



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:21 PM UTC

PDB ID : 3VI3 / pdb_00003vi3
Title : Crystal structure of alpha5beta1 integrin headpiece (ligand-free form)
Authors : Nagae, M.; Nogi, T.; Takagi, J.
Deposited on : 2011-09-21
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

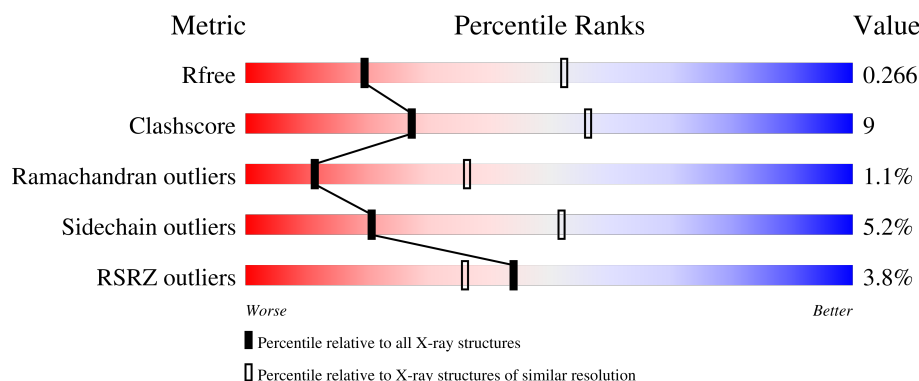
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



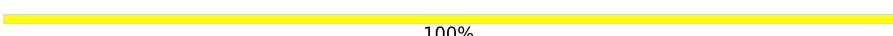
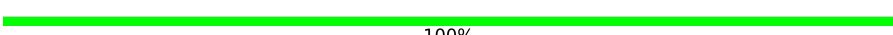
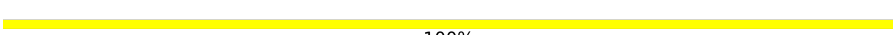
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	632	4% 72% 21% • 5%
1	C	632	5% 69% 22% • 7%
2	B	454	6% 71% 21% • 6%
2	D	454	3% 74% 20% • 5%
3	E	219	0% 75% 23% •

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Mol	Chain	Length	Quality of chain
3	L	219	
4	F	218	
4	H	218	
5	G	6	
5	K	6	
6	I	2	
6	J	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22803 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 Integrin alpha-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4567	2892	768	893	14			
1	C	589	Total	C	N	O	S	0	0	0
			4470	2832	748	876	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	624	GLY	-	expression tag	UNP P08648
A	625	GLY	-	expression tag	UNP P08648
A	626	LEU	-	expression tag	UNP P08648
A	627	GLU	-	expression tag	UNP P08648
A	628	ASN	-	expression tag	UNP P08648
A	629	LEU	-	expression tag	UNP P08648
A	630	TYR	-	expression tag	UNP P08648
A	631	PHE	-	expression tag	UNP P08648
A	632	GLN	-	expression tag	UNP P08648
C	624	GLY	-	expression tag	UNP P08648
C	625	GLY	-	expression tag	UNP P08648
C	626	LEU	-	expression tag	UNP P08648
C	627	GLU	-	expression tag	UNP P08648
C	628	ASN	-	expression tag	UNP P08648
C	629	LEU	-	expression tag	UNP P08648
C	630	TYR	-	expression tag	UNP P08648
C	631	PHE	-	expression tag	UNP P08648
C	632	GLN	-	expression tag	UNP P08648

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3327	2082	567	654	24			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	432	Total	C	N	O	S	0	0	0
			3367	2106	574	663	24			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	HIS	THR	SEE REMARK 999	UNP P05556
B	195	THR	SER	SEE REMARK 999	UNP P05556
B	446	GLY	-	expression tag	UNP P05556
B	447	GLY	-	expression tag	UNP P05556
B	448	LEU	-	expression tag	UNP P05556
B	449	GLU	-	expression tag	UNP P05556
B	450	ASN	-	expression tag	UNP P05556
B	451	LEU	-	expression tag	UNP P05556
B	452	TYR	-	expression tag	UNP P05556
B	453	PHE	-	expression tag	UNP P05556
B	454	GLN	-	expression tag	UNP P05556
D	92	HIS	THR	SEE REMARK 999	UNP P05556
D	195	THR	SER	SEE REMARK 999	UNP P05556
D	446	GLY	-	expression tag	UNP P05556
D	447	GLY	-	expression tag	UNP P05556
D	448	LEU	-	expression tag	UNP P05556
D	449	GLU	-	expression tag	UNP P05556
D	450	ASN	-	expression tag	UNP P05556
D	451	LEU	-	expression tag	UNP P05556
D	452	TYR	-	expression tag	UNP P05556
D	453	PHE	-	expression tag	UNP P05556
D	454	GLN	-	expression tag	UNP P05556

- Molecule 3 is a protein called SG/19 Fab fragment (Light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	219	Total	C	N	O	S	0	0	0
			1701	1066	292	335	8			
3	E	219	Total	C	N	O	S	0	0	0
			1701	1066	292	335	8			

- Molecule 4 is a protein called SG/19 Fab fragment (Heavy chain).

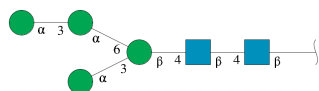
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	218	Total	C	N	O	S	0	0	0
			1651	1051	268	324	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	218	Total	C	N	O	S	0	0	0
			1651	1051	268	324	8			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	K	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

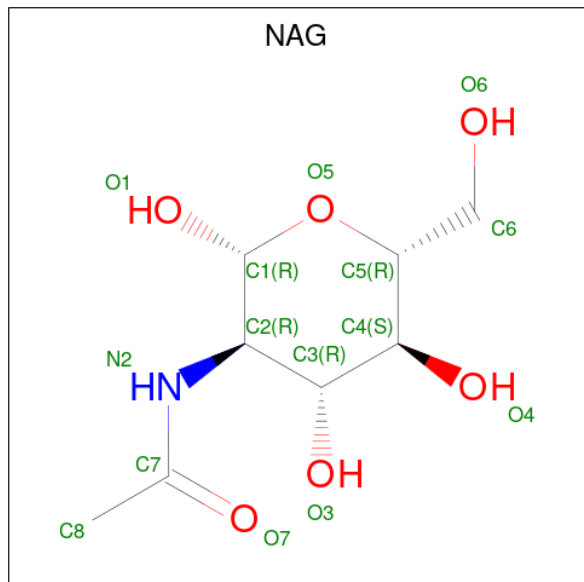


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Ca	0	0
			4	4		
7	B	2	Total	Ca	0	0
			2	2		
7	C	4	Total	Ca	0	0
			4	4		
7	D	2	Total	Ca	0	0
			2	2		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

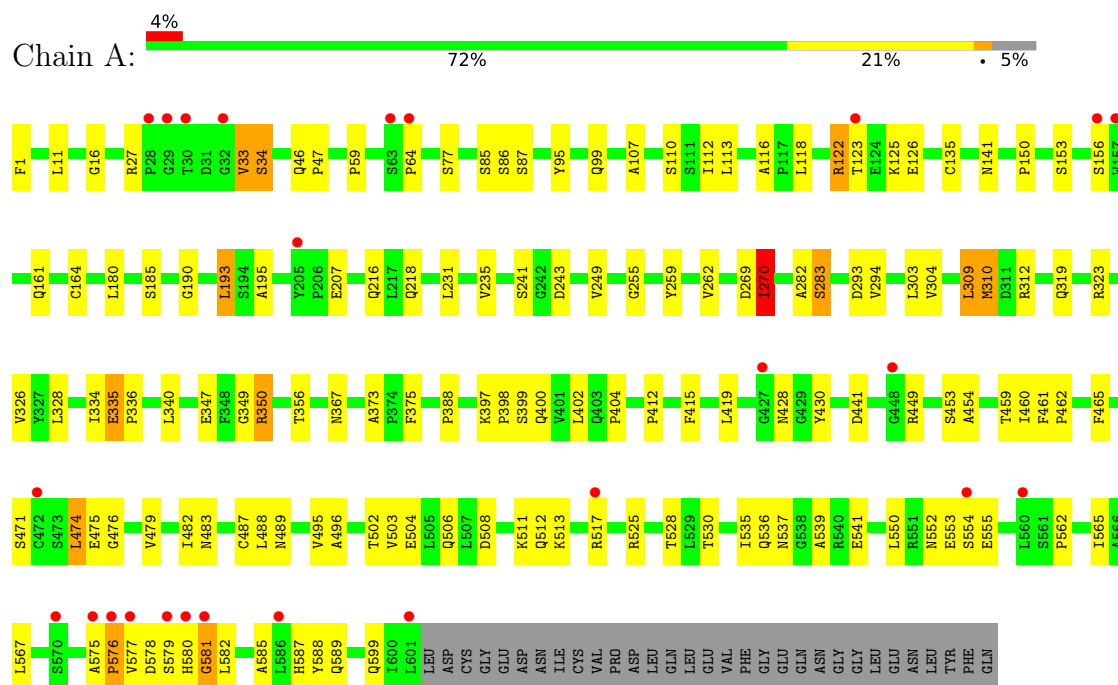
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total 1	Mg 1	0	0
9	D	1	Total 1	Mg 1	0	0

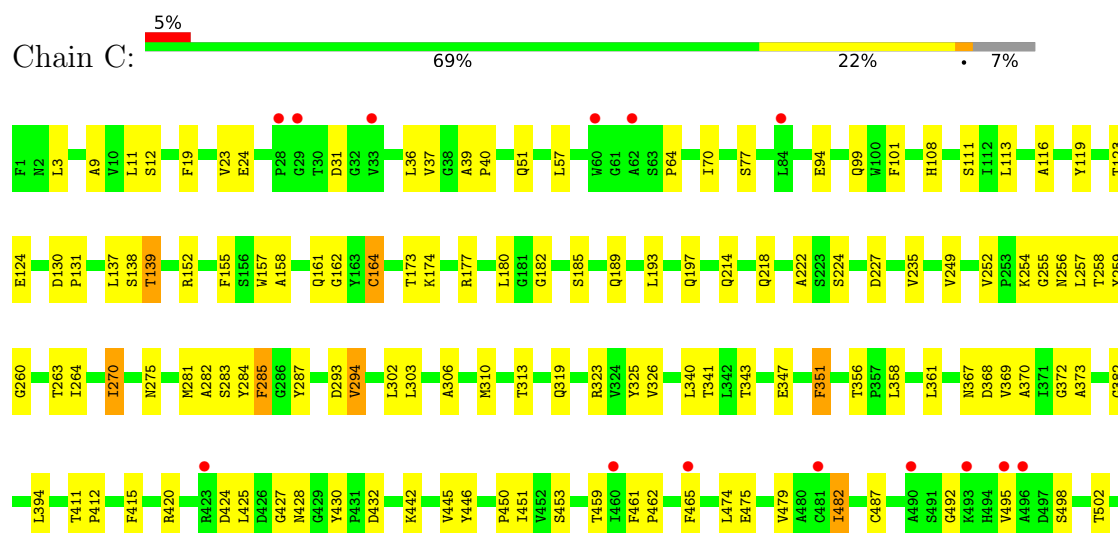
3 Residue-property plots

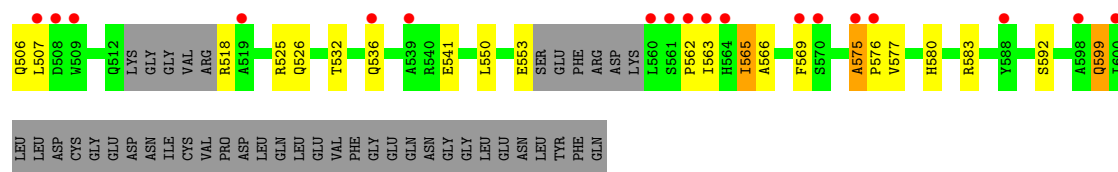
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Integrin alpha-5

