2	GAL	C1-O5-C5	2.86	116.06	112.19
3	F	1	GAL	C3-C4-C5	-2.84	105.17	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	2.83	116.02	112.19
3	F	1	GAL	O5-C5-C4	2.76	114.71	109.69
3	E	1	GAL	C3-C4-C5	2.46	114.63	110.24
3	E	1	GAL	C1-O5-C5	2.39	118.17	113.66
3	E	1	GAL	O2-C2-C3	2.25	115.56	110.35
3	F	2	GAL	O2-C2-C1	2.08	113.41	109.15
2	D	1	NAG	C1-O5-C5	2.02	114.93	112.19
2	C	1	NAG	O5-C5-C4	-2.02	106.03	109.69

There are no chirality outliers.

All (14) torsion outliers are listed below:

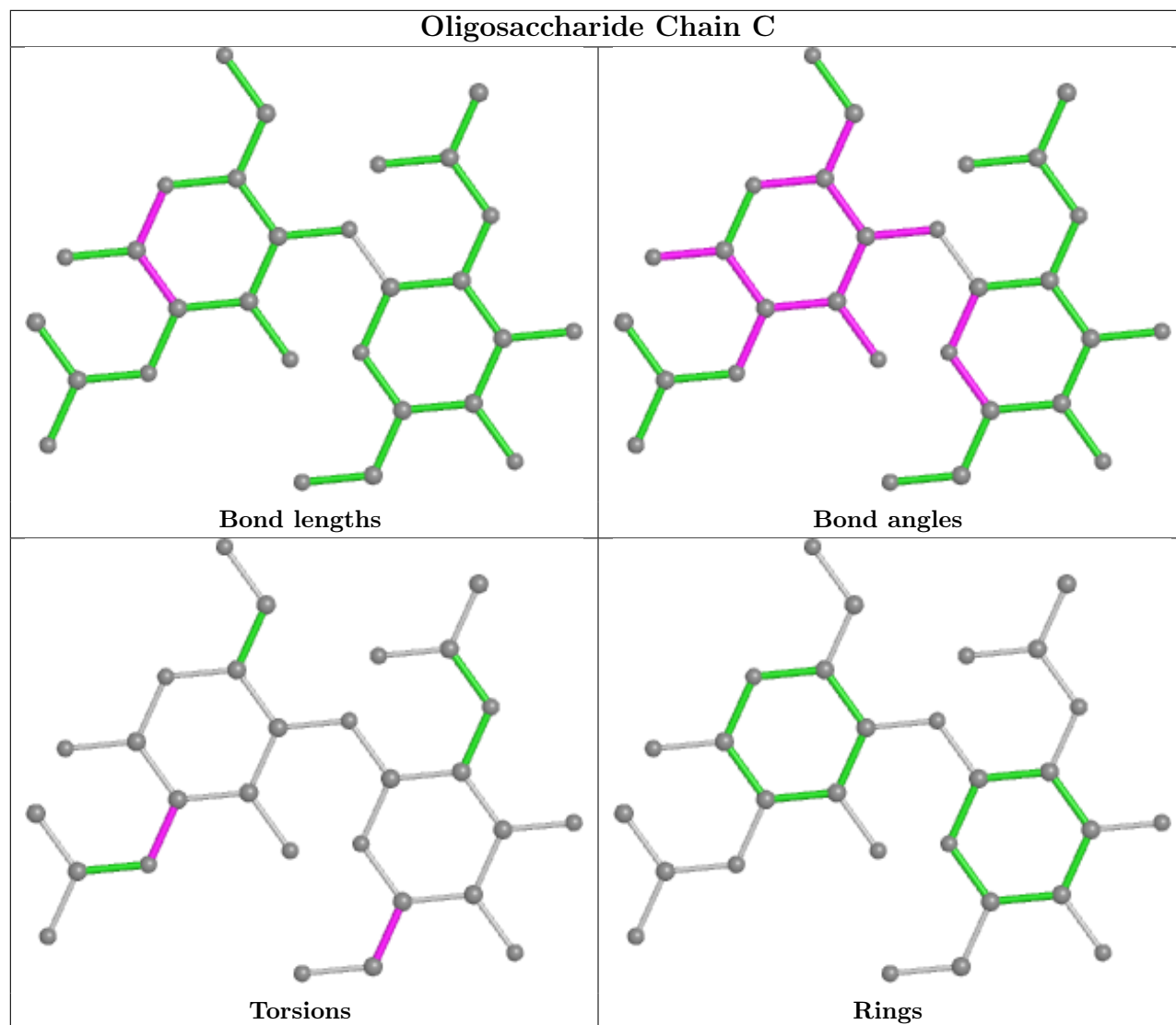
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	E	1	GAL	O5-C5-C6-O6
3	E	2	GAL	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	E	1	GAL	C4-C5-C6-O6
3	E	2	GAL	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	F	1	GAL	O5-C5-C6-O6
3	F	2	GAL	O5-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7
3	F	2	GAL	C4-C5-C6-O6

