



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:40 AM UTC

PDB ID : 3JWO / pdb_00003jwo
Title : Structure of HIV-1 gp120 with gp41-Interactive Region: Layered Architecture and Basis of Conformational Mobility
Authors : Pancera, M.; Majeed, S.; Huang, C.C.; Kwon, Y.D.; Zhou, T.; Robinson, J.E.; Sodroski, J.; Wyatt, R.; Kwong, P.D.
Deposited on : 2009-09-18
Resolution : 3.51 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

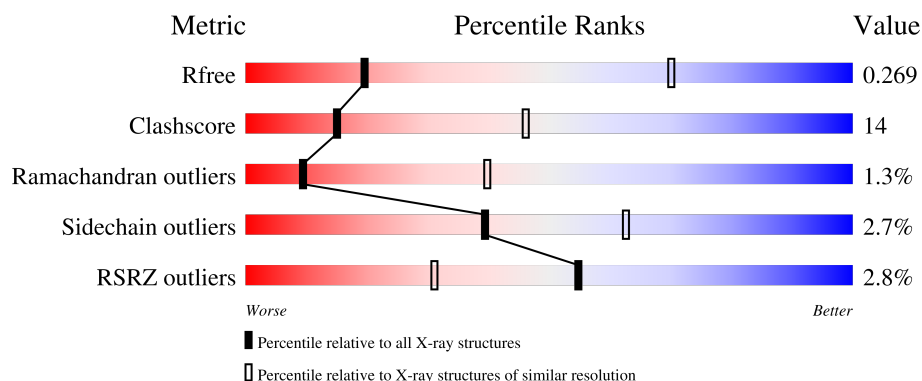
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	357	2% 66% 32% ..
2	C	184	2% 70% 28% .
3	L	209	3% 74% 25%
4	H	220	4% 74% 26%
5	B	2	50% 50%

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
5	NAG	B	1	X	-	-	-
6	NAG	A	734	X	-	-	-
6	NAG	A	948	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7597 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 HIV-1 GP120 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2747	1736	471	520	20			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	184	Total	C	N	O	S	0	0	0
			1432	896	250	281	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1000	MET	-	initiating methionine	UNP P01730

- Molecule 3 is a protein called FAB 48D LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	209	Total	C	N	O	S	0	0	0
			1600	1004	266	325	5			

- Molecule 4 is a protein called FAB 48D Heavy CHAIN.

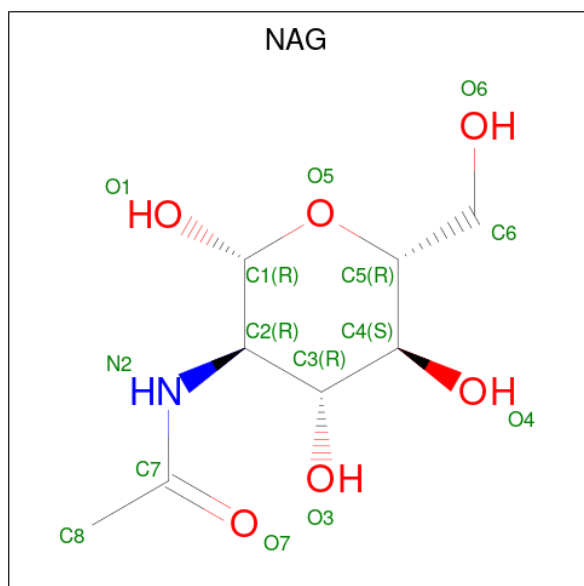
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	220	Total	C	N	O	S	0	0	0
			1654	1048	267	332	7			

- Molecule 5 is an oligosaccharide called beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	B	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