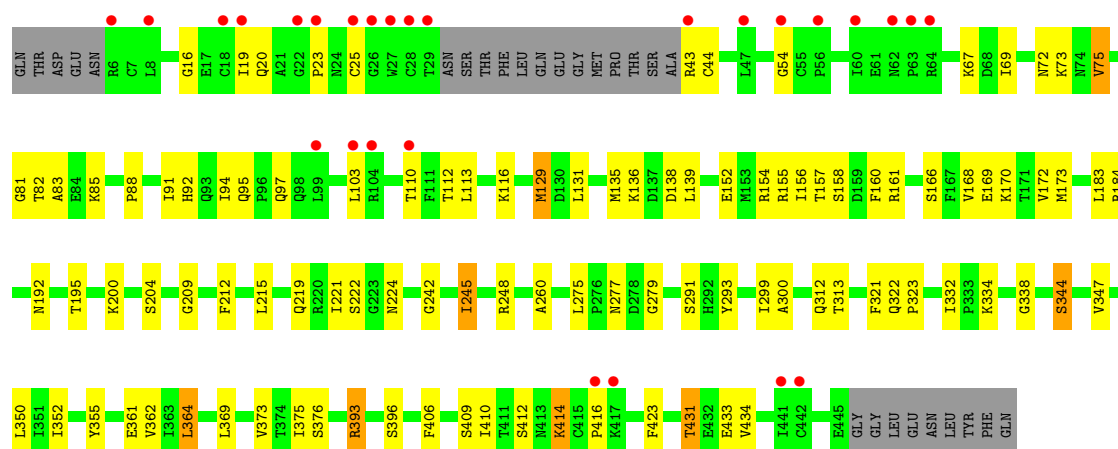


• Molecule 1: Integrin alpha-5

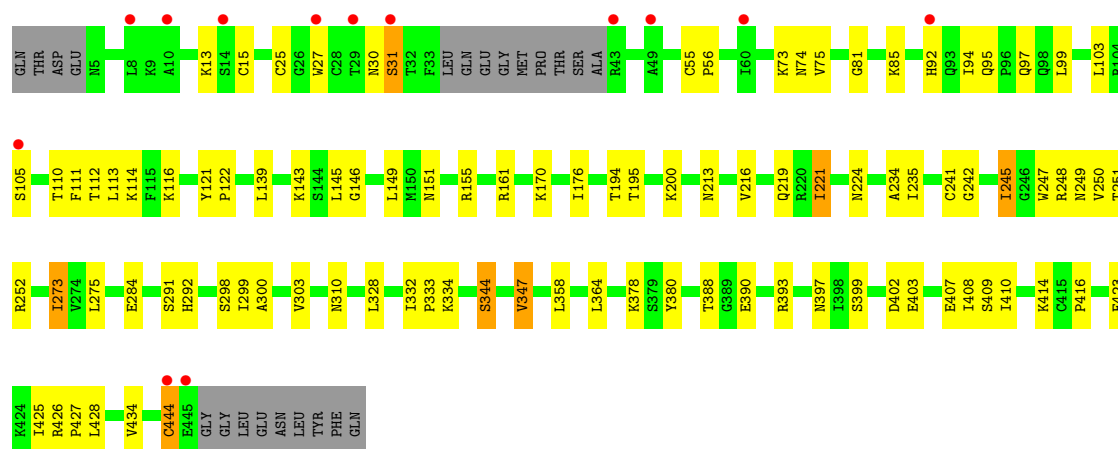
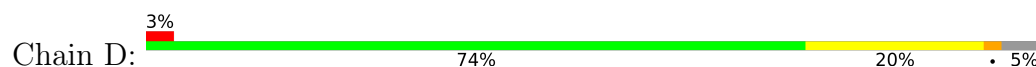




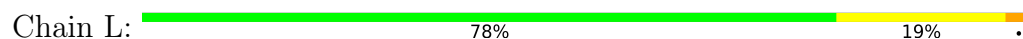
• Molecule 2: Integrin beta-1



• Molecule 2: Integrin beta-1

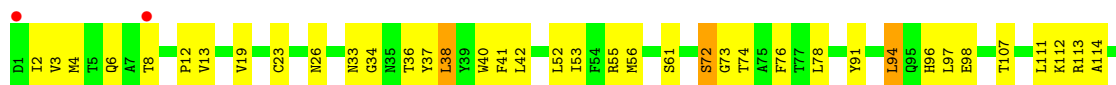
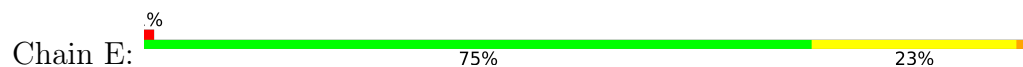


• Molecule 3: SG/19 Fab fragment (Light chain)





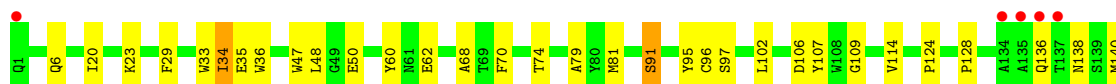
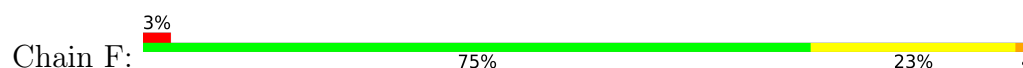
- Molecule 3: SG/19 Fab fragment (Light chain)



- Molecule 4: SG/19 Fab fragment (Heavy chain)



- Molecule 4: SG/19 Fab fragment (Heavy chain)



- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.96Å 102.81Å 125.08Å 76.10° 70.19° 71.28°	Depositor
Resolution (Å)	100.00 – 2.90 100.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (100.00-2.90) 98.9 (100.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.267 0.206 , 0.266	Depositor DCC
R_{free} test set	4551 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22803	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: NAG, BMA, CA, MAN, MG

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	0.57	0/4684	0.86	8/6374 (0.1%)
1	C	0.60	0/4584	0.90	12/6240 (0.2%)
2	B	0.55	0/3384	0.84	2/4565 (0.0%)
2	D	0.57	0/3425	0.90	0/4621
3	E	0.61	0/1741	0.87	1/2364 (0.0%)
3	L	0.64	0/1741	0.85	1/2364 (0.0%)
4	F	0.65	0/1698	0.86	1/2323 (0.0%)
4	H	0.68	0/1698	0.86	3/2323 (0.1%)
All	All	0.60	0/22955	0.87	28/31174 (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
1	C	0	1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	SER	N-CA-C	-7.09	103.08	112.72
1	A	259	TYR	N-CA-C	-7.01	99.44	109.96
1	C	139	THR	N-CA-C	6.78	121.80	112.04
2	B	332	ILE	N-CA-C	6.35	113.83	107.55
1	A	255	GLY	N-CA-C	6.30	120.12	112.49
1	C	214	GLN	N-CA-C	6.29	118.22	111.36
1	C	283	SER	N-CA-C	-6.28	100.55	109.96
1	A	283	SER	N-CA-C	-6.14	101.33	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	148	LYS	N-CA-C	6.01	118.21	109.07
1	C	259	TYR	N-CA-C	-6.01	100.94	109.96
3	E	34	GLY	N-CA-C	-5.97	107.97	115.08
1	C	257	LEU	N-CA-C	-5.95	98.12	110.80
1	A	335	GLU	CA-C-N	5.95	125.63	119.56
1	A	335	GLU	C-N-CA	5.95	125.63	119.56
1	C	182	GLY	CA-C-N	5.66	125.37	119.82
1	C	182	GLY	C-N-CA	5.66	125.37	119.82
4	H	148	LYS	N-CA-C	5.55	118.12	109.52
1	C	599	GLN	N-CA-C	5.53	116.66	108.86
4	H	204	HIS	CA-C-N	5.50	124.97	119.24
4	H	204	HIS	C-N-CA	5.50	124.97	119.24
1	A	537	ASN	N-CA-C	5.20	117.34	111.11
2	B	129	MET	N-CA-C	5.13	117.80	109.24
1	C	313	THR	CA-C-N	-5.13	114.46	119.64
1	C	313	THR	C-N-CA	-5.13	114.46	119.64
1	A	156	SER	N-CA-C	5.12	116.94	108.49
3	L	3	VAL	N-CA-C	5.09	115.19	107.75
1	C	39	ALA	CA-C-N	5.06	124.78	119.82
1	C	39	ALA	C-N-CA	5.06	124.78	119.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	155	PHE	Peptide

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	4567	0	4363	74	0
1	C	4470	0	4259	84	0
2	B	3327	0	3283	71	0
2	D	3367	0	3317	67	0
3	E	1701	0	1649	40	0
3	L	1701	0	1649	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1651	0	1610	33	0
4	H	1651	0	1610	31	0
5	G	72	0	61	0	0
5	K	72	0	61	0	0
6	I	28	0	25	0	0
6	J	28	0	25	0	0
7	A	4	0	0	0	0
7	B	2	0	0	0	0
7	C	4	0	0	0	0
7	D	2	0	0	0	0
8	A	70	0	65	3	0
8	B	14	0	13	0	0
8	C	56	0	52	0	0
8	D	14	0	13	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
All	All	22803	0	22055	406	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 9.