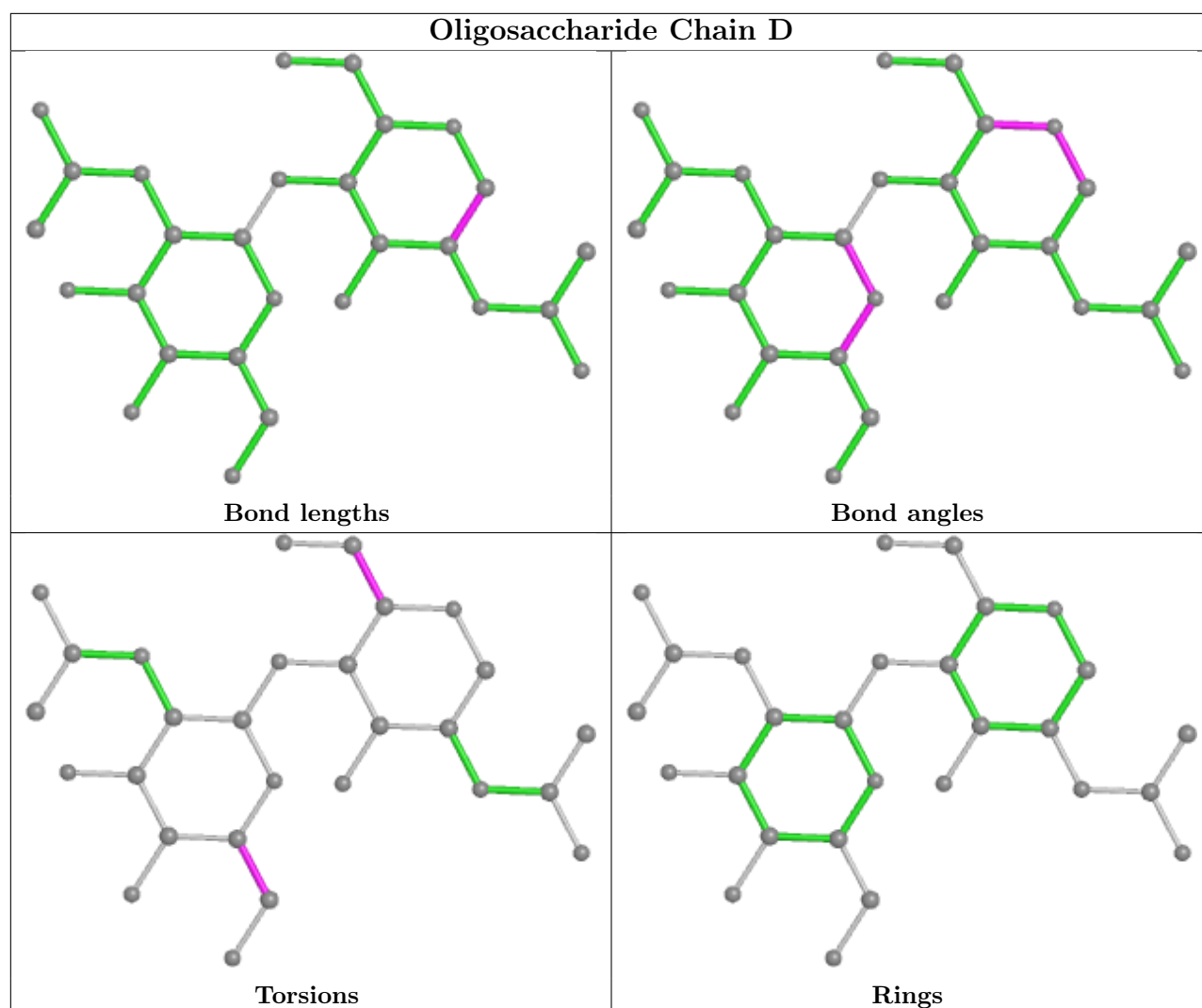
There are no ring outliers.

