



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:25 AM BST

PDB ID : 4PQK  
Title : C-Terminal domain of DNA binding protein  
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.K.  
Deposited on : 2014-03-03  
Resolution : 3.40 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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

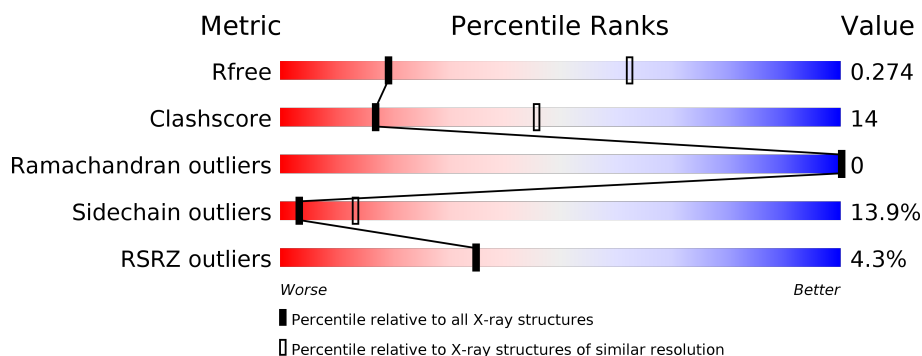
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	487	<div> <div>3%</div> <div>64%</div> <div>30%</div> <div>• •</div> </div>
1	B	487	<div> <div>4%</div> <div>70%</div> <div>26%</div> <div>• •</div> </div>
1	C	487	<div> <div>5%</div> <div>68%</div> <div>25%</div> <div>5% •</div> </div>
1	D	487	<div> <div>5%</div> <div>63%</div> <div>28%</div> <div>6% •</div> </div>
2	E	3	<div> <div>33%</div> <div>67%</div> </div>
2	F	3	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	3	 <div>67%33%</div>
2	H	3	 <div>100%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	E	3	-	-	X	-

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 14876 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 Maltose ABC transporter periplasmic protein, Truncated replication protein RepA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3700	2371	603	713	13			
1	B	479	Total	C	N	O	S	0	0	0
			3722	2392	615	703	12			
1	C	476	Total	C	N	O	S	0	0	0
			3648	2346	601	690	11			
1	D	472	Total	C	N	O	S	0	0	0
			3670	2351	601	707	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP U6NJU2
B	1	MET	-	expression tag	UNP U6NJU2
C	1	MET	-	expression tag	UNP U6NJU2
D	1	MET	-	expression tag	UNP U6NJU2

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



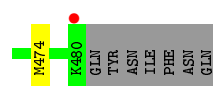
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			34	18	16			
2	F	3	Total	C	O	0	0	0
			34	18	16			
2	G	3	Total	C	O	0	0	0
			34	18	16			

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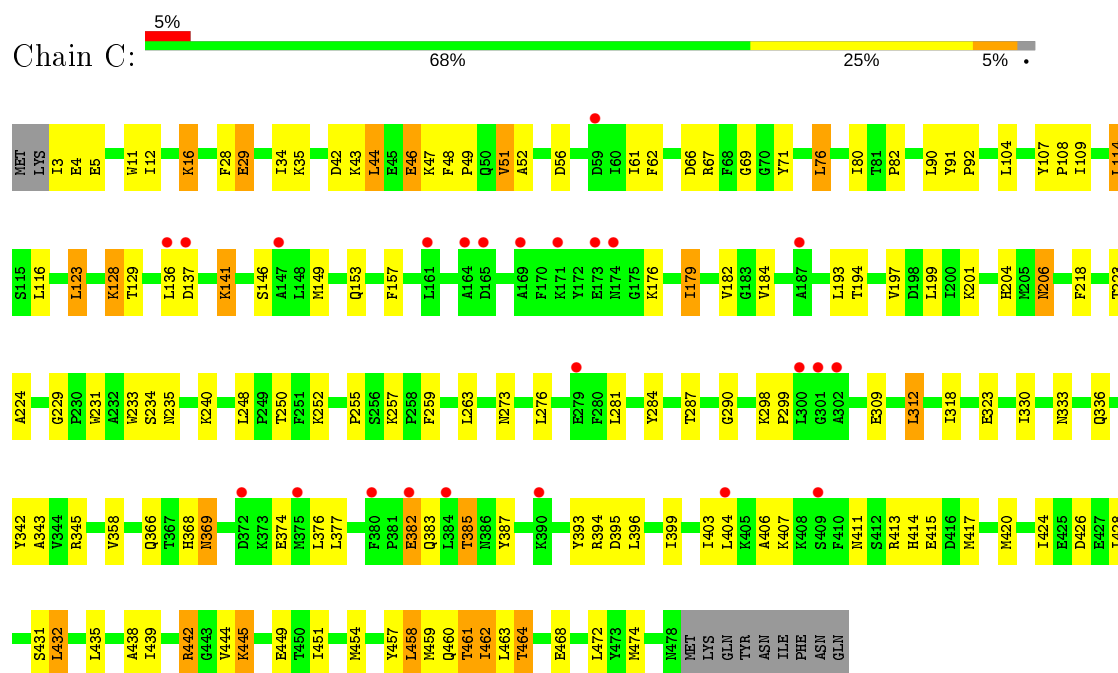
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	3	Total	C	O	0	0	0
			34	18	16			

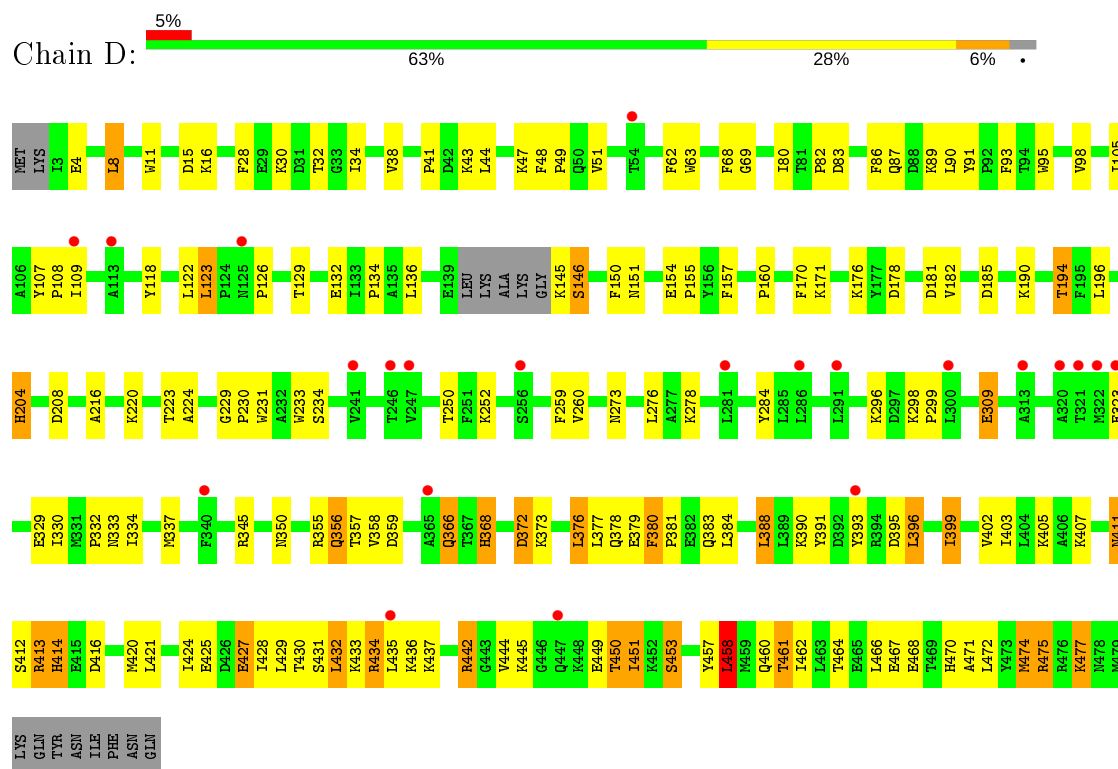




- Molecule 1: Maltose ABC transporter periplasmic protein, Truncated replication protein RepA



- Molecule 1: Maltose ABC transporter periplasmic protein, Truncated replication protein RepA



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranos
- e

Chain E:  33% 67%

GLC1  
GLC2  
GLC3

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:  100%

GLC1  
GLC2  
GLC3

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G:  67% 33%

GLC1  
GLC2  
GLC3

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H:  100%

GLC1  
GLC2  
GLC3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.22Å 93.67Å 100.81Å 107.67° 108.30° 84.93°	Depositor
Resolution (Å)	46.62 – 3.40 46.62 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.62-3.40) 67.2 (46.62-3.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.237 , 0.275 0.241 , 0.274	Depositor DCC
$R_{free}$ test set	1963 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.9	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 25.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	14876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/3784	0.57	0/5142
1	B	0.44	0/3805	0.54	0/5157
1	C	0.43	0/3730	0.63	1/5063 (0.0%)
1	D	0.45	0/3751	0.65	2/5090 (0.0%)
All	All	0.44	0/15070	0.60	3/20452 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	8	LEU	CA-CB-CG	5.36	127.62	115.30
1	D	458	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	463	LEU	CA-CB-CG	5.02	126.84	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	3700	0	3562	116	0
1	B	3722	0	3663	87	0
1	C	3648	0	3540	85	0
1	D	3670	0	3560	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	34	0	29	7	0
2	F	34	0	30	7	0
2	G	34	0	29	5	0
2	H	34	0	30	6	0
All	All	14876	0	14443	411	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 14.