All (406) 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)
2:B:94:ILE:HD11	2:B:113:LEU:HD21	1.52	0.91
2:D:110:THR:HG22	2:D:409:SER:CB	2.04	0.88
2:D:73:LYS:H	2:D:97:GLN:HE22	1.22	0.86
1:A:123:THR:HG22	1:A:126:GLU:O	1.76	0.84
1:C:99:GLN:HG3	1:C:116:ALA:HB1	1.59	0.84
4:H:10:GLU:HG2	4:H:18:VAL:HG21	1.58	0.84
1:A:34:SER:HB3	1:A:59:PRO:HA	1.59	0.83
1:C:282:ALA:HB3	2:D:299:ILE:HD12	1.62	0.80
1:C:575:ALA:HB3	1:C:576:PRO:HD3	1.63	0.80
2:D:110:THR:HG22	2:D:409:SER:HB3	1.64	0.80
1:A:512:GLN:HE22	1:A:517:ARG:HB3	1.47	0.80
2:B:85:LYS:HG2	3:E:37:TYR:CZ	2.17	0.80
4:F:70:PHE:CE1	4:F:81:MET:HE3	2.19	0.78
2:B:338:GLY:HA3	2:B:350:LEU:HD11	1.66	0.78
4:H:67:LYS:HE2	4:H:84:SER:O	1.85	0.77
1:A:303:LEU:HD23	1:A:326:VAL:HG22	1.66	0.77
3:L:111:LEU:H	3:L:171:GLN:HE22	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLN:HE22	1:C:222:ALA:H	1.35	0.74
4:F:153:GLU:HG2	4:F:154:PRO:HA	1.69	0.74
1:C:164:CYS:HB2	1:C:185:SER:OG	1.88	0.74
1:C:319:GLN:HB2	1:C:347:GLU:HG3	1.69	0.74
4:H:171:PHE:O	4:H:182:LEU:HD12	1.88	0.74
1:C:461:PHE:HB3	1:C:462:PRO:HD3	1.69	0.72
4:F:70:PHE:HE1	4:F:81:MET:HE3	1.53	0.72
1:A:310:MET:HG3	2:B:300:ALA:HB2	1.72	0.72
1:A:487:CYS:HB3	1:A:541:GLU:HG2	1.72	0.71
2:B:184:ARG:HA	2:B:195:THR:HG22	1.72	0.71
2:D:73:LYS:N	2:D:97:GLN:HE22	1.89	0.70
3:L:200:GLU:HG2	3:L:211:VAL:HG22	1.73	0.70
2:B:369:LEU:HD11	2:B:375:ILE:HG13	1.73	0.70
1:C:474:LEU:HD11	1:C:525:ARG:HD3	1.73	0.70
2:D:73:LYS:H	2:D:97:GLN:NE2	1.90	0.70
2:B:113:LEU:HD11	2:B:434:VAL:HG21	1.74	0.69
4:H:217:PRO:O	4:H:218:ARG:HB2	1.91	0.69
2:B:152:GLU:HG2	2:B:352:ILE:HD11	1.75	0.69
2:B:375:ILE:HG12	2:B:410:ILE:HG12	1.75	0.68
3:L:161:GLN:O	3:L:161:GLN:HG2	1.95	0.67
1:A:282:ALA:HB3	2:B:299:ILE:HD12	1.77	0.67
4:F:171:PHE:O	4:F:182:LEU:HD13	1.95	0.67
3:L:31:HIS:HD2	3:L:33:ASN:H	1.43	0.66
1:A:587:HIS:HD2	1:A:589:GLN:H	1.43	0.66
4:H:10:GLU:CG	4:H:18:VAL:HG21	2.26	0.66
1:A:506:GLN:HG2	1:A:528:THR:HG22	1.79	0.64
3:E:6:GLN:HE21	3:E:107:THR:HG23	1.62	0.64
3:E:198:THR:HG22	3:E:213:SER:CB	2.27	0.64
1:A:293:ASP:O	1:A:367:ASN:HB2	1.98	0.64
2:D:344:SER:O	2:D:347:VAL:HG22	1.98	0.64
2:D:145:LEU:HG	2:D:146:GLY:N	2.12	0.64
1:C:427:GLY:HA3	1:C:580:HIS:CE1	2.34	0.63
2:B:344:SER:O	2:B:347:VAL:HG23	1.98	0.63
1:A:110:SER:HB2	1:A:141:ASN:H	1.64	0.62
1:A:190:GLY:HA3	1:A:231:LEU:HB3	1.82	0.62
1:A:123:THR:HG23	1:A:125:LYS:H	1.64	0.62
1:C:562:PRO:HB3	1:C:599:GLN:HB3	1.82	0.62
3:L:42:LEU:HD13	3:L:91:TYR:CZ	2.34	0.62
3:E:13:VAL:HG21	3:E:19:VAL:CG2	2.31	0.61
1:A:562:PRO:HB3	1:A:599:GLN:HG2	1.83	0.61
2:D:110:THR:HG22	2:D:409:SER:HB2	1.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ARG:O	3:E:55:ARG:NH2	2.34	0.61
4:F:6:GLN:HE21	4:F:109:GLY:HA3	1.65	0.61
3:E:3:VAL:HB	3:E:26:ASN:HD22	1.65	0.61
1:C:111:SER:HA	1:C:138:SER:O	2.01	0.60
2:B:155:ARG:HH21	3:E:61:SER:N	2.00	0.60
1:C:487:CYS:HB3	1:C:541:GLU:HB3	1.84	0.60
2:B:170:LYS:HE3	2:B:291:SER:O	2.02	0.59
2:D:170:LYS:HE3	2:D:291:SER:O	2.02	0.59
2:D:241:CYS:HB2	2:D:245:ILE:CD1	2.33	0.59
1:C:193:LEU:HD23	1:C:218:GLN:HG2	1.84	0.59
1:C:427:GLY:HA3	1:C:580:HIS:HE1	1.67	0.59
4:H:177:SER:O	4:H:179:LEU:N	2.36	0.59
3:E:113:ARG:HG2	3:E:114:ALA:N	2.17	0.59
2:B:94:ILE:CD1	2:B:113:LEU:HD21	2.29	0.59
2:D:176:ILE:HG22	2:D:224:ASN:HB2	1.85	0.59
3:E:97:LEU:HG	3:E:98:GLU:HG2	1.84	0.58
2:B:131:LEU:HD12	2:B:166:SER:HB2	1.84	0.58
1:C:382:GLY:HA3	1:C:415:PHE:O	2.04	0.58
3:E:3:VAL:H	3:E:26:ASN:ND2	2.01	0.58
4:H:34:ILE:HD13	4:H:79:ALA:HB2	1.84	0.58
4:H:158:THR:HB	4:H:201:ASN:HB2	1.85	0.58
1:C:323:ARG:NH1	1:C:343:THR:OG1	2.36	0.58
1:C:424:ASP:OD2	1:C:428:ASN:O	2.22	0.58
2:D:81:GLY:HA2	4:H:33:TRP:CZ2	2.38	0.58
1:C:351:PHE:HA	1:C:373:ALA:HB2	1.86	0.57
1:C:425:LEU:CD2	1:C:445:VAL:HG11	2.34	0.57
2:B:131:LEU:HD12	2:B:166:SER:CB	2.33	0.57
1:C:157:TRP:CG	1:C:158:ALA:H	2.22	0.57
2:D:273:ILE:HD12	2:D:292:HIS:O	2.04	0.57
2:D:247:TRP:HB3	2:D:252:ARG:NE	2.20	0.57
1:C:137:LEU:HD21	1:C:197:GLN:HG2	1.86	0.57
2:B:152:GLU:CD	2:B:155:ARG:NH1	2.63	0.57
4:H:123:PRO:HB3	4:H:209:THR:HG21	1.86	0.57
1:A:193:LEU:HD23	1:A:218:GLN:HG2	1.87	0.57
3:L:17:GLU:HG2	3:L:18:SER:N	2.19	0.57
3:L:129:GLN:HE22	3:L:136:SER:HB2	1.70	0.56
1:A:107:ALA:CB	1:A:112:ILE:HG22	2.35	0.56
1:A:262:VAL:HG21	1:A:304:VAL:HG21	1.87	0.56
4:F:34:ILE:HD13	4:F:79:ALA:HB2	1.88	0.56
3:E:42:LEU:HD13	3:E:91:TYR:CZ	2.40	0.56
2:D:155:ARG:NH1	3:L:61:SER:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:GLY:HA2	2:B:19:ILE:HD12	1.86	0.56
2:D:161:ARG:HH12	2:D:248:ARG:HD3	1.70	0.56
1:A:350:ARG:O	1:A:373:ALA:HA	2.06	0.56
1:A:462:PRO:HD2	1:A:482:ILE:HG23	1.88	0.56
1:A:449:ARG:HE	1:A:585:ALA:HB2	1.71	0.55
1:C:502:THR:HG22	1:C:532:THR:HG22	1.87	0.55
1:C:506:GLN:HB2	1:C:566:ALA:HB3	1.88	0.55
4:H:177:SER:C	4:H:179:LEU:H	2.15	0.55
1:C:9:ALA:HB3	1:C:445:VAL:HB	1.88	0.55
1:C:465:PHE:CD1	1:C:550:LEU:HB2	2.42	0.55
1:A:319:GLN:HB2	1:A:347:GLU:HG3	1.89	0.55
3:E:198:THR:HG22	3:E:213:SER:HB2	1.89	0.55
4:F:6:GLN:HE22	4:F:95:TYR:HA	1.71	0.55
2:B:85:LYS:HG2	3:E:37:TYR:OH	2.07	0.55
4:H:6:GLN:HE21	4:H:109:GLY:HA3	1.71	0.55
4:H:148:LYS:HB3	4:H:181:THR:HG23	1.89	0.54
3:E:33:ASN:ND2	3:E:37:TYR:OH	2.40	0.54
1:C:351:PHE:O	1:C:372:GLY:O	2.24	0.54
4:H:91:SER:HA	4:H:114:VAL:O	2.08	0.54
4:H:153:GLU:HG3	4:H:154:PRO:HA	1.89	0.54
2:D:248:ARG:C	2:D:250:VAL:H	2.15	0.54
4:F:47:TRP:HZ2	4:F:50:GLU:HG2	1.73	0.54
1:A:27:ARG:HG3	1:A:33:VAL:HG13	1.90	0.54
3:E:2:ILE:HD11	3:E:98:GLU:HG3	1.90	0.53
2:D:85:LYS:HB2	3:L:31:HIS:CE1	2.43	0.53
3:E:6:GLN:NE2	3:E:107:THR:HG23	2.22	0.53
1:A:454:ALA:HA	1:A:489:ASN:O	2.08	0.53
1:C:518:ARG:HB3	1:C:563:ILE:HG12	1.89	0.53
4:F:48:LEU:HD12	4:F:81:MET:HE1	1.90	0.53
3:E:38:LEU:HD13	3:E:76:PHE:CD2	2.43	0.53
2:D:143:LYS:O	2:D:213:ASN:ND2	2.41	0.53
4:F:124:PRO:HB2	4:F:147:VAL:HG13	1.89	0.53
4:H:6:GLN:NE2	4:H:109:GLY:HA3	2.24	0.53
3:E:13:VAL:HG21	3:E:19:VAL:HG21	1.91	0.53
2:D:112:THR:HG22	2:D:407:GLU:HG3	1.89	0.52
1:A:474:LEU:HG	1:A:475:GLU:H	1.74	0.52
2:D:75:VAL:HG13	2:D:95:GLN:HG3	1.92	0.52
2:B:82:THR:HG22	3:E:96:HIS:CE1	2.45	0.52
1:C:465:PHE:HB3	1:C:550:LEU:HD22	1.92	0.52
3:E:198:THR:HG22	3:E:213:SER:OG	2.09	0.52
1:A:536:GLN:HB3	1:A:539:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:410:ILE:HD11	2:D:423:PHE:HZ	1.75	0.52
4:F:48:LEU:CD1	4:F:81:MET:HE1	2.39	0.52
2:D:247:TRP:HB3	2:D:252:ARG:HE	1.75	0.52
2:B:131:LEU:HD21	2:B:139:LEU:HD13	1.92	0.52
1:C:294:VAL:HG11	1:C:394:LEU:HB2	1.92	0.51
3:E:13:VAL:HG21	3:E:19:VAL:HG22	1.92	0.51
1:A:511:LYS:C	1:A:513:LYS:H	2.18	0.51
1:C:189:GLN:NE2	1:C:222:ALA:H	2.06	0.51
1:C:358:LEU:HB2	1:C:368:ASP:O	2.10	0.51
1:A:461:PHE:HB3	1:A:462:PRO:HD3	1.93	0.51
1:A:107:ALA:HB2	1:A:112:ILE:HG22	1.91	0.51
1:C:285:PHE:H	1:C:306:ALA:HA	1.75	0.51
4:H:11:LEU:O	4:H:12:MET:HE2	2.11	0.51
2:B:168:VAL:HG21	2:B:222:SER:HB3	1.93	0.51
2:B:312:GLN:HG2	2:B:334:LYS:HG3	1.91	0.51
1:C:575:ALA:CB	1:C:576:PRO:HD3	2.39	0.51
3:E:2:ILE:CD1	3:E:98:GLU:HG3	2.41	0.51
2:B:334:LYS:NZ	2:B:361:GLU:O	2.43	0.51
4:H:6:GLN:NE2	4:H:111:GLY:H	2.09	0.51
3:E:111:LEU:H	3:E:171:GLN:HE22	1.57	0.51
1:A:269:ASP:O	1:A:270:ILE:C	2.54	0.50
1:A:503:VAL:HG13	1:A:567:LEU:CD1	2.41	0.50
2:B:136:LYS:HG3	2:B:221:ILE:HG21	1.94	0.50
1:C:123:THR:HG22	1:C:124:GLU:H	1.76	0.50
2:B:275:LEU:HD23	2:B:293:TYR:CE2	2.46	0.50
1:C:249:VAL:HG22	1:C:264:ILE:HG12	1.93	0.50
2:D:414:LYS:O	2:D:416:PRO:HD3	2.10	0.50
3:L:29:LEU:HA	3:L:97:LEU:HD22	1.94	0.50
4:F:171:PHE:O	4:F:182:LEU:CD1	2.58	0.50
4:F:205:PRO:C	4:F:207:SER:H	2.19	0.50
1:A:262:VAL:HG21	1:A:304:VAL:CG2	2.42	0.50
2:B:161:ARG:HH11	2:B:248:ARG:HE	1.60	0.50
2:D:155:ARG:HH12	3:L:61:SER:HB3	1.77	0.50
1:A:309:LEU:HD22	1:A:323:ARG:HB2	1.93	0.50
1:A:349:GLY:HA2	1:A:375:PHE:HB2	1.94	0.50
2:B:155:ARG:O	4:F:102:LEU:HD11	2.11	0.50
2:B:209:GLY:O	2:B:212:PHE:HB3	2.12	0.50
2:D:145:LEU:HG	2:D:146:GLY:H	1.77	0.50
2:B:364:LEU:O	2:B:393:ARG:HD3	2.11	0.50
1:C:255:GLY:H	1:C:260:GLY:HA2	1.77	0.49
1:A:575:ALA:N	1:A:576:PRO:HD3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:SER:HB3	1:C:442:LYS:HG2	1.93	0.49
1:C:108:HIS:CE1	1:C:174:LYS:O	2.65	0.49
1:C:263:THR:HG22	1:C:275:ASN:OD1	2.11	0.49
2:D:85:LYS:HG2	3:L:37:TYR:CZ	2.47	0.49
4:H:193:TRP:CD1	4:H:194:PRO:HA	2.47	0.49
2:D:99:LEU:HD11	2:D:111:PHE:CG	2.47	0.49
2:D:410:ILE:CD1	2:D:423:PHE:HZ	2.25	0.49
1:C:173:THR:OG1	1:C:177:ARG:HB3	2.13	0.49
4:F:159:TRP:CZ3	4:F:200:CYS:HB3	2.47	0.49
2:B:113:LEU:HD22	2:B:364:LEU:HD21	1.93	0.49
2:B:113:LEU:CD1	2:B:434:VAL:HG21	2.41	0.49
2:B:83:ALA:HA	2:B:85:LYS:HZ3	1.78	0.49
3:L:113:ARG:HG2	3:L:114:ALA:N	2.27	0.49
2:D:121:TYR:CD2	2:D:122:PRO:HD2	2.48	0.49
2:B:375:ILE:HG22	2:B:376:SER:N	2.27	0.48
4:F:91:SER:HA	4:F:114:VAL:O	2.11	0.48
1:C:411:THR:HB	1:C:412:PRO:HD2	1.94	0.48
3:L:165:LEU:HD11	4:H:174:VAL:HB	1.95	0.48
3:E:40:TRP:HB2	3:E:53:ILE:HB	1.96	0.48
3:E:190:GLU:O	3:E:194:HIS:HD2	1.97	0.48
2:D:85:LYS:HG2	3:L:37:TYR:CE2	2.49	0.48
2:D:145:LEU:HD11	2:D:149:LEU:HB2	1.96	0.48
1:A:113:LEU:HD11	1:A:135:CYS:HB3	1.96	0.47
1:C:430:TYR:CE1	1:C:450:PRO:HA	2.47	0.47
2:B:81:GLY:HA2	4:F:33:TRP:CZ2	2.48	0.47
1:C:323:ARG:HD2	1:C:325:TYR:CZ	2.50	0.47
2:D:390:GLU:CD	2:D:390:GLU:H	2.22	0.47