4 monomers are involved in 8 short contacts:

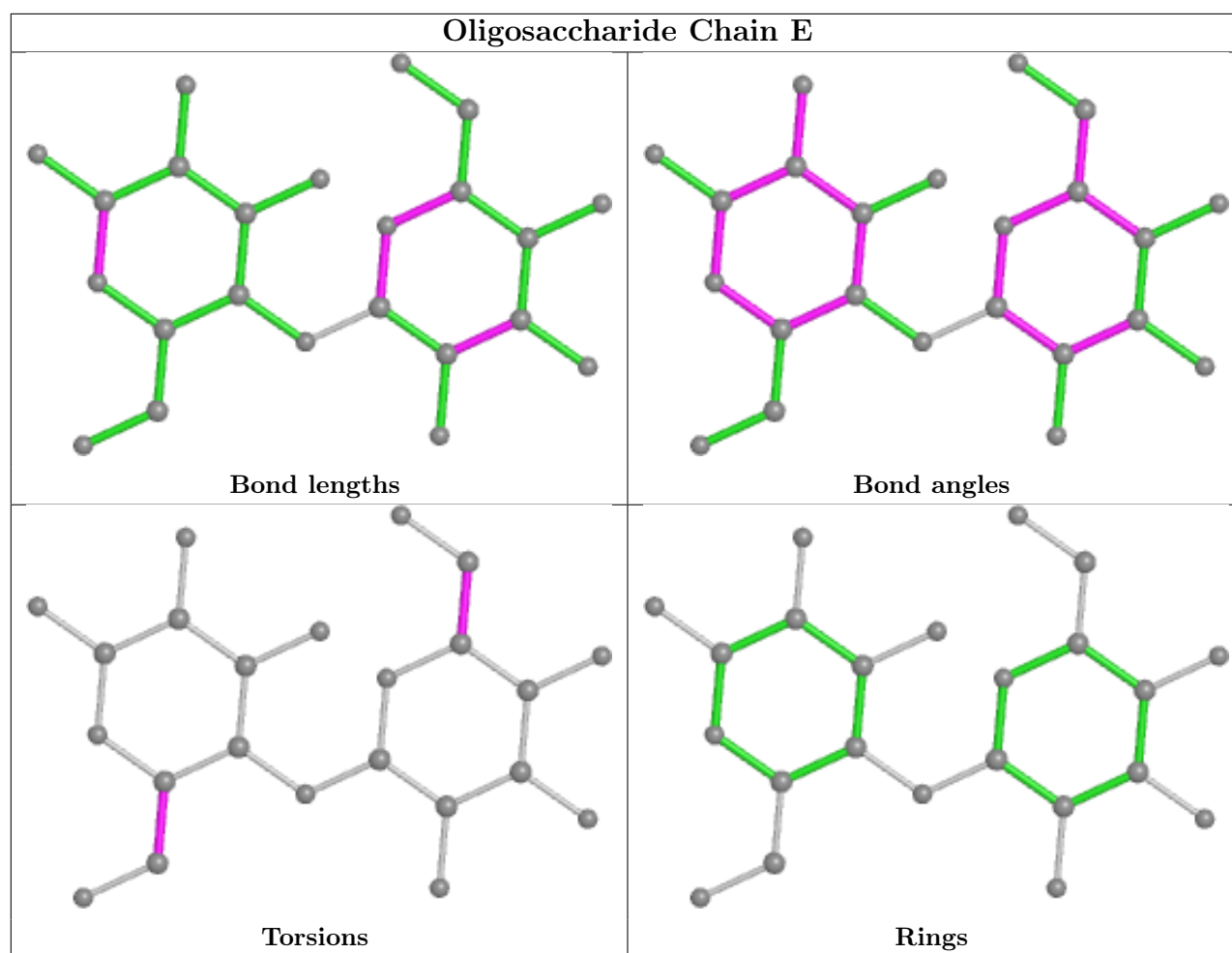
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	5	0
2	C	2	NAG	1	0
3	F	1	GAL	1	0
3	E	2	GAL	2	0

