



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:21 PM UTC

PDB ID : 3PHA / pdb_00003pha
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

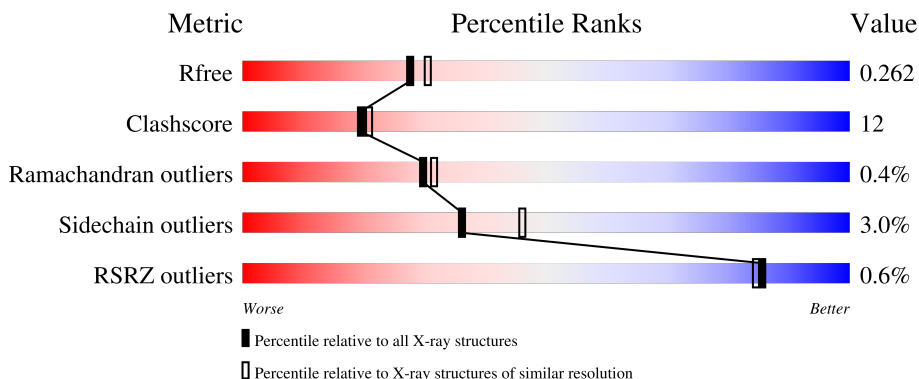
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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 style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">70% 27%</p>
1	B	666	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">75% 24%</p>
1	C	666	<div style="display: flex; align-items: center;"> <div style="width: 73%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">75% 23%</p>
1	D	666	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">75% 23%</p>
2	E	3	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background-color: yellow;"></div> </div> <p style="margin-left: 20px;">100%</p>

Continued on next page...

Continued from previous page...

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

2 Entry composition i

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

There are 16 discrepancies between the modelled and reference sequences:

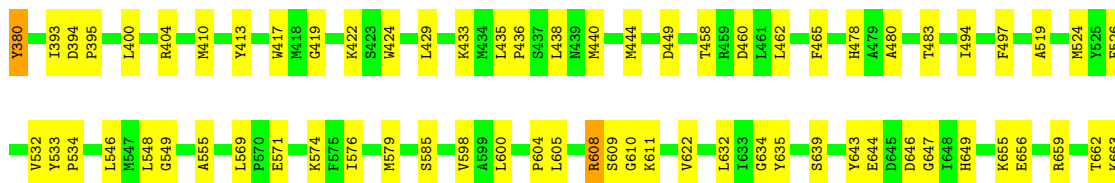
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A5ZY13
A	-1	ASN	-	expression tag	UNP A5ZY13
A	0	ALA	-	expression tag	UNP A5ZY13
A	169	TYR	TRP	engineered mutation	UNP A5ZY13
B	-2	SER	-	expression tag	UNP A5ZY13
B	-1	ASN	-	expression tag	UNP A5ZY13
B	0	ALA	-	expression tag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

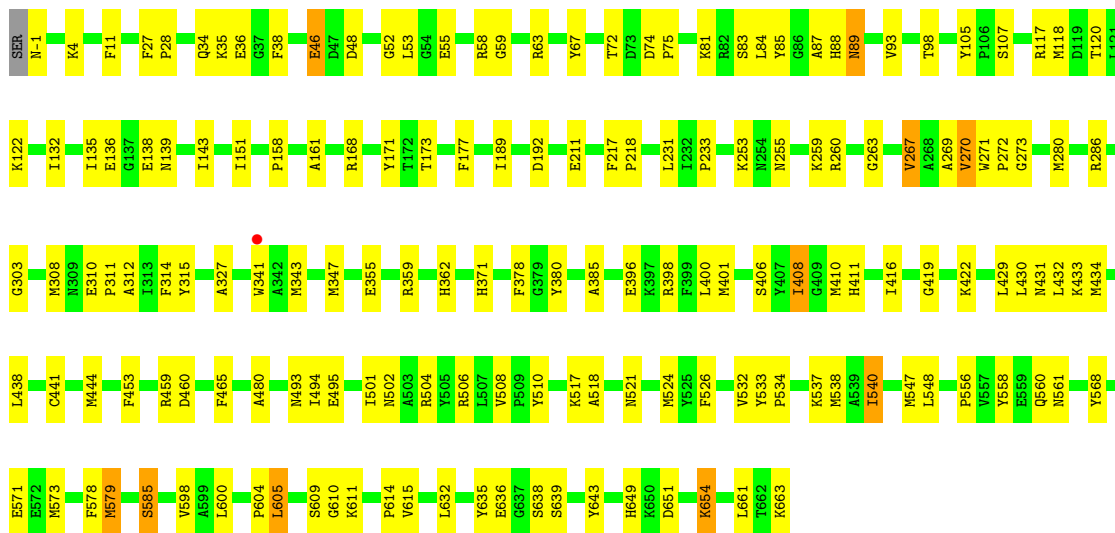
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	F	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	G	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	H	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 3 is water.

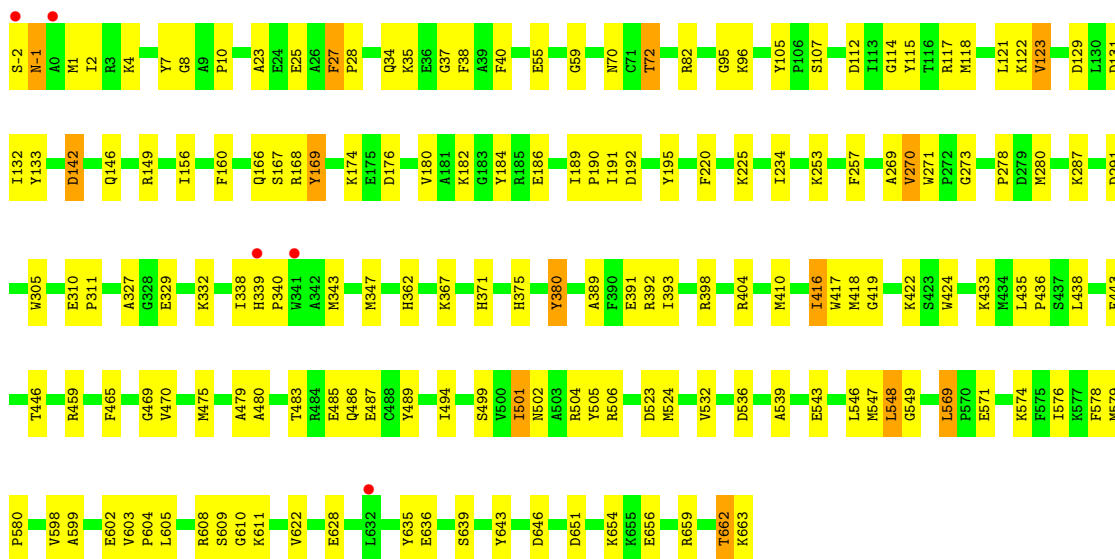
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total	O	0	0
			94	94		
3	B	120	Total	O	0	0
			120	120		
3	C	203	Total	O	0	0
			203	203		
3	D	184	Total	O	0	0
			184	184		




- Molecule 1: alpha-glucosidase



- Molecule 1: alpha-glucosidase



- 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 E:  100%

GLC1
GLC2
AC13

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

Chain F:  100%

GLC1
GLC2
AC13

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

Chain G:  33% 67%

GLC1
GLC2
AC13

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

Chain H:  100%

GLC1
GLC2
AC13

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.03Å 125.95Å 133.58Å 90.00° 107.72° 90.00°	Depositor
Resolution (Å)	42.41 – 2.17 42.41 – 2.17	Depositor EDS
% Data completeness (in resolution range)	90.4 (42.41-2.17) 97.9 (42.41-2.17)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.18Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.200 , 0.265 0.198 , 0.262	Depositor DCC
R_{free} test set	7172 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtrriage
Anisotropy	0.650	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22569	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GLC, AC1

