



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 05:03 PM BST

PDB ID : 3PHA  
Title : The crystal structure of the W169Y mutant of alpha-glucosidase (gh31 family) from *Ruminococcus obeum* atcc 29174 in complex with acarbose  
Authors : Tan, K.; Tesar, C.; Keigher, L.; Babnigg, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2010-11-03  
Resolution : 2.17 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	:	2.14.6
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)	:	2.14.6

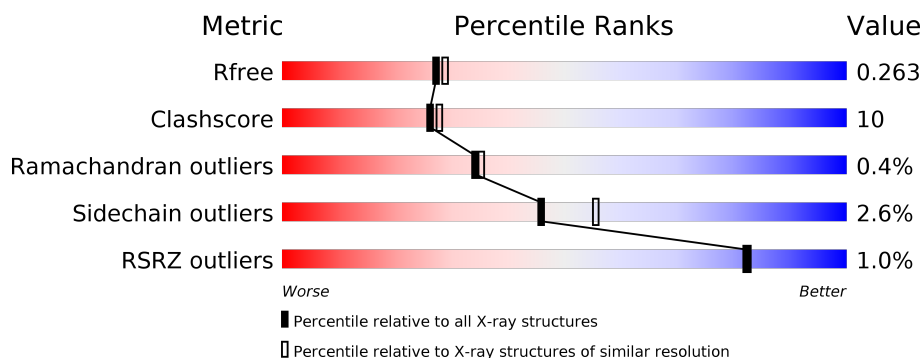
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 on 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	666	<div> <div></div> <div>72%</div> <div>26%</div> <div></div> </div>
1	B	666	<div> <div></div> <div>77%</div> <div>22%</div> <div></div> </div>
1	C	666	<div> <div></div> <div>78%</div> <div>21%</div> <div></div> </div>
1	D	666	<div> <div></div> <div>78%</div> <div>21%</div> <div></div> </div>
2	E	3	<div> <div></div> <div>100%</div> </div>
2	F	3	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	3	 33%67%
2	H	3	 100%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22569 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	1	0
			5440	3491	890	1024	35			
1	B	665	Total	C	N	O	S	0	1	0
			5447	3494	892	1026	35			
1	C	665	Total	C	N	O	S	0	1	0
			5448	3495	892	1026	35			
1	D	666	Total	C	N	O	S	0	1	0
			5457	3498	896	1028	35			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A5ZY13
A	-1	ASN	-	expression tag	UNP A5ZY13
A	0	ALA	-	expression tag	UNP A5ZY13
A	169	TYR	TRP	engineered mutation	UNP A5ZY13
B	-2	SER	-	expression tag	UNP A5ZY13
B	-1	ASN	-	expression tag	UNP A5ZY13
B	0	ALA	-	expression tag	UNP A5ZY13
B	169	TYR	TRP	engineered mutation	UNP A5ZY13
C	-2	SER	-	expression tag	UNP A5ZY13
C	-1	ASN	-	expression tag	UNP A5ZY13
C	0	ALA	-	expression tag	UNP A5ZY13
C	169	TYR	TRP	engineered mutation	UNP A5ZY13
D	-2	SER	-	expression tag	UNP A5ZY13
D	-1	ASN	-	expression tag	UNP A5ZY13
D	0	ALA	-	expression tag	UNP A5ZY13
D	169	TYR	TRP	engineered mutation	UNP A5ZY13

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	F	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	G	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	H	3	Total	C	N	O	0	0	0
			44	25	1	18			

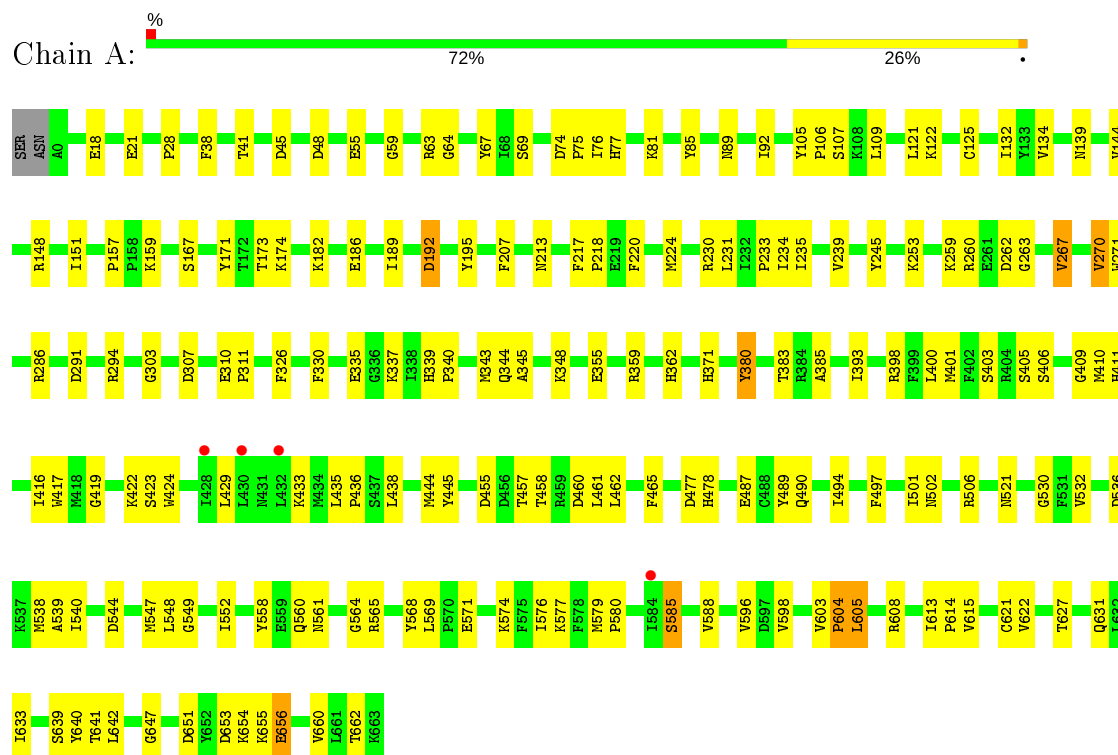
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total	O	0	0
			94	94		
3	B	120	Total	O	0	0
			120	120		
3	C	203	Total	O	0	0
			203	203		
3	D	184	Total	O	0	0
			184	184		

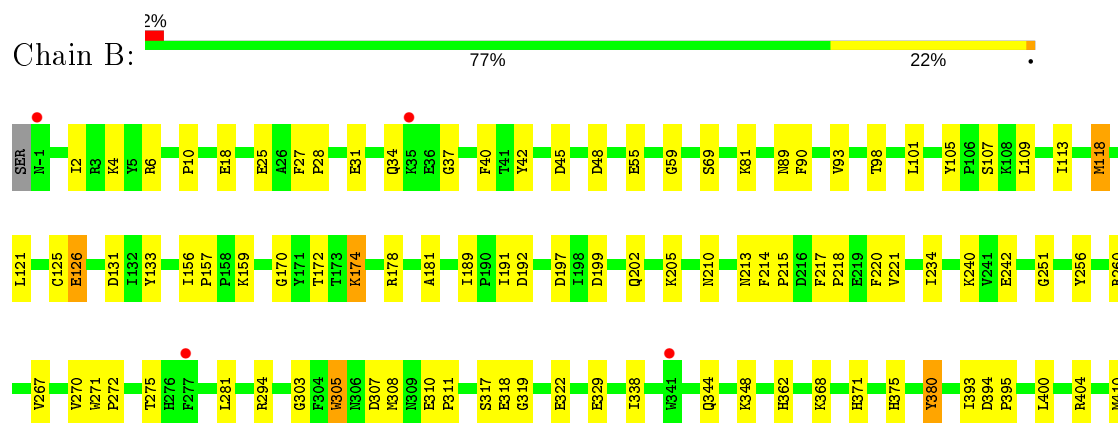
### 3 Residue-property plots

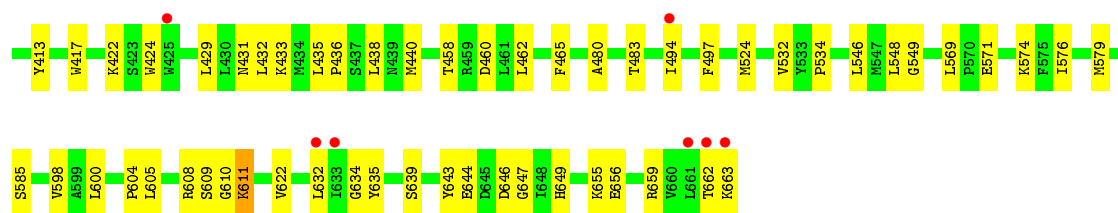
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: alpha-glucosidase