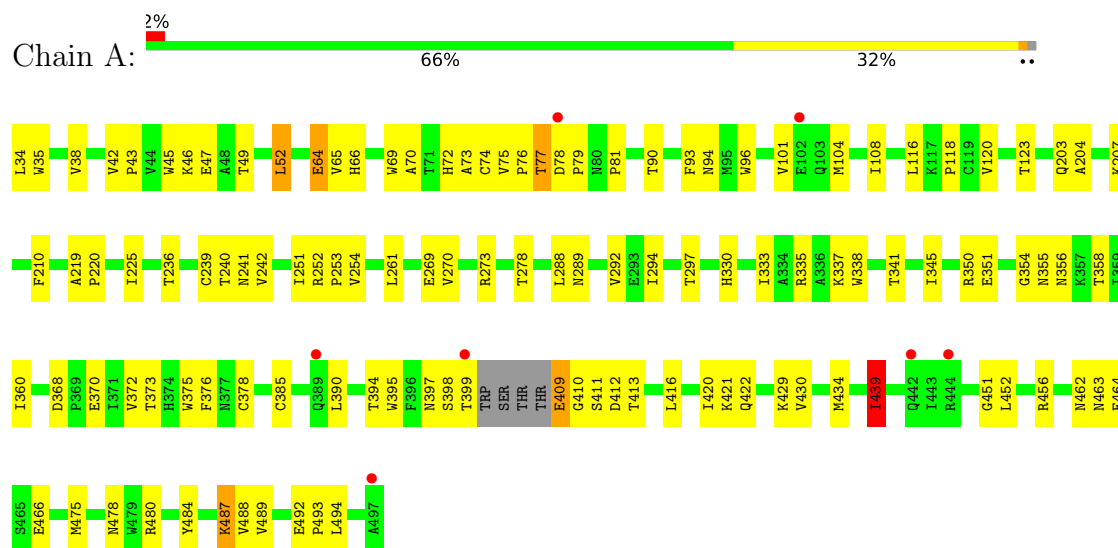


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

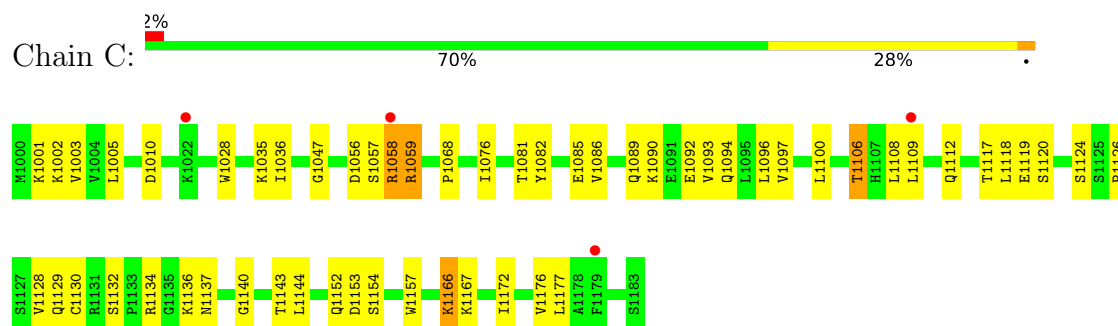
3 Residue-property plots

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.

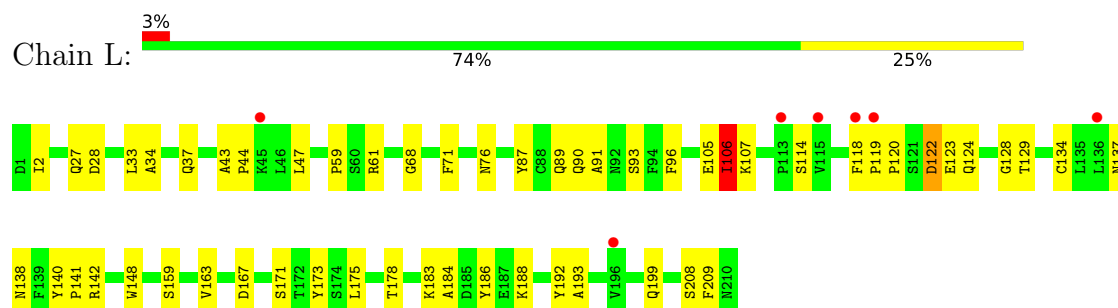
• Molecule 1: HIV-1 GP120 ENVELOPE GLYCOPROTEIN



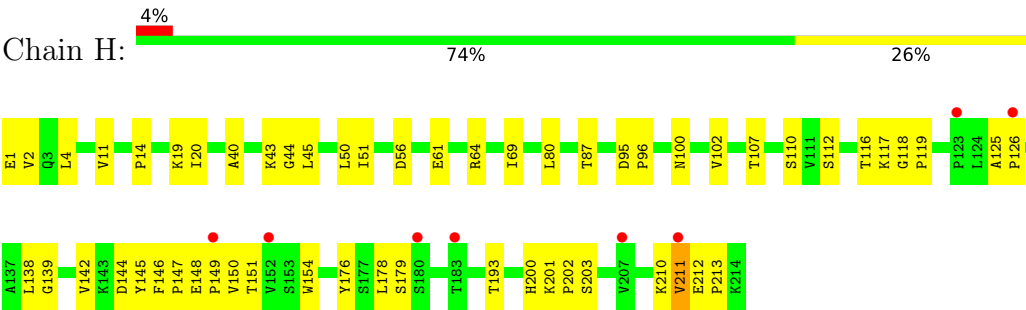
• Molecule 2: T-cell surface glycoprotein CD4



• Molecule 3: FAB 48D LIGHT CHAIN



● Molecule 4: FAB 48D Heavy CHAIN



● Molecule 5: beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	190.00Å 190.00Å 103.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.09 – 3.51 41.09 – 3.51	Depositor EDS
% Data completeness (in resolution range)	83.8 (41.09-3.51) 83.7 (41.09-3.51)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.257 , 0.273 0.252 , 0.269	Depositor DCC
R_{free} test set	2000 reflections (9.11%)	wwPDB-VP
Wilson B-factor (Å ²)	84.4	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 87.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7597	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: FUL, 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	0.30	0/2811	0.73	0/3827
2	C	0.36	1/1452 (0.1%)	0.77	3/1955 (0.2%)
3	L	0.30	0/1635	1.04	5/2221 (0.2%)
4	H	0.30	0/1695	0.72	2/2311 (0.1%)
All	All	0.31	1/7593 (0.0%)	0.81	10/10314 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1097	VAL	C-N	8.07	1.44	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	106	ILE	CA-C-N	-21.60	89.47	122.74
3	L	106	ILE	C-N-CA	-21.60	89.47	122.74
3	L	106	ILE	O-C-N	18.40	145.57	122.57
2	C	1120	SER	CA-C-N	6.91	124.70	119.66
2	C	1120	SER	C-N-CA	6.91	124.70	119.66
3	L	43	ALA	CA-C-N	5.30	125.24	119.78
3	L	43	ALA	C-N-CA	5.30	125.24	119.78
4	H	125	ALA	CA-C-N	5.11	125.03	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	125	ALA	C-N-CA	5.11	125.03	119.76
2	C	1097	VAL	O-C-N	-5.04	116.28	122.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	106	ILE	Mainchain

