



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 02:43 PM EDT

PDB ID : 1UKT  
Title : Crystal structure of Y100L mutant cyclodextrin glucanotransferase complexed with an acarbose  
Authors : Haga, K.; Kanai, R.; Sakamoto, O.; Harata, K.; Yamane, K.  
Deposited on : 2003-09-01  
Resolution : 2.20 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 : 2.23.2  
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) : 2.23.2

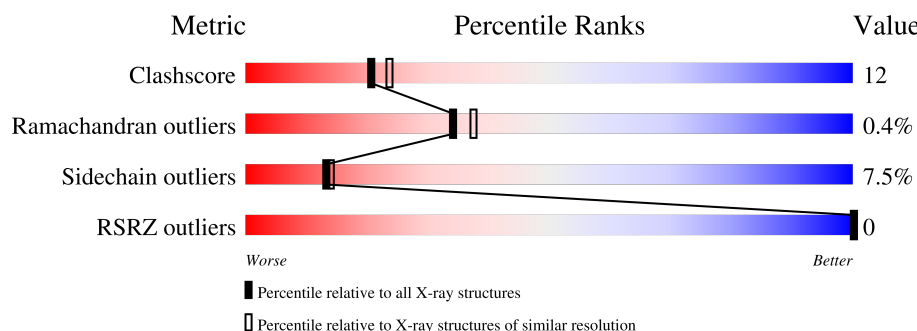
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



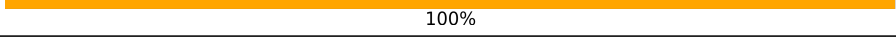

The reported resolution of this entry is 2.20 Å.

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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	686	
1	B	686	
2	C	3	
2	D	3	

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	GAL	C	1	X	-	-	X
2	GLC	C	2	-	-	-	X
2	GLD	C	3	-	-	-	X
2	GAL	D	1	X	-	-	-
2	GLD	D	3	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10961 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.

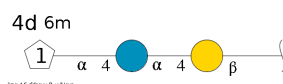
- Molecule 1 is a protein called Cyclomaltodextrin glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5308	3351	906	1035	16			
1	B	686	Total	C	N	O	S	0	0	0
			5308	3351	906	1035	16			

There are 6 discrepancies between the modelled and reference sequences:

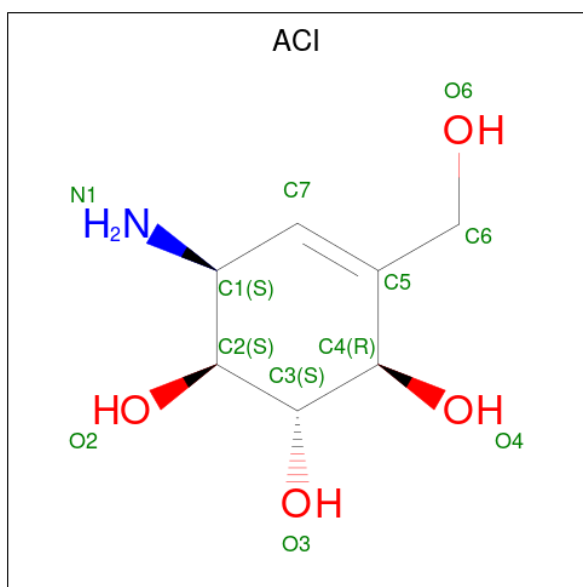
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	LEU	TYR	engineered mutation	UNP P05618
A	452	PRO	ARG	SEE REMARK 999	UNP P05618
A	454	GLY	ALA	SEE REMARK 999	UNP P05618
B	100	LEU	TYR	engineered mutation	UNP P05618
B	452	PRO	ARG	SEE REMARK 999	UNP P05618
B	454	GLY	ALA	SEE REMARK 999	UNP P05618

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-alpha-D-xylo-hexopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			32	18	14			
2	D	3	Total	C	O	0	0	0
			32	18	14			

- Molecule 3 is 6-AMINO-4-HYDROXYMETHYL-CYCLOHEX-4-ENE-1,2,3-TRIOL (three-letter code: ACI) (formula: C<sub>7</sub>H<sub>13</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	7	1	4		
3	B	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	B	2	Total	Ca	0	0
			2	2		

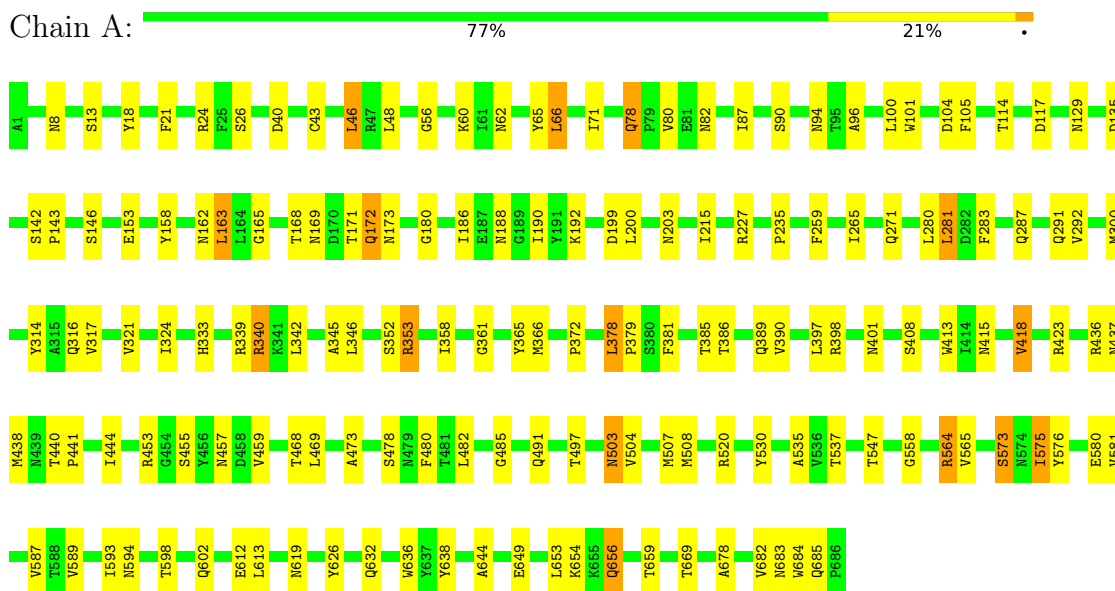
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	138	Total	O	0	0
			138	138		
5	B	115	Total	O	0	0
			115	115		