All (411) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3:GLC:O5	2:G:3:GLC:C5	1.63	1.46
2:E:3:GLC:O5	2:E:3:GLC:C5	1.64	1.45
2:H:3:GLC:O5	2:H:3:GLC:C5	1.64	1.43
2:F:3:GLC:C5	2:F:3:GLC:O5	1.64	1.41
2:F:3:GLC:C1	2:F:3:GLC:O5	1.72	1.38
2:E:3:GLC:O5	2:E:3:GLC:C1	1.73	1.37
2:G:3:GLC:C1	2:G:3:GLC:O5	1.71	1.36
2:H:3:GLC:O5	2:H:3:GLC:C1	1.71	1.36
1:A:155:PRO:HD3	1:A:345:ARG:HG3	1.36	1.05
1:C:413:ARG:HG2	1:C:414:HIS:CE1	1.93	1.03
1:A:129:THR:HG22	1:A:250:THR:OG1	1.61	1.00
1:A:272:PRO:HG2	1:A:273:ASN:ND2	1.79	0.97
1:B:144:GLY:O	1:B:145:LYS:NZ	2.03	0.91
1:B:377:LEU:HD21	1:B:396:LEU:HD21	1.52	0.90
1:C:403:ILE:HD12	1:C:428:ILE:HD13	1.52	0.89
2:E:3:GLC:C5	2:E:3:GLC:C1	2.51	0.88
1:A:420:MET:CE	1:A:420:MET:HA	2.06	0.85
2:G:3:GLC:C1	2:G:3:GLC:C5	2.54	0.85
2:F:3:GLC:C1	2:F:3:GLC:C5	2.56	0.84
1:A:420:MET:HE2	1:A:420:MET:HA	1.59	0.84
1:A:155:PRO:CD	1:A:345:ARG:HG3	2.07	0.83
1:B:424:ILE:HG22	1:B:428:ILE:HG13	1.60	0.83
1:A:421:LEU:HD12	1:A:421:LEU:H	1.42	0.83
1:D:80:ILE:HG22	1:D:82:PRO:HD3	1.62	0.80
1:C:16:LYS:NZ	1:C:263:LEU:HD22	1.96	0.80
1:A:376:LEU:HD11	1:A:400:LYS:HD2	1.63	0.79
2:H:3:GLC:C5	2:H:3:GLC:C1	2.60	0.78
1:B:170:PHE:CD2	1:B:334:ILE:HD11	2.18	0.78
1:C:11:TRP:HB3	1:C:44:LEU:HD12	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:HD3	1:A:345:ARG:CG	2.16	0.75
1:D:462:ILE:O	1:D:466:LEU:HD12	1.86	0.75
1:D:91:TYR:HE2	1:D:309:GLU:HG3	1.52	0.75
1:B:420:MET:HE3	1:B:421:LEU:H	1.52	0.75
1:B:407:LYS:O	1:B:411:ASN:ND2	2.20	0.74
1:B:296:LYS:HB3	1:B:296:LYS:HZ2	1.51	0.73
1:C:5:GLU:O	1:C:273:ASN:ND2	2.20	0.73
1:D:146:SER:HB2	1:D:223:THR:HG23	1.69	0.73
1:B:296:LYS:HB3	1:B:296:LYS:NZ	2.03	0.73
1:C:342:TYR:HD1	1:C:345:ARG:HH21	1.37	0.72
1:D:430:THR:O	1:D:434:ARG:HG2	1.88	0.72
1:C:16:LYS:HZ2	1:C:263:LEU:HD22	1.53	0.72
1:C:47:LYS:O	1:C:51:VAL:HG22	1.88	0.72
1:C:399:ILE:HD11	1:C:451:ILE:HG12	1.73	0.71
1:B:336:GLN:HE21	1:B:373:LYS:HG3	1.55	0.71
1:A:391:TYR:HB2	1:A:396:LEU:HD12	1.72	0.71
1:D:16:LYS:NZ	2:H:1:GLC:O2	2.24	0.70
1:D:368:HIS:O	1:D:368:HIS:ND1	2.23	0.70
1:D:402:VAL:HG11	1:D:458:LEU:HG	1.72	0.70
1:C:179:ILE:H	1:C:179:ILE:HD12	1.57	0.70
1:D:34:ILE:HD13	1:D:276:LEU:HD21	1.71	0.69
1:B:382:GLU:O	1:B:385:THR:HG22	1.92	0.69
1:B:80:ILE:HG22	1:B:82:PRO:HD3	1.74	0.68
1:D:388:LEU:HB3	1:D:396:LEU:HD11	1.75	0.68
1:D:414:HIS:HD2	1:D:470:HIS:CD2	2.11	0.68
1:B:240:LYS:HA	1:C:240:LYS:HG3	1.74	0.68
1:A:155:PRO:HG3	1:A:345:ARG:HA	1.77	0.67
1:B:378:GLN:HG2	1:B:379:GLU:HG2	1.75	0.66
1:C:431:SER:OG	1:C:462:ILE:HG22	1.95	0.66
1:A:168:TYR:CE1	1:A:183:GLY:HA3	2.31	0.65
1:B:391:TYR:H	1:B:391:TYR:HD2	1.44	0.65
1:B:303:VAL:HG22	1:B:312:LEU:HD12	1.79	0.65
1:A:67:ARG:NH2	2:E:3:GLC:O3	2.30	0.65
1:B:72:ALA:HB2	1:B:105:ILE:HG21	1.79	0.65
1:D:444:VAL:O	1:D:445:LYS:HB2	1.98	0.64
1:B:377:LEU:HD21	1:B:396:LEU:CD2	2.26	0.63
1:D:475:ARG:HH11	1:D:475:ARG:HG2	1.63	0.63
1:A:51:VAL:HB	1:A:56:ASP:OD2	1.98	0.63
1:B:97:ALA:HB2	1:B:330:ILE:HD11	1.81	0.63
1:C:206:ASN:N	1:C:206:ASN:OD1	2.31	0.62
1:A:129:THR:HG22	1:A:250:THR:HG1	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:ASP:OD1	1:C:451:ILE:CG2	2.48	0.62
1:A:410:PHE:HE2	1:A:419:TYR:CD1	2.18	0.62
1:B:129:THR:HG22	1:B:132:GLU:HG3	1.80	0.62
1:D:182:VAL:O	1:D:366:GLN:NE2	2.32	0.62
1:B:355:ARG:HG3	1:B:355:ARG:HH11	1.64	0.61
1:D:332:PRO:O	1:D:337:MET:HG3	2.01	0.61
1:D:403:ILE:HD12	1:D:428:ILE:HD13	1.81	0.61
1:D:413:ARG:HB2	1:D:414:HIS:ND1	2.15	0.61
1:A:410:PHE:HE2	1:A:419:TYR:CE1	2.18	0.61
1:D:69:GLY:HA3	1:D:333:ASN:O	2.01	0.61
1:D:384:LEU:HD23	1:D:425:GLU:HB2	1.82	0.61
1:A:376:LEU:HD13	1:A:376:LEU:O	2.01	0.60
1:B:424:ILE:CG2	1:B:428:ILE:HG13	2.30	0.60
1:D:98:VAL:O	1:D:105:ILE:HG13	2.01	0.60
1:A:450:THR:HG23	1:A:453:SER:H	1.66	0.60
1:C:137:ASP:OD2	1:C:204:HIS:HA	2.02	0.59
1:C:458:LEU:O	1:C:462:ILE:HG23	2.02	0.59
1:A:49:PRO:HG3	1:A:71:TYR:CE1	2.38	0.59
1:C:69:GLY:HA3	1:C:333:ASN:O	2.01	0.59
2:G:3:GLC:C6	2:G:3:GLC:O5	2.47	0.59
1:A:334:ILE:HG12	1:A:337:MET:HG2	1.84	0.59
1:C:343:ALA:HB2	1:C:369:ASN:ND2	2.18	0.59
1:C:80:ILE:HG22	1:C:82:PRO:HD3	1.84	0.59
1:D:462:ILE:HG22	1:D:466:LEU:HD11	1.85	0.59
1:A:345:ARG:NH2	2:E:3:GLC:O6	2.36	0.59
1:A:135:ALA:O	1:A:139:GLU:HG3	2.04	0.58
1:A:169:ALA:O	1:A:170:PHE:CD2	2.57	0.57
1:A:410:PHE:CE2	1:A:419:TYR:CD1	2.92	0.57
1:B:131:GLU:OE1	1:B:131:GLU:N	2.38	0.57
1:A:246:THR:OG1	1:A:247:VAL:N	2.36	0.57
1:B:380:PHE:HD1	1:B:384:LEU:HD12	1.70	0.57
1:A:391:TYR:HB2	1:A:396:LEU:CD1	2.34	0.57
1:D:414:HIS:CD2	1:D:470:HIS:CD2	2.91	0.57
1:D:4:GLU:O	1:D:273:ASN:ND2	2.30	0.57
1:C:182:VAL:HG12	1:C:184:VAL:HG23	1.87	0.56
1:D:414:HIS:NE2	1:D:467:GLU:OE2	2.35	0.56
1:C:34:ILE:HD13	1:C:276:LEU:HD21	1.88	0.56
1:A:350:ASN:HB3	1:A:356:GLN:HG2	1.88	0.56
1:A:410:PHE:CE2	1:A:419:TYR:CE1	2.94	0.56
1:D:442:ARG:HG2	1:D:449:GLU:HG2	1.87	0.56
1:A:130:TRP:HA	1:A:133:ILE:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLY:HA2	1:A:251:PHE:CE2	2.41	0.56
1:D:381:PRO:HG2	1:D:384:LEU:HB2	1.86	0.56
1:B:336:GLN:NE2	1:B:373:LYS:HG3	2.21	0.55
1:D:407:LYS:HG3	1:D:424:ILE:HD12	1.88	0.55
1:C:444:VAL:O	1:C:445:LYS:HD3	2.06	0.55
1:C:457:TYR:O	1:C:461:THR:OG1	2.23	0.55
1:C:48:PHE:HA	1:C:51:VAL:CG2	2.36	0.55
1:D:123:LEU:HD22	1:D:224:ALA:HB1	1.88	0.55
1:A:272:PRO:HG2	1:A:273:ASN:HD21	1.70	0.55
1:B:130:TRP:HB3	1:B:195:PHE:HE2	1.71	0.55
1:B:170:PHE:CE2	1:B:334:ILE:HD11	2.42	0.55
1:C:90:LEU:HD23	1:C:108:PRO:HG2	1.87	0.55
1:D:428:ILE:HG22	1:D:432:LEU:HD12	1.89	0.55
1:A:381:PRO:O	1:A:385:THR:HG23	2.07	0.54
1:D:134:PRO:HA	1:D:204:HIS:CD2	2.42	0.54
1:A:209:THR:HA	1:A:213:ILE:HD12	1.89	0.54
1:B:391:TYR:N	1:B:391:TYR:CD2	2.73	0.54
1:C:435:LEU:HD21	1:C:451:ILE:HD13	1.88	0.54
1:D:372:ASP:OD1	1:D:372:ASP:N	2.40	0.54
1:B:49:PRO:HG3	1:B:71:TYR:CE1	2.42	0.54
1:D:155:PRO:HG3	1:D:345:ARG:HA	1.89	0.54
1:D:185:ASP:O	1:D:190:LYS:NZ	2.41	0.54
1:D:399:ILE:HD11	1:D:451:ILE:HD11	1.90	0.54
1:B:172:TYR:HE1	1:B:175:GLY:HA2	1.73	0.54
1:B:65:HIS:CE1	1:B:331:MET:HB2	2.43	0.54
1:A:46:GLU:O	1:A:49:PRO:HD2	2.08	0.54
1:D:395:ASP:OD1	1:D:451:ILE:CG2	2.56	0.54
1:A:373:LYS:O	1:A:377:LEU:HG	2.07	0.53
1:B:443:GLY:HA2	1:B:447:GLN:O	2.07	0.53
1:B:218:PHE:HA	1:B:223:THR:HG22	1.89	0.53
1:C:229:GLY:HA3	1:C:231:TRP:CH2	2.44	0.53
1:B:65:HIS:CD2	1:B:97:ALA:HB1	2.43	0.53
1:C:16:LYS:HZ1	1:C:263:LEU:HD22	1.72	0.53
1:D:457:TYR:O	1:D:461:THR:OG1	2.25	0.53
1:B:66:ASP:OD1	1:B:66:ASP:N	2.40	0.53
1:C:439:ILE:HD11	1:C:454:MET:HG3	1.91	0.53
1:D:260:VAL:HB	1:D:330:ILE:HD13	1.91	0.53
1:D:129:THR:OG1	1:D:132:GLU:HG3	2.08	0.52
1:D:178:ASP:OD2	1:D:181:ASP:HB2	2.09	0.52
1:D:230:PRO:HA	1:D:233:TRP:CE2	2.44	0.52
1:C:29:GLU:HG3	1:C:35:LYS:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:PRO:HG3	1:B:71:TYR:HE1	1.74	0.52
1:D:118:TYR:CE1	1:D:126:PRO:HD3	2.45	0.52
1:D:378:GLN:O	1:D:379:GLU:HG2	2.09	0.52
1:B:378:GLN:NE2	1:B:379:GLU:H	2.07	0.52
1:B:414:HIS:NE2	1:B:467:GLU:OE2	2.39	0.52
1:C:128:LYS:HD2	1:C:128:LYS:N	2.24	0.52
1:D:384:LEU:O	1:D:388:LEU:HD12	2.10	0.52
1:B:287:THR:HG23	1:B:290:GLY:H	1.73	0.52
1:D:47:LYS:O	1:D:51:VAL:HG22	2.09	0.52
1:A:29:GLU:OE2	1:A:35:LYS:HD3	2.10	0.51
1:A:115:SER:OG	1:A:324:ASN:ND2	2.43	0.51
1:C:234:SER:HB3	1:C:299:PRO:HD3	1.93	0.51
1:C:116:LEU:HB2	1:C:248:LEU:HD23	1.92	0.51
1:C:406:ALA:HB3	1:C:462:ILE:HD11	1.93	0.51
1:B:129:THR:CG2	1:B:132:GLU:HG3	2.39	0.51
1:D:134:PRO:HA	1:D:204:HIS:HD2	1.75	0.51
1:D:471:ALA:O	1:D:475:ARG:HB2	2.11	0.51
2:E:2:GLC:O3	2:E:3:GLC:O2	2.28	0.51
1:C:312:LEU:HB3	1:C:318:ILE:HD13	1.93	0.51
2:H:3:GLC:O5	2:H:3:GLC:C6	2.51	0.51
1:D:407:LYS:O	1:D:411:ASN:HB2	2.11	0.51
1:D:424:ILE:O	1:D:427:GLU:HG2	2.11	0.51
1:A:155:PRO:CG	1:A:345:ARG:HG3	2.41	0.50
1:C:179:ILE:H	1:C:179:ILE:CD1	2.18	0.50
1:A:399:ILE:HG23	1:A:458:LEU:HD21	1.93	0.50
1:A:424:ILE:HG23	1:A:466:LEU:HD21	1.93	0.50
1:D:32:THR:HG22	1:D:34:ILE:HD12	1.93	0.50
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.46	0.50
1:A:155:PRO:HG3	1:A:345:ARG:CA	2.41	0.50
1:A:129:THR:HB	1:A:131:GLU:HG2	1.94	0.50
1:D:424:ILE:HD13	1:D:466:LEU:HD21	1.94	0.50
1:D:86:PHE:O	1:D:89:LYS:HB2	2.12	0.50
1:A:368:HIS:ND1	1:A:369:ASN:N	2.60	0.50
1:B:144:GLY:C	1:B:145:LYS:HZ3	2.11	0.50
1:A:192:GLY:HA2	1:A:251:PHE:HE2	1.76	0.50
1:B:69:GLY:HA3	1:B:333:ASN:O	2.11	0.50
1:B:399:ILE:O	1:B:403:ILE:HG12	2.12	0.50
1:C:413:ARG:HG2	1:C:414:HIS:ND1	2.25	0.49
1:C:407:LYS:O	1:C:411:ASN:HB2	2.12	0.49
1:A:182:VAL:HG12	1:A:184:VAL:HG23	1.94	0.49
1:A:148:LEU:HD22	1:A:150:PHE:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TRP:HB3	1:A:68:PHE:HE1	1.77	0.49
1:A:195:PHE:O	1:A:198:ASP:HB2	2.12	0.49
1:D:391:TYR:HB2	1:D:396:LEU:HD12	1.94	0.49
1:A:471:ALA:O	1:A:475:ARG:HG3	2.12	0.49
1:C:218:PHE:HA	1:C:223:THR:HG22	1.95	0.49
1:B:439:ILE:HG23	1:B:449:GLU:HB3	1.94	0.49
1:C:123:LEU:HD11	1:C:224:ALA:HB1	1.95	0.49
1:D:118:TYR:CE2	1:D:126:PRO:HG3	2.48	0.49
1:A:420:MET:CE	1:A:420:MET:CA	2.85	0.49
1:C:48:PHE:HA	1:C:51:VAL:HG23	1.95	0.49
1:C:49:PRO:HG3	1:C:71:TYR:CE1	2.48	0.49
1:A:376:LEU:CD1	1:A:400:LYS:HD2	2.38	0.48
1:D:474:MET:O	1:D:477:LYS:HD3	2.13	0.48
1:D:462:ILE:HG22	1:D:466:LEU:CD1	2.43	0.48
1:C:460:GLN:O	1:C:464:THR:OG1	2.31	0.48
1:D:350:ASN:HB3	1:D:356:GLN:HB2	1.95	0.48
1:A:155:PRO:HD2	2:E:2:GLC:O6	2.13	0.48
1:A:49:PRO:HG3	1:A:71:TYR:HE1	1.77	0.48
1:C:395:ASP:OD1	1:C:451:ILE:HG21	2.11	0.48