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	0.46	0/5585	0.82	7/7531 (0.1%)
1	B	0.47	0/5592	0.83	10/7541 (0.1%)
1	C	0.50	0/5593	0.83	5/7542 (0.1%)
1	D	0.51	0/5602	0.85	4/7553 (0.1%)
All	All	0.48	0/22372	0.83	26/30167 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	533	TYR	CA-C-N	6.99	127.14	119.87
1	C	533	TYR	C-N-CA	6.99	127.14	119.87
1	A	105	TYR	CA-C-N	6.48	127.94	119.84
1	A	105	TYR	C-N-CA	6.48	127.94	119.84
1	D	27	PHE	CA-C-N	6.33	125.75	118.85
1	D	27	PHE	C-N-CA	6.33	125.75	118.85
1	D	569	LEU	CA-C-N	6.21	126.33	119.87
1	D	569	LEU	C-N-CA	6.21	126.33	119.87
1	A	409	GLY	N-CA-C	-6.14	107.02	113.58
1	B	52	GLY	N-CA-C	6.09	117.71	111.56
1	C	406	SER	N-CA-C	6.00	116.47	108.38
1	B	555	ALA	CA-C-N	5.71	125.64	119.76
1	B	555	ALA	C-N-CA	5.71	125.64	119.76
1	A	613	ILE	CA-C-N	5.68	126.13	119.99
1	A	613	ILE	C-N-CA	5.68	126.13	119.99
1	B	533	TYR	CA-C-N	5.36	125.18	119.28
1	B	533	TYR	C-N-CA	5.36	125.18	119.28
1	B	375	HIS	N-CA-C	5.31	116.76	111.07
1	C	579	MET	CA-C-N	5.15	125.19	119.32
1	C	579	MET	C-N-CA	5.15	125.19	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	PHE	CA-C-N	5.14	124.94	119.28
1	B	27	PHE	C-N-CA	5.14	124.94	119.28
1	A	74	ASP	CA-C-N	5.13	126.14	120.45
1	A	74	ASP	C-N-CA	5.13	126.14	120.45
1	B	9	ALA	CA-C-N	5.04	124.95	119.76
1	B	9	ALA	C-N-CA	5.04	124.95	119.76