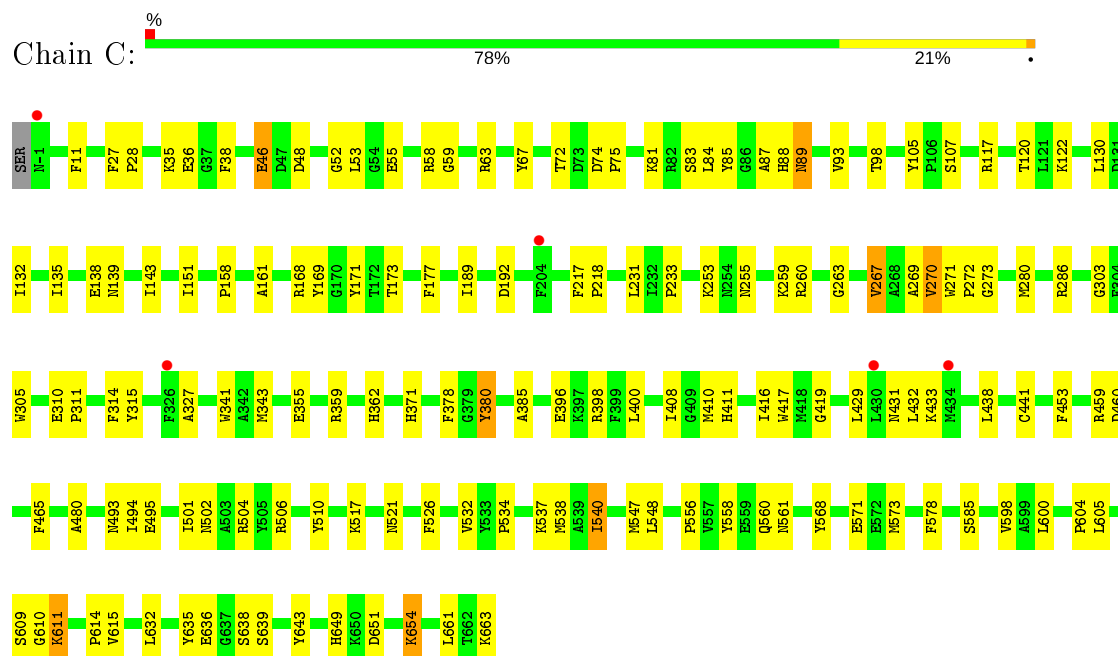


- Molecule 1: alpha-glucosidase

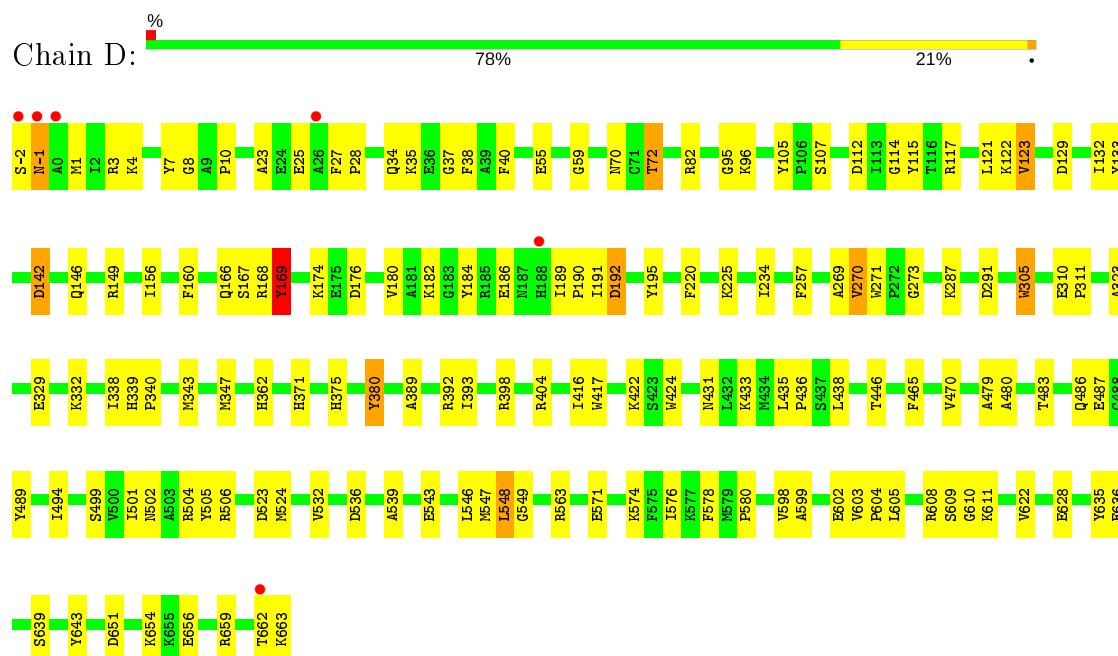




• Molecule 1: alpha-glucosidase



• Molecule 1: alpha-glucosidase



• Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:  100%

GLC1  
GLC2  
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain F:  100%

GLC1  
GLC2  
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain G:  33%  67%

GLC1  
GLC2  
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain H:  100%

GLC1  
GLC2  
AC13

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.03Å 125.95Å 133.58Å 90.00° 107.72° 90.00°	Depositor
Resolution (Å)	42.41 – 2.17 50.06 – 2.17	Depositor EDS
% Data completeness (in resolution range)	90.4 (42.41-2.17) 97.9 (50.06-2.17)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.200 , 0.265 0.198 , 0.263	Depositor DCC
$R_{free}$ test set	7170 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	22569	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4837e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: AC1, GLC

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	0.38	0/5585	0.54	0/7531
1	B	0.39	0/5592	0.54	1/7541 (0.0%)
1	C	0.41	0/5593	0.56	0/7542
1	D	0.42	0/5602	0.57	0/7553
All	All	0.40	0/22372	0.55	1/30167 (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	432	LEU	CA-CB-CG	5.63	128.25	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	5440	0	5213	135	0
1	B	5447	0	5217	108	0
1	C	5448	0	5219	105	0
1	D	5457	0	5226	100	0
2	E	44	0	30	0	0
2	F	44	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	44	0	30	1	0
2	H	44	0	30	3	0
3	A	94	0	0	5	0
3	B	120	0	0	4	0
3	C	203	0	0	11	0
3	D	184	0	0	4	0
All	All	22569	0	20995	448	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 10.