5.2 Too-close contacts ⓘ

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	2747	0	2664	98	0
2	C	1432	0	1460	39	0
3	L	1600	0	1552	33	0
4	H	1654	0	1613	40	0
5	B	24	0	22	0	0
6	A	140	0	130	3	0
All	All	7597	0	7441	206	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (206) 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:398:SER:HA	1:A:399:THR:C	1.48	1.27
3:L:106:ILE:CG2	3:L:107:LYS:H	1.50	1.16
3:L:106:ILE:HG22	3:L:107:LYS:H	0.99	1.13
3:L:106:ILE:HG22	3:L:107:LYS:N	1.66	1.04
1:A:398:SER:CA	1:A:399:THR:C	2.33	0.99
4:H:126:PRO:HD3	4:H:138:LEU:HD13	1.54	0.90
1:A:492:GLU:HB3	1:A:493:PRO:HD2	1.54	0.88
1:A:335:ARG:NE	1:A:411:SER:HB3	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:O	1:A:35:TRP:HB2	1.75	0.86
1:A:335:ARG:CZ	1:A:411:SER:HB3	2.07	0.84
2:C:1085:GLU:HG2	2:C:1090:LYS:HG3	1.57	0.84
3:L:106:ILE:CG2	3:L:107:LYS:N	2.22	0.83
2:C:1058:ARG:HH12	2:C:1059:ARG:HH11	1.24	0.82
1:A:204:ALA:HB2	3:L:28:ASP:HB3	1.62	0.82
1:A:45:TRP:CD1	1:A:489:VAL:HG21	2.16	0.80
2:C:1058:ARG:NH1	2:C:1059:ARG:HH11	1.79	0.79
2:C:1166:LYS:HD3	2:C:1167:LYS:H	1.49	0.77
1:A:351:GLU:HA	1:A:355:ASN:OD1	1.88	0.74
1:A:398:SER:HA	1:A:399:THR:O	1.88	0.72
4:H:116:THR:HG22	4:H:203:SER:HB3	1.72	0.72
3:L:89:GLN:NE2	3:L:96:PHE:HB3	2.05	0.71
2:C:1106:THR:HB	2:C:1112:GLN:HG3	1.73	0.71
1:A:335:ARG:NH2	1:A:411:SER:HB3	2.05	0.71
4:H:20:ILE:HG21	4:H:107:THR:HG21	1.75	0.69
3:L:89:GLN:HE21	3:L:96:PHE:HB3	1.60	0.67
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.77	0.67
1:A:492:GLU:HB3	1:A:493:PRO:CD	2.25	0.66
1:A:412:ASP:O	1:A:413:THR:CG2	2.43	0.66
4:H:200:HIS:CE1	4:H:202:PRO:HB2	2.30	0.66
1:A:207:LYS:HB3	1:A:439:ILE:HD11	1.76	0.66
4:H:116:THR:HA	4:H:146:PHE:O	1.94	0.66
1:A:398:SER:CA	1:A:399:THR:O	2.43	0.66
1:A:77:THR:HG22	1:A:78:ASP:H	1.61	0.65
2:C:1058:ARG:HH12	2:C:1059:ARG:NH1	1.94	0.65
1:A:64:GLU:OE2	1:A:66:HIS:HB2	1.96	0.65
2:C:1100:LEU:HD21	2:C:1172:ILE:HD11	1.79	0.65
1:A:420:ILE:HD12	1:A:420:ILE:H	1.64	0.63
1:A:360:ILE:HG12	1:A:394:THR:HG23	1.81	0.62
1:A:43:PRO:HA	1:A:494:LEU:HD23	1.82	0.62
1:A:412:ASP:C	1:A:413:THR:HG23	2.24	0.62
3:L:193:ALA:HB2	3:L:208:SER:HB3	1.82	0.62
1:A:78:ASP:HB2	1:A:79:PRO:HA	1.82	0.61
2:C:1134:ARG:HD3	2:C:1152:GLN:HB3	1.82	0.61
4:H:61:GLU:HA	4:H:64:ARG:NH1	2.15	0.61
4:H:138:LEU:HD11	4:H:211:VAL:HG11	1.82	0.61
2:C:1132:SER:HB3	2:C:1136:LYS:HB3	1.83	0.60
2:C:1086:VAL:O	2:C:1089:GLN:HG2	2.01	0.60
4:H:87:THR:HG23	4:H:110:SER:HA	1.82	0.60
4:H:119:PRO:HB3	4:H:142:VAL:CG1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TRP:HD1	1:A:489:VAL:HG21	1.66	0.59
1:A:207:LYS:CB	1:A:439:ILE:HD11	2.32	0.59
1:A:430:VAL:HG11	2:C:1059:ARG:HB2	1.83	0.58
2:C:1057:SER:HB2	2:C:1068:PRO:O	2.03	0.58
2:C:1140:GLY:HA3	2:C:1144:LEU:HG	1.85	0.58
1:A:335:ARG:HE	1:A:411:SER:HB3	1.63	0.58
1:A:451:GLY:C	1:A:452:LEU:HD12	2.29	0.58
1:A:108:ILE:HD12	1:A:253:PRO:HB3	1.83	0.58
2:C:1134:ARG:HH21	2:C:1136:LYS:HE2	1.69	0.57
1:A:269:GLU:HA	1:A:289:ASN:HD22	1.69	0.57
1:A:335:ARG:NH2	1:A:411:SER:CB	2.68	0.57
2:C:1003:VAL:HG22	2:C:1094:GLN:HB3	1.86	0.56
1:A:207:LYS:HG3	1:A:439:ILE:CG1	2.36	0.56
1:A:78:ASP:HB2	1:A:79:PRO:CA	2.37	0.55
1:A:207:LYS:CG	1:A:439:ILE:HD11	2.36	0.55
3:L:128:GLY:HA2	3:L:183:LYS:HD2	1.88	0.55
