



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2024 – 03:35 PM EST

PDB ID : 3T5O  
Title : Crystal Structure of human Complement Component C6  
Authors : Aleshin, A.E.; Stec, B.; Bankston, L.A.; DiScipio, R.G.; Liddington, R.C.  
Deposited on : 2011-07-27  
Resolution : 2.87 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.

The types of validation reports are described at

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

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

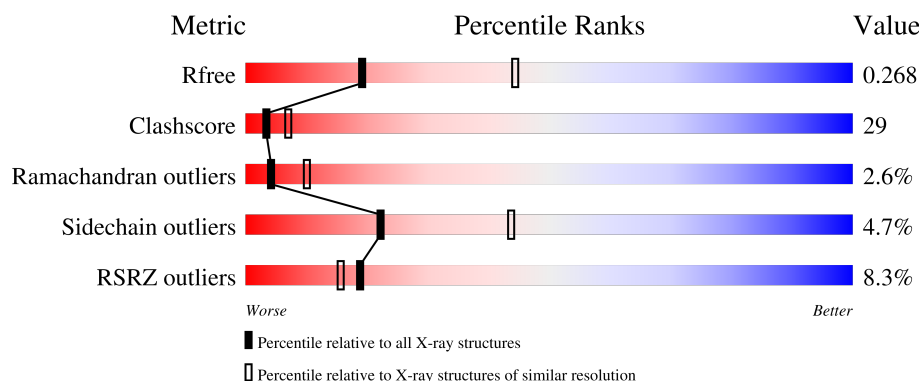
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.87 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))
$R_{free}$	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	913	 8% 52% 38% 5% 5%
2	B	2	 100%
3	C	2	 50% 50%

## 2 Entry composition [i](#)

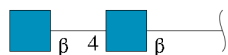
There are 6 unique types of molecules in this entry. The entry contains 6934 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 component C6.

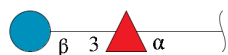
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	871	Total	C	N	O	S	0	0	0
			6830	4222	1203	1336	69			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose.

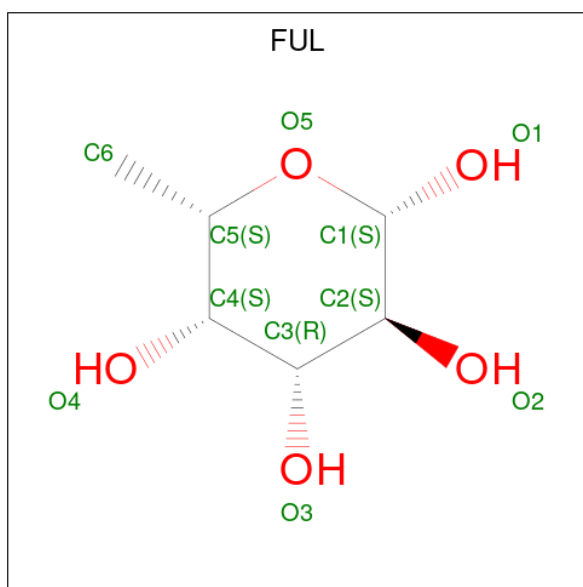


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

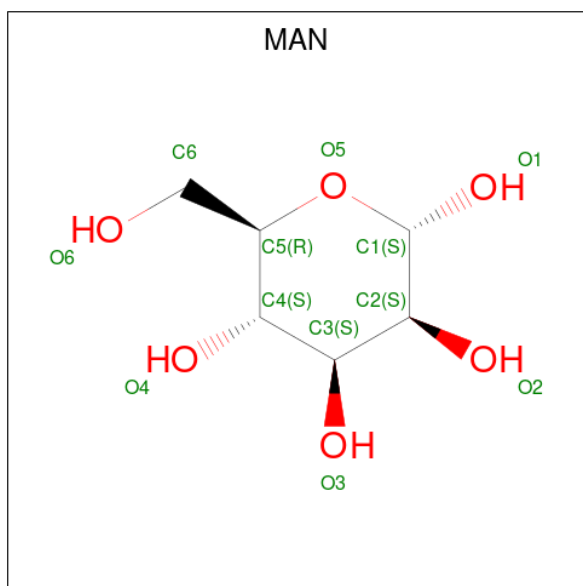
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cd	0	0
			1	1		

- Molecule 5 is beta-L-fucopyranose (three-letter code: FUL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		

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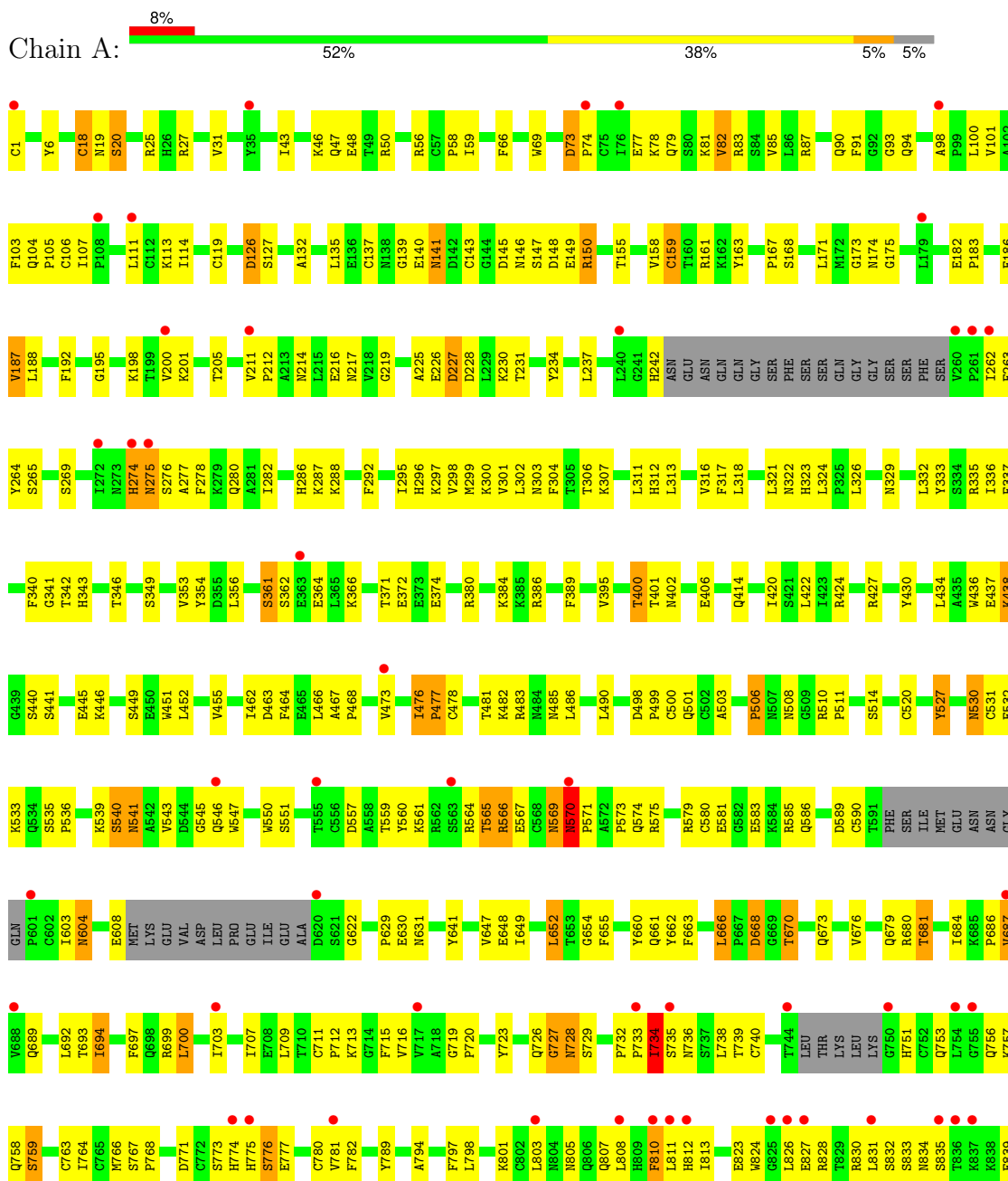
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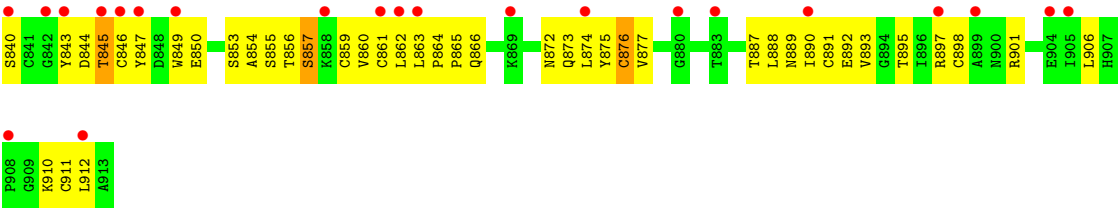
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