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	147	0
1	B	5447	0	5217	119	0
1	C	5448	0	5219	121	0
1	D	5457	0	5226	113	0
2	E	44	0	30	0	0
2	F	44	0	30	3	0
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	5	0
3	C	203	0	0	11	0
3	D	184	0	0	4	0
All	All	22569	0	20995	498	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 (498) 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:C:343:MET:HE3	1:D:343:MET:HE2	1.40	1.02
1:A:270:VAL:HG12	1:A:271:TRP:H	1.24	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:PHE:HB2	1:A:343:MET:HE3	1.49	0.95
1:C:327:ALA:HA	1:C:343:MET:HE1	1.49	0.94
1:D:343:MET:HE3	1:D:347:MET:HE3	1.52	0.89
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	2.13	0.78
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:579:MET:HE2	1:A:585:SER:HB3	1.66	0.75
1:A:576:ILE:HB	1:A:605:LEU:HD13	1.68	0.75
1:C:327:ALA:CA	1:C:343:MET:HE1	2.16	0.74
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: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:C:430:LEU:HG	1:C:434:MET:HE2	1.72	0.71
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:NH2	1:B:267[B]:VAL:HG12	2.05	0.70
1:B:260:ARG:HH21	1:B:267[B]:VAL:HG12	1.55	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
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:A:270:VAL:HG12	1:A:271:TRP:N	2.01	0.68
1:A:323:ALA:HB1	1:A:347:MET:HE1	1.74	0.67
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:A:460:ASP:HB3	1:B:118:MET:HE1	1.78	0.66
1:D:343:MET:CE	1:D:347:MET:HE3	2.23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:TYR:CE2	1:B:107:SER:HB3	2.31	0.65
1:C:327:ALA:CB	1:C:343:MET:HE1	2.27	0.65
1:A:362:HIS:NE2	1:A:371:HIS:HD2	1.94	0.65
1:A:444:MET:HE1	1:A:518:ALA:HB3	1.78	0.65
1:B:267[B]:VAL:HG11	1:B:317:SER:OG	1.95	0.65
1:C:347:MET:HE2	1:D:343:MET:HB3	1.78	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:59:GLY:HA2	1:D:433:LYS:HD3	1.79	0.62
1:D:310:GLU:N	1:D:311:PRO:HA	2.14	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: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:327:ALA:HB2	1:D:343:MET:HE1	1.81	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:327:ALA:HA	1:C:343:MET:CE	2.28	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:-1:ASN:C	1:D:1:MET:H	2.09	0.60
1:D:339:HIS:ND1	1:D:340:PRO:HD2	2.17	0.59
1:D:548:LEU:HD12	1:D:548:LEU:C	2.27	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
1:B:109:LEU:HD12	1:B:125:CYS:HB3	1.85	0.59
1:A:45:ASP:HB3	1:A:48:ASP:CG	2.28	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ALA:C	1:C:88:HIS:HD2	2.11	0.58
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:D:278:PRO:HB2	1:D:280:MET:HE2	1.83	0.58
1:A:460:ASP:HB3	1:B:118:MET:CE	2.33	0.58
1:C:579:MET:HE2	1:C:585:SER:CB	2.33	0.58
1:B:234:ILE:HD11	1:B:307:ASP:CB	2.32	0.58
1:B:417:TRP:CD1	1:B:419:GLY:H	2.22	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:C:610:GLY:C	1:C:611:LYS:HD2	2.29	0.57
1:A:655:LYS:HG3	1:A:656:GLU:OE2	2.04	0.57
1:D:1:MET:HE3	1:D:146:GLN:HE22	1.69	0.57
1:D:40:PHE:HB3	1:D:123:VAL:HG13	1.85	0.57
1:A:224:MET:HA	1:A:224:MET:HE2	1.86	0.57
1:B:404:ARG:HB2	1:B:417:TRP:CH2	2.39	0.57
1:D:639:SER:HG	1:D:662:THR:HG23	1.70	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:A:574:LYS:HG2	1:A:588:VAL:HG22	1.86	0.56
1:B:6:ARG:HD3	1:B:131:ASP:OD1	2.05	0.56
1:B:362:HIS:NE2	1:B:371:HIS:HD2	2.03	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:B:524:MET:HE2	1:B:526:PHE: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:B:126:GLU:CD	1:B:126:GLU:H	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:PHE:C	1:A:38:PHE:CD2	2.85	0.55
1:A:654:LYS:HD2	1:A:654:LYS:N	2.21	0.55
1:C:643:TYR:C	1:C:643:TYR:CD2	2.84	0.55
1:C:231:LEU:O	1:C:233:PRO:HD3	2.07	0.54
1:C:308:MET:HE3	1:C:312:ALA:HB3	1.89	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
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:B:6:ARG:HD2	1:B:10:PRO:HG2	1.90	0.54
1:C:89:ASN:N	1:C:89:ASN:ND2	2.52	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:C:460:ASP:HB3	1:D:118:MET:HE1	1.90	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:B:532:VAL:C	1:B:534:PRO:HD3	2.34	0.53
1:D:610:GLY:C	1:D:611:LYS:HD2	2.34	0.53
1:A:38:PHE:CZ	1:A:132:ILE:HD11	2.43	0.53
1:A:182:LYS:HG3	1:A:186:GLU:CD	2.33	0.53
1:A:306:ASN:CG	1:A:382:MET:HE2	2.34	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:C:579:MET:HE2	1:C:585:SER:HB3	1.90	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:343:MET:HE3	1:B:347:MET:HE3	1.90	0.53
1:B:435:LEU:HB2	1:B:436:PRO:HD3	1.91	0.53
1:A:286:ARG:CG	1:A:385:ALA:HB2	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:579:MET:HE2	1:B:585:SER:OG	2.09	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:A:278:PRO:HB2	1:A:280:MET:HE2	1.92	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:D:380:TYR:CD1	1:D:380:TYR:C	2.88	0.51
1:A:532:VAL:HG21	1:A:547:MET:HG3	1.93	0.51
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:D:-1:ASN:C	1:D:1:MET:N	2.66	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:D:579:MET:HE1	1:D:602:GLU:OE2	2.11	0.51
1:C:35:LYS:HG3	1:C:36:GLU:N	2.26	0.51
1:C:87:ALA:C	1:C:88:HIS:CD2	2.89	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:318:GLU:O	1:B:322:GLU:HG3	2.11	0.51
1:B:610:GLY:C	1:B:611:LYS:HD2	2.37	0.50
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:D:38:PHE:CZ	1:D:132:ILE:HD11	2.46	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:C:444:MET:HE1	1:C:518:ALA:CB	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:VAL:HG21	1:A:633:ILE:HD12	1.94	0.50
1:C:72:THR:HA	3:C:763:HOH:O	2.10	0.50
1:C:638:SER:HB3	3:C:703:HOH:O	2.12	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:D:160:PHE:CD1	1:D:160:PHE:C	2.89	0.49
1:A:121:LEU:HD12	1:A:122:LYS:N	2.27	0.49
1:C:416:ILE:C	1:C:416:ILE:HD12	2.38	0.49
1:B:380:TYR:C	1:B:380:TYR:CD1	2.90	0.49
1:B:444:MET:HE1	1:B:519:ALA:HB2	1.94	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:55:GLU:O	1:D:55:GLU:HG2	2.12	0.49
1:D:329:GLU:HA	1:D:332:LYS:NZ	2.27	0.49
1:A:76:ILE:HG13	1:A:76:ILE:O	2.13	0.49
1:B:323:ALA:HB1	1:B:347:MET:HE1	1.95	0.49
1:C:444:MET:HE1	1:C:518:ALA:HB3	1.95	0.49
1:A:653:ASP:C	1:A:654:LYS:HD2	2.38	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:D:643:TYR:C	1:D:643:TYR:CD2	2.91	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
1:A:568:TYR:C	1:A:569:LEU:HD23	2.38	0.48
1:B:605:LEU:C	1:B:605:LEU:HD12	2.38	0.48
1:C:408:ILE:HD13	1:C:441:CYS:HB3	1.93	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: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:C:38:PHE:C	1:C:38:PHE:CD2	2.91	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:B:643:TYR:C	1:B:643:TYR:CD2	2.91	0.48
1:A:380:TYR:CD1	1:A:380:TYR:C	2.91	0.48
1:A:579:MET:HE2	1:A:585:SER:CB	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:SER:O	1:C:84:LEU:HD23	2.14	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: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:A:28:PRO:HG2	1:A:134:VAL:HG11	1.97	0.47
1:B:267[B]:VAL:CG1	1:B:317:SER:OG	2.62	0.47
1:C:579:MET:HE2	1:C:585:SER:HB2	1.97	0.47
1:B:25:GLU:H	1:B:25:GLU:CD	2.21	0.47
1:B:93:VAL:O	1:B:98:THR:HA	2.15	0.47
1:B:655:LYS:HE2	1:B:656:GLU:OE1	2.15	0.47
1:B:45:ASP:HB3	1:B:48:ASP:OD1	2.14	0.47
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.74	0.47
1:D:501:ILE:O	1:D:504:ARG:HB3	2.15	0.47
1:D:605:LEU:C	1:D:605:LEU:HD12	2.40	0.47
1:A:38:PHE:HZ	1:A:132:ILE:HD11	1.80	0.47
1:A:260:ARG:C	1:A:262:ASP:H	2.22	0.47
1:A:335:GLU:HB2	1:A:337:LYS:HG3	1.97	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
1:D:95:GLY:O	1:D:96:LYS:C	2.58	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:B:197:ASP:OD1	2:F:3:AC1:O4	2.31	0.46
1:C:74:ASP:HA	1:C:75:PRO:HD3	1.74	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: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:524:MET:HE2	1:C:526:PHE:O	2.16	0.46
1:D:176:ASP:O	1:D:180:VAL:HG23	2.15	0.46
1:A:76:ILE:O	1:A:81:LYS:HE3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LYS:HG2	1:A:220:PHE:CE1	2.50	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:11:PHE:C	1:C:11:PHE:CD2	2.94	0.46
1:C:118:MET:HE2	1:D:459:ARG:HH11	1.81	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:D:169:TYR:CD1	1:D:169:TYR:C	2.92	0.46
1:A:48:ASP:O	1:A:63:ARG:HD2	2.16	0.46
1:A:544:ASP:CG	1:A:565:ARG:HH22	2.23	0.46
1:A:418:MET:HE1	1:A:435:LEU:CD2	2.46	0.45
1:B:634:GLY:N	1:B:663:LYS:HE3	2.31	0.45
1:D:417:TRP:CD1	1:D:419:GLY:H	2.33	0.45
1:D:418:MET:HE2	1:D:438:LEU:HD12	1.99	0.45
1:B:271:TRP:HB2	1:B:272:PRO:HD3	1.99	0.45
1:A:418:MET:HE1	1:A:435:LEU:HD23	1.98	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:A:423:SER:C	1:A:461:LEU:HD21	2.40	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:A:477:ASP:C	1:A:477:ASP:OD1	2.60	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: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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:GLY:C	1:D:10:PRO:HD3	2.42	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:C:67:TYR:CD2	1:C:67:TYR:N	2.85	0.44
1:C:270:VAL:HG12	1:C:271:TRP:N	2.30	0.44
1:C:502:ASN:O	1:C:506:ARG:HG3	2.17	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:B:259:LYS:NZ	3:B:700:HOH:O	2.51	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:A:45:ASP:HB3	1:A:48:ASP:OD1	2.17	0.44
1:C:259:LYS:CE	1:C:263:GLY:O	2.65	0.44
1:C:654:LYS:HE3	1:C:654:LYS:CA	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: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:67:TYR:N	1:A:67:TYR:CD2	2.86	0.44
1:A:105:TYR:CE2	1:A:107:SER:HB3	2.53	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: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:A:651:ASP:CG	1:A:654:LYS:HD3	2.44	0.43
1:C:396:GLU:O	1:C:649:HIS:HA	2.17	0.43
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:A:326:PHE:CD2	1:A:343:MET:HE2	2.53	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:PRO:HD2	1:A:303:GLY:O	2.19	0.43
1:A:270:VAL:CG1	1:A:271:TRP:N	2.72	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:8:GLY:C	1:B:10:PRO:HD3	2.44	0.43
1:B:571:GLU:OE2	1:B:608:ARG:HD2	2.18	0.43
1:D:578:PHE:HB3	3:D:675:HOH:O	2.18	0.43
1:C:52:GLY:O	1:C:53:LEU:HB2	2.18	0.43
1:D:4:LYS:HD3	1:D:131:ASP:CG	2.44	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: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:HD12	1:A:462:LEU:O	2.19	0.42
1:C:88:HIS:CD2	1:C:88:HIS:N	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: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:159:LYS:HB2	1:B:647:GLY:HA3	2.01	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:D:4:LYS:HG3	1:D:133:TYR:CZ	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:173:THR:HG22	1:A:213:ASN:ND2	2.34	0.42
1:A:210:ASN:OD1	1:A:210:ASN:C	2.63	0.42
1:C:34:GLN:O	1:C:35:LYS:C	2.63	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: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:53:LEU:O	1:B:54:GLY:C	2.63	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: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:A:330:PHE:CG	1:A:343:MET:HE3	2.56	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:D:646:ASP:OD1	1:D:646:ASP:C	2.63	0.41
1:A:64:GLY:O	1:B:458:THR:HG21	2.21	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
1:B:174:LYS:HG3	1:B:220:PHE:CE1	2.55	0.41
1:B:600:LEU:HD23	1:B:600:LEU:HA	1.87	0.41
1:C:280:MET:O	1:C:286:ARG:HD3	2.19	0.41
1:C:548:LEU:C	1:C:548:LEU:HD23	2.44	0.41
1:C:632:LEU:HD11	1:C:661:LEU:HB3	2.02	0.41
1:D:410:MET:HE2	1:D:443:PHE:HE1	1.85	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:257:PHE:HB2	3:D:758:HOH:O	2.21	0.41
1:A:159:LYS:HG2	1:A:622:VAL:HG11	2.03	0.41
1:A:548:LEU:HB3	1:A:552:ILE:CG1	2.51	0.41
1:C:506:ARG:HB3	1:C:615:VAL:HG13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:GLN:HA	1:D:37:GLY:O	2.19	0.41
1:A:77:HIS:CD2	1:A:77:HIS:N	2.89	0.41
1:A:530:GLY:HA2	1:A:540:ILE:HG22	2.01	0.41
1:A:548:LEU:HD23	1:A:548:LEU:C	2.46	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:B:449:ASP:CG	1:B:478:HIS:HB3	2.46	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:69:SER:OG	1:A:89:ASN:ND2	2.54	0.41
1:A:175:GLU:O	1:A:176:ASP:C	2.63	0.41
1:A:457:THR:HG22	1:A:458:THR:N	2.34	0.41
1:B:310:GLU:H	1:B:310:GLU:CD	2.29	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:D:469:GLY:C	1:D:475:MET:HG3	2.46	0.41
1:A:429:LEU:HD22	1:A:558:TYR:CE1	2.56	0.40
1:B:394:ASP:C	1:B:394:ASP:OD1	2.63	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:A:239:VAL:HG12	1:A:245:TYR:HE2	1.86	0.40
1:B:319:GLY:HA3	3:B:767:HOH:O	2.21	0.40
1:B:548:LEU:HD23	1:B:548:LEU:C	2.46	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:87:ALA:C	1:A:88:HIS:CD2	2.99	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
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: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:A:260:ARG:C	1:A:262:ASP:N	2.79	0.40
1:B:81:LYS:HA	1:B:81:LYS:HD3	1.90	0.40
1:B:532:VAL:O	1:B:534:PRO:HD3	2.21	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%)	36	39
1	B	664/666 (100%)	615 (93%)	48 (7%)	1 (0%)	43	49
1	C	664/666 (100%)	622 (94%)	39 (6%)	3 (0%)	24	25
1	D	665/666 (100%)	627 (94%)	34 (5%)	4 (1%)	21	20
All	All	2656/2664 (100%)	2481 (93%)	165 (6%)	10 (0%)	30	31

