



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:51 AM UTC

PDB ID : 4LN4 / pdb_00004ln4
Title : The crystal structure of hemagglutinin form a h7n9 influenza virus
(a/shanghai/1/2013) in complex with lstb
Authors : Yang, H.; Carney, P.J.; Chang, J.C.; Villanueva, J.M.; Stevens, J.
Deposited on : 2013-07-11
Resolution : 3.10 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

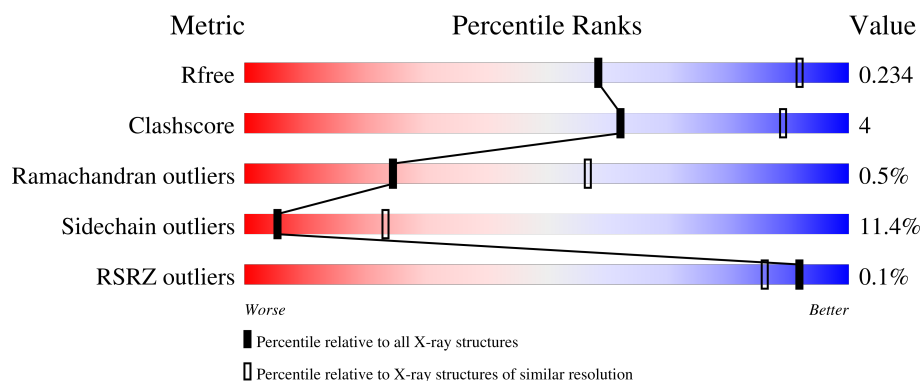
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	325	
1	C	325	
1	E	325	
1	G	325	
1	I	325	

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Mol	Chain	Length	Quality of chain
1	K	325	 79% 15% . .
2	B	181	 80% 11% . 8%
2	D	181	 77% 14% . 8%
2	F	181	 77% 14% . 8%
2	H	181	 76% 13% . 9%
2	J	181	 76% 13% . 9%
2	L	181	 76% 13% . 9%
3	M	3	 100%
3	N	3	 100%
3	O	3	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22827 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2410	1494	435	466	15			
1	C	316	Total	C	N	O	S	0	0	0
			2410	1494	435	466	15			
1	E	316	Total	C	N	O	S	0	0	0
			2410	1494	435	466	15			
1	G	316	Total	C	N	O	S	0	0	0
			2410	1494	435	466	15			
1	I	316	Total	C	N	O	S	0	0	0
			2410	1494	435	466	15			
1	K	316	Total	C	N	O	S	0	0	0
			2410	1494	435	466	15			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1359	838	237	277	7			
2	D	167	Total	C	N	O	S	0	0	0
			1359	838	237	277	7			
2	F	167	Total	C	N	O	S	0	0	0
			1359	838	237	277	7			
2	H	164	Total	C	N	O	S	0	0	0
			1335	823	231	274	7			
2	J	164	Total	C	N	O	S	0	0	0
			1335	823	231	274	7			
2	L	164	Total	C	N	O	S	0	0	0
			1335	823	231	274	7			

- Molecule 3 is an oligosaccharide called 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
3	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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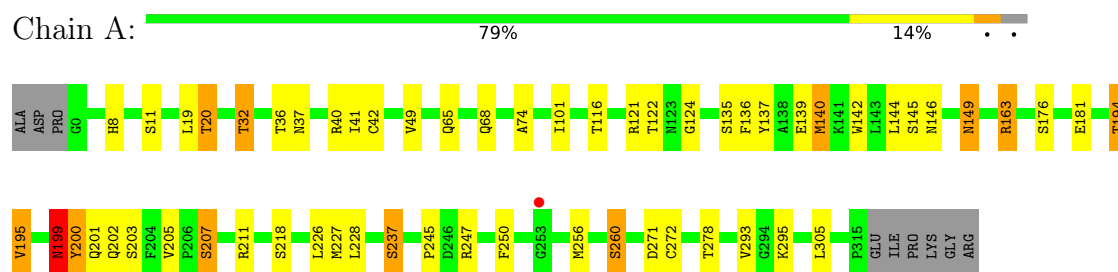
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	J	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		

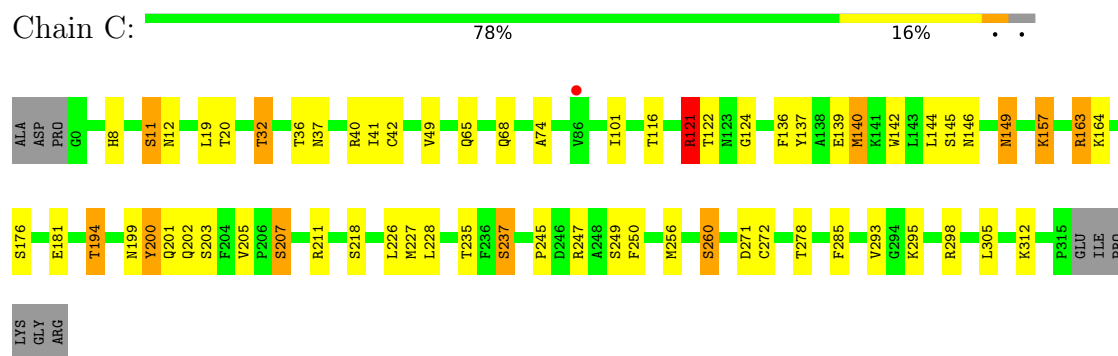
3 Residue-property plots

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.

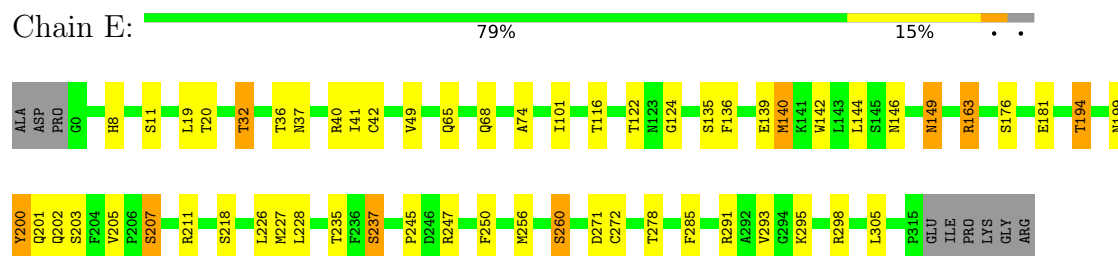
• Molecule 1: Hemagglutinin



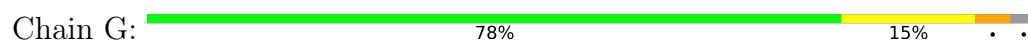
• Molecule 1: Hemagglutinin

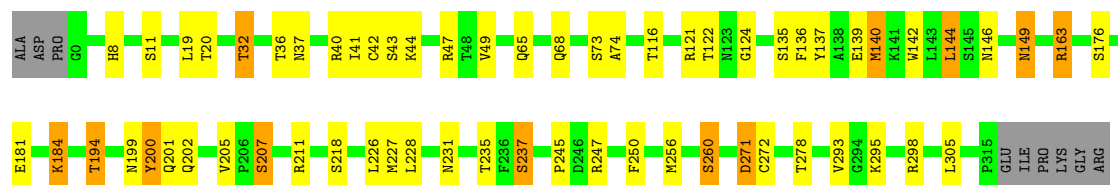


• Molecule 1: Hemagglutinin



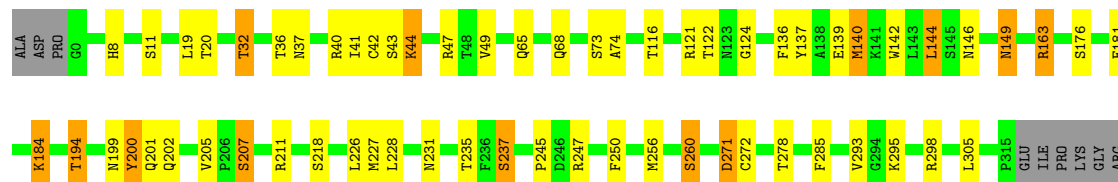
• Molecule 1: Hemagglutinin





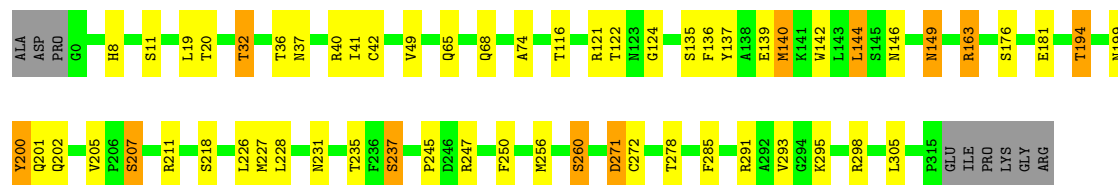
• Molecule 1: Hemagglutinin

Chain I: 78% 15% . .



