



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:09 PM UTC

PDB ID : 3T5O / pdb_00003t5o
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

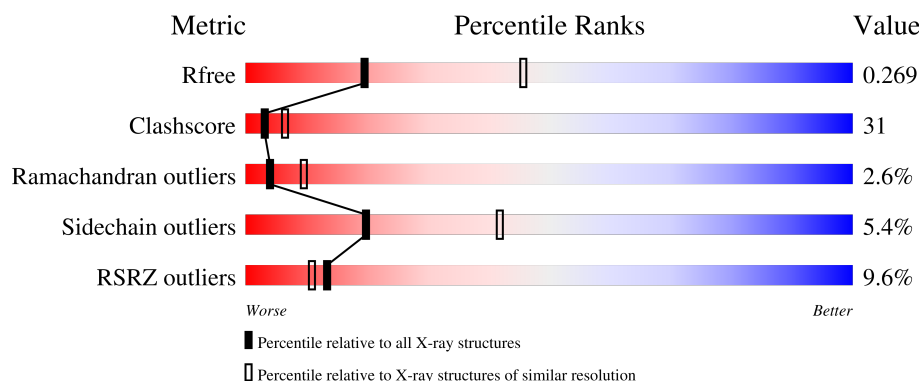
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

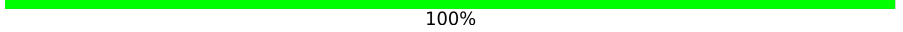
The reported resolution of this entry is 2.87 Å.

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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (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 ≥ 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	

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.

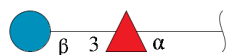
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	871	Total	C	N	O	S	0	0	0
			6830	4222	1203	1336	69			

- 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.

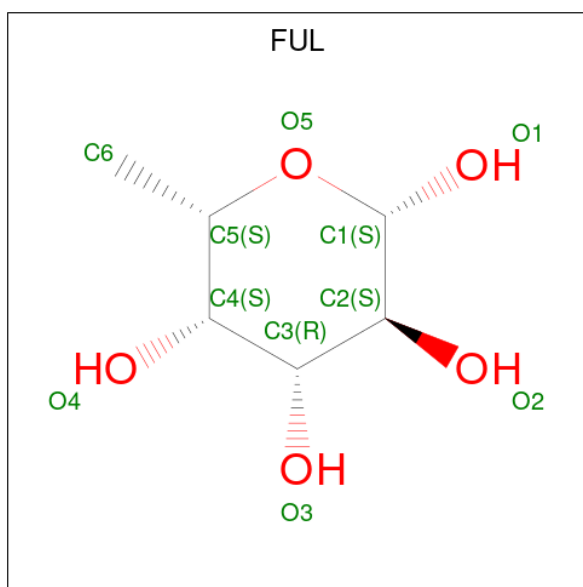


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 4 is CADMIUM ION (CCD ID: CD) (formula: Cd).

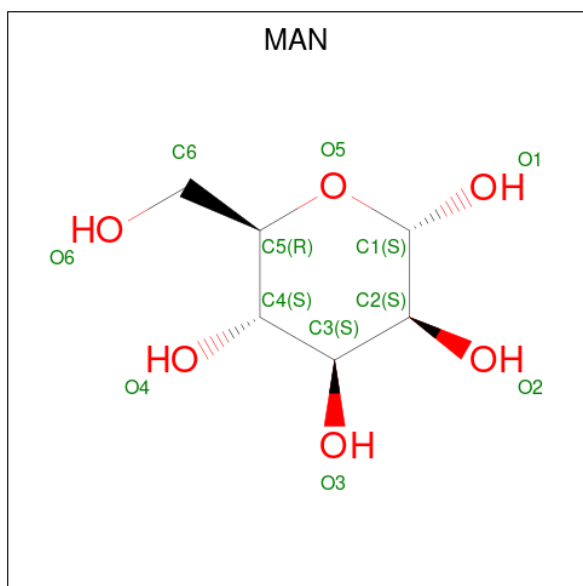
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cd	0	0
			1	1		

- Molecule 5 is beta-L-fucopyranose (CCD ID: FUL) (formula: C₆H₁₂O₅).



