



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:24 AM BST

PDB ID : 3T5O
Title : Crystal Structure of human Complement Component C6
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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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

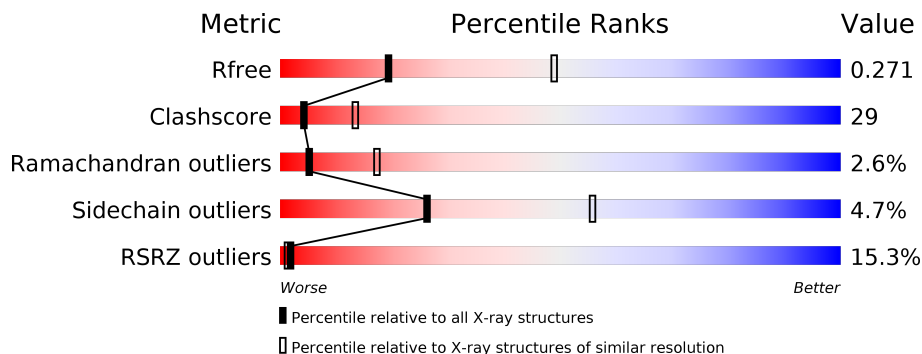
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 ≥ 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	
2	B	2	
3	C	2	

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	NAG	B	2	-	-	-	X

2 Entry composition i

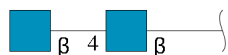
There are 6 unique types of molecules in this entry. The entry contains 6934 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

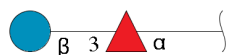
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	871	6830	4222	1203	1336	69	0	0	0

- 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
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

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

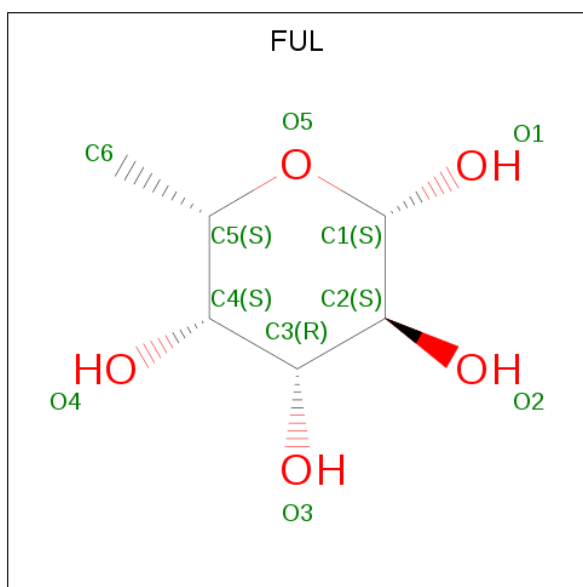


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	C	2	21	12	9	0	0	0

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

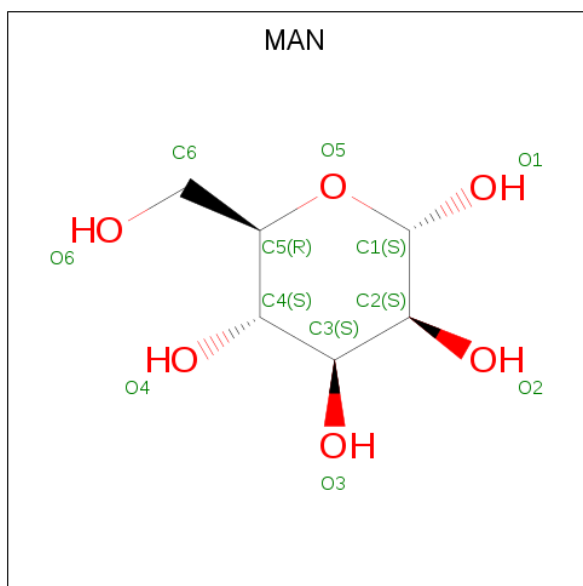
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cd	0	0
			1	1		

- Molecule 5 is beta-L-fucopyranose (three-letter code: FUL) (formula: C₆H₁₂O₅).