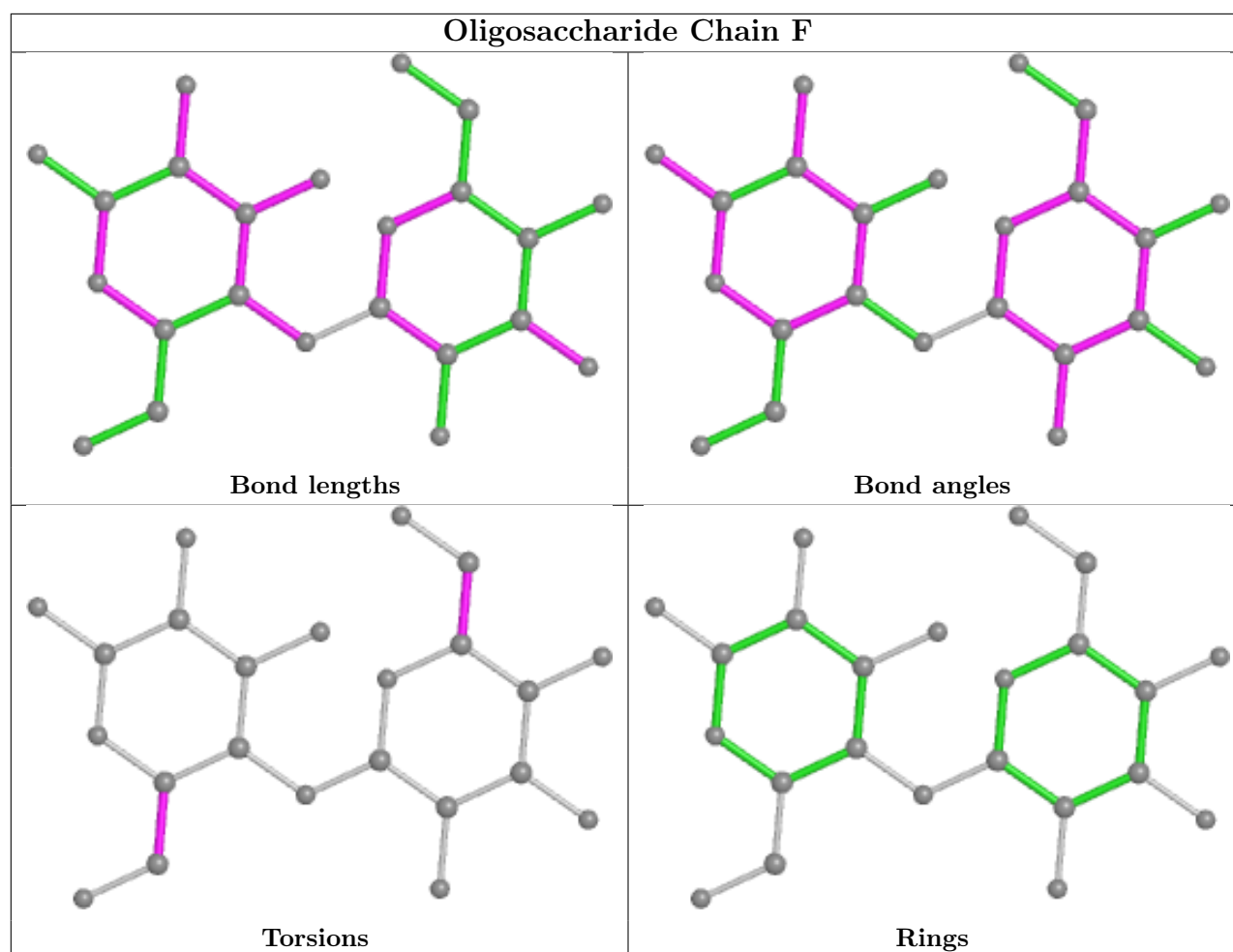
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	B	801	1	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	A	805	1	14,14,15	2.40	1 (7%)	17,19,21	2.51	1 (5%)