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

- Molecule 6 is alpha-D-mannopyranose (CCD ID: 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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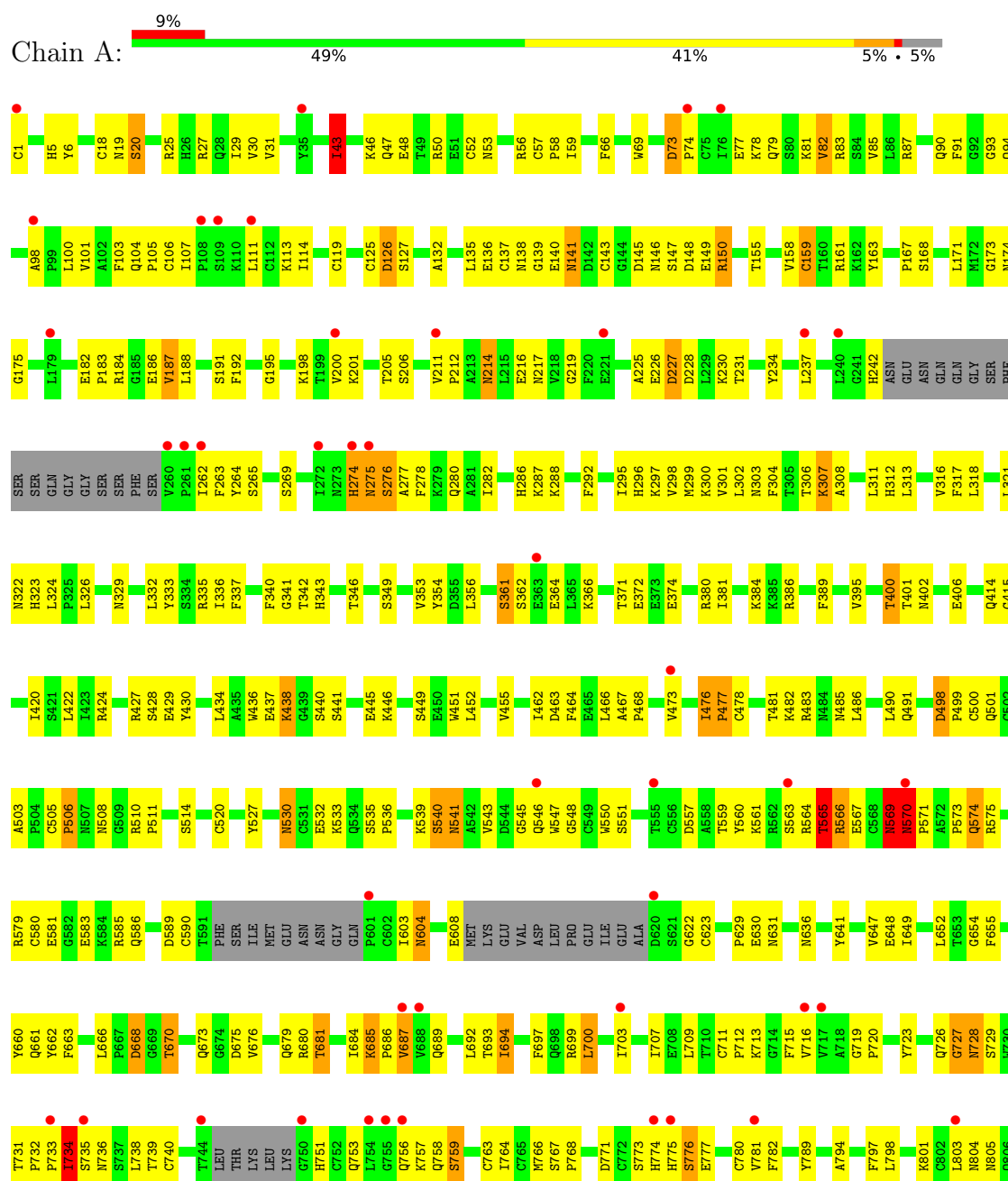
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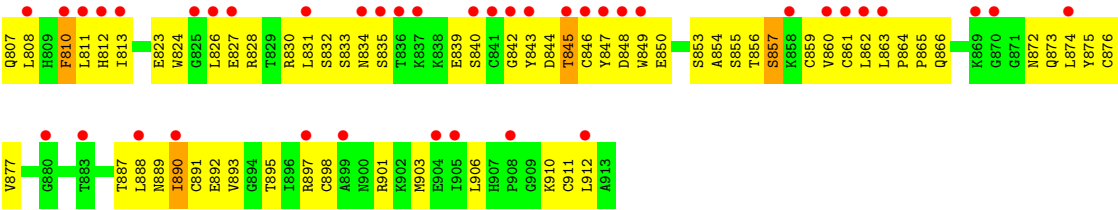
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

