



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:21 PM BST

PDB ID : 1GPZ  
Title : THE CRYSTAL STRUCTURE OF THE ZYMOGEN CATALYTIC DOMAIN  
OF COMPLEMENT PROTEASE C1R  
Authors : Budayova-Spano, M.; Fontecilla-Camps, J.C.; Gaboriaud, C.  
Deposited on : 2001-11-15  
Resolution : 2.90 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

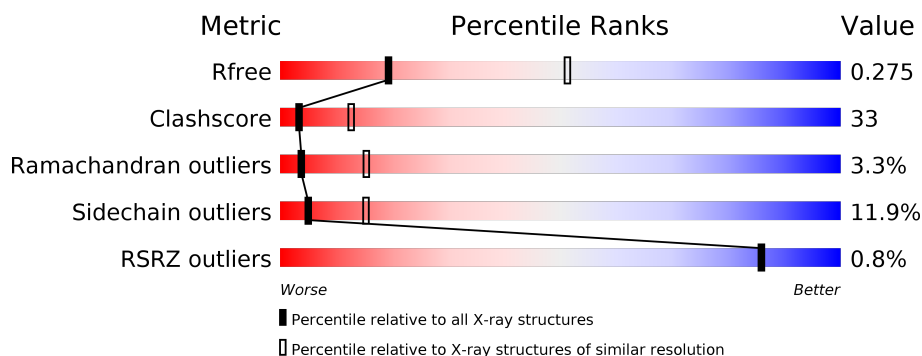
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	399	
1	B	399	
2	C	3	
3	D	4	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	2	X	-	-	X
3	MAN	D	3	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5970 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.

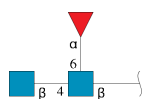
- Molecule 1 is a protein called COMPLEMENT C1R COMPONENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	172	0	1
			2932	1857	516	537	22			
1	B	368	Total	C	N	O	S	116	0	1
			2923	1852	515	534	22			

There are 2 discrepancies between the modelled and reference sequences:

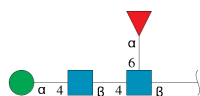
Chain	Residue	Modelled	Actual	Comment	Reference
A	446	GLN	ARG	engineered mutation	UNP P00736
B	446	GLN	ARG	engineered mutation	UNP P00736

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



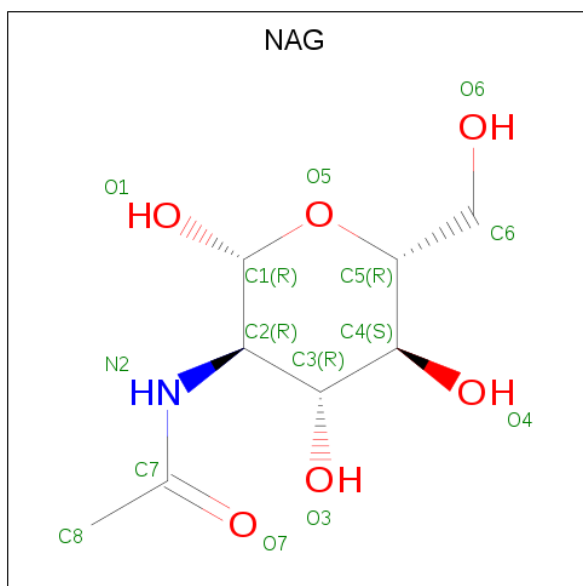
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

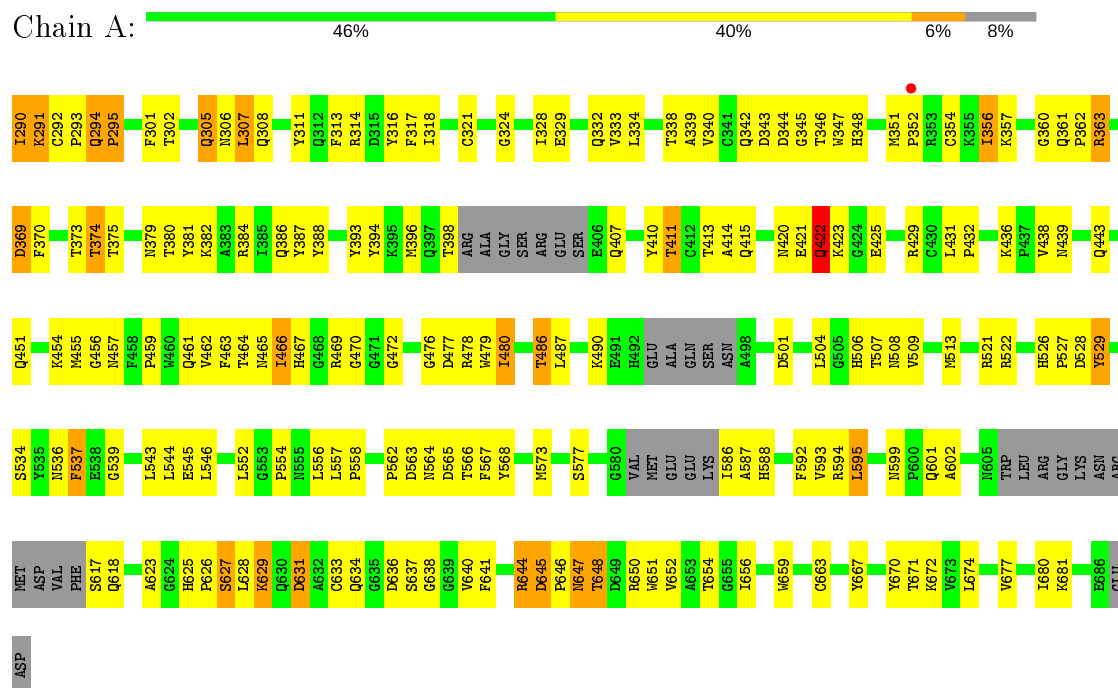
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	6	Total	O	0	0
			6	6		

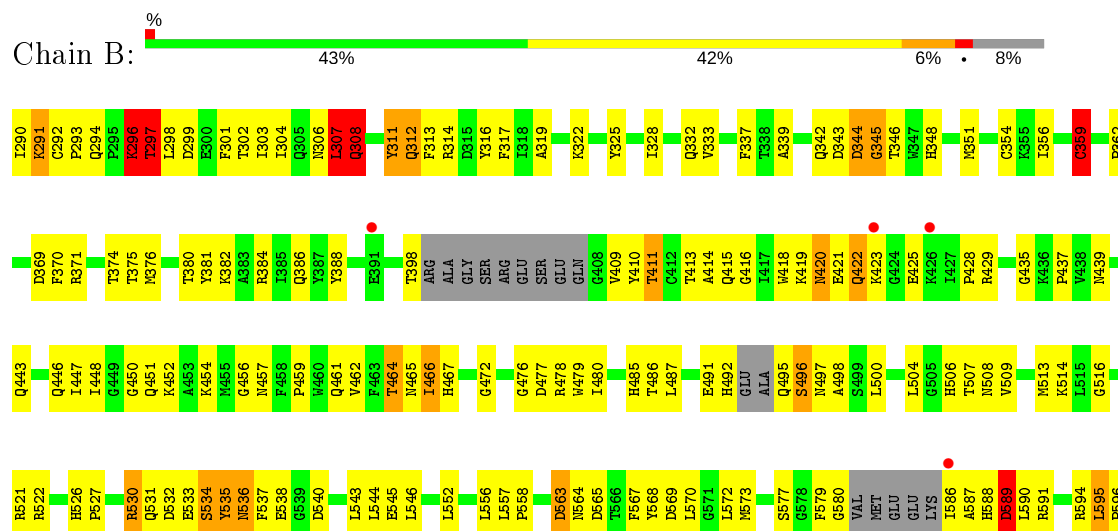
### 3 Residue-property plots

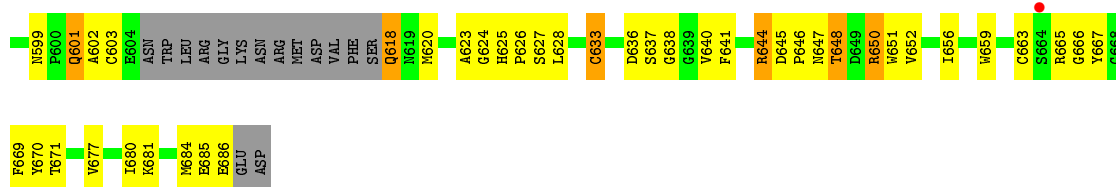
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: COMPLEMENT C1R COMPONENT