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.48	0.48
1:A:149:MET:HB2	1:A:223:THR:HG21	1.96	0.48
1:A:152:LEU:HD12	1:A:207:ALA:HA	1.95	0.48
1:A:376:LEU:HD11	1:A:400:LYS:CD	2.40	0.48
1:B:355:ARG:NH1	1:B:355:ARG:HG3	2.28	0.48
1:A:129:THR:OG1	1:A:132:GLU:HG2	2.13	0.48
1:A:168:TYR:CE1	1:A:183:GLY:N	2.82	0.48
1:C:233:TRP:HB2	1:C:299:PRO:HG2	1.95	0.48
1:C:255:PRO:HG2	1:C:257:LYS:NZ	2.28	0.48
1:C:395:ASP:OD1	1:C:451:ILE:HG22	2.14	0.48
1:B:382:GLU:HA	1:B:385:THR:HG22	1.96	0.48
1:D:384:LEU:HD11	1:D:428:ILE:HG21	1.95	0.48
1:A:168:TYR:CE1	1:A:183:GLY:CA	2.96	0.48
1:C:428:ILE:O	1:C:432:LEU:HD12	2.14	0.48
2:F:3:GLC:C6	2:F:3:GLC:O5	2.50	0.48
1:B:248:LEU:HB3	1:B:256:SER:HB2	1.96	0.47
1:B:16:LYS:NZ	2:F:1:GLC:O2	2.39	0.47
1:D:190:LYS:HD2	1:D:359:ASP:OD2	2.13	0.47
1:C:439:ILE:CD1	1:C:454:MET:HG3	2.44	0.47
1:D:435:LEU:HD22	1:D:458:LEU:HD22	1.96	0.47
1:D:442:ARG:HG2	1:D:449:GLU:CG	2.44	0.47
1:B:91:TYR:HE2	1:B:309:GLU:HG2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:LYS:O	1:D:194:THR:OG1	2.32	0.47
1:A:90:LEU:CD1	1:A:108:PRO:HG2	2.45	0.47
1:A:410:PHE:CE2	1:A:419:TYR:HD1	2.32	0.47
1:A:421:LEU:N	1:A:421:LEU:HD12	2.22	0.47
1:B:41:PRO:HG2	1:B:44:LEU:HB3	1.97	0.47
1:A:424:ILE:HG22	1:A:428:ILE:HG13	1.96	0.47
1:A:159:TRP:CH2	1:A:340:PHE:HZ	2.33	0.46
1:A:151:ASN:HB3	1:A:211:TYR:N	2.29	0.46
1:A:83:ASP:N	1:A:83:ASP:OD1	2.48	0.46
1:B:312:LEU:HB3	1:B:318:ILE:HD13	1.97	0.46
1:A:123:LEU:HA	1:A:123:LEU:HD13	1.68	0.46
1:A:19:ASN:HB2	1:A:297:ASP:OD2	2.15	0.46
1:B:391:TYR:HB2	1:B:396:LEU:HD12	1.98	0.46
1:D:475:ARG:NH1	1:D:475:ARG:HG2	2.29	0.46
1:B:42:ASP:N	1:B:42:ASP:OD2	2.48	0.46
1:C:114:LEU:HD21	1:C:157:PHE:CD2	2.51	0.46
1:D:414:HIS:ND1	1:D:414:HIS:N	2.63	0.46
1:A:168:TYR:CD1	1:A:168:TYR:C	2.89	0.46
1:D:170:PHE:CD2	1:D:334:ILE:HD11	2.51	0.46
1:A:3:ILE:HG13	1:A:57:GLY:O	2.16	0.46
1:A:456:ALA:O	1:A:460:GLN:HG3	2.15	0.46
1:C:28:PHE:HD1	1:C:284:TYR:CD2	2.34	0.46
1:C:287:THR:HG23	1:C:290:GLY:H	1.79	0.46
1:D:91:TYR:CE2	1:D:309:GLU:HG3	2.42	0.46
1:A:472:LEU:O	1:A:476:ARG:HB2	2.16	0.46
1:B:155:PRO:HD3	1:B:345:ARG:HG3	1.97	0.45
1:B:130:TRP:HB3	1:B:195:PHE:CE2	2.50	0.45
1:C:229:GLY:HA3	1:C:231:TRP:CZ3	2.51	0.45
1:C:396:LEU:HA	1:C:396:LEU:HD23	1.80	0.45
1:D:28:PHE:HA	1:D:284:TYR:CE1	2.51	0.45
1:D:458:LEU:O	1:D:462:ILE:HG13	2.16	0.45
1:B:114:LEU:HA	1:B:114:LEU:HD12	1.76	0.45
1:B:315:ASP:HA	1:B:316:PRO:HD2	1.83	0.45
1:B:296:LYS:NZ	1:B:296:LYS:CB	2.73	0.45
1:B:67:ARG:NH2	2:F:3:GLC:O3	2.36	0.45
1:A:200:ILE:HD13	1:A:207:ALA:HB2	1.98	0.45
1:A:457:TYR:O	1:A:461:THR:OG1	2.32	0.45
1:A:90:LEU:HB2	1:A:95:TRP:NE1	2.32	0.45
1:B:116:LEU:HB2	1:B:248:LEU:HD12	1.97	0.45
1:C:107:TYR:CD1	1:C:281:LEU:HD13	2.51	0.45
1:A:172:TYR:O	1:A:172:TYR:CG	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:GLU:OE1	2:H:2:GLC:O6	2.21	0.45
1:B:252:LYS:HB3	1:B:252:LYS:HE2	1.78	0.45
1:C:194:THR:HA	1:C:358:VAL:HG21	1.99	0.45
1:C:382:GLU:HA	1:C:385:THR:OG1	2.16	0.45
1:B:145:LYS:HZ2	1:B:145:LYS:HA	1.82	0.45
1:D:32:THR:CG2	1:D:34:ILE:HD12	2.46	0.45
1:C:382:GLU:O	1:C:385:THR:OG1	2.29	0.45
1:D:194:THR:HA	1:D:358:VAL:HG21	1.98	0.45
1:B:61:ILE:HG13	1:B:62:PHE:N	2.31	0.45
1:A:145:LYS:HD2	1:A:221:GLY:O	2.17	0.44
1:C:411:ASN:O	1:C:414:HIS:O	2.34	0.44
1:A:162:ILE:HG23	1:A:189:ALA:HB1	1.99	0.44
1:B:193:LEU:O	1:B:197:VAL:HG23	2.18	0.44
1:D:63:TRP:HB3	1:D:68:PHE:HE1	1.82	0.44
1:A:384:LEU:O	1:A:388:LEU:HD23	2.17	0.44
1:B:91:TYR:CE1	1:B:306:LYS:HG2	2.51	0.44
1:A:158:THR:HG21	1:A:196:LEU:HD22	1.99	0.44
1:C:407:LYS:HE3	1:C:420:MET:SD	2.58	0.44
1:B:424:ILE:O	1:B:424:ILE:HG22	2.16	0.44
1:A:69:GLY:HA3	1:A:333:ASN:O	2.17	0.44
1:B:273:ASN:HB3	1:B:276:LEU:HB2	2.00	0.44
1:C:43:LYS:HB3	1:C:46:GLU:HG3	1.99	0.44
1:C:67:ARG:NH2	2:G:3:GLC:O3	2.34	0.44
1:A:131:GLU:H	1:A:131:GLU:HG2	1.42	0.44
1:A:168:TYR:CD1	1:A:168:TYR:O	2.70	0.44
1:A:84:LYS:NZ	1:A:88:ASP:OD2	2.51	0.44
1:D:395:ASP:OD1	1:D:451:ILE:HG22	2.17	0.44
1:D:429:LEU:O	1:D:433:LYS:HG3	2.18	0.44
1:A:169:ALA:O	1:A:170:PHE:CG	2.71	0.44
1:C:449:GLU:HA	1:C:449:GLU:OE2	2.18	0.44
1:B:172:TYR:CE1	1:B:175:GLY:HA2	2.53	0.43
1:D:129:THR:HG22	1:D:250:THR:OG1	2.18	0.43
1:D:384:LEU:HD11	1:D:428:ILE:CG2	2.48	0.43
1:D:384:LEU:HD12	1:D:388:LEU:HD11	1.99	0.43
1:D:450:THR:O	1:D:453:SER:N	2.50	0.43
1:D:150:PHE:HZ	1:D:196:LEU:HD11	1.83	0.43
1:A:383:GLN:HB3	1:A:425:GLU:OE2	2.18	0.43
1:B:12:ILE:HA	1:B:62:PHE:HB2	1.99	0.43
1:A:154:GLU:HA	1:A:155:PRO:HD3	1.85	0.43
1:D:383:GLN:NE2	1:D:425:GLU:OE1	2.51	0.43
1:A:210:ASP:H	1:A:213:ILE:HD12	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LEU:HB3	1:B:318:ILE:CD1	2.48	0.43
1:B:414:HIS:HD2	1:B:470:HIS:CD2	2.35	0.43
1:D:151:ASN:HB3	1:D:157:PHE:CD1	2.53	0.43
1:A:169:ALA:C	1:A:170:PHE:CD2	2.92	0.43
1:B:122:LEU:HD23	1:B:224:ALA:HB2	1.99	0.43
1:D:427:GLU:N	1:D:427:GLU:OE2	2.52	0.43
1:D:41:PRO:HB2	1:D:47:LYS:NZ	2.34	0.43
1:B:114:LEU:HG	1:B:227:ILE:HG22	2.00	0.43
1:B:112:GLU:HG2	1:B:261:GLY:O	2.18	0.43
1:C:29:GLU:CG	1:C:35:LYS:HA	2.48	0.43
1:D:41:PRO:HG2	1:D:44:LEU:HB3	2.00	0.43
1:A:372:ASP:HB3	1:A:375:MET:HB3	2.01	0.43
1:A:10:ILE:HB	1:A:38:VAL:HG22	2.00	0.43
1:C:377:LEU:HD23	1:C:377:LEU:C	2.39	0.43
1:D:229:GLY:HA3	1:D:231:TRP:CH2	2.53	0.43
1:C:49:PRO:HG3	1:C:71:TYR:HE1	1.82	0.43
1:A:421:LEU:H	1:A:421:LEU:CD1	2.20	0.43
1:A:43:LYS:HD3	1:A:46:GLU:OE2	2.18	0.43
1:A:185:ASP:CB	1:A:366:GLN:OE1	2.67	0.42
1:D:157:PHE:O	1:D:160:PRO:HD2	2.19	0.42
1:A:84:LYS:HA	1:A:84:LYS:HD2	1.81	0.42
1:B:202:ASN:O	1:B:203:LYS:HB2	2.19	0.42
1:D:107:TYR:OH	1:D:278:LYS:HD3	2.19	0.42
1:B:128:LYS:HE2	1:B:128:LYS:HB3	1.88	0.42
1:C:255:PRO:HG2	1:C:257:LYS:HZ2	1.83	0.42
1:A:427:GLU:HG3	1:A:466:LEU:HD23	2.00	0.42
1:B:134:PRO:HB3	1:B:204:HIS:NE2	2.35	0.42
1:B:392:ASP:OD1	1:B:392:ASP:N	2.52	0.42
1:C:438:ALA:O	1:C:442:ARG:HB2	2.19	0.42
1:D:62:PHE:HE1	1:D:109:ILE:HG13	1.83	0.42
1:D:83:ASP:N	1:D:83:ASP:OD1	2.52	0.42
1:A:315:ASP:HB3	1:A:318:ILE:HG12	2.01	0.42
1:B:259:PHE:HA	1:B:259:PHE:HD1	1.71	0.42
1:A:410:PHE:CE2	1:A:419:TYR:HE1	2.38	0.42
1:D:155:PRO:HG3	1:D:345:ARG:CA	2.49	0.42
1:A:420:MET:HE3	1:A:420:MET:HA	1.98	0.42
1:C:141:LYS:HE2	1:C:141:LYS:HB2	1.79	0.42
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.81	0.42
1:A:65:HIS:CE1	1:A:331:MET:HB2	2.55	0.42
1:B:155:PRO:HD2	2:F:2:GLC:O6	2.20	0.42
1:D:424:ILE:HG21	1:D:424:ILE:HD13	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:ASP:OD1	1:D:451:ILE:HG21	2.19	0.42
1:C:250:THR:HG22	1:C:255:PRO:HA	2.02	0.42
1:D:298:LYS:HA	1:D:299:PRO:HD3	1.89	0.42
1:D:431:SER:HA	1:D:434:ARG:HG3	2.01	0.42
1:C:12:ILE:HA	1:C:62:PHE:HB2	2.02	0.41
1:D:43:LYS:HE3	1:D:43:LYS:HB2	1.89	0.41
1:B:117:ILE:HG22	1:B:218:PHE:CZ	2.54	0.41
1:C:377:LEU:HD21	1:C:385:THR:CG2	2.50	0.41
1:A:159:TRP:NE1	1:A:163:ALA:HB2	2.35	0.41
1:A:196:LEU:O	1:A:196:LEU:HG	2.20	0.41
1:D:87:GLN:HG3	1:D:95:TRP:CE2	2.55	0.41
1:B:463:LEU:HD23	1:B:463:LEU:HA	1.90	0.41
1:A:123:LEU:HD13	1:A:124:PRO:HD2	2.02	0.41
1:C:66:ASP:HA	1:C:333:ASN:HA	2.02	0.41
1:C:91:TYR:HA	1:C:92:PRO:HD3	1.89	0.41
1:D:154:GLU:HA	1:D:155:PRO:HD3	1.96	0.41
1:D:11:TRP:HB3	1:D:44:LEU:HD13	2.03	0.41
1:B:380:PHE:HD1	1:B:384:LEU:CD1	2.34	0.41
1:C:407:LYS:HE3	1:C:420:MET:HA	2.02	0.41
1:A:308:TYR:CE2	1:A:312:LEU:HD11	2.56	0.41
1:C:393:TYR:CE2	1:C:394:ARG:NH1	2.89	0.41
1:C:424:ILE:O	1:C:428:ILE:HG13	2.21	0.41
1:C:76:LEU:HD13	1:C:76:LEU:N	2.36	0.41
1:D:373:LYS:HG3	1:D:393:TYR:HD1	1.85	0.41
1:D:107:TYR:HA	1:D:108:PRO:HD3	1.87	0.41
1:D:170:PHE:HE1	1:D:182:VAL:HG22	1.85	0.41
1:A:404:LEU:HA	1:A:404:LEU:HD12	1.88	0.41
1:D:216:ALA:HB1	1:D:220:LYS:NZ	2.36	0.41
1:D:424:ILE:HG22	1:D:428:ILE:HG13	2.03	0.41
1:A:168:TYR:CD1	1:A:183:GLY:HA3	2.55	0.41
1:A:405:LYS:HE3	1:A:459:MET:HE2	2.03	0.41
1:B:194:THR:HA	1:B:358:VAL:HG21	2.02	0.41
1:D:48:PHE:HB3	1:D:49:PRO:HD3	2.03	0.41
1:A:184:VAL:HG12	1:A:362:LEU:HD22	2.02	0.40
1:A:368:HIS:C	1:A:368:HIS:ND1	2.74	0.40
1:C:179:ILE:CG2	1:C:336:GLN:HG2	2.50	0.40
1:C:382:GLU:H	1:C:382:GLU:HG2	1.45	0.40
1:D:90:LEU:HB2	1:D:95:TRP:NE1	2.36	0.40
1:A:11:TRP:HB3	1:A:44:LEU:HD13	2.03	0.40
1:B:168:TYR:CE2	1:B:183:GLY:HA3	2.56	0.40
1:C:52:ALA:HA	1:C:56:ASP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:PHE:HB3	1:D:105:ILE:HD13	2.03	0.40
1:A:61:ILE:HG13	1:A:62:PHE:N	2.35	0.40
1:B:271:SER:HA	1:B:272:PRO:HD3	1.83	0.40
1:D:377:LEU:O	1:D:380:PHE:HB2	2.22	0.40
1:A:167:GLY:HA3	1:A:189:ALA:HB2	2.04	0.40
1:B:233:TRP:HB2	1:B:299:PRO:HG2	2.04	0.40
1:C:109:ILE:HD13	1:C:109:ILE:HA	1.84	0.40
1:C:193:LEU:O	1:C:197:VAL:HG23	2.21	0.40
1:C:47:LYS:HB2	1:C:47:LYS:HE3	1.82	0.40
1:D:170:PHE:CE1	1:D:182:VAL:HG22	2.57	0.40
1:A:232:ALA:O	1:A:236:ILE:HG13	2.21	0.40
1:C:235:ASN:OD1	1:C:298:LYS:HE3	2.21	0.40
1:D:376:LEU:HD23	1:D:396:LEU:HD23	2.03	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	476/487 (98%)	463 (97%)	13 (3%)	0	100	100
1	B	477/487 (98%)	472 (99%)	5 (1%)	0	100	100
1	C	474/487 (97%)	469 (99%)	5 (1%)	0	100	100
1	D	468/487 (96%)	464 (99%)	4 (1%)	0	100	100
All	All	1895/1948 (97%)	1868 (99%)	27 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	375/407 (92%)	326 (87%)	49 (13%)	4	15
1	B	380/407 (93%)	337 (89%)	43 (11%)	6	21
1	C	363/407 (89%)	308 (85%)	55 (15%)	3	11
1	D	375/407 (92%)	315 (84%)	60 (16%)	2	10
All	All	1493/1628 (92%)	1286 (86%)	207 (14%)	3	13