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

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

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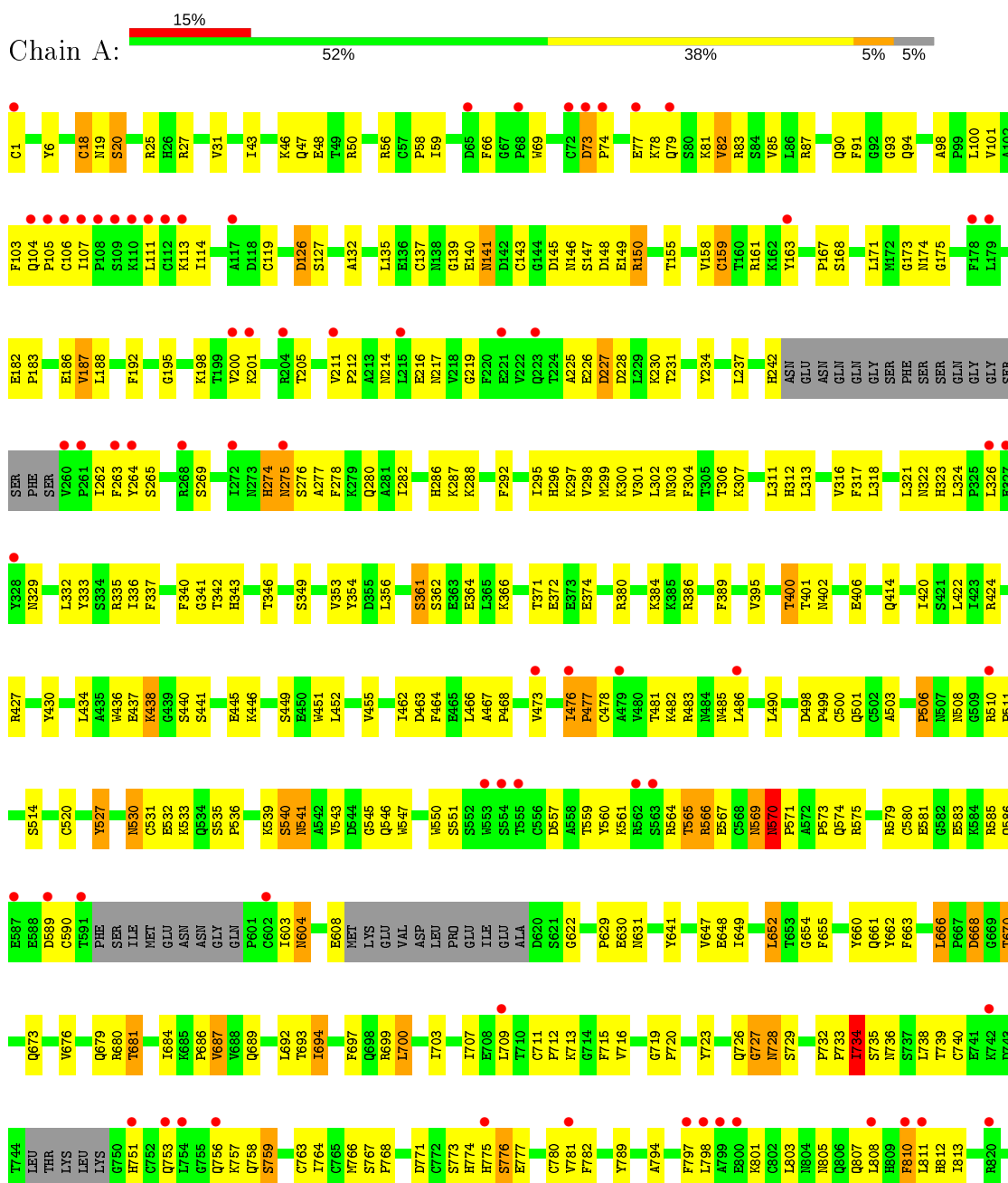
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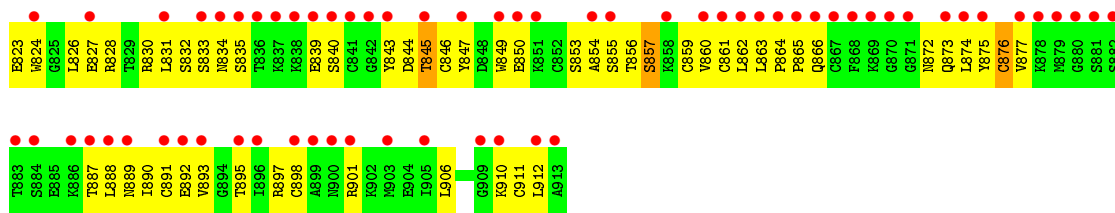
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	11	6	5	0	0