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	801	1	-	4/6/23/26	0/1/1/1
5	NAG	A	805	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	805	NAG	O5-C1	8.76	1.57	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	805	NAG	C1-O5-C5	9.73	125.38	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	801	NAG	C8-C7-N2-C2
5	B	801	NAG	O7-C7-N2-C2
5	B	801	NAG	O5-C5-C6-O6
5	B	801	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	801	NAG	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	705/718 (98%)	0.30	41 (5%)	23 15	37, 52, 88, 117	0
1	B	705/718 (98%)	0.16	27 (3%)	40 30	32, 51, 80, 104	0
All	All	1410/1436 (98%)	0.23	68 (4%)	30 21	32, 52, 84, 117	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	600	SER	7.2
1	A	486	GLY	7.0
1	A	599	SER	5.2
1	A	571	GLY	5.0
1	A	623	PHE	4.6
1	B	483	LEU	4.4
1	A	484	LYS	4.3
1	A	604	TRP	4.3
1	B	507	LYS	4.1
1	A	597	SER	4.0
1	A	610	MET	3.8
1	A	572	SER	3.7
1	B	609	LEU	3.6
1	B	614	GLN	3.6
1	B	610	MET	3.6
1	B	485	ASN	3.6
1	A	418	GLN	3.4
1	A	602	VAL	3.3
1	A	483	LEU	3.0
1	B	348	TYR	3.0
1	B	623	PHE	3.0
1	B	448	THR	3.0
1	A	478	SER	3.0
1	B	625	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	609	LEU	2.9
1	B	606	ARG	2.8
1	A	697	LEU	2.8
1	A	429	GLY	2.8
1	A	605	VAL	2.7
1	A	452	ASN	2.7
1	A	705	VAL	2.7
1	B	202	GLN	2.6
1	B	608	SER	2.6
1	A	620	LYS	2.6
1	A	598	GLY	2.6
1	B	486	GLY	2.6
1	B	383	VAL	2.6
1	A	487	LYS	2.5
1	B	482	PHE	2.5
1	A	627	GLY	2.5
1	B	713	ASN	2.5
1	A	479	ASN	2.5
1	B	489	PRO	2.4
1	A	455	TRP	2.4
1	B	700	SER	2.4
1	A	335	LYS	2.4
1	A	485	ASN	2.4
1	A	703	LEU	2.3
1	A	416	ASN	2.3
1	A	603	GLU	2.3
1	A	434	GLN	2.3
1	A	419	SER	2.3
1	A	477	ALA	2.3
1	A	567	GLY	2.3
1	B	452	ASN	2.3
1	A	331	ARG	2.2
1	A	568	LEU	2.2
1	B	134	PRO	2.2
1	B	217	LYS	2.2
1	B	701	GLY	2.1
1	A	629	ASN	2.1
1	A	454	LEU	2.1
1	B	431	LEU	2.1
1	B	670	ALA	2.1
1	A	608	SER	2.1
1	A	453	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	476	ILE	2.1
1	B	726	ALA	2.1