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	30	LYS
1	A	44	LEU
1	A	61	ILE
1	A	88	ASP
1	A	114	LEU
1	A	115	SER
1	A	131	GLU
1	A	136	LEU
1	A	148	LEU
1	A	158	THR
1	A	171	LYS
1	A	179	ILE
1	A	199	LEU
1	A	208	ASP
1	A	212	SER
1	A	223	THR
1	A	228	ASN
1	A	234	SER
1	A	259	PHE
1	A	273	ASN
1	A	323	GLU
1	A	330	ILE
1	A	346	THR

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Mol	Chain	Res	Type
1	A	360	GLU
1	A	368	HIS
1	A	369	ASN
1	A	373	LYS
1	A	375	MET
1	A	376	LEU
1	A	386	ASN
1	A	392	ASP
1	A	396	LEU
1	A	404	LEU
1	A	413	ARG
1	A	417	MET
1	A	418	HIS
1	A	420	MET
1	A	422	GLU
1	A	427	GLU
1	A	429	LEU
1	A	431	SER
1	A	436	LYS
1	A	442	ARG
1	A	454	MET
1	A	465	GLU
1	A	472	LEU
1	A	474	MET
1	A	476	ARG
1	B	37	THR
1	B	42	ASP
1	B	59	ASP
1	B	61	ILE
1	B	76	LEU
1	B	81	THR
1	B	101	ASN
1	B	105	ILE
1	B	114	LEU
1	B	143	LYS
1	B	173	GLU
1	B	182	VAL
1	B	186	ASN
1	B	205	MET
1	B	234	SER
1	B	248	LEU
1	B	259	PHE

