



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 11:15 AM EDT

PDB ID : 3M6S
Title : Crystal structure of H1N1pdm Hemagglutinin
Authors : Yang, H.; Carney, P.J.; Stevens, J.
Deposited on : 2010-03-16
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

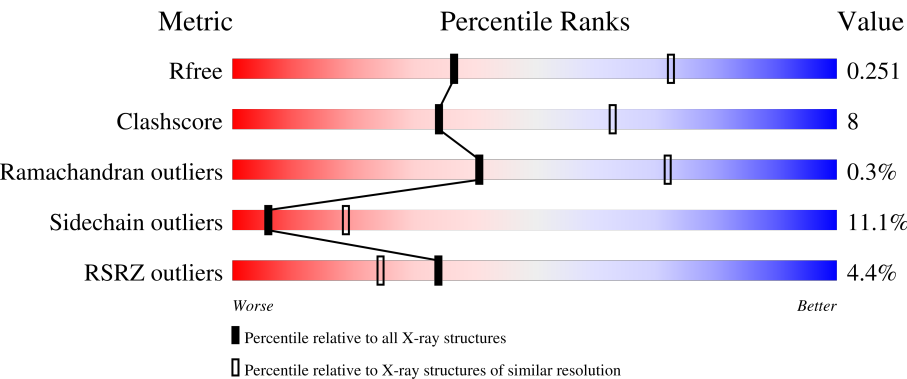
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	331	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>79%16% . .</div></div>
1	C	331	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>76%18% . .</div></div>
1	E	331	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>77%17% . .</div></div>
1	G	331	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>78%15% . . .</div></div>
1	I	331	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>79%15% . .</div></div>

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Mol	Chain	Length	Quality of chain
1	K	331	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	
3	M	2	
3	O	2	
3	P	2	
3	Q	2	
4	N	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	N	3	X	-	-	-
5	NAG	G	331	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 23587 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	325	Total	C	N	O	S	0	0	0
			2533	1602	435	485	11			
1	C	323	Total	C	N	O	S	0	0	0
			2518	1593	433	481	11			
1	E	323	Total	C	N	O	S	0	0	0
			2518	1593	433	481	11			
1	G	322	Total	C	N	O	S	0	0	0
			2514	1591	432	480	11			
1	I	322	Total	C	N	O	S	0	0	0
			2511	1588	432	480	11			
1	K	321	Total	C	N	O	S	0	0	0
			2506	1587	431	477	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP C5MV42
A	-2	ASP	-	expression tag	UNP C5MV42
A	-1	PRO	-	expression tag	UNP C5MV42
A	0	GLY	-	expression tag	UNP C5MV42
C	-3	ALA	-	expression tag	UNP C5MV42
C	-2	ASP	-	expression tag	UNP C5MV42
C	-1	PRO	-	expression tag	UNP C5MV42
C	0	GLY	-	expression tag	UNP C5MV42
E	-3	ALA	-	expression tag	UNP C5MV42
E	-2	ASP	-	expression tag	UNP C5MV42
E	-1	PRO	-	expression tag	UNP C5MV42
E	0	GLY	-	expression tag	UNP C5MV42
G	-3	ALA	-	expression tag	UNP C5MV42
G	-2	ASP	-	expression tag	UNP C5MV42
G	-1	PRO	-	expression tag	UNP C5MV42
G	0	GLY	-	expression tag	UNP C5MV42
I	-3	ALA	-	expression tag	UNP C5MV42

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	ASP	-	expression tag	UNP C5MV42
I	-1	PRO	-	expression tag	UNP C5MV42
I	0	GLY	-	expression tag	UNP C5MV42
K	-3	ALA	-	expression tag	UNP C5MV42
K	-2	ASP	-	expression tag	UNP C5MV42
K	-1	PRO	-	expression tag	UNP C5MV42
K	0	GLY	-	expression tag	UNP C5MV42

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	5	0	0
			1368	860	232	270	6			
2	D	171	Total	C	N	O	S	0	0	0
			1386	870	234	276	6			
2	F	171	Total	C	N	O	S	0	0	0
			1386	870	234	276	6			
2	H	170	Total	C	N	O	S	0	0	0
			1377	865	233	273	6			
2	J	170	Total	C	N	O	S	0	0	0
			1377	865	233	273	6			
2	L	171	Total	C	N	O	S	0	0	0
			1386	870	234	276	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	GLY	engineered mutation	UNP C5MV42
B	176	GLY	VAL	engineered mutation	UNP C5MV42
B	177	ARG	LYS	engineered mutation	UNP C5MV42
B	179	VAL	-	expression tag	UNP C5MV42
B	180	PRO	-	expression tag	UNP C5MV42
B	181	ARG	-	expression tag	UNP C5MV42
D	175	SER	GLY	engineered mutation	UNP C5MV42
D	176	GLY	VAL	engineered mutation	UNP C5MV42
D	177	ARG	LYS	engineered mutation	UNP C5MV42
D	179	VAL	-	expression tag	UNP C5MV42
D	180	PRO	-	expression tag	UNP C5MV42
D	181	ARG	-	expression tag	UNP C5MV42
F	175	SER	GLY	engineered mutation	UNP C5MV42
F	176	GLY	VAL	engineered mutation	UNP C5MV42
F	177	ARG	LYS	engineered mutation	UNP C5MV42

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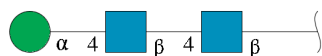
Chain	Residue	Modelled	Actual	Comment	Reference
F	179	VAL	-	expression tag	UNP C5MV42
F	180	PRO	-	expression tag	UNP C5MV42
F	181	ARG	-	expression tag	UNP C5MV42
H	175	SER	GLY	engineered mutation	UNP C5MV42
H	176	GLY	VAL	engineered mutation	UNP C5MV42
H	177	ARG	LYS	engineered mutation	UNP C5MV42
H	179	VAL	-	expression tag	UNP C5MV42
H	180	PRO	-	expression tag	UNP C5MV42
H	181	ARG	-	expression tag	UNP C5MV42
J	175	SER	GLY	engineered mutation	UNP C5MV42
J	176	GLY	VAL	engineered mutation	UNP C5MV42
J	177	ARG	LYS	engineered mutation	UNP C5MV42
J	179	VAL	-	expression tag	UNP C5MV42
J	180	PRO	-	expression tag	UNP C5MV42
J	181	ARG	-	expression tag	UNP C5MV42
L	175	SER	GLY	engineered mutation	UNP C5MV42
L	176	GLY	VAL	engineered mutation	UNP C5MV42
L	177	ARG	LYS	engineered mutation	UNP C5MV42
L	179	VAL	-	expression tag	UNP C5MV42
L	180	PRO	-	expression tag	UNP C5MV42
L	181	ARG	-	expression tag	UNP C5MV42