### 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 component C6

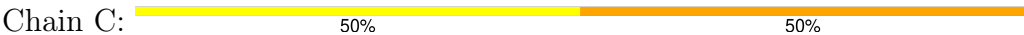




● Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 3: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.81Å 180.15Å 60.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.06 – 2.87 43.06 – 2.87	Depositor EDS
% Data completeness (in resolution range)	94.9 (43.06-2.87) 94.9 (43.06-2.87)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.222 , 0.276 0.215 , 0.268	Depositor DCC
$R_{free}$ test set	2179 reflections (6.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 107.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6934	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: FUL, FUC, BGC, CD, MAN, NAG

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	0.50	1/6973 (0.0%)	0.67	3/9409 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	CYS	CB-SG	5.23	1.91	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	LEU	CA-CB-CG	-6.84	99.56	115.30
1	A	570	ASN	N-CA-C	-5.68	95.67	111.00
1	A	666	LEU	CA-CB-CG	-5.07	103.64	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	6830	0	6498	398	0
2	B	28	0	25	0	0
3	C	21	0	19	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	10	0	10	3	0
6	A	44	0	40	7	0
All	All	6934	0	6592	398	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 29.

All (398) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ASN:HB3	1:A:571:PRO:CD	1.40	1.41
1:A:824:TRP:HE1	1:A:901:ARG:HD2	1.06	1.17
1:A:570:ASN:HB3	1:A:571:PRO:HD3	1.30	1.13
1:A:476:ILE:HB	1:A:477:PRO:HD2	1.29	1.11
1:A:570:ASN:HB3	1:A:571:PRO:HD2	1.22	1.08
1:A:333:TYR:HE2	1:A:485:ASN:HB3	1.16	1.06
1:A:734:ILE:HD13	1:A:734:ILE:H	0.96	1.06
1:A:570:ASN:CB	1:A:571:PRO:CD	2.33	1.05
1:A:734:ILE:H	1:A:734:ILE:CD1	1.75	0.99
1:A:734:ILE:HD13	1:A:734:ILE:N	1.78	0.98
1:A:715:PHE:HB3	1:A:740:CYS:HB3	1.46	0.98
1:A:1:CYS:HB3	1:A:43:ILE:HD11	1.43	0.97
1:A:333:TYR:CE2	1:A:485:ASN:HB3	2.00	0.96
1:A:567:GLU:O	1:A:569:ASN:OD1	1.84	0.96
1:A:560:TYR:HB3	1:A:589:ASP:HB2	1.51	0.93
1:A:205:THR:HG22	1:A:205:THR:O	1.68	0.90
1:A:840:SER:HA	1:A:844:ASP:HB2	1.52	0.90
1:A:336:ILE:HD11	1:A:486:LEU:HD11	1.53	0.88
1:A:853:SER:HB2	1:A:856:THR:HB	1.54	0.88
1:A:734:ILE:HG13	1:A:738:LEU:HB2	1.56	0.87
1:A:801:LYS:HA	1:A:805:ASN:HB2	1.55	0.87
1:A:824:TRP:NE1	1:A:901:ARG:HD2	1.90	0.85
1:A:756:GLN:HB2	1:A:763:CYS:HB3	1.57	0.85
1:A:546:GLN:HB2	1:A:571:PRO:CG	2.07	0.84
1:A:476:ILE:HB	1:A:477:PRO:CD	2.08	0.83
1:A:757:LYS:HE2	1:A:766:MET:HA	1.61	0.82
1:A:863:LEU:HB3	1:A:865:PRO:HD2	1.59	0.82
1:A:893:VAL:HG12	1:A:897:ARG:CZ	2.11	0.81
1:A:566:ARG:HD2	1:A:583:GLU:O	1.81	0.80
1:A:400:THR:HG22	1:A:401:THR:HG23	1.64	0.80
1:A:560:TYR:CB	1:A:589:ASP:HB2	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:ARG:O	1:A:700:LEU:HD13	1.82	0.79
1:A:79:GLN:HG3	1:A:106:CYS:HB2	1.65	0.78
1:A:824:TRP:O	1:A:828:ARG:HG2	1.84	0.77
1:A:719:GLY:H	1:A:738:LEU:HD13	1.48	0.77
1:A:73:ASP:H	1:A:74:PRO:HD3	1.50	0.76
1:A:126:ASP:OD1	1:A:150:ARG:NH2	2.19	0.76
1:A:570:ASN:CB	1:A:571:PRO:HD3	2.10	0.75
1:A:545:GLY:HA3	1:A:573:PRO:HG3	1.67	0.75
1:A:73:ASP:N	1:A:74:PRO:HD3	2.02	0.75
1:A:342:THR:HG22	1:A:343:HIS:ND1	2.02	0.74
1:A:853:SER:CB	1:A:856:THR:HB	2.17	0.74
1:A:143:CYS:SG	1:A:148:ASP:HB3	2.27	0.73
1:A:476:ILE:HD12	1:A:482:LYS:HE3	1.69	0.73
1:A:874:LEU:HD22	1:A:890:ILE:HG22	1.71	0.72
1:A:372:GLU:H	5:A:1004:FUL:C1	2.03	0.72
1:A:734:ILE:HG13	1:A:738:LEU:CB	2.20	0.72
1:A:581:GLU:OE1	1:A:581:GLU:HA	1.89	0.71
1:A:141:ASN:ND2	1:A:146:ASN:HB2	2.05	0.71
1:A:231:THR:HG22	1:A:295:ILE:HG13	1.73	0.71
1:A:274:HIS:HB3	1:A:277:ALA:HB3	1.73	0.71
1:A:476:ILE:CD1	1:A:482:LYS:HE3	2.21	0.70
1:A:560:TYR:HA	1:A:590:CYS:O	1.92	0.70
1:A:570:ASN:CB	1:A:571:PRO:HD2	2.11	0.69
1:A:482:LYS:HA	1:A:485:ASN:HB2	1.73	0.69
1:A:897:ARG:HA	1:A:901:ARG:HA	1.75	0.69
1:A:297:LYS:HG2	1:A:299:MET:HE2	1.71	0.69
1:A:380:ARG:HG2	1:A:380:ARG:HH11	1.55	0.69
1:A:66:PHE:HB3	1:A:81:LYS:HE2	1.73	0.69
1:A:876:CYS:SG	1:A:906:LEU:HD12	2.33	0.68
1:A:79:GLN:O	1:A:103:PHE:HA	1.94	0.68
1:A:828:ARG:HG3	1:A:847:TYR:CZ	2.28	0.67
1:A:668:ASP:HB3	1:A:670:THR:HB	1.77	0.67
1:A:801:LYS:O	1:A:805:ASN:HB2	1.95	0.67
1:A:843:TYR:N	1:A:844:ASP:HA	2.10	0.67
1:A:547:TRP:H	6:A:1010:MAN:H2	1.60	0.67
1:A:274:HIS:HB3	1:A:277:ALA:CB	2.24	0.67
1:A:187:VAL:HG13	1:A:188:LEU:HD13	1.76	0.67
1:A:692:LEU:HD12	1:A:692:LEU:H	1.59	0.67
1:A:277:ALA:HB1	1:A:422:LEU:CD2	2.25	0.66
1:A:546:GLN:HB2	1:A:571:PRO:HG3	1.78	0.66
1:A:801:LYS:CA	1:A:805:ASN:HB2	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PHE:HD1	1:A:530:ASN:ND2	1.93	0.66
1:A:780:CYS:O	1:A:811:LEU:HB3	1.95	0.66