• Molecule 1: Hemagglutinin

Chain K: 79% 15% . .



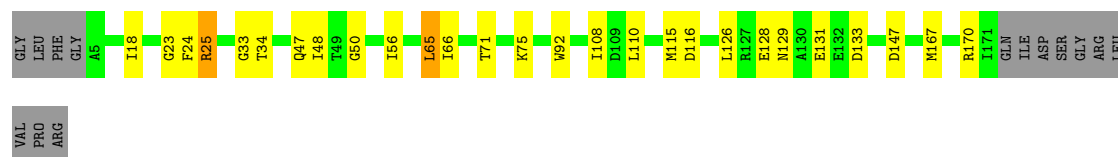
• Molecule 2: Hemagglutinin

Chain B: 80% 11% 8%



• Molecule 2: Hemagglutinin

Chain D: 77% 14% 8%



• Molecule 2: Hemagglutinin

Chain F: 77% 14% 8%



PRO
ARG

• Molecule 2: Hemagglutinin

Chain H:  76% 13% • 9%

GLY LEU PHE GLY ALA I6 I18 G23 F24 R25 G33 Q47 I48 I56 L65 I66 T71 E74 K75 W92 L110 M115 D116 L126 N129 D133 F141 D147 E164 E165 A166 M167 Q168 N169 ARG ILE ILE GLN ASP ILE ILE SER ARG GLY ARG LEU

VAL
PRO
ARG

• Molecule 2: Hemagglutinin

Chain J:  76% 13% • 9%

GLY LEU PHE GLY ALA I6 I18 G23 F24 R25 G33 T34 Q47 I48 I56 L65 I66 T71 E74 K75 W92 L110 M115 D116 L126 N129 D133 D147 E164 M167 Q168 N169 ARG ILE ILE GLN ASP ILE ILE SER ARG GLY ARG LEU VAL PRO

ARG

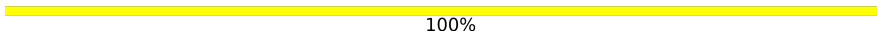
• Molecule 2: Hemagglutinin

Chain L:  76% 13% • 9%

GLY LEU PHE GLY ALA I6 I18 G23 F24 R25 Q47 I48 I56 L65 I66 D67 T71 E72 V73 E74 K75 W92 L110 M115 D116 L126 N129 D133 F141 D147 E164 E165 A166 M167 Q168 N169 ARG ILE ILE GLN ASP ILE ILE SER ARG GLY ARG LEU

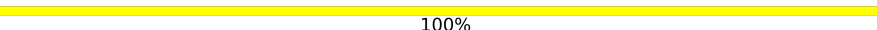
VAL
PRO
ARG

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

MAG1
MAG2
BMA3

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2
BMA3

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

MAG1
MAG2
BOL3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	154.01Å 153.96Å 153.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 3.10 48.75 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.75-3.10) 99.5 (48.75-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.201 , 0.239 0.200 , 0.234	Depositor DCC
R_{free} test set	3385 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	86.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l 0.023 for -l,-k,-h 0.023 for -h,l,k 0.439 for l,h,k 0.439 for k,l,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22827	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: BMA, 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	0.72	0/2455	0.95	2/3316 (0.1%)
1	C	0.73	0/2455	0.99	6/3316 (0.2%)
1	E	0.72	0/2455	0.95	2/3316 (0.1%)
1	G	0.71	0/2455	0.96	1/3316 (0.0%)
1	I	0.71	0/2455	0.96	1/3316 (0.0%)
1	K	0.70	0/2455	0.96	1/3316 (0.0%)
2	B	0.77	0/1382	0.98	2/1863 (0.1%)
2	D	0.77	0/1382	0.97	1/1863 (0.1%)
2	F	0.78	0/1382	0.97	1/1863 (0.1%)
2	H	0.71	0/1358	0.94	1/1831 (0.1%)
2	J	0.70	0/1358	0.94	1/1831 (0.1%)
2	L	0.71	0/1358	0.94	1/1831 (0.1%)
All	All	0.72	0/22950	0.96	20/30978 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	SER	N-CA-C	-8.07	98.54	110.48
1	C	157	LYS	CG-CD-CE	6.73	126.77	111.30
1	C	121	ARG	CG-CD-NE	6.25	125.76	112.00
1	C	260	SER	N-CA-C	5.60	117.35	108.79
2	B	59	THR	N-CA-CB	5.59	118.19	109.97
1	G	260	SER	N-CA-C	5.49	117.19	108.79
1	A	260	SER	N-CA-C	5.43	117.32	109.07
1	E	260	SER	N-CA-C	5.37	117.24	109.07
1	I	260	SER	N-CA-C	5.36	116.98	108.79
2	L	23	GLY	N-CA-C	5.34	118.94	111.19
2	H	23	GLY	N-CA-C	5.34	118.94	111.19
1	K	260	SER	N-CA-C	5.31	116.92	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	ILE	CB-CA-C	-5.26	105.24	111.81
2	J	23	GLY	N-CA-C	5.22	118.76	111.19
1	A	101	ILE	CB-CA-C	-5.20	105.31	111.81
1	C	12	ASN	CA-C-O	5.18	128.51	122.03
2	F	23	GLY	N-CA-C	5.18	118.70	111.19
2	D	23	GLY	N-CA-C	5.14	118.65	111.19
2	B	23	GLY	N-CA-C	5.13	118.62	111.19
1	E	101	ILE	CB-CA-C	-5.02	105.54	111.81

There are no chirality outliers.

There are no planarity outliers.

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	2410	0	2361	27	1
1	C	2410	0	2361	23	1
1	E	2410	0	2361	21	1
1	G	2410	0	2362	22	1
1	I	2410	0	2362	22	1
1	K	2410	0	2362	22	1
2	B	1359	0	1263	9	0
2	D	1359	0	1263	12	0
2	F	1359	0	1263	12	0
2	H	1335	0	1234	10	0
2	J	1335	0	1234	10	0
2	L	1335	0	1234	11	0
3	M	39	0	34	0	0
3	N	39	0	34	0	0
3	O	39	0	34	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	14	0	13	0	0
4	H	14	0	13	0	0
4	I	14	0	13	0	0
4	J	14	0	13	0	0
4	K	14	0	13	0	0
4	L	14	0	13	1	0
All	All	22827	0	21918	183	3

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 4.