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

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

## 6.3 Carbohydrates [i](#)

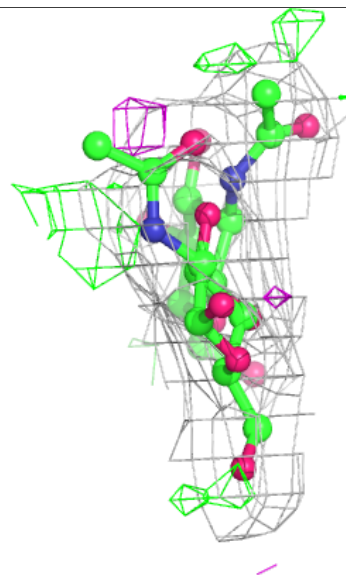
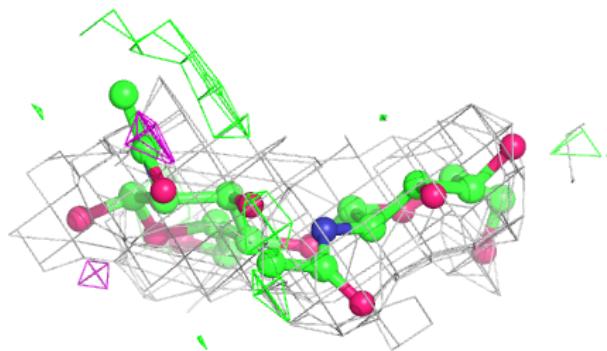
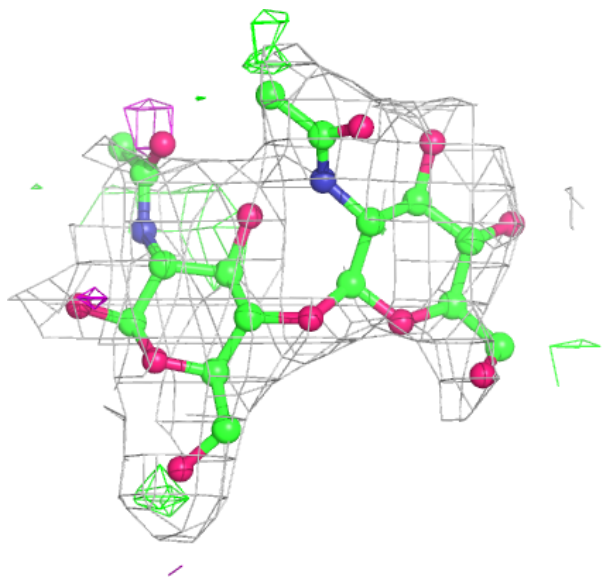
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GAL	F	1	12/12	0.33	0.77	79,97,104,106	0
2	NAG	C	2	14/15	0.78	0.19	77,88,97,98	0
2	NAG	D	2	14/15	0.80	0.28	62,84,95,97	0
3	GAL	E	1	12/12	0.82	0.23	56,72,81,83	0
2	NAG	C	1	15/15	0.84	0.24	45,71,89,93	0
3	GAL	F	2	11/12	0.91	0.24	43,51,61,64	0
3	GAL	E	2	11/12	0.94	0.17	45,51,55,56	0
2	NAG	D	1	14/15	0.96	0.20	49,59,68,71	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.