All (448) 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:270:VAL:HG12	1:A:271:TRP:H	1.24	1.00
1:A:330:PHE:HB2	1:A:343:MET:HE3	1.48	0.95
1:C:327:ALA:HA	1:C:343:MET:HE1	1.53	0.88
1:C:429:LEU:HD22	1:C:558:TYR:CE1	2.09	0.87
1:A:59:GLY:HA2	1:A:433:LYS:HD3	1.60	0.82
1:A:330:PHE:CB	1:A:343:MET:HE3	2.12	0.79
1:D:4:LYS:HG3	1:D:133:TYR:CE1	2.18	0.78
1:D:436:PRO:HG3	1:D:546:LEU:HD21	1.66	0.77
1:A:576:ILE:HB	1:A:605:LEU:HD13	1.68	0.75
1:D:270:VAL:HG12	1:D:271:TRP:H	1.52	0.74
1:D:548:LEU:HD12	1:D:549:GLY:N	2.02	0.74
1:A:270:VAL:HG12	1:A:271:TRP:N	2.01	0.74
1:A:310:GLU:N	1:A:311:PRO:HA	2.03	0.73
1:A:21:GLU:HG2	3:A:675:HOH:O	1.88	0.73
1:B:598:VAL:HG11	1:B:604:PRO:HG3	1.71	0.72
1:A:571:GLU:OE2	1:A:608:ARG:HD2	1.90	0.72
1:A:641:THR:HG22	1:A:660:VAL:HG12	1.71	0.71
1:D:651:ASP:OD1	1:D:654:LYS:HE3	1.91	0.71
1:B:210:ASN:HB3	1:B:213:ASN:HB2	1.72	0.70
1:C:432[B]:LEU:HD12	1:C:556:PRO:HG2	1.74	0.70
1:D:532:VAL:HG21	1:D:547:MET:HG3	1.72	0.70
1:B:260:ARG:HH21	1:B:267[B]:VAL:HG12	1.55	0.70
1:B:260:ARG:NH2	1:B:267[B]:VAL:HG12	2.05	0.70
1:D:70:ASN:O	1:D:72:THR:HG22	1.90	0.70
1:B:632:LEU:O	1:B:663:LYS:HE2	1.91	0.70
1:D:362:HIS:NE2	1:D:371:HIS:HD2	1.91	0.69
1:C:310:GLU:N	1:C:311:PRO:HA	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:HE3	1:B:215:PRO:HD2	1.76	0.68
1:C:59:GLY:HA2	1:C:433:LYS:HD3	1.75	0.68
1:D:55:GLU:HB2	1:D:438:LEU:HD21	1.77	0.67
1:A:598:VAL:HG11	1:A:604:PRO:HG3	1.77	0.66
1:C:609:SER:HA	1:C:635:TYR:CE2	2.30	0.66
1:B:4:LYS:HG3	1:B:133:TYR:CE1	2.31	0.66
1:C:35:LYS:HG3	1:C:36:GLU:H	1.60	0.66
1:A:639:SER:HB3	1:A:662:THR:HG22	1.77	0.65
1:B:105:TYR:CE2	1:B:107:SER:HB3	2.31	0.65
1:A:362:HIS:NE2	1:A:371:HIS:HD2	1.94	0.65
1:B:267[B]:VAL:HG11	1:B:317:SER:OG	1.95	0.65
1:C:408:ILE:CD1	1:C:441:CYS:HB3	2.27	0.65
1:D:436:PRO:HG3	1:D:546:LEU:CD2	2.26	0.65
1:C:270:VAL:HG12	1:C:271:TRP:H	1.62	0.64
1:B:639:SER:HA	3:B:759:HOH:O	1.96	0.64
1:B:436:PRO:HG3	1:B:546:LEU:HD21	1.80	0.64
3:D:841:HOH:O	2:H:2:GLC:H3	1.99	0.63
1:D:310:GLU:N	1:D:311:PRO:HA	2.14	0.62
1:D:59:GLY:HA2	1:D:433:LYS:HD3	1.79	0.62
1:B:234:ILE:HD11	1:B:307:ASP:HB2	1.81	0.62
1:B:59:GLY:HA2	1:B:433:LYS:HD3	1.81	0.62
1:C:327:ALA:HA	1:C:343:MET:CE	2.28	0.62
1:C:560:GLN:O	1:C:561:ASN:HB2	1.99	0.62
1:A:330:PHE:HB2	1:A:343:MET:CE	2.28	0.62
1:A:345:ALA:HA	1:A:348:LYS:HE3	1.82	0.61
1:D:571:GLU:OE2	1:D:608:ARG:HD3	2.01	0.61
1:B:380:TYR:HA	1:B:410:MET:HG3	1.83	0.61
1:C:89:ASN:HD22	1:C:89:ASN:N	1.99	0.61
1:B:294:ARG:HG3	1:B:393:ILE:HD13	1.82	0.61
1:B:436:PRO:HG3	1:B:546:LEU:CD2	2.31	0.61
1:A:55:GLU:HB2	1:A:438:LEU:HD21	1.83	0.60
1:B:2:ILE:O	1:B:2:ILE:HG22	2.02	0.60
1:D:479:ALA:HB1	1:D:483:THR:HG21	1.82	0.60
1:A:344:GLN:HG2	1:A:348:LYS:HE2	1.84	0.60
1:B:240:LYS:HA	1:B:275:THR:HG22	1.83	0.60
1:B:371:HIS:HE1	1:B:375:HIS:ND1	1.99	0.60
1:D:339:HIS:ND1	1:D:340:PRO:HD2	2.17	0.59
1:B:55:GLU:HB2	1:B:438:LEU:HD21	1.84	0.59
1:A:409:GLY:H	1:A:411:HIS:HD2	1.51	0.59
1:A:422:LYS:HD3	1:A:455:ASP:OD2	2.02	0.59
1:C:286:ARG:HG3	1:C:385:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:HD12	1:B:125:CYS:HB3	1.85	0.59
1:A:403:SER:O	1:A:416:ILE:HD13	2.03	0.58
1:C:93:VAL:O	1:C:98:THR:HA	2.01	0.58
1:C:651:ASP:OD2	1:C:654:LYS:HD2	2.04	0.58
1:A:231:LEU:O	1:A:233:PRO:HD3	2.03	0.58
1:D:182:LYS:O	1:D:186:GLU:HB2	2.04	0.58
1:A:460:ASP:HB3	1:B:118:MET:CE	2.33	0.58
1:B:234:ILE:HD11	1:B:307:ASP:CB	2.32	0.58
1:C:89:ASN:N	1:C:89:ASN:ND2	2.52	0.58
1:A:260:ARG:NH2	1:A:267:VAL:HG12	2.19	0.58
1:B:172:THR:HG22	1:B:213:ASN:HD21	1.69	0.58
1:B:105:TYR:CZ	1:B:107:SER:HB3	2.39	0.57
1:D:435:LEU:HB2	1:D:436:PRO:HD3	1.85	0.57
1:A:655:LYS:HG3	1:A:656:GLU:OE2	2.04	0.57
1:D:40:PHE:HB3	1:D:123:VAL:HG13	1.85	0.57
1:D:323:ALA:HB1	1:D:347:MET:HE1	1.87	0.57
1:B:404:ARG:HB2	1:B:417:TRP:CH2	2.39	0.57
1:B:303:GLY:HA3	1:B:400:LEU:HB3	1.86	0.56
1:A:171:TYR:HB2	3:A:696:HOH:O	2.05	0.56
1:D:599:ALA:HB3	1:D:602:GLU:HG3	1.86	0.56
1:B:362:HIS:NE2	1:B:371:HIS:HD2	2.03	0.56
1:B:6:ARG:HD3	1:B:131:ASP:OD1	2.05	0.56
1:A:574:LYS:HG2	1:A:588:VAL:HG22	1.86	0.56
1:D:156:ILE:HG22	1:D:398:ARG:HD3	1.86	0.56
1:B:202:GLN:OE1	1:B:210:ASN:HA	2.04	0.56
1:B:310:GLU:N	1:B:311:PRO:HA	2.20	0.56
1:A:538:MET:HG2	1:A:568:TYR:CE1	2.41	0.56
1:B:436:PRO:O	1:B:440:MET:HG3	2.06	0.56
1:C:431:ASN:HB2	3:C:858:HOH:O	2.06	0.56
1:A:286:ARG:HG2	1:A:385:ALA:HB2	1.87	0.55
1:A:560:GLN:O	1:A:561:ASN:HB2	2.05	0.55
1:C:260:ARG:HH22	1:C:267:VAL:HG12	1.70	0.55
1:C:526:PHE:CE1	1:C:548:LEU:HD12	2.41	0.55
1:A:310:GLU:N	1:A:311:PRO:CA	2.69	0.55
1:D:-1:ASN:C	1:D:1:MET:H	2.09	0.55
1:A:654:LYS:HD2	1:A:654:LYS:N	2.21	0.55
1:D:548:LEU:HD12	1:D:548:LEU:C	2.27	0.55
1:C:231:LEU:O	1:C:233:PRO:HD3	2.07	0.54
1:D:329:GLU:HB3	1:D:338:ILE:CD1	2.36	0.54
1:B:174:LYS:HD2	1:B:214:PHE:CD1	2.43	0.54
1:B:609:SER:HA	1:B:635:TYR:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LYS:HE3	1:C:263:GLY:O	2.07	0.54
1:B:308:MET:HA	1:B:404:ARG:NH1	2.23	0.54
1:A:45:ASP:HB3	1:A:48:ASP:CG	2.28	0.54
1:B:6:ARG:HD2	1:B:10:PRO:HG2	1.90	0.54
1:C:87:ALA:C	1:C:88:HIS:HD2	2.11	0.54
1:D:329:GLU:HB3	1:D:338:ILE:HD11	1.90	0.54
1:A:157:PRO:HG3	1:A:445:TYR:CD1	2.42	0.54
1:B:644:GLU:OE2	1:B:659:ARG:NH1	2.41	0.54
1:C:362:HIS:NE2	1:C:371:HIS:HD2	2.05	0.53
1:C:460:ASP:HB3	1:C:600:LEU:HD11	1.91	0.53
1:D:480:ALA:O	1:D:483:THR:HG22	2.09	0.53
1:D:639:SER:OG	1:D:662:THR:HG23	2.08	0.53
1:C:48:ASP:O	1:C:63:ARG:HD2	2.09	0.53
1:D:-1:ASN:N	1:D:-1:ASN:HD22	2.06	0.53
1:D:105:TYR:CE2	1:D:107:SER:HB3	2.44	0.53
1:D:121:LEU:HD12	1:D:122:LYS:N	2.24	0.53
1:A:38:PHE:CZ	1:A:132:ILE:HD11	2.43	0.53
1:A:564:GLY:HA3	1:A:596:VAL:O	2.09	0.53
1:A:651:ASP:OD1	1:A:654:LYS:HD3	2.09	0.53
1:B:371:HIS:CE1	1:B:375:HIS:ND1	2.77	0.53
1:C:171:TYR:HB2	3:C:808:HOH:O	2.07	0.53
1:D:416:ILE:HG12	1:D:446:THR:HG22	1.90	0.53
1:D:610:GLY:O	1:D:611:LYS:HD2	2.08	0.53
1:B:435:LEU:HB2	1:B:436:PRO:HD3	1.91	0.53
1:C:610:GLY:C	1:C:611:LYS:HD2	2.29	0.53
1:A:286:ARG:CG	1:A:385:ALA:HB2	2.39	0.52
1:A:383:THR:HG23	1:A:401:MET:HE2	1.91	0.52
1:B:202:GLN:O	1:B:205:LYS:HD3	2.09	0.52
1:A:189:ILE:HD11	1:A:494:ILE:HD11	1.91	0.52
1:B:460:ASP:HB3	1:B:600:LEU:HD11	1.91	0.52
1:D:112:ASP:OD1	1:D:115:TYR:HB3	2.10	0.52
1:B:422:LYS:HD3	1:B:424:TRP:CZ2	2.43	0.52
1:A:230:ARG:HA	3:A:733:HOH:O	2.10	0.52
1:B:646:ASP:OD2	1:B:649:HIS:ND1	2.36	0.52
1:A:303:GLY:HA2	1:A:400:LEU:O	2.10	0.52
1:A:85:TYR:CE2	1:A:419:GLY:HA3	2.44	0.52
1:B:202:GLN:OE1	1:B:202:GLN:HA	2.10	0.52
1:D:167:SER:HB2	1:D:195:TYR:HB2	1.92	0.51
1:C:105:TYR:CE2	1:C:107:SER:HB3	2.46	0.51
1:C:117:ARG:HD3	3:C:783:HOH:O	2.09	0.51
1:A:532:VAL:HG21	1:A:547:MET:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ARG:NH2	1:C:267:VAL:HG12	2.24	0.51