4:F:148:LYS:HB3	4:F:181:THR:HG23	1.96	0.47
2:B:172:VAL:HG12	2:B:173:MET:O	2.14	0.47
1:C:282:ALA:HB3	2:D:299:ILE:CD1	2.38	0.47
2:D:399:SER:O	2:D:402:ASP:HB2	2.13	0.47
3:L:38:LEU:HD13	3:L:76:PHE:CD2	2.49	0.47
1:C:99:GLN:HG3	1:C:116:ALA:CB	2.40	0.47
2:B:88:PRO:HA	2:B:91:ILE:HD12	1.95	0.47
1:A:460:ILE:HG23	1:A:482:ILE:CG2	2.45	0.47
1:A:512:GLN:NE2	1:A:517:ARG:HB3	2.22	0.47
2:B:75:VAL:CG1	2:B:116:LYS:HD3	2.45	0.47
4:F:29:PHE:CE1	4:F:34:ILE:HD11	2.49	0.47
4:F:170:THR:HG22	4:F:182:LEU:HD11	1.96	0.47
1:A:578:ASP:CG	1:A:579:SER:H	2.23	0.47
3:L:14:THR:HG23	3:L:112:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:10:GLU:HG3	4:H:12:MET:HE3	1.97	0.47
3:L:24:ARG:HA	3:L:74:THR:O	2.15	0.47
1:C:498:SER:HB3	1:C:536:GLN:HE21	1.80	0.46
2:D:380:TYR:HE2	2:D:407:GLU:HB2	1.80	0.46
1:C:19:PHE:CE1	1:C:37:VAL:HG11	2.50	0.46
1:C:77:SER:HB2	1:C:94:GLU:HG3	1.97	0.46
1:A:356:THR:CG2	1:A:419:LEU:HB3	2.46	0.46
2:B:375:ILE:HD11	2:B:423:PHE:CE1	2.49	0.46
3:L:17:GLU:HG2	3:L:18:SER:H	1.77	0.46
2:B:69:ILE:HG21	2:B:72:ASN:HD22	1.81	0.46
2:B:169:GLU:HG3	2:B:170:LYS:N	2.30	0.46
4:F:128:PRO:HB3	4:F:215:ILE:HG22	1.98	0.46
1:A:153:SER:OG	1:A:161:GLN:NE2	2.48	0.46
2:B:157:THR:CG2	2:B:160:PHE:HB2	2.46	0.46
1:C:310:MET:HG3	2:D:300:ALA:HB2	1.97	0.46
1:C:462:PRO:HD2	1:C:482:ILE:HG23	1.98	0.46
4:H:3:HIS:NE2	4:H:5:GLN:HG2	2.31	0.46
3:E:113:ARG:HG2	3:E:114:ALA:H	1.81	0.46
1:A:465:PHE:CE1	1:A:550:LEU:HB2	2.50	0.46
1:C:323:ARG:HD3	1:C:341:THR:HB	1.98	0.46
1:C:382:GLY:HA3	1:C:415:PHE:HB3	1.97	0.46
1:C:161:GLN:O	1:C:164:CYS:HB3	2.16	0.45
1:C:303:LEU:HG	1:C:326:VAL:HG22	1.99	0.45
2:B:152:GLU:HA	2:B:155:ARG:NH1	2.30	0.45
2:B:338:GLY:CA	2:B:350:LEU:HD11	2.42	0.45
1:C:57:LEU:HB2	1:C:70:ILE:HD11	1.97	0.45
1:C:258:THR:OG1	1:C:281:MET:HE2	2.16	0.45
4:H:30:THR:HA	4:H:53:PRO:HB2	1.98	0.45
2:D:94:ILE:HD12	2:D:434:VAL:HG23	1.97	0.45
2:D:161:ARG:NH1	2:D:248:ARG:HD3	2.31	0.45
3:L:31:HIS:CD2	3:L:33:ASN:H	2.29	0.45
1:A:460:ILE:HG23	1:A:482:ILE:HG21	1.99	0.45
1:A:508:ASP:O	1:A:512:GLN:HG2	2.16	0.45
2:B:376:SER:HB3	2:B:409:SER:HB3	1.98	0.45
1:C:453:SER:H	1:C:492:GLY:HA3	1.81	0.45
2:B:138:ASP:OD2	2:B:344:SER:HB2	2.16	0.45
2:D:30:ASN:O	2:D:31:SER:HB3	2.16	0.45
2:D:221:ILE:H	2:D:221:ILE:HG13	1.31	0.45
1:A:164:CYS:HB2	1:A:185:SER:OG	2.17	0.45
1:A:412:PRO:HG2	2:B:275:LEU:HD11	1.98	0.45
2:B:112:THR:HA	2:B:406:PHE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:LYS:NZ	2:D:219:GLN:HE22	2.15	0.45
1:A:241:SER:CB	8:A:2008:NAG:H82	2.47	0.45
1:A:99:GLN:HG3	1:A:116:ALA:HB1	1.99	0.45
2:B:277:ASN:HD22	2:B:279:GLY:H	1.65	0.45
2:D:408:ILE:HD13	2:D:425:ILE:HD13	1.99	0.45
3:E:4:MET:HE3	3:E:23:CYS:SG	2.56	0.45
4:F:138:ASN:C	4:F:140:MET:H	2.25	0.45
2:B:200:LYS:NZ	2:B:219:GLN:HE22	2.15	0.44
1:C:119:TYR:OH	1:C:152:ARG:NH1	2.49	0.44
4:H:17:SER:HB2	4:H:84:SER:HA	1.99	0.44
1:A:16:GLY:N	1:A:441:ASP:OD1	2.48	0.44
1:A:335:GLU:HA	1:A:336:PRO:HD3	1.80	0.44
2:B:110:THR:HG22	2:B:409:SER:OG	2.18	0.44
1:C:224:SER:HA	1:C:227:ASP:OD2	2.17	0.44
1:C:284:TYR:HB3	1:C:287:TYR:HB2	1.99	0.44
2:D:143:LYS:HA	2:D:216:VAL:HG13	1.98	0.44
3:L:218:GLU:O	3:L:219:CYS:SG	2.76	0.44
2:B:312:GLN:HG2	2:B:334:LYS:CG	2.46	0.44
4:F:136:GLN:HG3	4:F:138:ASN:O	2.18	0.44
2:B:431:THR:O	2:B:433:GLU:HG3	2.17	0.44
1:C:361:LEU:HB3	1:C:368:ASP:OD1	2.18	0.44
2:D:252:ARG:HH11	2:D:310:ASN:H	1.66	0.44
1:A:428:ASN:ND2	1:A:430:TYR:HB2	2.33	0.44
1:A:504:GLU:HG3	1:A:530:THR:HG22	1.98	0.44
2:B:158:SER:HA	3:E:55:ARG:NH1	2.33	0.44
2:D:94:ILE:HA	2:D:114:LYS:O	2.17	0.44
3:E:165:LEU:HD12	3:E:165:LEU:HA	1.90	0.44
1:A:460:ILE:HD11	1:A:565:ILE:HG13	1.99	0.44
4:H:140:MET:HB3	4:H:187:THR:HG22	2.00	0.44
4:F:160:ASN:C	4:F:162:GLY:H	2.26	0.44
1:A:503:VAL:HG13	1:A:567:LEU:HD11	2.00	0.43
2:B:25:CYS:HB3	2:B:44:CYS:SG	2.58	0.43
1:C:382:GLY:CA	1:C:415:PHE:HB3	2.48	0.43
3:L:111:LEU:H	3:L:171:GLN:NE2	2.08	0.43
1:A:474:LEU:HD12	1:A:525:ARG:HD3	2.00	0.43
2:D:103:LEU:HD21	2:D:410:ILE:HG22	2.00	0.43
2:D:344:SER:O	2:D:347:VAL:CG2	2.66	0.43
1:C:3:LEU:HD22	1:C:446:TYR:HB3	1.99	0.43
3:E:171:GLN:OE1	3:E:176:SER:HB2	2.18	0.43
2:B:129:MET:HE3	2:B:135:MET:HE3	2.01	0.43
3:L:39:TYR:HD1	3:L:51:LEU:HD11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:334:LYS:HG3	2:D:428:LEU:HB3	2.00	0.43
3:E:72:SER:OG	3:E:73:GLY:N	2.52	0.43
1:A:195:ALA:HB2	1:A:216:GLN:HG3	2.00	0.43
1:A:235:VAL:HA	1:A:249:VAL:O	2.19	0.43
1:C:99:GLN:HB2	1:C:119:TYR:HA	2.00	0.43
1:C:358:LEU:HD11	1:C:370:ALA:HB2	2.00	0.43
2:D:194:THR:HG22	2:D:195:THR:O	2.18	0.43
2:D:334:LYS:NZ	2:D:358:LEU:O	2.51	0.43
4:H:60:TYR:CE2	4:H:70:PHE:CD2	3.06	0.43
3:E:154:LYS:HB2	3:E:198:THR:OG1	2.19	0.43
2:B:72:ASN:OD1	2:B:95:GLN:HG3	2.19	0.43
1:C:157:TRP:CG	1:C:158:ALA:N	2.85	0.43
4:F:35:GLU:O	4:F:96:CYS:HA	2.19	0.43
4:F:60:TYR:CE2	4:F:70:PHE:CD2	3.07	0.43
4:F:97:SER:HB2	4:F:107:TYR:O	2.18	0.43
1:A:1:PHE:HA	1:A:400:GLN:HB2	2.00	0.43
1:A:241:SER:HB2	8:A:2008:NAG:C8	2.48	0.43
1:A:580:HIS:O	1:A:582:LEU:N	2.52	0.43
2:B:73:LYS:HD3	2:B:92:HIS:CD2	2.53	0.43
1:C:258:THR:OG1	1:C:281:MET:HG3	2.18	0.43
4:F:143:LEU:HB3	4:F:215:ILE:HD12	2.00	0.43
1:C:24:GLU:HB3	1:C:36:LEU:HB2	2.01	0.43
4:H:217:PRO:O	4:H:218:ARG:CB	2.65	0.42
1:A:453:SER:HB3	1:A:587:HIS:HB2	2.01	0.42
2:D:75:VAL:HG22	2:D:95:GLN:HE21	1.84	0.42
2:D:378:LYS:HG2	2:D:388:THR:HG22	2.00	0.42
1:C:130:ASP:OD1	1:C:162:GLY:HA3	2.19	0.42
2:D:95:GLN:HB2	2:D:114:LYS:HB2	2.01	0.42
3:L:145:TYR:CG	3:L:146:PRO:HA	2.55	0.42
4:F:68:ALA:HB1	4:F:81:MET:HE2	2.01	0.42
1:A:85:SER:O	1:A:87:SER:N	2.52	0.42
1:A:95:TYR:OH	1:A:122:ARG:HB2	2.19	0.42
1:C:264:ILE:HD11	1:C:302:LEU:HD22	2.00	0.42
3:E:42:LEU:HB2	3:E:52:LEU:HD11	2.01	0.42
3:E:200:GLU:HG2	3:E:211:VAL:HG22	2.00	0.42
4:H:156:THR:OG1	4:H:203:ALA:HB3	2.19	0.42
1:C:19:PHE:CZ	1:C:37:VAL:HG11	2.55	0.42
2:D:74:ASN:HA	2:D:95:GLN:CD	2.45	0.42
3:E:180:MET:HG2	3:E:181:SER:N	2.35	0.42
1:A:474:LEU:CG	1:A:475:GLU:H	2.33	0.42
1:C:553:GLU:H	1:C:553:GLU:CD	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:ASN:HD21	3:L:59:LEU:H	1.66	0.42
2:D:332:ILE:HA	2:D:333:PRO:HD3	1.86	0.42
3:L:124:PRO:HB3	3:L:214:PHE:CZ	2.55	0.42
2:D:299:ILE:O	2:D:303:VAL:HG23	2.19	0.42
3:E:112:PRO:HB2	3:E:112:LYS:HG3	2.01	0.42
3:E:172:ASP:O	3:E:176:SER:HA	2.19	0.42
1:C:23:VAL:HG23	1:C:420:ARG:HB2	2.02	0.42
1:C:356:THR:HG22	1:C:370:ALA:HB3	2.02	0.42
3:E:41:PHE:HE2	3:E:94:LEU:HB3	1.84	0.42
1:C:569:PHE:HB2	1:C:592:SER:HB2	2.02	0.41
1:C:577:VAL:HG22	1:C:583:ARG:HE	1.85	0.41
3:E:190:GLU:O	3:E:194:HIS:CD2	2.73	0.41
4:F:186:VAL:HG22	4:F:188:VAL:HG23	2.02	0.41
2:B:156:ILE:HG21	2:B:355:TYR:CE2	2.56	0.41
2:D:298:SER:O	2:D:299:ILE:C	2.64	0.41
1:A:241:SER:HB2	8:A:2008:NAG:H82	2.03	0.41
1:C:108:HIS:HE1	1:C:174:LYS:O	2.03	0.41
2:B:260:ALA:HA	2:B:321:PHE:CE2	2.55	0.41
4:F:36:TRP:CZ3	4:F:96:CYS:HB3	2.54	0.41
4:F:124:PRO:HA	4:F:150:TYR:HB3	2.02	0.41
1:A:150:PRO:HB3	1:A:216:GLN:OE1	2.20	0.41
1:C:293:ASP:O	1:C:367:ASN:HB2	2.21	0.41
1:C:507:LEU:HD23	1:C:565:ILE:HD13	2.02	0.41
2:D:15:CYS:HB3	2:D:444:CYS:HB2	1.97	0.41
1:A:123:THR:CG2	1:A:126:GLU:O	2.58	0.41
1:A:388:PRO:HD3	1:A:399:SER:HB3	2.01	0.41
2:B:375:ILE:CG2	2:B:376:SER:N	2.83	0.41
1:C:323:ARG:HH11	1:C:323:ARG:HG3	1.86	0.41
2:B:20:GLN:O	2:B:414:LYS:HE2	2.20	0.41
1:C:131:PRO:O	1:C:164:CYS:O	2.39	0.41
2:D:426:ARG:HA	2:D:427:PRO:HD3	1.99	0.41
1:A:479:VAL:HG12	1:A:552:ASN:HB2	2.02	0.41
1:A:495:VAL:HG12	1:A:496:ALA:H	1.85	0.41
2:B:103:LEU:HD21	2:B:412:SER:HB3	2.03	0.41
2:B:152:GLU:CD	2:B:155:ARG:HH11	2.28	0.41
2:B:277:ASN:ND2	2:B:279:GLY:H	2.18	0.41
2:D:55:CYS:HA	2:D:56:PRO:HD3	1.86	0.41
2:D:234:ALA:O	2:D:235:ILE:C	2.63	0.41
2:D:328:LEU:HG	2:D:332:ILE:HD12	2.03	0.41
3:L:14:THR:O	3:L:17:GLU:HB3	2.21	0.41
3:L:141:LEU:N	3:L:141:LEU:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLN:HA	1:A:47:PRO:HD2	1.91	0.41
1:C:40:PRO:HA	1:C:101:PHE:O	2.20	0.41
2:D:116:LYS:HB2	2:D:403:GLU:HG2	2.02	0.41
4:H:39:GLN:HB2	4:H:45:LEU:HD23	2.02	0.41
4:H:47:TRP:CH2	4:H:49:GLY:HA2	2.56	0.40
1:A:397:LYS:HA	1:A:398:PRO:HD3	1.82	0.40
1:A:404:PRO:HD3	1:A:415:PHE:CG	2.56	0.40
2:B:204:SER:HB2	2:B:245:ILE:O	2.21	0.40
2:B:322:GLN:N	2:B:323:PRO:HD2	2.37	0.40
1:C:356:THR:CG2	1:C:370:ALA:HB3	2.51	0.40
2:D:161:ARG:HH12	2:D:248:ARG:CD	2.33	0.40
1:A:577:VAL:HG13	1:A:581:GLY:HA2	2.04	0.40
1:C:340:LEU:HG	1:C:341:THR:N	2.36	0.40
1:A:553:GLU:C	1:A:555:GLU:H	2.29	0.40
2:B:67:LYS:HD3	2:B:110:THR:O	2.21	0.40
4:F:150:TYR:CE1	4:F:180:TYR:HB2	2.57	0.40
2:B:43:ARG:HH11	2:B:43:ARG:HA	1.86	0.40
2:B:369:LEU:HD13	2:B:373:VAL:HG12	2.04	0.40
4:H:176:GLN:C	4:H:177:SER:O	2.60	0.40
3:E:94:LEU:HD13	3:E:94:LEU:C	2.47	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	599/632 (95%)	538 (90%)	53 (9%)	8 (1%)	9	32
1	C	583/632 (92%)	515 (88%)	59 (10%)	9 (2%)	8	28
2	B	423/454 (93%)	380 (90%)	39 (9%)	4 (1%)	14	41
2	D	428/454 (94%)	381 (89%)	42 (10%)	5 (1%)	10	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	217/219 (99%)	210 (97%)	6 (3%)	1 (0%)	24	54
3	L	217/219 (99%)	204 (94%)	11 (5%)	2 (1%)	14	41
4	F	216/218 (99%)	192 (89%)	23 (11%)	1 (0%)	24	54
4	H	216/218 (99%)	198 (92%)	16 (7%)	2 (1%)	14	41
All	All	2899/3046 (95%)	2618 (90%)	249 (9%)	32 (1%)	11	36