3 Residue-property plots

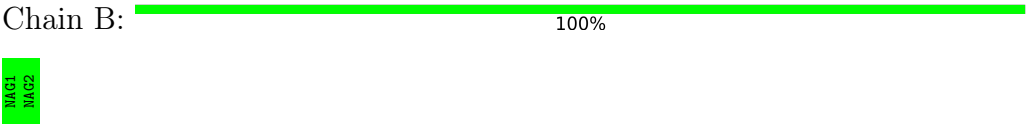
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.222 , 0.276 0.216 , 0.269	Depositor DCC
R_{free} test set	2179 reflections (5.78%)	wwPDB-VP
Wilson B-factor (Å ²)	82.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 107.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CD, FUL, NAG, MAN, BGC, FUC

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	0.62	0/6973	1.02	31/9409 (0.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	ASP	CA-C-N	8.96	129.19	119.87
1	A	498	ASP	C-N-CA	8.96	129.19	119.87
1	A	57	CYS	CA-C-N	7.94	129.76	119.84
1	A	57	CYS	C-N-CA	7.94	129.76	119.84
1	A	842	GLY	N-CA-C	-7.02	106.13	114.48
1	A	505	CYS	CA-C-N	6.40	127.84	119.84
1	A	505	CYS	C-N-CA	6.40	127.84	119.84
1	A	570	ASN	N-CA-C	-6.40	95.67	109.81
1	A	636	ASN	N-CA-C	6.39	117.90	107.23
1	A	548	GLY	N-CA-C	-6.01	102.20	112.30
1	A	623	CYS	CA-C-N	5.84	126.31	120.52
1	A	623	CYS	C-N-CA	5.84	126.31	120.52
1	A	191	SER	N-CA-C	-5.84	106.28	113.41
1	A	731	THR	N-CA-C	5.77	118.57	108.75
1	A	685	LYS	CA-C-N	5.70	126.97	119.84
1	A	685	LYS	C-N-CA	5.70	126.97	119.84
1	A	574	GLN	N-CA-C	5.70	117.73	109.07
1	A	206	SER	CB-CA-C	-5.53	110.22	116.63
1	A	415	GLY	N-CA-C	-5.48	107.11	115.66
1	A	563	SER	N-CA-C	5.47	117.50	109.24
1	A	43	ILE	N-CA-C	5.46	119.94	113.22
1	A	569	ASN	CA-C-O	5.36	121.05	117.94
1	A	184	ARG	N-CA-C	5.33	113.87	108.75
1	A	308	ALA	N-CA-C	5.31	117.15	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	ASN	CB-CA-C	-5.23	109.54	117.07
1	A	675	ASP	CA-C-N	-5.10	115.62	122.91
1	A	675	ASP	C-N-CA	-5.10	115.62	122.91
1	A	565	THR	N-CA-C	5.08	117.62	108.48
1	A	125	CYS	N-CA-C	-5.07	103.35	110.50
1	A	276	SER	N-CA-C	-5.04	107.78	114.04
1	A	29	ILE	N-CA-C	5.04	115.95	108.23

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	420	0
2	B	28	0	25	0	0
3	C	21	0	19	1	0
4	A	1	0	0	0	0
5	A	10	0	10	3	0
6	A	44	0	40	7	0
All	All	6934	0	6592	420	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 31.