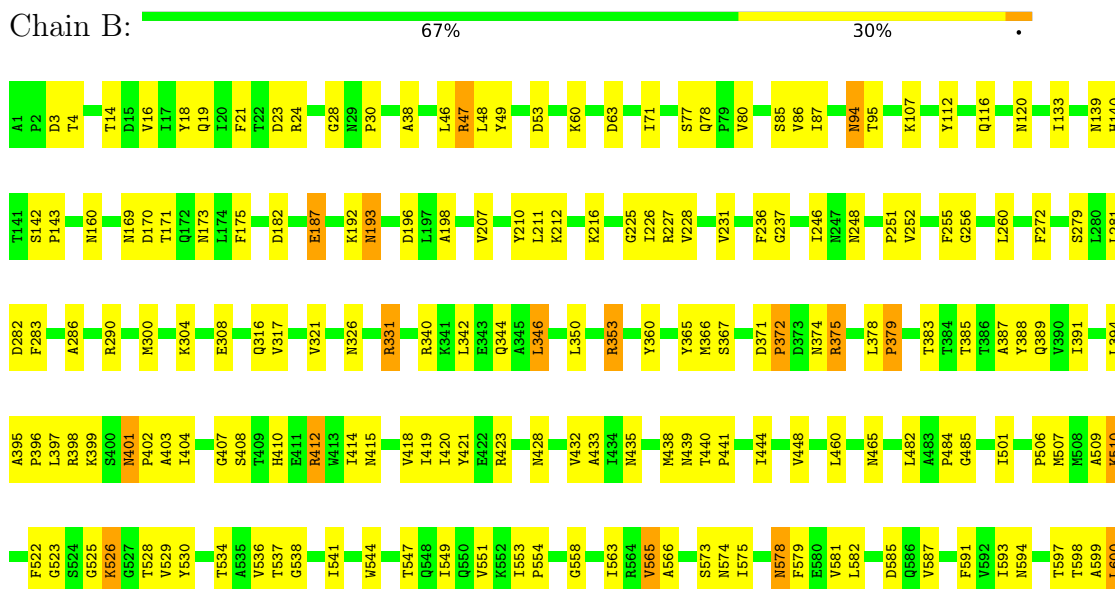
### 3 Residue-property plots

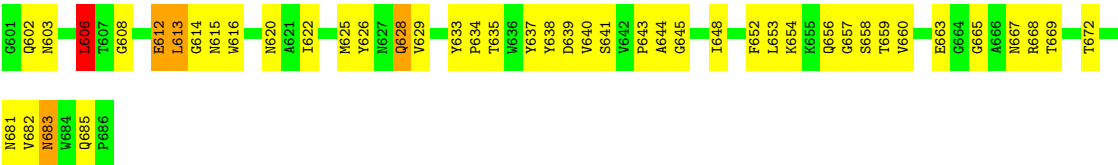
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



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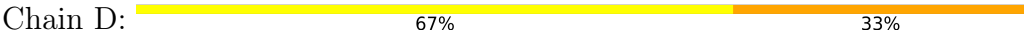




- Molecule 2: 4,6-dideoxy-alpha-D-xylo-hexopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-galactopyranose



- Molecule 2: 4,6-dideoxy-alpha-D-xylo-hexopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-galactopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.68Å 74.47Å 80.10Å 85.29° 105.59° 100.81°	Depositor
Resolution (Å)	10.00 – 2.20 77.11 – 2.02	Depositor EDS
% Data completeness (in resolution range)	56.7 (10.00-2.20) 73.2 (77.11-2.02)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.02Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.173 , 0.276 0.201 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 64.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10961	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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, GLD, CA, GLC, ACI

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	0/5441	0.70	0/7422
1	B	0.43	0/5441	0.69	1/7422 (0.0%)
All	All	0.44	0/10882	0.69	1/14844 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	606	LEU	CA-CB-CG	5.02	126.85	115.30

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	5308	0	5052	90	0
1	B	5308	0	5052	160	0
2	C	32	0	29	5	0
2	D	32	0	29	3	0
3	A	12	0	12	0	0
3	B	12	0	11	3	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	138	0	0	4	0
5	B	115	0	0	2	0
All	All	10961	0	10185	257	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 12.