1:A:733:PRO:O	1:A:735:SER:N	2.28	0.66
1:A:498:ASP:O	1:A:501:GLN:HG3	1.96	0.65
1:A:342:THR:HG22	1:A:343:HIS:CE1	2.31	0.65
1:A:111:LEU:O	1:A:113:LYS:HG2	1.95	0.65
1:A:569:ASN:OD1	1:A:569:ASN:N	2.30	0.65
1:A:301:VAL:O	1:A:302:LEU:HD12	1.97	0.65
1:A:801:LYS:HG3	1:A:805:ASN:CG	2.17	0.65
1:A:333:TYR:O	1:A:336:ILE:HG12	1.97	0.65
1:A:726:GLN:O	1:A:728:ASN:N	2.30	0.64
1:A:887:THR:C	1:A:888:LEU:HD22	2.18	0.64
1:A:140:GLU:CD	1:A:158:VAL:HG21	2.17	0.64
1:A:237:LEU:HD21	1:A:292:PHE:CE1	2.32	0.64
1:A:739:THR:HG22	1:A:740:CYS:N	2.13	0.64
1:A:205:THR:O	1:A:205:THR:CG2	2.42	0.63
1:A:66:PHE:CB	1:A:81:LYS:HE2	2.29	0.63
1:A:893:VAL:HG12	1:A:897:ARG:NH2	2.14	0.63
1:A:104:GLN:HB3	1:A:105:PRO:HD2	1.79	0.62
1:A:532:GLU:HG2	1:A:533:LYS:N	2.14	0.62
1:A:681:THR:OG1	1:A:703:ILE:HD11	2.00	0.62
1:A:888:LEU:HD12	1:A:892:GLU:CD	2.20	0.61
1:A:875:TYR:HB2	1:A:910:LYS:HA	1.83	0.61
1:A:757:LYS:HG2	1:A:766:MET:HB3	1.82	0.61
1:A:728:ASN:OD1	1:A:728:ASN:C	2.38	0.60
1:A:329:ASN:HD22	1:A:332:LEU:HB2	1.65	0.60
1:A:498:ASP:CG	1:A:499:PRO:HD2	2.22	0.60
1:A:798:LEU:O	1:A:801:LYS:HB3	2.01	0.60
1:A:59:ILE:O	1:A:93:GLY:HA3	2.00	0.60
1:A:211:VAL:HG12	1:A:212:PRO:O	2.02	0.60
1:A:139:GLY:N	1:A:149:GLU:OE2	2.35	0.60
1:A:73:ASP:N	1:A:74:PRO:CD	2.65	0.59
1:A:876:CYS:HA	1:A:911:CYS:HB2	1.84	0.59
1:A:296:HIS:HA	1:A:354:TYR:O	2.03	0.59
1:A:343:HIS:HB3	1:A:466:LEU:HB3	1.85	0.59
1:A:875:TYR:CG	1:A:910:LYS:HA	2.37	0.59
1:A:557:ASP:HB2	1:A:561:LYS:O	2.02	0.59
1:A:288:LYS:HA	1:A:527:TYR:CD1	2.38	0.59
1:A:216:GLU:HB2	1:A:307:LYS:HB2	1.85	0.59
1:A:716:VAL:O	1:A:740:CYS:HA	2.02	0.59
1:A:715:PHE:CB	1:A:740:CYS:HB3	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:HH12	1:A:414:GLN:NE2	2.01	0.58
1:A:550:TRP:CE3	1:A:564:ARG:HG2	2.38	0.58
1:A:464:PHE:O	1:A:464:PHE:CD1	2.57	0.58
1:A:689:GLN:NE2	1:A:736:ASN:HA	2.19	0.58
1:A:694:ILE:CG2	1:A:709:LEU:HD11	2.34	0.58
1:A:274:HIS:O	1:A:276:SER:N	2.37	0.58
1:A:532:GLU:HG2	1:A:533:LYS:H	1.69	0.58
1:A:81:LYS:O	1:A:101:VAL:HG23	2.05	0.57
1:A:630:GLU:O	1:A:631:ASN:HB2	2.05	0.57
1:A:69:TRP:HZ3	1:A:79:GLN:O	1.88	0.57
1:A:77:GLU:O	1:A:77:GLU:HG3	2.03	0.57
1:A:887:THR:O	1:A:888:LEU:HD13	2.04	0.57
1:A:810:PHE:CD2	1:A:811:LEU:N	2.73	0.57
1:A:580:CYS:HB2	6:A:1010:MAN:H3	1.87	0.57
1:A:756:GLN:CB	1:A:763:CYS:HB3	2.32	0.56
1:A:313:LEU:HD12	1:A:318:LEU:HD13	1.88	0.56
1:A:386:ARG:HH12	1:A:414:GLN:HE21	1.54	0.56
1:A:389:PHE:CE1	1:A:445:GLU:HB3	2.41	0.56
1:A:876:CYS:HA	1:A:911:CYS:CB	2.30	0.56
1:A:546:GLN:HB2	1:A:571:PRO:CD	2.36	0.56
1:A:875:TYR:CB	1:A:910:LYS:HA	2.35	0.56
1:A:440:SER:OG	1:A:441:SER:N	2.39	0.56
1:A:876:CYS:CA	1:A:911:CYS:HB2	2.36	0.56
1:A:847:TYR:HB3	1:A:849:TRP:CE2	2.41	0.55
1:A:402:ASN:O	1:A:406:GLU:HB2	2.07	0.55
1:A:82:VAL:HG22	1:A:101:VAL:HB	1.88	0.55
1:A:322:ASN:C	1:A:324:LEU:H	2.10	0.55
1:A:863:LEU:H	1:A:866:GLN:HE21	1.53	0.55
1:A:872:ASN:H	1:A:890:ILE:HD13	1.71	0.55
1:A:336:ILE:HD11	1:A:486:LEU:CD1	2.34	0.55
1:A:227:ASP:O	1:A:230:LYS:HE2	2.07	0.54
1:A:280:GLN:NE2	1:A:420:ILE:HG23	2.22	0.54
1:A:300:LYS:HG2	1:A:349:SER:HB3	1.89	0.54
1:A:812:HIS:CD2	1:A:813:ILE:O	2.60	0.54
1:A:564:ARG:NH2	1:A:586:GLN:OE1	2.40	0.54
1:A:689:GLN:HE21	1:A:736:ASN:HA	1.72	0.54
1:A:839:GLU:HG3	1:A:846:CYS:HB3	1.89	0.54
1:A:307:LYS:O	1:A:311:LEU:HD21	2.08	0.53
1:A:877:VAL:CG2	1:A:888:LEU:HD23	2.38	0.53
1:A:832:SER:OG	1:A:833:SER:N	2.39	0.53
1:A:6:TYR:O	1:A:27:ARG:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:LYS:NZ	1:A:844:ASP:OD1	2.40	0.53
1:A:498:ASP:OD2	1:A:499:PRO:HD2	2.09	0.53
1:A:132:ALA:N	1:A:135:LEU:HD12	2.23	0.53
1:A:82:VAL:CG2	1:A:101:VAL:HB	2.39	0.53
1:A:663:PHE:CD1	1:A:673:GLN:HG2	2.43	0.53
1:A:354:TYR:CE1	1:A:434:LEU:HD13	2.43	0.53
1:A:298:VAL:HG23	1:A:353:VAL:HG22	1.91	0.52
1:A:751:HIS:O	1:A:753:GLN:HG3	2.10	0.52
1:A:372:GLU:HB2	5:A:1004:FUL:O2	2.10	0.52
1:A:774:HIS:O	1:A:775:HIS:C	2.48	0.52
1:A:776:SER:HB2	1:A:794:ALA:HB3	1.90	0.52
1:A:161:ARG:HD3	1:A:163:TYR:HE2	1.74	0.52
1:A:168:SER:HB3	1:A:171:LEU:HD22	1.90	0.52
1:A:100:LEU:HD12	1:A:100:LEU:H	1.74	0.52
1:A:833:SER:O	1:A:834:ASN:HB2	2.09	0.52
1:A:175:GLY:HA3	1:A:340:PHE:O	2.09	0.52
1:A:694:ILE:HG22	1:A:709:LEU:CD1	2.39	0.52
1:A:739:THR:HG22	1:A:740:CYS:H	1.75	0.52
1:A:182:GLU:HG2	1:A:183:PRO:HD2	1.91	0.52
1:A:47:GLN:HG2	1:A:48:GLU:N	2.24	0.52
1:A:173:GLY:O	1:A:187:VAL:HG12	2.09	0.52
1:A:337:PHE:HA	1:A:341:GLY:O	2.10	0.51
1:A:451:TRP:O	1:A:455:VAL:HG23	2.10	0.51
1:A:856:THR:O	1:A:857:SER:HB2	2.10	0.51
1:A:726:GLN:NE2	1:A:729:SER:OG	2.29	0.51
1:A:901:ARG:O	1:A:901:ARG:HG2	2.10	0.51
1:A:476:ILE:CB	1:A:477:PRO:HD2	2.19	0.51
1:A:567:GLU:C	1:A:569:ASN:OD1	2.48	0.51
1:A:336:ILE:CD1	1:A:486:LEU:HD11	2.33	0.51