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
1	A	604	PRO
1	D	270	VAL
1	C	598	VAL
1	D	191	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	574/575 (100%)	557 (97%)	17 (3%)	36	46
1	B	575/575 (100%)	564 (98%)	11 (2%)	50	63
1	C	575/575 (100%)	554 (96%)	21 (4%)	30	38
1	D	576/575 (100%)	556 (96%)	20 (4%)	32	40
All	All	2300/2300 (100%)	2231 (97%)	69 (3%)	36	46

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	121	LEU
1	A	175	GLU
1	A	185	ARG
1	A	239	VAL
1	A	253	LYS
1	A	267	VAL
1	A	364	VAL
1	A	380	TYR
1	A	405	SER
1	A	417	TRP
1	A	465	PHE
1	A	521	ASN
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	126	GLU
1	B	174	LYS
1	B	253	LYS
1	B	270	VAL
1	B	305	TRP
1	B	380	TYR
1	B	465	PHE
1	B	569	LEU
1	B	608	ARG
1	C	-1	ASN
1	C	4	LYS
1	C	46	GLU
1	C	89	ASN
1	C	136	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	192	ASP
1	C	211	GLU
1	C	267	VAL
1	C	341	TRP
1	C	401	MET
1	C	408	ILE
1	C	422	LYS
1	C	465	PHE
1	C	495	GLU
1	C	508	VAL
1	C	540	ILE
1	C	585	SER
1	C	604	PRO
1	C	605	LEU
1	C	636	GLU
1	C	654	LYS
1	D	-2	SER
1	D	-1	ASN
1	D	2	ILE
1	D	35	LYS
1	D	72	THR
1	D	123	VAL
1	D	142	ASP
1	D	253	LYS
1	D	367	LYS
1	D	380	TYR
1	D	391	GLU
1	D	416	ILE
1	D	465	PHE
1	D	485	GLU
1	D	501	ILE
1	D	548	LEU
1	D	569	LEU
1	D	628	GLU
1	D	659	ARG
1	D	662	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	127	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	166	GLN
1	A	344	GLN
1	A	371	HIS
1	A	411	HIS
1	A	521	ASN
1	A	550	ASN
1	A	631	GLN
1	B	89	ASN
1	B	127	ASN
1	B	146	GLN
1	B	213	ASN
1	B	227	GLN
1	B	282	ASN
1	B	306	ASN
1	B	344	GLN
1	B	371	HIS
1	B	431	ASN
1	C	-1	ASN
1	C	34	GLN
1	C	88	HIS
1	C	89	ASN
1	C	166	GLN
1	C	188	HIS
1	C	202	GLN
1	C	344	GLN
1	C	371	HIS
1	C	493	ASN
1	C	550	ASN
1	C	561	ASN
1	D	34	GLN
1	D	77	HIS
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 [i](#)