All (420) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:801:LYS:HG3	1:A:805:ASN:CG	2.17	0.69
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: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:140:GLU:CD	1:A:158:VAL:HG21	2.17	0.69
1:A:887:THR:C	1:A:888:LEU:HD22	2.18	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:888:LEU:HD12	1:A:892:GLU:CD	2.20	0.66
1:A:801:LYS:CA	1:A:805:ASN:HB2	2.23	0.66
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:728:ASN:OD1	1:A:728:ASN:C	2.38	0.65
1:A:498:ASP:CG	1:A:499:PRO:HD2	2.22	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:329:ASN:HD22	1:A:332:LEU:HB2	1.65	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:322:ASN:C	1:A:324:LEU:H	2.10	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
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:774:HIS:O	1:A:775:HIS:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:567:GLU:C	1:A:569:ASN:OD1	2.48	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:297:LYS:HG2	1:A:299:MET:HE2	1.87	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: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:734:ILE:O	1:A:735:SER:C	2.51	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:6:TYR:O	1:A:27:ARG:HD3	2.09	0.53
1:A:147:SER:C	1:A:149:GLU:H	2.16	0.53
1:A:297:LYS:HE3	1:A:299:MET:HE2	1.91	0.53
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:832:SER:OG	1:A:833:SER:N	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:173:GLY:O	1:A:187:VAL:HG12	2.09	0.52
1:A:805:ASN:C	1:A:807:GLN:H	2.17	0.52
1:A:776:SER:O	1:A:777:GLU:C	2.53	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:569:ASN:O	1:A:570:ASN:C	2.52	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: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:863:LEU:C	1:A:865:PRO:HD2	2.35	0.51
1:A:473:VAL:O	1:A:483:ARG:HG3	2.10	0.51
1:A:47:GLN:HG2	1:A:48:GLU:N	2.24	0.50
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
1:A:380:ARG:HH11	1:A:380:ARG:CG	2.23	0.50
1:A:877:VAL:HB	1:A:903:MET:HE2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:527:TYR:N	1:A:527:TYR:CD2	2.80	0.49
1:A:106:CYS:SG	1:A:107:ILE:N	2.85	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: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: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: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
1:A:559:THR:C	1:A:561:LYS:N	2.71	0.48
1:A:801:LYS:C	1:A:805:ASN:HB2	2.38	0.48
1:A:828:ARG:HD2	1:A:849:TRP:HZ2	1.79	0.48
1:A:697:PHE:C	1:A:697:PHE:CD2	2.92	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:629:PRO:O	1:A:630:GLU:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:LYS:O	1:A:114:ILE:HD13	2.14	0.47
1:A:436:TRP:C	1:A:437:GLU:HG3	2.38	0.47
1:A:437:GLU:O	1:A:438:LYS:C	2.56	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:303:ASN:O	1:A:304:PHE:HB3	2.14	0.47
1:A:462:ILE:O	1:A:463:ASP:C	2.57	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: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:322:ASN:C	1:A:324:LEU:N	2.72	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:226:GLU:O	1:A:227:ASP:C	2.57	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
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:445:GLU:O	1:A:446:LYS:C	2.60	0.45
1:A:274:HIS:O	1:A:275:ASN:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:SER:O	1:A:429:GLU:C	2.58	0.45
1:A:486:LEU:HD12	1:A:486:LEU:HA	1.76	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:138:ASN:OD1	1:A:138:ASN:C	2.60	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:699:ARG:C	1:A:700:LEU:HD13	2.42	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:304:PHE:CD1	1:A:304:PHE:C	2.95	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:797:PHE:O	1:A:798:LEU:C	2.60	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:875:TYR:CG	1:A:887:THR:HG23	2.54	0.43
1:A:137:CYS:C	1:A:155:THR:HG22	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:751:HIS:C	1:A:753:GLN:N	2.76	0.43
1:A:354:TYR:CZ	1:A:356:LEU:HD11	2.54	0.43
1:A:508:ASN:OD1	1:A:543:VAL:HA	2.19	0.43
1:A:559:THR:C	1:A:561:LYS:H	2.26	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:804:ASN:HB3	1:A:807:GLN:CD	2.44	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:136:GLU:O	1:A:137:CYS:C	2.61	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:52:CYS:O	1:A:53:ASN:C	2.61	0.42
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:733:PRO:C	1:A:735:SER:H	2.27	0.42
1:A:455:VAL:O	1:A:455:VAL:HG12	2.19	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:608:GLU:H	1:A:608:GLU:HG2	1.67	0.42
1:A:274:HIS:ND1	1:A:274:HIS:C	2.77	0.42
1:A:324:LEU:HB3	1:A:333:TYR:CE1	2.54	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: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:728:ASN:O	1:A:728:ASN:CG	2.63	0.41
1:A:847:TYR:O	1:A:848:ASP:C	2.61	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:736:ASN:C	1:A:738:LEU:H	2.29	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:810:PHE:CD2	1:A:810:PHE:C	2.99	0.41
1:A:147:SER:C	1:A:149:GLU:N	2.79	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:226:GLU:C	1:A:228:ASP:N	2.79	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:464:PHE:CE1	1:A:466:LEU:HD21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASN:ND2	1:A:186:GLU:HA	2.36	0.40
1:A:322:ASN:O	1:A:324:LEU:N	2.54	0.40
1:A:539:LYS:O	1:A:540:SER:C	2.63	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%)	4 9

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

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Mol	Chain	Res	Type
1	A	476	ILE
1	A	477	PRO
1	A	73	ASP
1	A	732	PRO

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	772/810 (95%)	730 (95%)	42 (5%)	20	42

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	30	VAL
1	A	43	ILE
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	214	ASN
1	A	274	HIS
1	A	307	LYS
1	A	361	SER
1	A	381	ILE
1	A	384	LYS
1	A	395	VAL
1	A	400	THR
1	A	491	GLN
1	A	506	PRO
1	A	514	SER
1	A	530	ASN