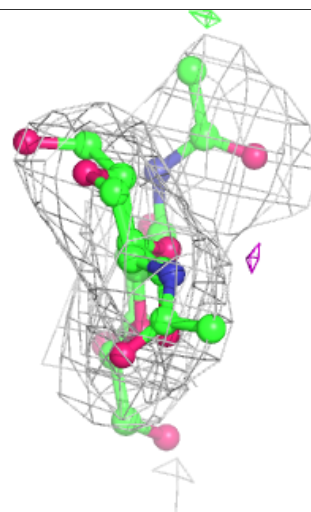
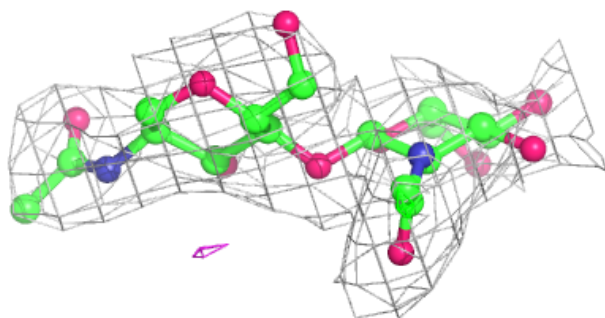
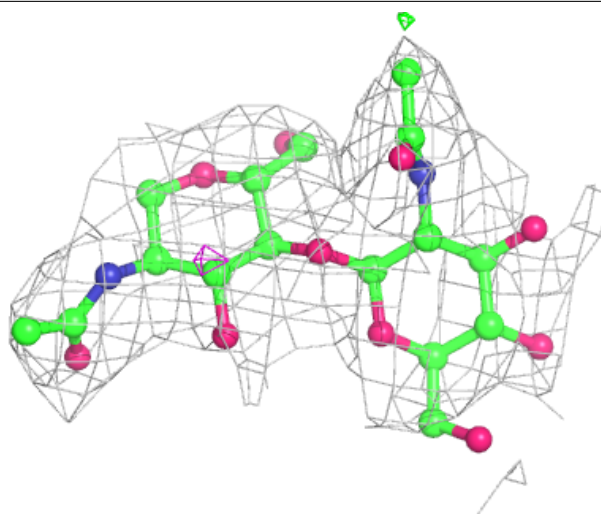
**Electron density around Chain C:**

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



**Electron density around Chain D:**

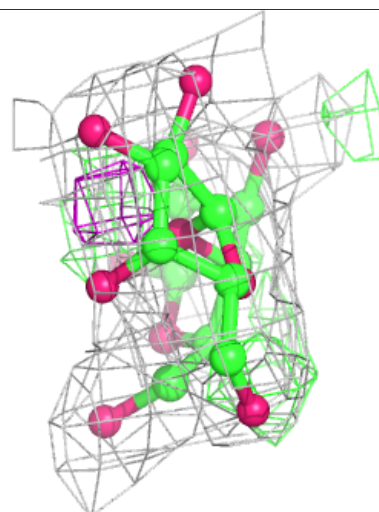
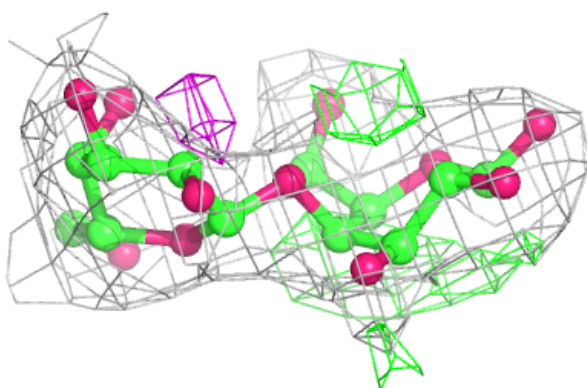
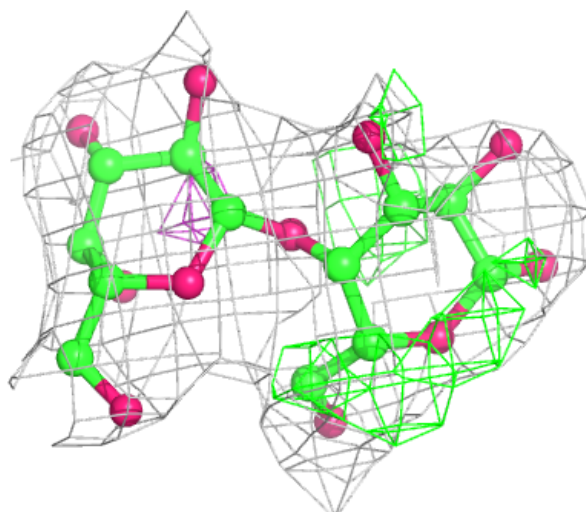
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