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

5.5 Carbohydrates [i](#)

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	0.57	0	17,17,17	1.40	4 (23%)
2	GLC	E	2	2	11,11,12	0.46	0	15,15,17	1.49	2 (13%)
2	AC1	E	3	2	21,22,23	0.62	0	22,32,34	1.19	1 (4%)
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	1.40	2 (13%)
2	AC1	F	3	2	21,22,23	0.76	0	22,32,34	1.53	4 (18%)
2	GLC	G	1	2	12,12,12	0.55	0	17,17,17	1.33	4 (23%)
2	GLC	G	2	2	11,11,12	0.48	0	15,15,17	1.54	1 (6%)
2	AC1	G	3	2	21,22,23	0.68	0	22,32,34	1.23	1 (4%)
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	2.02	4 (26%)
2	AC1	H	3	2	21,22,23	0.85	0	22,32,34	1.54	5 (22%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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 (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	GLC	C1-O5-C5	5.13	119.06	112.19
2	G	2	GLC	C1-O5-C5	4.77	118.58	112.19
2	H	2	GLC	C1-C2-C3	4.15	115.69	109.64
2	E	2	GLC	C1-O5-C5	4.02	117.57	112.19
2	F	2	GLC	C1-O5-C5	3.92	117.44	112.19
2	F	1	GLC	C1-C2-C3	3.83	118.16	110.36
2	H	3	AC1	C1-O5-C5	3.74	121.80	112.97
2	E	3	AC1	C1-O5-C5	3.66	121.60	112.97
2	F	1	GLC	O5-C1-C2	3.66	116.73	110.30
2	F	3	AC1	C1-O5-C5	3.53	121.30	112.97
2	G	3	AC1	C1-O5-C5	3.49	121.21	112.97
2	H	1	GLC	O1-C1-O5	-3.27	100.70	110.41
2	F	3	AC1	O3-C3-C4	3.21	115.97	109.58
2	G	1	GLC	C1-O5-C5	3.02	119.50	113.65
2	H	3	AC1	O2B-C2B-C1B	2.94	114.87	109.08
2	F	2	GLC	C1-C2-C3	2.93	113.92	109.64
2	E	1	GLC	O1-C1-O5	-2.88	101.85	110.41
2	F	1	GLC	O1-C1-O5	-2.68	102.45	110.41
2	G	1	GLC	O1-C1-O5	-2.67	102.49	110.41
2	H	3	AC1	C5-C4-N4A	2.55	118.75	111.74
2	E	1	GLC	O5-C1-C2	2.45	114.61	110.30
2	H	2	GLC	C3-C4-C5	2.33	114.46	110.23
2	G	1	GLC	O5-C1-C2	2.33	114.40	110.30
2	E	1	GLC	C1-C2-C3	2.32	115.08	110.36
2	H	3	AC1	C1-C2-C3	2.28	112.97	109.64
2	E	2	GLC	C1-C2-C3	2.19	112.83	109.64
2	H	2	GLC	C2-C3-C4	2.18	114.69	110.86
2	F	1	GLC	C1-O5-C5	2.18	117.86	113.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	GLC	C1-C2-C3	2.09	114.61	110.36
2	H	3	AC1	O3B-C3B-C2B	2.08	115.28	110.38
2	F	3	AC1	C5-C4-N4A	2.08	117.47	111.74
2	F	3	AC1	O2B-C2B-C1B	2.06	113.13	109.08
2	E	1	GLC	C1-O5-C5	2.01	117.54	113.65

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

There are no ring outliers.

8 monomers are involved in 7 short contacts:

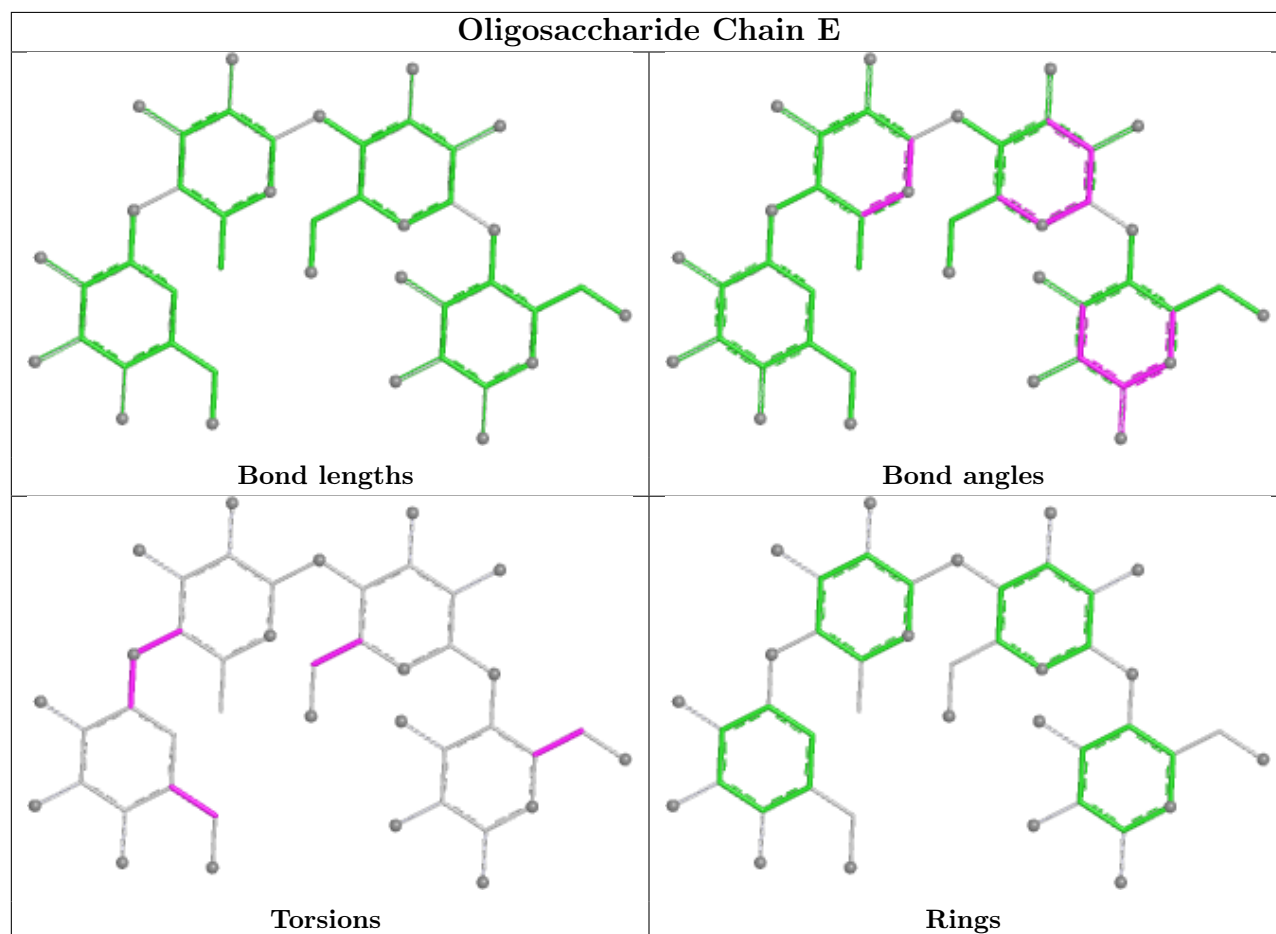
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	AC1	1	0
2	H	2	GLC	2	0