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Mol	Chain	Res	Type
1	B	279	GLU
1	B	289	GLU
1	B	296	LYS
1	B	310	GLU
1	B	368	HIS
1	B	370	PHE
1	B	374	GLU
1	B	375	MET
1	B	376	LEU
1	B	384	LEU
1	B	391	TYR
1	B	392	ASP
1	B	394	ARG
1	B	396	LEU
1	B	413	ARG
1	B	416	ASP
1	B	417	MET
1	B	418	HIS
1	B	421	LEU
1	B	426	ASP
1	B	430	THR
1	B	436	LYS
1	B	444	VAL
1	B	460	GLN
1	B	468	GLU
1	B	474	MET
1	C	3	ILE
1	C	4	GLU
1	C	16	LYS
1	C	29	GLU
1	C	42	ASP
1	C	44	LEU
1	C	46	GLU
1	C	51	VAL
1	C	61	ILE
1	C	76	LEU
1	C	104	LEU
1	C	114	LEU
1	C	123	LEU
1	C	128	LYS
1	C	129	THR
1	C	136	LEU

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Mol	Chain	Res	Type
1	C	141	LYS
1	C	146	SER
1	C	149	MET
1	C	153	GLN
1	C	176	LYS
1	C	179	ILE
1	C	199	LEU
1	C	201	LYS
1	C	206	ASN
1	C	252	LYS
1	C	259	PHE
1	C	309	GLU
1	C	312	LEU
1	C	323	GLU
1	C	330	ILE
1	C	366	GLN
1	C	368	HIS
1	C	369	ASN
1	C	374	GLU
1	C	376	LEU
1	C	382	GLU
1	C	383	GLN
1	C	385	THR
1	C	387	TYR
1	C	404	LEU
1	C	415	GLU
1	C	417	MET
1	C	426	ASP
1	C	432	LEU
1	C	442	ARG
1	C	445	LYS
1	C	458	LEU
1	C	459	MET
1	C	461	THR
1	C	462	ILE
1	C	464	THR
1	C	468	GLU
1	C	472	LEU
1	C	474	MET
1	D	8	LEU
1	D	15	ASP
1	D	30	LYS

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Mol	Chain	Res	Type
1	D	38	VAL
1	D	93	PHE
1	D	122	LEU
1	D	123	LEU
1	D	136	LEU
1	D	145	LYS
1	D	146	SER
1	D	171	LYS
1	D	176	LYS
1	D	194	THR
1	D	204	HIS
1	D	208	ASP
1	D	234	SER
1	D	252	LYS
1	D	259	PHE
1	D	296	LYS
1	D	309	GLU
1	D	323	GLU
1	D	329	GLU
1	D	355	ARG
1	D	356	GLN
1	D	357	THR
1	D	366	GLN
1	D	368	HIS
1	D	372	ASP
1	D	376	LEU
1	D	380	PHE
1	D	388	LEU
1	D	390	LYS
1	D	396	LEU
1	D	399	ILE
1	D	405	LYS
1	D	411	ASN
1	D	412	SER
1	D	413	ARG
1	D	414	HIS
1	D	416	ASP
1	D	420	MET
1	D	421	LEU
1	D	427	GLU
1	D	432	LEU
1	D	434	ARG

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Mol	Chain	Res	Type
1	D	436	LYS
1	D	437	LYS
1	D	442	ARG
1	D	450	THR
1	D	451	ILE
1	D	453	SER
1	D	458	LEU
1	D	460	GLN
1	D	461	THR
1	D	464	THR
1	D	468	GLU
1	D	472	LEU
1	D	474	MET
1	D	475	ARG
1	D	477	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	ASN
1	B	336	GLN
1	B	378	GLN
1	C	369	ASN
1	D	470	HIS

### 5.3.3 RNA [i](#)

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	1.27	1 (8%)	17,17,17	1.61	4 (23%)
2	GLC	E	2	2	11,11,12	2.03	4 (36%)	15,15,17	1.72	5 (33%)
2	GLC	E	3	2	11,11,12	7.45	7 (63%)	15,15,17	4.87	8 (53%)
2	GLC	F	1	2	12,12,12	1.22	0	17,17,17	1.31	3 (17%)
2	GLC	F	2	2	11,11,12	1.70	3 (27%)	15,15,17	1.23	1 (6%)
2	GLC	F	3	2	11,11,12	7.22	8 (72%)	15,15,17	3.45	5 (33%)
2	GLC	G	1	2	12,12,12	1.21	2 (16%)	17,17,17	1.80	5 (29%)
2	GLC	G	2	2	11,11,12	1.72	3 (27%)	15,15,17	1.71	4 (26%)
2	GLC	G	3	2	11,11,12	7.07	7 (63%)	15,15,17	3.77	4 (26%)
2	GLC	H	1	2	12,12,12	1.25	1 (8%)	17,17,17	1.41	2 (11%)
2	GLC	H	2	2	11,11,12	1.77	3 (27%)	15,15,17	1.12	2 (13%)
2	GLC	H	3	2	11,11,12	7.14	8 (72%)	15,15,17	2.89	5 (33%)