All (183) 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:128:GLU:O	2:B:170:ARG:NH1	1.83	1.11
1:C:121:ARG:NH1	1:C:145:SER:O	1.99	0.95
1:G:139:GLU:OE1	1:G:247:ARG:HD3	1.73	0.89
1:A:139:GLU:OE1	1:A:247:ARG:HD3	1.73	0.89
1:C:139:GLU:OE1	1:C:247:ARG:HD3	1.73	0.88
1:E:139:GLU:OE1	1:E:247:ARG:HD3	1.72	0.88
1:I:139:GLU:OE1	1:I:247:ARG:HD3	1.73	0.88
1:K:139:GLU:OE1	1:K:247:ARG:HD3	1.73	0.87
1:G:32:THR:HB	1:G:305:LEU:O	1.89	0.73
1:E:32:THR:HB	1:E:305:LEU:O	1.89	0.72
1:I:32:THR:HB	1:I:305:LEU:O	1.89	0.72
1:C:32:THR:HB	1:C:305:LEU:O	1.89	0.72
1:A:32:THR:HB	1:A:305:LEU:O	1.89	0.72
1:A:195:VAL:HG12	1:A:195:VAL:O	1.89	0.71
1:K:32:THR:HB	1:K:305:LEU:O	1.89	0.71
1:C:293:VAL:HG11	2:D:65:LEU:HD13	1.74	0.70
1:A:207:SER:CB	1:C:203:SER:OG	2.43	0.67
1:I:293:VAL:HG11	2:J:65:LEU:HD13	1.77	0.66
1:A:195:VAL:HG12	1:A:200:TYR:HE2	1.60	0.66
1:A:293:VAL:HG11	2:B:65:LEU:HD13	1.77	0.66
1:K:293:VAL:HG11	2:L:65:LEU:HD13	1.79	0.64
1:E:293:VAL:HG11	2:F:65:LEU:HD13	1.79	0.64
2:F:131:GLU:OE1	2:F:170:ARG:NH1	2.30	0.64
1:G:293:VAL:HG11	2:H:65:LEU:HD13	1.79	0.64
1:C:140:MET:HE2	1:C:245:PRO:HA	1.81	0.63
1:E:140:MET:HE2	1:E:245:PRO:HA	1.80	0.63
1:K:207:SER:O	1:K:211:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:MET:HE2	1:A:245:PRO:HA	1.80	0.63
2:B:56:ILE:CG2	2:B:56:ILE:O	2.47	0.62
2:D:56:ILE:O	2:D:56:ILE:CG2	2.48	0.62
1:C:207:SER:CB	1:E:203:SER:OG	2.48	0.62
1:E:207:SER:O	1:E:211:ARG:NH2	2.32	0.61
1:G:40:ARG:O	1:G:278:THR:HG22	2.00	0.61
1:K:140:MET:HE2	1:K:245:PRO:HA	1.81	0.61
2:D:131:GLU:OE1	2:D:170:ARG:NH1	2.31	0.61
2:F:56:ILE:CG2	2:F:56:ILE:O	2.48	0.61
1:I:40:ARG:O	1:I:278:THR:HG22	2.01	0.61
1:G:140:MET:HE2	1:G:245:PRO:HA	1.81	0.61
1:I:124:GLY:HA3	1:I:142:TRP:HB3	1.82	0.61
1:I:140:MET:HE2	1:I:245:PRO:HA	1.82	0.60
1:A:203:SER:OG	1:E:207:SER:CB	2.49	0.60
1:G:207:SER:O	1:G:211:ARG:NH2	2.32	0.60
1:K:40:ARG:O	1:K:278:THR:HG22	2.00	0.60
1:K:124:GLY:HA3	1:K:142:TRP:HB3	1.83	0.60
1:C:121:ARG:HH11	1:C:121:ARG:HG3	1.66	0.60
2:H:56:ILE:O	2:H:56:ILE:CG2	2.50	0.60
1:A:207:SER:O	1:A:211:ARG:NH2	2.32	0.60
1:G:124:GLY:HA3	1:G:142:TRP:HB3	1.82	0.60
2:L:56:ILE:O	2:L:56:ILE:CG2	2.49	0.60
1:C:40:ARG:O	1:C:278:THR:HG22	2.02	0.59
1:C:207:SER:O	1:C:211:ARG:NH2	2.32	0.59
1:E:40:ARG:O	1:E:278:THR:HG22	2.01	0.59
1:A:40:ARG:O	1:A:278:THR:HG22	2.02	0.59
2:J:56:ILE:CG2	2:J:56:ILE:O	2.50	0.58
1:C:124:GLY:HA3	1:C:142:TRP:HB3	1.85	0.58
1:I:207:SER:O	1:I:211:ARG:NH2	2.32	0.58
1:E:124:GLY:HA3	1:E:142:TRP:HB3	1.85	0.58
1:A:124:GLY:HA3	1:A:142:TRP:HB3	1.86	0.57
2:J:169:ASN:N	2:J:169:ASN:OD1	2.37	0.57
2:L:169:ASN:N	2:L:169:ASN:OD1	2.37	0.57
1:G:47:ARG:NH1	1:G:73:SER:OG	2.38	0.56
2:H:169:ASN:N	2:H:169:ASN:OD1	2.38	0.56
1:I:47:ARG:NH1	1:I:73:SER:OG	2.39	0.56
1:G:298:ARG:HG2	2:H:92:TRP:CE2	2.41	0.56
1:G:163:ARG:HG3	1:G:250:PHE:CZ	2.41	0.55
1:I:163:ARG:HG3	1:I:250:PHE:CZ	2.42	0.55
1:K:163:ARG:HG3	1:K:250:PHE:CZ	2.41	0.55
1:C:163:ARG:HG3	1:C:250:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:HG3	1:A:250:PHE:CZ	2.43	0.54
1:K:298:ARG:HG2	2:L:92:TRP:CE2	2.42	0.54
1:E:163:ARG:HG3	1:E:250:PHE:CZ	2.43	0.54
2:D:128:GLU:HG3	2:D:170:ARG:HH21	1.73	0.54
2:F:128:GLU:HG3	2:F:170:ARG:HH21	1.73	0.53
1:A:195:VAL:HG12	1:A:200:TYR:CE2	2.44	0.53
2:D:47:GLN:CD	2:D:110:LEU:HD11	2.34	0.53
1:I:298:ARG:HG2	2:J:92:TRP:CE2	2.44	0.52
2:B:141:PHE:CD1	2:B:170:ARG:HD2	2.44	0.52
2:D:115:MET:HE3	2:D:115:MET:HA	1.90	0.52
2:B:56:ILE:O	2:B:56:ILE:HG22	2.10	0.52
2:J:47:GLN:CD	2:J:110:LEU:HD11	2.35	0.52
2:F:56:ILE:O	2:F:56:ILE:HG22	2.10	0.51
1:A:200:TYR:CD2	1:A:200:TYR:C	2.88	0.51
1:A:195:VAL:CG1	1:A:200:TYR:HE2	2.23	0.51
2:F:47:GLN:CD	2:F:110:LEU:HD11	2.35	0.51
2:H:47:GLN:CD	2:H:110:LEU:HD11	2.36	0.50
2:L:47:GLN:CD	2:L:110:LEU:HD11	2.36	0.50
2:B:115:MET:HE3	2:B:115:MET:HA	1.92	0.50
2:F:115:MET:HE3	2:F:115:MET:HA	1.93	0.50
2:H:115:MET:HE3	2:H:115:MET:HA	1.94	0.50
2:B:47:GLN:CD	2:B:110:LEU:HD11	2.36	0.50
2:D:56:ILE:O	2:D:56:ILE:HG22	2.10	0.50
1:G:200:TYR:CD2	1:G:200:TYR:C	2.90	0.49
1:I:200:TYR:CD2	1:I:200:TYR:C	2.90	0.49
2:J:115:MET:HA	2:J:115:MET:HE3	1.94	0.49
2:L:115:MET:HE3	2:L:115:MET:HA	1.94	0.48
1:I:226:LEU:HD12	1:I:226:LEU:C	2.38	0.48
1:K:200:TYR:C	1:K:200:TYR:CD2	2.91	0.48
1:A:195:VAL:CG1	1:A:200:TYR:CE2	2.97	0.48
2:J:56:ILE:O	2:J:56:ILE:HG22	2.14	0.48
1:K:194:THR:HG23	1:K:237:SER:HB3	1.95	0.48
1:I:194:THR:HG23	1:I:237:SER:HB2	1.96	0.48
1:C:200:TYR:C	1:C:200:TYR:CD2	2.92	0.47
1:A:194:THR:HG23	1:A:237:SER:HB3	1.96	0.47
1:C:194:THR:HG23	1:C:237:SER:HB3	1.97	0.47
1:K:49:VAL:HG23	1:K:74:ALA:HB2	1.97	0.47
1:E:194:THR:HG23	1:E:237:SER:HB3	1.96	0.46
1:A:42:CYS:SG	1:A:278:THR:HG21	2.56	0.46
1:G:226:LEU:C	1:G:226:LEU:HD12	2.40	0.46
1:G:194:THR:HG23	1:G:237:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:ILE:O	2:H:56:ILE:HG22	2.14	0.46
2:L:56:ILE:O	2:L:56:ILE:HG22	2.15	0.46
1:A:199:ASN:ND2	1:A:199:ASN:C	2.74	0.46
1:K:42:CYS:SG	1:K:278:THR:HG21	2.56	0.45
1:C:49:VAL:HG23	1:C:74:ALA:HB2	1.98	0.45
1:I:49:VAL:HG23	1:I:74:ALA:HB2	1.97	0.45
1:G:42:CYS:SG	1:G:278:THR:HG21	2.57	0.45
1:E:200:TYR:C	1:E:200:TYR:CD2	2.94	0.45
1:A:49:VAL:HG23	1:A:74:ALA:HB2	1.98	0.45
1:C:42:CYS:SG	1:C:278:THR:HG21	2.56	0.45
1:G:49:VAL:HG23	1:G:74:ALA:HB2	1.97	0.45
1:A:20:THR:O	2:D:50:GLY:HA3	2.16	0.45
1:E:42:CYS:SG	1:E:278:THR:HG21	2.56	0.45
2:B:6:ILE:HD11	2:B:25:ARG:HB3	2.00	0.44
2:J:6:ILE:HD11	2:J:25:ARG:HB3	2.00	0.44
2:L:72:GLU:OE2	4:L:500:NAG:H83	2.17	0.44
1:E:41:ILE:HD11	1:E:260:SER:OG	2.18	0.44
1:E:49:VAL:HG23	1:E:74:ALA:HB2	1.98	0.44
2:L:6:ILE:HD11	2:L:25:ARG:HB3	1.99	0.44
1:I:42:CYS:SG	1:I:278:THR:HG21	2.57	0.44
1:K:226:LEU:C	1:K:226:LEU:HD12	2.42	0.44
1:I:121:ARG:NH2	1:I:144:LEU:HD23	2.33	0.43
1:E:226:LEU:HD12	1:E:226:LEU:C	2.43	0.43
1:G:121:ARG:NH2	1:G:144:LEU:HD23	2.33	0.43
1:A:121:ARG:HD3	1:A:145:SER:O	2.17	0.43
2:D:25:ARG:HA	2:D:33:GLY:O	2.19	0.43
2:B:25:ARG:HA	2:B:33:GLY:O	2.18	0.43
1:C:226:LEU:C	1:C:226:LEU:HD12	2.44	0.43
2:F:6:ILE:HD11	2:F:25:ARG:HB3	1.99	0.43
1:G:41:ILE:HD11	1:G:260:SER:OG	2.19	0.43
1:K:121:ARG:NH2	1:K:144:LEU:HD23	2.34	0.43
1:E:298:ARG:HG2	2:F:92:TRP:CE2	2.54	0.43
2:H:6:ILE:HD11	2:H:25:ARG:HB3	2.00	0.43
1:I:272:CYS:HB2	1:I:295:LYS:O	2.19	0.43
1:K:41:ILE:HD11	1:K:260:SER:OG	2.19	0.43
1:C:272:CYS:HB2	1:C:295:LYS:O	2.19	0.43
1:C:32:THR:HG23	1:C:285:PHE:HD1	1.84	0.42
1:K:136:PHE:CG	1:K:137:TYR:N	2.87	0.42
1:C:312:LYS:HG3	2:D:108:ILE:HG23	2.01	0.42
1:I:41:ILE:HD11	1:I:260:SER:OG	2.18	0.42
1:A:41:ILE:HD11	1:A:260:SER:OG	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:LYS:O	1:G:184:LYS:HG3	2.19	0.42
1:G:272:CYS:HB2	1:G:295:LYS:O	2.19	0.42
1:A:272:CYS:HB2	1:A:295:LYS:O	2.19	0.42
1:C:41:ILE:HD11	1:C:260:SER:OG	2.18	0.42
1:K:272:CYS:HB2	1:K:295:LYS:O	2.19	0.42
2:F:25:ARG:HA	2:F:33:GLY:O	2.19	0.42
1:I:184:LYS:O	1:I:184:LYS:HG3	2.19	0.42
1:G:136:PHE:CG	1:G:137:TYR:N	2.88	0.42
1:A:136:PHE:CG	1:A:137:TYR:N	2.88	0.42
2:J:25:ARG:HA	2:J:33:GLY:O	2.20	0.42
1:E:272:CYS:HB2	1:E:295:LYS:O	2.19	0.41
1:I:136:PHE:CG	1:I:137:TYR:N	2.89	0.41
1:E:32:THR:HG23	1:E:285:PHE:HD1	1.84	0.41
1:C:298:ARG:HG2	2:D:92:TRP:CE2	2.55	0.41
1:A:226:LEU:HD12	1:A:226:LEU:C	2.45	0.41
1:K:291:ARG:HH21	2:L:67:ASP:HB3	1.86	0.41
2:D:24:PHE:O	2:D:34:THR:HA	2.21	0.41
2:F:119:TYR:OH	2:F:132:GLU:OE2	2.31	0.41
1:C:136:PHE:CG	1:C:137:TYR:N	2.89	0.41
1:E:135:SER:OG	1:E:136:PHE:N	2.54	0.41
1:G:135:SER:OG	1:G:136:PHE:N	2.54	0.41
2:H:25:ARG:HA	2:H:33:GLY:O	2.20	0.41
1:K:32:THR:HG23	1:K:285:PHE:HD1	1.86	0.41
1:A:135:SER:OG	1:A:136:PHE:N	2.53	0.40
1:K:135:SER:OG	1:K:136:PHE:N	2.53	0.40
2:L:141:PHE:O	2:L:166:ALA:HA	2.21	0.40
2:J:24:PHE:O	2:J:34:THR:HA	2.22	0.40
2:H:141:PHE:O	2:H:166:ALA:HA	2.21	0.40
1:I:32:THR:HG23	1:I:285:PHE:HD1	1.85	0.40
1:I:43:SER:O	1:I:44:LYS:C	2.65	0.40
1:E:291:ARG:HH21	2:F:67:ASP:HB3	1.86	0.40
1:G:43:SER:O	1:G:44:LYS:C	2.65	0.40
1:K:49:VAL:CG2	1:K:74:ALA:HB2	2.52	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ASN:OD1	1:G:149:ASN:OD1[2_654]	2.13	0.07
1:A:149:ASN:OD1	1:I:149:ASN:OD1[4_545]	2.14	0.06
1:E:149:ASN:OD1	1:K:149:ASN:OD1[3_644]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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	314/325 (97%)	293 (93%)	19 (6%)	2 (1%)	21	52
1	C	314/325 (97%)	291 (93%)	21 (7%)	2 (1%)	21	52
1	E	314/325 (97%)	293 (93%)	19 (6%)	2 (1%)	21	52
1	G	314/325 (97%)	292 (93%)	19 (6%)	3 (1%)	12	41
1	I	314/325 (97%)	292 (93%)	19 (6%)	3 (1%)	12	41
1	K	314/325 (97%)	292 (93%)	19 (6%)	3 (1%)	12	41
2	B	165/181 (91%)	154 (93%)	11 (7%)	0	100	100
2	D	165/181 (91%)	155 (94%)	10 (6%)	0	100	100
2	F	165/181 (91%)	155 (94%)	10 (6%)	0	100	100
2	H	162/181 (90%)	153 (94%)	9 (6%)	0	100	100
2	J	162/181 (90%)	151 (93%)	11 (7%)	0	100	100
2	L	162/181 (90%)	151 (93%)	11 (7%)	0	100	100
All	All	2865/3036 (94%)	2672 (93%)	178 (6%)	15 (0%)	24	57