1:D:532:VAL:CG2	1:D:547:MET:HG3	2.40	0.51
1:C:310:GLU:N	1:C:311:PRO:CA	2.73	0.51
1:C:271:TRP:HB2	1:C:272:PRO:HD3	1.93	0.51
1:C:408:ILE:HD11	1:C:441:CYS:HB3	1.91	0.51
1:D:23:ALA:HB1	1:D:25:GLU:OE2	2.09	0.51
1:D:389:ALA:O	1:D:393:ILE:HG13	2.11	0.51
1:C:35:LYS:HG3	1:C:36:GLU:N	2.26	0.51
1:D:-1:ASN:N	1:D:-1:ASN:ND2	2.59	0.51
1:A:76:ILE:HG13	1:A:81:LYS:HE3	1.93	0.51
1:B:126:GLU:CD	1:B:126:GLU:H	2.13	0.51
1:B:318:GLU:O	1:B:322:GLU:HG3	2.11	0.51
1:D:114:GLY:HA2	1:D:117:ARG:O	2.10	0.50
1:D:636:GLU:OE2	1:D:663:LYS:HE3	2.10	0.50
1:A:260:ARG:HH22	1:A:267:VAL:HG12	1.75	0.50
1:B:189:ILE:HD11	1:B:494:ILE:HD11	1.92	0.50
1:C:355:GLU:O	1:C:359:ARG:HG3	2.12	0.50
1:A:291:ASP:HB3	1:A:294:ARG:NH2	2.27	0.50
1:A:38:PHE:CD2	1:A:38:PHE:C	2.85	0.50
1:D:38:PHE:CZ	1:D:132:ILE:HD11	2.46	0.50
1:C:643:TYR:CD2	1:C:643:TYR:C	2.84	0.50
1:C:217:PHE:HB3	1:C:218:PRO:HD3	1.94	0.50
1:B:90:PHE:HD1	1:B:101:LEU:O	1.95	0.50
1:C:168:ARG:HD2	3:C:848:HOH:O	2.11	0.50
1:A:615:VAL:HG21	1:A:633:ILE:HD12	1.94	0.50
1:C:638:SER:HB3	3:C:703:HOH:O	2.12	0.50
1:C:72:THR:HA	3:C:763:HOH:O	2.10	0.50
1:A:502:ASN:O	1:A:506:ARG:HG3	2.12	0.50
1:C:517:LYS:O	1:C:521:ASN:HB2	2.11	0.50
1:A:286:ARG:HG2	1:A:385:ALA:CB	2.42	0.49
1:A:121:LEU:HD12	1:A:122:LYS:N	2.27	0.49
1:A:435:LEU:HB2	1:A:436:PRO:HD3	1.94	0.49
1:B:69:SER:OG	1:B:89:ASN:ND2	2.46	0.49
1:D:329:GLU:HA	1:D:332:LYS:NZ	2.27	0.49
1:D:55:GLU:O	1:D:55:GLU:HG2	2.12	0.49
1:A:76:ILE:HG13	1:A:76:ILE:O	2.13	0.49
1:A:18:GLU:HB2	3:A:667:HOH:O	2.11	0.49
1:D:536:ASP:HB3	1:D:539:ALA:HB3	1.94	0.49
1:D:142:ASP:O	1:D:146:GLN:HG3	2.13	0.48
1:B:192:ASP:OD2	1:B:622:VAL:HG23	2.13	0.48
1:C:534:PRO:HB2	3:C:758:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-1:ASN:C	1:D:1:MET:N	2.66	0.48
1:C:408:ILE:HD13	1:C:441:CYS:HB3	1.93	0.48
1:C:343:MET:CE	1:D:343:MET:HE2	2.42	0.48
1:B:532:VAL:C	1:B:534:PRO:HD3	2.34	0.48
1:C:158:PRO:HG3	1:C:398:ARG:O	2.14	0.48
1:D:598:VAL:HG11	1:D:604:PRO:HG3	1.95	0.48
1:A:105:TYR:HA	1:A:106:PRO:HD3	1.66	0.48
1:A:139:ASN:HB2	3:A:694:HOH:O	2.14	0.48
1:A:182:LYS:HG3	1:A:186:GLU:CD	2.33	0.48
1:A:174:LYS:HG2	1:A:220:PHE:CD1	2.49	0.48
1:B:113:ILE:HG23	1:B:121:LEU:HD13	1.95	0.48
1:D:502:ASN:O	1:D:506:ARG:HG3	2.13	0.48
1:D:654:LYS:HB3	1:D:656:GLU:HG2	1.96	0.48
1:B:574:LYS:HE3	1:B:634:GLY:O	2.14	0.48
1:D:610:GLY:C	1:D:611:LYS:HD2	2.34	0.48
2:G:1:GLC:H62	2:G:2:GLC:O5	2.14	0.48
1:A:548:LEU:HD23	1:A:549:GLY:N	2.29	0.47
1:D:40:PHE:HD2	1:D:123:VAL:CG1	2.26	0.47
1:D:166:GLN:NE2	1:D:184:TYR:OH	2.45	0.47
1:B:251:GLY:HA2	1:B:256:TYR:HB2	1.95	0.47
1:C:122:LYS:HG2	3:C:686:HOH:O	2.12	0.47
1:C:269:ALA:HA	1:C:273:GLY:O	2.14	0.47
1:C:83:SER:O	1:C:84:LEU:HD23	2.14	0.47
1:A:460:ASP:HB3	1:B:118:MET:HE3	1.96	0.47
1:D:192:ASP:OD2	1:D:622:VAL:HG23	2.14	0.47
1:D:174:LYS:HG2	1:D:220:PHE:CD1	2.49	0.47
1:A:497:PHE:O	1:A:501:ILE:HG12	2.14	0.47
1:B:27:PHE:HA	1:B:28:PRO:HD3	1.78	0.47
1:A:457:THR:HG22	1:A:458:THR:H	1.80	0.47
1:B:267[B]:VAL:CG1	1:B:317:SER:OG	2.62	0.47
1:A:224:MET:HA	1:A:224:MET:HE2	1.96	0.47
1:A:28:PRO:HG2	1:A:134:VAL:HG11	1.97	0.47
1:B:655:LYS:HE2	1:B:656:GLU:OE1	2.15	0.47
1:B:93:VAL:O	1:B:98:THR:HA	2.15	0.47
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.74	0.47
1:B:45:ASP:HB3	1:B:48:ASP:OD1	2.14	0.47
1:D:501:ILE:O	1:D:504:ARG:HB3	2.15	0.47
1:A:335:GLU:HB2	1:A:337:LYS:HG3	1.97	0.47
1:A:38:PHE:HZ	1:A:132:ILE:HD11	1.80	0.47
1:B:6:ARG:CD	1:B:10:PRO:HG2	2.44	0.47
1:D:7:TYR:O	1:D:129:ASP:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:TYR:C	1:D:380:TYR:CD1	2.88	0.47
1:C:138:GLU:HG3	1:C:139:ASN:H	1.79	0.46
1:D:523:ASP:OD1	1:D:524:MET:N	2.44	0.46
1:C:161:ALA:CB	1:C:400:LEU:HD13	2.45	0.46
1:C:189:ILE:HD11	1:C:494:ILE:HD11	1.96	0.46
1:C:74:ASP:HA	1:C:75:PRO:HD3	1.74	0.46
1:B:197:ASP:OD1	2:F:3:AC1:O4	2.31	0.46
1:B:197:ASP:O	1:B:199:ASP:N	2.49	0.46
1:C:639:SER:HB2	1:C:661:LEU:O	2.15	0.46
1:C:151:ILE:HD12	1:C:411:HIS:CE1	2.50	0.46
1:C:87:ALA:C	1:C:88:HIS:CD2	2.89	0.46
1:D:176:ASP:O	1:D:180:VAL:HG23	2.15	0.46
1:A:174:LYS:HG2	1:A:220:PHE:CE1	2.50	0.46
1:A:76:ILE:O	1:A:81:LYS:HE3	2.15	0.46
1:C:537:LYS:HD2	1:C:540:ILE:HD11	1.97	0.46
1:B:40:PHE:CZ	1:B:42:TYR:HB2	2.50	0.46
1:C:253:LYS:HE3	1:C:253:LYS:HB2	1.83	0.46
1:A:253:LYS:HB2	1:A:253:LYS:HE2	1.47	0.46
1:A:521:ASN:N	1:A:521:ASN:HD22	2.14	0.46
1:C:255:ASN:HA	3:C:799:HOH:O	2.15	0.46
1:D:269:ALA:HA	1:D:273:GLY:O	2.16	0.46
1:A:576:ILE:HB	1:A:605:LEU:CD1	2.41	0.46
1:C:85:TYR:CE2	1:C:419:GLY:HA3	2.51	0.46
1:A:48:ASP:O	1:A:63:ARG:HD2	2.16	0.46
1:B:610:GLY:C	1:B:611:LYS:HD2	2.37	0.46
1:B:634:GLY:N	1:B:663:LYS:HE3	2.31	0.45
1:B:271:TRP:HB2	1:B:272:PRO:HD3	1.99	0.45
1:C:501:ILE:O	1:C:504:ARG:HB3	2.16	0.45
1:C:537:LYS:HA	1:C:540:ILE:CD1	2.46	0.45
2:F:1:GLC:H61	2:F:2:GLC:H5	1.99	0.45
1:D:168:ARG:HH22	1:D:483:THR:HG22	1.82	0.45
1:A:294:ARG:HG3	1:A:393:ILE:CD1	2.47	0.45
1:B:329:GLU:HB3	1:B:338:ILE:CD1	2.46	0.45
1:C:432[B]:LEU:HD12	1:C:556:PRO:CG	2.43	0.45
1:D:189:ILE:HD11	1:D:494:ILE:HG12	1.98	0.45
1:B:109:LEU:CD1	1:B:125:CYS:HB3	2.45	0.45
1:C:55:GLU:HB2	1:C:438:LEU:HD21	1.99	0.45
1:D:160:PHE:C	1:D:160:PHE:CD1	2.89	0.45
1:C:105:TYR:CZ	1:C:107:SER:HB3	2.52	0.45
1:C:459:ARG:NH2	1:C:493:ASN:HB2	2.32	0.45
1:B:191:ILE:HG12	1:B:192:ASP:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:PHE:O	1:B:221:VAL:HG23	2.16	0.45
2:H:1:GLC:H61	2:H:2:GLC:O5	2.17	0.45
1:A:217:PHE:HB3	1:A:218:PRO:HD3	1.99	0.45
1:A:45:ASP:HB3	1:A:48:ASP:OD1	2.17	0.45
1:A:564:GLY:CA	1:A:596:VAL:O	2.65	0.45
1:B:240:LYS:HE3	1:B:242:GLU:HB2	1.98	0.45
1:D:146:GLN:O	1:D:149[A]:ARG:HB2	2.17	0.45
1:A:259:LYS:HE3	1:A:263:GLY:O	2.16	0.44
1:B:380:TYR:C	1:B:380:TYR:CD1	2.90	0.44
1:C:270:VAL:HG12	1:C:271:TRP:N	2.30	0.44
1:C:416:ILE:HD12	1:C:416:ILE:C	2.38	0.44
1:C:502:ASN:O	1:C:506:ARG:HG3	2.17	0.44
1:C:67:TYR:CD2	1:C:67:TYR:N	2.85	0.44
1:D:270:VAL:HG12	1:D:271:TRP:N	2.26	0.44
1:A:422:LYS:HD2	1:A:424:TRP:CZ2	2.53	0.44
1:A:653:ASP:C	1:A:654:LYS:HD2	2.38	0.44
1:B:294:ARG:HG3	1:B:393:ILE:CD1	2.46	0.44
1:A:234:ILE:HD11	1:A:307:ASP:CB	2.48	0.44
1:B:574:LYS:O	1:B:576:ILE:HG12	2.18	0.44
1:D:603:VAL:HA	1:D:604:PRO:HD3	1.87	0.44
1:C:259:LYS:CE	1:C:263:GLY:O	2.65	0.44
1:C:654:LYS:CA	1:C:654:LYS:HE3	2.47	0.44
1:B:344:GLN:HG2	1:B:348:LYS:HE3	1.98	0.44
1:B:662:THR:HG23	3:B:759:HOH:O	2.17	0.44
1:A:217:PHE:N	1:A:218:PRO:CD	2.80	0.44
1:B:217:PHE:HB3	1:B:218:PRO:HD3	1.99	0.44
1:D:643:TYR:CD2	1:D:643:TYR:C	2.91	0.44
1:A:380:TYR:CD1	1:A:380:TYR:C	2.91	0.44
1:A:59:GLY:CA	1:A:433:LYS:HD3	2.41	0.44
1:B:305:TRP:CD1	1:B:305:TRP:N	2.86	0.44