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	SER
2	B	416	PRO
1	C	256	ASN
1	C	285	PHE
1	C	575	ALA
2	D	31	SER
2	D	105	SER
4	H	178	ASP
3	E	72	SER
1	A	350	ARG
1	A	476	GLY
1	A	576	PRO
1	A	581	GLY
2	B	242	GLY
1	C	51	GLN
2	D	242	GLY
1	A	64	PRO
2	D	249	ASN
3	L	26	ASN
3	L	72	SER
4	F	206	ALA
1	A	243	ASP
1	A	270	ILE
2	B	54	GLY
1	C	31	ASP
1	C	64	PRO
2	D	13	LYS
4	H	176	GLN
1	C	351	PHE
2	B	23	PRO
1	C	270	ILE
1	C	495	VAL

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	486/513 (95%)	459 (94%)	27 (6%)	19	50
1	C	476/513 (93%)	457 (96%)	19 (4%)	28	62
2	B	379/402 (94%)	364 (96%)	15 (4%)	28	62
2	D	384/402 (96%)	367 (96%)	17 (4%)	25	59
3	E	194/194 (100%)	183 (94%)	11 (6%)	18	49
3	L	194/194 (100%)	179 (92%)	15 (8%)	12	35
4	F	186/186 (100%)	175 (94%)	11 (6%)	18	48
4	H	186/186 (100%)	173 (93%)	13 (7%)	14	40
All	All	2485/2590 (96%)	2357 (95%)	128 (5%)	21	52

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	33	VAL
1	A	34	SER
1	A	77	SER
1	A	118	LEU
1	A	122	ARG
1	A	180	LEU
1	A	193	LEU
1	A	207	GLU
1	A	270	ILE
1	A	283	SER
1	A	294	VAL
1	A	309	LEU
1	A	310	MET
1	A	312	ARG
1	A	328	LEU
1	A	334	ILE
1	A	340	LEU
1	A	402	LEU

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Mol	Chain	Res	Type
1	A	459	THR
1	A	471	SER
1	A	474	LEU
1	A	483	ASN
1	A	488	LEU
1	A	502	THR
1	A	535	ILE
1	A	588	TYR
2	B	75	VAL
2	B	97	GLN
2	B	183	LEU
2	B	192	ASN
2	B	215	LEU
2	B	224	ASN
2	B	245	ILE
2	B	313	THR
2	B	344	SER
2	B	362	VAL
2	B	364	LEU
2	B	393	ARG
2	B	396	SER
2	B	414	LYS
2	B	431	THR
1	C	11	LEU
1	C	113	LEU
1	C	139	THR
1	C	164	CYS
1	C	180	LEU
1	C	235	VAL
1	C	252	VAL
1	C	254	LYS
1	C	270	ILE
1	C	294	VAL
1	C	369	VAL
1	C	432	ASP
1	C	451	ILE
1	C	459	THR
1	C	475	GLU
1	C	479	VAL
1	C	482	ILE
1	C	526	GLN
1	C	565	ILE

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Mol	Chain	Res	Type
2	D	25	CYS
2	D	27	TRP
2	D	92	HIS
2	D	113	LEU
2	D	139	LEU
2	D	221	ILE
2	D	245	ILE
2	D	251	THR
2	D	273	ILE
2	D	275	LEU
2	D	284	GLU
2	D	344	SER
2	D	347	VAL
2	D	364	LEU
2	D	393	ARG
2	D	397	ASN
2	D	444	CYS
3	L	14	THR
3	L	19	VAL
3	L	38	LEU
3	L	44	ARG
3	L	53	ILE
3	L	57	SER
3	L	61	SER
3	L	72	SER
3	L	94	LEU
3	L	107	THR
3	L	109	LEU
3	L	160	ARG
3	L	161	GLN
3	L	165	LEU
3	L	198	THR
4	H	7	SER
4	H	34	ILE
4	H	67	LYS
4	H	69	THR
4	H	74	THR
4	H	91	SER
4	H	106	ASP
4	H	118	SER
4	H	145	CYS
4	H	166	SER

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Mol	Chain	Res	Type
4	H	182	LEU
4	H	195	SER
4	H	216	VAL
3	E	8	THR
3	E	36	THR
3	E	38	LEU
3	E	56	MET
3	E	74	THR
3	E	78	LEU
3	E	94	LEU
3	E	121	SER
3	E	127	SER
3	E	165	LEU
3	E	186	LEU
4	F	20	ILE
4	F	23	LYS
4	F	34	ILE
4	F	62	GLU
4	F	74	THR
4	F	91	SER
4	F	106	ASP
4	F	177	SER
4	F	182	LEU
4	F	191	SER
4	F	215	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	400	GLN
1	A	512	GLN
1	A	587	HIS
2	B	11	ASN
2	B	92	HIS
2	B	109	GLN
2	B	151	ASN
2	B	219	GLN
2	B	277	ASN
2	B	292	HIS
2	B	312	GLN
2	B	343	ASN

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Mol	Chain	Res	Type
2	B	349	GLN
1	C	108	HIS
1	C	165	GLN
1	C	189	GLN
1	C	197	GLN
1	C	400	GLN
1	C	489	ASN
1	C	531	GLN
1	C	580	HIS
2	D	20	GLN
2	D	62	ASN
2	D	95	GLN
2	D	97	GLN
2	D	151	ASN
2	D	219	GLN
2	D	309	ASN
2	D	312	GLN
2	D	349	GLN
2	D	366	ASN
2	D	383	ASN
3	L	31	HIS
3	L	129	GLN
3	L	171	GLN
3	L	195	ASN
4	H	6	GLN
3	E	6	GLN
3	E	26	ASN
3	E	33	ASN
3	E	35	ASN
3	E	47	GLN
3	E	129	GLN
3	E	150	ASN
3	E	171	GLN
4	F	5	GLN
4	F	6	GLN
4	F	169	HIS

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 ⓘ

16 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	G	1	1,5	14,14,15	0.78	0	17,19,21	1.12	1 (5%)
5	NAG	G	2	5	14,14,15	0.61	0	17,19,21	2.45	5 (29%)
5	BMA	G	3	5	11,11,12	0.39	0	15,15,17	0.59	0
5	MAN	G	4	5	11,11,12	0.59	0	15,15,17	1.05	2 (13%)
5	MAN	G	5	5	11,11,12	0.63	0	15,15,17	1.03	1 (6%)
5	MAN	G	6	5	11,11,12	0.61	0	15,15,17	0.71	0
6	NAG	I	1	2,6	14,14,15	0.55	0	17,19,21	0.74	0
6	NAG	I	2	6	14,14,15	0.53	0	17,19,21	0.84	0
6	NAG	J	1	6,1	14,14,15	0.59	0	17,19,21	1.10	1 (5%)
6	NAG	J	2	6	14,14,15	0.52	0	17,19,21	0.97	1 (5%)
5	NAG	K	1	1,5	14,14,15	0.63	0	17,19,21	1.28	3 (17%)
5	NAG	K	2	5	14,14,15	0.52	0	17,19,21	2.94	4 (23%)
5	BMA	K	3	5	11,11,12	0.43	0	15,15,17	0.99	1 (6%)
5	MAN	K	4	5	11,11,12	0.67	0	15,15,17	1.43	3 (20%)
5	MAN	K	5	5	11,11,12	0.55	0	15,15,17	1.21	1 (6%)
5	MAN	K	6	5	11,11,12	0.69	0	15,15,17	1.17	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
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	0/1/1/1
5	MAN	G	6	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	1/6/23/26	0/1/1/1
6	NAG	J	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	3/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	2/2/19/22	0/1/1/1
5	MAN	K	5	5	-	1/2/19/22	0/1/1/1
5	MAN	K	6	5	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	2	NAG	C1-O5-C5	6.95	121.51	112.19
5	G	2	NAG	C2-N2-C7	6.41	131.50	122.90
5	K	2	NAG	C2-N2-C7	6.27	131.31	122.90
5	K	2	NAG	C4-C3-C2	-5.89	102.39	111.02
5	G	2	NAG	C4-C3-C2	-5.81	102.50	111.02
5	K	5	MAN	C1-O5-C5	3.64	117.06	112.19
5	G	2	NAG	O5-C1-C2	-3.39	106.05	111.29
5	K	4	MAN	C1-C2-C3	3.30	114.45	109.64
5	K	2	NAG	O5-C5-C4	3.09	118.34	110.83
5	K	1	NAG	C1-O5-C5	2.88	116.05	112.19
5	G	4	MAN	C1-O5-C5	2.76	115.89	112.19
5	K	4	MAN	O5-C5-C6	2.61	112.74	107.66
5	K	4	MAN	C2-C3-C4	2.56	115.37	110.86
5	G	1	NAG	O5-C1-C2	-2.54	107.36	111.29
5	K	6	MAN	C3-C4-C5	2.34	114.47	110.23
6	J	2	NAG	C1-O5-C5	2.30	115.27	112.19
5	K	1	NAG	C3-C4-C5	2.27	114.35	110.23
6	J	1	NAG	C1-O5-C5	2.23	115.17	112.19
5	K	3	BMA	C1-C2-C3	-2.18	106.47	109.64
5	G	5	MAN	C1-O5-C5	2.18	115.11	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	2	NAG	O3-C3-C2	2.17	113.91	109.40
5	G	2	NAG	C1-O5-C5	2.13	115.04	112.19
5	K	1	NAG	C4-C3-C2	2.07	114.05	111.02
5	G	4	MAN	O5-C5-C6	2.06	111.68	107.66
5	K	6	MAN	C2-C3-C4	2.06	114.48	110.86

There are no chirality outliers.