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



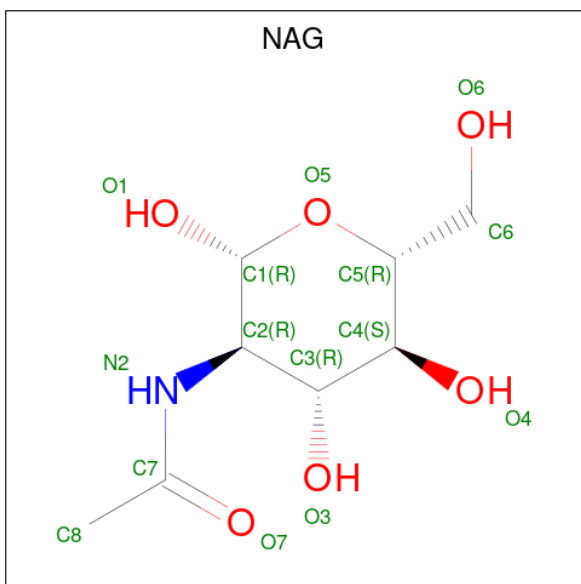
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-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
4	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

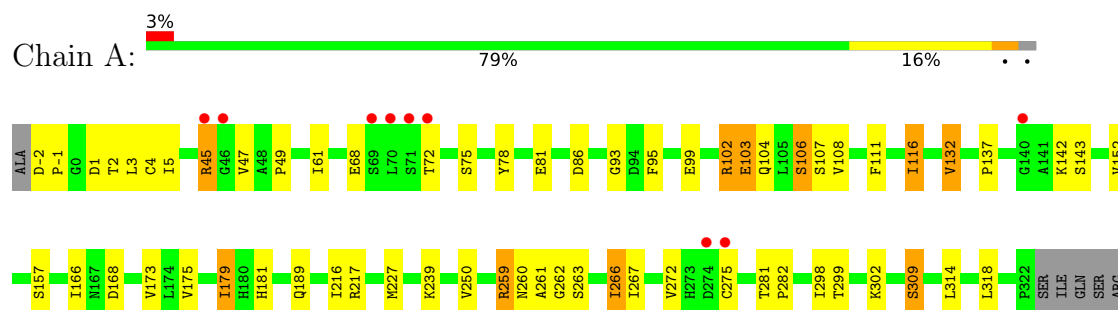


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

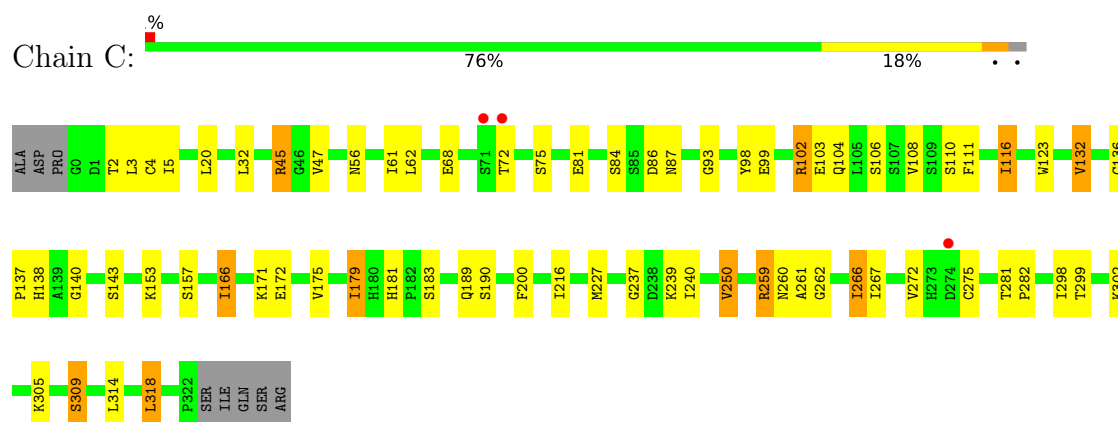
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