4:H:1:GLU:HG3	4:H:2:VAL:H	1.70	0.55
1:A:335:ARG:HH21	1:A:411:SER:CB	2.20	0.55
1:A:104:MET:HE1	1:A:251:ILE:CG2	2.37	0.54
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.42	0.54
2:C:1089:GLN:C	2:C:1090:LYS:HD2	2.32	0.54
1:A:412:ASP:O	1:A:413:THR:HG22	2.07	0.54
1:A:398:SER:HB2	1:A:399:THR:O	2.09	0.53
1:A:412:ASP:C	1:A:413:THR:CG2	2.81	0.53
1:A:412:ASP:O	1:A:413:THR:HG23	2.08	0.53
4:H:138:LEU:HD11	4:H:211:VAL:CG1	2.39	0.53
1:A:207:LYS:HG3	1:A:439:ILE:HG12	1.91	0.52
2:C:1130:CYS:SG	2:C:1144:LEU:HD22	2.50	0.52
2:C:1118:LEU:HD22	2:C:1128:VAL:HG22	1.90	0.52
2:C:1154:SER:HB2	2:C:1176:VAL:HG12	1.90	0.52
1:A:398:SER:CB	1:A:399:THR:O	2.58	0.52
4:H:4:LEU:HD11	4:H:102:VAL:HG23	1.91	0.52
3:L:192:TYR:HB2	3:L:209:PHE:CE2	2.44	0.52
3:L:59:PRO:HB3	3:L:61:ARG:NH1	2.25	0.51
1:A:207:LYS:HG3	1:A:439:ILE:HD11	1.93	0.51
2:C:1076:ILE:HG13	2:C:1119:GLU:CD	2.35	0.51
4:H:193:THR:HG23	4:H:210:LYS:HE3	1.93	0.51
3:L:91:ALA:HB1	4:H:100:ASN:O	2.11	0.50
4:H:117:LYS:HD3	4:H:118:GLY:N	2.26	0.50
4:H:148:GLU:HB3	4:H:149:PRO:HA	1.94	0.50
1:A:420:ILE:HD12	1:A:420:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:HE2	1:A:492:GLU:OE2	2.11	0.50
1:A:90:THR:OG1	1:A:240:THR:HG22	2.12	0.50
1:A:341:THR:O	1:A:345:ILE:HG13	2.12	0.50
3:L:167:ASP:O	3:L:171:SER:HA	2.12	0.49
1:A:294:ILE:HD12	1:A:333:ILE:HD11	1.95	0.49
1:A:350:ARG:HG2	1:A:355:ASN:HA	1.94	0.49
4:H:200:HIS:HE1	4:H:202:PRO:HB2	1.78	0.49
2:C:1153:ASP:HB3	2:C:1157:TRP:HZ2	1.77	0.49
3:L:184:ALA:O	3:L:188:LYS:HD3	2.12	0.49
3:L:90:GLN:O	3:L:96:PHE:HA	2.12	0.49
4:H:145:TYR:HD1	4:H:200:HIS:HE2	1.61	0.48
1:A:104:MET:HE1	1:A:251:ILE:HG22	1.93	0.48
6:A:730:NAG:HN2	6:A:730:NAG:H5	1.77	0.48
2:C:1132:SER:CB	2:C:1136:LYS:HB3	2.43	0.48
1:A:47:GLU:HG2	1:A:487:LYS:HE3	1.94	0.48
4:H:119:PRO:CB	4:H:142:VAL:HG13	2.43	0.48
1:A:70:ALA:O	1:A:74:CYS:HB2	2.13	0.48
1:A:75:VAL:HG13	1:A:76:PRO:HD2	1.96	0.47
1:A:338:TRP:CE2	1:A:390:LEU:HD22	2.49	0.47
3:L:33:LEU:HG	3:L:34:ALA:N	2.29	0.47
4:H:50:LEU:HD12	4:H:50:LEU:C	2.40	0.47
2:C:1082:TYR:O	2:C:1093:VAL:HG12	2.15	0.47
1:A:42:VAL:HG13	1:A:43:PRO:HD2	1.97	0.47
1:A:219:ALA:HB2	1:A:225:ILE:HG13	1.97	0.47
1:A:94:ASN:HA	1:A:236:THR:HG22	1.97	0.46
1:A:373:THR:HB	1:A:385:CYS:O	2.15	0.46
1:A:270:VAL:HG22	1:A:288:LEU:HA	1.98	0.46
3:L:140:TYR:CG	3:L:141:PRO:HA	2.51	0.46
1:A:72:HIS:O	1:A:72:HIS:CG	2.69	0.46
2:C:1166:LYS:CD	2:C:1167:LYS:H	2.24	0.46
4:H:51:ILE:HA	4:H:56:ASP:O	2.15	0.46
4:H:148:GLU:OE1	4:H:149:PRO:HA	2.16	0.46
1:A:108:ILE:CD1	1:A:253:PRO:HB3	2.46	0.46
1:A:52:LEU:HD12	1:A:52:LEU:N	2.31	0.46
1:A:77:THR:HG22	1:A:78:ASP:N	2.27	0.45
4:H:14:PRO:HD3	4:H:112:SER:O	2.15	0.45
2:C:1058:ARG:HD3	2:C:1058:ARG:HA	1.49	0.45
4:H:11:VAL:HG22	4:H:147:PRO:HG2	1.98	0.45
4:H:69:ILE:HG12	4:H:80:LEU:HD13	1.98	0.45
1:A:420:ILE:HG22	1:A:421:LYS:N	2.32	0.44
2:C:1124:SER:O	2:C:1126:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1154:SER:HB2	2:C:1176:VAL:CG1	2.47	0.44
1:A:96:TRP:HD1	1:A:236:THR:HG21	1.82	0.44
1:A:219:ALA:HA	1:A:220:PRO:HD3	1.79	0.44
3:L:124:GLN:HG2	3:L:129:THR:O	2.18	0.44
1:A:335:ARG:HE	1:A:411:SER:CB	2.30	0.44
1:A:292:VAL:HG13	1:A:337:LYS:HE3	1.99	0.44
1:A:422:GLN:O	1:A:434:MET:HA	2.17	0.44
3:L:159:SER:HA	3:L:178:THR:O	2.16	0.44