1:A:105:TYR:CE2	1:A:107:SER:HB3	2.53	0.44
1:A:67:TYR:CD2	1:A:67:TYR:N	2.86	0.44
1:C:38:PHE:CZ	1:C:132:ILE:HD11	2.53	0.44
1:C:46:GLU:HA	3:C:727:HOH:O	2.17	0.44
1:C:52:GLY:O	1:C:53:LEU:HB2	2.18	0.44
1:A:568:TYR:C	1:A:569:LEU:HD23	2.38	0.43
1:A:69:SER:CB	1:A:89:ASN:HD21	2.31	0.43
1:B:317:SER:HA	3:B:709:HOH:O	2.18	0.43
1:D:479:ALA:HB2	1:D:486:GLN:HG3	2.00	0.43
1:B:605:LEU:C	1:B:605:LEU:HD12	2.38	0.43
1:C:396:GLU:O	1:C:649:HIS:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:MET:HG2	1:C:568:TYR:CE1	2.53	0.43
1:A:536:ASP:HB3	1:A:539:ALA:HB3	1.99	0.43
1:C:135:ILE:CG2	1:C:143:ILE:HG23	2.48	0.43
1:C:314:PHE:O	1:C:315:TYR:HB3	2.18	0.43
1:D:433:LYS:HE2	1:D:543:GLU:HB3	2.01	0.43
1:A:167:SER:HB2	1:A:195:TYR:HB2	1.99	0.43
1:B:34:GLN:HA	1:B:37:GLY:O	2.17	0.43
1:C:578:PHE:HE1	1:C:605:LEU:HD21	1.83	0.43
1:A:192:ASP:OD2	1:A:621:CYS:HA	2.18	0.43
1:A:270:VAL:CG1	1:A:271:TRP:N	2.72	0.43
1:A:233:PRO:HD2	1:A:303:GLY:O	2.19	0.43
1:C:38:PHE:CD2	1:C:38:PHE:C	2.91	0.43
1:D:422:LYS:HD3	1:D:424:TRP:CZ2	2.54	0.43
1:D:487:GLU:HB3	1:D:489:TYR:CE1	2.53	0.43
1:A:487:GLU:HB2	1:A:490:GLN:HG2	1.99	0.43
1:A:603:VAL:HA	1:A:604:PRO:HD3	1.78	0.43
1:B:571:GLU:OE2	1:B:608:ARG:HD2	2.18	0.43
1:B:643:TYR:C	1:B:643:TYR:CD2	2.91	0.43
1:D:578:PHE:HB3	3:D:675:HOH:O	2.18	0.43
1:A:613:ILE:HA	1:A:614:PRO:HD3	1.79	0.43
1:D:225:LYS:HE3	1:D:225:LYS:HB2	1.76	0.43
1:A:339:HIS:CG	1:A:340:PRO:HD2	2.53	0.43
1:A:409:GLY:N	1:A:411:HIS:HD2	2.14	0.43
1:A:536:ASP:OD1	1:A:538:MET:HB3	2.19	0.42
1:B:178:ARG:O	1:B:181:ALA:HB3	2.19	0.42
1:B:462:LEU:HD23	1:B:497:PHE:CE1	2.54	0.42
1:D:329:GLU:HA	1:D:332:LYS:HZ3	1.84	0.42
1:D:416:ILE:O	1:D:446:THR:HA	2.19	0.42
1:A:167:SER:HG	1:A:478:HIS:CE1	2.36	0.42
1:B:25:GLU:CD	1:B:25:GLU:H	2.21	0.42
1:C:453:PHE:CZ	1:C:480:ALA:HB2	2.54	0.42
1:C:571:GLU:O	1:C:573:MET:HG3	2.19	0.42
1:A:462:LEU:O	1:A:462:LEU:HD12	2.19	0.42
1:C:88:HIS:N	1:C:88:HIS:CD2	2.87	0.42
2:F:1:GLC:H61	2:F:2:GLC:C5	2.49	0.42
1:A:577:LYS:HA	1:A:603:VAL:O	2.19	0.42
1:B:6:ARG:HH11	1:B:10:PRO:HG2	1.84	0.42
1:B:174:LYS:O	1:B:178:ARG:HG3	2.19	0.42
1:C:532:VAL:HG21	1:C:547:MET:HG3	2.01	0.42
1:A:487:GLU:HB3	1:A:489:TYR:CE1	2.55	0.42
1:A:579:MET:HE2	1:A:585:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:LEU:HG	1:B:433:LYS:HE2	1.99	0.42
1:C:378:PHE:HB2	3:C:762:HOH:O	2.19	0.42
1:C:611:LYS:HD2	1:C:611:LYS:N	2.34	0.42
1:A:92:ILE:HD11	1:A:144:VAL:HG22	2.01	0.42
1:D:499:SER:OG	1:D:580:PRO:HA	2.19	0.42
1:D:574:LYS:O	1:D:576:ILE:HG12	2.19	0.42
1:A:406:SER:HB3	1:A:416:ILE:HD11	2.02	0.42
1:B:394:ASP:HA	1:B:395:PRO:HD3	1.79	0.42
1:B:462:LEU:HD23	1:B:497:PHE:HE1	1.85	0.42
1:B:159:LYS:HB2	1:B:647:GLY:HA3	2.01	0.42
1:D:4:LYS:HG3	1:D:133:TYR:CZ	2.55	0.42
1:D:605:LEU:C	1:D:605:LEU:HD12	2.40	0.42
1:D:82:ARG:HA	3:D:788:HOH:O	2.18	0.42
1:A:109:LEU:HD12	1:A:125:CYS:HB3	2.01	0.42
1:A:260:ARG:C	1:A:262:ASP:H	2.22	0.42
1:D:95:GLY:O	1:D:96:LYS:C	2.58	0.42
1:A:173:THR:HG22	1:A:213:ASN:ND2	2.34	0.42
1:D:404:ARG:NH2	2:H:3:AC1:HCB1	2.34	0.42
1:A:631:GLN:HE21	1:A:633:ILE:HG12	1.85	0.42
1:B:524:MET:HE2	1:B:524:MET:HB3	1.93	0.42
1:C:510:TYR:HB2	1:C:614:PRO:HD2	2.01	0.42
1:A:355:GLU:O	1:A:359:ARG:HG3	2.20	0.41
1:C:168:ARG:HB3	1:C:171:TYR:CZ	2.55	0.41
1:A:380:TYR:HA	1:A:410:MET:HG3	2.02	0.41
1:B:480:ALA:HB3	1:B:483:THR:CG2	2.51	0.41
1:C:380:TYR:HA	1:C:410:MET:HG3	2.01	0.41
1:D:38:PHE:HZ	1:D:132:ILE:HD11	1.85	0.41
1:D:343:MET:HE1	1:D:347:MET:CE	2.49	0.41
1:D:371:HIS:HE1	1:D:375:HIS:ND1	2.18	0.41
1:A:76:ILE:HG13	1:A:81:LYS:CE	2.49	0.41
1:B:579:MET:HE3	1:B:585:SER:HB3	2.02	0.41
1:C:343:MET:HE2	1:D:343:MET:HE2	2.03	0.41
1:C:453:PHE:CE2	1:C:480:ALA:HB2	2.55	0.41
1:B:156:ILE:HA	1:B:157:PRO:HD3	1.91	0.41
1:B:548:LEU:HD23	1:B:549:GLY:N	2.34	0.41
1:C:27:PHE:HA	1:C:28:PRO:HD3	1.82	0.41
1:C:303:GLY:HA2	1:C:400:LEU:O	2.20	0.41
1:D:609:SER:HA	1:D:635:TYR:CE2	2.56	0.41
1:A:239:VAL:HG12	1:A:245:TYR:CE2	2.55	0.41
1:A:398:ARG:NH1	1:A:647:GLY:HA2	2.35	0.41
1:A:409:GLY:H	1:A:411:HIS:CD2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:HG3	1:B:220:PHE:CE1	2.55	0.41
1:A:64:GLY:O	1:B:458:THR:HG21	2.21	0.41
1:B:600:LEU:HD23	1:B:600:LEU:HA	1.87	0.41
1:C:11:PHE:C	1:C:11:PHE:CD2	2.94	0.41
1:C:280:MET:O	1:C:286:ARG:HD3	2.19	0.41
1:C:632:LEU:HD11	1:C:661:LEU:HB3	2.02	0.41
1:A:148:ARG:NH2	1:A:444:MET:SD	2.94	0.41
1:A:207:PHE:CE1	1:A:235:ILE:HD12	2.56	0.41
1:D:169:TYR:C	1:D:169:TYR:CD1	2.92	0.41
1:D:257:PHE:HB2	3:D:758:HOH:O	2.21	0.41
1:A:544:ASP:CG	1:A:565:ARG:HH22	2.23	0.41
1:A:548:LEU:HB3	1:A:552:ILE:CG1	2.51	0.41
1:A:159:LYS:HG2	1:A:622:VAL:HG11	2.03	0.41
1:C:506:ARG:HB3	1:C:615:VAL:HG13	2.03	0.41
1:D:34:GLN:HA	1:D:37:GLY:O	2.19	0.41
1:A:77:HIS:N	1:A:77:HIS:CD2	2.89	0.41
1:A:530:GLY:HA2	1:A:540:ILE:HG22	2.01	0.41
1:A:640:TYR:CE2	1:A:642:LEU:HA	2.56	0.41
1:B:172:THR:CG2	1:B:213:ASN:HD21	2.33	0.41
1:B:368:LYS:HB3	1:B:368:LYS:HE2	1.93	0.41
1:D:105:TYR:CZ	1:D:107:SER:HB3	2.56	0.41
1:D:291:ASP:OD1	1:D:392:ARG:NH2	2.46	0.41
1:A:423:SER:C	1:A:461:LEU:HD21	2.40	0.41
1:A:457:THR:HG22	1:A:458:THR:N	2.34	0.41
1:A:69:SER:OG	1:A:89:ASN:ND2	2.54	0.41
1:C:81:LYS:HA	1:C:81:LYS:HD3	1.81	0.41
1:D:167:SER:CB	1:D:195:TYR:HB2	2.51	0.41
1:A:429:LEU:HD22	1:A:558:TYR:CE1	2.56	0.40
1:C:117:ARG:HB2	1:C:120:THR:HB	2.03	0.40
1:D:27:PHE:HA	1:D:28:PRO:HD3	1.75	0.40
1:D:8:GLY:C	1:D:10:PRO:HD3	2.42	0.40
1:A:239:VAL:HG12	1:A:245:TYR:HE2	1.86	0.40
1:A:326:PHE:CD2	1:A:343:MET:HE2	2.56	0.40
1:B:319:GLY:HA3	3:B:767:HOH:O	2.21	0.40
1:C:260:ARG:NH2	1:C:267:VAL:CG1	2.84	0.40
1:D:190:PRO:HB2	1:D:505:TYR:CE1	2.56	0.40
1:A:151:ILE:HG13	1:A:411:HIS:CE1	2.57	0.40
1:A:579:MET:HA	1:A:580:PRO:HD3	1.90	0.40
1:C:173:THR:O	1:C:177:PHE:HD2	2.04	0.40
1:C:654:LYS:HE3	1:C:654:LYS:HA	2.03	0.40
1:D:182:LYS:HG3	1:D:186:GLU:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ILE:HB	1:D:305:TRP:CE2	2.57	0.40
1:A:234:ILE:HG12	1:A:235:ILE:N	2.36	0.40
1:A:477:ASP:C	1:A:477:ASP:OD1	2.60	0.40
1:B:413:TYR:CD2	1:B:413:TYR:N	2.90	0.40
1:D:287:LYS:HG3	1:D:392:ARG:NH2	2.35	0.40
1:A:74:ASP:HA	1:A:75:PRO:HD3	1.71	0.40
1:B:532:VAL:O	1:B:534:PRO:HD3	2.21	0.40
1:B:81:LYS:HD3	1:B:81:LYS:HA	1.90	0.40
1:C:632:LEU:O	1:C:663:LYS:HE2	2.21	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	663/666 (100%)	617 (93%)	44 (7%)	2 (0%)	41	43
1	B	664/666 (100%)	615 (93%)	48 (7%)	1 (0%)	47	52
1	C	664/666 (100%)	622 (94%)	39 (6%)	3 (0%)	29	28
1	D	665/666 (100%)	627 (94%)	34 (5%)	4 (1%)	25	24
All	All	2656/2664 (100%)	2481 (93%)	165 (6%)	10 (0%)	34	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	58	ARG
1	D	169	TYR
1	C	270	VAL
1	B	170	GLY
1	A	270	VAL
1	D	470	VAL