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Mol	Chain	Res	Type
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	685	LYS
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
1	A	890	ILE

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	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	275	ASN
1	A	280	GLN
1	A	286	HIS
1	A	296	HIS
1	A	312	HIS
1	A	329	ASN
1	A	408	HIS
1	A	414	GLN
1	A	530	ASN
1	A	541	ASN
1	A	574	GLN

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Mol	Chain	Res	Type
1	A	604	ASN
1	A	625	GLN
1	A	679	GLN
1	A	753	GLN
1	A	756	GLN
1	A	804	ASN
1	A	806	GLN
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	1,2	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	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	-3.20	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
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

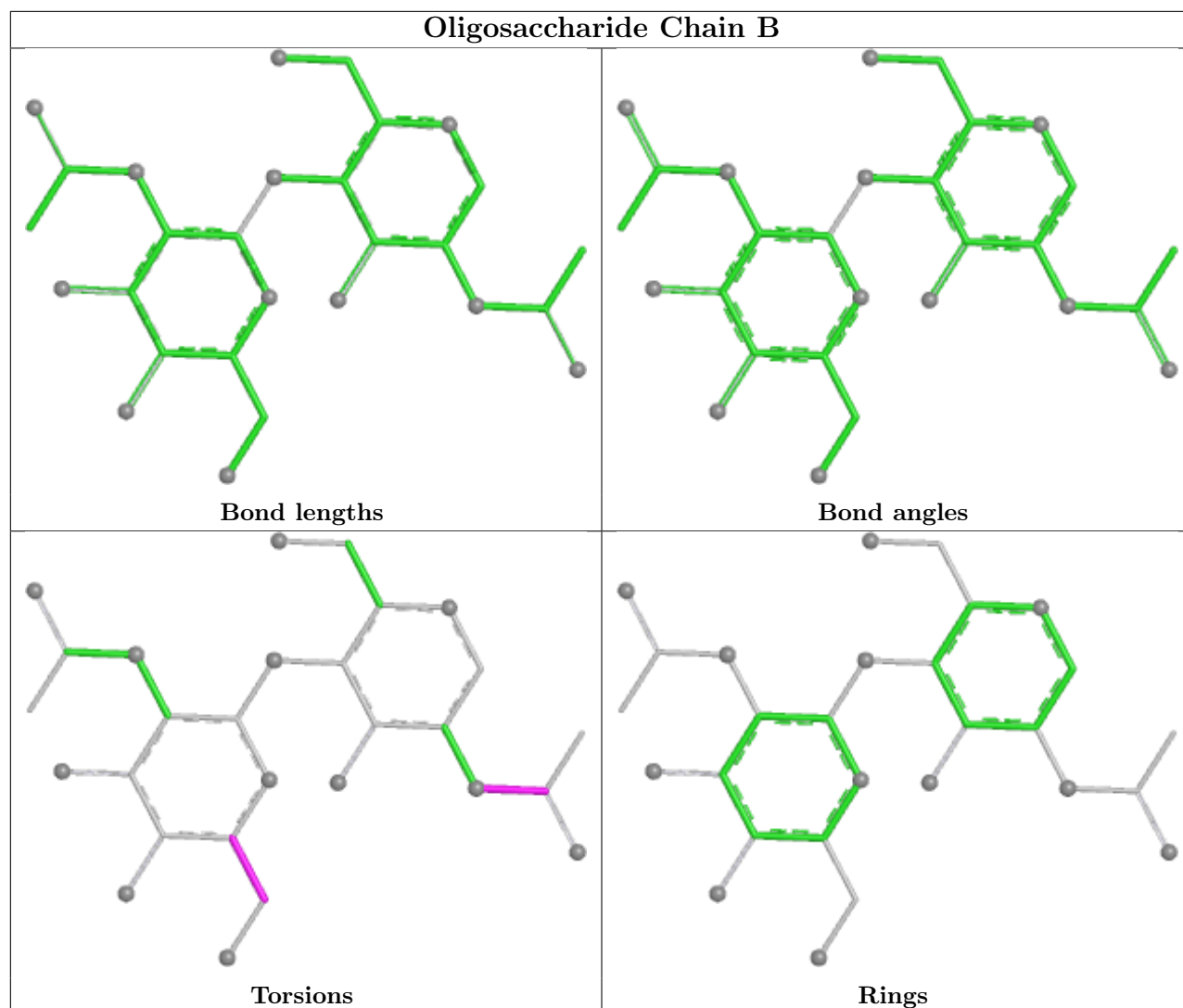
There are no ring outliers.