3 Residue-property plots i

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

Chain B: 100%

MAG1
MAG2

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

Chain C: 50% 50%

FUC1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	146.81Å 180.15Å 60.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.06 – 2.87 47.53 – 2.87	Depositor EDS
% Data completeness (in resolution range)	94.9 (43.06-2.87) 94.9 (47.53-2.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.86Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.222 , 0.276 0.219 , 0.271	Depositor DCC
R_{free} test set	2179 reflections (6.10%)	wwPDB-VP
Wilson B-factor (Å ²)	82.3	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 81.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6934	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, NAG, CD, FUC, FUL, 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	0.50	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:O	1:A:205:THR:HG22	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:HA	1:A:581:GLU:OE1	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:HH11	1:A:380:ARG:HG2	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:C	1:A:728:ASN:OD1	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:630:GLU:O	1:A:631:ASN:HB2	2.05	0.57
1:A:81:LYS:O	1:A:101:VAL:HG23	2.05	0.57
1:A:77:GLU:O	1:A:77:GLU:HG3	2.03	0.57
1:A:69:TRP:HZ3	1:A:79:GLN:O	1.88	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:663:PHE:CD1	1:A:673:GLN:HG2	2.43	0.53
1:A:82:VAL:CG2	1:A:101:VAL:HB	2.39	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:H	1:A:100:LEU:HD12	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:173:GLY:O	1:A:187:VAL:HG12	2.09	0.52
1:A:47:GLN:HG2	1:A:48:GLU:N	2.24	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:473:VAL:HG13	1:A:473:VAL:O	2.11	0.51
1:A:336:ILE:CD1	1:A:486:LEU:HD11	2.33	0.51
1:A:850:GLU:HB3	1:A:859:CYS:HB3	1.93	0.51
1:A:739:THR:CG2	1:A:740:CYS:N	2.74	0.51
1:A:85:VAL:HG23	1:A:85:VAL:O	2.11	0.51
1:A:59:ILE:CG2	1:A:87:ARG:HD2	2.41	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:278:PHE:CE2	1:A:282:ILE:HD11	2.46	0.50
1:A:380:ARG:HH11	1:A:380:ARG:CG	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:NH2	1:A:98:ALA:O	2.45	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:CG	1:A:751:HIS:O	2.65	0.50
1:A:234:TYR:HB2	1:A:292:PHE:HB2	1.93	0.50
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:56:ARG:O	1:A:58:PRO:HD3	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:CD2	1:A:527:TYR:N	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:547:TRP:HE1	6:A:1010:MAN:H5	1.78	0.48
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: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:78:LYS:HD3	1:A:103:PHE:CE1	2.50	0.47
1:A:27:ARG:HG3	1:A:46:LYS:HA	1.96	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:776:SER:O	1:A:777:GLU:C	2.53	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: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:N	1:A:912:LEU:HD12	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:NH1	1:A:380:ARG:CG	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:H	1:A:912:LEU:HD12	1.80	0.46
1:A:326:LEU:N	1:A:326:LEU:HD12	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:HG12	1:A:31:VAL:O	2.15	0.45
1:A:380:ARG:NH1	1:A:380:ARG:HG2	2.26	0.45
1:A:692:LEU:HD12	1:A:692:LEU:N	2.31	0.45
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:18:CYS:SG	3:C:1:FUC:H5	2.57	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:HA	1:A:335:ARG:HD2	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:H	1:A:214:ASN:HD22	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:CD2	1:A:697:PHE:C	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:HA	1:A:561:LYS:HD3	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:HG12	1:A:455:VAL:O	2.19	0.42
1:A:437:GLU:O	1:A:438:LYS:C	2.56	0.42
1:A:452:LEU:HA	1:A:452:LEU:HD12	1.76	0.42
1:A:226:GLU:O	1:A:227:ASP:C	2.57	0.42
1:A:219:GLY:O	1:A:302:LEU:HA	2.19	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:ND2	1:A:604:ASN:H	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:286:HIS:HE1	1:A:520:CYS:O	2.04	0.41
1:A:90:GLN:HE22	1:A:503:ALA:N	2.18	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:HB2	1:A:201:LYS:HE3	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: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:81:LYS:O	1:A:101:VAL:HA	2.20	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:550:TRP:HB2	6:A:1009:MAN:C5	2.51	0.41
1:A:225:ALA:O	1:A:228:ASP:HB2	2.20	0.41
1:A:263:PHE:N	1:A:263:PHE:CD2	2.88	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:N	1:A:100:LEU:HD12	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%)	5 17

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%)	26 56

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

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

Mol	Chain	Res	Type
1	A	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 [i](#)

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

5.5 Carbohydrates [i](#)

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	1,2	14,14,15	0.62	0	17,19,21	0.77	0
2	NAG	B	2	2	14,14,15	0.53	0	17,19,21	0.68	0
3	FUC	C	1	1,3	10,10,11	0.81	0	14,14,16	1.62	4 (28%)
3	BGC	C	2	3	11,11,12	1.18	1 (9%)	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
2	NAG	B	1	1,2	-	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	-3.38	1.38	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	BGC	C1-C2-C3	-3.80	104.99	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FUC	C6-C5-C4	-2.91	107.70	113.07
3	C	1	FUC	O5-C5-C6	2.71	113.17	107.33
3	C	1	FUC	C1-C2-C3	2.38	112.59	109.67
3	C	2	BGC	O5-C1-C2	-2.24	107.32	110.77
3	C	1	FUC	O4-C4-C5	-2.20	104.78	109.67
3	C	2	BGC	C3-C4-C5	-2.13	106.44	110.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