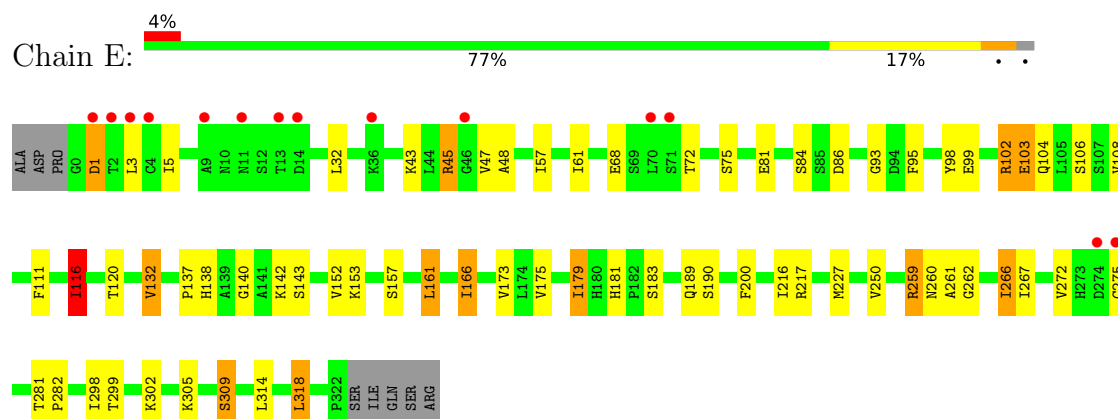
• Molecule 1: Hemagglutinin



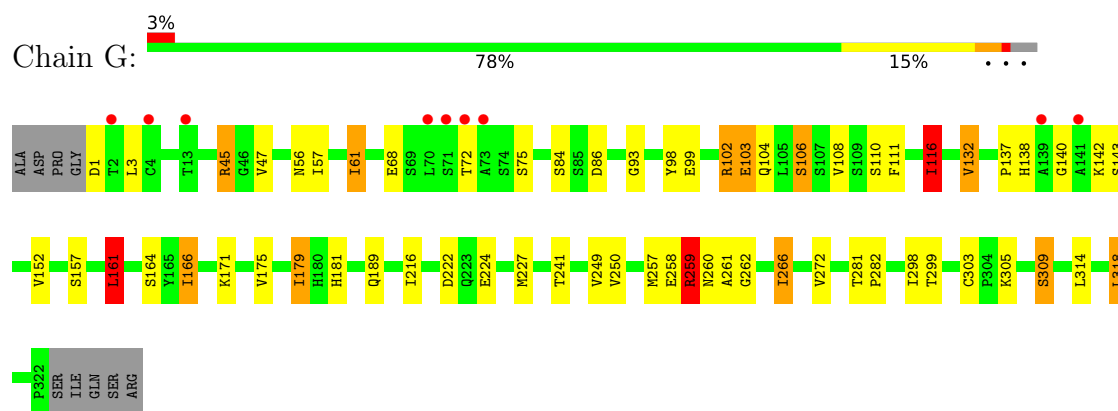
• Molecule 1: Hemagglutinin



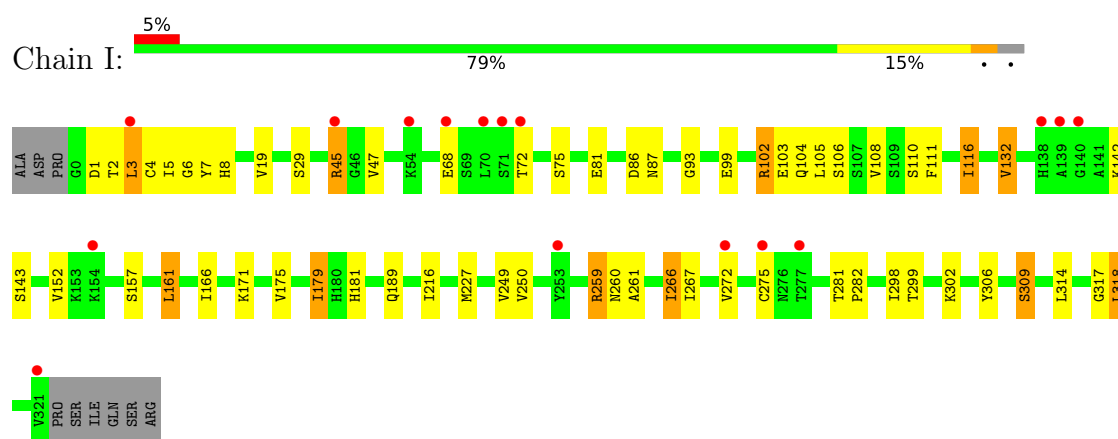
• Molecule 1: Hemagglutinin



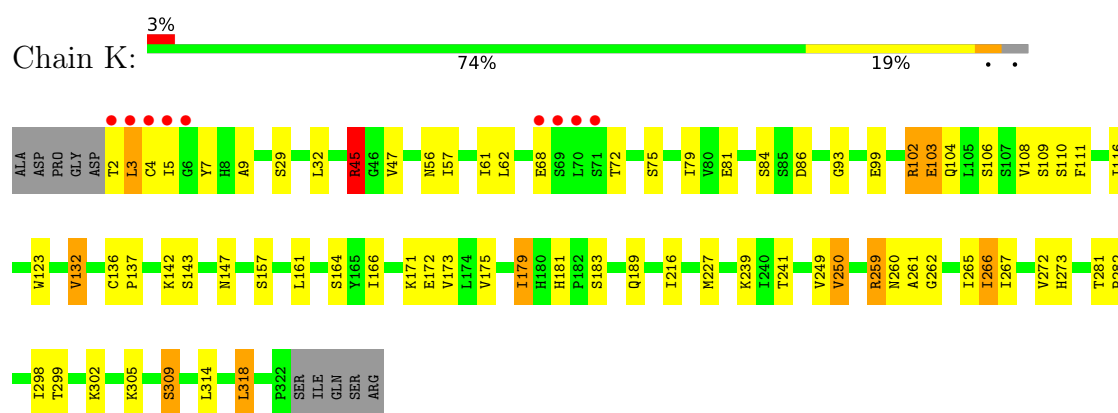
• Molecule 1: Hemagglutinin



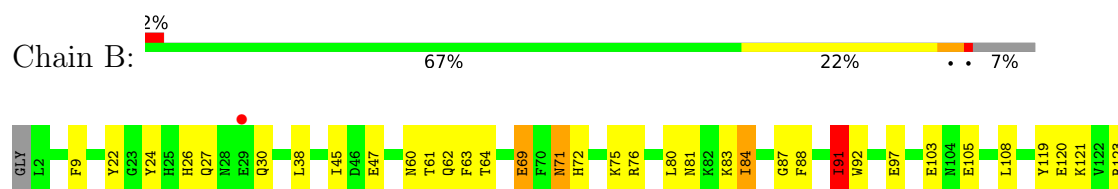
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin



• Molecule 2: Hemagglutinin





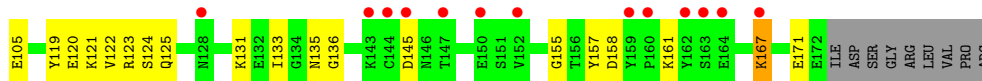
• Molecule 2: Hemagglutinin

Chain D: 70% 20% 6%



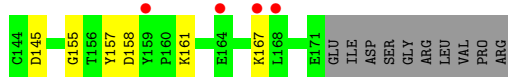
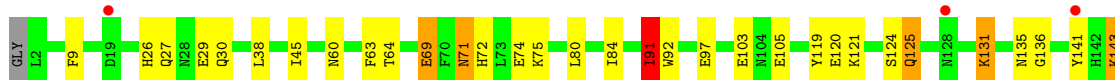
• Molecule 2: Hemagglutinin