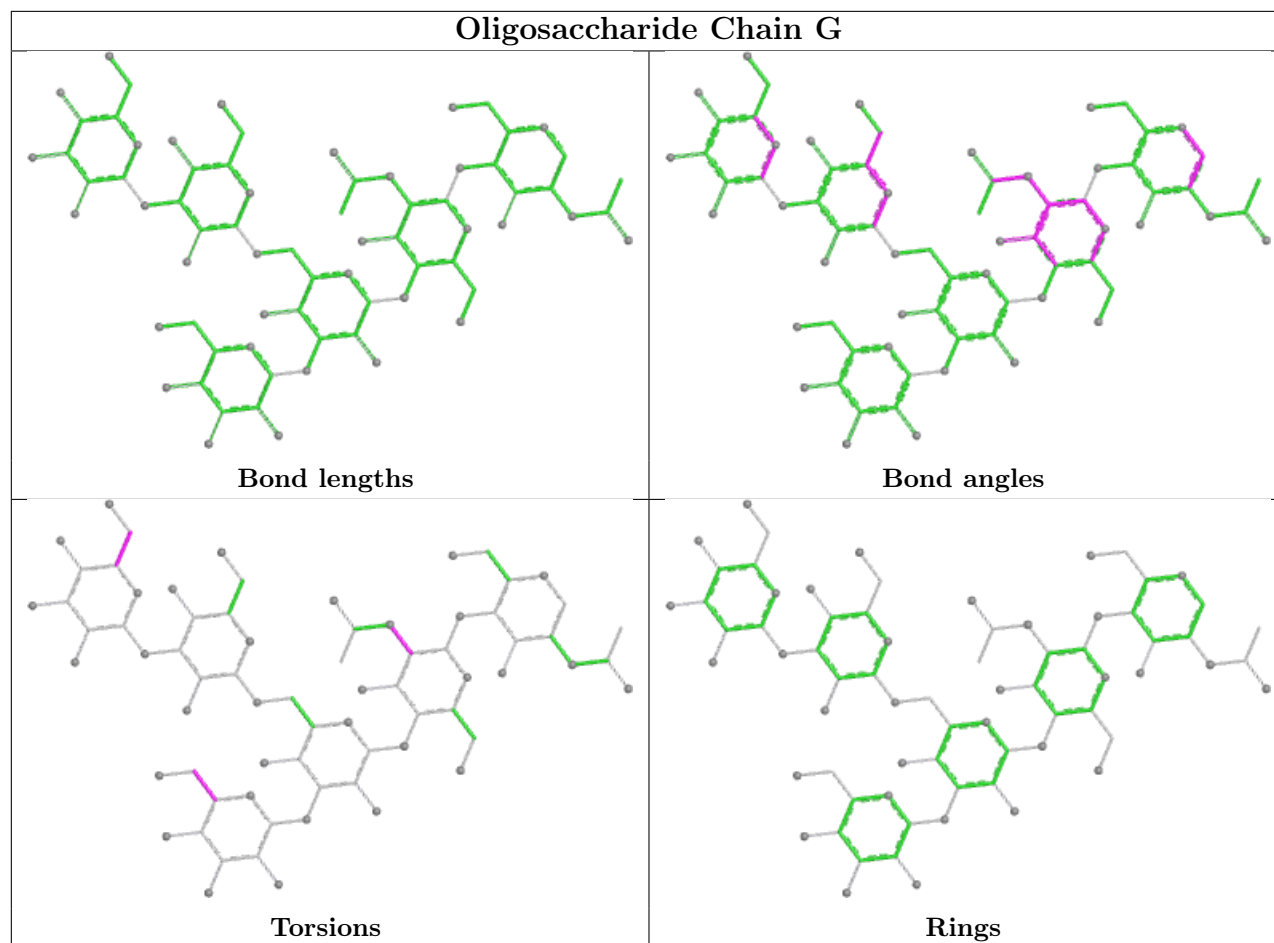
All (18) torsion outliers are listed below:

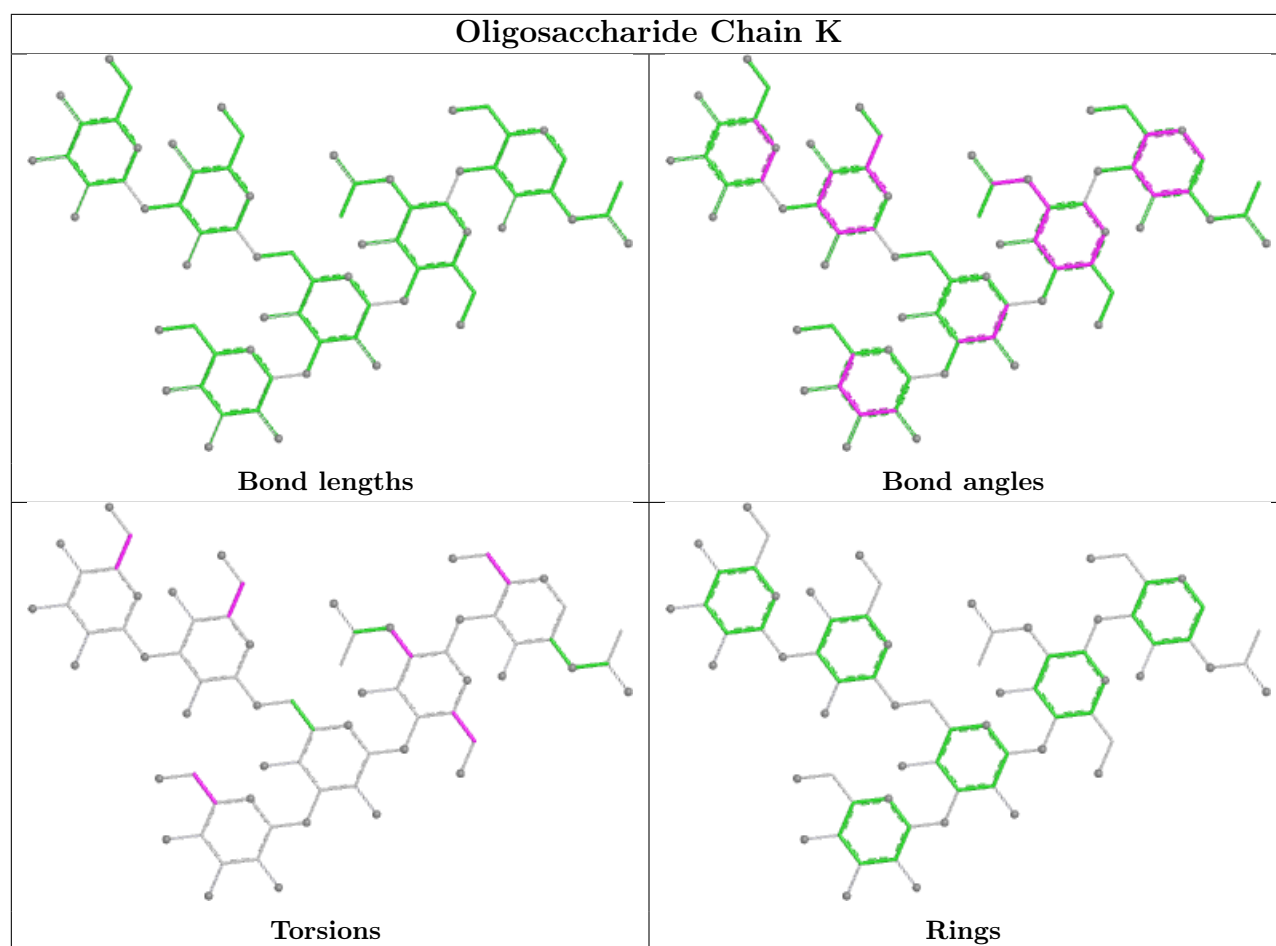
Mol	Chain	Res	Type	Atoms
6	J	2	NAG	O5-C5-C6-O6
5	K	6	MAN	O5-C5-C6-O6
5	G	6	MAN	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	K	6	MAN	C4-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
5	G	6	MAN	C4-C5-C6-O6
5	K	4	MAN	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	K	5	MAN	O5-C5-C6-O6
5	K	4	MAN	O5-C5-C6-O6
5	G	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C3-C2-N2-C7
5	G	5	MAN	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6

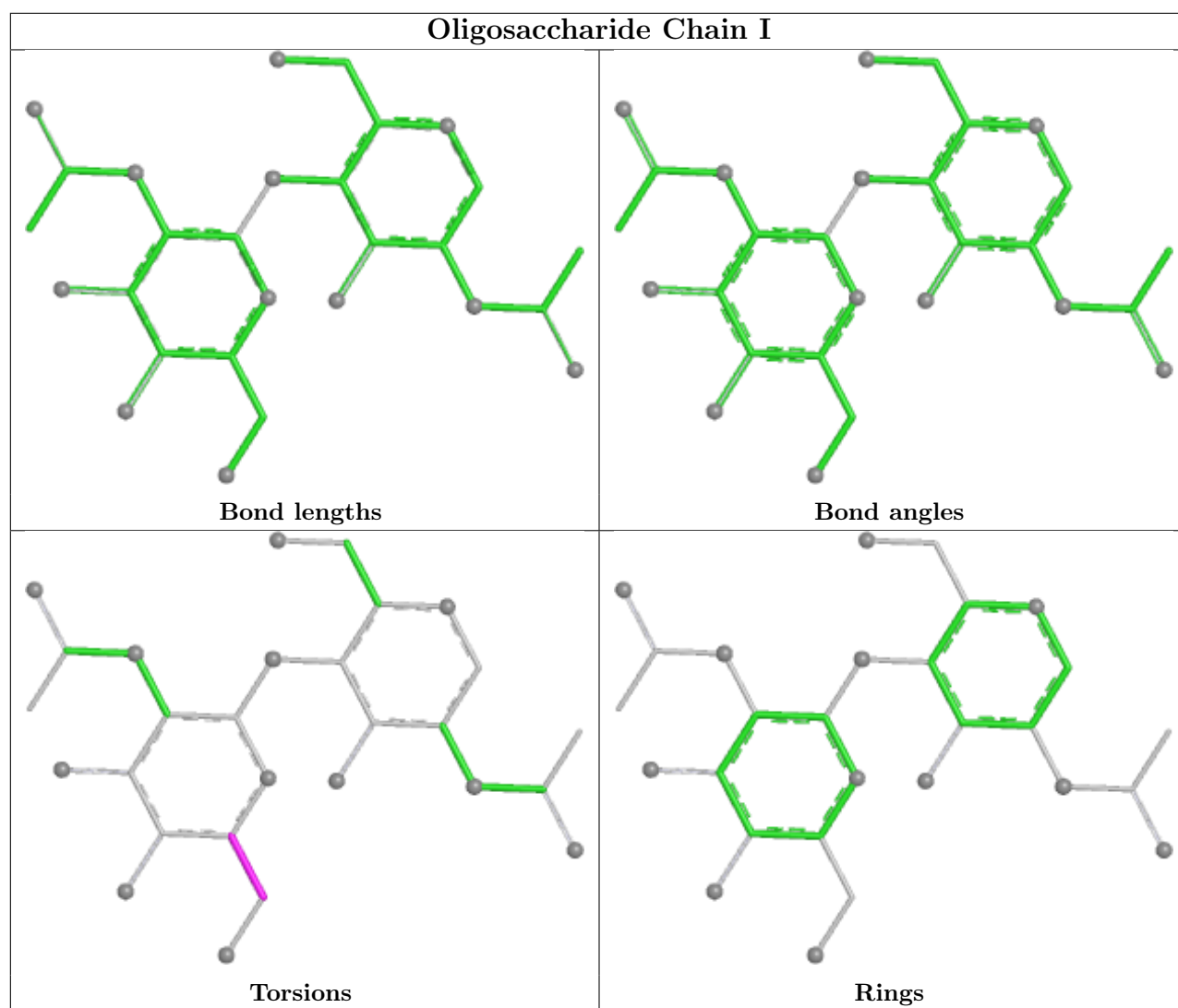
There are no ring outliers.