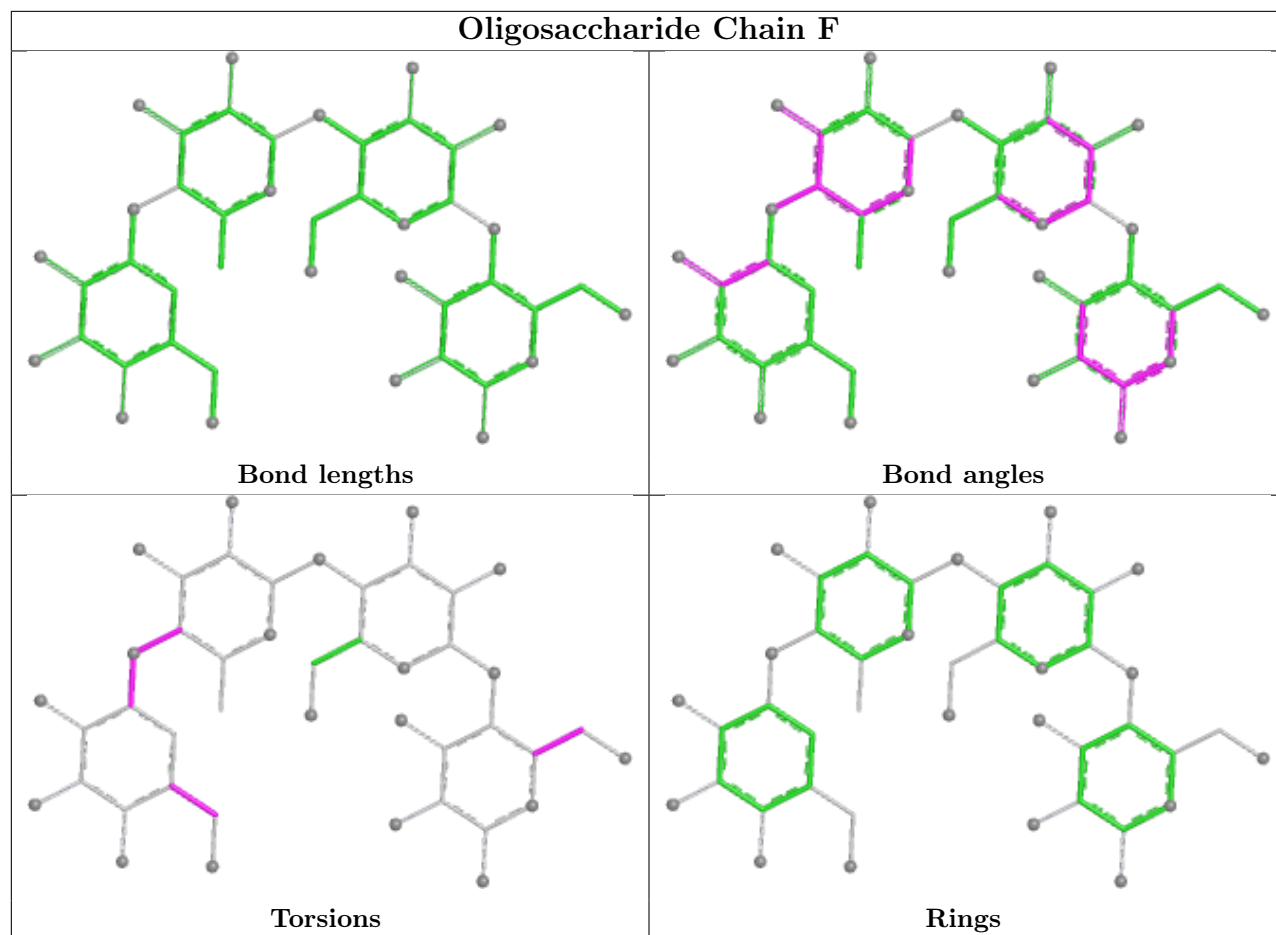
Continued on next page...

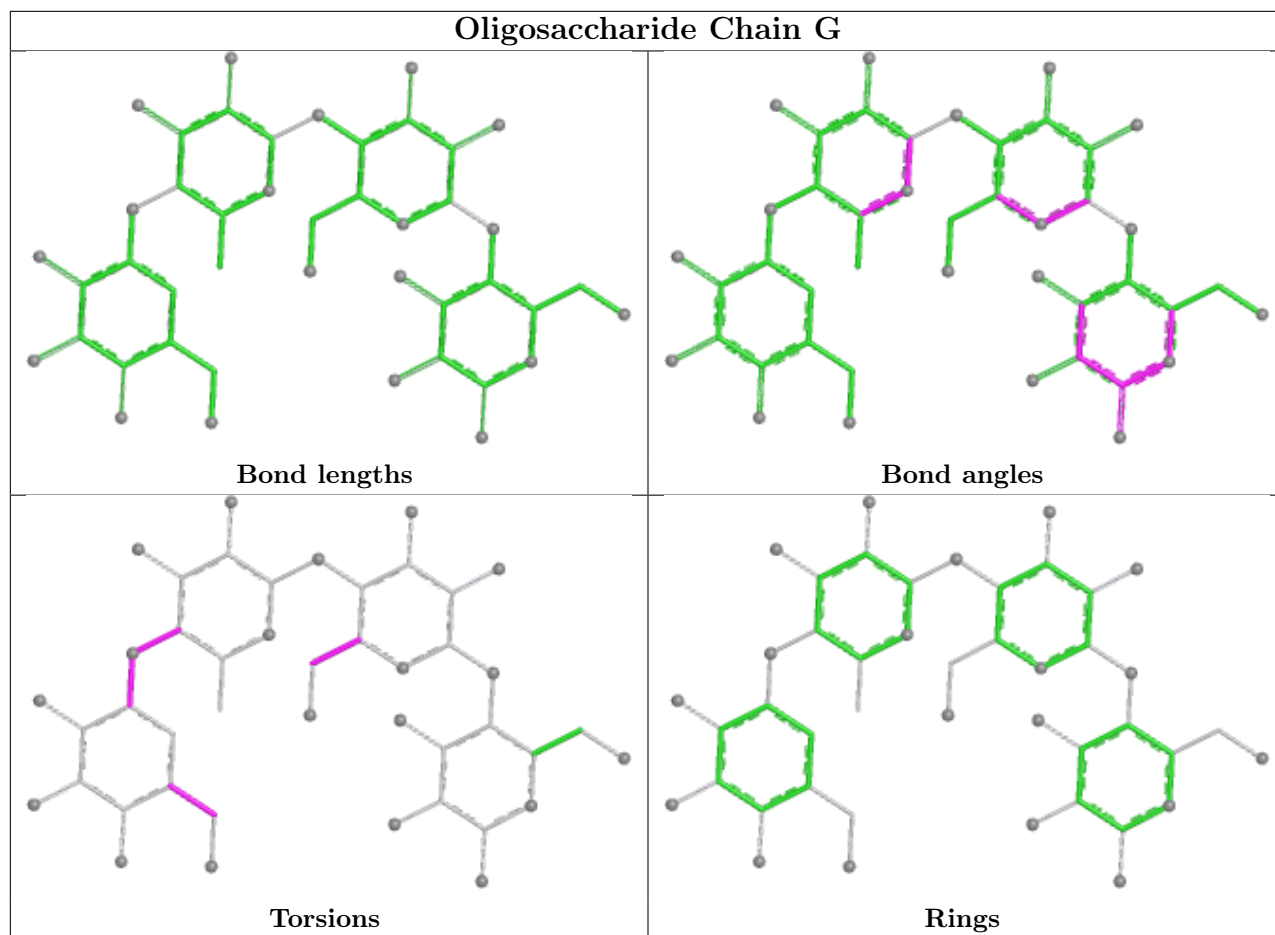
Continued from previous page...