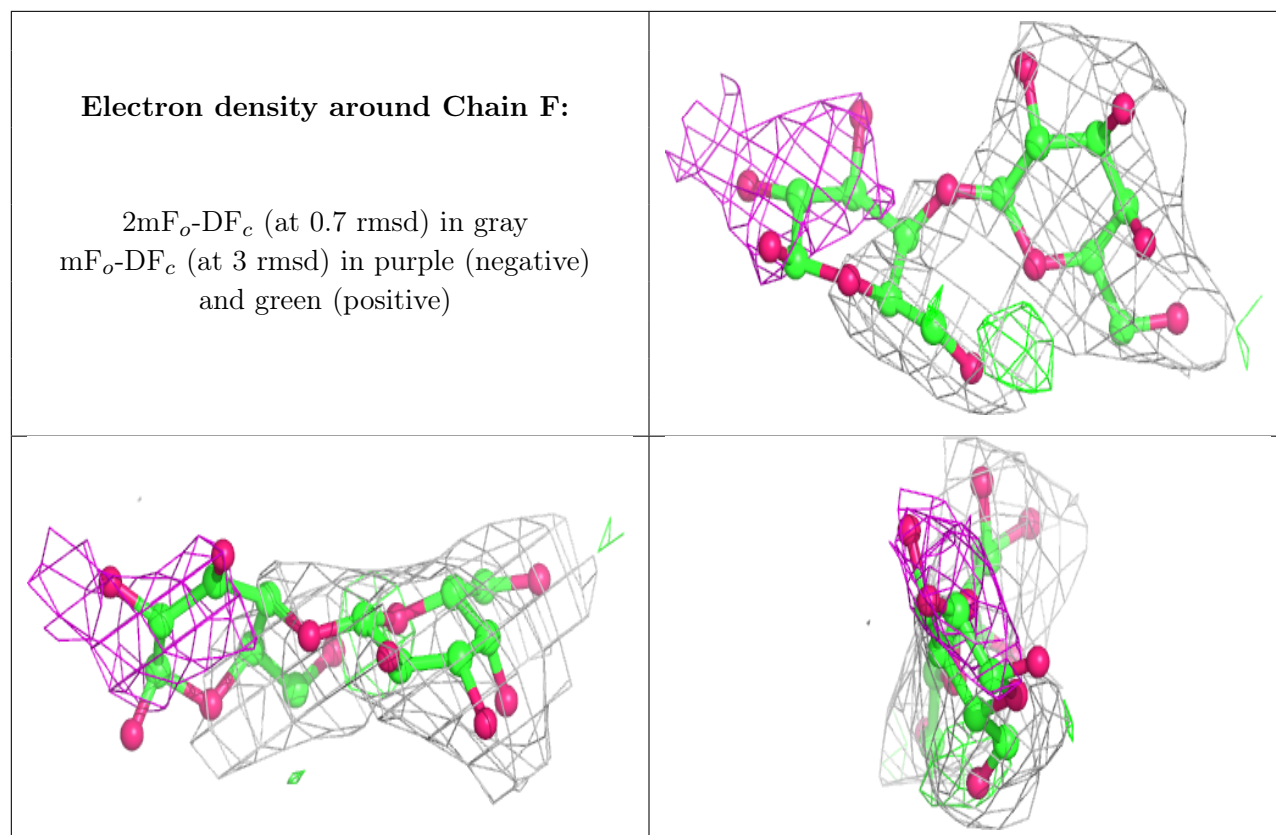




**Electron density around Chain E:**

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





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	A	805	14/15	0.68	0.38	79,91,105,106	0
5	NAG	B	801	14/15	0.83	0.23	75,88,95,99	0
4	CL	A	804	1/1	0.99	0.11	40,40,40,40	0
4	CL	B	805	1/1	0.99	0.20	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.