All (257) 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:314:TYR:HB2	1:A:317:VAL:HG22	1.59	0.85
1:A:82:ASN:HD22	1:A:96:ALA:HB1	1.41	0.84
1:B:536:VAL:HG21	1:B:554:PRO:HG3	1.60	0.83
1:A:453:ARG:HH22	1:A:473:ALA:HB2	1.48	0.78
1:B:528:THR:HG23	1:B:566:ALA:HB3	1.66	0.78
1:A:60:LYS:HE2	1:A:60:LYS:HA	1.69	0.73
1:B:14:THR:HG22	1:B:399:LYS:HG2	1.71	0.73
1:B:375:ARG:HD2	1:B:375:ARG:H	1.51	0.72
1:B:378:LEU:HD12	1:B:379:PRO:HD2	1.72	0.72
1:B:612:GLU:HG3	1:B:643:PRO:HD3	1.72	0.72
1:B:522:PHE:CE2	1:B:565:VAL:HG11	2.25	0.71
1:A:594:ASN:HB2	1:A:683:ASN:HD22	1.55	0.71
1:B:78:GLN:HG2	1:B:80:VAL:HG22	1.71	0.71
2:C:1:GAL:H5	2:C:2:GLC:O2	1.91	0.70
1:A:287:GLN:O	1:A:291:GLN:HG3	1.92	0.69
1:B:231:VAL:HG11	1:B:256:GLY:HA3	1.75	0.68
1:B:526:LYS:NZ	1:B:537:THR:HB	2.09	0.68
1:B:598:THR:HB	1:B:602:GLN:HB3	1.77	0.67
1:B:139:ASN:HD22	1:B:140:HIS:HD2	1.40	0.66
1:B:286:ALA:O	1:B:290:ARG:HG3	1.95	0.66
1:B:3:ASP:HB3	1:B:547:THR:O	1.95	0.65
1:B:435:ASN:O	1:B:485:GLY:HA2	1.97	0.65
1:A:530:TYR:CE2	1:A:535:ALA:HB2	2.32	0.65
1:A:26:SER:O	1:A:56:GLY:HA3	1.96	0.65
1:A:564:ARG:HG3	1:A:575:ILE:HG13	1.79	0.64
1:B:28:GLY:O	1:B:30:PRO:HD3	1.98	0.64
1:B:47:ARG:HD2	1:B:372:PRO:HG3	1.80	0.63
1:A:457:ASN:HA	1:A:468:THR:HG22	1.80	0.62
3:B:705:ACI:H1	2:D:3:GLD:H63	1.81	0.62
1:B:316:GLN:HG2	1:B:507:MET:HE3	1.82	0.62
1:A:397:LEU:HD11	1:A:459:VAL:HG11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ILE:HG22	1:B:551:VAL:HG23	1.81	0.61
1:A:508:MET:HA	1:A:580:GLU:O	2.00	0.60
1:B:441:PRO:HB3	1:B:484:PRO:HD3	1.83	0.59
1:A:352:SER:O	1:A:398:ARG:NH2	2.35	0.59
1:A:378:LEU:HD23	1:A:379:PRO:HD2	1.84	0.59
1:B:316:GLN:HE22	1:B:578:ASN:HB3	1.67	0.59
1:B:300:MET:HB2	1:B:415:ASN:O	2.02	0.59
1:A:18:TYR:HB2	1:A:71:ILE:HG12	1.83	0.59
1:B:394:LEU:HD21	1:B:460:LEU:CD2	2.34	0.58
1:B:522:PHE:HE2	1:B:565:VAL:HG11	1.68	0.58
1:B:414:ILE:HG13	1:B:415:ASN:H	1.69	0.58
1:B:653:LEU:HD13	1:B:660:VAL:HG13	1.85	0.58
1:B:606:LEU:CD1	1:B:622:ILE:HB	2.33	0.58
1:B:575:ILE:HD12	1:B:575:ILE:H	1.69	0.57
1:A:281:LEU:HD12	1:A:321:VAL:HB	1.86	0.57
1:B:187:GLU:OE2	1:B:626:TYR:HB3	2.05	0.57
1:A:453:ARG:NH2	1:A:473:ALA:HB2	2.19	0.57
1:A:503:ASN:HD22	1:A:504:VAL:N	2.03	0.57
1:B:317:VAL:HG22	1:B:353:ARG:HE	1.70	0.57
1:B:212:LYS:O	1:B:216:LYS:HG2	2.04	0.57
1:B:401:ASN:ND2	1:B:403:ALA:H	2.02	0.57
1:B:47:ARG:HG2	1:B:94:ASN:ND2	2.20	0.56
1:B:187:GLU:HG2	1:B:628:GLN:NE2	2.20	0.56
1:B:606:LEU:HD13	1:B:622:ILE:HB	1.88	0.56
1:B:394:LEU:HD21	1:B:460:LEU:HD22	1.88	0.55
1:B:526:LYS:HZ3	1:B:537:THR:HB	1.68	0.55
1:B:663:GLU:HG2	1:B:685:GLN:HB2	1.88	0.55
1:B:529:VAL:HG22	1:B:565:VAL:HG23	1.87	0.55
1:B:554:PRO:HA	5:B:1237:HOH:O	2.07	0.55
1:A:602:GLN:NE2	1:A:656:GLN:NE2	2.54	0.54
1:A:602:GLN:NE2	1:A:656:GLN:HE22	2.05	0.54
1:A:316:GLN:NE2	1:A:507:MET:HG3	2.22	0.54
1:B:207:VAL:O	1:B:211:LEU:HD23	2.07	0.54
1:B:482:LEU:HD12	5:B:1087:HOH:O	2.08	0.54
1:B:16:VAL:HG11	1:B:395:ALA:HB1	1.88	0.54
1:A:80:VAL:HG13	1:A:104:ASP:O	2.09	0.53
1:A:186:ILE:O	1:A:190:ILE:HG13	2.08	0.53
1:B:536:VAL:CG2	1:B:554:PRO:HG3	2.35	0.53
1:A:507:MET:SD	1:A:576:TYR:HE2	2.32	0.53
1:A:342:LEU:HD23	1:A:365:TYR:CD1	2.44	0.53
1:B:414:ILE:HG13	1:B:415:ASN:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:THR:HB	1:A:602:GLN:HB3	1.91	0.53
1:B:587:VAL:HG13	1:B:644:ALA:HB2	1.92	0.52
3:B:705:ACI:H1	2:D:3:GLD:C6	2.40	0.52
1:B:143:PRO:HB3	1:B:196:ASP:OD1	2.10	0.52
1:B:231:VAL:CG1	1:B:256:GLY:HA3	2.40	0.52
1:B:608:GLY:N	1:B:613:LEU:HB3	2.24	0.52
1:B:616:TRP:CZ2	1:B:667:ASN:ND2	2.78	0.52
1:A:40:ASP:HB2	1:A:48:LEU:HD22	1.92	0.52
1:B:187:GLU:HG2	1:B:628:GLN:HE22	1.75	0.52
1:A:593:ILE:HG13	1:A:682:VAL:HG23	1.92	0.51
1:B:387:ALA:O	1:B:391:ILE:HG13	2.11	0.51
1:A:114:THR:H	1:A:117:ASP:HB2	1.76	0.51