#### • Molecule 1: COMPLEMENT C1R COMPONENT





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 33% 67%



- Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.30 Å 101.80 Å 122.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.90 29.68 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (12.00-2.90) 98.4 (29.68-2.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.34	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.90 Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.242 , 0.290 0.226 , 0.275	Depositor DCC
$R_{free}$ test set	1360 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 85.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: FUC, NAG, MAN

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	0.70	0/3007	0.84	1/4074 (0.0%)
1	B	0.70	0/2998	0.89	4/4062 (0.1%)
All	All	0.70	0/6005	0.86	5/8136 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	CYS	CA-CB-SG	-11.25	93.75	114.00
1	B	563	ASP	CB-CA-C	-5.83	98.73	110.40
1	B	633	CYS	CA-CB-SG	5.50	123.90	114.00
1	B	466	ILE	N-CA-C	-5.31	96.66	111.00
1	A	633	CYS	CA-CB-SG	5.21	123.37	114.00

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	2932	0	2815	172	0
1	B	2923	0	2807	190	0
2	C	38	0	34	8	0
3	D	49	0	43	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	13	0	0
5	A	8	0	0	0	0
5	B	6	0	0	0	0
All	All	5970	0	5712	361	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 33.

All (361) 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:B:648:THR:HG23	1:B:650:ARG:HG2	1.29	1.09
1:A:480:ILE:HD11	1:A:544:LEU:HD12	1.12	1.07
1:B:480:ILE:HD11	1:B:544:LEU:HD12	1.12	1.05
1:B:648:THR:CG2	1:B:650:ARG:HG2	1.93	0.99
1:B:618:GLN:HE22	1:B:620:MET:HG3	1.25	0.97
1:B:567:PHE:CE1	1:B:572:LEU:HD13	2.02	0.95
1:A:506:HIS:HD2	1:A:508:ASN:H	1.03	0.94
1:A:480:ILE:CD1	1:A:544:LEU:HD12	1.99	0.93
1:B:506:HIS:CD2	1:B:508:ASN:H	1.87	0.92
1:B:480:ILE:CD1	1:B:544:LEU:HD12	1.99	0.92
1:B:506:HIS:HD2	1:B:508:ASN:H	1.04	0.92
2:C:1:NAG:H61	2:C:2:NAG:HN2	1.34	0.91
1:B:374:THR:HG22	1:B:375:THR:H	1.34	0.91
1:A:506:HIS:CD2	1:A:508:ASN:H	1.88	0.90
1:A:464:THR:HG22	1:A:470:GLY:C	1.93	0.88
1:B:307:LEU:O	1:B:308:GLN:HB2	1.74	0.88
1:A:466:ILE:HD11	1:A:487:LEU:HA	1.52	0.88
1:B:297:THR:O	1:B:298:LEU:HD23	1.74	0.88
1:B:454:LYS:H	1:B:457:ASN:ND2	1.76	0.84
1:B:480:ILE:HD11	1:B:544:LEU:CD1	2.05	0.84
1:B:636:ASP:O	1:B:637:SER:HB3	1.78	0.83
1:B:625:HIS:HD2	1:B:627:SER:OG	1.62	0.83
1:A:420:ASN:C	1:A:422:GLN:H	1.82	0.83
1:A:636:ASP:O	1:A:637:SER:HB3	1.77	0.82
1:B:480:ILE:HG12	1:B:544:LEU:HB2	1.63	0.81
1:A:438:VAL:HG11	1:A:554:PRO:HB3	1.63	0.80
1:B:506:HIS:HD2	1:B:508:ASN:N	1.78	0.80
1:A:432:PRO:HB3	1:A:552:LEU:HD11	1.62	0.80
1:A:529:TYR:HB2	1:A:539:GLY:O	1.81	0.80
1:A:506:HIS:HD2	1:A:508:ASN:N	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:LEU:H	1:B:595:LEU:HD12	1.48	0.79
1:B:410:TYR:OH	1:B:423:LYS:HE2	1.82	0.79
1:B:618:GLN:NE2	1:B:620:MET:HG3	1.98	0.78
1:A:595:LEU:H	1:A:595:LEU:HD12	1.48	0.77
1:A:593:VAL:HG23	1:A:634:GLN:HG3	1.66	0.77
1:A:370:PHE:HB3	1:A:387:TYR:CD2	2.20	0.77
1:B:410:TYR:HA	1:B:419:LYS:O	1.86	0.76
1:A:305:GLN:HB2	1:A:318:ILE:HG22	1.69	0.75
1:A:480:ILE:HG12	1:A:544:LEU:HB2	1.69	0.75
1:B:495:GLN:HG2	1:B:495:GLN:O	1.87	0.74
1:B:599:ASN:HD22	1:B:601:GLN:HB2	1.51	0.74
1:A:480:ILE:HD11	1:A:544:LEU:CD1	2.05	0.74
1:B:304:ILE:HD11	1:B:351:MET:HE1	1.69	0.74
1:B:409:VAL:O	1:B:420:ASN:HB2	1.87	0.74
1:B:446:GLN:O	1:B:448:ILE:HG13	1.89	0.73
1:A:291:LYS:O	1:A:345:GLY:HA2	1.88	0.73
1:A:420:ASN:O	1:A:422:GLN:N	2.20	0.73
1:B:314:ARG:HH11	1:B:314:ARG:HG3	1.54	0.73
1:B:374:THR:HG22	1:B:375:THR:N	2.04	0.73
1:A:420:ASN:HB3	1:A:423:LYS:H	1.52	0.73
1:B:304:ILE:HD11	1:B:351:MET:CE	2.18	0.72
2:C:1:NAG:H61	2:C:2:NAG:N2	2.03	0.72
1:B:599:ASN:ND2	1:B:601:GLN:HB2	2.05	0.71
1:A:291:LYS:O	1:A:345:GLY:CA	2.39	0.71
1:A:644:ARG:HB3	1:A:644:ARG:HH11	1.55	0.71
1:B:466:ILE:O	1:B:467:HIS:HB2	1.90	0.71
1:B:356:ILE:HD11	1:B:381:TYR:HB3	1.73	0.70
1:A:373:THR:O	1:A:373:THR:HG22	1.91	0.70
1:B:567:PHE:CD1	1:B:572:LEU:HD13	2.26	0.70
1:A:317:PHE:CE2	1:A:339:ALA:HB3	2.27	0.70
1:A:388:TYR:HA	1:A:396:MET:HE3	1.75	0.69
1:B:302:THR:HA	1:B:354:CYS:SG	2.34	0.68
1:B:625:HIS:CD2	1:B:627:SER:OG	2.47	0.67
1:A:436:LYS:HE3	1:A:650:ARG:HG2	1.76	0.66
1:A:573:MET:HE2	1:A:594:ARG:HG2	1.77	0.66