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	199	ASN
1	E	199	ASN
1	G	199	ASN
1	I	199	ASN
1	K	199	ASN
1	G	149	ASN
1	A	149	ASN
1	C	149	ASN
1	E	149	ASN
1	I	149	ASN
1	K	149	ASN
1	A	199	ASN

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Mol	Chain	Res	Type
1	G	271	ASP
1	I	271	ASP
1	K	271	ASP

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	264/271 (97%)	233 (88%)	31 (12%)	5	22
1	C	264/271 (97%)	230 (87%)	34 (13%)	4	18
1	E	264/271 (97%)	234 (89%)	30 (11%)	5	23
1	G	264/271 (97%)	232 (88%)	32 (12%)	5	20
1	I	264/271 (97%)	231 (88%)	33 (12%)	4	19
1	K	264/271 (97%)	233 (88%)	31 (12%)	5	22
2	B	144/155 (93%)	131 (91%)	13 (9%)	9	33
2	D	144/155 (93%)	131 (91%)	13 (9%)	9	33
2	F	144/155 (93%)	131 (91%)	13 (9%)	9	33
2	H	142/155 (92%)	126 (89%)	16 (11%)	5	23
2	J	142/155 (92%)	126 (89%)	16 (11%)	5	23
2	L	142/155 (92%)	125 (88%)	17 (12%)	5	21
All	All	2442/2556 (96%)	2163 (89%)	279 (11%)	5	23

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	11	SER
1	A	19	LEU
1	A	20	THR
1	A	32	THR
1	A	36	THR
1	A	37	ASN

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Mol	Chain	Res	Type
1	A	65	GLN
1	A	68	GLN
1	A	116	THR
1	A	122	THR
1	A	140	MET
1	A	144	LEU
1	A	146	ASN
1	A	163	ARG
1	A	176	SER
1	A	181	GLU
1	A	194	THR
1	A	195	VAL
1	A	199	ASN
1	A	200	TYR
1	A	201	GLN
1	A	202	GLN
1	A	205	VAL
1	A	207	SER
1	A	218	SER
1	A	227	MET
1	A	228	LEU
1	A	237	SER
1	A	256	MET
1	A	271	ASP
2	B	18	ILE
2	B	25	ARG
2	B	48	ILE
2	B	59	THR
2	B	65	LEU
2	B	66	ILE
2	B	71	THR
2	B	75	LYS
2	B	116	ASP
2	B	126	LEU
2	B	129	ASN
2	B	133	ASP
2	B	147	ASP
1	C	8	HIS
1	C	11	SER
1	C	19	LEU
1	C	20	THR
1	C	32	THR