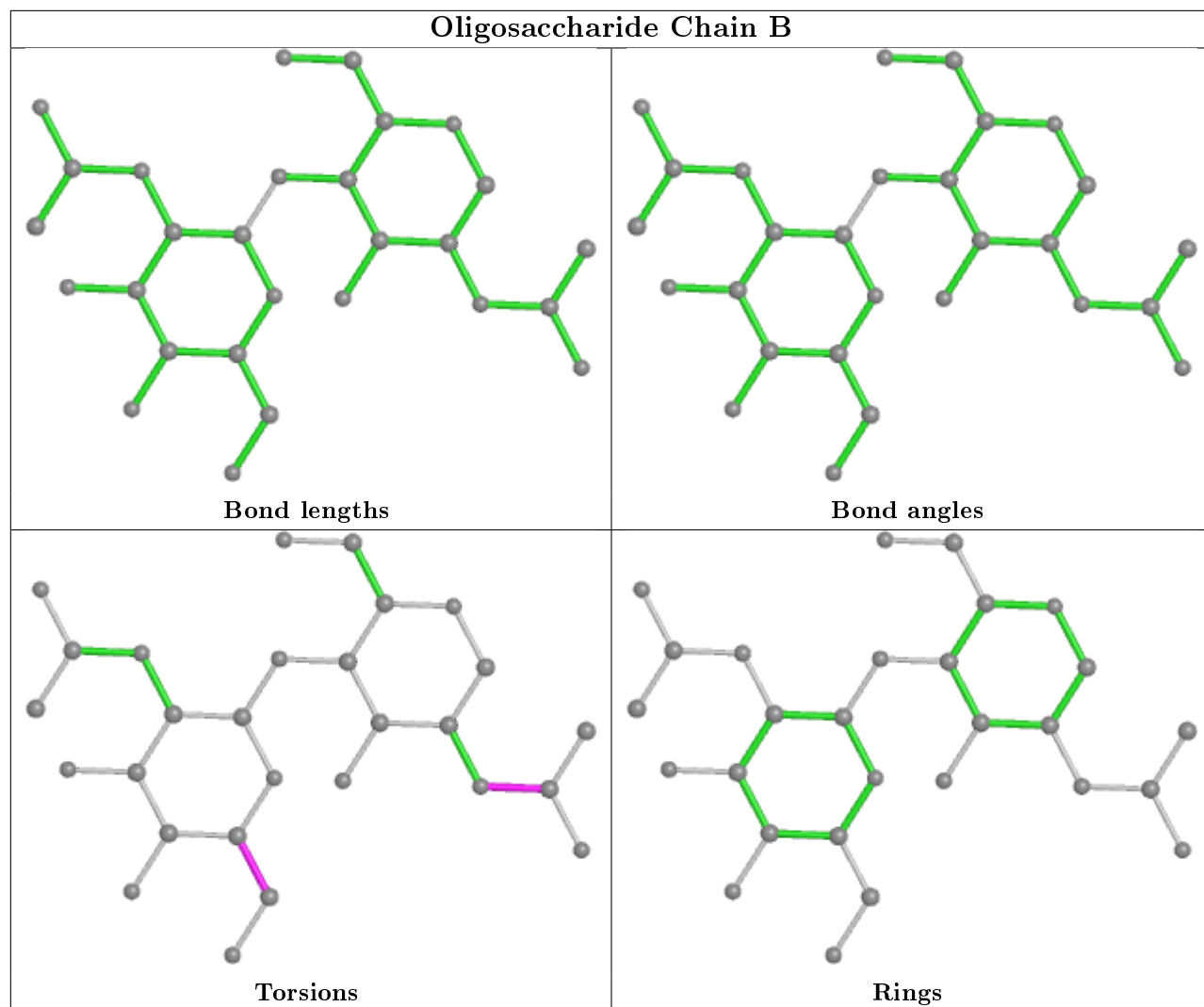
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	C	2	BGC	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
3	C	2	BGC	C4-C5-C6-O6