1:B:344:ASP:O	1:B:346:THR:HG23	1.95	0.66
1:A:454:LYS:H	1:A:457:ASN:ND2	1.93	0.66
1:B:304:ILE:HG23	1:B:317:PHE:HD1	1.60	0.66
1:A:595:LEU:N	1:A:595:LEU:HD12	2.11	0.66
1:A:407:GLN:HG2	1:A:407:GLN:O	1.94	0.66
1:B:313:PHE:CE2	1:B:314:ARG:HG2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:VAL:HG21	1:A:631:ASP:O	1.96	0.65
1:B:296:LYS:HD2	1:B:351:MET:HB3	1.79	0.65
1:B:648:THR:HG21	1:B:650:ARG:HH11	1.60	0.65
1:B:313:PHE:O	1:B:314:ARG:HB2	1.96	0.65
1:A:381:TYR:O	1:A:382:LYS:HB2	1.97	0.65
1:B:497:ASN:OD1	3:D:1:NAG:H2	1.97	0.65
1:B:644:ARG:HB3	1:B:644:ARG:HH11	1.61	0.65
1:A:351:MET:SD	1:A:352:PRO:HD2	2.37	0.65
1:A:293:PRO:O	1:A:295:PRO:HD3	1.96	0.64
1:B:595:LEU:HD12	1:B:595:LEU:N	2.12	0.64
1:A:490:LYS:NZ	1:A:536:ASN:H	1.96	0.64
1:A:490:LYS:NZ	1:A:537:PHE:H	1.96	0.63
1:B:625:HIS:CD2	1:B:627:SER:H	2.16	0.63
1:B:291:LYS:HB2	1:B:311:TYR:O	1.98	0.63
1:A:677:VAL:HG12	1:A:681:LYS:HD2	1.81	0.63
1:A:307:LEU:HA	1:A:311:TYR:OH	1.99	0.63
1:A:567:PHE:CE2	2:C:3:FUC:H62	2.35	0.62
1:A:663:CYS:HA	1:A:667:TYR:O	1.98	0.62
1:B:344:ASP:O	1:B:346:THR:N	2.33	0.62
1:B:304:ILE:HD12	1:B:317:PHE:CE1	2.35	0.62
1:A:373:THR:O	1:A:373:THR:CG2	2.48	0.61
1:A:487:LEU:HD11	1:A:544:LEU:HD21	1.82	0.61
1:B:536:ASN:C	1:B:538:GLU:H	2.02	0.61
1:B:602:ALA:HB1	1:B:667:TYR:CE1	2.35	0.61
1:A:420:ASN:C	1:A:422:GLN:N	2.53	0.61
1:B:304:ILE:HG23	1:B:317:PHE:CD1	2.36	0.61
1:A:306:ASN:H	3:D:4:FUC:H63	1.66	0.61
1:B:447:ILE:HG12	1:B:596:PRO:HD3	1.82	0.60
2:C:1:NAG:C6	2:C:2:NAG:HN2	2.09	0.60
1:B:648:THR:HG23	1:B:650:ARG:H	1.66	0.60
1:A:526:HIS:CG	1:A:527:PRO:HD2	2.37	0.60
1:B:435:GLY:O	1:B:437:PRO:HD3	2.01	0.60
1:B:526:HIS:CG	1:B:527:PRO:HD2	2.36	0.60
1:B:454:LYS:H	1:B:457:ASN:HD22	1.48	0.60
1:B:487:LEU:HD11	1:B:544:LEU:HD21	1.83	0.60
1:A:587:ALA:O	1:A:588:HIS:HB2	2.01	0.59
1:A:420:ASN:HB3	1:A:423:LYS:N	2.17	0.59
1:B:568:TYR:HA	1:B:572:LEU:HD22	1.84	0.59
1:A:464:THR:HG22	1:A:470:GLY:CA	2.33	0.59
1:B:595:LEU:HD13	1:B:641:PHE:HE1	1.66	0.59
1:A:529:TYR:H	1:A:539:GLY:HA3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ASN:ND2	1:A:455:MET:O	2.33	0.58
1:B:466:ILE:HG12	1:B:500:LEU:HA	1.85	0.58
1:B:536:ASN:O	1:B:538:GLU:N	2.36	0.58
1:A:436:LYS:HE3	1:A:650:ARG:CG	2.33	0.58
1:B:645:ASP:HB3	1:B:648:THR:HG22	1.86	0.58
1:A:625:HIS:HB3	1:A:628:LEU:HD12	1.84	0.58
1:B:573:MET:HE2	1:B:594:ARG:HG2	1.85	0.58
1:B:567:PHE:HE1	1:B:572:LEU:HD13	1.67	0.58
1:A:305:GLN:HB3	1:A:318:ILE:HB	1.86	0.57
1:A:476:GLY:O	1:A:558:PRO:HG3	2.04	0.57
1:B:648:THR:CG2	1:B:650:ARG:H	2.17	0.57
1:A:564:ASN:HD22	2:C:1:NAG:C7	2.17	0.57
1:A:344:ASP:OD1	1:A:346:THR:HG22	2.05	0.57
1:B:293:PRO:O	1:B:294:GLN:C	2.42	0.57
1:A:595:LEU:HD13	1:A:641:PHE:HE1	1.69	0.57
1:A:636:ASP:O	1:A:637:SER:CB	2.48	0.56
1:B:586:ILE:HG22	1:B:587:ALA:N	2.21	0.56
1:A:302:THR:HA	1:A:354:CYS:SG	2.46	0.56
1:A:363:ARG:CZ	1:A:363:ARG:HB3	2.35	0.56
1:A:454:LYS:H	1:A:457:ASN:HD22	1.52	0.56
1:A:593:VAL:HG23	1:A:634:GLN:CG	2.35	0.56
1:A:363:ARG:NH1	1:A:363:ARG:HB3	2.20	0.56
1:A:568:TYR:CE2	1:A:672:LYS:HG3	2.41	0.55
1:A:306:ASN:HA	3:D:4:FUC:H2	1.88	0.55
1:A:311:TYR:HD2	1:A:347:TRP:HH2	1.53	0.55
1:B:568:TYR:C	1:B:568:TYR:CD2	2.79	0.55
1:B:677:VAL:HG12	1:B:681:LYS:HD2	1.86	0.55
1:B:291:LYS:O	1:B:291:LYS:HD2	2.06	0.55
1:B:626:PRO:HD3	1:B:667:TYR:OH	2.06	0.55
1:A:425:GLU:O	1:A:425:GLU:HG2	2.07	0.55
1:B:595:LEU:HB3	1:B:628:LEU:HD11	1.87	0.54
1:B:476:GLY:O	1:B:558:PRO:HG3	2.08	0.54
1:B:303:ILE:HG22	1:B:304:ILE:N	2.23	0.54
1:B:307:LEU:O	1:B:308:GLN:CB	2.52	0.54
1:B:381:TYR:O	1:B:382:LYS:HB2	2.05	0.54
1:B:648:THR:CG2	1:B:650:ARG:CG	2.80	0.54
1:A:305:GLN:CB	1:A:318:ILE:HG22	2.36	0.54
1:B:533:GLU:O	1:B:535:TYR:N	2.41	0.54
1:B:527:PRO:O	1:B:530:ARG:NH2	2.39	0.54
1:A:388:TYR:HA	1:A:396:MET:CE	2.36	0.54
1:B:291:LYS:CD	1:B:291:LYS:C	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:PRO:O	1:A:295:PRO:CD	2.56	0.53
1:B:466:ILE:O	1:B:467:HIS:CB	2.53	0.53
1:B:423:LYS:HE3	1:B:428:PRO:CA	2.39	0.53
1:B:328:ILE:HD13	1:B:333:VAL:HA	1.90	0.53
1:A:466:ILE:CG1	1:A:467:HIS:N	2.71	0.53
1:A:564:ASN:ND2	2:C:1:NAG:C7	2.72	0.53
1:A:526:HIS:CD2	1:A:527:PRO:HD2	2.44	0.53
1:B:314:ARG:NH1	1:B:314:ARG:HG3	2.22	0.53
1:B:443:GLN:CD	1:B:644:ARG:NH2	2.62	0.52
1:B:625:HIS:HD2	1:B:627:SER:CB	2.21	0.52
1:A:301:PHE:O	1:A:321:CYS:HA	2.09	0.52
1:A:456:GLY:O	1:A:459:PRO:HD3	2.08	0.52