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Mol	Chain	Res	Type
1	A	604	PRO
1	D	270	VAL
1	C	598	VAL
1	D	191	ILE

### 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	574/575 (100%)	563 (98%)	11 (2%)	57	68
1	B	575/575 (100%)	563 (98%)	12 (2%)	53	64
1	C	575/575 (100%)	557 (97%)	18 (3%)	40	48
1	D	576/575 (100%)	558 (97%)	18 (3%)	40	48
All	All	2300/2300 (100%)	2241 (97%)	59 (3%)	46	55

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	192	ASP
1	A	267	VAL
1	A	380	TYR
1	A	405	SER
1	A	417	TRP
1	A	465	PHE
1	A	585	SER
1	A	605	LEU
1	A	627	THR
1	A	656	GLU
1	B	18	GLU
1	B	31	GLU
1	B	118	MET
1	B	126	GLU
1	B	174	LYS
1	B	270	VAL

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Mol	Chain	Res	Type
1	B	305	TRP
1	B	380	TYR
1	B	431	ASN
1	B	465	PHE
1	B	569	LEU
1	B	611	LYS
1	C	46	GLU
1	C	89	ASN
1	C	130	LEU
1	C	169	TYR
1	C	192	ASP
1	C	267	VAL
1	C	305	TRP
1	C	341	TRP
1	C	380	TYR
1	C	417	TRP
1	C	465	PHE
1	C	495	GLU
1	C	540	ILE
1	C	585	SER
1	C	604	PRO
1	C	611	LYS
1	C	636	GLU
1	C	654	LYS
1	D	-2	SER
1	D	-1	ASN
1	D	3	ARG
1	D	35	LYS
1	D	72	THR
1	D	123	VAL
1	D	142	ASP
1	D	169	TYR
1	D	192	ASP
1	D	305	TRP
1	D	380	TYR
1	D	417	TRP
1	D	431	ASN
1	D	465	PHE
1	D	548	LEU
1	D	563	ARG
1	D	628	GLU
1	D	659	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	127	ASN
1	A	166	GLN
1	A	227	GLN
1	A	344	GLN
1	A	371	HIS
1	A	411	HIS
1	A	521	ASN
1	A	631	GLN
1	B	89	ASN
1	B	146	GLN
1	B	166	GLN
1	B	213	ASN
1	B	306	ASN
1	B	344	GLN
1	B	371	HIS
1	C	-1	ASN
1	C	88	HIS
1	C	89	ASN
1	C	202	GLN
1	C	306	ASN
1	C	344	GLN
1	C	371	HIS
1	D	34	GLN
1	D	89	ASN
1	D	166	GLN
1	D	306	ASN
1	D	371	HIS
1	D	431	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 ⓘ

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	E	1	2	12,12,12	0.56	0	17,17,17	1.40	4 (23%)
2	GLC	E	2	2	11,11,12	0.46	0	15,15,17	1.62	4 (26%)
2	AC1	E	3	2	21,22,23	0.63	0	22,32,34	1.55	3 (13%)
2	GLC	F	1	2	12,12,12	0.59	0	17,17,17	1.73	4 (23%)
2	GLC	F	2	2	11,11,12	0.50	0	15,15,17	1.49	2 (13%)
2	AC1	F	3	2	21,22,23	0.77	0	22,32,34	1.84	5 (22%)
2	GLC	G	1	2	12,12,12	0.54	0	17,17,17	1.34	4 (23%)
2	GLC	G	2	2	11,11,12	0.48	0	15,15,17	1.59	2 (13%)
2	AC1	G	3	2	21,22,23	0.69	0	22,32,34	1.58	2 (9%)
2	GLC	H	1	2	12,12,12	0.51	0	17,17,17	1.05	1 (5%)
2	GLC	H	2	2	11,11,12	0.40	0	15,15,17	2.17	4 (26%)
2	AC1	H	3	2	21,22,23	0.86	0	22,32,34	1.99	6 (27%)

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	GLC	E	1	2	-	2/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	AC1	E	3	2	-	4/6/43/46	0/2/2/2
2	GLC	F	1	2	-	2/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	AC1	F	3	2	-	5/6/43/46	0/2/2/2
2	GLC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AC1	G	3	2	-	4/6/43/46	0/2/2/2
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	1/2/19/22	0/1/1/1
2	AC1	H	3	2	-	2/6/43/46	0/2/2/2

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	AC1	C2-C3-C4	-5.62	105.67	110.63
2	H	2	GLC	C1-O5-C5	5.07	119.06	112.19
2	H	2	GLC	C1-C2-C3	4.90	115.69	109.67
2	F	3	AC1	C2-C3-C4	-4.81	106.39	110.63
2	G	2	GLC	C1-O5-C5	4.71	118.58	112.19
2	G	3	AC1	C2-C3-C4	-4.27	106.86	110.63
2	E	3	AC1	C2-C3-C4	-4.09	107.02	110.63
2	H	3	AC1	C1-O5-C5	3.98	121.80	112.78
2	E	2	GLC	C1-O5-C5	3.97	117.57	112.19
2	E	3	AC1	C1-O5-C5	3.89	121.60	112.78
2	F	2	GLC	C1-O5-C5	3.87	117.44	112.19
2	F	1	GLC	C1-C2-C3	3.78	118.16	110.31
2	F	3	AC1	C1-O5-C5	3.76	121.30	112.78
2	G	3	AC1	C1-O5-C5	3.72	121.21	112.78
2	F	1	GLC	O5-C1-C2	3.61	116.73	110.28
2	F	2	GLC	C1-C2-C3	3.46	113.92	109.67
2	H	1	GLC	O1-C1-O5	-3.23	100.70	110.38
2	F	3	AC1	O3-C3-C4	3.13	115.97	109.66
2	G	1	GLC	C1-O5-C5	3.09	119.50	113.66
2	H	3	AC1	O2B-C2B-C1B	2.86	114.87	109.12
2	E	1	GLC	O1-C1-O5	-2.84	101.85	110.38
2	H	3	AC1	C1-C2-C3	2.68	112.97	109.67
2	F	1	GLC	O1-C1-O5	-2.64	102.45	110.38
2	G	1	GLC	O1-C1-O5	-2.63	102.49	110.38
2	E	2	GLC	C1-C2-C3	2.57	112.83	109.67
2	H	3	AC1	C5-C4-N4A	2.55	118.75	111.74
2	E	1	GLC	O5-C1-C2	2.42	114.61	110.28
2	H	2	GLC	C3-C4-C5	2.37	114.46	110.24
2	G	1	GLC	O5-C1-C2	2.31	114.40	110.28
2	E	1	GLC	C1-C2-C3	2.30	115.08	110.31
2	G	2	GLC	C1-C2-C3	2.29	112.48	109.67
2	F	1	GLC	C1-O5-C5	2.22	117.86	113.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	GLC	C2-C3-C4	2.19	114.69	110.89
2	H	3	AC1	O3B-C3B-C2B	2.13	115.28	110.35
2	F	3	AC1	C5-C4-N4A	2.08	117.47	111.74
2	E	3	AC1	C1-C2-C3	2.08	112.22	109.67
2	G	1	GLC	C1-C2-C3	2.07	114.61	110.31
2	E	1	GLC	C1-O5-C5	2.06	117.54	113.66
2	E	2	GLC	C3-C4-C5	-2.02	106.64	110.24
2	F	3	AC1	O3B-C3B-C2B	2.02	115.01	110.35
2	E	2	GLC	O5-C5-C6	2.00	110.34	107.20

There are no chirality outliers.

All (24) torsion outliers are listed below:

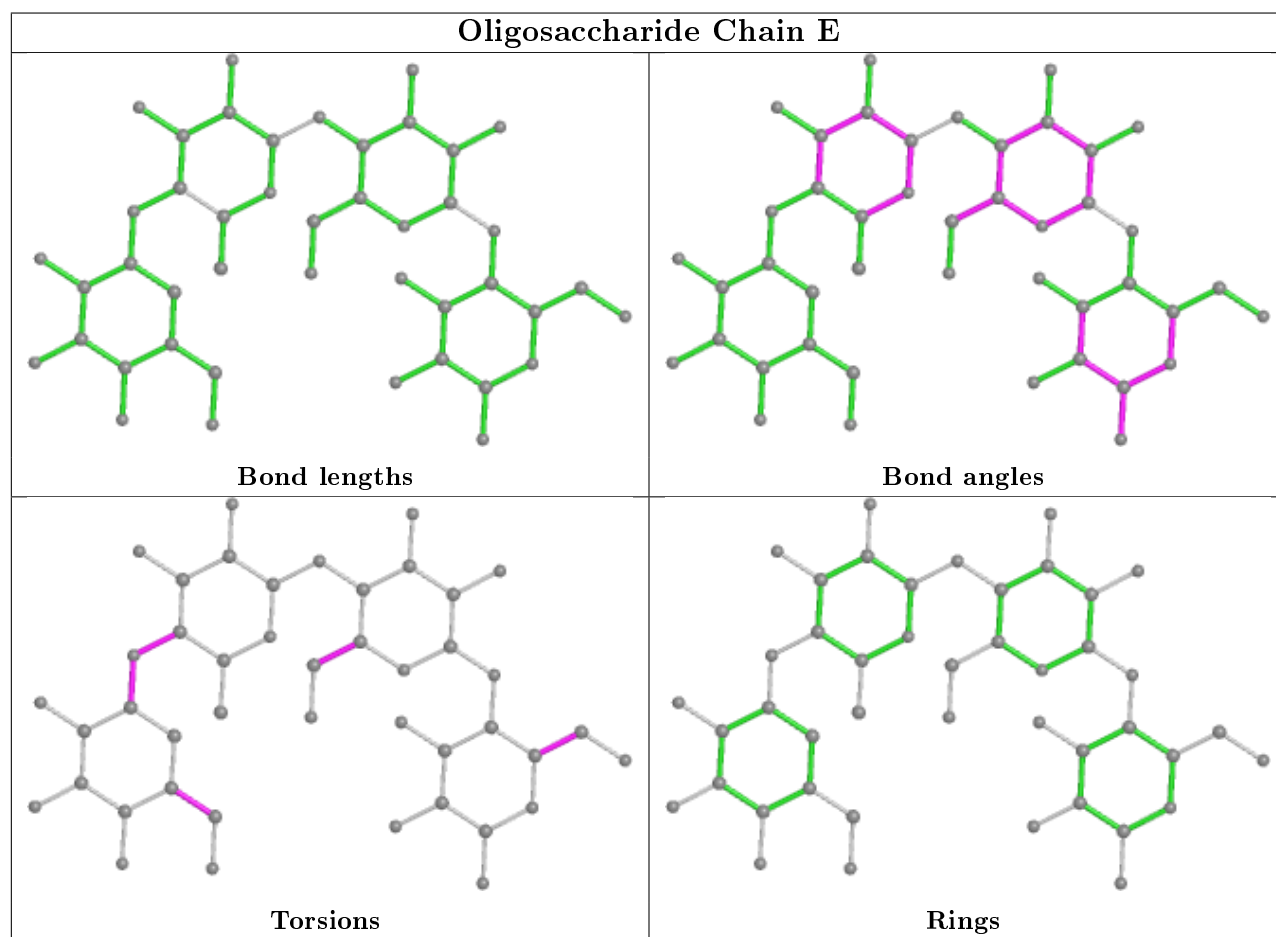
Mol	Chain	Res	Type	Atoms
2	F	3	AC1	C7B-C1B-N4A-C4
2	F	3	AC1	C7B-C5B-C6B-O6B
2	H	3	AC1	C7B-C1B-N4A-C4
2	E	3	AC1	C7B-C1B-N4A-C4
2	E	3	AC1	C4A-C5B-C6B-O6B
2	E	3	AC1	C7B-C5B-C6B-O6B
2	G	3	AC1	C7B-C1B-N4A-C4
2	G	3	AC1	C7B-C5B-C6B-O6B
2	E	2	GLC	O5-C5-C6-O6
2	G	2	GLC	O5-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	G	2	GLC	C4-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
2	F	3	AC1	C3-C4-N4A-C1B
2	H	3	AC1	C3-C4-N4A-C1B
2	E	3	AC1	C3-C4-N4A-C1B
2	G	3	AC1	C3-C4-N4A-C1B
2	G	3	AC1	C5-C4-N4A-C1B
2	F	3	AC1	C4A-C5B-C6B-O6B
2	E	1	GLC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	F	3	AC1	C5-C4-N4A-C1B