Chain F: 70% 22% 6%



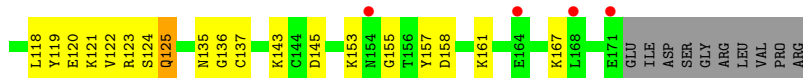
• Molecule 2: Hemagglutinin

Chain H: 73% 18% 6%



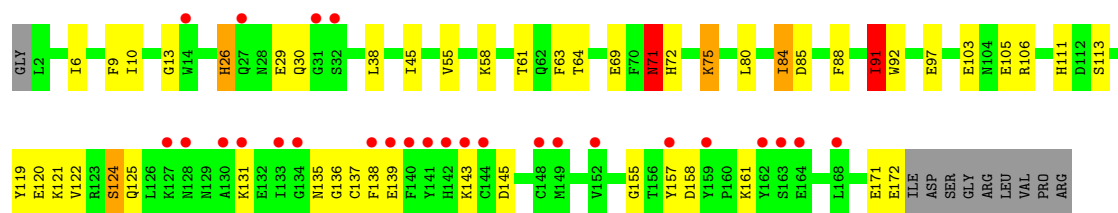
• Molecule 2: Hemagglutinin

Chain J: 66% 25% 6%



• Molecule 2: Hemagglutinin

Chain L: 67% 24% 6%



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

Chain M: 50%



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

Chain O: 100%



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

Chain P: 50%



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

Chain Q: 100%



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

Chain N: 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.98Å 109.71Å 129.90Å 86.25° 74.68° 75.10°	Depositor
Resolution (Å)	50.00 – 2.80 48.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.80) 98.1 (48.87-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.230 , 0.256 0.227 , 0.251	Depositor DCC
R_{free} test set	4608 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23587	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, 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	0.75	0/2597	0.83	1/3530 (0.0%)
1	C	0.79	1/2581 (0.0%)	0.84	2/3507 (0.1%)
1	E	0.71	0/2581	0.80	2/3507 (0.1%)
1	G	0.86	1/2577 (0.0%)	0.88	4/3502 (0.1%)
1	I	0.68	0/2573	0.78	1/3495 (0.0%)
1	K	0.75	0/2569	0.82	2/3491 (0.1%)
2	B	0.71	0/1396	0.79	3/1881 (0.2%)
2	D	0.77	0/1414	0.78	2/1905 (0.1%)
2	F	0.68	0/1414	0.73	1/1905 (0.1%)
2	H	0.75	1/1405 (0.1%)	0.72	1/1893 (0.1%)
2	J	0.77	1/1405 (0.1%)	0.75	2/1893 (0.1%)
2	L	0.73	0/1414	0.74	3/1905 (0.2%)
All	All	0.75	4/23926 (0.0%)	0.80	24/32414 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	258	GLU	CG-CD	6.18	1.61	1.51
1	C	4	CYS	CB-SG	-5.94	1.72	1.81
2	J	137	CYS	CB-SG	5.78	1.92	1.82
2	H	74	GLU	CG-CD	5.42	1.60	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	LYS	CB-CA-C	9.40	129.19	110.40
2	L	91	ILE	CG1-CB-CG2	-8.03	93.73	111.40
2	B	91	ILE	CG1-CB-CG2	-7.20	95.55	111.40
2	D	91	ILE	CG1-CB-CG2	-6.26	97.62	111.40
2	H	91	ILE	CG1-CB-CG2	-6.16	97.85	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	45	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	K	56	ASN	CB-CA-C	-6.02	98.36	110.40
2	F	91	ILE	CG1-CB-CG2	-5.95	98.31	111.40
1	G	56	ASN	CB-CA-C	-5.71	98.99	110.40
2	B	143	LYS	CA-CB-CG	5.56	125.63	113.40
1	G	161	LEU	CB-CG-CD1	-5.50	101.64	111.00
2	J	91	ILE	CG1-CB-CG2	-5.39	99.54	111.40
1	A	116	ILE	CB-CA-C	-5.36	100.87	111.60
2	L	71	ASN	CB-CA-C	5.35	121.10	110.40
1	G	116	ILE	CB-CA-C	-5.31	100.99	111.60
2	L	75	LYS	CD-CE-NZ	5.20	123.67	111.70
1	G	259	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	116	ILE	CB-CA-C	-5.14	101.33	111.60
1	E	116	ILE	CB-CA-C	-5.11	101.37	111.60
2	J	71	ASN	N-CA-CB	-5.09	101.44	110.60
1	C	56	ASN	CB-CA-C	-5.06	100.28	110.40
1	E	161	LEU	CA-CB-CG	5.06	126.93	115.30
2	D	71	ASN	CB-CA-C	5.03	120.47	110.40
1	I	161	LEU	CA-CB-CG	5.02	126.85	115.30

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	2533	0	2483	40	1
1	C	2518	0	2472	52	0
1	E	2518	0	2472	43	1
1	G	2514	0	2466	36	2
1	I	2511	0	2464	62	0
1	K	2506	0	2460	59	1
2	B	1368	0	1293	36	3
2	D	1386	0	1305	41	0
2	F	1386	0	1305	38	0
2	H	1377	0	1299	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1377	0	1299	56	0
2	L	1386	0	1305	45	0
3	M	28	0	25	2	0
3	O	28	0	24	2	0
3	P	28	0	25	1	0
3	Q	28	0	25	0	0
4	N	39	0	34	1	0
5	A	14	0	13	1	0
5	E	14	0	13	1	0
5	G	28	0	26	0	0
All	All	23587	0	22808	390	4

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 8.