1:A:587:VAL:HG13	1:A:644:ALA:HB2	1.92	0.51
1:B:403:ALA:O	1:B:407:GLY:HA3	2.11	0.51
1:B:408:SER:O	1:B:423:ARG:HA	2.11	0.51
1:B:350:LEU:O	1:B:398:ARG:NH1	2.44	0.51
1:A:316:GLN:HG2	1:A:507:MET:HE2	1.92	0.51
1:A:340:ARG:HB3	1:A:438:MET:HE1	1.93	0.50
1:B:410:HIS:ND1	1:B:412:ARG:NE	2.60	0.50
1:A:565:VAL:HB	1:A:573:SER:OG	2.10	0.50
1:B:558:GLY:HA2	1:B:581:VAL:HG23	1.92	0.50
1:A:339:ARG:HB3	1:A:365:TYR:CE1	2.47	0.50
1:A:60:LYS:HD3	1:A:381:PHE:CE1	2.47	0.49
1:A:353:ARG:H	1:A:353:ARG:HD3	1.77	0.49
1:B:594:ASN:HB2	1:B:683:ASN:OD1	2.12	0.49
1:B:597:THR:HG22	1:B:633:TYR:OH	2.12	0.49
1:B:415:ASN:HB3	1:B:418:VAL:HB	1.93	0.49
1:B:528:THR:CG2	1:B:566:ALA:HB3	2.40	0.49
1:B:47:ARG:HG2	1:B:94:ASN:HD21	1.77	0.49
1:B:304:LYS:O	1:B:308:GLU:HG3	2.12	0.49
1:A:520:ARG:HD3	1:A:547:THR:HG22	1.94	0.49
1:B:625:MET:HG2	1:B:638:TYR:HB2	1.94	0.49
1:B:19:GLN:O	1:B:360:TYR:HB3	2.13	0.49
1:B:331:ARG:NH1	1:B:366:MET:HB3	2.28	0.49
1:A:82:ASN:HD21	1:A:101:TRP:H	1.61	0.49
1:B:193:ASN:N	1:B:193:ASN:HD22	2.11	0.48
1:A:13:SER:O	1:A:398:ARG:NH1	2.46	0.48
1:A:80:VAL:CG1	1:A:105:PHE:HA	2.43	0.48
1:B:372:PRO:HA	1:B:375:ARG:HD3	1.94	0.48
1:B:585:ASP:O	1:B:643:PRO:HA	2.13	0.48
1:B:4:THR:O	1:B:4:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:PRO:HA	1:B:196:ASP:O	2.13	0.48
1:B:541:ILE:HG23	1:B:551:VAL:HG22	1.96	0.48
1:B:665:GLY:HA3	1:B:685:GLN:OE1	2.14	0.48
1:A:361:GLY:HA3	1:A:366:MET:SD	2.54	0.47
2:C:2:GLC:H3	2:C:3:GLD:H5	1.95	0.47
1:A:401:ASN:HD22	1:A:491:GLN:NE2	2.12	0.47
1:B:192:LYS:HE3	1:B:629:VAL:HG22	1.95	0.47
1:B:501:ILE:N	1:B:574:ASN:HD21	2.11	0.47
1:A:415:ASN:HB3	1:A:418:VAL:HG13	1.97	0.47
1:A:408:SER:O	1:A:423:ARG:HA	2.14	0.47
1:B:228:VAL:O	1:B:256:GLY:HA2	2.15	0.47
1:B:593:ILE:CD1	1:B:682:VAL:HG23	2.45	0.47
1:A:188:ASN:O	1:A:192:LYS:HB2	2.15	0.47
1:A:346:LEU:HD22	1:A:358:ILE:HD12	1.97	0.47
2:C:1:GAL:C5	2:C:2:GLC:O2	2.62	0.47
1:A:480:PHE:HE1	1:A:482:LEU:HD13	1.79	0.47
1:B:170:ASP:OD1	1:B:173:ASN:HA	2.15	0.47
1:B:342:LEU:O	1:B:346:LEU:HB2	2.15	0.47
1:B:444:ILE:HD12	1:B:444:ILE:N	2.29	0.47
1:B:575:ILE:HD12	1:B:575:ILE:N	2.29	0.47
1:A:114:THR:N	1:A:117:ASP:HB2	2.30	0.47
1:A:146:SER:HA	1:A:168:THR:OG1	2.16	0.46
1:A:180:GLY:O	1:A:192:LYS:HD3	2.15	0.46
1:B:87:ILE:O	1:B:94:ASN:N	2.48	0.46
1:B:509:ALA:O	1:B:581:VAL:HA	2.15	0.46
1:B:529:VAL:HG21	1:B:551:VAL:HG21	1.96	0.46
1:A:455:SER:HA	1:A:469:LEU:O	2.16	0.46
1:B:236:PHE:HD2	1:B:272:PHE:HD1	1.63	0.46
1:B:614:GLY:HA3	1:B:620:ASN:O	2.16	0.46
1:A:158:TYR:HA	1:A:162:ASN:O	2.16	0.46
1:A:649:GLU:HG2	1:A:669:THR:HG22	1.98	0.46
1:B:579:PHE:HE2	1:B:581:VAL:HG12	1.80	0.46
1:A:292:VAL:HG13	1:A:436:ARG:NH1	2.31	0.46
1:B:365:TYR:HE2	1:B:385:THR:HB	1.81	0.46
1:B:652:PHE:HD2	1:B:668:ARG:HH22	1.64	0.46
1:A:413:TRP:CZ3	1:A:415:ASN:HB2	2.51	0.46
1:B:526:LYS:HZ3	1:B:538:GLY:H	1.64	0.45
1:A:235:PRO:HG3	5:A:1032:HOH:O	2.17	0.45
1:B:395:ALA:HB3	1:B:396:PRO:HD3	1.97	0.45
1:B:210:TYR:HD2	1:B:211:LEU:HD22	1.81	0.45
1:B:236:PHE:CD2	1:B:272:PHE:HD1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:LYS:HE2	1:B:538:GLY:HA2	1.98	0.45
1:B:656:GLN:O	1:B:658:SER:N	2.50	0.45
1:A:340:ARG:HD3	1:A:340:ARG:HA	1.76	0.45
1:B:24:ARG:NH2	1:B:48:LEU:O	2.50	0.45
1:A:78:GLN:HG2	1:A:135:ASP:O	2.17	0.44
1:B:225:GLY:HA2	1:B:252:VAL:HG13	1.98	0.44
1:B:317:VAL:CG2	1:B:353:ARG:HE	2.28	0.44
1:B:196:ASP:O	1:B:196:ASP:CG	2.56	0.44
1:B:227:ARG:HG2	1:B:255:PHE:CE1	2.52	0.44
1:B:530:TYR:HA	1:B:534:THR:O	2.18	0.44
1:B:139:ASN:HD22	1:B:140:HIS:CD2	2.29	0.44
1:B:236:PHE:HD2	1:B:272:PHE:CD1	2.35	0.44
1:B:412:ARG:HA	1:B:412:ARG:HD2	1.83	0.44
1:A:65:TYR:HD2	1:A:66:LEU:HD13	1.83	0.44
1:A:172:GLN:O	1:A:172:GLN:NE2	2.51	0.44
1:A:333:HIS:HD2	5:A:1114:HOH:O	2.01	0.44