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	-	1/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	2/2/19/22	0/1/1/1
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	GLC	F	3	2	-	2/2/19/22	0/1/1/1
2	GLC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	1/2/19/22	0/1/1/1
2	GLC	G	3	2	-	2/2/19/22	0/1/1/1
2	GLC	H	1	2	-	2/2/22/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	3	2	-	2/2/19/22	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	GLC	O5-C1	18.58	1.73	1.43
2	F	3	GLC	O5-C1	17.70	1.72	1.43
2	G	3	GLC	O5-C1	17.43	1.71	1.43
2	H	3	GLC	O5-C1	17.42	1.71	1.43
2	H	3	GLC	O5-C5	10.51	1.64	1.43
2	F	3	GLC	O5-C5	10.39	1.64	1.43
2	E	3	GLC	O5-C5	10.15	1.64	1.43
2	G	3	GLC	O5-C5	9.89	1.63	1.43
2	H	3	GLC	O3-C3	8.29	1.62	1.43
2	E	3	GLC	O3-C3	8.18	1.62	1.43
2	F	3	GLC	O3-C3	8.17	1.62	1.43
2	G	3	GLC	O3-C3	7.98	1.61	1.43
2	E	3	GLC	C2-C3	-7.13	1.42	1.52
2	F	3	GLC	C2-C3	-6.81	1.42	1.52
2	G	3	GLC	C2-C3	-6.66	1.42	1.52
2	H	3	GLC	C2-C3	-6.13	1.43	1.52
2	E	3	GLC	C4-C3	-5.05	1.39	1.52
2	G	3	GLC	C4-C3	-4.37	1.41	1.52
2	H	3	GLC	C4-C3	-4.08	1.41	1.52
2	F	3	GLC	C4-C3	-4.06	1.42	1.52
2	E	2	GLC	O5-C1	3.79	1.49	1.43
2	G	2	GLC	O5-C1	3.77	1.49	1.43
2	H	2	GLC	O5-C1	3.77	1.49	1.43
2	F	2	GLC	O5-C1	3.68	1.49	1.43
2	E	2	GLC	C2-C3	-3.20	1.47	1.52
2	E	3	GLC	O2-C2	3.12	1.50	1.43
2	H	3	GLC	O2-C2	3.04	1.49	1.43
2	G	3	GLC	O2-C2	2.96	1.49	1.43
2	F	3	GLC	O2-C2	2.75	1.49	1.43
2	H	3	GLC	O4-C4	2.72	1.49	1.43
2	E	2	GLC	O5-C5	2.69	1.48	1.43
2	E	1	GLC	O5-C1	2.67	1.49	1.42
2	G	3	GLC	C6-C5	-2.64	1.43	1.51
2	E	2	GLC	O4-C4	2.61	1.49	1.43
2	F	3	GLC	C6-C5	-2.57	1.43	1.51
2	F	3	GLC	O4-C4	2.50	1.48	1.43
2	E	3	GLC	C6-C5	-2.45	1.43	1.51
2	F	2	GLC	O5-C5	2.45	1.48	1.43
2	H	3	GLC	C6-C5	-2.45	1.43	1.51
2	F	2	GLC	C2-C3	-2.42	1.48	1.52
2	H	2	GLC	O5-C5	2.35	1.48	1.43
2	H	2	GLC	O4-C4	2.23	1.48	1.43
2	H	1	GLC	O5-C1	2.22	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	GLC	O5-C5	2.19	1.47	1.43
2	G	2	GLC	C2-C3	-2.18	1.49	1.52
2	G	1	GLC	O2-C2	2.18	1.48	1.43
2	G	1	GLC	O3-C3	2.14	1.48	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	GLC	C1-O5-C5	-11.46	96.66	112.19
2	E	3	GLC	C2-C3-C4	10.20	128.55	110.89
2	G	3	GLC	C1-O5-C5	-9.80	98.92	112.19
2	F	3	GLC	C1-O5-C5	-9.59	99.20	112.19
2	G	3	GLC	C2-C3-C4	8.63	125.83	110.89
2	H	3	GLC	C1-O5-C5	-7.60	101.90	112.19
2	F	3	GLC	C2-C3-C4	7.26	123.46	110.89
2	E	3	GLC	O5-C5-C6	7.11	118.34	107.20
2	H	3	GLC	C2-C3-C4	6.60	122.32	110.89
2	G	3	GLC	O3-C3-C2	-5.11	100.21	109.99
2	E	3	GLC	O3-C3-C2	-4.43	101.50	109.99
2	F	3	GLC	O3-C3-C2	-3.81	102.70	109.99
2	G	1	GLC	C4-C3-C2	3.53	116.98	110.82
2	G	2	GLC	C1-C2-C3	3.51	113.98	109.67
2	E	3	GLC	C1-C2-C3	3.46	113.92	109.67
2	E	2	GLC	O3-C3-C2	-3.45	103.38	109.99
2	E	3	GLC	C6-C5-C4	-3.41	105.03	113.00
2	G	3	GLC	C1-C2-C3	3.08	113.45	109.67
2	E	1	GLC	O5-C5-C4	3.05	115.23	109.69
2	F	2	GLC	O4-C4-C3	-3.01	103.39	110.35
2	H	2	GLC	C1-O5-C5	2.95	116.19	112.19
2	F	1	GLC	O4-C4-C3	-2.92	103.59	110.35
2	E	3	GLC	O3-C3-C4	-2.89	103.67	110.35
2	E	2	GLC	C1-O5-C5	2.89	116.10	112.19
2	G	1	GLC	C1-C2-C3	2.84	116.20	110.31
2	H	1	GLC	O5-C5-C4	2.82	114.81	109.69
2	E	3	GLC	O2-C2-C1	2.80	114.87	109.15
2	H	3	GLC	O3-C3-C2	-2.79	104.65	109.99
2	G	1	GLC	C1-O5-C5	-2.76	108.46	113.66
2	G	2	GLC	O5-C5-C4	2.74	117.50	110.83
2	F	1	GLC	C1-O5-C5	-2.65	108.66	113.66
2	G	2	GLC	O4-C4-C5	-2.65	102.73	109.30
2	H	1	GLC	C4-C3-C2	2.63	115.42	110.82
2	G	1	GLC	C3-C4-C5	2.59	114.86	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	GLC	O5-C5-C4	2.56	114.34	109.69
2	E	2	GLC	C2-C3-C4	2.55	115.31	110.89
2	F	3	GLC	O5-C5-C4	2.47	116.83	110.83
2	E	1	GLC	C1-C2-C3	2.40	115.29	110.31
2	H	3	GLC	O5-C5-C4	2.29	116.41	110.83
2	F	1	GLC	O1-C1-O5	-2.26	103.59	110.38
2	E	1	GLC	O3-C3-C2	-2.22	105.22	110.35
2	E	1	GLC	C6-C5-C4	-2.20	107.85	113.00
2	E	2	GLC	O5-C5-C6	2.18	110.62	107.20
2	H	3	GLC	C6-C5-C4	-2.16	107.95	113.00
2	E	2	GLC	O2-C2-C3	-2.13	105.87	110.14
2	G	2	GLC	C1-O5-C5	2.11	115.05	112.19
2	F	3	GLC	C6-C5-C4	-2.10	108.08	113.00
2	H	2	GLC	O5-C5-C4	2.07	115.87	110.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3	GLC	O5-C5-C6-O6
2	G	3	GLC	O5-C5-C6-O6
2	H	3	GLC	O5-C5-C6-O6
2	E	3	GLC	O5-C5-C6-O6
2	F	3	GLC	C4-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	G	3	GLC	C4-C5-C6-O6
2	E	3	GLC	C4-C5-C6-O6
2	H	1	GLC	C4-C5-C6-O6
2	H	3	GLC	C4-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	G	2	GLC	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 25 short contacts:

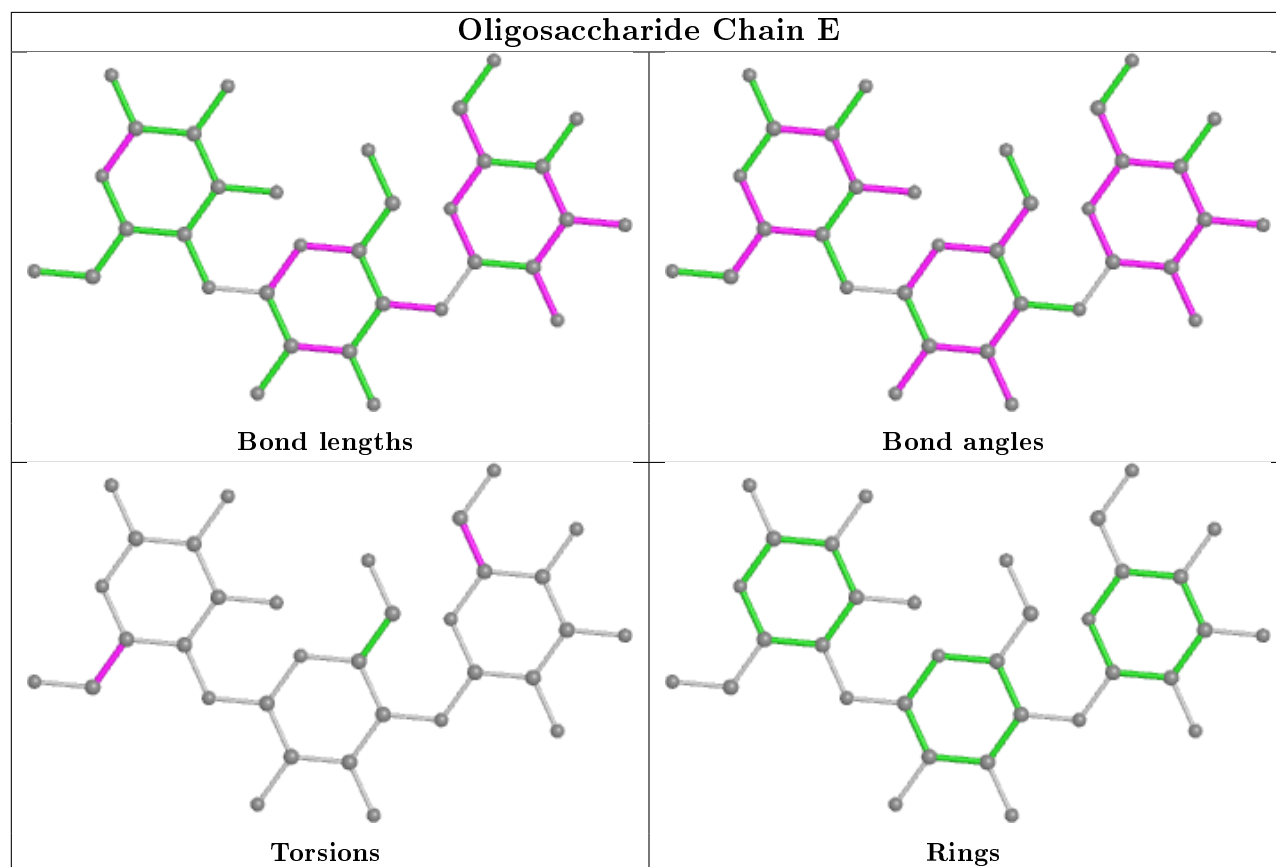
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	GLC	1	0
2	F	3	GLC	5	0
2	H	3	GLC	4	0

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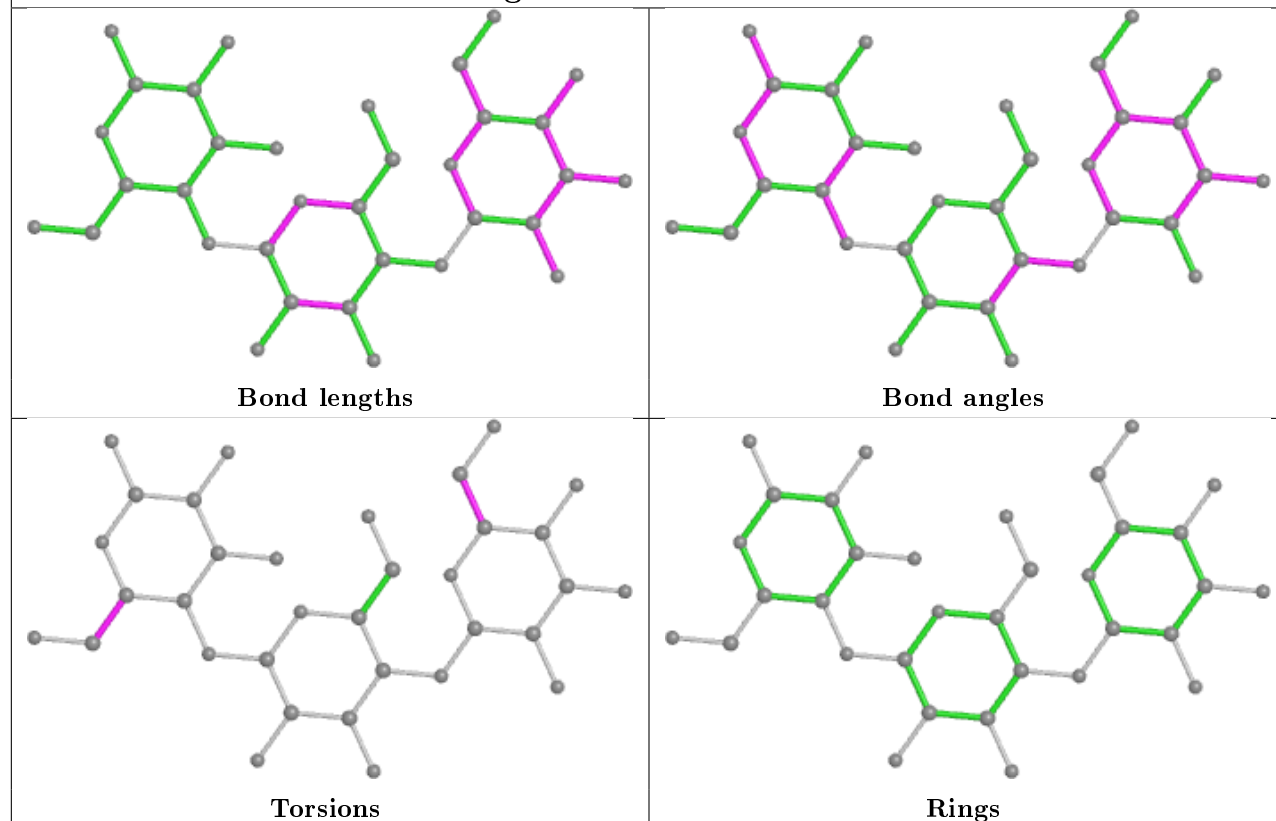
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	GLC	6	0
2	E	2	GLC	2	0
2	F	2	GLC	1	0
2	F	1	GLC	1	0
2	G	3	GLC	5	0
2	H	2	GLC	1	0