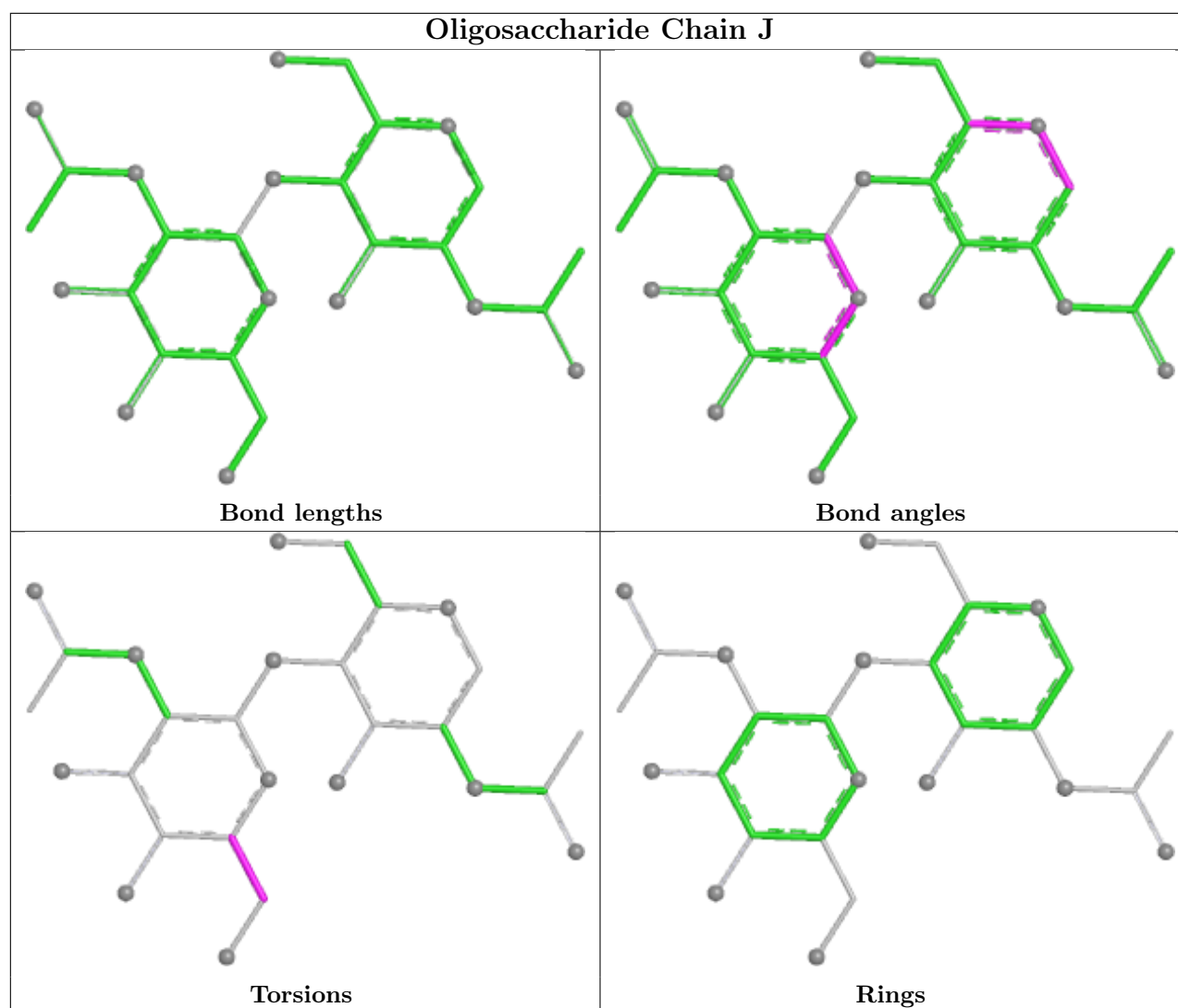
No monomer is involved in short contacts.

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](#)

Of 25 ligands modelled in this entry, 14 are monoatomic - leaving 11 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	$\# Z > 2$
8	NAG	A	2007	1	14,14,15	0.46	0	17,19,21	0.96	0
8	NAG	A	2006	1	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
8	NAG	C	2007	1	14,14,15	0.51	0	17,19,21	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	C	2009	1	14,14,15	0.61	0	17,19,21	0.95	0
8	NAG	A	2015	1	14,14,15	0.44	0	17,19,21	1.83	1 (5%)
8	NAG	D	2004	2	14,14,15	0.48	0	17,19,21	1.16	1 (5%)
8	NAG	A	2008	1	14,14,15	0.37	0	17,19,21	1.91	2 (11%)
8	NAG	C	2016	1	14,14,15	0.44	0	17,19,21	1.30	1 (5%)
8	NAG	A	2005	1	14,14,15	0.56	0	17,19,21	0.94	0
8	NAG	B	2004	2	14,14,15	0.54	0	17,19,21	1.20	1 (5%)
8	NAG	C	2008	1	14,14,15	0.53	0	17,19,21	1.16	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
8	NAG	A	2007	1	-	0/6/23/26	0/1/1/1
8	NAG	A	2006	1	-	1/6/23/26	0/1/1/1
8	NAG	C	2007	1	-	1/6/23/26	0/1/1/1
8	NAG	C	2009	1	-	2/6/23/26	0/1/1/1
8	NAG	A	2015	1	-	2/6/23/26	0/1/1/1
8	NAG	D	2004	2	-	0/6/23/26	0/1/1/1
8	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	C	2016	1	-	2/6/23/26	0/1/1/1
8	NAG	A	2005	1	-	2/6/23/26	0/1/1/1
8	NAG	B	2004	2	-	1/6/23/26	0/1/1/1
8	NAG	C	2008	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2008	NAG	C1-O5-C5	6.47	120.86	112.19
8	A	2015	NAG	C1-O5-C5	6.38	120.73	112.19
8	C	2016	NAG	C1-O5-C5	4.32	117.98	112.19
8	C	2008	NAG	C1-O5-C5	4.06	117.62	112.19
8	B	2004	NAG	C1-O5-C5	3.87	117.38	112.19
8	D	2004	NAG	C1-O5-C5	3.76	117.23	112.19
8	C	2007	NAG	C1-O5-C5	3.27	116.56	112.19
8	A	2006	NAG	C1-O5-C5	2.10	115.00	112.19
8	A	2008	NAG	C6-C5-C4	-2.09	107.88	113.02

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	2009	NAG	O5-C5-C6-O6
8	A	2015	NAG	C4-C5-C6-O6
8	C	2009	NAG	C4-C5-C6-O6
8	A	2015	NAG	O5-C5-C6-O6
8	C	2016	NAG	O5-C5-C6-O6
8	A	2005	NAG	O5-C5-C6-O6
8	A	2005	NAG	C4-C5-C6-O6
8	C	2007	NAG	O5-C5-C6-O6
8	A	2006	NAG	C1-C2-N2-C7
8	C	2016	NAG	C4-C5-C6-O6
8	B	2004	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2008	NAG	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	601/632 (95%)	0.18	25 (4%)	40	32	44, 68, 119, 155	0
1	C	589/632 (93%)	0.30	32 (5%)	31	24	40, 67, 140, 189	0
2	B	427/454 (94%)	0.25	27 (6%)	26	20	43, 66, 161, 185	0
2	D	432/454 (95%)	0.10	13 (3%)	52	43	40, 59, 136, 158	0
3	E	219/219 (100%)	-0.03	3 (1%)	73	65	47, 64, 84, 97	0
3	L	219/219 (100%)	-0.14	0	100	100	40, 57, 77, 91	0
4	F	218/218 (100%)	0.15	6 (2%)	55	46	44, 67, 101, 117	0
4	H	218/218 (100%)	0.04	6 (2%)	55	46	38, 60, 99, 117	0
All	All	2923/3046 (95%)	0.15	112 (3%)	44	36	38, 64, 127, 189	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	28	CYS	6.9
1	C	519	ALA	5.9
1	C	588	TYR	5.5
4	F	137	THR	5.4
2	B	441	ILE	5.2
1	C	576	PRO	5.0
4	F	135	ALA	4.4
4	H	137	THR	4.3
1	A	601	LEU	4.2
1	C	600	ILE	4.1
1	C	563	ILE	4.0
1	C	569	PHE	3.9
2	B	60	ILE	3.8
1	C	508	ASP	3.7
1	A	575	ALA	3.7
2	B	19	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	205	TYR	3.6
2	D	31	SER	3.6
1	C	560	LEU	3.6
4	F	134	ALA	3.5
1	C	29	GLY	3.5
1	C	84	LEU	3.4
1	A	579	SER	3.4
2	D	27	TRP	3.4
1	A	577	VAL	3.3
1	C	465	PHE	3.3
2	B	23	PRO	3.3
2	D	8	LEU	3.3
4	H	134	ALA	3.2
1	C	495	VAL	3.2
1	C	570	SER	3.2
2	B	8	LEU	3.1
1	A	581	GLY	3.1
1	A	29	GLY	3.1
1	C	509	TRP	3.0
2	D	14	SER	3.0
1	C	598	ALA	3.0
1	A	32	GLY	2.9
2	B	104	ARG	2.9
2	B	47	LEU	2.9
2	B	26	GLY	2.9
2	B	27	TRP	2.9
1	C	423	ARG	2.8
1	A	580	HIS	2.8
2	B	442	CYS	2.8
1	A	427	GLY	2.8
2	B	22	GLY	2.8
1	A	64	PRO	2.7
1	C	575	ALA	2.7
2	D	29	THR	2.7
1	A	576	PRO	2.6
2	D	105	SER	2.6
1	C	507	LEU	2.6
1	C	62	ALA	2.6
1	C	564	HIS	2.6
2	D	43	ARG	2.6
2	B	54	GLY	2.6
1	A	570	SER	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	136	GLN	2.5
1	C	561	SER	2.5
2	B	62	ASN	2.5
2	B	63	PRO	2.5
2	D	10	ALA	2.5
4	H	176	GLN	2.5
1	C	562	PRO	2.4
2	D	49	ALA	2.4
2	B	110	THR	2.4
3	E	1	ASP	2.4
1	A	554	SER	2.4
1	C	490	ALA	2.4
4	H	200	CYS	2.4
2	B	417	LYS	2.4
4	H	135	ALA	2.4
1	A	448	GLY	2.4
1	A	30	THR	2.4
2	B	416	PRO	2.4
2	D	60	ILE	2.3
2	B	29	THR	2.3
2	B	25	CYS	2.3
1	C	28	PRO	2.3
4	F	1	GLN	2.2
1	C	60	TRP	2.2
1	C	33	VAL	2.2
2	B	64	ARG	2.2
1	C	496	ALA	2.2
3	E	8	THR	2.2
1	C	493	LYS	2.2
2	B	99	LEU	2.2
4	F	164	LEU	2.2
2	D	445	GLU	2.2
2	B	43	ARG	2.2
1	A	28	PRO	2.2
1	A	123	THR	2.2
1	C	481	CYS	2.2
1	C	539	ALA	2.2
1	A	517	ARG	2.1
2	B	56	PRO	2.1
2	B	103	LEU	2.1
3	E	119	THR	2.1
2	D	444	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	6	ARG	2.1
1	A	63	SER	2.1
1	A	156	SER	2.1
2	B	18	CYS	2.1
4	H	212	ASP	2.1
2	D	92	HIS	2.0
1	A	586	LEU	2.0
1	C	536	GLN	2.0
1	A	472	CYS	2.0
1	A	560	LEU	2.0
1	C	460	ILE	2.0
1	A	157	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