1:B:291:LYS:HD2	1:B:291:LYS:C	2.30	0.52
1:A:644:ARG:CB	1:A:644:ARG:HH11	2.22	0.52
1:A:490:LYS:HZ3	1:A:536:ASN:H	1.56	0.52
1:B:317:PHE:CE2	1:B:339:ALA:HB3	2.44	0.52
1:B:297:THR:C	1:B:298:LEU:HD23	2.30	0.52
1:B:586:ILE:O	1:B:587:ALA:HB3	2.10	0.52
1:A:292:CYS:HA	1:A:345:GLY:O	2.09	0.52
1:A:374:THR:O	1:A:375:THR:C	2.44	0.51
1:A:465:ASN:O	1:A:501:ASP:HB2	2.11	0.51
1:B:307:LEU:HD12	1:B:311:TYR:OH	2.10	0.51
1:B:526:HIS:CD2	1:B:527:PRO:HD2	2.45	0.51
1:A:528:ASP:O	1:A:529:TYR:C	2.48	0.51
1:A:647:ASN:O	1:A:648:THR:HB	2.09	0.51
1:B:359:CYS:HB3	1:B:416:GLY:C	2.30	0.51
1:A:369:ASP:HB3	1:A:388:TYR:CZ	2.46	0.51
1:B:648:THR:HG21	1:B:650:ARG:HG2	1.89	0.50
1:A:490:LYS:HZ2	1:A:537:PHE:H	1.58	0.50
1:A:623:ALA:HB3	1:A:670:TYR:CE1	2.46	0.50
1:A:629:LYS:N	1:A:629:LYS:HD2	2.25	0.50
1:A:645:ASP:CG	1:A:648:THR:HG22	2.31	0.50
1:B:656:ILE:HB	1:B:671:THR:HB	1.94	0.50
1:A:432:PRO:HB3	1:A:552:LEU:CD1	2.38	0.50
1:B:450:GLY:HA3	1:B:591:ARG:HH12	1.76	0.50
1:B:313:PHE:HD1	1:B:342:GLN:C	2.16	0.50
1:B:325:TYR:CD2	1:B:356:ILE:HA	2.47	0.50
1:A:356:ILE:HD11	1:A:381:TYR:HB3	1.92	0.49
1:B:485:HIS:ND1	1:B:540:ASP:OD2	2.39	0.49
1:A:356:ILE:CG1	1:A:381:TYR:HB3	2.42	0.49
1:B:291:LYS:HA	1:B:312:GLN:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:THR:HG22	1:A:414:ALA:N	2.28	0.49
1:A:413:THR:HG22	1:A:415:GLN:H	1.78	0.49
1:B:302:THR:HG22	1:B:303:ILE:N	2.27	0.49
1:A:568:TYR:CZ	1:A:672:LYS:HG3	2.47	0.49
1:B:413:THR:HG22	1:B:415:GLN:H	1.78	0.49
1:B:464:THR:HG23	1:B:465:ASN:N	2.27	0.49
1:B:665:ARG:O	1:B:665:ARG:HG3	2.13	0.49
1:A:438:VAL:HG11	1:A:554:PRO:CB	2.39	0.49
1:A:466:ILE:CD1	1:A:487:LEU:HA	2.35	0.49
1:B:304:ILE:HD11	1:B:351:MET:HE3	1.94	0.49
1:B:589:ASP:OD2	1:B:589:ASP:N	2.44	0.49
1:B:567:PHE:HD2	1:B:647:ASN:ND2	2.10	0.49
1:B:290:ILE:O	1:B:290:ILE:HG13	2.11	0.49
1:A:340:VAL:HG21	1:B:514:LYS:HG3	1.93	0.49
1:B:580:GLY:HA2	1:B:587:ALA:HB2	1.94	0.49
1:B:636:ASP:O	1:B:637:SER:CB	2.48	0.49
1:A:360:GLY:O	1:A:379:ASN:HB3	2.13	0.48
1:A:343:ASP:C	1:A:345:GLY:H	2.16	0.48
1:B:599:ASN:HD21	1:B:601:GLN:CD	2.16	0.48
1:B:623:ALA:HB3	1:B:670:TYR:CE1	2.48	0.48
1:A:625:HIS:CD2	1:A:627:SER:HB2	2.48	0.48
1:B:369:ASP:HB3	1:B:388:TYR:CZ	2.48	0.48
1:A:398:THR:HA	1:A:407:GLN:OE1	2.13	0.48
1:B:290:ILE:HD11	1:B:345:GLY:H	1.78	0.48
1:A:344:ASP:CG	1:A:346:THR:HG22	2.34	0.48
1:A:461:GLN:NE2	1:A:577:SER:OG	2.46	0.48
1:A:501:ASP:OD2	1:B:316:TYR:OH	2.24	0.48
1:B:588:HIS:O	1:B:589:ASP:O	2.32	0.48
1:B:423:LYS:HE3	1:B:428:PRO:HA	1.96	0.47
1:A:568:TYR:CZ	1:A:672:LYS:CG	2.97	0.47
1:B:413:THR:HG22	1:B:414:ALA:N	2.29	0.47
1:A:370:PHE:HA	1:A:387:TYR:HA	1.96	0.47
1:B:303:ILE:CG2	1:B:304:ILE:N	2.77	0.47
1:B:356:ILE:CD1	1:B:381:TYR:HB3	2.44	0.47
1:A:316:TYR:CD2	1:B:513:MET:SD	3.08	0.47
1:A:305:GLN:O	1:A:306:ASN:HB3	2.15	0.47
1:B:292:CYS:HA	1:B:345:GLY:O	2.14	0.47
1:A:307:LEU:O	1:A:307:LEU:HD12	2.15	0.47
1:A:479:TRP:CH2	1:A:545:GLU:HG3	2.50	0.47
1:A:324:GLY:O	1:A:357:LYS:HG3	2.14	0.47
1:B:533:GLU:O	1:B:534:SER:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:THR:HG21	1:B:650:ARG:NH1	2.29	0.46
1:B:624:GLY:HA3	1:B:666:GLY:O	2.15	0.46
1:B:479:TRP:CH2	1:B:545:GLU:HG3	2.49	0.46
1:B:462:VAL:HG22	1:B:504:LEU:HD23	1.97	0.46
1:A:644:ARG:CG	1:A:644:ARG:HH11	2.28	0.46
1:B:306:ASN:O	1:B:307:LEU:C	2.53	0.46
1:B:472:GLY:HA2	1:B:638:GLY:O	2.14	0.46
1:B:644:ARG:HG2	1:B:651:TRP:CE2	2.50	0.46
1:B:644:ARG:CB	1:B:644:ARG:HH11	2.26	0.46
1:A:342:GLN:HB2	1:A:346:THR:O	2.15	0.46
1:B:306:ASN:O	1:B:307:LEU:O	2.33	0.46
1:B:313:PHE:CD2	1:B:314:ARG:HG2	2.49	0.46
1:A:308:GLN:N	1:A:311:TYR:OH	2.39	0.46
1:A:644:ARG:HG2	1:A:651:TRP:CE2	2.50	0.46
1:B:648:THR:HG23	1:B:650:ARG:CG	2.22	0.46
1:B:603:CYS:HB3	1:B:669:PHE:CZ	2.51	0.46
1:A:370:PHE:HA	1:A:386:GLN:O	2.16	0.45
1:A:656:ILE:HB	1:A:671:THR:HB	1.98	0.45
1:B:299:ASP:OD1	1:B:301:PHE:HB2	2.17	0.45
1:B:410:TYR:CA	1:B:419:LYS:O	2.62	0.45
1:B:663:CYS:HA	1:B:667:TYR:O	2.17	0.45
1:A:291:LYS:HG3	1:A:292:CYS:N	2.31	0.45
1:A:563:ASP:HA	1:A:674:LEU:HD13	1.99	0.45
1:B:311:TYR:N	1:B:311:TYR:CD1	2.85	0.45
1:A:384:ARG:HG2	1:A:411:THR:HG22	1.99	0.45
1:B:374:THR:CG2	1:B:375:THR:H	2.05	0.45
1:A:291:LYS:HB2	1:A:291:LYS:HE3	1.67	0.45
1:A:563:ASP:C	1:A:563:ASP:OD1	2.54	0.44
1:A:625:HIS:O	1:A:628:LEU:HB2	2.18	0.44
1:A:311:TYR:CD2	1:A:347:TRP:HH2	2.33	0.44
1:B:595:LEU:CD1	1:B:641:PHE:HE1	2.31	0.44