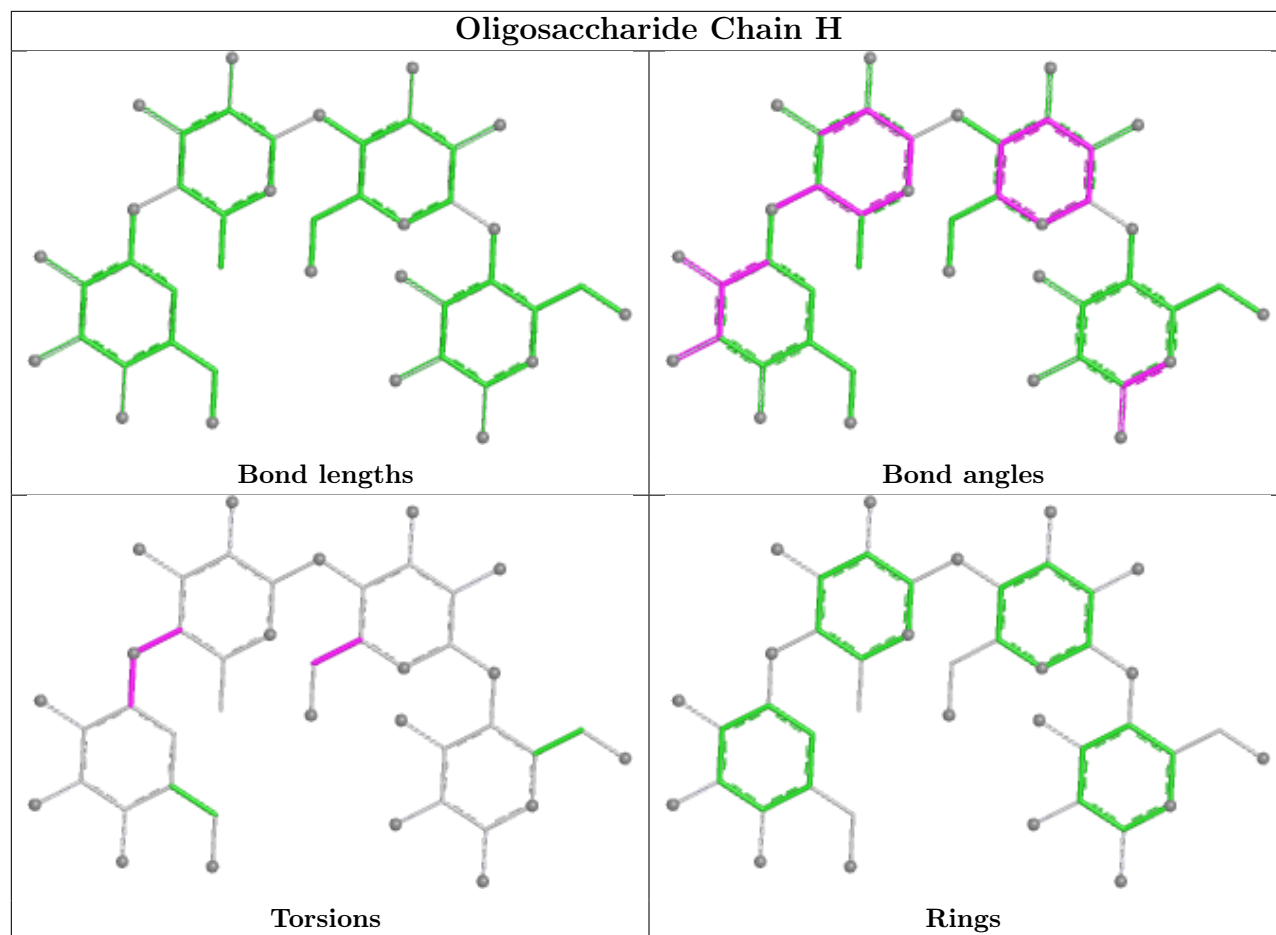
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	GLC	1	0
2	F	2	GLC	2	0
2	G	2	GLC	1	0
2	H	3	AC1	1	0
2	G	1	GLC	1	0
2	F	1	GLC	2	0

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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	664/666 (99%)	0.21	7 (1%) 78 77	32, 50, 78, 116	1 (0%)
1	B	665/666 (99%)	0.17	4 (0%) 85 84	27, 48, 76, 108	2 (0%)
1	C	665/666 (99%)	-0.14	1 (0%) 91 90	19, 38, 64, 103	2 (0%)
1	D	666/666 (100%)	-0.16	5 (0%) 82 82	22, 38, 68, 111	2 (0%)
All	All	2660/2664 (99%)	0.02	17 (0%) 85 84	19, 44, 74, 116	7 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-2	SER	3.9
1	A	1	MET	2.9
1	D	0	ALA	2.8
1	B	0	ALA	2.8
1	D	341	TRP	2.7
1	A	0	ALA	2.7
1	A	341	TRP	2.7
1	D	339	HIS	2.5
1	B	277	PHE	2.5
1	B	341	TRP	2.5
1	D	632	LEU	2.2
1	C	341	TRP	2.2
1	A	584	ILE	2.1
1	A	369[A]	ILE	2.1
1	B	191	ILE	2.1
1	A	9	ALA	2.1
1	A	343	MET	2.0

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

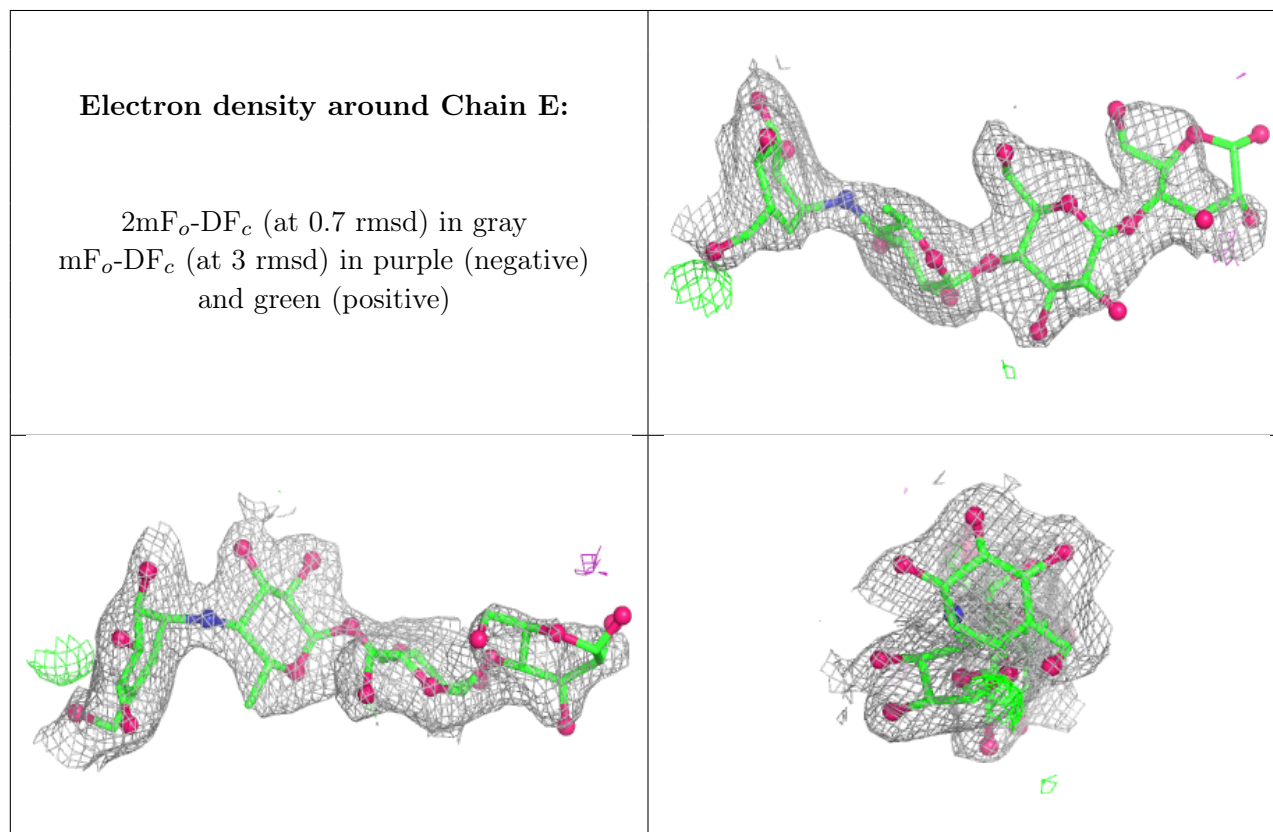
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