1:A:358:THR:HG23	1:A:395:TRP:O	2.18	0.44
2:C:1129:GLN:NE2	2:C:1137:ASN:HB3	2.32	0.44
1:A:118:PRO:HD2	1:A:203:GLN:NE2	2.32	0.44
3:L:122:ASP:OD2	3:L:123:GLU:HG3	2.18	0.43
3:L:128:GLY:CA	3:L:183:LYS:HD2	2.47	0.43
4:H:145:TYR:CZ	4:H:176:TYR:HB2	2.53	0.43
1:A:207:LYS:HG3	1:A:439:ILE:CD1	2.48	0.43
1:A:101:VAL:HG21	1:A:480:ARG:HG2	2.00	0.43
2:C:1117:THR:HG23	2:C:1143:THR:HG22	2.00	0.43
1:A:294:ILE:O	1:A:294:ILE:HG23	2.19	0.43
2:C:1005:LEU:CD2	2:C:1096:LEU:HB2	2.48	0.43
3:L:163:VAL:HG22	3:L:175:LEU:HD12	2.00	0.43
4:H:119:PRO:HB3	4:H:142:VAL:HG12	2.01	0.43
4:H:119:PRO:HB3	4:H:142:VAL:HG13	2.01	0.43
1:A:65:VAL:HG21	1:A:210:PHE:CD1	2.53	0.43
4:H:95:ASP:N	4:H:96:PRO:HD3	2.33	0.42
3:L:87:TYR:OH	4:H:44:GLY:HA2	2.19	0.42
1:A:34:LEU:N	1:A:34:LEU:HD22	2.34	0.42
2:C:1118:LEU:HD22	2:C:1128:VAL:CG2	2.48	0.42
1:A:456:ARG:HD2	1:A:466:GLU:OE1	2.20	0.42
1:A:475:MET:HA	1:A:478:ASN:OD1	2.19	0.42
2:C:1035:LYS:O	2:C:1047:GLY:HA3	2.20	0.42
1:A:78:ASP:CG	1:A:81:PRO:HG3	2.44	0.42
6:A:730:NAG:H62	6:A:734:NAG:O7	2.20	0.42
1:A:123:THR:HG21	1:A:429:LYS:HE3	2.02	0.42
1:A:394:THR:HG22	1:A:397:ASN:HB2	2.01	0.42
2:C:1134:ARG:NH1	2:C:1152:GLN:HB2	2.35	0.42
1:A:368:ASP:O	1:A:372:VAL:HG23	2.19	0.42
1:A:330:HIS:HA	1:A:416:LEU:O	2.20	0.42
1:A:252:ARG:HA	1:A:253:PRO:HD3	1.76	0.42
3:L:120:PRO:HG2	3:L:186:TYR:CZ	2.55	0.42
1:A:69:TRP:O	1:A:73:ALA:HB3	2.20	0.41
1:A:350:ARG:NH2	1:A:356:ASN:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLU:HA	1:A:375:TRP:HB2	2.01	0.41
3:L:118:PHE:HA	3:L:119:PRO:HD3	1.87	0.41
4:H:146:PHE:HA	4:H:147:PRO:HA	1.77	0.41
4:H:212:GLU:HA	4:H:213:PRO:HD3	1.75	0.41
1:A:480:ARG:O	1:A:484:TYR:HB3	2.20	0.41
2:C:1001:LYS:HG2	2:C:1002:LYS:N	2.35	0.41
3:L:44:PRO:CG	4:H:45:LEU:HD11	2.49	0.41
1:A:254:VAL:HG11	1:A:261:LEU:HB2	2.02	0.41
2:C:1108:LEU:O	2:C:1109:LEU:HB2	2.20	0.41
3:L:114:SER:HB2	3:L:137:ASN:HB3	2.03	0.41
1:A:273:ARG:NH2	1:A:484:TYR:CE2	2.89	0.41
1:A:463:ASN:O	1:A:464:GLU:HB2	2.20	0.41
3:L:28:ASP:OD1	3:L:68:GLY:HA2	2.20	0.41
3:L:134:CYS:HB2	3:L:148:TRP:CZ2	2.55	0.41
2:C:1028:TRP:O	2:C:1036:ILE:HB	2.21	0.41
4:H:178:LEU:HD12	4:H:179:SER:N	2.36	0.41
4:H:201:LYS:N	4:H:202:PRO:CD	2.83	0.41
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.89	0.41
1:A:278:THR:HG22	6:A:776:NAG:H62	2.03	0.41
1:A:376:PHE:HE2	1:A:378:CYS:HB2	1.84	0.41
2:C:1081:THR:CG2	2:C:1092:GLU:HG2	2.51	0.41
4:H:19:LYS:HA	4:H:80:LEU:O	2.21	0.41
4:H:116:THR:CG2	4:H:203:SER:HB3	2.46	0.41
1:A:96:TRP:CD1	1:A:236:THR:HG21	2.56	0.41
2:C:1144:LEU:HD12	2:C:1144:LEU:N	2.36	0.41
1:A:207:LYS:HD3	1:A:207:LYS:HA	1.93	0.40
1:A:368:ASP:OD2	2:C:1059:ARG:NH2	2.40	0.40
4:H:118:GLY:HA2	4:H:119:PRO:HD3	1.91	0.40
4:H:139:GLY:HA2	4:H:154:TRP:CH2	2.55	0.40
1:A:409:GLU:HA	1:A:410:GLY:HA3	1.62	0.40
3:L:2:ILE:HD12	3:L:27:GLN:HB2	2.03	0.40
1:A:93:PHE:HE2	1:A:239:CYS:HB3	1.85	0.40
3:L:142:ARG:HB2	3:L:173:TYR:CE1	2.57	0.40
4:H:40:ALA:HB3	4:H:43:LYS:HB2	2.04	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	349/357 (98%)	300 (86%)	44 (13%)	5 (1%)	9	38
2	C	182/184 (99%)	168 (92%)	13 (7%)	1 (0%)	24	58
3	L	207/209 (99%)	190 (92%)	14 (7%)	3 (1%)	9	38
4	H	218/220 (99%)	193 (88%)	22 (10%)	3 (1%)	9	38
All	All	956/970 (99%)	851 (89%)	93 (10%)	12 (1%)	9	40