1:A:462:VAL:HG22	1:A:504:LEU:HD23	1.99	0.44
1:B:312:GLN:HE21	1:B:312:GLN:HB3	1.64	0.44
1:B:291:LYS:O	1:B:345:GLY:HA2	2.17	0.44
1:B:579:PHE:HB3	1:B:587:ALA:HB1	1.99	0.44
1:A:393:TYR:OH	1:A:554:PRO:HD3	2.17	0.44
1:B:456:GLY:O	1:B:459:PRO:HD3	2.16	0.44
1:A:466:ILE:HG12	1:A:467:HIS:H	1.81	0.44
1:A:563:ASP:HA	1:A:674:LEU:CD1	2.48	0.44
1:B:531:GLN:HG2	1:B:532:ASP:N	2.33	0.44
1:B:568:TYR:HA	1:B:572:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:ARG:CG	1:B:644:ARG:HH11	2.29	0.44
1:B:659:TRP:O	1:B:669:PHE:HB2	2.18	0.44
1:A:443:GLN:NE2	1:A:644:ARG:NH2	2.65	0.44
1:B:567:PHE:CD2	1:B:646:PRO:HD2	2.53	0.44
1:B:308:GLN:HB2	1:B:311:TYR:CZ	2.53	0.44
1:B:563:ASP:CB	1:B:565:ASP:H	2.31	0.44
1:A:629:LYS:HD2	1:A:629:LYS:H	1.82	0.43
1:A:529:TYR:N	1:A:539:GLY:HA3	2.33	0.43
1:A:601:GLN:O	1:A:602:ALA:C	2.56	0.43
1:B:425:GLU:HG2	1:B:425:GLU:O	2.18	0.43
1:A:472:GLY:HA2	1:A:638:GLY:O	2.17	0.43
1:B:302:THR:HG22	1:B:303:ILE:H	1.84	0.43
1:A:599:ASN:HD22	1:A:601:GLN:HB2	1.83	0.43
1:B:314:ARG:NH1	1:B:314:ARG:CG	2.80	0.43
1:B:319:ALA:HB3	1:B:337:PHE:HB3	2.00	0.43
1:A:528:ASP:HB2	1:A:539:GLY:HA3	2.00	0.43
1:A:313:PHE:CD1	1:A:343:ASP:N	2.87	0.43
1:A:466:ILE:HD11	1:A:486:THR:O	2.19	0.43
1:A:313:PHE:CE1	1:A:343:ASP:N	2.87	0.43
1:A:543:LEU:HD11	1:A:680:ILE:HG23	2.01	0.43
1:B:478:ARG:HA	1:B:546:LEU:HD12	2.01	0.43
1:B:602:ALA:HB1	1:B:667:TYR:CD1	2.54	0.43
1:A:328:ILE:HD13	1:A:333:VAL:HA	2.01	0.42
1:A:478:ARG:HA	1:A:546:LEU:HD12	2.00	0.42
1:B:304:ILE:HD12	1:B:317:PHE:CD1	2.54	0.42
1:B:464:THR:CG2	1:B:465:ASN:N	2.80	0.42
1:B:498:ALA:HA	3:D:4:FUC:O3	2.19	0.42
1:A:311:TYR:CD2	1:A:347:TRP:CH2	3.07	0.42
1:A:521:ARG:HG2	1:A:522:ARG:HG3	2.00	0.42
1:A:617:SER:OG	1:A:618:GLN:N	2.51	0.42
1:A:626:PRO:C	1:A:628:LEU:H	2.22	0.42
1:B:509:VAL:O	1:B:513:MET:HG3	2.19	0.42
1:B:625:HIS:CD2	1:B:627:SER:CB	3.01	0.42
1:B:496:SER:OG	3:D:1:NAG:C8	2.67	0.42
1:A:648:THR:HG23	1:A:650:ARG:HB2	2.01	0.42
1:B:370:PHE:HA	1:B:386:GLN:O	2.19	0.42
1:B:384:ARG:HG2	1:B:411:THR:HG22	2.01	0.42
1:A:566:THR:OG1	2:C:1:NAG:H62	2.20	0.42
1:B:344:ASP:OD1	1:B:344:ASP:N	2.53	0.42
1:B:435:GLY:O	1:B:651:TRP:HD1	2.03	0.42
1:A:329:GLU:HB2	1:A:334:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:TYR:HA	1:A:339:ALA:O	2.19	0.42
1:A:344:ASP:OD2	1:A:346:THR:HG22	2.19	0.42
1:A:394:TYR:HA	1:A:431:LEU:O	2.20	0.42
1:B:410:TYR:N	1:B:410:TYR:CD1	2.88	0.42
1:B:552:LEU:HB3	1:B:557:LEU:HD23	2.01	0.42
1:B:344:ASP:C	1:B:346:THR:H	2.22	0.42
1:B:375:THR:O	1:B:376:MET:C	2.57	0.42
1:B:665:ARG:O	1:B:665:ARG:CG	2.67	0.42
1:A:313:PHE:O	1:A:314:ARG:HB2	2.20	0.42
1:A:338:THR:HB	1:B:516:GLY:HA2	2.02	0.42
1:A:595:LEU:N	1:A:595:LEU:CD1	2.82	0.41
1:A:599:ASN:ND2	1:A:601:GLN:HB2	2.34	0.41
1:B:292:CYS:HB3	1:B:293:PRO:HD2	2.02	0.41
1:B:356:ILE:HG23	1:B:356:ILE:O	2.19	0.41
1:B:521:ARG:HG2	1:B:522:ARG:HG3	2.01	0.41
1:A:451:GLN:HB2	1:A:592:PHE:CE2	2.56	0.41
1:B:563:ASP:HB2	1:B:565:ASP:H	1.85	0.41
1:A:567:PHE:CD2	2:C:3:FUC:H62	2.55	0.41
1:A:509:VAL:O	1:A:513:MET:HG3	2.20	0.41
1:A:645:ASP:OD2	1:A:648:THR:CG2	2.69	0.41
1:B:296:LYS:HB2	1:B:297:THR:H	1.43	0.41
1:B:322:LYS:HB3	1:B:322:LYS:HE2	1.81	0.41
1:B:579:PHE:CB	1:B:587:ALA:HB1	2.51	0.41
1:B:543:LEU:HD11	1:B:680:ILE:HG23	2.01	0.41
1:A:361:GLN:NE2	1:A:362:PRO:HD2	2.35	0.41
1:A:463:PHE:CZ	1:A:469:ARG:HG3	2.56	0.41
1:B:420:ASN:O	1:B:422:GLN:N	2.50	0.41
1:B:684:MET:O	1:B:686:GLU:N	2.53	0.41
1:A:410:TYR:N	1:A:410:TYR:CD1	2.88	0.41
1:A:420:ASN:HB3	1:A:423:LYS:CA	2.50	0.41
1:B:451:GLN:HB3	1:B:451:GLN:HE21	1.63	0.41
1:A:305:GLN:CB	1:A:318:ILE:CG2	3.00	0.40
1:A:398:THR:CB	1:A:407:GLN:OE1	2.69	0.40
1:A:552:LEU:HB3	1:A:557:LEU:HD23	2.03	0.40
1:A:290:ILE:O	1:A:290:ILE:HG23	2.20	0.40
1:A:293:PRO:O	1:A:295:PRO:N	2.54	0.40
1:A:466:ILE:HG12	1:A:467:HIS:N	2.36	0.40
1:B:362:PRO:HG3	1:B:418:TRP:CE2	2.56	0.40
1:B:496:SER:OG	3:D:1:NAG:H81	2.21	0.40
1:A:628:LEU:O	1:A:629:LYS:C	2.59	0.40
1:B:521:ARG:NH1	1:B:545:GLU:OE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:THR:HG22	1:A:470:GLY:O	2.19	0.40
1:B:461:GLN:NE2	1:B:577:SER:OG	2.54	0.40
1:A:641:PHE:HD2	1:A:654:THR:OG1	2.05	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	359/399 (90%)	316 (88%)	34 (10%)	9 (2%)	5	21
1	B	358/399 (90%)	310 (87%)	33 (9%)	15 (4%)	3	10
All	All	717/798 (90%)	626 (87%)	67 (9%)	24 (3%)	4	15