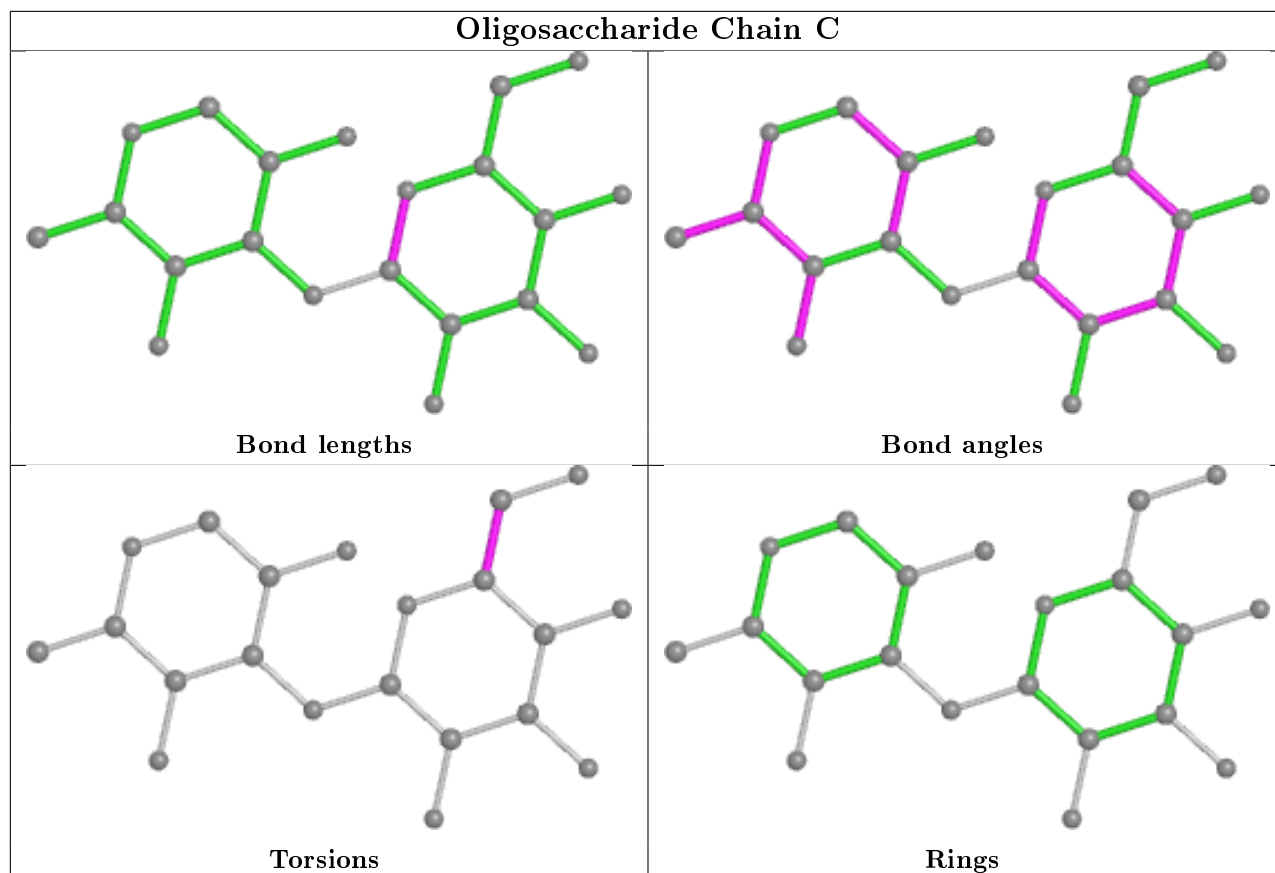
There are no ring outliers.

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	1010	1	11,11,12	0.47	0	15,15,17	1.35	2 (13%)
6	MAN	A	1007	1	11,11,12	0.90	0	15,15,17	1.35	3 (20%)
5	FUL	A	1004	1	10,10,11	0.66	0	14,14,16	1.03	1 (7%)
6	MAN	A	1008	1	11,11,12	1.18	0	15,15,17	1.77	4 (26%)
6	MAN	A	1009	1	11,11,12	0.65	0	15,15,17	1.51	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	1010	1	-	0/2/19/22	0/1/1/1
5	FUL	A	1004	1	-	-	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
6	MAN	A	1009	1	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1008	MAN	C1-C2-C3	-3.22	105.70	109.67
6	A	1010	MAN	C2-C3-C4	-3.18	105.40	110.89
6	A	1009	MAN	C3-C4-C5	3.18	115.90	110.24
6	A	1008	MAN	O4-C4-C3	-3.11	103.16	110.35
6	A	1009	MAN	C1-O5-C5	2.93	116.17	112.19
6	A	1008	MAN	O5-C5-C6	2.59	111.27	107.20
6	A	1007	MAN	O5-C5-C6	2.54	111.19	107.20
6	A	1007	MAN	O4-C4-C3	-2.46	104.65	110.35
6	A	1007	MAN	O5-C1-C2	-2.39	107.08	110.77
6	A	1008	MAN	O4-C4-C5	-2.39	103.37	109.30
6	A	1010	MAN	C1-C2-C3	-2.20	106.96	109.67
6	A	1009	MAN	O5-C1-C2	-2.17	107.42	110.77
5	A	1004	FUL	C1-C2-C3	2.05	112.18	109.67