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Mol	Chain	Res	Type
1	C	36	THR
1	C	37	ASN
1	C	65	GLN
1	C	68	GLN
1	C	116	THR
1	C	121	ARG
1	C	122	THR
1	C	140	MET
1	C	144	LEU
1	C	146	ASN
1	C	157	LYS
1	C	163	ARG
1	C	164	LYS
1	C	176	SER
1	C	181	GLU
1	C	194	THR
1	C	200	TYR
1	C	201	GLN
1	C	202	GLN
1	C	205	VAL
1	C	207	SER
1	C	218	SER
1	C	227	MET
1	C	228	LEU
1	C	235	THR
1	C	237	SER
1	C	249	SER
1	C	256	MET
1	C	271	ASP
2	D	18	ILE
2	D	25	ARG
2	D	48	ILE
2	D	65	LEU
2	D	66	ILE
2	D	71	THR
2	D	75	LYS
2	D	116	ASP
2	D	126	LEU
2	D	129	ASN
2	D	133	ASP
2	D	147	ASP
2	D	167	MET

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Mol	Chain	Res	Type
1	E	8	HIS
1	E	11	SER
1	E	19	LEU
1	E	20	THR
1	E	32	THR
1	E	36	THR
1	E	37	ASN
1	E	65	GLN
1	E	68	GLN
1	E	116	THR
1	E	122	THR
1	E	140	MET
1	E	144	LEU
1	E	146	ASN
1	E	163	ARG
1	E	176	SER
1	E	181	GLU
1	E	194	THR
1	E	200	TYR
1	E	201	GLN
1	E	202	GLN
1	E	205	VAL
1	E	207	SER
1	E	218	SER
1	E	227	MET
1	E	228	LEU
1	E	235	THR
1	E	237	SER
1	E	256	MET
1	E	271	ASP
2	F	18	ILE
2	F	25	ARG
2	F	48	ILE
2	F	65	LEU
2	F	66	ILE
2	F	71	THR
2	F	75	LYS
2	F	116	ASP
2	F	126	LEU
2	F	129	ASN
2	F	133	ASP
2	F	147	ASP

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Mol	Chain	Res	Type
2	F	167	MET
1	G	8	HIS
1	G	11	SER
1	G	19	LEU
1	G	20	THR
1	G	32	THR
1	G	36	THR
1	G	37	ASN
1	G	65	GLN
1	G	68	GLN
1	G	116	THR
1	G	122	THR
1	G	140	MET
1	G	144	LEU
1	G	146	ASN
1	G	163	ARG
1	G	176	SER
1	G	181	GLU
1	G	184	LYS
1	G	194	THR
1	G	200	TYR
1	G	201	GLN
1	G	202	GLN
1	G	205	VAL
1	G	207	SER
1	G	218	SER
1	G	227	MET
1	G	228	LEU
1	G	231	ASN
1	G	235	THR
1	G	237	SER
1	G	256	MET
1	G	271	ASP
2	H	18	ILE
2	H	25	ARG
2	H	48	ILE
2	H	65	LEU
2	H	66	ILE
2	H	71	THR
2	H	74	GLU
2	H	75	LYS
2	H	116	ASP

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Mol	Chain	Res	Type
2	H	126	LEU
2	H	129	ASN
2	H	133	ASP
2	H	147	ASP
2	H	164	GLU
2	H	167	MET
2	H	169	ASN
1	I	8	HIS
1	I	11	SER
1	I	19	LEU
1	I	20	THR
1	I	32	THR
1	I	36	THR
1	I	37	ASN
1	I	44	LYS
1	I	65	GLN
1	I	68	GLN
1	I	116	THR
1	I	122	THR
1	I	140	MET
1	I	144	LEU
1	I	146	ASN
1	I	163	ARG
1	I	176	SER
1	I	181	GLU
1	I	184	LYS
1	I	194	THR
1	I	200	TYR
1	I	201	GLN
1	I	202	GLN
1	I	205	VAL
1	I	207	SER
1	I	218	SER
1	I	227	MET
1	I	228	LEU
1	I	231	ASN
1	I	235	THR
1	I	237	SER
1	I	256	MET
1	I	271	ASP
2	J	18	ILE
2	J	25	ARG

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Mol	Chain	Res	Type
2	J	48	ILE
2	J	65	LEU
2	J	66	ILE
2	J	71	THR
2	J	74	GLU
2	J	75	LYS
2	J	116	ASP
2	J	126	LEU
2	J	129	ASN
2	J	133	ASP
2	J	147	ASP
2	J	164	GLU
2	J	167	MET
2	J	169	ASN
1	K	8	HIS
1	K	11	SER
1	K	19	LEU
1	K	20	THR
1	K	32	THR
1	K	36	THR
1	K	37	ASN
1	K	65	GLN
1	K	68	GLN
1	K	116	THR
1	K	122	THR
1	K	140	MET
1	K	144	LEU
1	K	146	ASN
1	K	163	ARG
1	K	176	SER
1	K	181	GLU
1	K	194	THR
1	K	200	TYR
1	K	201	GLN
1	K	202	GLN
1	K	205	VAL
1	K	207	SER
1	K	218	SER
1	K	227	MET
1	K	228	LEU
1	K	231	ASN
1	K	235	THR

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Mol	Chain	Res	Type
1	K	237	SER
1	K	256	MET
1	K	271	ASP
2	L	18	ILE
2	L	25	ARG
2	L	48	ILE
2	L	56	ILE
2	L	65	LEU
2	L	66	ILE
2	L	71	THR
2	L	74	GLU
2	L	75	LYS
2	L	116	ASP
2	L	126	LEU
2	L	129	ASN
2	L	133	ASP
2	L	147	ASP
2	L	164	GLU
2	L	167	MET
2	L	169	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	A	199	ASN
2	B	62	GLN
2	B	155	ASN
2	B	159	HIS
2	D	27	GLN
2	D	62	GLN
2	D	155	ASN
1	E	165	ASN
2	F	62	GLN
2	F	155	ASN
2	F	159	HIS
2	H	47	GLN
2	H	62	GLN
2	H	155	ASN
2	H	159	HIS
1	I	161	ASN
2	J	62	GLN

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Mol	Chain	Res	Type
2	J	155	ASN
2	J	159	HIS
1	K	161	ASN
1	K	231	ASN
2	L	62	GLN
2	L	155	ASN
2	L	159	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 ⓘ

9 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	$\# Z > 2$
3	NAG	M	1	1,3	14,14,15	0.58	0	17,19,21	0.94	1 (5%)
3	NAG	M	2	3	14,14,15	0.86	0	17,19,21	1.40	3 (17%)
3	BMA	M	3	3	11,11,12	0.71	0	15,15,17	1.33	2 (13%)
3	NAG	N	1	1,3	14,14,15	0.59	0	17,19,21	1.12	1 (5%)
3	NAG	N	2	3	14,14,15	0.61	0	17,19,21	1.84	4 (23%)
3	BMA	N	3	3	11,11,12	0.73	0	15,15,17	1.64	2 (13%)
3	NAG	O	1	1,3	14,14,15	0.65	0	17,19,21	1.56	2 (11%)
3	NAG	O	2	3	14,14,15	0.72	0	17,19,21	1.79	4 (23%)
3	BMA	O	3	3	11,11,12	0.84	0	15,15,17	1.37	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
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	BMA	M	3	3	-	2/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	BMA	O	3	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1	NAG	C1-C2-N2	-4.86	102.78	110.43
3	N	2	NAG	C1-O5-C5	4.16	117.76	112.19
3	O	2	NAG	O4-C4-C5	3.82	118.73	109.32
3	N	2	NAG	O4-C4-C5	3.43	117.77	109.32
3	N	3	BMA	O5-C5-C6	3.33	114.14	107.66
3	N	3	BMA	C1-C2-C3	-3.20	104.98	109.64
3	M	3	BMA	C3-C4-C5	2.98	115.64	110.23
3	M	3	BMA	C1-C2-C3	-2.91	105.41	109.64
3	O	2	NAG	C1-C2-N2	2.77	114.80	110.43
3	O	2	NAG	C4-C3-C2	-2.70	107.05	111.02
3	M	2	NAG	C2-N2-C7	2.56	126.33	122.90
3	O	3	BMA	C3-C4-C5	2.53	114.83	110.23
3	N	2	NAG	C4-C3-C2	-2.51	107.34	111.02
3	N	1	NAG	C1-O5-C5	2.46	115.48	112.19
3	O	2	NAG	O7-C7-C8	-2.32	117.92	122.05
3	N	2	NAG	O7-C7-C8	-2.30	117.96	122.05
3	O	3	BMA	O5-C5-C6	2.29	112.12	107.66
3	O	1	NAG	C6-C5-C4	2.28	118.61	113.02
3	M	2	NAG	O7-C7-C8	-2.26	118.03	122.05
3	M	2	NAG	C6-C5-C4	2.13	118.26	113.02
3	M	1	NAG	O5-C5-C4	-2.01	105.94	110.83

There are no chirality outliers.