1:A:473:VAL:O	1:A:473:VAL:HG13	2.11	0.51
1:A:850:GLU:HB3	1:A:859:CYS:HB3	1.93	0.51
1:A:59:ILE:CG2	1:A:87:ARG:HD2	2.41	0.51
1:A:85:VAL:HG23	1:A:85:VAL:O	2.11	0.51
1:A:739:THR:CG2	1:A:740:CYS:N	2.74	0.51
1:A:546:GLN:O	1:A:571:PRO:HD2	2.11	0.51
1:A:473:VAL:O	1:A:483:ARG:HG3	2.10	0.51
1:A:274:HIS:O	1:A:277:ALA:N	2.45	0.50
1:A:287:LYS:O	1:A:288:LYS:HB3	2.10	0.50
1:A:306:THR:HB	1:A:346:THR:O	2.11	0.50
1:A:83:ARG:NH2	1:A:98:ALA:O	2.45	0.50
1:A:278:PHE:CE2	1:A:282:ILE:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ARG:HH11	1:A:380:ARG:CG	2.23	0.50
1:A:808:LEU:HD12	1:A:808:LEU:N	2.27	0.50
1:A:876:CYS:N	1:A:911:CYS:HB2	2.27	0.50
1:A:751:HIS:O	1:A:751:HIS:CG	2.65	0.50
1:A:234:TYR:HB2	1:A:292:PHE:HB2	1.93	0.50
1:A:56:ARG:O	1:A:58:PRO:HD3	2.11	0.49
1:A:301:VAL:O	1:A:302:LEU:CD1	2.60	0.49
1:A:362:SER:O	1:A:366:LYS:HG3	2.11	0.49
1:A:242:HIS:CE1	1:A:269:SER:HA	2.47	0.49
1:A:276:SER:O	1:A:280:GLN:HG3	2.12	0.49
1:A:333:TYR:HE2	1:A:485:ASN:CB	2.07	0.49
1:A:427:ARG:HB2	1:A:430:TYR:HD2	1.76	0.49
1:A:372:GLU:N	5:A:1004:FUL:C1	2.75	0.49
1:A:158:VAL:HG23	1:A:159:CYS:N	2.27	0.49
1:A:371:THR:HG22	1:A:374:GLU:HG3	1.94	0.49
1:A:106:CYS:SG	1:A:107:ILE:N	2.85	0.49
1:A:527:TYR:N	1:A:527:TYR:CD2	2.80	0.49
1:A:478:CYS:HB3	1:A:481:THR:HB	1.94	0.49
1:A:663:PHE:CG	1:A:673:GLN:HG2	2.48	0.49
1:A:734:ILE:O	1:A:735:SER:C	2.51	0.49
1:A:477:PRO:HG2	1:A:478:CYS:H	1.78	0.49
1:A:727:GLY:O	1:A:728:ASN:OD1	2.30	0.49
1:A:873:GLN:NE2	1:A:875:TYR:CE1	2.81	0.49
1:A:198:LYS:HG3	1:A:211:VAL:HB	1.95	0.49
1:A:147:SER:C	1:A:149:GLU:H	2.16	0.48
1:A:263:PHE:H	1:A:263:PHE:HD2	1.61	0.48
1:A:547:TRP:HE1	6:A:1010:MAN:H5	1.78	0.48
1:A:541:ASN:O	1:A:575:ARG:HD2	2.14	0.48
1:A:263:PHE:HB3	1:A:468:PRO:HD3	1.95	0.48
1:A:874:LEU:CD2	1:A:890:ILE:HG22	2.43	0.48
1:A:303:ASN:O	1:A:304:PHE:HB3	2.14	0.48
1:A:354:TYR:HE1	1:A:434:LEU:HD13	1.79	0.48
1:A:550:TRP:HB2	6:A:1009:MAN:H5	1.94	0.48
1:A:78:LYS:HA	1:A:104:GLN:O	2.14	0.48
1:A:107:ILE:HG13	1:A:107:ILE:O	2.14	0.48
1:A:336:ILE:HD11	1:A:486:LEU:HD21	1.95	0.48
1:A:371:THR:HG23	1:A:374:GLU:H	1.77	0.48
1:A:476:ILE:CB	1:A:477:PRO:CD	2.87	0.48
1:A:498:ASP:OD1	1:A:500:CYS:HB3	2.14	0.48
1:A:758:GLN:HG2	1:A:759:SER:N	2.28	0.48
1:A:158:VAL:HG11	1:A:195:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:ARG:HD2	1:A:849:TRP:HZ2	1.79	0.48
1:A:735:SER:O	1:A:736:ASN:HB2	2.13	0.48
1:A:739:THR:CG2	1:A:740:CYS:H	2.27	0.48
1:A:803:LEU:N	1:A:803:LEU:HD12	2.29	0.48
1:A:324:LEU:HB3	1:A:333:TYR:HE1	1.79	0.47
1:A:684:ILE:O	1:A:686:PRO:HD3	2.15	0.47
1:A:27:ARG:HG3	1:A:46:LYS:HA	1.96	0.47
1:A:78:LYS:HD3	1:A:103:PHE:CE1	2.50	0.47
1:A:876:CYS:CA	1:A:911:CYS:CB	2.93	0.47
1:A:50:ARG:HH22	6:A:1007:MAN:H5	1.78	0.47
1:A:719:GLY:H	1:A:738:LEU:CD1	2.21	0.47
1:A:805:ASN:C	1:A:807:GLN:H	2.17	0.47
1:A:863:LEU:C	1:A:865:PRO:HD2	2.35	0.47
1:A:113:LYS:O	1:A:114:ILE:HD13	2.14	0.47
1:A:546:GLN:N	1:A:571:PRO:HG2	2.29	0.47
1:A:776:SER:O	1:A:777:GLU:C	2.53	0.47
1:A:827:GLU:HA	1:A:830:ARG:NH1	2.30	0.47
1:A:889:ASN:O	1:A:893:VAL:HG23	2.14	0.47
1:A:756:GLN:HE21	1:A:763:CYS:CB	2.28	0.47
1:A:864:PRO:N	1:A:865:PRO:HD2	2.30	0.47
1:A:875:TYR:CE2	1:A:910:LYS:HG2	2.50	0.47
1:A:569:ASN:O	1:A:570:ASN:C	2.52	0.47
1:A:694:ILE:HG23	1:A:709:LEU:HD11	1.96	0.47
1:A:912:LEU:HD12	1:A:912:LEU:N	2.30	0.47
1:A:264:TYR:CD1	1:A:265:SER:O	2.68	0.46
1:A:343:HIS:HA	1:A:467:ALA:O	2.15	0.46
1:A:579:ARG:H	1:A:579:ARG:HG3	1.52	0.46
1:A:380:ARG:CG	1:A:380:ARG:NH1	2.79	0.46
1:A:569:ASN:O	1:A:571:PRO:HD2	2.15	0.46
1:A:237:LEU:HD21	1:A:292:PHE:CD1	2.50	0.46
1:A:603:ILE:HG22	1:A:604:ASN:O	2.16	0.46
1:A:400:THR:HG22	1:A:401:THR:CG2	2.42	0.46
1:A:546:GLN:CB	1:A:571:PRO:CG	2.87	0.46
1:A:317:PHE:CE1	1:A:321:LEU:HD22	2.50	0.46
1:A:912:LEU:HD12	1:A:912:LEU:H	1.80	0.46
1:A:326:LEU:HD12	1:A:326:LEU:N	2.31	0.45
1:A:782:PHE:CD1	1:A:789:TYR:HB3	2.51	0.45
1:A:69:TRP:CE3	1:A:79:GLN:HB3	2.51	0.45
1:A:386:ARG:HH22	1:A:414:GLN:NE2	2.14	0.45
1:A:862:LEU:O	1:A:895:THR:HB	2.16	0.45
1:A:535:SER:HB2	1:A:536:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:GLU:HB2	1:A:662:TYR:CE1	2.52	0.45
1:A:389:PHE:HZ	1:A:449:SER:HB2	1.81	0.45
1:A:839:GLU:HG3	1:A:846:CYS:CB	2.46	0.45
1:A:187:VAL:HG13	1:A:188:LEU:CD1	2.46	0.45
1:A:486:LEU:HD12	1:A:486:LEU:HA	1.76	0.45
1:A:629:PRO:O	1:A:630:GLU:C	2.55	0.45
1:A:31:VAL:O	1:A:31:VAL:HG12	2.15	0.45
1:A:380:ARG:HG2	1:A:380:ARG:NH1	2.26	0.45
1:A:692:LEU:HD12	1:A:692:LEU:N	2.31	0.45
1:A:18:CYS:SG	3:C:1:FUC:H5	2.57	0.44
1:A:302:LEU:O	1:A:349:SER:HB3	2.17	0.44
1:A:873:GLN:HB3	1:A:875:TYR:CE1	2.52	0.44
1:A:654:GLY:O	1:A:681:THR:HG23	2.18	0.44
1:A:192:PHE:CE2	1:A:312:HIS:CD2	3.05	0.44