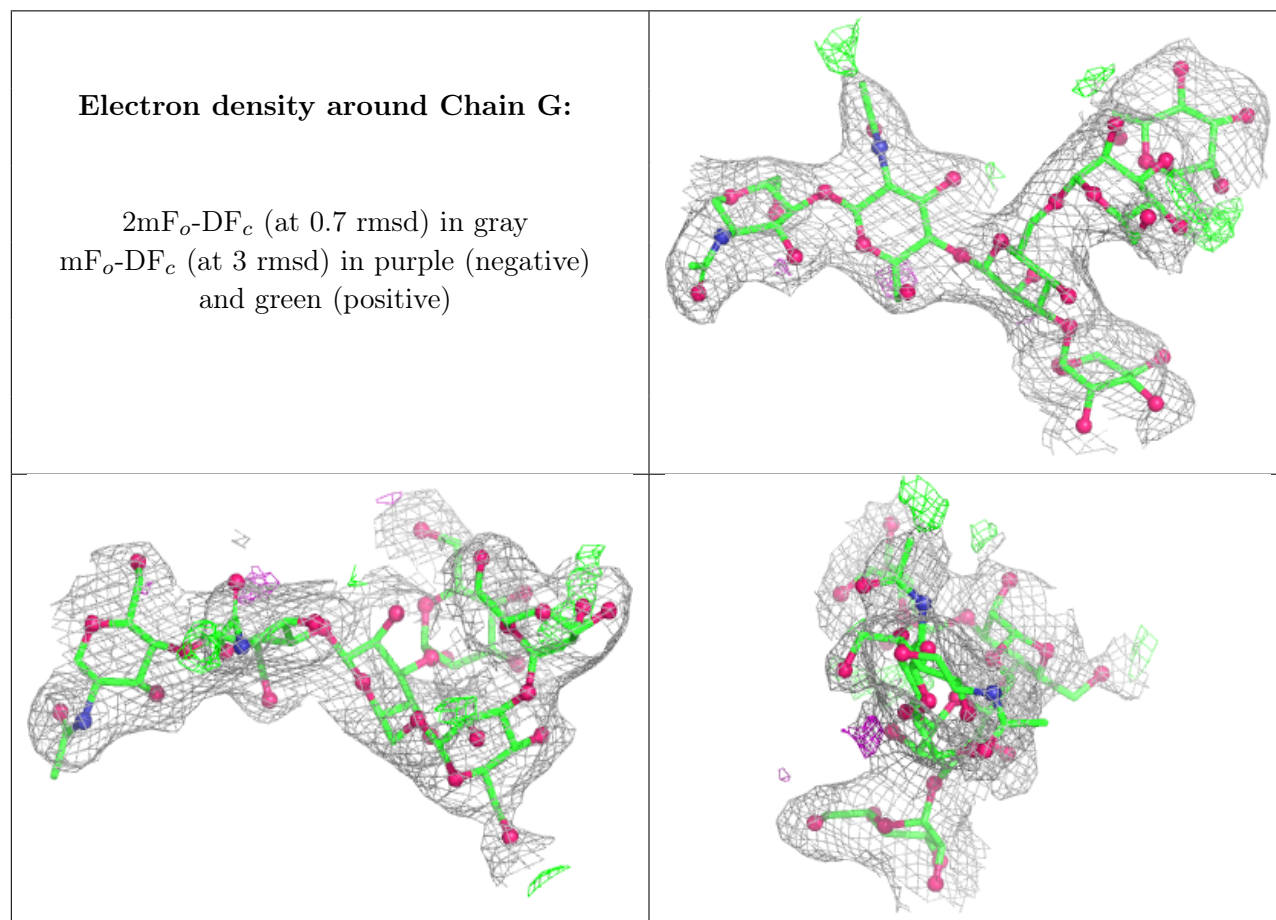
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

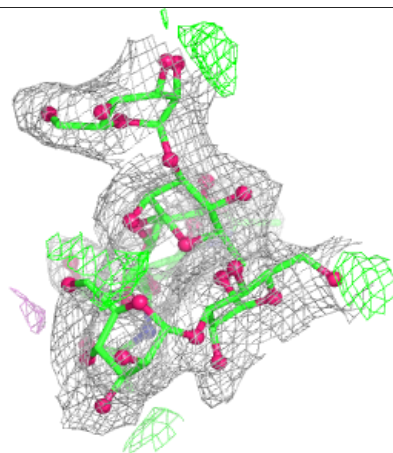
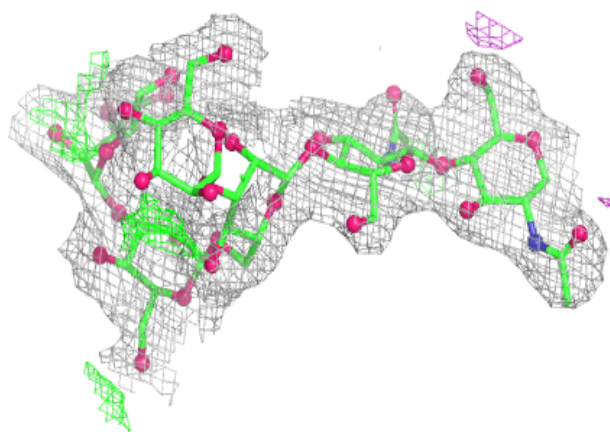
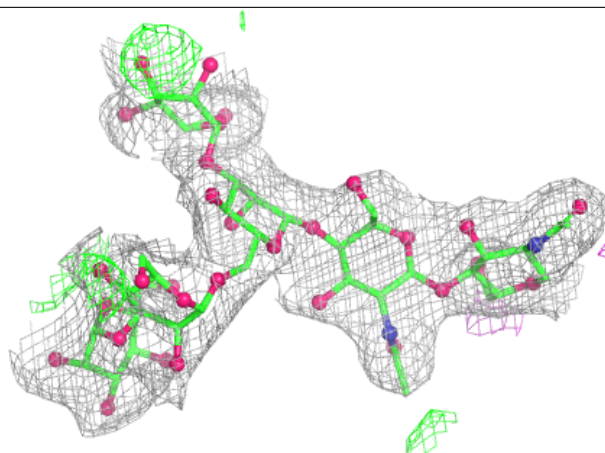
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	G	1	14/15	-	-	53,56,65,66	0
5	NAG	G	2	14/15	-	-	58,63,70,71	0
5	BMA	G	3	11/12	-	-	75,83,90,92	0
5	MAN	G	4	11/12	-	-	98,101,108,108	0
5	MAN	G	5	11/12	-	-	78,85,91,92	0
5	MAN	G	6	11/12	-	-	88,100,105,105	0
5	NAG	K	2	14/15	0.61	0.12	55,59,64,71	0
6	NAG	J	2	14/15	0.81	0.10	108,116,118,121	0
5	BMA	K	3	11/12	-	-	66,73,76,77	0
5	MAN	K	4	11/12	-	-	80,85,91,94	0
5	MAN	K	5	11/12	-	-	77,85,95,96	0
5	MAN	K	6	11/12	-	-	69,84,89,90	0
6	NAG	I	2	14/15	0.87	0.11	97,105,111,113	0
6	NAG	J	1	14/15	0.88	0.08	74,82,90,100	0
5	NAG	K	1	14/15	0.93	0.08	50,54,59,59	0
6	NAG	I	1	14/15	0.95	0.08	74,81,87,92	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.



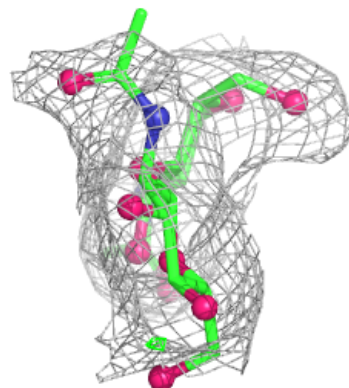
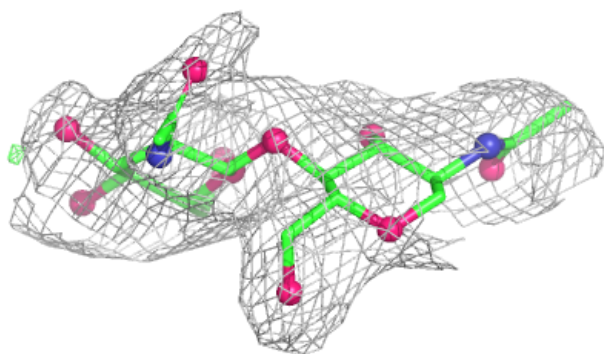
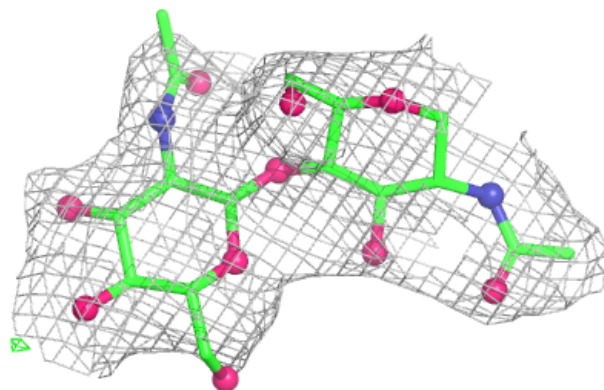
Electron density around Chain K:

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

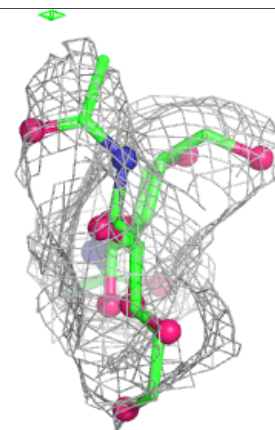
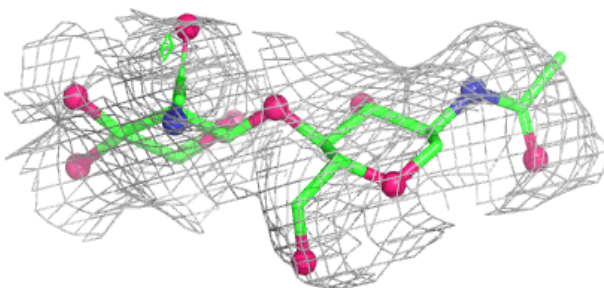
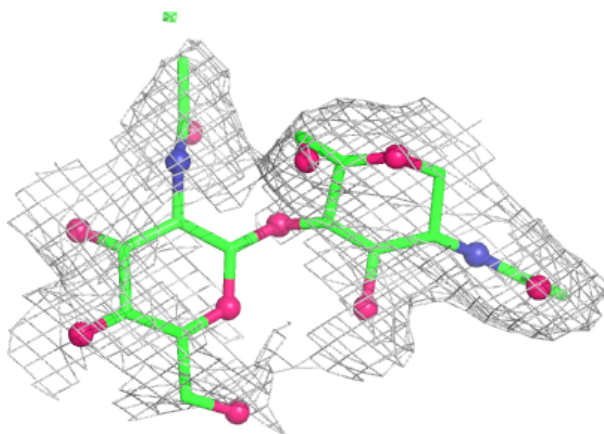


Electron density around Chain I:

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

**Electron density around Chain J:**

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



6.4 Ligands

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
8	NAG	A	2015	14/15	0.74	0.14	82,93,103,112	0
8	NAG	C	2007	14/15	0.75	0.13	87,102,110,111	0
9	MG	D	2003	1/1	0.77	0.21	57,57,57,57	0
8	NAG	A	2006	14/15	0.80	0.11	92,104,108,108	0
8	NAG	C	2016	14/15	0.81	0.12	100,110,118,124	0
8	NAG	A	2007	14/15	0.82	0.14	92,99,101,104	0
9	MG	B	2003	1/1	0.84	0.21	62,62,62,62	0
8	NAG	D	2004	14/15	0.84	0.10	68,71,73,73	0
8	NAG	C	2008	14/15	0.85	0.13	97,101,105,105	0
8	NAG	A	2008	14/15	0.88	0.10	62,68,71,72	0
8	NAG	C	2009	14/15	0.89	0.09	64,70,74,75	0
8	NAG	A	2005	14/15	0.90	0.08	73,78,86,86	0
7	CA	A	2002	1/1	0.93	0.06	84,84,84,84	0
8	NAG	B	2004	14/15	0.93	0.08	66,71,77,78	0
7	CA	B	2001	1/1	0.93	0.06	69,69,69,69	0
7	CA	D	2001	1/1	0.96	0.06	65,65,65,65	0
7	CA	A	2001	1/1	0.97	0.06	69,69,69,69	0
7	CA	C	2002	1/1	0.97	0.04	75,75,75,75	0
7	CA	A	2003	1/1	0.97	0.05	78,78,78,78	0
7	CA	A	2004	1/1	0.97	0.05	88,88,88,88	0
7	CA	B	2002	1/1	0.98	0.08	62,62,62,62	0
7	CA	C	2004	1/1	0.99	0.04	81,81,81,81	0
7	CA	C	2001	1/1	0.99	0.02	63,63,63,63	0
7	CA	D	2002	1/1	0.99	0.03	54,54,54,54	0
7	CA	C	2003	1/1	0.99	0.03	84,84,84,84	0

6.5 Other polymers

There are no such residues in this entry.