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	76	ASN
3	L	138	ASN
4	H	130	SER
4	H	144	ASP
1	A	241	ASN
1	A	354	GLY
2	C	1056	ASP
3	L	93	SER
4	H	131	THR
1	A	439	ILE
1	A	462	ASN
1	A	487	LYS

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	309/313 (99%)	298 (96%)	11 (4%)	31	57
2	C	166/166 (100%)	160 (96%)	6 (4%)	31	57
3	L	182/182 (100%)	179 (98%)	3 (2%)	55	70
4	H	185/185 (100%)	182 (98%)	3 (2%)	55	70
All	All	842/846 (100%)	819 (97%)	23 (3%)	39	62

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	49	THR
1	A	52	LEU
1	A	64	GLU
1	A	77	THR
1	A	120	VAL
1	A	242	VAL
1	A	297	THR
1	A	409	GLU
1	A	439	ILE
1	A	488	VAL
2	C	1010	ASP
2	C	1058	ARG
2	C	1059	ARG
2	C	1106	THR
2	C	1166	LYS
2	C	1177	LEU
3	L	105	GLU
3	L	122	ASP
3	L	199	GLN
4	H	150	VAL
4	H	151	THR
4	H	211	VAL

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

Mol	Chain	Res	Type
1	A	332	ASN
1	A	344	GLN
1	A	422	GLN
2	C	1107	HIS
3	L	90	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 ⓘ

2 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	$\# Z > 2$
5	NAG	B	1	5,1	14,14,15	0.54	0	17,19,21	1.44	2 (11%)
5	FUL	B	2	5	10,10,11	0.65	0	14,14,16	0.51	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
5	NAG	B	1	5,1	1/1/5/7	2/6/23/26	0/1/1/1
5	FUL	B	2	5	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	NAG	O5-C1-C2	4.10	117.64	111.29
5	B	1	NAG	O5-C5-C6	2.62	112.77	107.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1	NAG	C1