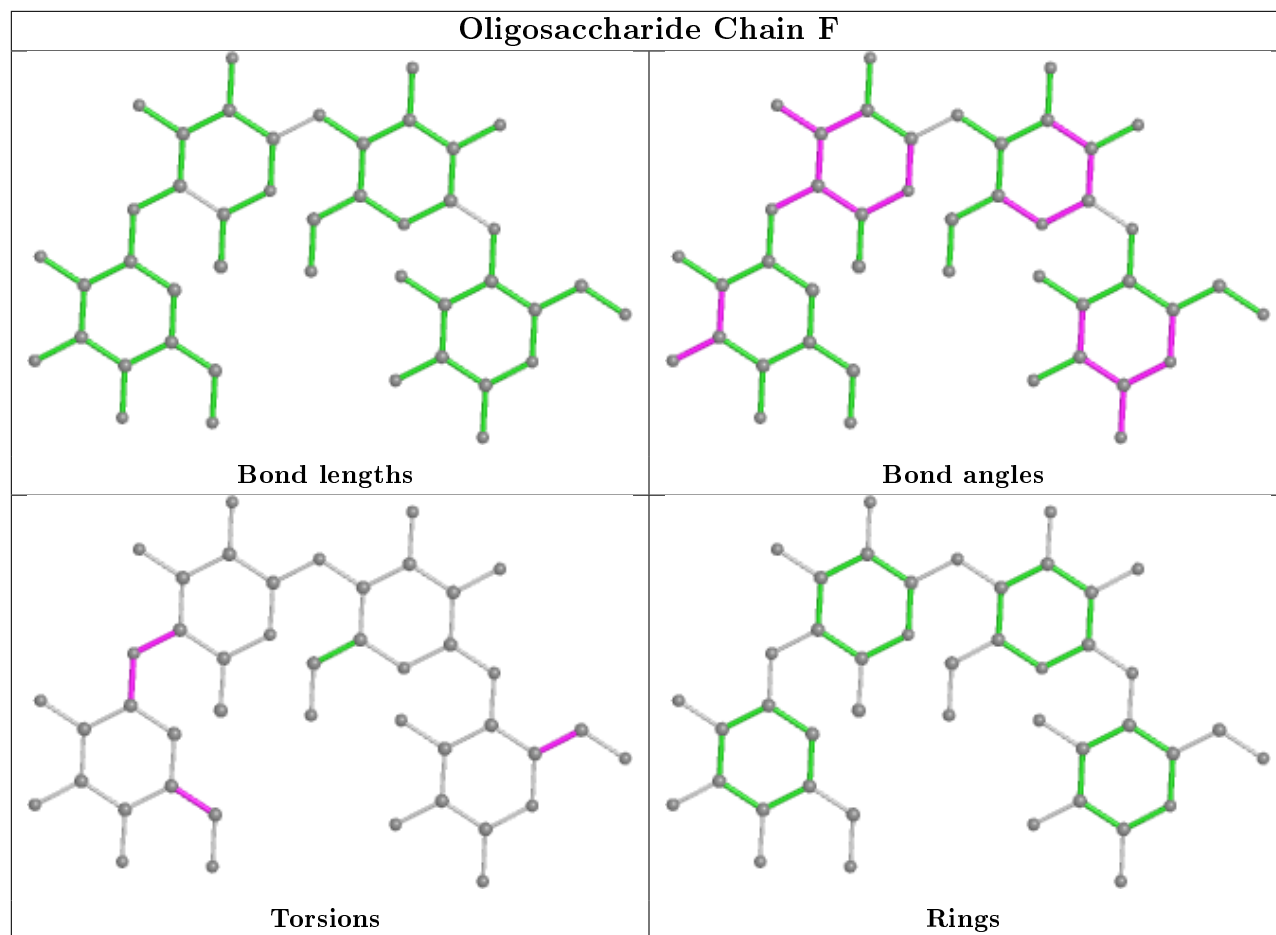
There are no ring outliers.

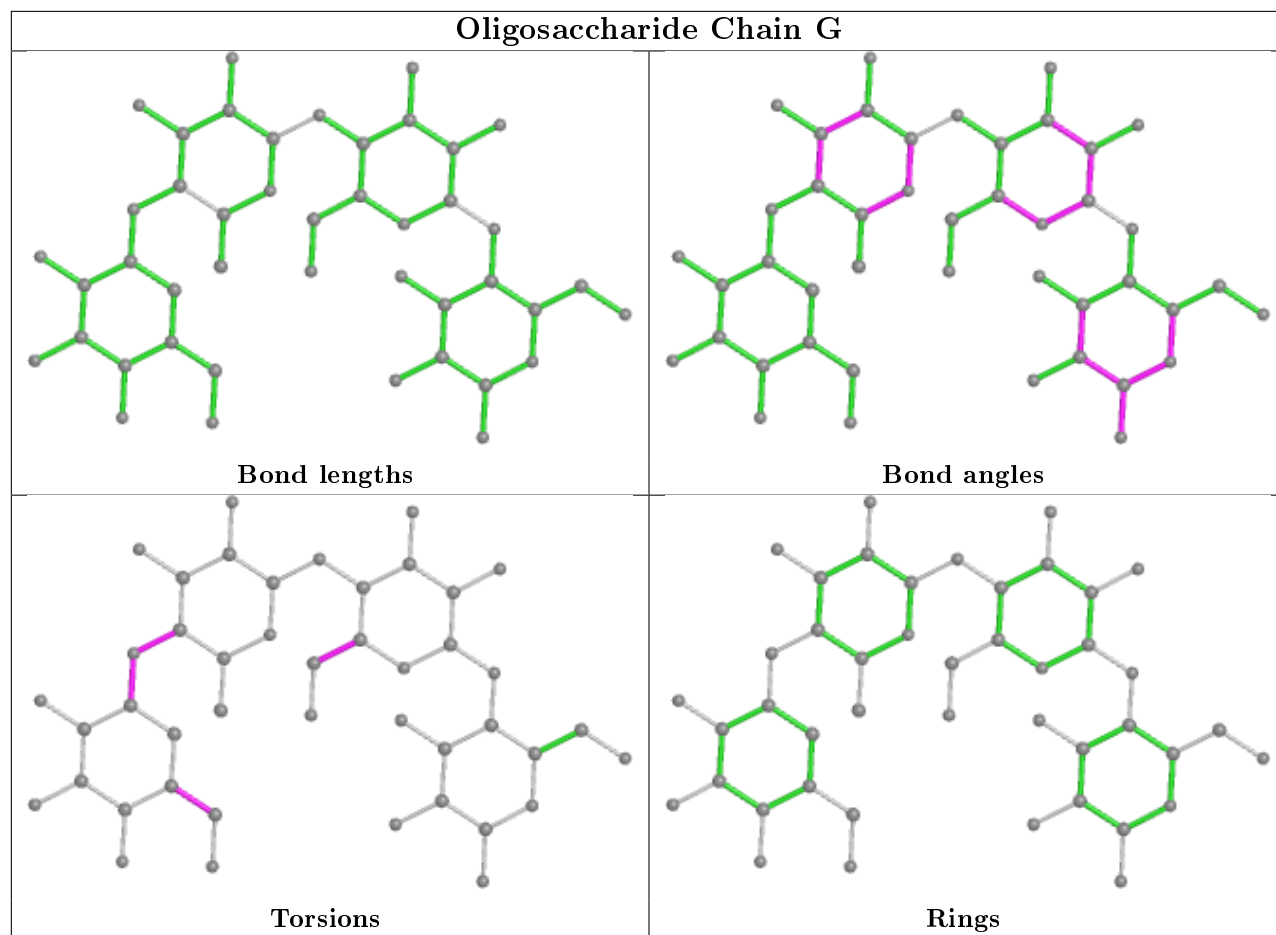
8 monomers are involved in 7 short contacts:

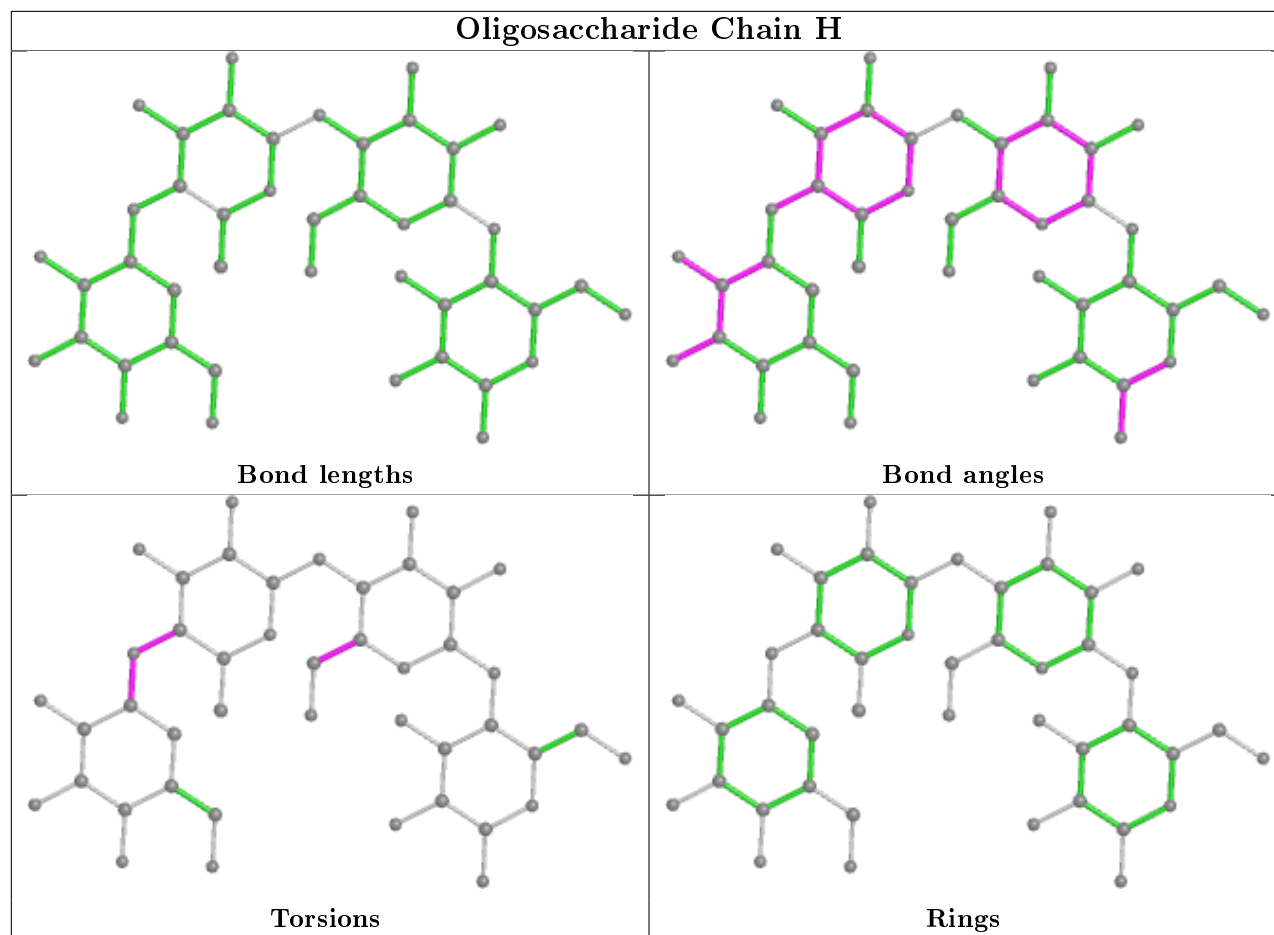
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	AC1	1	0
2	G	1	GLC	1	0
2	F	2	GLC	2	0
2	G	2	GLC	1	0
2	H	3	AC1	1	0
2	H	1	GLC	1	0
2	F	1	GLC	2	0
2	H	2	GLC	2	0

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](#)

There are no ligands in this entry.