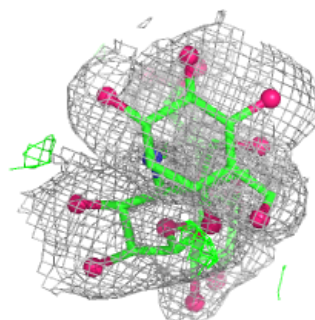
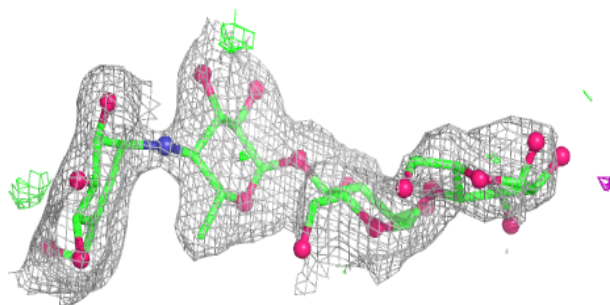
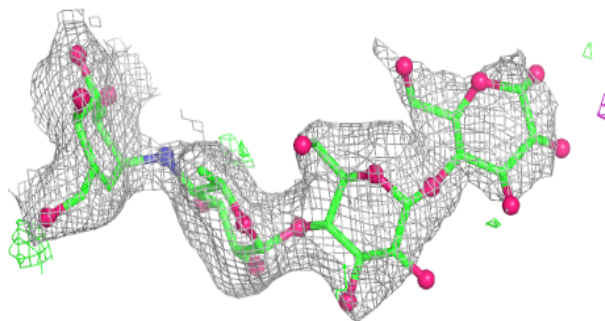
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	F	1	12/12	0.69	0.15	100,107,110,111	0
2	GLC	G	1	12/12	0.77	0.16	92,109,125,128	0
2	GLC	H	1	12/12	0.78	0.14	102,117,121,124	0
2	GLC	E	1	12/12	0.82	0.12	95,112,120,120	0
2	GLC	H	2	11/12	0.82	0.12	58,79,93,94	0
2	GLC	E	2	11/12	0.83	0.10	64,70,84,84	0
2	GLC	F	2	11/12	0.85	0.11	51,71,86,88	0
2	GLC	G	2	11/12	0.85	0.10	55,71,80,81	0
2	AC1	F	3	21/22	0.92	0.08	38,48,61,65	0
2	AC1	H	3	21/22	0.92	0.08	29,35,44,54	0
2	AC1	G	3	21/22	0.94	0.08	31,39,44,48	0
2	AC1	E	3	21/22	0.94	0.08	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.

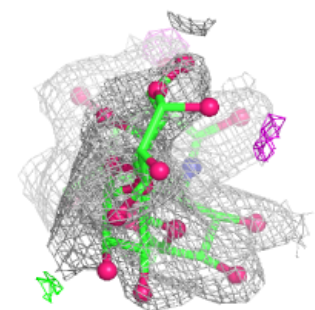
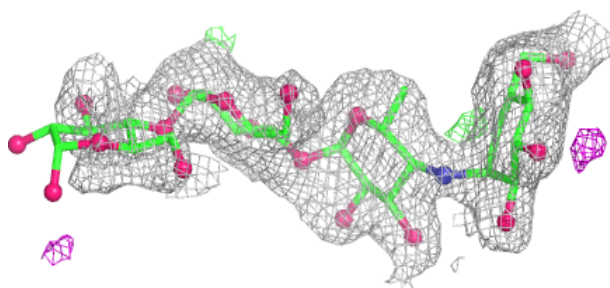
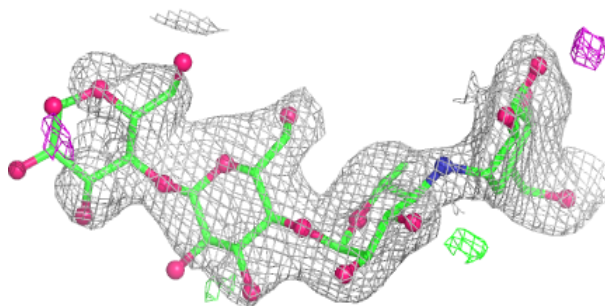


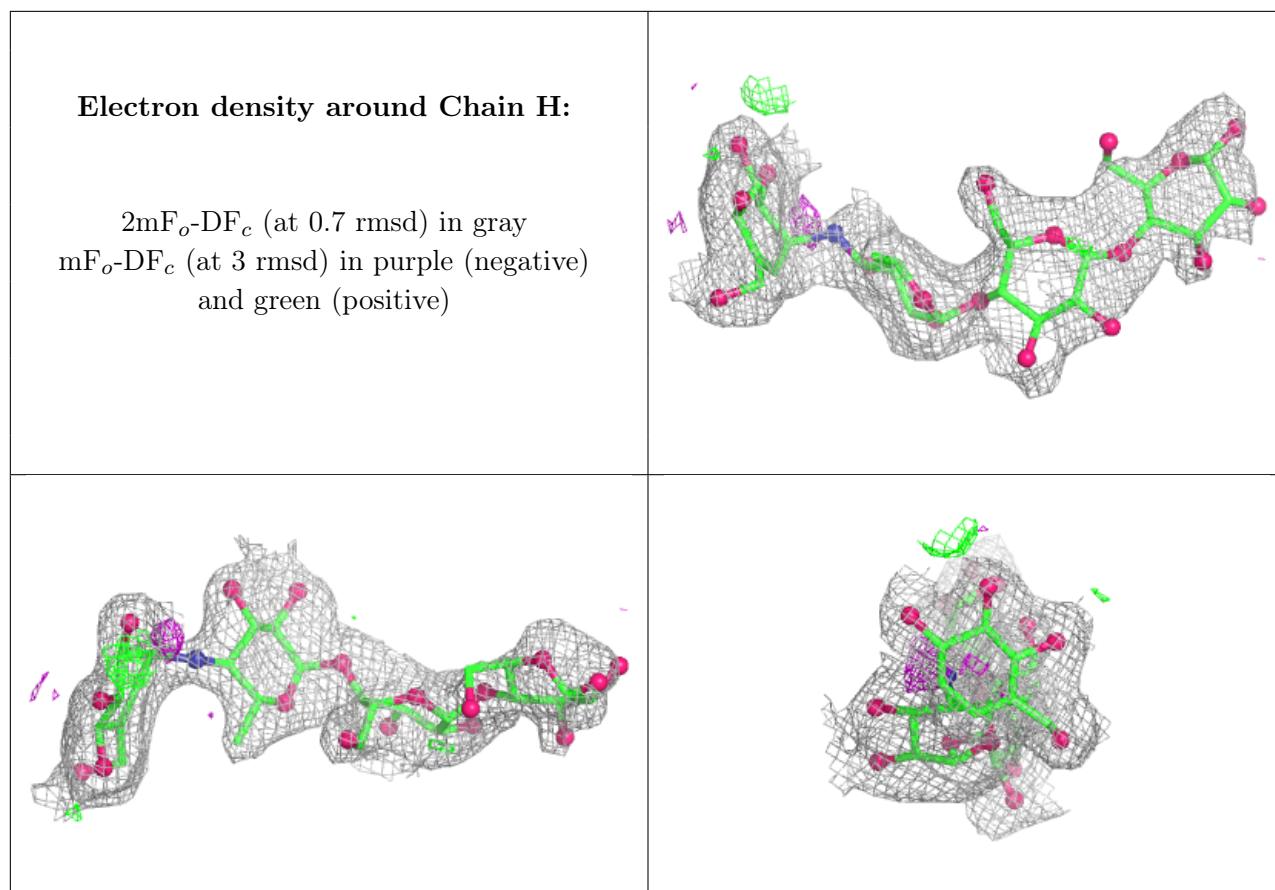
Electron density around Chain F:

$2mF_o-DF_c$ (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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.