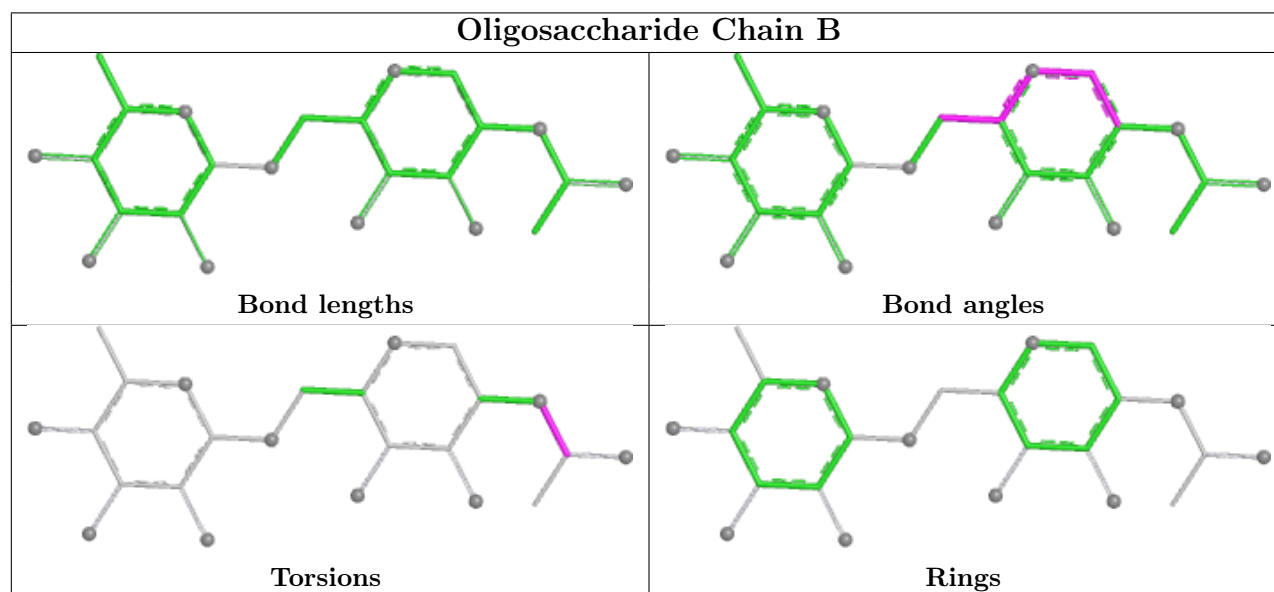
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1	NAG	C8-C7-N2-C2
5	B	1	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

10 ligands 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	$\# Z > 2$
6	NAG	A	948	1	14,14,15	0.52	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	762	1	14,14,15	0.49	0	17,19,21	0.88	0
6	NAG	A	588	1	14,14,15	0.53	0	17,19,21	1.35	2 (11%)
6	NAG	A	730	1	14,14,15	0.47	0	17,19,21	0.82	1 (5%)
6	NAG	A	886	1	14,14,15	0.50	0	17,19,21	0.75	0
6	NAG	A	897	1	14,14,15	0.52	0	17,19,21	0.87	0
6	NAG	A	741	1	14,14,15	0.52	0	17,19,21	0.81	1 (5%)
6	NAG	A	734	1	14,14,15	0.50	0	17,19,21	0.76	0
6	NAG	A	892	1	14,14,15	0.53	0	17,19,21	1.08	2 (11%)
6	NAG	A	776	1	14,14,15	0.49	0	17,19,21	0.70	1 (5%)

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	NAG	A	948	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	A	762	1	-	2/6/23/26	0/1/1/1
6	NAG	A	588	1	-	2/6/23/26	0/1/1/1
6	NAG	A	730	1	-	3/6/23/26	0/1/1/1
6	NAG	A	886	1	-	2/6/23/26	0/1/1/1
6	NAG	A	897	1	-	3/6/23/26	0/1/1/1
6	NAG	A	741	1	-	2/6/23/26	0/1/1/1
6	NAG	A	734	1	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	A	892	1	-	0/6/23/26	0/1/1/1
6	NAG	A	776	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	588	NAG	C1-O5-C5	4.31	117.96	112.19
6	A	892	NAG	C1-O5-C5	2.74	115.86	112.19
6	A	948	NAG	C1-O5-C5	2.64	115.73	112.19
6	A	588	NAG	O5-C1-C2	2.46	115.10	111.29
6	A	892	NAG	O5-C1-C2	2.23	114.74	111.29
6	A	730	NAG	C1-O5-C5	2.11	115.01	112.19
6	A	776	NAG	C1-O5-C5	2.04	114.92	112.19
6	A	741	NAG	C1-O5-C5	2.04	114.92	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	734	NAG	C1
6	A	948	NAG	C1

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	588	NAG	C8-C7-N2-C2
6	A	588	NAG	O7-C7-N2-C2
6	A	734	NAG	C1-C2-N2-C7
6	A	734	NAG	C8-C7-N2-C2
6	A	734	NAG	O7-C7-N2-C2
6	A	741	NAG	C8-C7-N2-C2
6	A	741	NAG	O7-C7-N2-C2
6	A	886	NAG	C8-C7-N2-C2
6	A	886	NAG	O7-C7-N2-C2
6	A	897	NAG	C3-C2-N2-C7
6	A	897	NAG	C8-C7-N2-C2
6	A	897	NAG	O7-C7-N2-C2
6	A	762	NAG	O5-C5-C6-O6
6	A	776	NAG	C8-C7-N2-C2
6	A	730	NAG	C8-C7-N2-C2
6	A	730	NAG	O7-C7-N2-C2
6	A	776	NAG	O7-C7-N2-C2
6	A	730	NAG	O5-C5-C6-O6
6	A	762	NAG	C4-C5-C6-O6
6	A	948	NAG	C8-C7-N2-C2
6	A	948	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	730	NAG	2	0
6	A	734	NAG	1	0
6	A	776	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	353/357 (98%)	0.35	7 (1%) 65 37	68, 98, 161, 262	0
2	C	184/184 (100%)	0.24	4 (2%) 62 35	86, 121, 182, 234	0
3	L	209/209 (100%)	0.38	7 (3%) 49 27	105, 173, 260, 460	0
4	H	220/220 (100%)	0.51	9 (4%) 41 22	95, 164, 306, 365	0
All	All	966/970 (99%)	0.37	27 (2%) 55 31	68, 124, 257, 460	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	183	THR	4.6
3	L	115	VAL	4.0
2	C	1179	PHE	3.4
4	H	152	VAL	3.3
3	L	118	PHE	3.1
4	H	123	PRO	3.1
4	H	126	PRO	2.9
4	H	136	ALA	2.8
3	L	113	PRO	2.8
4	H	211	VAL	2.8
3	L	119	PRO	2.7
3	L	136	LEU	2.7
3	L	196	VAL	2.6
4	H	149	PRO	2.5
2	C	1109	LEU	2.3
1	A	399	THR	2.3
1	A	497	ALA	2.3
1	A	78	ASP	2.2
1	A	444	ARG	2.2
2	C	1058	ARG	2.2
4	H	180	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	442	GLN	2.1
4	H	207	VAL	2.0
2	C	1022	LYS	2.0
3	L	45	LYS	2.0
1	A	102	GLU	2.0
1	A	389	GLN	2.0