1:B:60:LYS:HA	1:B:63:ASP:OD2	2.17	0.44
1:B:526:LYS:HE2	1:B:538:GLY:CA	2.48	0.44
1:B:648:ILE:O	1:B:669:THR:HA	2.18	0.44
1:A:386:THR:O	1:A:390:VAL:HG23	2.18	0.44
1:B:385:THR:OG1	1:B:388:TYR:HB2	2.18	0.44
1:B:401:ASN:C	1:B:401:ASN:HD22	2.21	0.44
1:B:565:VAL:HG12	1:B:573:SER:OG	2.17	0.44
1:B:440:THR:HA	1:B:441:PRO:HD2	1.91	0.43
1:A:142:SER:HB2	1:A:143:PRO:CD	2.49	0.43
1:B:18:TYR:HB2	1:B:71:ILE:HD12	2.00	0.43
1:B:553:ILE:HA	1:B:554:PRO:HD3	1.85	0.43
1:B:251:PRO:HB3	1:B:506:PRO:HD3	2.00	0.43
1:A:503:ASN:ND2	1:A:504:VAL:H	2.15	0.43
1:A:46:LEU:HB3	1:A:372:PRO:HB2	2.01	0.43
1:B:420:ILE:HA	1:B:432:VAL:O	2.18	0.43
1:A:142:SER:HB2	1:A:143:PRO:HD2	2.01	0.43
1:B:645:GLY:HA2	1:B:672:THR:O	2.18	0.43
1:A:324:ILE:HG21	1:A:345:ALA:HB1	2.00	0.43
1:B:401:ASN:HD21	1:B:428:ASN:HB3	1.84	0.43
1:B:608:GLY:HA3	1:B:613:LEU:HD23	2.01	0.43
1:B:439:ASN:O	1:B:441:PRO:HD3	2.18	0.43
1:A:80:VAL:HG13	1:A:105:PHE:HA	2.01	0.42
1:A:503:ASN:HD22	1:A:504:VAL:H	1.65	0.42
1:A:589:VAL:HG22	1:A:678:ALA:HB3	2.01	0.42
1:A:594:ASN:HB2	1:A:683:ASN:ND2	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:TYR:O	1:A:636:TRP:HA	2.20	0.42
1:B:633:TYR:CD1	1:B:634:PRO:HA	2.54	0.42
1:B:38:ALA:O	1:B:49:TYR:HB2	2.20	0.42
1:B:53:ASP:HB2	1:B:112:TYR:O	2.19	0.42
1:B:522:PHE:CD2	1:B:565:VAL:HG11	2.53	0.42
2:C:2:GLC:H3	2:C:3:GLD:C5	2.48	0.42
1:A:24:ARG:N	1:A:24:ARG:HD2	2.34	0.42
1:A:215:ILE:HD12	1:A:215:ILE:HA	1.81	0.42
1:B:260:LEU:HB2	1:B:283:PHE:HB3	2.01	0.42
1:B:331:ARG:HH12	1:B:366:MET:HB3	1.83	0.42
1:A:82:ASN:ND2	1:A:96:ALA:HB1	2.22	0.42
1:A:444:ILE:N	1:A:444:ILE:HD12	2.34	0.42
1:B:23:ASP:OD1	1:B:49:TYR:HD1	2.03	0.42
1:B:421:TYR:CD1	1:B:421:TYR:N	2.87	0.42
1:A:654:LYS:HE3	1:A:684:TRP:CZ2	2.55	0.42
1:B:237:GLY:HA3	1:B:639:ASP:O	2.19	0.42
1:B:226:ILE:HD12	1:B:246:ILE:HD13	2.02	0.42
1:B:236:PHE:CD2	1:B:272:PHE:CD1	3.07	0.42
1:A:440:THR:HA	1:A:441:PRO:HD3	1.77	0.42
1:B:371:ASP:HA	1:B:372:PRO:HA	1.88	0.42
1:B:175:PHE:CD2	1:B:198:ALA:HB1	2.54	0.41
1:B:420:ILE:HG12	1:B:433:ALA:CB	2.50	0.41
1:A:385:THR:O	1:A:389:GLN:HG2	2.20	0.41
1:B:116:GLN:O	1:B:120:ASN:HB2	2.20	0.41
1:A:656:GLN:HG2	1:A:659:THR:HB	2.02	0.41
1:A:656:GLN:HG2	1:A:656:GLN:O	2.21	0.41
1:B:255:PHE:HD1	1:B:281:LEU:HD22	1.84	0.41
1:B:394:LEU:HD21	1:B:460:LEU:HD21	2.01	0.41
1:B:397:LEU:HB3	1:B:404:ILE:HD12	2.02	0.41
1:B:597:THR:HA	1:B:633:TYR:OH	2.20	0.41
1:B:603:ASN:O	1:B:654:LYS:HA	2.20	0.41
1:B:633:TYR:HA	1:B:635:THR:H	1.85	0.41
1:A:163:LEU:HD22	1:A:165:GLY:H	1.84	0.41
1:A:259:PHE:HE2	5:A:1195:HOH:O	2.02	0.41
1:B:401:ASN:HA	1:B:402:PRO:HD2	1.99	0.41
1:A:558:GLY:HA2	1:A:581:VAL:HG22	2.03	0.41
1:B:526:LYS:HZ1	1:B:537:THR:HB	1.81	0.41
1:B:544:TRP:CD1	1:B:544:TRP:C	2.94	0.41
1:B:255:PHE:CE1	1:B:321:VAL:HG21	2.56	0.41
1:B:340:ARG:HG2	1:B:438:MET:HE1	2.03	0.41
1:A:87:ILE:O	1:A:94:ASN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PHE:CG	2:C:2:GLC:H2	2.55	0.41
1:A:437:ASN:O	1:A:485:GLY:N	2.54	0.41
1:B:465:ASN:N	1:B:465:ASN:HD22	2.19	0.41
1:B:593:ILE:HD12	1:B:682:VAL:HG23	2.01	0.41
1:A:613:LEU:HD23	1:A:613:LEU:HA	1.91	0.41
1:B:46:LEU:HD23	1:B:372:PRO:O	2.20	0.41
1:A:8:ASN:HB3	5:A:1019:HOH:O	2.20	0.40
1:B:248:ASN:ND2	1:B:510:LYS:HD2	2.36	0.40
1:B:523:GLY:O	1:B:544:TRP:CD1	2.74	0.40
1:B:591:PHE:O	1:B:637:TYR:HA	2.20	0.40
1:B:80:VAL:HA	1:B:107:LYS:O	2.22	0.40
1:B:340:ARG:O	1:B:344:GLN:HG3	2.21	0.40
1:B:412:ARG:HG3	1:B:448:VAL:O	2.22	0.40
1:B:211:LEU:HD13	1:B:211:LEU:HA	1.80	0.40
3:B:705:ACI:C1	2:D:3:GLD:H63	2.49	0.40
1:A:259:PHE:CD1	1:A:283:PHE:CE1	3.09	0.40
1:B:599:ALA:O	1:B:602:GLN:HB2	2.21	0.40
1:B:38:ALA:HB2	1:B:86:VAL:CG2	2.51	0.40
1:B:414:ILE:HD12	1:B:419:ILE:HG13	2.03	0.40
1:B:501:ILE:H	1:B:574:ASN:ND2	2.19	0.40
1:B:652:PHE:HE2	1:B:682:VAL:HG21	1.86	0.40