1:A:652:LEU:HA	1:A:652:LEU:HD23	1.56	0.44
1:A:831:LEU:HD12	1:A:835:SER:HB2	1.98	0.44
1:A:226:GLU:O	1:A:228:ASP:N	2.51	0.44
1:A:354:TYR:CZ	1:A:356:LEU:CD1	3.01	0.44
1:A:277:ALA:HB1	1:A:422:LEU:HD23	1.99	0.44
1:A:335:ARG:HD2	1:A:335:ARG:HA	1.78	0.44
1:A:560:TYR:O	1:A:590:CYS:N	2.51	0.44
1:A:694:ILE:H	1:A:694:ILE:HG12	1.53	0.44
1:A:767:SER:HA	1:A:768:PRO:HD3	1.88	0.44
1:A:214:ASN:HD22	1:A:214:ASN:H	1.66	0.44
1:A:329:ASN:ND2	1:A:332:LEU:HB2	2.31	0.44
1:A:361:SER:OG	1:A:364:GLU:HG2	2.18	0.44
1:A:550:TRP:CD2	1:A:566:ARG:HG2	2.53	0.44
1:A:19:ASN:O	1:A:20:SER:HB3	2.16	0.44
1:A:424:ARG:HH11	1:A:424:ARG:HG2	1.83	0.44
1:A:767:SER:N	1:A:771:ASP:OD2	2.48	0.44
1:A:545:GLY:O	1:A:580:CYS:HB3	2.18	0.43
1:A:810:PHE:CG	1:A:811:LEU:N	2.86	0.43
1:A:127:SER:HB3	1:A:145:ASP:OD1	2.18	0.43
1:A:622:GLY:HA3	1:A:641:TYR:O	2.19	0.43
1:A:856:THR:O	1:A:857:SER:CB	2.66	0.43
1:A:264:TYR:HD1	1:A:265:SER:O	2.01	0.43
1:A:828:ARG:HG3	1:A:847:TYR:CE2	2.53	0.43
1:A:891:CYS:O	1:A:895:THR:HG23	2.18	0.43
1:A:171:LEU:CD1	1:A:171:LEU:N	2.81	0.43
1:A:559:THR:C	1:A:561:LYS:N	2.71	0.43
1:A:801:LYS:C	1:A:805:ASN:HB2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:PHE:C	1:A:697:PHE:CD2	2.92	0.43
1:A:875:TYR:CG	1:A:887:THR:HG23	2.54	0.43
1:A:216:GLU:O	1:A:217:ASN:ND2	2.51	0.43
1:A:550:TRP:CZ2	1:A:566:ARG:NE	2.87	0.43
1:A:666:LEU:HA	1:A:666:LEU:HD23	1.46	0.43
1:A:694:ILE:CG2	1:A:709:LEU:CD1	2.95	0.43
1:A:354:TYR:CZ	1:A:356:LEU:HD11	2.54	0.43
1:A:436:TRP:C	1:A:437:GLU:HG3	2.38	0.43
1:A:508:ASN:OD1	1:A:543:VAL:HA	2.19	0.43
1:A:585:ARG:HG2	1:A:586:GLN:N	2.34	0.43
1:A:641:TYR:CE1	1:A:647:VAL:HG11	2.54	0.43
1:A:781:VAL:HG11	1:A:797:PHE:CD1	2.54	0.43
1:A:843:TYR:HD2	1:A:845:THR:O	2.02	0.43
1:A:860:VAL:HG12	1:A:861:CYS:N	2.34	0.43
1:A:560:TYR:HB3	1:A:589:ASP:CB	2.36	0.43
1:A:561:LYS:HD3	1:A:561:LYS:HA	1.68	0.43
1:A:655:PHE:CE1	1:A:680:ARG:HG3	2.54	0.42
1:A:864:PRO:N	1:A:865:PRO:CD	2.81	0.42
1:A:756:GLN:HB3	1:A:764:ILE:O	2.19	0.42
1:A:543:VAL:HB	1:A:574:GLN:HB2	2.01	0.42
1:A:455:VAL:O	1:A:455:VAL:HG12	2.19	0.42
1:A:437:GLU:O	1:A:438:LYS:C	2.56	0.42
1:A:452:LEU:HD12	1:A:452:LEU:HA	1.76	0.42
1:A:219:GLY:O	1:A:302:LEU:HA	2.19	0.42
1:A:226:GLU:O	1:A:227:ASP:C	2.57	0.42
1:A:608:GLU:H	1:A:608:GLU:HG2	1.67	0.42
1:A:324:LEU:HB3	1:A:333:TYR:CE1	2.54	0.42
1:A:462:ILE:O	1:A:463:ASP:C	2.57	0.42
1:A:823:GLU:O	1:A:826:LEU:HB3	2.18	0.42
1:A:551:SER:HB2	1:A:565:THR:O	2.20	0.42
1:A:843:TYR:CB	1:A:844:ASP:HA	2.50	0.42
1:A:158:VAL:HB	1:A:195:GLY:O	2.20	0.42
1:A:322:ASN:C	1:A:324:LEU:N	2.72	0.42
1:A:604:ASN:H	1:A:604:ASN:ND2	2.17	0.42
1:A:776:SER:CB	1:A:794:ALA:HB3	2.50	0.42
1:A:25:ARG:HH12	6:A:1008:MAN:H61	1.84	0.41
1:A:302:LEU:O	1:A:349:SER:HA	2.20	0.41
1:A:90:GLN:HE22	1:A:503:ALA:N	2.18	0.41
1:A:286:HIS:HE1	1:A:520:CYS:O	2.04	0.41
1:A:854:ALA:O	1:A:855:SER:HB2	2.19	0.41
1:A:873:GLN:NE2	1:A:875:TYR:HE1	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:PRO:O	1:A:168:SER:HB2	2.20	0.41
1:A:337:PHE:CZ	1:A:490:LEU:HB2	2.55	0.41
1:A:510:ARG:HA	1:A:511:PRO:HD2	1.96	0.41
1:A:539:LYS:O	1:A:540:SER:O	2.38	0.41
1:A:201:LYS:HE3	1:A:201:LYS:HB2	1.83	0.41
1:A:550:TRP:CE3	1:A:566:ARG:HG2	2.55	0.41
1:A:603:ILE:N	1:A:603:ILE:HD12	2.35	0.41
1:A:893:VAL:HG12	1:A:897:ARG:NE	2.35	0.41
1:A:158:VAL:HG23	1:A:159:CYS:HB2	2.01	0.41
1:A:853:SER:HB3	1:A:856:THR:HB	2.01	0.41
1:A:81:LYS:O	1:A:101:VAL:HA	2.20	0.41
1:A:298:VAL:CG2	1:A:462:ILE:HD12	2.50	0.41
1:A:686:PRO:HG2	1:A:707:ILE:CD1	2.50	0.41
1:A:687:VAL:HG21	1:A:735:SER:HA	2.02	0.41
1:A:773:SER:OG	1:A:774:HIS:N	2.53	0.41
1:A:801:LYS:HG3	1:A:805:ASN:CB	2.50	0.41
1:A:137:CYS:HB3	1:A:155:THR:HG22	2.02	0.41
1:A:262:ILE:HG22	1:A:263:PHE:CD2	2.55	0.41
1:A:316:VAL:HG13	1:A:317:PHE:N	2.36	0.41
1:A:332:LEU:O	1:A:335:ARG:HB2	2.21	0.41
1:A:434:LEU:HA	1:A:434:LEU:HD23	1.84	0.41
1:A:545:GLY:O	1:A:546:GLN:HG2	2.21	0.41
1:A:713:LYS:HD3	1:A:713:LYS:N	2.35	0.41
1:A:225:ALA:O	1:A:228:ASP:HB2	2.20	0.41
1:A:263:PHE:CD2	1:A:263:PHE:N	2.88	0.41
1:A:550:TRP:HB2	6:A:1009:MAN:C5	2.51	0.41
1:A:666:LEU:HB2	1:A:670:THR:O	2.21	0.41
1:A:720:PRO:HG2	1:A:723:TYR:CZ	2.56	0.41
1:A:875:TYR:HB3	1:A:911:CYS:H	1.86	0.41
1:A:100:LEU:HD12	1:A:100:LEU:N	2.35	0.40
1:A:660:TYR:O	1:A:676:VAL:HB	2.21	0.40
1:A:843:TYR:N	1:A:844:ASP:CA	2.83	0.40
1:A:801:LYS:O	1:A:805:ASN:CB	2.67	0.40
1:A:828:ARG:NH2	1:A:898:CYS:HA	2.35	0.40
1:A:445:GLU:O	1:A:446:LYS:C	2.60	0.40
1:A:464:PHE:CE1	1:A:466:LEU:HD21	2.57	0.40
1:A:174:ASN:ND2	1:A:186:GLU:HA	2.36	0.40
1:A:274:HIS:O	1:A:275:ASN:C	2.60	0.40
1:A:322:ASN:O	1:A:324:LEU:N	2.54	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	861/913 (94%)	734 (85%)	105 (12%)	22 (3%)	<b>4</b> <b>10</b>