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	1010	MAN	3	0
6	A	1007	MAN	1	0
5	A	1004	FUL	3	0
6	A	1008	MAN	1	0
6	A	1009	MAN	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	871/913 (95%)	0.95	133 (15%) 2 1	41, 107, 238, 291	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	840	SER	14.8
1	A	861	CYS	11.7
1	A	892	GLU	10.2
1	A	913	ALA	10.2
1	A	879	MET	9.7
1	A	843	TYR	9.5
1	A	870	GLY	9.5
1	A	834	ASN	9.4
1	A	888	LEU	9.3
1	A	842	GLY	9.3
1	A	865	PRO	8.8
1	A	873	GLN	8.5
1	A	838	LYS	7.7
1	A	111	LEU	7.5
1	A	862	LEU	7.5
1	A	775	HIS	7.5
1	A	871	GLY	7.4
1	A	860	VAL	7.4
1	A	73	ASP	6.8
1	A	105	PRO	6.7
1	A	899	ALA	6.6
1	A	875	TYR	6.6
1	A	880	GLY	6.6
1	A	893	VAL	6.6
1	A	264	TYR	6.6
1	A	905	ILE	6.6
1	A	753	GLN	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	874	LEU	6.4
1	A	110	LYS	6.1
1	A	882	SER	6.0
1	A	903	MET	5.6
1	A	864	PRO	5.6
1	A	836	THR	5.4
1	A	555	THR	5.3
1	A	835	SER	5.2
1	A	887	THR	5.2
1	A	884	SER	5.0
1	A	563	SER	5.0
1	A	820	ARG	4.9
1	A	889	ASN	4.9
1	A	847	TYR	4.8
1	A	754	LEU	4.8
1	A	839	GLU	4.8
1	A	808	LEU	4.7
1	A	896	ILE	4.7
1	A	756	GLN	4.6
1	A	827	GLU	4.6
1	A	200	VAL	4.5
1	A	912	LEU	4.5
1	A	868	PHE	4.4
1	A	591	THR	4.3
1	A	473	VAL	4.3
1	A	112	CYS	4.2
1	A	854	ALA	4.2
1	A	878	LYS	4.2
1	A	117	ALA	4.2
1	A	824	TRP	4.1
1	A	811	LEU	4.1
1	A	831	LEU	4.1
1	A	107	ILE	4.0
1	A	223	GLN	4.0
1	A	866	GLN	4.0
1	A	869	LYS	3.9
1	A	742	LYS	3.8
1	A	72	CYS	3.8
1	A	877	VAL	3.8
1	A	833	SER	3.7
1	A	587	GLU	3.7
1	A	895	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	204	ARG	3.5
1	A	562	ARG	3.4
1	A	106	CYS	3.4
1	A	851	LYS	3.3
1	A	553	TRP	3.2
1	A	910	LYS	3.2
1	A	797	PHE	3.2
1	A	602	CYS	3.1
1	A	909	GLY	3.1
1	A	275	ASN	3.1
1	A	221	GLU	3.1
1	A	837	LYS	3.1
1	A	104	GLN	3.1
1	A	268	ARG	3.0
1	A	900	ASN	3.0
1	A	261	PRO	2.9
1	A	891	CYS	2.8
1	A	800	GLU	2.8
1	A	486	LEU	2.8
1	A	479	ALA	2.7
1	A	326	LEU	2.7
1	A	798	LEU	2.7
1	A	77	GLU	2.7
1	A	849	TRP	2.7
1	A	109	SER	2.6
1	A	867	CYS	2.6
1	A	260	VAL	2.6
1	A	781	VAL	2.5
1	A	179	LEU	2.5
1	A	263	PHE	2.5
1	A	810	PHE	2.5
1	A	841	CYS	2.5
1	A	858	LYS	2.4
1	A	215	LEU	2.4
1	A	328	TYR	2.4
1	A	476	ILE	2.4
1	A	211	VAL	2.4
1	A	272	ILE	2.4
1	A	65	ASP	2.4
1	A	845	THR	2.4
1	A	113	LYS	2.4
1	A	68	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	327	GLU	2.4
1	A	201	LYS	2.4
1	A	886	LYS	2.3
1	A	850	GLU	2.3
1	A	589	ASP	2.3
1	A	709	LEU	2.3
1	A	178	PHE	2.3
1	A	883	THR	2.2
1	A	1	CYS	2.2
1	A	881	SER	2.2
1	A	799	ALA	2.2
1	A	79	GLN	2.2
1	A	751	HIS	2.1
1	A	510	ARG	2.1
1	A	163	TYR	2.1
1	A	108	PRO	2.1
1	A	554	SER	2.0
1	A	863	LEU	2.0
1	A	901	ARG	2.0
1	A	855	SER	2.0
1	A	898	CYS	2.0
1	A	74	PRO	2.0