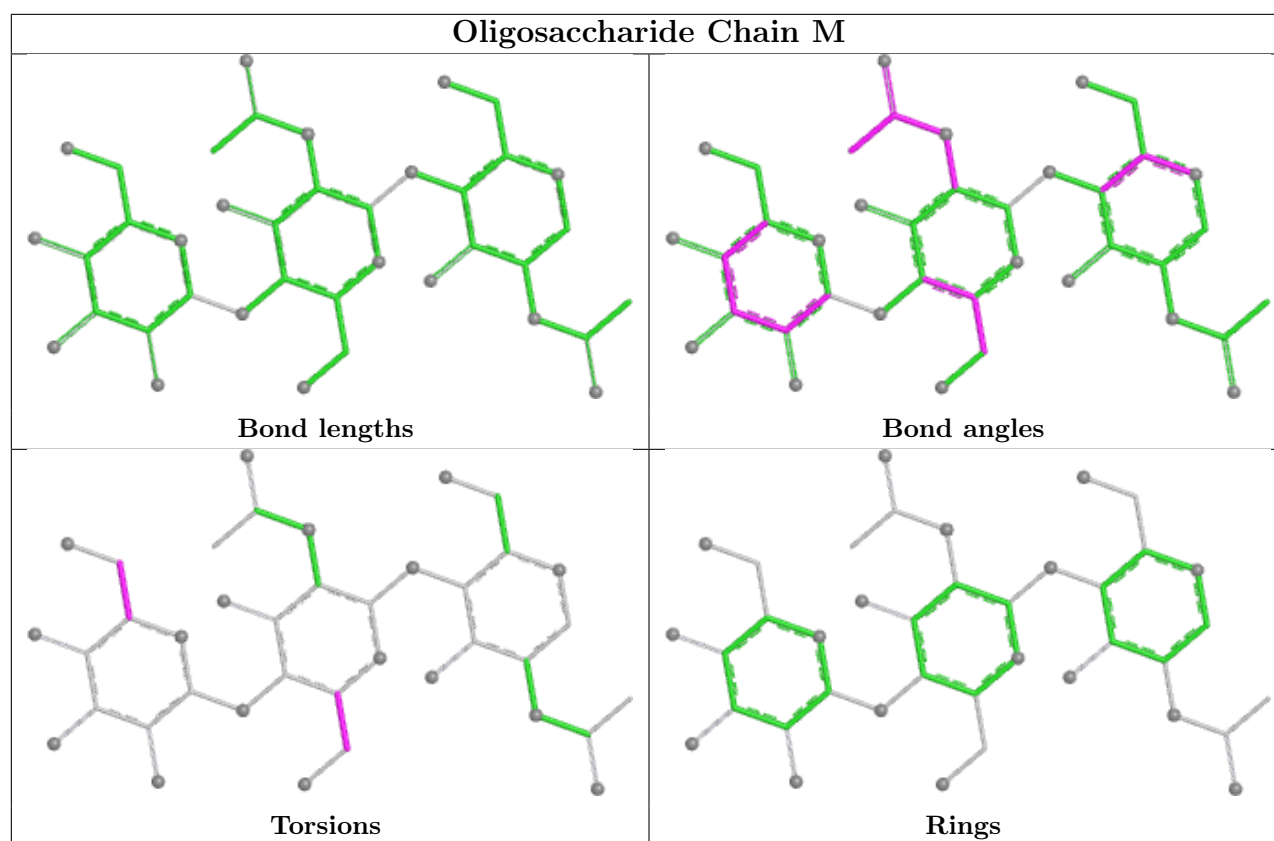
All (8) torsion outliers are listed below:

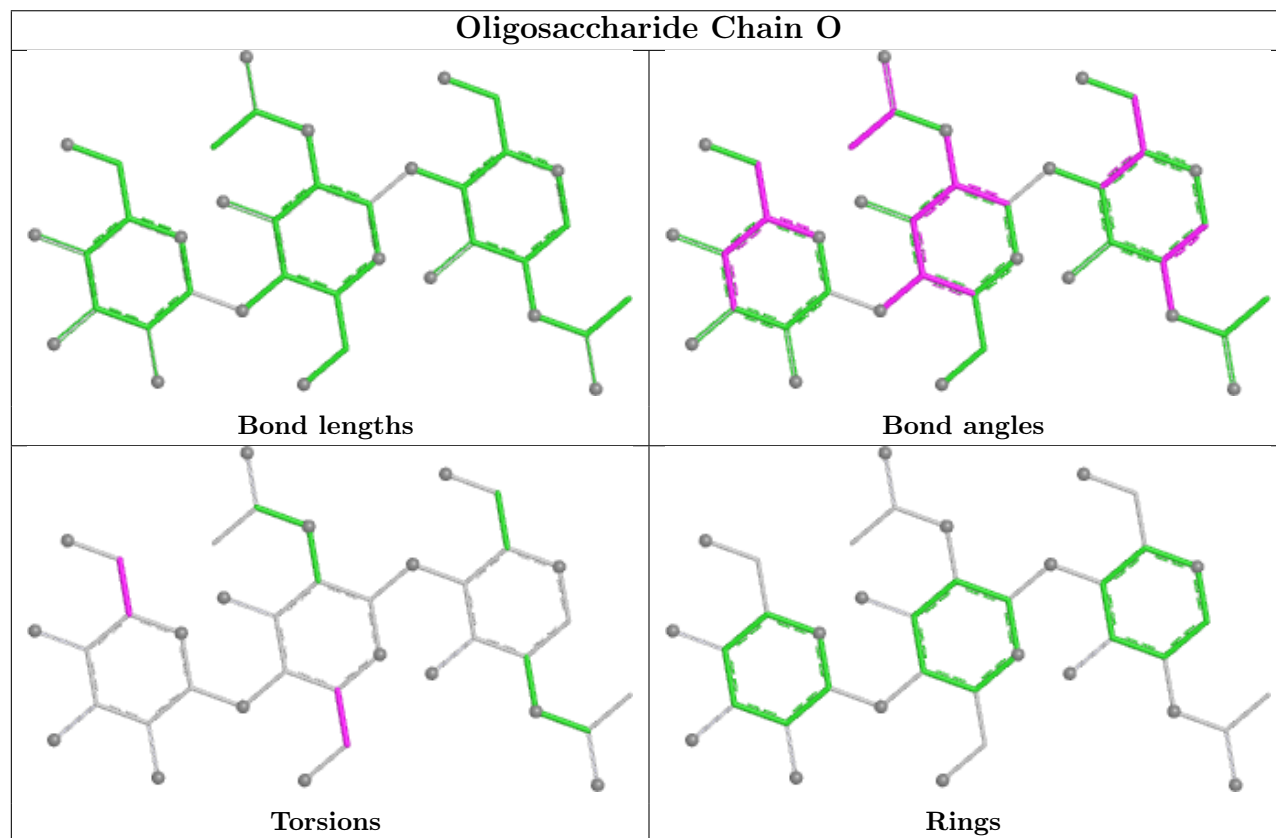
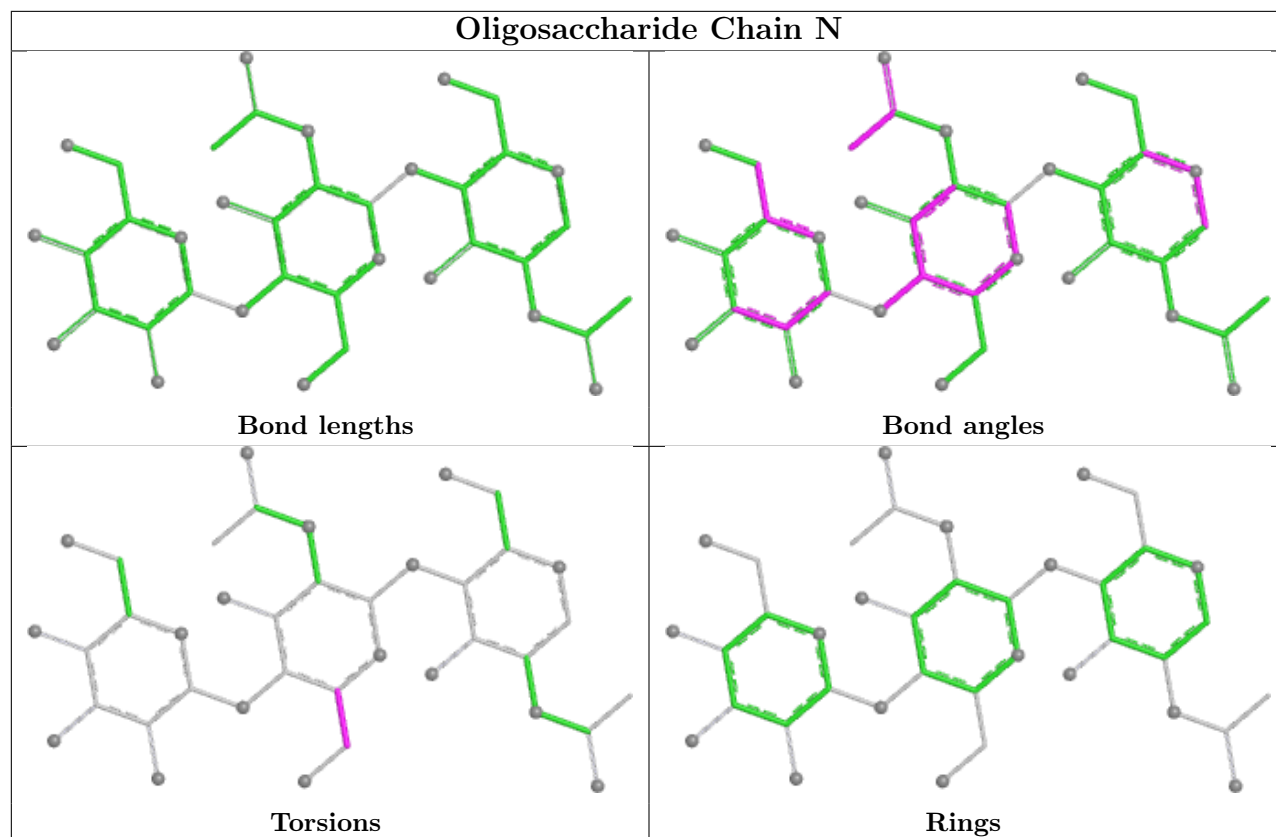
Mol	Chain	Res	Type	Atoms
3	M	2	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	M	3	BMA	O5-C5-C6-O6
3	M	3	BMA	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6