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ARG
1	A	540	SER
1	A	570	ASN
1	A	712	PRO
1	A	727	GLY
1	A	734	ILE
1	A	141	ASN
1	A	275	ASN
1	A	323	HIS
1	A	668	ASP
1	A	857	SER
1	A	227	ASP
1	A	810	PHE
1	A	438	LYS
1	A	759	SER
1	A	506	PRO
1	A	687	VAL
1	A	20	SER
1	A	476	ILE
1	A	477	PRO
1	A	73	ASP
1	A	732	PRO

### 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	772/810 (95%)	736 (95%)	36 (5%)	22	44

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	CYS
1	A	82	VAL
1	A	94	GLN
1	A	119	CYS
1	A	126	ASP
1	A	159	CYS
1	A	187	VAL
1	A	200	VAL
1	A	274	HIS
1	A	361	SER
1	A	384	LYS
1	A	395	VAL
1	A	400	THR
1	A	506	PRO
1	A	514	SER
1	A	527	TYR
1	A	530	ASN
1	A	541	ASN
1	A	565	THR
1	A	566	ARG
1	A	569	ASN
1	A	604	ASN
1	A	649	ILE
1	A	661	GLN
1	A	670	THR
1	A	679	GLN
1	A	681	THR
1	A	693	THR
1	A	694	ILE
1	A	700	LEU
1	A	711	CYS
1	A	728	ASN
1	A	734	ILE
1	A	776	SER
1	A	845	THR

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Mol	Chain	Res	Type
1	A	876	CYS

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

Mol	Chain	Res	Type
1	A	36	GLN
1	A	79	GLN
1	A	90	GLN
1	A	174	ASN
1	A	190	ASN
1	A	207	ASN
1	A	223	GLN
1	A	242	HIS
1	A	271	ASN
1	A	275	ASN
1	A	280	GLN
1	A	286	HIS
1	A	296	HIS
1	A	312	HIS
1	A	329	ASN
1	A	377	HIS
1	A	408	HIS
1	A	414	GLN
1	A	530	ASN
1	A	574	GLN
1	A	604	ASN
1	A	679	GLN
1	A	753	GLN
1	A	756	GLN
1	A	804	ASN
1	A	812	HIS
1	A	817	GLN
1	A	866	GLN
1	A	873	GLN

### 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 ⓘ

4 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	B	1	2,1	14,14,15	0.60	0	17,19,21	0.76	0
2	NAG	B	2	2	14,14,15	0.53	0	17,19,21	0.60	0
3	FUC	C	1	1,3	10,10,11	0.78	0	14,14,16	1.54	4 (28%)
3	BGC	C	2	3	11,11,12	1.14	1 (9%)	15,15,17	1.43	2 (13%)

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	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
3	FUC	C	1	1,3	-	-	0/1/1/1
3	BGC	C	2	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	BGC	O5-C1	-3.20	1.38	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	BGC	C1-C2-C3	-3.20	104.99	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FUC	C6-C5-C4	-2.94	107.70	113.08
3	C	1	FUC	O5-C5-C6	2.66	113.17	107.40
3	C	1	FUC	O4-C4-C5	-2.24	104.78	109.74
3	C	2	BGC	C3-C4-C5	-2.09	106.44	110.23
3	C	1	FUC	C1-C2-C3	2.02	112.59	109.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	C	2	BGC	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
3	C	2	BGC	C4-C5-C6-O6