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

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

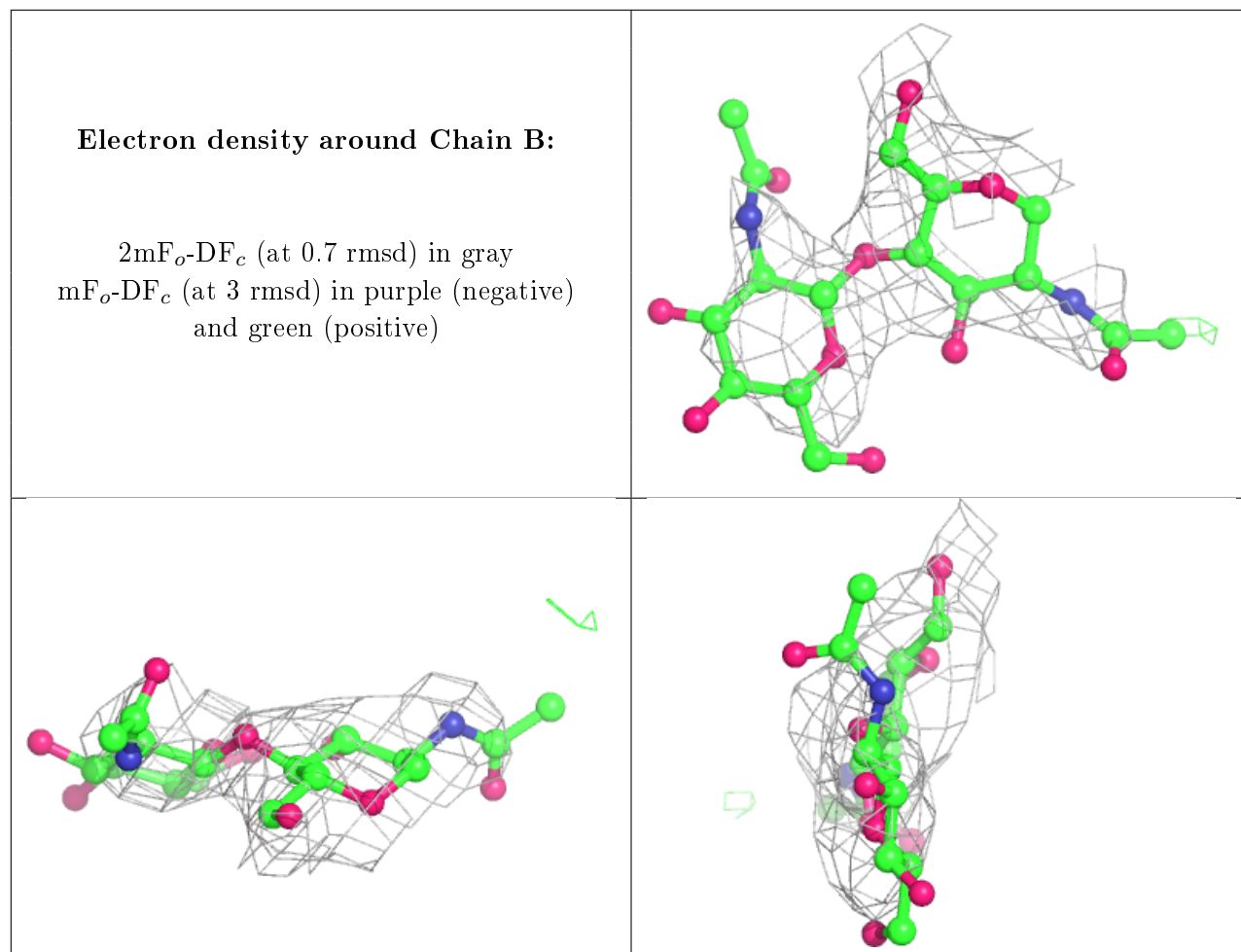
6.3 Carbohydrates [i](#)