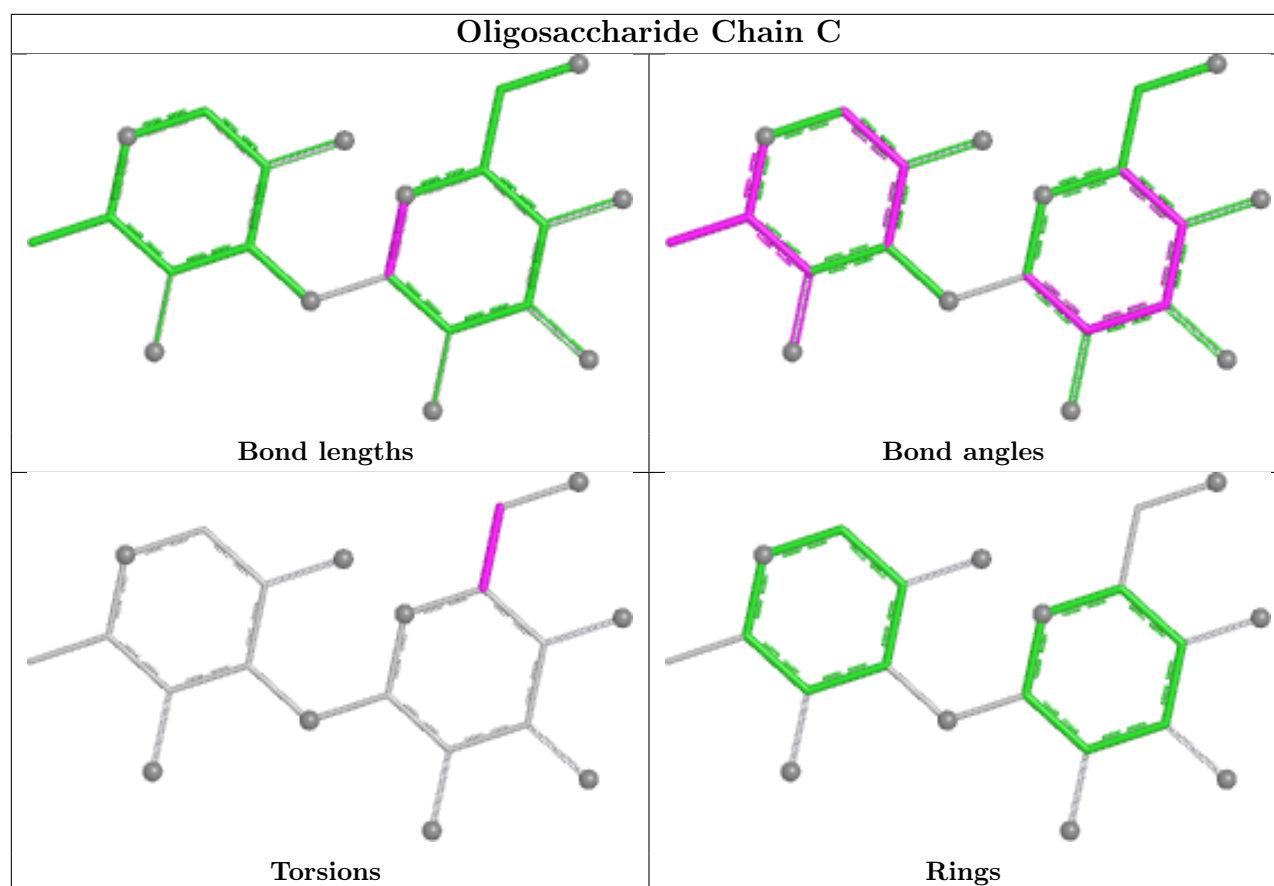
1 monomer is involved in 1 short contact:

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	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	1009	1	11,11,12	0.63	0	15,15,17	1.43	2 (13%)
6	MAN	A	1008	1	11,11,12	1.15	0	15,15,17	1.62	3 (20%)
5	FUL	A	1004	1	10,10,11	0.64	0	14,14,16	0.89	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
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	1009	1	-	1/2/19/22	0/1/1/1
6	MAN	A	1008	1	-	2/2/19/22	1/1/1/1
5	FUL	A	1004	1	-	-	0/1/1/1