## 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	664/666 (99%)	0.12	4 (0%) 89 89	32, 50, 78, 116	1 (0%)
1	B	665/666 (99%)	0.09	11 (1%) 70 70	27, 48, 76, 108	1 (0%)
1	C	665/666 (99%)	-0.15	5 (0%) 86 86	23, 38, 64, 103	2 (0%)
1	D	666/666 (100%)	-0.15	6 (0%) 84 84	22, 38, 68, 111	1 (0%)
All	All	2660/2664 (99%)	-0.02	26 (0%) 82 82	22, 44, 74, 116	5 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-2	SER	8.2
1	C	-1	ASN	3.6
1	B	-1	ASN	3.5
1	B	661	LEU	3.4
1	A	584	ILE	3.2
1	C	326	PHE	3.0
1	C	204	PHE	3.0
1	C	434	MET	2.7
1	D	0	ALA	2.6
1	D	662	THR	2.5
1	B	633	ILE	2.4
1	B	662	THR	2.4
1	B	632	LEU	2.4
1	C	430	LEU	2.3
1	B	341	TRP	2.3
1	D	26	ALA	2.3
1	A	428	ILE	2.2
1	B	35	LYS	2.2
1	B	425	TRP	2.2
1	D	-1	ASN	2.1
1	B	494	ILE	2.1

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	B	277	PHE	2.1
1	A	430	LEU	2.1
1	A	432	LEU	2.0
1	D	188	HIS	2.0
1	B	663	LYS	2.0

## 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](#)

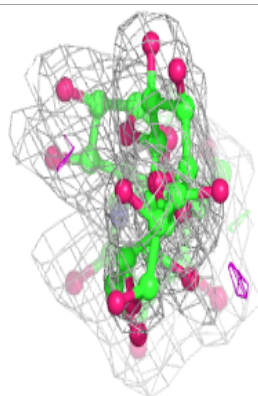
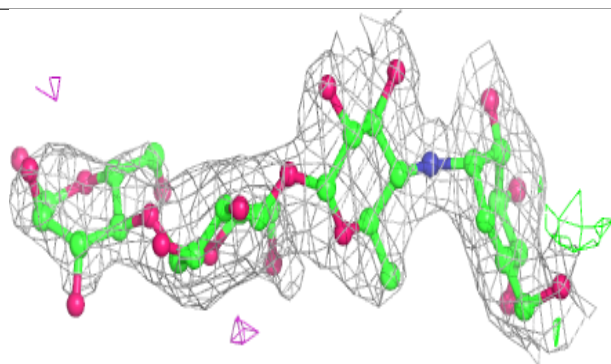
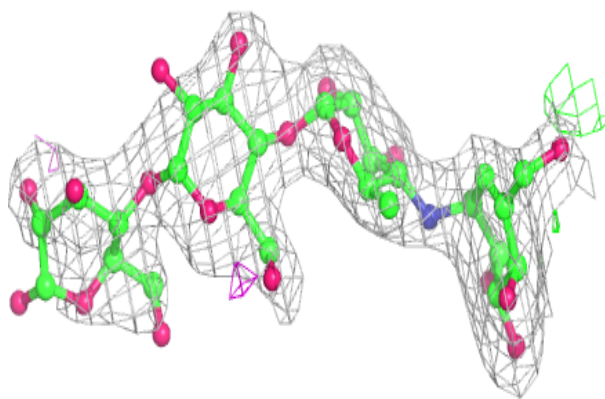
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	GLC	G	1	12/12	0.74	0.26	92,109,125,128	0
2	GLC	F	1	12/12	0.83	0.24	100,107,110,111	0
2	GLC	E	1	12/12	0.84	0.18	95,112,120,120	0
2	GLC	H	1	12/12	0.87	0.23	102,117,121,124	0
2	GLC	F	2	11/12	0.89	0.15	51,71,86,88	0
2	GLC	H	2	11/12	0.90	0.15	58,79,93,94	0
2	GLC	E	2	11/12	0.92	0.11	64,70,84,84	0
2	GLC	G	2	11/12	0.92	0.11	55,71,80,81	0
2	AC1	F	3	21/22	0.94	0.12	38,48,61,65	0
2	AC1	H	3	21/22	0.94	0.13	29,35,44,54	0
2	AC1	G	3	21/22	0.95	0.10	31,39,44,48	0
2	AC1	E	3	21/22	0.97	0.11	32,50,55,65	0

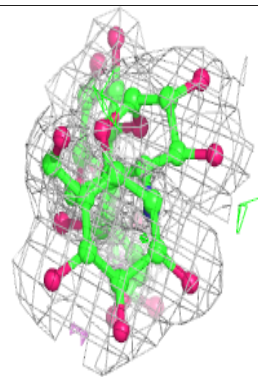
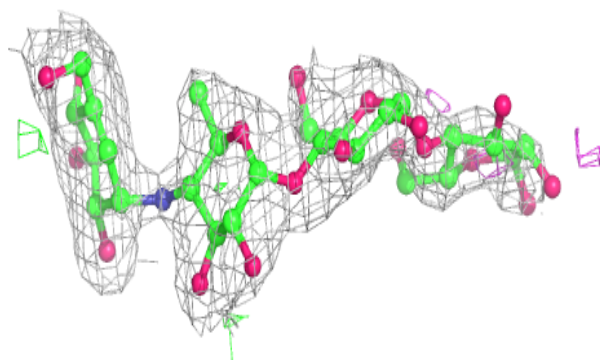
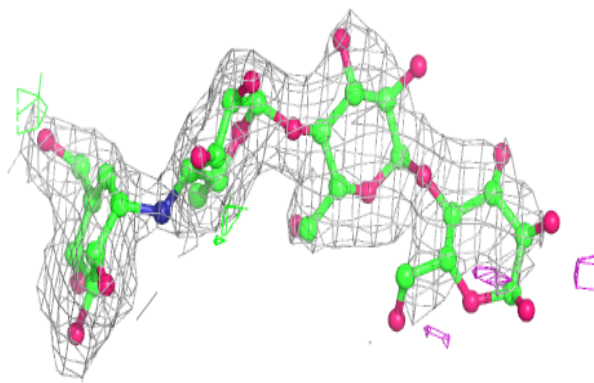
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain E:**

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

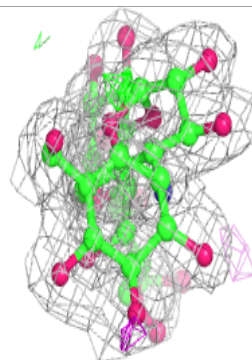
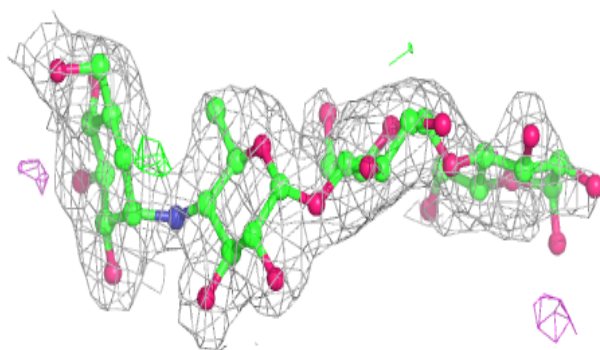
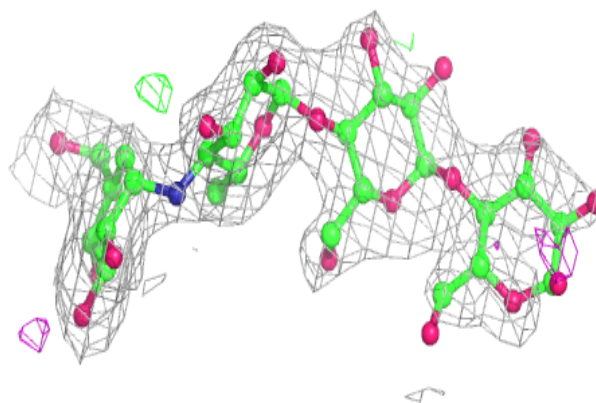
**Electron density around Chain F:**

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

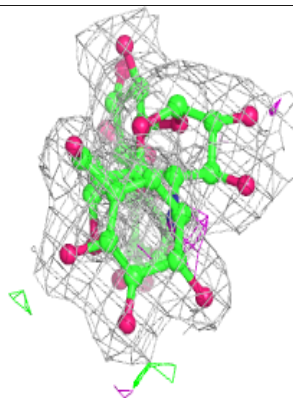
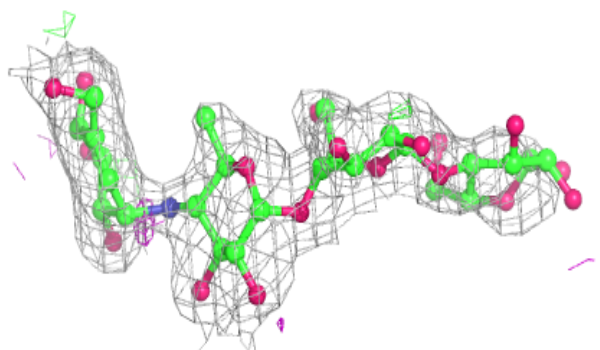
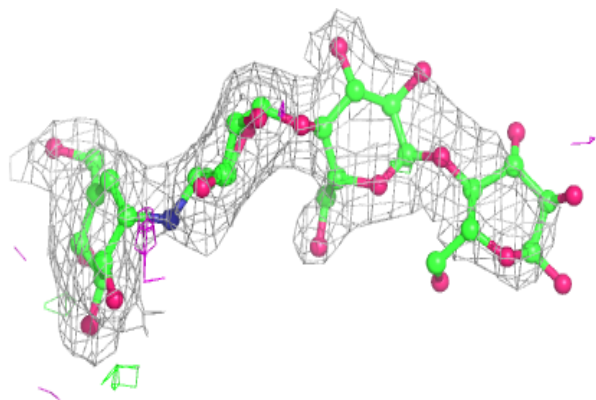


**Electron density around Chain G:**

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

**Electron density around Chain H:**

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



## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.