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	421	GLU
1	A	422	GLN
1	A	534	SER
1	A	648	THR
1	B	296	LYS
1	B	297	THR
1	B	307	LEU
1	B	308	GLN
1	B	496	SER
1	B	534	SER
1	B	535	TYR
1	B	536	ASN
1	B	685	GLU
1	B	345	GLY

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Mol	Chain	Res	Type
1	B	422	GLN
1	B	537	PHE
1	A	537	PHE
1	B	421	GLU
1	B	491	GLU
1	B	589	ASP
1	A	529	TYR
1	A	627	SER
1	A	631	ASP

### 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	315/342 (92%)	281 (89%)	34 (11%)	6	20
1	B	314/342 (92%)	273 (87%)	41 (13%)	4	12
All	All	629/684 (92%)	554 (88%)	75 (12%)	5	15

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	ILE
1	A	291	LYS
1	A	294	GLN
1	A	295	PRO
1	A	305	GLN
1	A	307	LEU
1	A	332	GLN
1	A	348	HIS
1	A	356	ILE
1	A	363	ARG
1	A	369	ASP
1	A	374	THR
1	A	380	THR
1	A	411	THR

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Mol	Chain	Res	Type
1	A	422	GLN
1	A	429	ARG
1	A	466	ILE
1	A	477	ASP
1	A	480	ILE
1	A	486	THR
1	A	507	THR
1	A	556	LEU
1	A	562	PRO
1	A	565	ASP
1	A	586	ILE
1	A	595	LEU
1	A	629	LYS
1	A	640	VAL
1	A	644	ARG
1	A	645	ASP
1	A	646	PRO
1	A	647	ASN
1	A	652	VAL
1	A	659	TRP
1	B	291	LYS
1	B	296	LYS
1	B	297	THR
1	B	307	LEU
1	B	308	GLN
1	B	311	TYR
1	B	312	GLN
1	B	332	GLN
1	B	343	ASP
1	B	344	ASP
1	B	348	HIS
1	B	359	CYS
1	B	371	ARG
1	B	380	THR
1	B	398	THR
1	B	411	THR
1	B	420	ASN
1	B	429	ARG
1	B	439	ASN
1	B	452	LYS
1	B	464	THR
1	B	477	ASP

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Mol	Chain	Res	Type
1	B	486	THR
1	B	492	HIS
1	B	507	THR
1	B	530	ARG
1	B	556	LEU
1	B	564	ASN
1	B	569	ASP
1	B	570	LEU
1	B	589	ASP
1	B	590	LEU
1	B	595	LEU
1	B	601	GLN
1	B	618	GLN
1	B	633	CYS
1	B	640	VAL
1	B	644	ARG
1	B	648	THR
1	B	650	ARG
1	B	652	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	326	GLN
1	A	332	GLN
1	A	361	GLN
1	A	443	GLN
1	A	457	ASN
1	A	461	GLN
1	A	506	HIS
1	A	548	ASN
1	A	599	ASN
1	B	305	GLN
1	B	306	ASN
1	B	312	GLN
1	B	326	GLN
1	B	439	ASN
1	B	451	GLN
1	B	457	ASN
1	B	461	GLN
1	B	465	ASN

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Mol	Chain	Res	Type
1	B	506	HIS
1	B	555	ASN
1	B	599	ASN
1	B	625	HIS
1	B	647	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

7 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	C	1	1,2	14,14,15	0.69	0	17,19,21	1.28	2 (11%)
2	NAG	C	2	2	14,14,15	0.74	0	17,19,21	0.67	0
2	FUC	C	3	2	10,10,11	0.77	1 (10%)	14,14,16	0.50	0
3	NAG	D	1	1,3	14,14,15	0.82	0	17,19,21	1.00	2 (11%)
3	NAG	D	2	3	14,14,15	0.76	0	17,19,21	1.03	2 (11%)
3	MAN	D	3	3	11,11,12	0.76	0	15,15,17	1.18	3 (20%)
3	FUC	D	4	3	10,10,11	0.67	0	14,14,16	0.94	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	C	2	2	1/1/5/7	4/6/23/26	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	MAN	D	3	3	-	2/2/19/22	0/1/1/1
3	FUC	D	4	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	FUC	C2-C3	2.02	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C4-C3-C2	-3.63	105.69	111.02
3	D	1	NAG	C2-N2-C7	-2.79	118.93	122.90
3	D	2	NAG	C4-C3-C2	-2.71	107.05	111.02
2	C	1	NAG	C2-N2-C7	-2.63	119.16	122.90
3	D	3	MAN	C1-O5-C5	2.53	115.62	112.19
3	D	3	MAN	C1-C2-C3	2.49	112.73	109.67
3	D	3	MAN	O5-C1-C2	2.44	114.54	110.77
3	D	4	FUC	C1-C2-C3	-2.07	107.12	109.67
3	D	2	NAG	C2-N2-C7	-2.06	119.97	122.90
3	D	1	NAG	C1-O5-C5	2.04	114.96	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2	NAG	C1