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	684/686 (100%)	638 (93%)	45 (7%)	1 (0%)	51	60
1	B	684/686 (100%)	626 (92%)	53 (8%)	5 (1%)	22	22
All	All	1368/1372 (100%)	1264 (92%)	98 (7%)	6 (0%)	34	37



All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	600	LEU
1	B	379	PRO
1	B	578	ASN
1	A	90	SER
1	B	657	GLY
1	B	525	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	564/564 (100%)	523 (93%)	41 (7%)	14	15
1	B	564/564 (100%)	520 (92%)	44 (8%)	12	13
All	All	1128/1128 (100%)	1043 (92%)	85 (8%)	13	14

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	PHE
1	A	43	CYS
1	A	46	LEU
1	A	62	ASN
1	A	66	LEU
1	A	78	GLN
1	A	100	LEU
1	A	129	ASN
1	A	153	GLU
1	A	163	LEU
1	A	169	ASN
1	A	171	THR
1	A	172	GLN
1	A	173	ASN
1	A	199	ASP
1	A	200	LEU
1	A	203	ASN

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Mol	Chain	Res	Type
1	A	227	ARG
1	A	265	ILE
1	A	271	GLN
1	A	280	LEU
1	A	281	LEU
1	A	300	MET
1	A	340	ARG
1	A	353	ARG
1	A	378	LEU
1	A	418	VAL
1	A	478	SER
1	A	497	THR
1	A	503	ASN
1	A	537	THR
1	A	564	ARG
1	A	573	SER
1	A	575	ILE
1	A	612	GLU
1	A	619	ASN
1	A	632	GLN
1	A	638	TYR
1	A	653	LEU
1	A	656	GLN
1	A	685	GLN
1	B	21	PHE
1	B	47	ARG
1	B	77	SER
1	B	85	SER
1	B	94	ASN
1	B	95	THR
1	B	133	ILE
1	B	142	SER
1	B	160	ASN
1	B	169	ASN
1	B	171	THR
1	B	182	ASP
1	B	187	GLU
1	B	193	ASN
1	B	279	SER
1	B	282	ASP
1	B	326	ASN
1	B	331	ARG

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Mol	Chain	Res	Type
1	B	346	LEU
1	B	353	ARG
1	B	367	SER
1	B	372	PRO
1	B	374	ASN
1	B	375	ARG
1	B	383	THR
1	B	389	GLN
1	B	401	ASN
1	B	412	ARG
1	B	510	LYS
1	B	526	LYS
1	B	563	ILE
1	B	565	VAL
1	B	582	LEU
1	B	600	LEU
1	B	606	LEU
1	B	612	GLU
1	B	613	LEU
1	B	615	ASN
1	B	628	GLN
1	B	640	VAL
1	B	641	SER
1	B	659	THR
1	B	681	ASN
1	B	683	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	82	ASN
1	A	88	ASN
1	A	93	ASN
1	A	94	ASN
1	A	126	HIS
1	A	129	ASN
1	A	160	ASN
1	A	177	HIS
1	A	247	ASN
1	A	316	GLN
1	A	327	HIS

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Mol	Chain	Res	Type
1	A	410	HIS
1	A	457	ASN
1	A	465	ASN
1	A	467	ASN
1	A	491	GLN
1	A	503	ASN
1	A	548	GLN
1	A	586	GLN
1	A	594	ASN
1	A	602	GLN
1	A	619	ASN
1	A	656	GLN
1	A	683	ASN
1	A	685	GLN
1	B	59	ASN
1	B	62	ASN
1	B	94	ASN
1	B	116	GLN
1	B	172	GLN
1	B	193	ASN
1	B	239	GLN
1	B	316	GLN
1	B	326	ASN
1	B	392	GLN
1	B	401	ASN
1	B	439	ASN
1	B	457	ASN
1	B	465	ASN
1	B	550	GLN
1	B	574	ASN
1	B	681	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