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

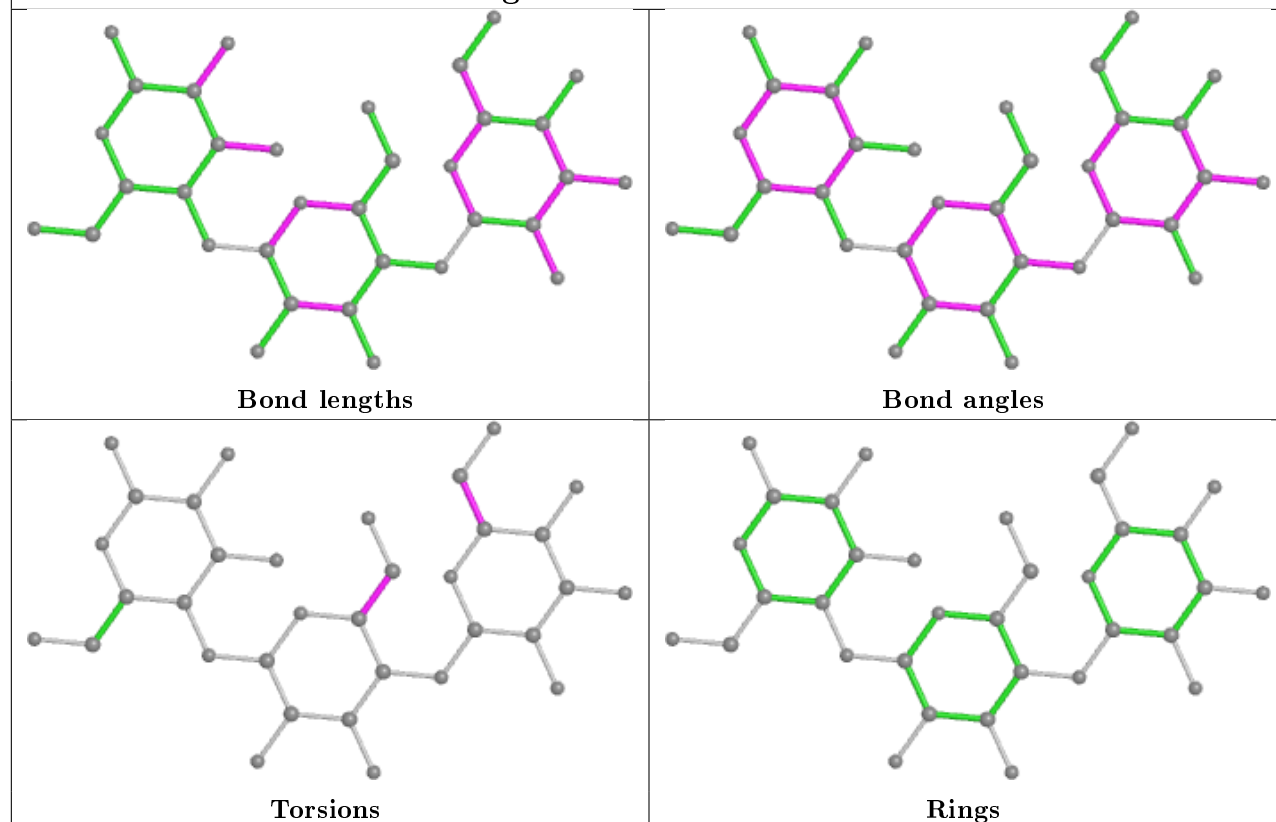


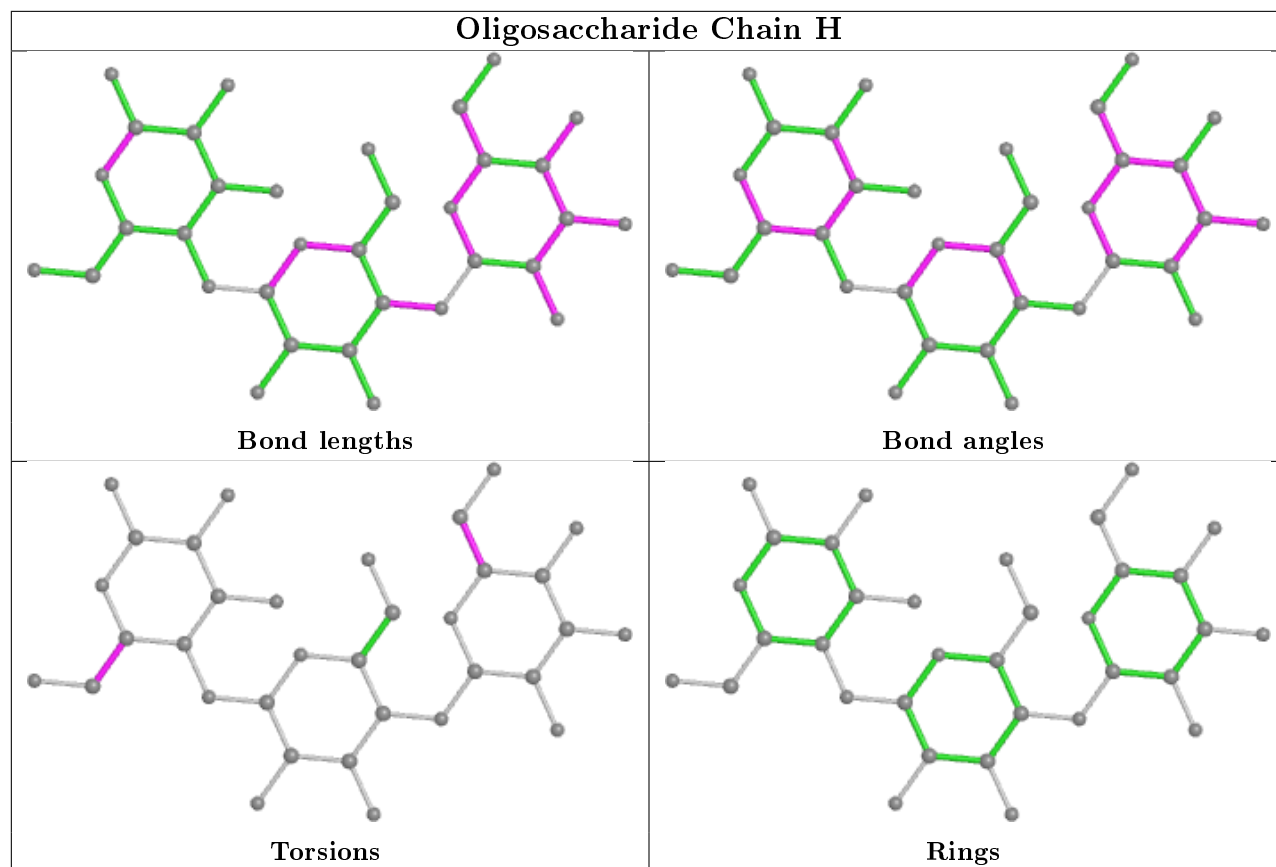


## Oligosaccharide Chain F



## Oligosaccharide Chain G





## 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	478/487 (98%)	0.08	17 (3%) 42 42	31, 61, 95, 121	0
1	B	479/487 (98%)	0.10	19 (3%) 38 37	39, 66, 99, 135	0
1	C	476/487 (97%)	0.06	24 (5%) 28 29	41, 68, 105, 140	0
1	D	472/487 (96%)	0.15	22 (4%) 31 31	45, 73, 100, 138	0
All	All	1905/1948 (97%)	0.10	82 (4%) 35 35	31, 67, 101, 140	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	125	ASN	4.9
1	C	165	ASP	4.6
1	C	375	MET	4.5
1	C	372	ASP	4.4
1	C	173	GLU	4.3
1	C	404	LEU	4.2
1	C	382	GLU	4.1
1	D	54	THR	4.1
1	B	416	ASP	4.0
1	A	167	GLY	4.0
1	C	174	ASN	3.9
1	B	371	ASP	3.6
1	C	380	PHE	3.6
1	B	143	LYS	3.5
1	D	247	VAL	3.5
1	B	174	ASN	3.4
1	B	210	ASP	3.4
1	B	449	GLU	3.4
1	A	321	THR	3.3
1	C	147	ALA	3.2
1	C	161	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	281	LEU	3.2
1	D	300	LEU	3.2
1	D	320	ALA	3.2
1	D	435	LEU	3.1
1	C	301	GLY	3.1
1	D	313	ALA	3.1
1	B	386	ASN	3.1
1	B	69	GLY	3.0
1	C	384	LEU	3.0
1	A	145	LYS	2.9
1	B	173	GLU	2.9
1	A	82	PRO	2.8
1	B	392	ASP	2.8
1	B	393	TYR	2.8
1	D	109	ILE	2.8
1	C	171	LYS	2.8
1	D	322	MET	2.8
1	B	372	ASP	2.8
1	C	187	ALA	2.7
1	B	125	ASN	2.7
1	B	323	GLU	2.7
1	D	321	THR	2.6
1	D	256	SER	2.6
1	B	417	MET	2.6
1	B	480	LYS	2.5
1	C	169	ALA	2.5
1	C	136	LEU	2.5
1	B	324	ASN	2.5
1	A	264	SER	2.5
1	D	447	GLN	2.5
1	A	244	GLY	2.4
1	C	164	ALA	2.4
1	D	393	TYR	2.4
1	C	137	ASP	2.4
1	C	390	LYS	2.4
1	D	246	THR	2.4
1	A	78	ALA	2.4
1	C	302	ALA	2.3
1	A	391	TYR	2.3
1	A	323	GLU	2.3
1	B	68	PHE	2.2
1	D	241	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	398	ILE	2.2
1	C	279	GLU	2.2
1	A	416	ASP	2.2
1	A	296	LYS	2.2
1	D	291	LEU	2.1
1	C	59	ASP	2.1
1	A	224	ALA	2.1
1	A	166	GLY	2.1
1	B	59	ASP	2.1
1	C	300	LEU	2.1
1	A	383	GLN	2.1
1	C	409	SER	2.1
1	D	286	LEU	2.1
1	D	323	GLU	2.1
1	D	113	ALA	2.1
1	A	258	PRO	2.0
1	D	365	ALA	2.0
1	D	340	PHE	2.0
1	A	415	GLU	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.