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

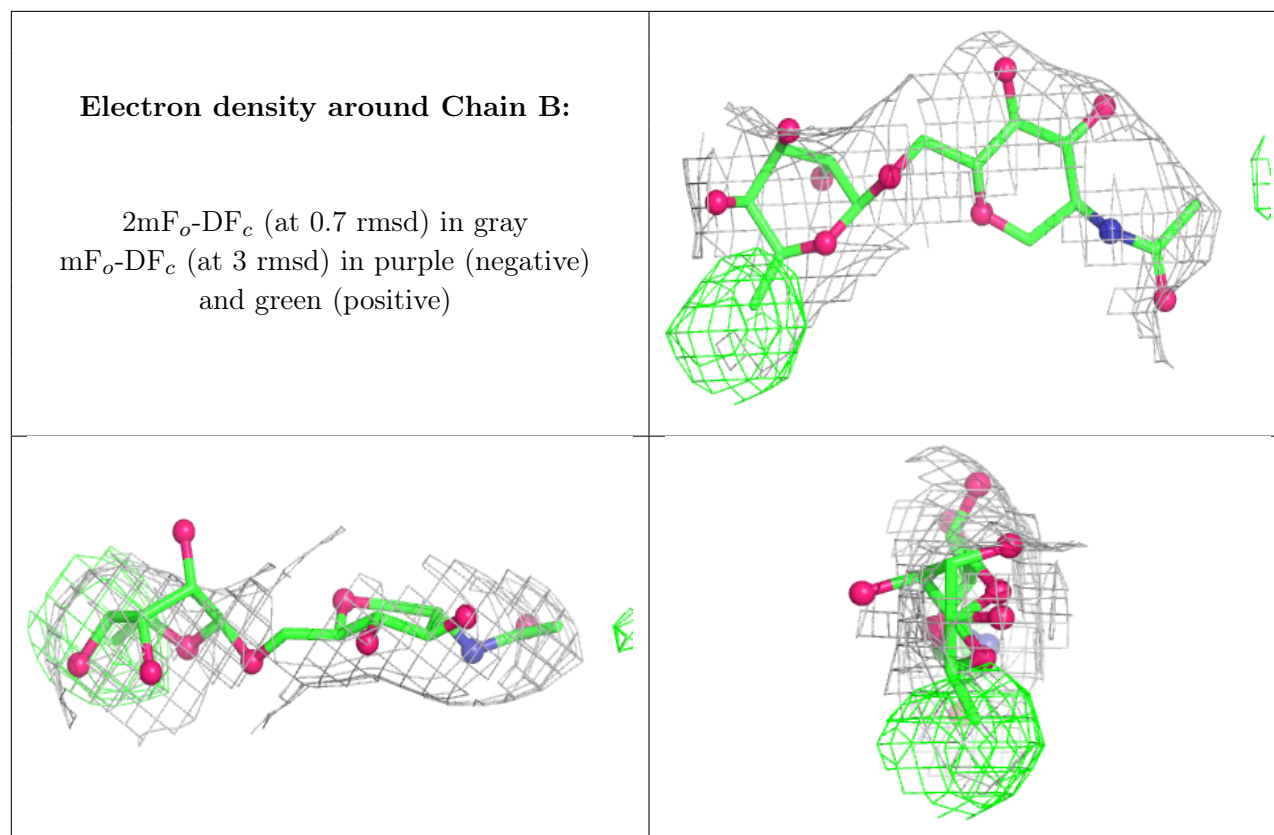
There are no non-standard protein/DNA/RNA residues in this entry.

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
5	NAG	B	1	14/15	-	-	84,111,141,166	0
5	FUL	B	2	10/11	-	-	197,211,231,236	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.



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
6	NAG	A	730	14/15	0.47	0.18	232,249,275,286	0
6	NAG	A	741	14/15	0.55	0.18	215,224,236,239	0
6	NAG	A	897	14/15	0.61	0.14	139,208,226,240	0
6	NAG	A	588	14/15	0.67	0.13	95,145,161,167	0
6	NAG	A	948	14/15	0.72	0.17	134,155,186,195	0
6	NAG	A	892	14/15	0.73	0.15	102,144,192,206	0
6	NAG	A	734	14/15	0.79	0.15	145,167,194,207	0
6	NAG	A	776	14/15	0.81	0.12	112,131,168,180	0
6	NAG	A	762	14/15	0.90	0.11	75,80,100,100	0
6	NAG	A	886	14/15	0.92	0.11	75,115,154,164	0

6.5 Other polymers [i](#)

There are no such residues in this entry.