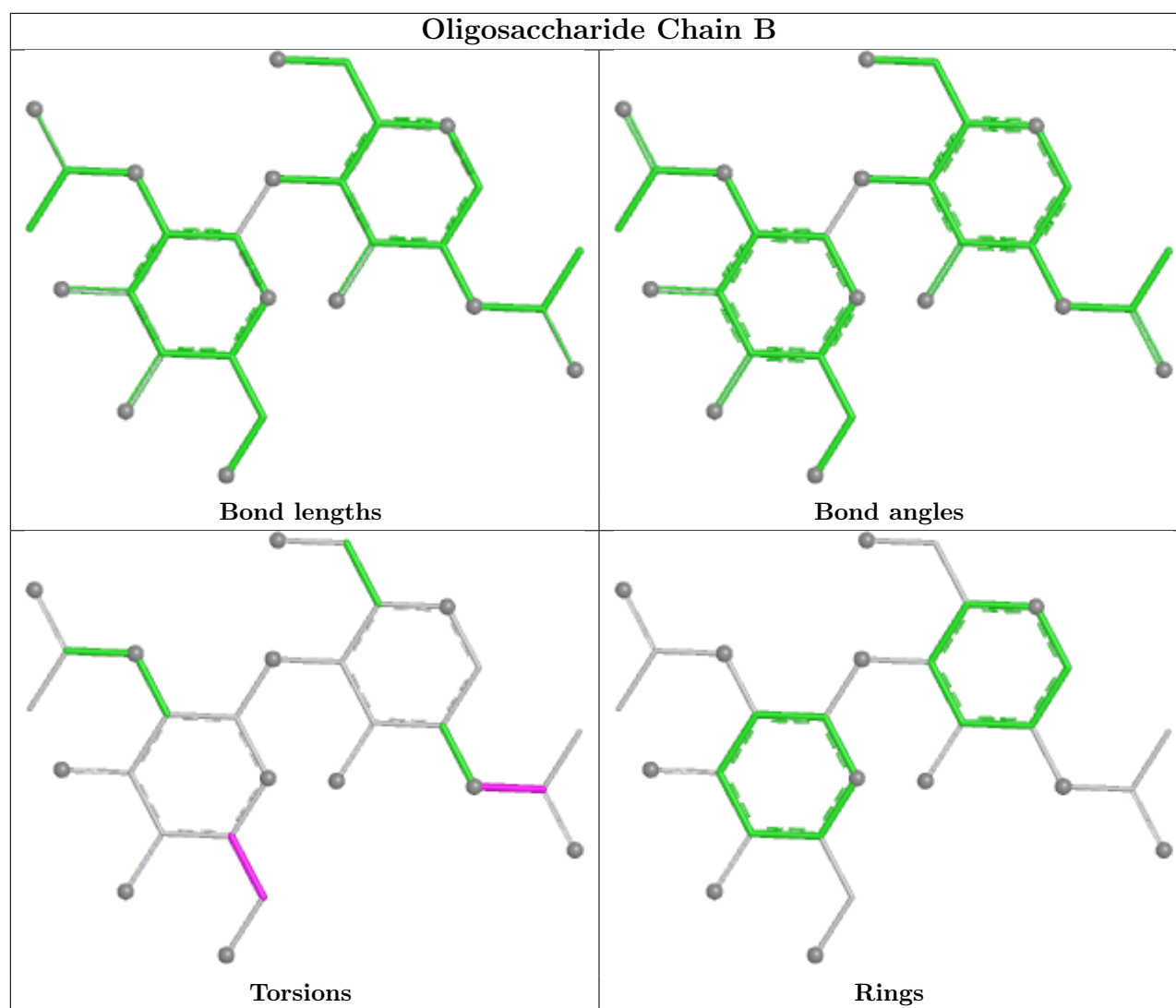
There are no ring outliers.

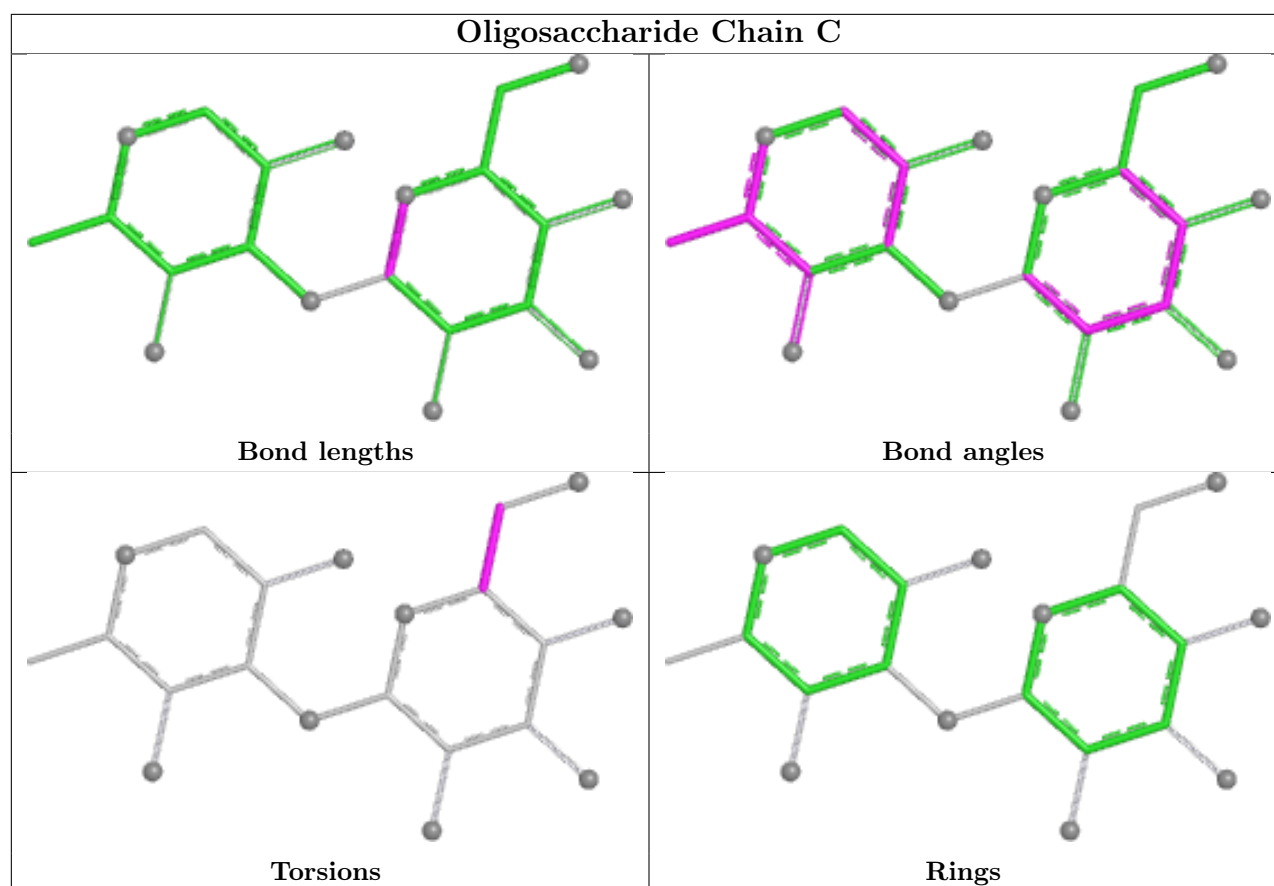
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	FUC	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.







## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	MAN	A	1009	1	11,11,12	0.63	0	15,15,17	1.43	2 (13%)
5	FUL	A	1004	1	10,10,11	0.64	0	14,14,16	0.89	0
6	MAN	A	1010	1	11,11,12	0.46	0	15,15,17	1.24	1 (6%)
6	MAN	A	1007	1	11,11,12	0.88	0	15,15,17	1.15	1 (6%)
6	MAN	A	1008	1	11,11,12	1.15	0	15,15,17	1.62	3 (20%)

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
6	MAN	A	1009	1	-	1/2/19/22	0/1/1/1
5	FUL	A	1004	1	-	-	0/1/1/1
6	MAN	A	1010	1	-	0/2/19/22	0/1/1/1
6	MAN	A	1007	1	-	0/2/19/22	0/1/1/1
6	MAN	A	1008	1	-	2/2/19/22	1/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1009	MAN	C3-C4-C5	3.13	115.90	110.23
6	A	1010	MAN	C2-C3-C4	-3.11	105.40	110.86
6	A	1008	MAN	O4-C4-C3	-3.06	103.16	110.38
6	A	1009	MAN	C1-O5-C5	2.97	116.17	112.19
6	A	1008	MAN	C1-C2-C3	-2.71	105.70	109.64
6	A	1007	MAN	O4-C4-C3	-2.43	104.65	110.38
6	A	1008	MAN	O4-C4-C5	-2.42	103.37	109.32