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	1010	MAN	3	0
6	A	1007	MAN	1	0
6	A	1009	MAN	2	0
6	A	1008	MAN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1004	FUL	3	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%)	0.48	84 (9%) 13 11	41, 107, 238, 291	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	843	TYR	6.4
1	A	811	LEU	5.7
1	A	831	LEU	5.5
1	A	842	GLY	5.5
1	A	601	PRO	5.3
1	A	847	TYR	5.0
1	A	755	GLY	4.9
1	A	897	ARG	4.8
1	A	835	SER	4.5
1	A	111	LEU	4.5
1	A	775	HIS	4.3
1	A	754	LEU	4.3
1	A	750	GLY	3.8
1	A	810	PHE	3.6
1	A	908	PRO	3.6
1	A	272	ILE	3.5
1	A	687	VAL	3.4
1	A	274	HIS	3.4
1	A	905	ILE	3.4
1	A	744	THR	3.4
1	A	874	LEU	3.4
1	A	733	PRO	3.4
1	A	826	LEU	3.3
1	A	845	THR	3.2
1	A	803	LEU	3.1
1	A	240	LEU	3.1
1	A	912	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	880	GLY	3.0
1	A	260	VAL	2.9
1	A	555	THR	2.9
1	A	262	ILE	2.9
1	A	861	CYS	2.9
1	A	108	PRO	2.8
1	A	808	LEU	2.8
1	A	812	HIS	2.7
1	A	904	GLU	2.7
1	A	862	LEU	2.6
1	A	620	ASP	2.6
1	A	774	HIS	2.6
1	A	563	SER	2.5
1	A	261	PRO	2.5
1	A	200	VAL	2.5
1	A	717	VAL	2.5
1	A	899	ALA	2.5
1	A	570	ASN	2.5
1	A	98	ALA	2.5
1	A	363	GLU	2.5
1	A	883	THR	2.5
1	A	74	PRO	2.4
1	A	735	SER	2.4
1	A	840	SER	2.4
1	A	858	LYS	2.4
1	A	863	LEU	2.4
1	A	890	ILE	2.4
1	A	211	VAL	2.4
1	A	1	CYS	2.3
1	A	849	TRP	2.3
1	A	275	ASN	2.3
1	A	35	TYR	2.3
1	A	703	ILE	2.2
1	A	846	CYS	2.2
1	A	836	THR	2.2
1	A	825	GLY	2.2
1	A	179	LEU	2.2
1	A	837	LYS	2.2
1	A	76	ILE	2.2
1	A	546	GLN	2.2
1	A	827	GLU	2.2
1	A	688	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	781	VAL	2.1
1	A	869	LYS	2.1
1	A	841	CYS	2.1
1	A	473	VAL	2.1
1	A	870	GLY	2.1
1	A	716	VAL	2.1
1	A	848	ASP	2.1
1	A	888	LEU	2.1
1	A	109	SER	2.1
1	A	237	LEU	2.0
1	A	834	ASN	2.0
1	A	813	ILE	2.0
1	A	221	GLU	2.0
1	A	756	GLN	2.0
1	A	860	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](#)

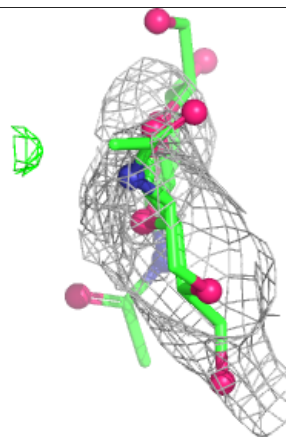
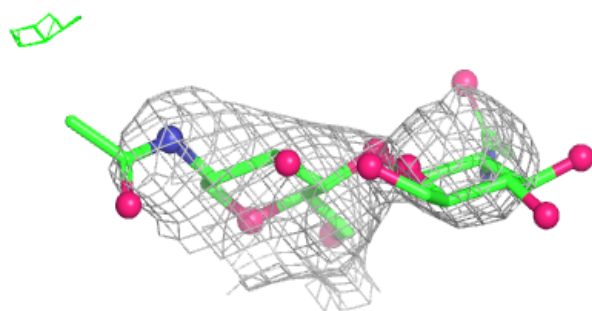
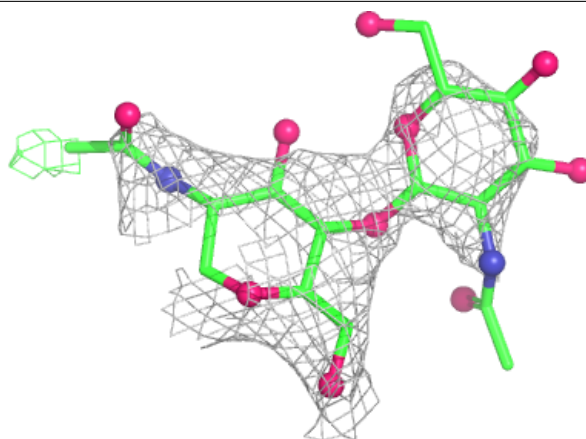
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