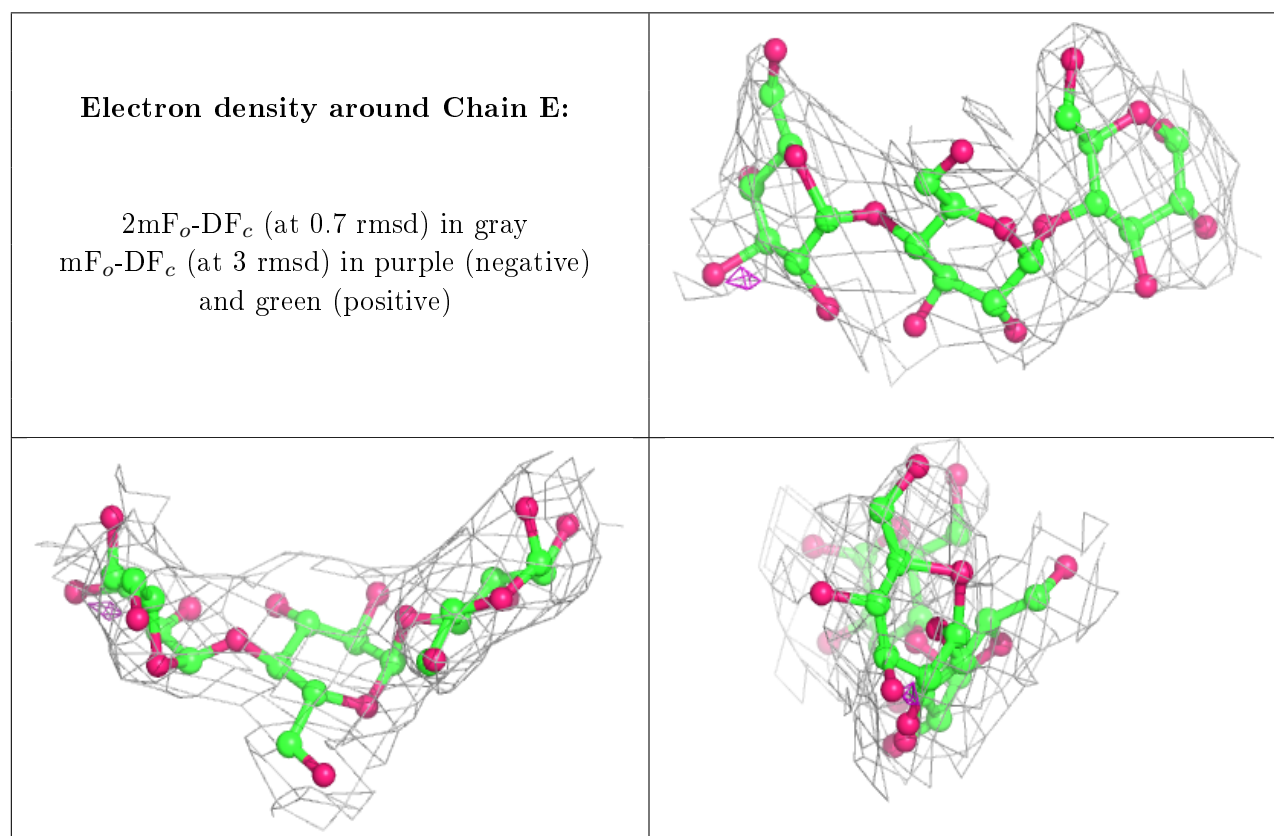
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	H	3	11/12	0.79	0.35	45,65,74,74	0
2	GLC	H	1	12/12	0.85	0.27	49,60,68,72	0
2	GLC	F	1	12/12	0.88	0.35	47,52,59,61	0
2	GLC	E	3	11/12	0.89	0.45	37,55,66,76	0
2	GLC	H	2	11/12	0.89	0.17	47,55,59,66	0
2	GLC	F	3	11/12	0.90	0.16	52,61,67,76	0
2	GLC	F	2	11/12	0.91	0.23	33,47,57,60	0
2	GLC	G	3	11/12	0.93	0.16	61,67,79,81	0
2	GLC	G	1	12/12	0.93	0.28	57,64,72,78	0

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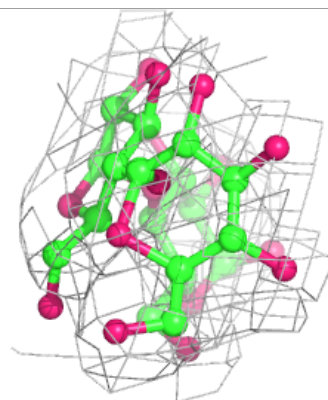
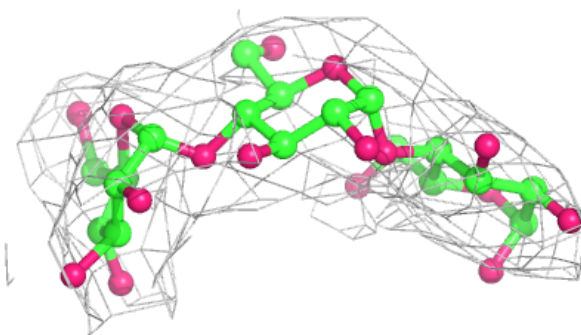
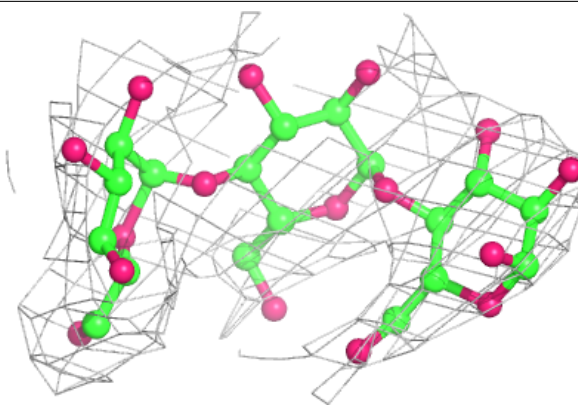
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	E	1	12/12	0.94	0.19	36,44,53,54	0
2	GLC	E	2	11/12	0.94	0.14	30,33,36,37	0
2	GLC	G	2	11/12	0.95	0.12	53,60,69,70	0

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.

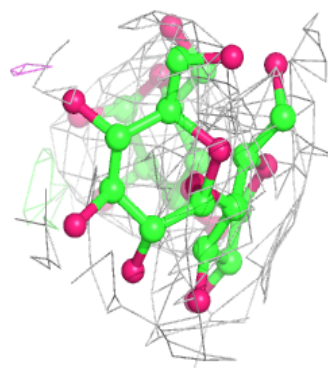
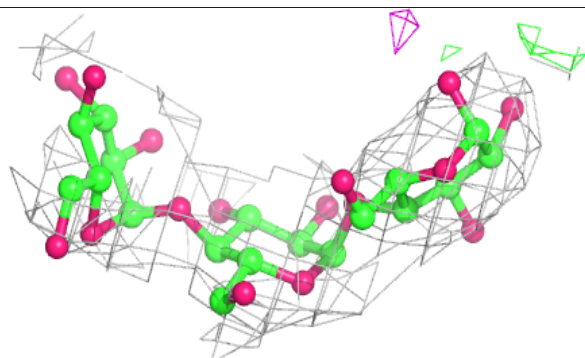
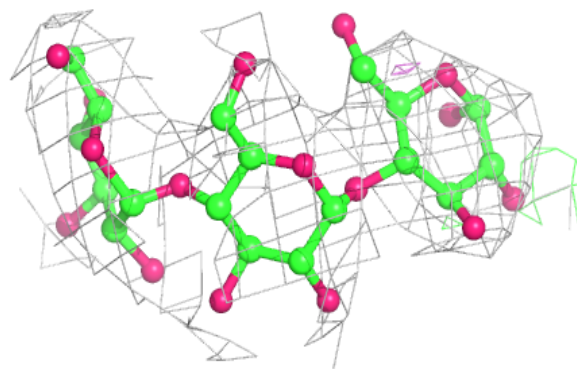


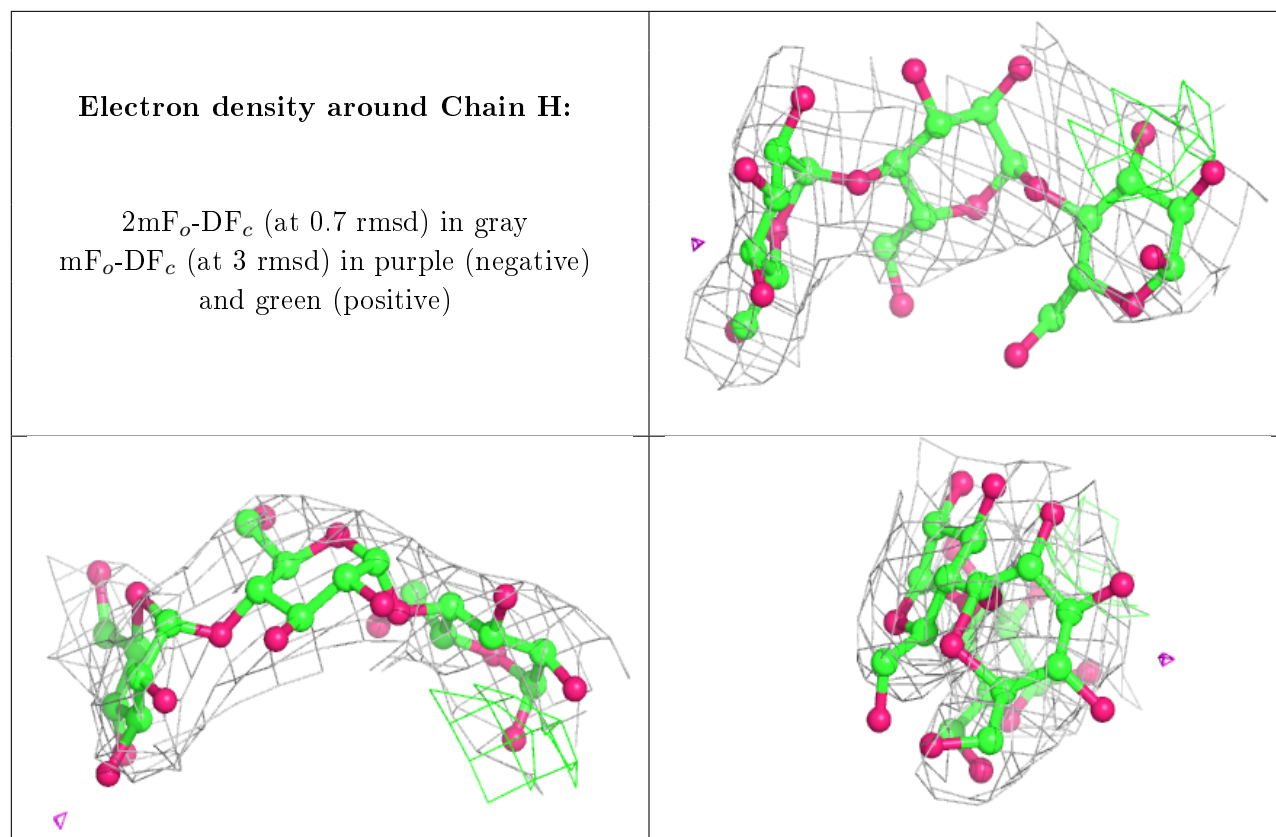
**Electron density around Chain F:**

$2mF_o-DF_c$  (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.