6 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	GAL	C	1	2	12,12,12	0.63	0	17,17,17	1.10	1 (5%)
2	GLC	C	2	2	11,11,12	0.58	0	15,15,17	1.99	1 (6%)
2	GLD	C	3	2,3	9,9,10	1.16	0	10,12,14	1.28	2 (20%)
2	GAL	D	1	2	12,12,12	0.97	1 (8%)	17,17,17	2.18	2 (11%)
2	GLC	D	2	2	11,11,12	0.67	0	15,15,17	2.20	4 (26%)
2	GLD	D	3	2,3	9,9,10	1.25	1 (11%)	10,12,14	1.08	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
2	GAL	C	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLD	C	3	2,3	-	-	0/1/1/1
2	GAL	D	1	2	1/1/5/5	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLD	D	3	2,3	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	GAL	C4-C5	2.45	1.58	1.53
2	D	3	GLD	C3-C2	2.20	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GAL	C1-O5-C5	7.97	128.69	113.66
2	D	2	GLC	C1-O5-C5	7.03	121.71	112.19
2	C	2	GLC	C1-O5-C5	6.68	121.24	112.19
2	C	1	GAL	C1-O5-C5	3.00	119.32	113.66
2	D	1	GAL	C3-C4-C5	2.61	114.90	110.24
2	D	2	GLC	C3-C4-C5	2.49	114.68	110.24
2	D	2	GLC	O5-C1-C2	-2.41	107.05	110.77
2	C	3	GLD	C4-C3-C2	-2.39	107.31	110.27
2	D	3	GLD	C4-C3-C2	2.15	112.93	110.27
2	D	2	GLC	C6-C5-C4	-2.04	108.23	113.00
2	C	3	GLD	C3-C4-C5	-2.02	107.98	111.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	GAL	C4
2	D	1	GAL	C4

All (2) torsion outliers are listed below:

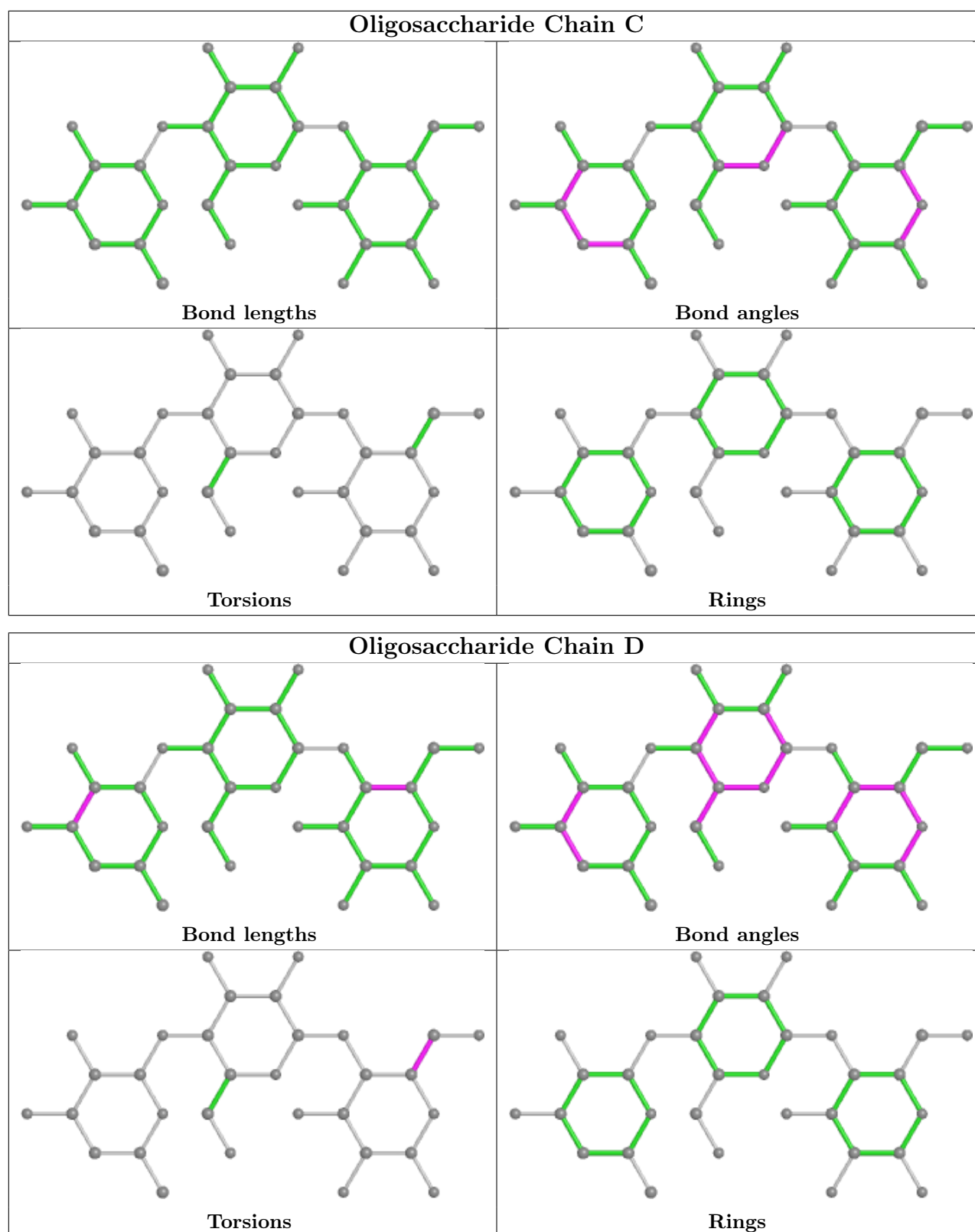
Mol	Chain	Res	Type	Atoms
2	D	1	GAL	O5-C5-C6-O6
2	D	1	GAL	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	GLD	3	0
2	C	3	GLD	2	0
2	C	1	GAL	2	0
2	C	2	GLC	5	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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	ACI	B	705	2	12,12,12	2.27	3 (25%)	11,17,17	1.07	1 (9%)
3	ACI	A	701	2	12,12,12	2.42	3 (25%)	11,17,17	0.85	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
3	ACI	B	705	2	-	1/2/22/22	0/1/1/1
3	ACI	A	701	2	-	1/2/22/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ACI	C7-C5	7.32	1.43	1.32
3	B	705	ACI	C7-C5	6.80	1.42	1.32
3	A	701	ACI	C4-C5	2.79	1.53	1.51
3	A	701	ACI	C1-C7	2.64	1.56	1.50
3	B	705	ACI	C1-C7	2.60	1.56	1.50
3	B	705	ACI	C2-C1	2.31	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	705	ACI	C4-C5-C7	-2.70	117.80	122.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	ACI	C7-C5-C6-O6
3	B	705	ACI	C7-C5-C6-O6