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2

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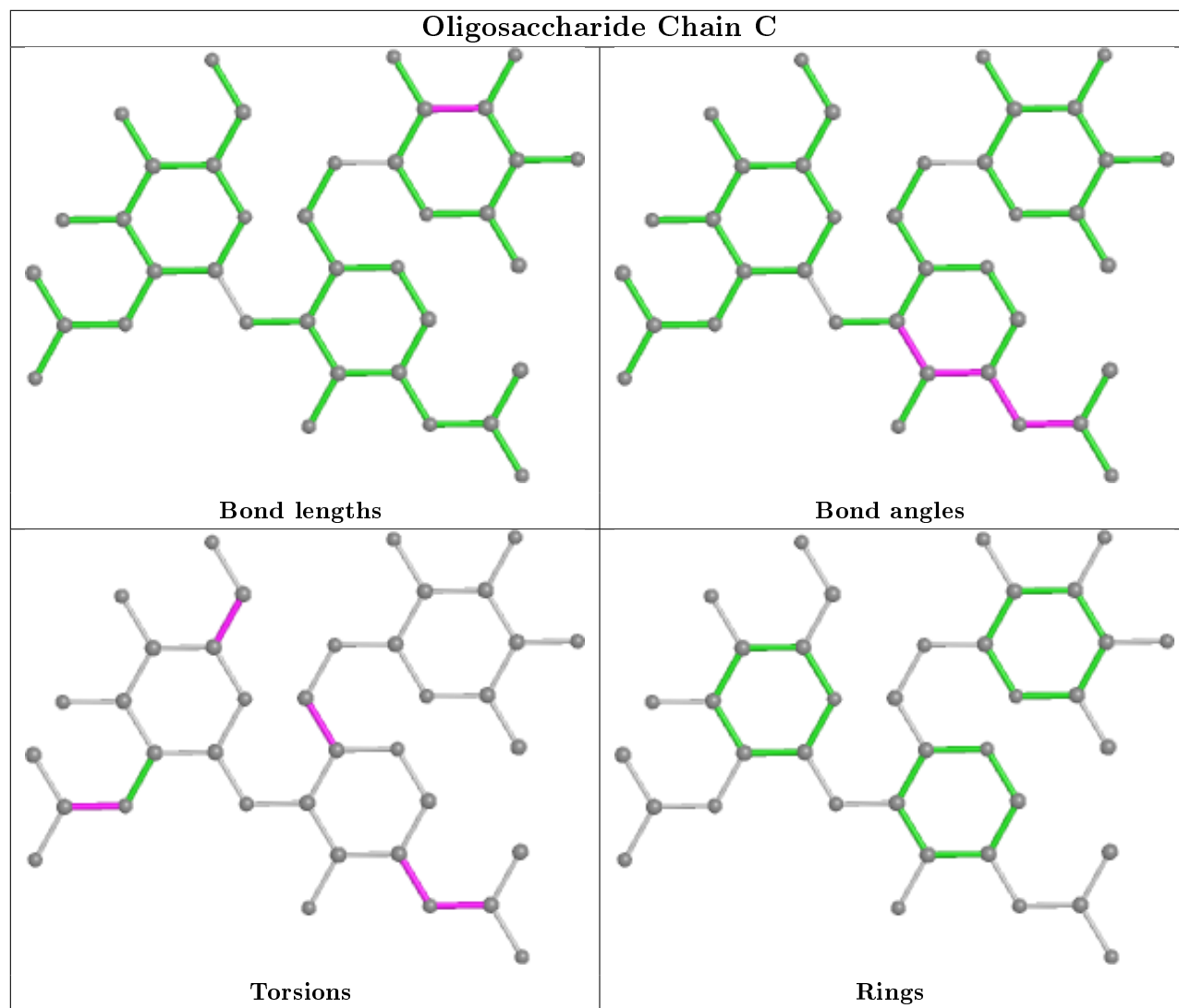
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	3	MAN	C4-C5-C6-O6
3	D	3	MAN	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7

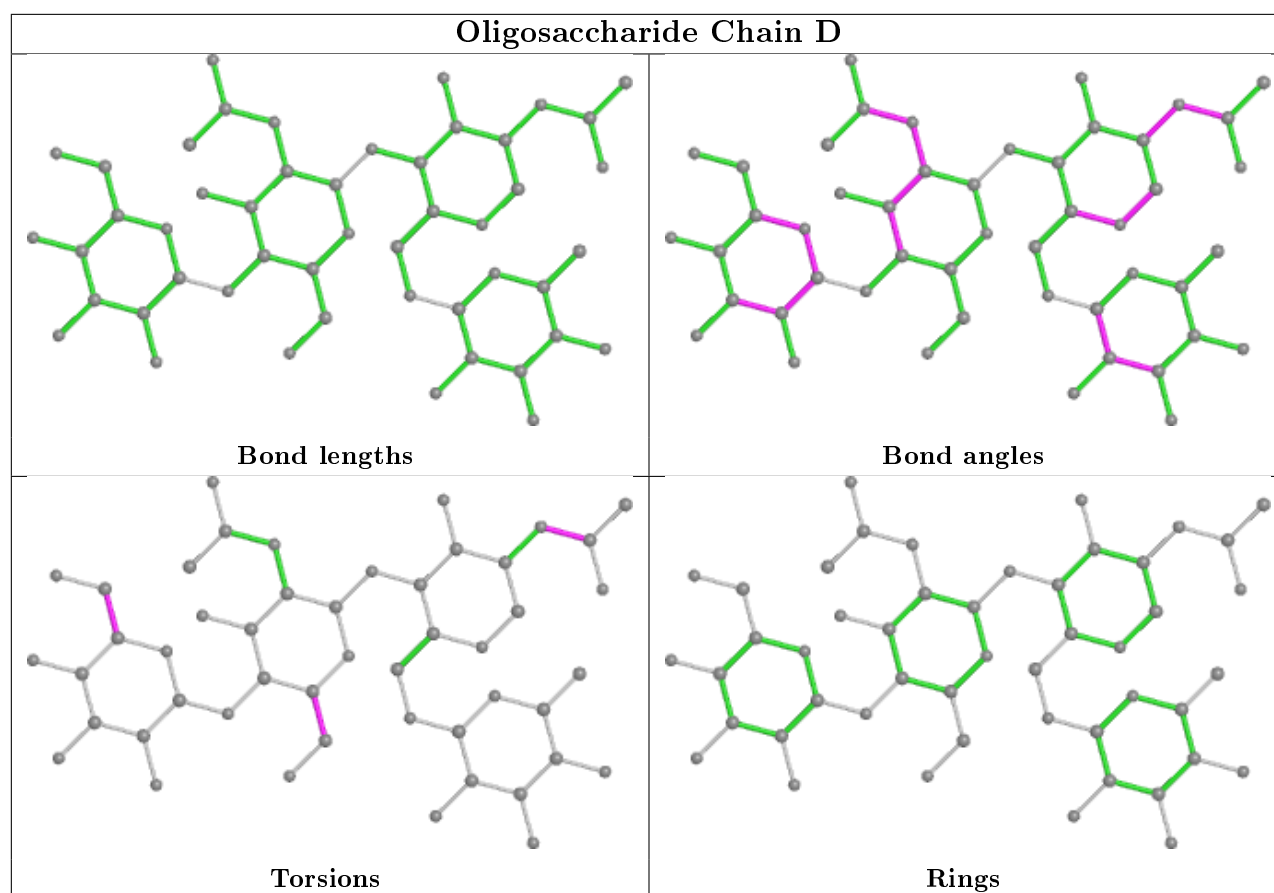
There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	3	0
2	C	1	NAG	6	0
2	C	2	NAG	3	0
3	D	4	FUC	3	0
2	C	3	FUC	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](#)

1 ligand is 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	$\# Z  > 2$
4	NAG	B	1005	1	14,14,15	1.02	1 (7%)	17,19,21	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1005	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1005	NAG	C1-C2	2.90	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1005	NAG	C8-C7-N2-C2
4	B	1005	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	369/399 (92%)	0.02	1 (0%) 94 94	31, 54, 88, 135	38 (10%)
1	B	368/399 (92%)	0.10	5 (1%) 75 75	25, 53, 84, 129	30 (8%)
All	All	737/798 (92%)	0.06	6 (0%) 86 86	25, 53, 87, 135	68 (9%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	586	ILE	4.7
1	B	423	LYS	4.0
1	A	352	PRO	3.1
1	B	426	LYS	2.8
1	B	664	SER	2.2
1	B	391	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(Å <sup>2</sup> )	Q<0.9
3	MAN	D	3	11/12	0.49	0.42	97,106,112,113	0
2	NAG	C	2	14/15	0.74	0.61	138,145,150,150	0
2	NAG	C	1	14/15	0.78	0.26	99,107,117,126	0