All (390) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:45:ARG:HG3	1:I:45:ARG:HH11	1.07	1.10
1:E:45:ARG:HG3	1:E:45:ARG:HH11	1.09	1.10
1:I:5:ILE:HD13	2:J:24:TYR:CD1	1.87	1.09
1:I:4:CYS:O	2:J:24:TYR:HA	1.52	1.09
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.14	1.08
1:G:45:ARG:HG3	1:G:45:ARG:HH11	1.17	1.07
1:I:5:ILE:CD1	2:J:24:TYR:CE1	2.39	1.05
2:J:91:ILE:HG22	2:L:92:TRP:CZ2	1.91	1.04
1:C:45:ARG:HG3	1:C:45:ARG:HH11	1.21	1.03
1:I:309:SER:HB3	2:J:97:GLU:OE2	1.66	0.96
1:K:5:ILE:HG13	2:L:119:TYR:HA	1.45	0.96
1:K:45:ARG:HG3	1:K:45:ARG:HH11	1.31	0.95
1:I:45:ARG:HG3	1:I:45:ARG:NH1	1.80	0.93
1:K:2:THR:HA	2:L:138:PHE:O	1.70	0.91
2:D:84:ILE:HD11	2:F:83:LYS:HE3	1.52	0.91
2:D:92:TRP:CZ2	2:F:91:ILE:HG22	2.06	0.90
1:I:5:ILE:HD13	2:J:24:TYR:HD1	1.37	0.89
1:A:45:ARG:HG3	1:A:45:ARG:NH1	1.87	0.88
2:B:92:TRP:CZ2	2:D:91:ILE:HG22	2.09	0.88
1:I:5:ILE:CD1	2:J:24:TYR:HE1	1.81	0.86
1:G:45:ARG:HG3	1:G:45:ARG:NH1	1.89	0.86
1:I:5:ILE:HD12	2:J:24:TYR:CE1	2.11	0.86
2:B:76:ARG:HG2	1:E:103:GLU:HG3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:309:SER:HB3	2:L:97:GLU:OE2	1.76	0.85
1:E:45:ARG:HG3	1:E:45:ARG:NH1	1.82	0.85
1:E:309:SER:HB3	2:F:97:GLU:OE2	1.78	0.83
1:C:45:ARG:HG3	1:C:45:ARG:NH1	1.92	0.83
1:C:259:ARG:HH11	1:C:259:ARG:HG2	1.43	0.82
2:B:83:LYS:HE3	2:F:84:ILE:HD11	1.59	0.82
1:E:259:ARG:HG2	1:E:259:ARG:HH11	1.44	0.82
2:B:91:ILE:HG22	2:F:92:TRP:CZ2	2.14	0.81
1:I:45:ARG:HH11	1:I:45:ARG:CG	1.90	0.81
1:G:309:SER:HB3	2:H:97:GLU:OE2	1.80	0.80
2:D:167:LYS:O	2:D:171:GLU:HG3	1.81	0.80
1:I:4:CYS:O	2:J:24:TYR:CA	2.29	0.80
1:I:5:ILE:HD11	2:J:122:VAL:HG21	1.64	0.80
1:I:99:GLU:CD	2:J:71:ASN:HB2	2.02	0.80
1:I:259:ARG:HG2	1:I:259:ARG:HH11	1.47	0.80
2:J:91:ILE:HG22	2:L:92:TRP:CE2	2.17	0.80
1:G:45:ARG:HH11	1:G:45:ARG:CG	1.95	0.79
2:B:84:ILE:HD11	2:D:83:LYS:HE3	1.64	0.79
1:K:259:ARG:HG2	1:K:259:ARG:HH11	1.50	0.77
1:A:309:SER:HB3	2:B:97:GLU:OE2	1.86	0.76
1:C:166:ILE:HD11	1:K:260:ASN:OD1	1.86	0.76
1:A:45:ARG:HH11	1:A:45:ARG:CG	1.97	0.76
1:K:45:ARG:HG3	1:K:45:ARG:NH1	2.00	0.75
1:E:45:ARG:HH11	1:E:45:ARG:CG	1.94	0.75
2:L:125:GLN:OE1	2:L:155:GLY:HA2	1.88	0.74
1:A:259:ARG:HG2	1:A:259:ARG:HH11	1.52	0.73
2:J:83:LYS:HE3	2:L:84:ILE:HD11	1.71	0.72
1:A:103:GLU:HG3	2:D:76:ARG:HG2	1.71	0.72
2:B:76:ARG:CG	1:E:103:GLU:HG3	2.20	0.72
2:D:92:TRP:CE2	2:F:91:ILE:HG22	2.23	0.72
1:E:137:PRO:HD2	5:E:328:NAG:H83	1.71	0.72
1:G:93:GLY:HA3	1:G:227:MET:O	1.88	0.72
1:I:1:ASP:O	1:I:2:THR:HG23	1.90	0.71
1:C:302:LYS:HG2	2:D:61:THR:HG23	1.72	0.71
1:I:6:GLY:N	2:J:23:GLY:O	2.23	0.71
1:C:166:ILE:HG12	1:K:109:SER:CB	2.23	0.69
2:F:167:LYS:O	2:F:171:GLU:HG3	1.93	0.68
2:D:88:PHE:CZ	2:F:87:GLY:HA3	2.28	0.68
1:I:19:VAL:HG11	2:J:102:LEU:HD23	1.75	0.68
2:D:84:ILE:CD1	2:F:83:LYS:HE3	2.23	0.68
1:K:3:LEU:O	2:L:138:PHE:N	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLU:HG3	2:D:76:ARG:CG	2.24	0.68
1:C:102:ARG:NE	2:D:69:GLU:OE1	2.23	0.68
1:I:1:ASP:O	1:I:2:THR:CG2	2.42	0.68
1:G:102:ARG:NE	2:H:69:GLU:OE1	2.25	0.67
2:B:92:TRP:CE2	2:D:91:ILE:HG22	2.28	0.67
1:I:8:HIS:HB2	2:J:20:GLY:O	1.95	0.66
1:I:1:ASP:C	1:I:2:THR:HG23	2.14	0.66
1:E:93:GLY:HA3	1:E:227:MET:O	1.95	0.66
1:C:45:ARG:HH11	1:C:45:ARG:CG	2.03	0.66
1:E:5:ILE:HD11	2:F:122:VAL:HG21	1.78	0.66
1:C:166:ILE:HG12	1:K:109:SER:HB3	1.78	0.66
1:C:309:SER:HB3	2:D:97:GLU:OE2	1.96	0.66
1:G:259:ARG:HG2	1:G:259:ARG:HH11	1.59	0.66