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1008	MAN	O5-C5-C6-O6
6	A	1008	MAN	C4-C5-C6-O6
6	A	1009	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1008	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1009	MAN	2	0
5	A	1004	FUL	3	0
6	A	1010	MAN	3	0
6	A	1007	MAN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1008	MAN	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	871/913 (95%)	0.34	72 (8%) 19 16	41, 107, 238, 291	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	843	TYR	6.3
1	A	811	LEU	5.6
1	A	831	LEU	5.4
1	A	842	GLY	5.4
1	A	601	PRO	5.2
1	A	847	TYR	4.9
1	A	755	GLY	4.8
1	A	897	ARG	4.8
1	A	835	SER	4.5
1	A	111	LEU	4.4
1	A	775	HIS	4.3
1	A	754	LEU	4.2
1	A	750	GLY	3.7
1	A	810	PHE	3.5
1	A	908	PRO	3.4
1	A	272	ILE	3.4
1	A	687	VAL	3.3
1	A	274	HIS	3.3
1	A	905	ILE	3.3
1	A	744	THR	3.3
1	A	874	LEU	3.3
1	A	733	PRO	3.2
1	A	826	LEU	3.2
1	A	845	THR	3.1
1	A	803	LEU	3.0
1	A	240	LEU	3.0
1	A	912	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	880	GLY	2.8
1	A	260	VAL	2.8
1	A	555	THR	2.8
1	A	262	ILE	2.8
1	A	861	CYS	2.7
1	A	108	PRO	2.7
1	A	808	LEU	2.6
1	A	812	HIS	2.6
1	A	904	GLU	2.6
1	A	620	ASP	2.5
1	A	774	HIS	2.5
1	A	862	LEU	2.5
1	A	563	SER	2.4
1	A	200	VAL	2.4
1	A	717	VAL	2.4
1	A	570	ASN	2.4
1	A	899	ALA	2.4
1	A	261	PRO	2.4
1	A	363	GLU	2.4
1	A	98	ALA	2.4
1	A	883	THR	2.4
1	A	735	SER	2.3
1	A	840	SER	2.3
1	A	858	LYS	2.3
1	A	74	PRO	2.3
1	A	211	VAL	2.3
1	A	890	ILE	2.3
1	A	863	LEU	2.3
1	A	1	CYS	2.2
1	A	849	TRP	2.2
1	A	275	ASN	2.2
1	A	703	ILE	2.1
1	A	836	THR	2.1
1	A	35	TYR	2.1
1	A	837	LYS	2.1
1	A	825	GLY	2.1
1	A	546	GLN	2.1
1	A	179	LEU	2.1
1	A	76	ILE	2.1
1	A	846	CYS	2.1
1	A	827	GLU	2.1
1	A	869	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	688	VAL	2.0
1	A	781	VAL	2.0
1	A	473	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

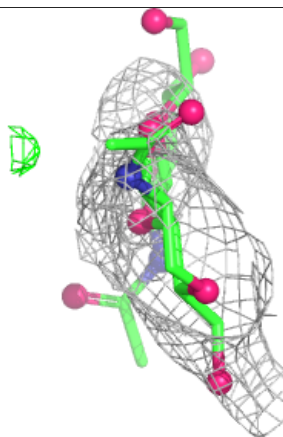
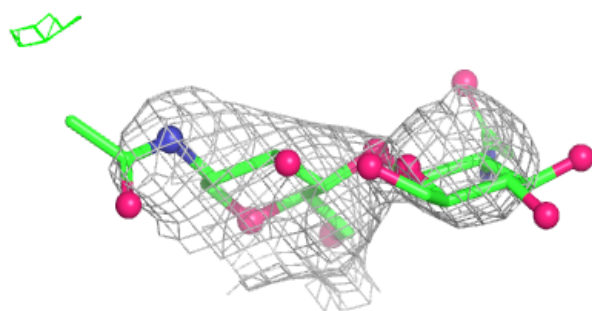
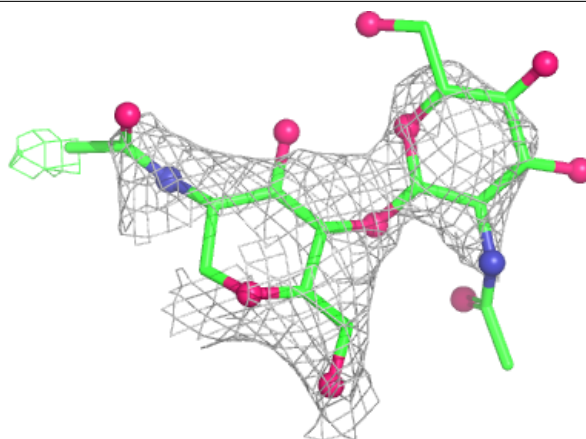
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	B	1	14/15	0.55	0.13	120,151,163,169	0
2	NAG	B	2	14/15	0.65	0.10	148,174,183,187	0
3	BGC	C	2	11/12	0.96	0.07	51,62,72,80	0
3	FUC	C	1	10/11	0.97	0.05	47,56,68,78	0

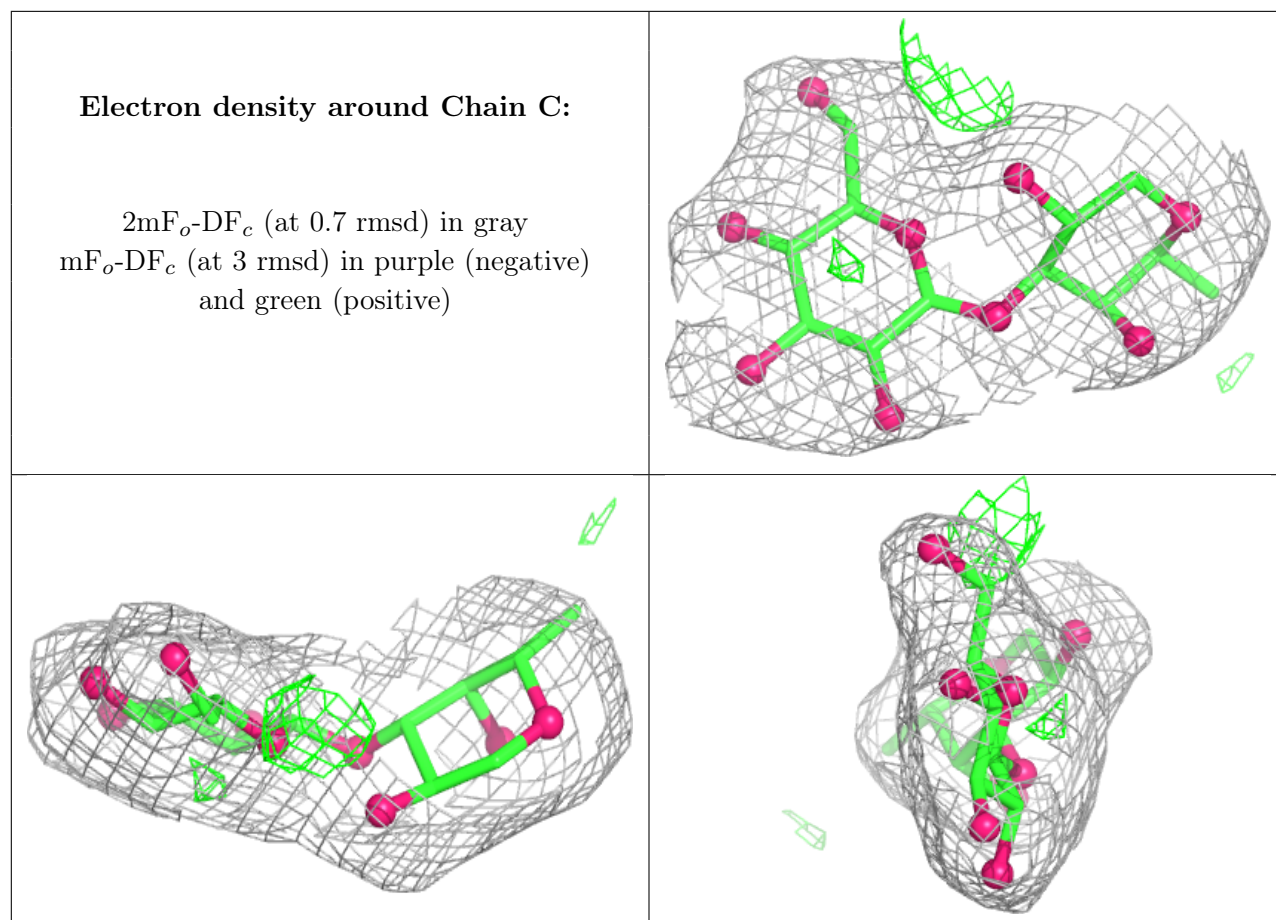
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain B:**

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







## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	FUL	A	1004	10/11	0.59	0.15	154,162,169,172	0
6	MAN	A	1010	11/12	0.79	0.11	127,137,142,143	0
6	MAN	A	1009	11/12	0.84	0.13	152,162,169,172	0
6	MAN	A	1007	11/12	0.86	0.15	73,87,95,102	0
6	MAN	A	1008	11/12	0.94	0.11	58,71,81,107	0
4	CD	A	1001	1/1	0.99	0.03	133,133,133,133	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.