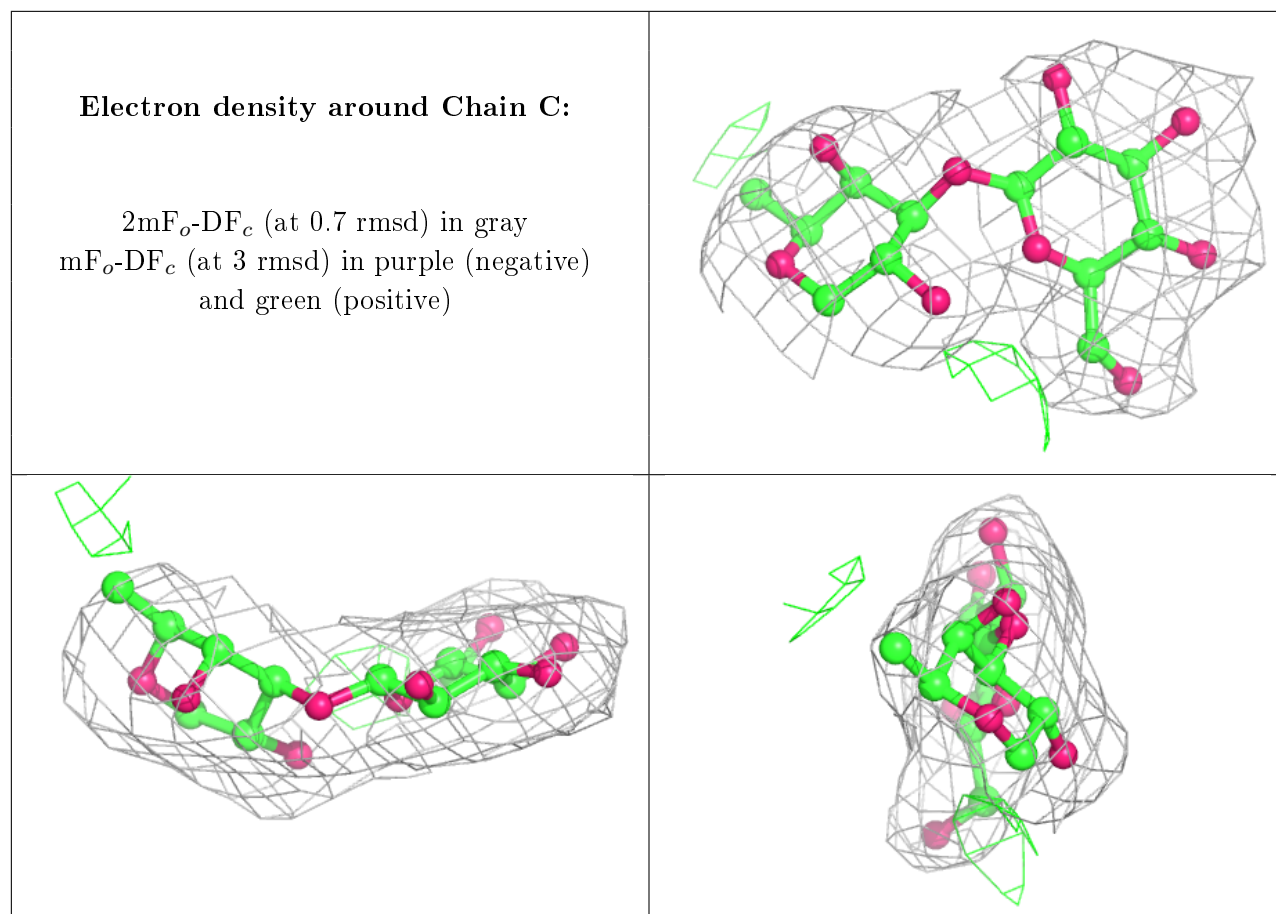
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.77	0.54	148,174,183,187	0
2	NAG	B	1	14/15	0.90	0.25	120,151,163,169	0
3	BGC	C	2	11/12	0.97	0.20	51,62,72,80	0
3	FUC	C	1	10/11	0.98	0.19	47,56,68,78	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.





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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FUL	A	1004	10/11	0.81	0.32	154,162,169,172	0
6	MAN	A	1010	11/12	0.88	0.23	127,137,142,143	0
6	MAN	A	1009	11/12	0.92	0.19	152,162,169,172	0
6	MAN	A	1007	11/12	0.95	0.22	73,87,95,102	0
6	MAN	A	1008	11/12	0.96	0.22	58,71,81,107	0
4	CD	A	1001	1/1	0.97	0.18	133,133,133,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.