1:C:93:GLY:HA3	1:C:227:MET:O	1.96	0.66
1:G:266:ILE:HD12	1:G:282:PRO:HA	1.78	0.66
2:H:29:GLU:OE1	2:H:143:LYS:HE2	1.95	0.65
1:I:132:VAL:HG22	1:I:143:SER:HA	1.79	0.64
1:C:266:ILE:HD12	1:C:282:PRO:HA	1.80	0.64
2:D:84:ILE:HD11	2:F:83:LYS:HG2	1.81	0.63
1:G:132:VAL:HG22	1:G:143:SER:HA	1.81	0.63
1:I:2:THR:O	2:J:26:HIS:HA	1.99	0.63
1:C:200:PHE:HZ	1:E:217:ARG:HG3	1.64	0.62
1:E:132:VAL:HG22	1:E:143:SER:CA	2.29	0.62
1:C:166:ILE:CG1	1:K:109:SER:HB3	2.30	0.62
1:I:259:ARG:HG2	1:I:259:ARG:NH1	2.15	0.62
1:K:302:LYS:HG2	2:L:61:THR:HG23	1.81	0.62
2:F:125:GLN:OE1	2:F:155:GLY:HA2	2.00	0.61
1:A:298:ILE:O	1:A:298:ILE:HG13	2.00	0.61
2:B:47:GLU:HB3	1:C:20:LEU:HB3	1.81	0.61
2:D:81:ASN:HB2	2:F:80:LEU:HD11	1.83	0.61
1:A:132:VAL:HG22	1:A:143:SER:HA	1.83	0.60
1:A:179:ILE:HD11	1:A:181:HIS:CE1	2.36	0.60
1:E:132:VAL:HG22	1:E:143:SER:HA	1.82	0.60
1:I:5:ILE:CD1	2:J:24:TYR:CD1	2.62	0.60
1:I:5:ILE:HD12	2:J:24:TYR:HE1	1.55	0.60
1:C:259:ARG:HG2	1:C:259:ARG:NH1	2.14	0.60
1:K:2:THR:CA	2:L:138:PHE:O	2.45	0.59
1:C:179:ILE:HD11	1:C:181:HIS:CE1	2.37	0.59
1:A:132:VAL:HG22	1:A:143:SER:CA	2.33	0.59
1:I:132:VAL:HG22	1:I:143:SER:CA	2.33	0.59
1:A:266:ILE:HD12	1:A:282:PRO:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:298:ILE:O	1:K:298:ILE:HG13	2.01	0.59
1:C:262:GLY:O	2:D:63:PHE:HE1	1.85	0.59
1:I:302:LYS:HE2	2:J:63:PHE:HB2	1.83	0.59
1:E:302:LYS:HG2	2:F:61:THR:HG23	1.84	0.59
1:E:305:LYS:HG3	2:F:92:TRP:CE2	2.38	0.58
1:G:262:GLY:O	2:H:63:PHE:HE1	1.85	0.58
1:C:281:THR:HG22	1:C:299:THR:HG22	1.85	0.58
2:H:63:PHE:CD1	2:H:63:PHE:C	2.77	0.58
1:I:99:GLU:OE1	2:J:71:ASN:HB2	2.02	0.58
1:K:4:CYS:HA	2:L:136:GLY:O	2.04	0.58
1:E:99:GLU:HA	1:E:102:ARG:HG3	1.86	0.57
2:B:91:ILE:HG22	2:F:92:TRP:CE2	2.39	0.57
2:D:125:GLN:OE1	2:D:155:GLY:HA2	2.04	0.57
1:G:132:VAL:HG22	1:G:143:SER:CA	2.34	0.57
1:K:266:ILE:HD12	1:K:282:PRO:HA	1.86	0.57
1:I:99:GLU:HA	1:I:102:ARG:HG3	1.85	0.57
1:A:2:THR:OG1	2:B:27:GLN:HB3	2.04	0.57
1:G:104:GLN:HG2	1:G:259:ARG:HH12	1.70	0.57
1:I:108:VAL:HG21	1:I:111:PHE:HB2	1.87	0.57
1:E:102:ARG:NE	2:F:69:GLU:OE1	2.28	0.56
1:E:266:ILE:HD12	1:E:282:PRO:HA	1.85	0.56
1:G:99:GLU:HA	1:G:102:ARG:HG3	1.87	0.56
1:G:281:THR:HG22	1:G:299:THR:HG22	1.87	0.56
2:B:84:ILE:CD1	2:D:83:LYS:HE3	2.36	0.56
1:K:305:LYS:HG3	2:L:92:TRP:CE2	2.40	0.56
1:C:200:PHE:CZ	1:E:217:ARG:HG3	2.41	0.56
1:I:19:VAL:HG11	2:J:102:LEU:CD2	2.36	0.56
1:I:266:ILE:HD12	1:I:282:PRO:HA	1.88	0.55
1:K:32:LEU:HD21	2:L:55:VAL:HG11	1.86	0.55
1:E:259:ARG:HG2	1:E:259:ARG:NH1	2.15	0.55
1:E:32:LEU:HD21	2:F:55:VAL:HG11	1.88	0.55
1:K:9:ALA:HB2	2:L:13:GLY:HA3	1.87	0.55
1:I:93:GLY:HA3	1:I:227:MET:O	2.05	0.55
1:A:108:VAL:HG21	1:A:111:PHE:HB2	1.89	0.55
2:B:71:ASN:OD1	2:B:72:HIS:N	2.40	0.55
2:F:125:GLN:HG2	2:F:157:TYR:HB3	1.89	0.55
1:K:259:ARG:HG2	1:K:259:ARG:NH1	2.17	0.55
1:K:93:GLY:HA3	1:K:227:MET:O	2.07	0.54
1:C:103:GLU:HG3	2:F:76:ARG:CG	2.37	0.54
1:I:281:THR:HG22	1:I:299:THR:HG22	1.89	0.54
1:G:298:ILE:HG13	1:G:298:ILE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:9:PHE:O	2:J:135:ASN:HA	2.08	0.54
1:C:132:VAL:HG22	1:C:143:SER:HA	1.90	0.54
1:E:108:VAL:HG21	1:E:111:PHE:HB2	1.90	0.54
1:A:2:THR:O	2:B:27:GLN:N	2.39	0.54
2:L:125:GLN:HG2	2:L:157:TYR:HB3	1.90	0.53
2:B:71:ASN:OD1	2:B:71:ASN:C	2.47	0.53
1:K:2:THR:HG22	2:L:139:GLU:HA	1.90	0.53
1:E:5:ILE:HG13	2:F:119:TYR:HA	1.90	0.53
2:L:29:GLU:OE1	2:L:143:LYS:HE3	2.08	0.53