There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	705	ACI	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	686/686 (100%)	-0.68	0 100 100	6, 18, 32, 50	0
1	B	686/686 (100%)	-0.60	0 100 100	7, 24, 40, 56	0
All	All	1372/1372 (100%)	-0.64	0 100 100	6, 21, 38, 56	0

There are no RSRZ outliers to report.

### 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](#)

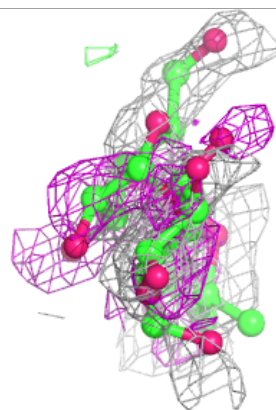
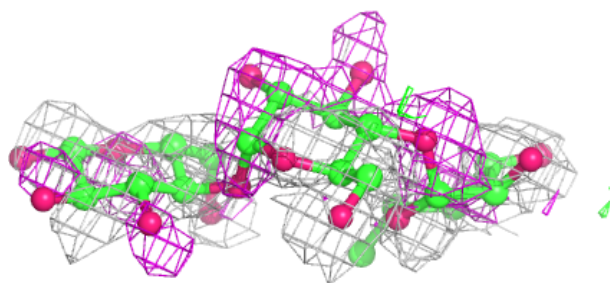
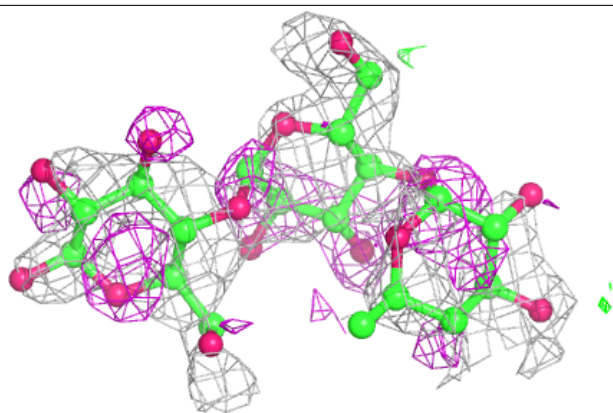
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 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
2	GAL	D	1	12/12	0.51	0.40	46,54,55,56	0
2	GLC	C	2	11/12	0.61	0.59	52,56,59,59	0
2	GLD	D	3	9/10	0.61	0.49	44,49,52,52	0
2	GLD	C	3	9/10	0.65	0.42	51,55,56,57	0
2	GAL	C	1	12/12	0.66	0.46	52,54,56,57	0
2	GLC	D	2	11/12	0.68	0.31	44,50,53,55	0

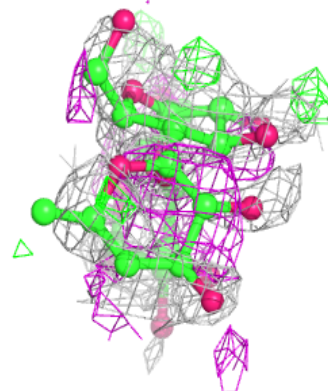
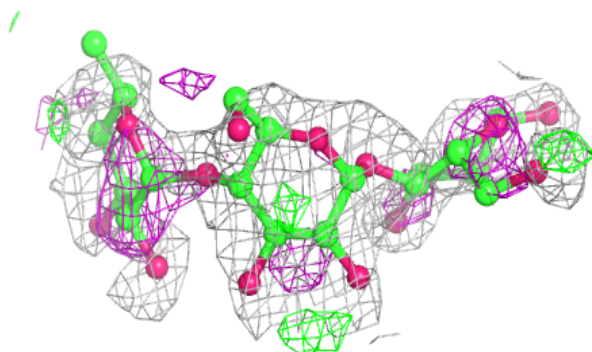
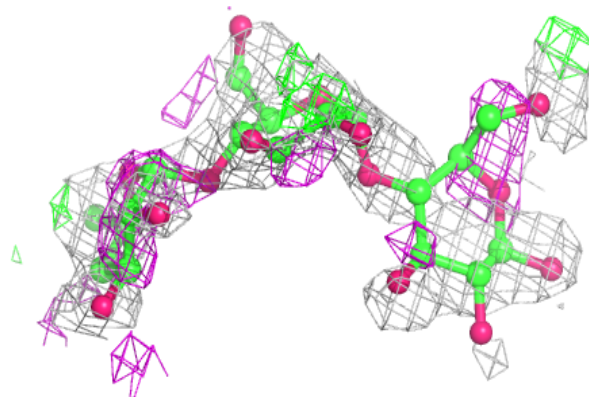
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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)



## 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
3	ACI	A	701	12/12	0.61	0.27	46,51,53,53	0
3	ACI	B	705	12/12	0.71	0.28	43,46,49,50	0
4	CA	A	687	1/1	0.86	0.09	24,24,24,24	0
4	CA	A	688	1/1	0.95	0.11	21,21,21,21	0
4	CA	B	689	1/1	0.97	0.09	28,28,28,28	0
4	CA	B	690	1/1	0.97	0.12	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.