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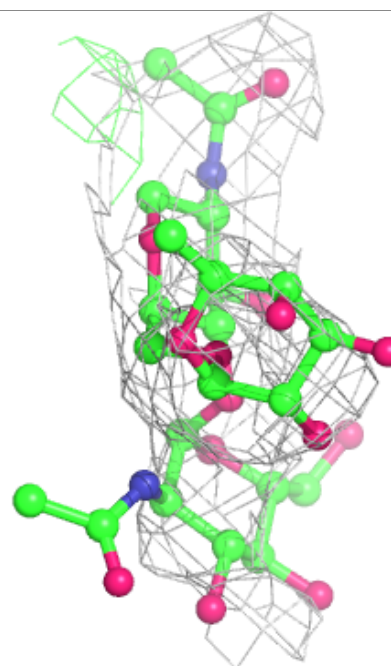
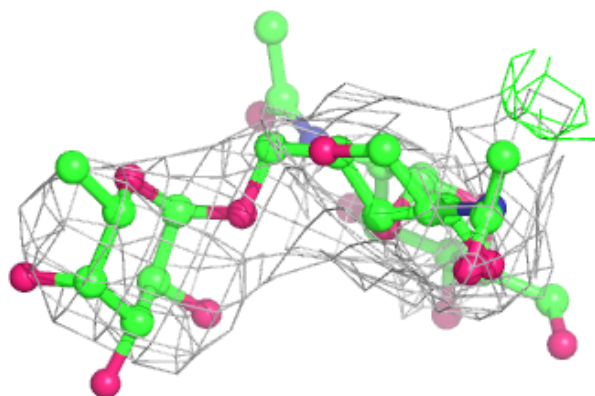
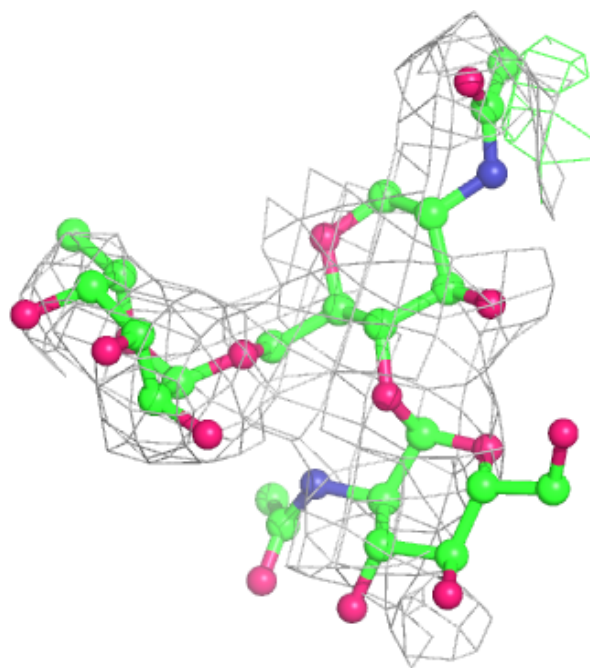
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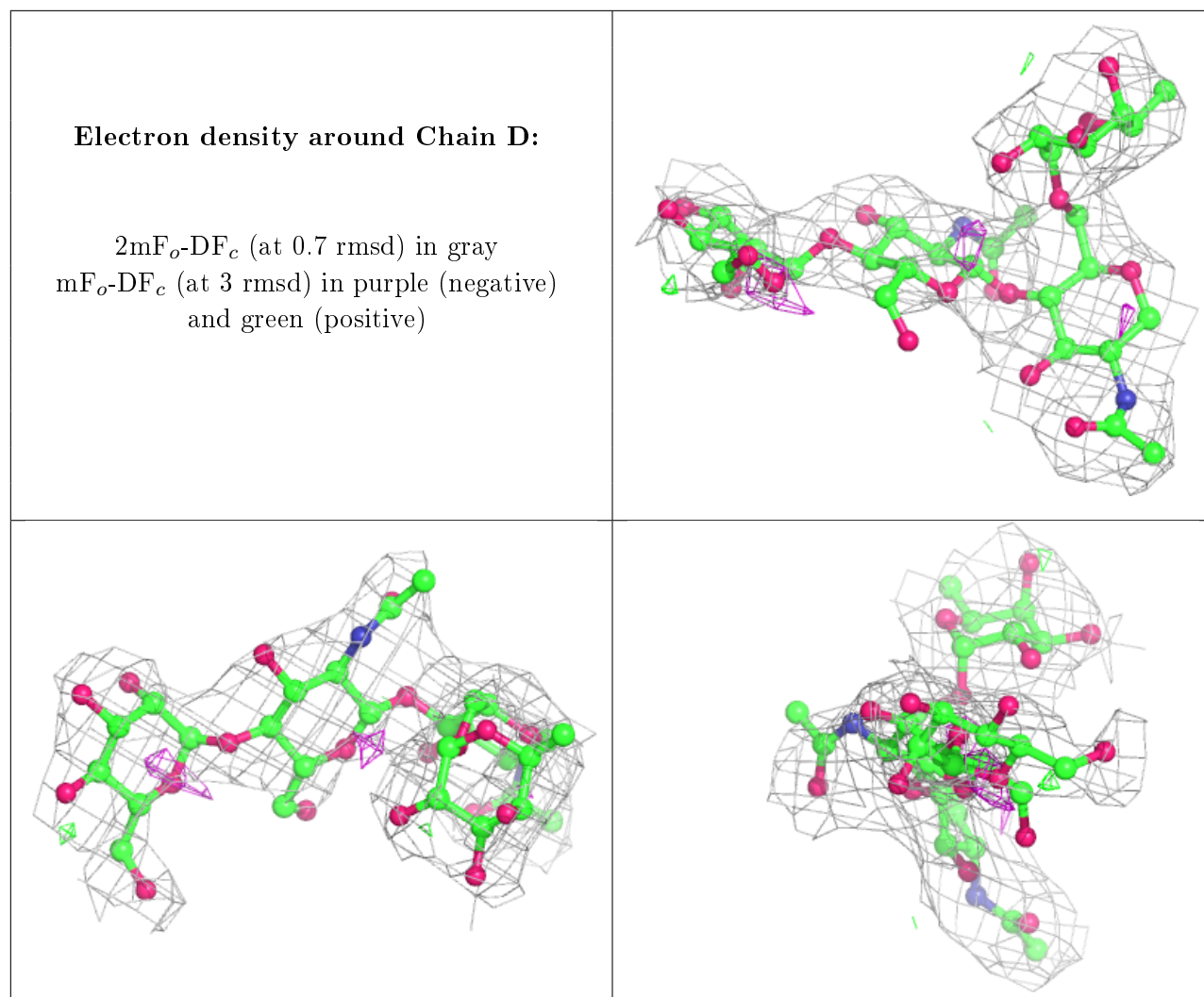
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	2	14/15	0.85	0.41	91,96,100,101	0
2	FUC	C	3	10/11	0.89	0.44	105,113,115,115	0
3	NAG	D	1	14/15	0.91	0.19	64,77,82,88	0
3	FUC	D	4	10/11	0.92	0.14	77,79,85,87	0

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

**Electron density around Chain C:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	1005	14/15	0.85	0.18	77,82,85,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.