2:D:30:GLN:OE1	2:D:145:ASP:HB2	2.08	0.53
2:J:63:PHE:CD1	2:J:63:PHE:C	2.81	0.53
1:K:179:ILE:HD11	1:K:181:HIS:CE1	2.43	0.53
1:C:2:THR:HA	2:D:138:PHE:O	2.09	0.53
1:A:281:THR:HG22	1:A:299:THR:HG22	1.91	0.53
2:L:30:GLN:OE1	2:L:145:ASP:HB2	2.09	0.53
1:K:132:VAL:HG22	1:K:143:SER:HA	1.91	0.53
1:A:-2:ASP:HB2	1:A:-1:PRO:HD3	1.90	0.52
2:D:125:GLN:HG2	2:D:157:TYR:HB3	1.91	0.52
2:F:30:GLN:OE1	2:F:145:ASP:HB2	2.09	0.52
1:K:172:GLU:OE2	1:K:259:ARG:NE	2.36	0.52
1:E:262:GLY:O	2:F:63:PHE:HE1	1.92	0.52
1:I:132:VAL:HG13	1:I:142:LYS:HB3	1.91	0.52
1:A:102:ARG:NE	2:B:69:GLU:OE1	2.28	0.52
1:I:7:TYR:HA	2:J:22:TYR:HA	1.91	0.52
1:A:93:GLY:HA3	1:A:227:MET:O	2.08	0.52
1:K:137:PRO:HD2	3:P:1:NAG:H83	1.92	0.52
1:I:6:GLY:HA3	2:J:14:TRP:CZ3	2.44	0.52
1:E:281:THR:HG22	1:E:299:THR:HG22	1.91	0.52
1:K:3:LEU:N	2:L:138:PHE:O	2.42	0.52
1:C:108:VAL:HG21	1:C:111:PHE:HB2	1.91	0.52
1:K:123:TRP:CZ2	1:K:250:VAL:HG11	2.44	0.52
1:E:81:GLU:O	1:E:267:ILE:HA	2.09	0.52
1:A:104:GLN:HG2	1:A:259:ARG:HH12	1.75	0.51
2:B:125:GLN:HG2	2:B:157:TYR:HB3	1.92	0.51
1:K:7:TYR:CE2	2:L:6:ILE:HA	2.45	0.51
3:O:1:NAG:H62	3:O:2:NAG:C1	2.40	0.51
1:I:318:LEU:HD21	2:J:21:TRP:CD1	2.45	0.51
1:I:318:LEU:HD23	1:I:318:LEU:N	2.25	0.51
1:I:298:ILE:O	1:I:298:ILE:HG13	2.10	0.51
1:I:5:ILE:HA	2:J:23:GLY:O	2.12	0.50
1:A:132:VAL:HG13	1:A:142:LYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:ILE:O	1:E:179:ILE:HG13	2.11	0.50
1:A:81:GLU:O	1:A:267:ILE:HA	2.12	0.50
1:I:3:LEU:HD21	2:J:153:LYS:HE2	1.93	0.50
1:C:61:ILE:HD12	1:C:62:LEU:N	2.27	0.50
2:B:84:ILE:HD11	2:D:83:LYS:HG2	1.94	0.50
1:E:132:VAL:CG2	1:E:143:SER:HA	2.41	0.50
1:A:259:ARG:HG2	1:A:259:ARG:NH1	2.21	0.50
2:J:87:GLY:HA3	2:L:88:PHE:CZ	2.47	0.50
1:K:45:ARG:HH11	1:K:45:ARG:CG	2.13	0.50
1:G:138:HIS:O	1:G:140:GLY:N	2.43	0.50
2:D:120:GLU:O	2:D:124:SER:HB2	2.12	0.49
2:H:30:GLN:OE1	2:H:145:ASP:HB2	2.11	0.49
1:K:132:VAL:HG22	1:K:143:SER:CA	2.42	0.49
1:C:103:GLU:HG3	2:F:76:ARG:HG3	1.95	0.49
2:F:119:TYR:CE1	2:F:136:GLY:HA2	2.47	0.49
1:K:99:GLU:HA	1:K:102:ARG:HG3	1.94	0.49
1:A:4:CYS:O	2:B:24:TYR:HA	2.12	0.49
1:C:318:LEU:H	1:C:318:LEU:HD23	1.76	0.49
1:C:298:ILE:O	1:C:298:ILE:HG13	2.12	0.49
1:I:104:GLN:HG2	1:I:259:ARG:HH12	1.78	0.49
2:B:81:ASN:HB2	2:D:80:LEU:HD11	1.95	0.49
1:G:108:VAL:HG21	1:G:111:PHE:HB2	1.93	0.49
2:L:91:ILE:HG23	2:L:91:ILE:HD13	1.41	0.49
1:G:259:ARG:HG2	1:G:259:ARG:NH1	2.26	0.48
2:B:88:PHE:CZ	2:D:87:GLY:HA3	2.48	0.48
2:B:120:GLU:O	2:B:124:SER:HB2	2.14	0.48
2:J:71:ASN:HB3	2:J:74:GLU:OE1	2.14	0.48
1:C:104:GLN:HG2	1:C:259:ARG:HH12	1.78	0.48
2:L:71:ASN:OD1	2:L:72:HIS:N	2.46	0.48
1:I:1:ASP:C	1:I:2:THR:CG2	2.79	0.48
1:K:262:GLY:O	2:L:63:PHE:HE1	1.97	0.48
1:E:138:HIS:O	1:E:140:GLY:N	2.43	0.48
2:J:71:ASN:OD1	2:J:72:HIS:N	2.47	0.48
1:E:179:ILE:HD11	1:E:181:HIS:CE1	2.48	0.48
1:C:153:LYS:HE2	1:C:190:SER:O	2.14	0.47
1:K:108:VAL:HG21	1:K:111:PHE:HB2	1.96	0.47
2:F:120:GLU:O	2:F:124:SER:HB2	2.15	0.47
1:G:98:TYR:O	1:G:102:ARG:HG2	2.14	0.47
1:G:179:ILE:HD11	1:G:181:HIS:CE1	2.49	0.47
1:C:318:LEU:HD23	1:C:318:LEU:N	2.29	0.47
1:E:98:TYR:O	1:E:102:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:305:LYS:HG3	2:H:92:TRP:CE2	2.50	0.47
2:J:30:GLN:OE1	2:J:145:ASP:HB2	2.14	0.47
1:C:32:LEU:HD21	2:D:55:VAL:HG11	1.96	0.47
1:C:104:GLN:HG2	1:C:259:ARG:NH1	2.29	0.47
2:F:63:PHE:CD1	2:F:63:PHE:C	2.87	0.47
2:F:158:ASP:OD1	2:F:161:LYS:HB2	2.14	0.47