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

12 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
4	NAG	L	500	2	14,14,15	0.90	1 (7%)	17,19,21	1.78	4 (23%)
4	NAG	E	404	1	14,14,15	0.91	1 (7%)	17,19,21	1.37	2 (11%)
4	NAG	C	404	1	14,14,15	0.82	1 (7%)	17,19,21	1.75	3 (17%)
4	NAG	B	500	2	14,14,15	0.83	1 (7%)	17,19,21	2.59	6 (35%)
4	NAG	J	500	2	14,14,15	0.92	1 (7%)	17,19,21	1.64	2 (11%)
4	NAG	K	800	1	14,14,15	0.43	0	17,19,21	1.04	2 (11%)
4	NAG	G	800	1	14,14,15	0.47	0	17,19,21	1.93	5 (29%)
4	NAG	D	500	2	14,14,15	0.78	1 (7%)	17,19,21	2.38	4 (23%)
4	NAG	A	404	1	14,14,15	0.60	0	17,19,21	2.04	5 (29%)
4	NAG	I	800	1	14,14,15	0.42	0	17,19,21	1.25	2 (11%)
4	NAG	H	500	2	14,14,15	0.87	1 (7%)	17,19,21	1.89	2 (11%)
4	NAG	F	500	2	14,14,15	0.78	0	17,19,21	1.77	4 (23%)

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
4	NAG	L	500	2	-	0/6/23/26	0/1/1/1
4	NAG	E	404	1	-	3/6/23/26	0/1/1/1
4	NAG	C	404	1	-	1/6/23/26	0/1/1/1
4	NAG	B	500	2	-	1/6/23/26	0/1/1/1
4	NAG	J	500	2	-	2/6/23/26	0/1/1/1
4	NAG	K	800	1	-	1/6/23/26	0/1/1/1
4	NAG	G	800	1	-	0/6/23/26	0/1/1/1
4	NAG	D	500	2	-	0/6/23/26	0/1/1/1
4	NAG	A	404	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	800	1	-	0/6/23/26	0/1/1/1
4	NAG	H	500	2	-	0/6/23/26	0/1/1/1
4	NAG	F	500	2	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	500	NAG	C1-C2	2.83	1.56	1.52
4	J	500	NAG	C1-C2	2.59	1.55	1.52
4	H	500	NAG	C1-C2	2.50	1.55	1.52
4	E	404	NAG	C1-C2	2.47	1.55	1.52
4	B	500	NAG	C1-C2	2.44	1.55	1.52
4	C	404	NAG	C1-C2	2.34	1.55	1.52
4	D	500	NAG	C1-C2	2.03	1.55	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	500	NAG	C1-O5-C5	8.08	123.01	112.19
4	D	500	NAG	C1-O5-C5	7.71	122.52	112.19
4	H	500	NAG	C1-O5-C5	6.01	120.24	112.19
4	C	404	NAG	O5-C1-C2	-5.02	103.52	111.29
4	A	404	NAG	C4-C3-C2	-4.62	104.25	111.02
4	G	800	NAG	C1-C2-N2	-4.36	103.56	110.43
4	J	500	NAG	O5-C5-C6	4.24	115.91	107.66
4	L	500	NAG	C1-O5-C5	4.20	117.81	112.19
4	F	500	NAG	C1-O5-C5	4.11	117.70	112.19
4	G	800	NAG	C1-O5-C5	3.58	116.98	112.19
4	G	800	NAG	C4-C3-C2	-3.57	105.78	111.02
4	A	404	NAG	O5-C5-C6	3.56	114.60	107.66
4	L	500	NAG	O5-C5-C6	3.28	114.04	107.66
4	F	500	NAG	C3-C4-C5	-3.18	104.46	110.23
4	J	500	NAG	C1-O5-C5	3.17	116.43	112.19
4	A	404	NAG	C1-O5-C5	3.02	116.24	112.19
4	I	800	NAG	C1-O5-C5	2.93	116.11	112.19
4	B	500	NAG	O3-C3-C2	2.78	115.17	109.40
4	I	800	NAG	C4-C3-C2	-2.77	106.96	111.02
4	E	404	NAG	C4-C3-C2	2.77	115.08	111.02
4	B	500	NAG	C3-C4-C5	-2.75	105.24	110.23
4	B	500	NAG	O5-C5-C4	2.69	117.38	110.83
4	L	500	NAG	C6-C5-C4	-2.68	106.44	113.02
4	D	500	NAG	O5-C5-C4	2.62	117.19	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	NAG	O7-C7-C8	-2.49	117.62	122.05
4	D	500	NAG	C3-C4-C5	-2.45	105.80	110.23
4	C	404	NAG	C1-O5-C5	2.43	115.44	112.19
4	F	500	NAG	O4-C4-C5	2.37	115.17	109.32
4	E	404	NAG	C2-N2-C7	2.36	126.06	122.90
4	B	500	NAG	C1-C2-N2	2.32	114.09	110.43
4	C	404	NAG	C4-C3-C2	2.30	114.39	111.02
4	B	500	NAG	C4-C3-C2	-2.29	107.66	111.02
4	D	500	NAG	O3-C3-C2	2.26	114.10	109.40
4	G	800	NAG	C3-C4-C5	-2.23	106.19	110.23
4	K	800	NAG	C1-C2-N2	-2.17	107.02	110.43
4	A	404	NAG	O3-C3-C2	2.15	113.88	109.40
4	K	800	NAG	C4-C3-C2	-2.14	107.88	111.02
4	H	500	NAG	C1-C2-N2	2.13	113.79	110.43
4	F	500	NAG	O3-C3-C4	2.12	115.37	110.38
4	G	800	NAG	O4-C4-C5	2.06	114.39	109.32
4	L	500	NAG	O5-C1-C2	-2.01	108.19	111.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	404	NAG	C3-C2-N2-C7
4	J	500	NAG	O5-C5-C6-O6
4	A	404	NAG	O5-C5-C6-O6
4	J	500	NAG	C4-C5-C6-O6
4	A	404	NAG	C4-C5-C6-O6
4	E	404	NAG	O5-C5-C6-O6
4	F	500	NAG	O5-C5-C6-O6
4	C	404	NAG	O5-C5-C6-O6
4	E	404	NAG	C4-C5-C6-O6
4	K	800	NAG	C4-C5-C6-O6
4	B	500	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	500	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	316/325 (97%)	-0.38	1 (0%) 90 80	63, 96, 124, 151	1 (0%)
1	C	316/325 (97%)	-0.43	1 (0%) 90 80	60, 95, 120, 141	1 (0%)
1	E	316/325 (97%)	-0.46	0 100 100	62, 95, 122, 148	1 (0%)
1	G	316/325 (97%)	-0.37	0 100 100	72, 99, 129, 152	1 (0%)
1	I	316/325 (97%)	-0.38	0 100 100	71, 100, 126, 146	1 (0%)
1	K	316/325 (97%)	-0.43	0 100 100	73, 100, 127, 155	1 (0%)
2	B	167/181 (92%)	-0.39	0 100 100	58, 101, 127, 156	0
2	D	167/181 (92%)	-0.42	0 100 100	61, 98, 129, 155	0
2	F	167/181 (92%)	-0.43	0 100 100	56, 98, 124, 159	0
2	H	164/181 (90%)	-0.49	0 100 100	69, 107, 130, 168	0
2	J	164/181 (90%)	-0.45	0 100 100	73, 109, 130, 169	0
2	L	164/181 (90%)	-0.42	0 100 100	68, 110, 131, 170	0
All	All	2889/3036 (95%)	-0.42	2 (0%) 92 86	56, 100, 127, 170	6 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	86	VAL	2.8
1	A	253	GLY	2.1