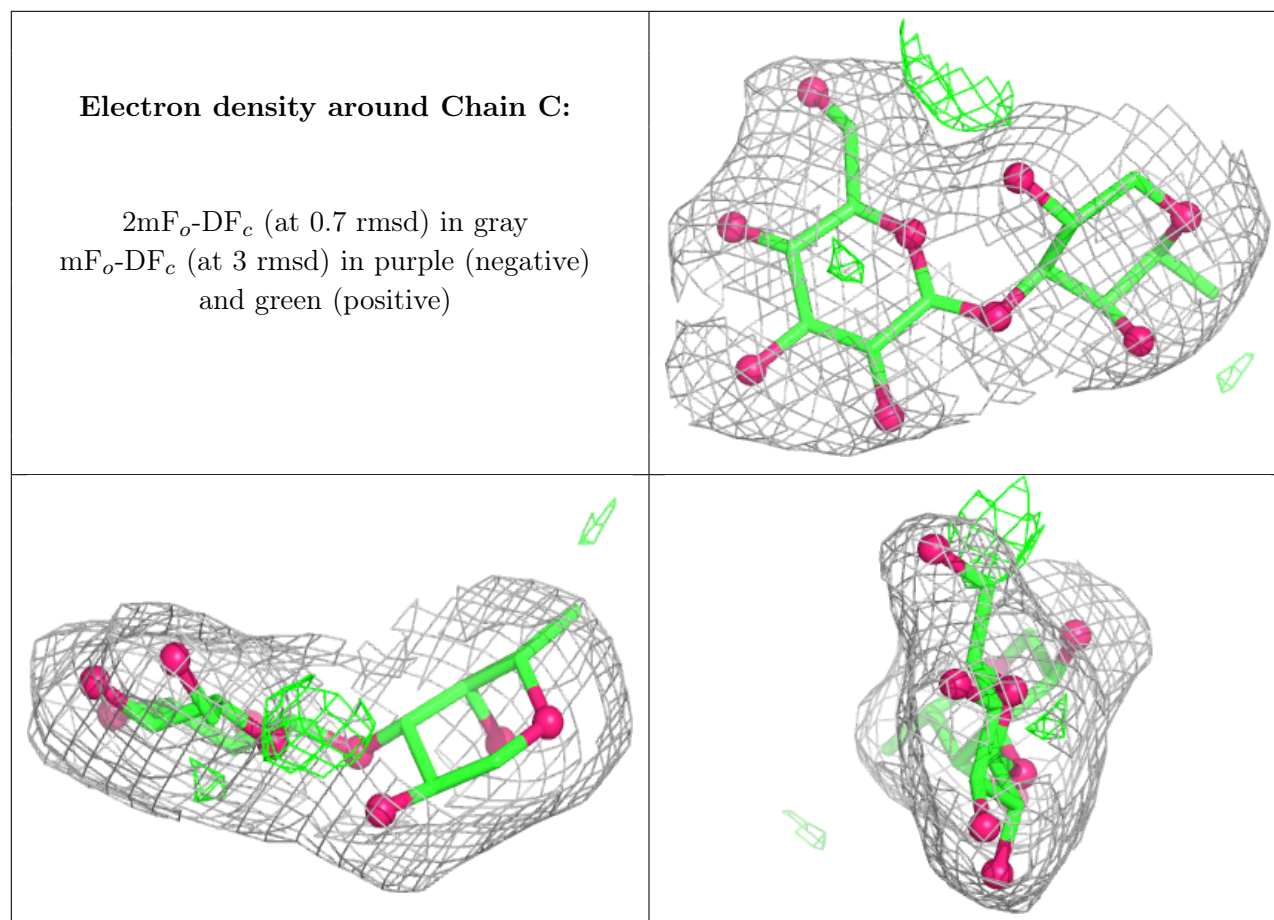
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	1	14/15	0.55	0.13	120,151,163,169	0
2	NAG	B	2	14/15	0.65	0.10	148,174,183,187	0
3	BGC	C	2	11/12	0.96	0.07	51,62,72,80	0
3	FUC	C	1	10/11	0.97	0.05	47,56,68,78	0

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, 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($\text{\AA}^2$)	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.