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

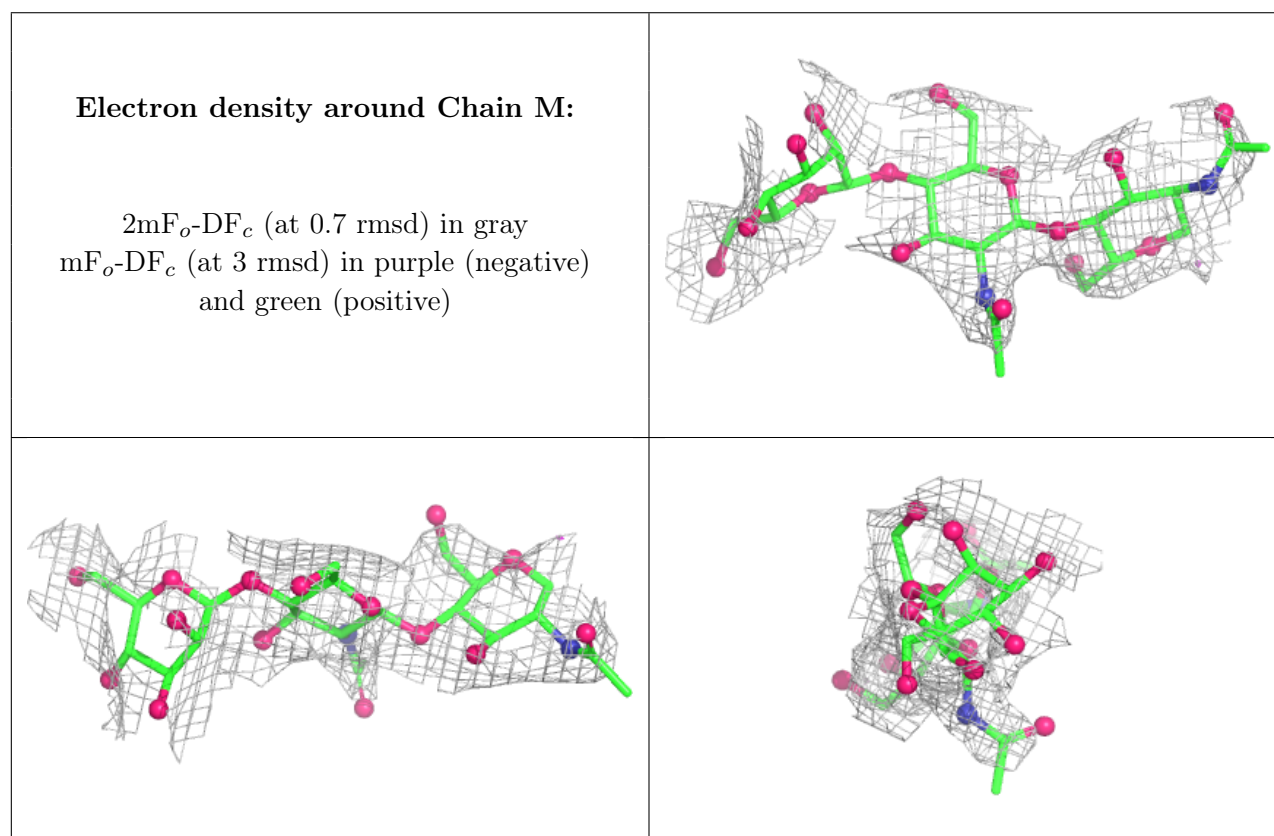
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

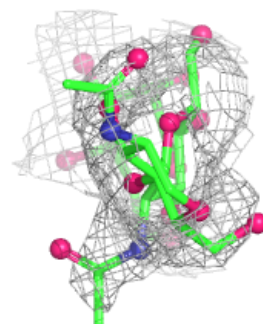
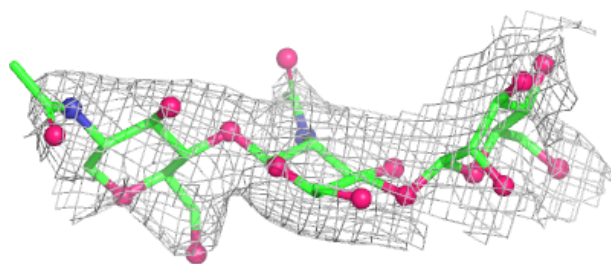
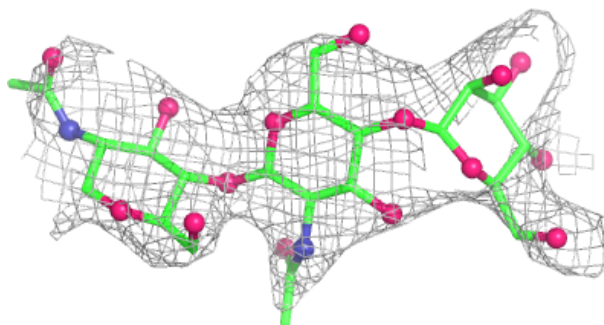
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	N	3	11/12	0.64	0.09	136,159,178,192	0
3	BMA	M	3	11/12	0.66	0.10	116,160,169,170	0
3	BMA	O	3	11/12	0.75	0.07	123,149,159,160	0
3	NAG	M	2	14/15	0.81	0.09	119,151,159,164	0
3	NAG	N	2	14/15	0.84	0.09	115,144,152,161	0
3	NAG	M	1	14/15	0.86	0.09	118,129,139,139	0
3	NAG	O	2	14/15	0.87	0.07	113,137,144,149	0
3	NAG	N	1	14/15	0.88	0.09	116,126,131,141	0
3	NAG	O	1	14/15	0.88	0.09	105,119,132,132	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.

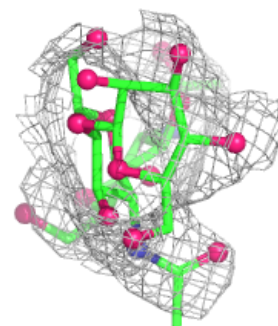
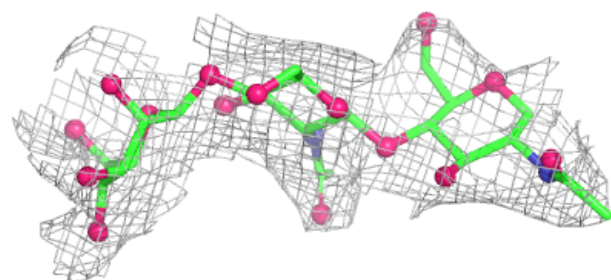
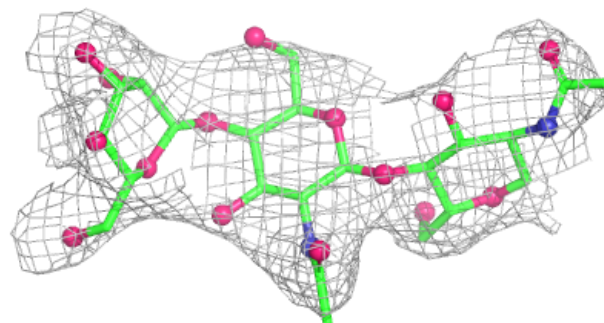


Electron density around Chain N:

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

**Electron density around Chain O:**

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
4	NAG	E	404	14/15	0.63	0.09	134,158,166,166	0
4	NAG	A	404	14/15	0.66	0.09	152,160,169,171	0
4	NAG	C	404	14/15	0.75	0.09	137,151,158,159	0
4	NAG	D	500	14/15	0.79	0.11	96,116,128,129	0
4	NAG	L	500	14/15	0.79	0.09	106,113,126,128	0
4	NAG	J	500	14/15	0.80	0.08	104,114,124,125	0
4	NAG	H	500	14/15	0.80	0.09	108,116,123,127	0
4	NAG	F	500	14/15	0.81	0.09	91,108,123,132	0
4	NAG	B	500	14/15	0.82	0.10	91,115,128,136	0
4	NAG	K	800	14/15	0.86	0.09	119,143,151,152	0
4	NAG	I	800	14/15	0.88	0.08	114,134,143,143	0
4	NAG	G	800	14/15	0.89	0.07	107,131,141,146	0

6.5 Other polymers

There are no such residues in this entry.