1:I:7:TYR:HA	2:J:21:TRP:O	2.14	0.47
2:L:91:ILE:HD12	2:L:91:ILE:HG21	1.41	0.47
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.50	0.47
1:K:57:ILE:O	1:K:61:ILE:HG13	2.14	0.47
1:K:164:SER:OG	1:K:241:THR:HG22	2.15	0.47
1:I:5:ILE:CG2	2:J:118:LEU:HD23	2.45	0.47
1:I:132:VAL:CG2	1:I:143:SER:HA	2.45	0.47
2:J:76:ARG:HG2	1:K:103:GLU:HG3	1.97	0.47
1:I:317:GLY:HA2	2:J:21:TRP:CZ2	2.49	0.47
2:L:120:GLU:O	2:L:124:SER:HB2	2.15	0.46
2:B:30:GLN:OE1	2:B:145:ASP:HB2	2.16	0.46
2:B:9:PHE:O	2:B:135:ASN:HA	2.15	0.46
1:E:298:ILE:HG13	1:E:298:ILE:O	2.15	0.46
1:G:257:MET:HE1	1:G:259:ARG:HD2	1.98	0.46
2:J:83:LYS:HG2	2:L:84:ILE:HD11	1.96	0.46
1:E:104:GLN:HG2	1:E:259:ARG:HH12	1.80	0.46
1:G:104:GLN:HG2	1:G:259:ARG:NH1	2.29	0.46
2:J:105:GLU:HG2	2:L:106:ARG:HH22	1.80	0.46
2:L:158:ASP:OD1	2:L:161:LYS:HB2	2.16	0.46
1:A:302:LYS:HG2	2:B:61:THR:HG23	1.97	0.46
1:C:103:GLU:HG3	2:F:76:ARG:HG2	1.97	0.46
1:I:5:ILE:HG23	2:J:118:LEU:HD23	1.98	0.46
2:B:158:ASP:OD1	2:B:161:LYS:HB2	2.15	0.46
1:A:103:GLU:HG3	2:D:76:ARG:HG3	1.98	0.46
1:E:1:ASP:HB3	2:F:28:ASN:HA	1.97	0.46
2:H:9:PHE:O	2:H:135:ASN:HA	2.16	0.46
1:K:5:ILE:HD11	2:L:122:VAL:HG21	1.98	0.46
1:K:7:TYR:CZ	2:L:6:ILE:HA	2.50	0.46
2:H:158:ASP:OD1	2:H:161:LYS:HB2	2.15	0.46
1:I:2:THR:OG1	2:J:27:GLN:HB3	2.16	0.45
1:C:166:ILE:HG12	1:K:109:SER:HB2	1.97	0.45
1:G:110:SER:OG	1:G:171:LYS:HE3	2.17	0.45
1:G:318:LEU:HD23	1:G:318:LEU:H	1.81	0.45
2:H:125:GLN:OE1	2:H:155:GLY:HA2	2.17	0.45
1:I:3:LEU:CD2	2:J:24:TYR:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:GLU:HG2	2:B:123:ARG:NH2	2.32	0.45
2:D:63:PHE:CD1	2:D:63:PHE:C	2.89	0.45
2:J:119:TYR:CE1	2:J:136:GLY:HA2	2.51	0.45
2:J:158:ASP:OD1	2:J:161:LYS:HB2	2.16	0.45
2:D:158:ASP:OD1	2:D:161:LYS:HB2	2.17	0.45
2:H:120:GLU:O	2:H:124:SER:HB2	2.17	0.45
2:H:131:LYS:HG3	2:H:141:TYR:OH	2.17	0.45
2:L:75:LYS:HB2	2:L:75:LYS:HE2	1.82	0.45
1:E:318:LEU:HD23	1:E:318:LEU:H	1.82	0.45
1:I:179:ILE:HD11	1:I:181:HIS:CE1	2.52	0.45
2:J:2:LEU:O	2:L:113:SER:OG	2.27	0.45
1:K:281:THR:HG22	1:K:299:THR:HG22	1.99	0.45
2:J:120:GLU:O	2:J:124:SER:HB2	2.16	0.45
1:C:132:VAL:HG22	1:C:143:SER:CA	2.46	0.45
2:F:120:GLU:HG2	2:F:123:ARG:NH2	2.31	0.45
1:A:262:GLY:O	2:B:63:PHE:HE1	1.99	0.44
1:I:318:LEU:HD23	1:I:318:LEU:H	1.82	0.44
1:K:110:SER:OG	1:K:171:LYS:HE3	2.18	0.44
1:A:49:PRO:HB3	1:A:78:TYR:CE1	2.52	0.44
1:G:103:GLU:O	1:G:106:SER:HB2	2.17	0.44
1:G:318:LEU:HD23	1:G:318:LEU:N	2.32	0.44
1:C:5:ILE:HG13	2:D:119:TYR:HA	2.00	0.44
1:K:318:LEU:HB3	2:L:111:HIS:CG	2.53	0.44
2:L:26:HIS:HD1	2:L:26:HIS:C	2.21	0.44
1:C:136:CYS:O	1:C:143:SER:HB3	2.18	0.44
1:I:3:LEU:HD22	2:J:24:TYR:HB3	1.99	0.44
1:A:217:ARG:HG3	1:E:200:PHE:HZ	1.81	0.44
2:B:63:PHE:CD1	2:B:63:PHE:C	2.91	0.44
2:D:133:ILE:O	2:D:133:ILE:CG2	2.66	0.44
1:K:2:THR:HG22	2:L:139:GLU:CA	2.48	0.44
2:H:91:ILE:HD12	2:H:91:ILE:HG21	1.42	0.43
1:K:4:CYS:HA	2:L:137:CYS:HA	1.99	0.43
1:K:61:ILE:HG13	1:K:61:ILE:H	1.62	0.43
1:K:81:GLU:O	1:K:267:ILE:HA	2.18	0.43
2:J:120:GLU:HG2	2:J:123:ARG:NH2	2.33	0.43
2:L:71:ASN:OD1	2:L:71:ASN:C	2.57	0.43
1:A:5:ILE:HD13	2:B:24:TYR:HD1	1.83	0.43
1:C:99:GLU:HA	1:C:102:ARG:HG3	2.00	0.43
2:D:9:PHE:O	2:D:135:ASN:HA	2.19	0.43
1:C:240:ILE:HG23	1:C:240:ILE:O	2.19	0.43
1:E:116:ILE:HD13	1:E:116:ILE:HG21	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:318:LEU:HD23	1:E:318:LEU:N	2.34	0.43
2:D:131:LYS:HG3	2:D:141:TYR:OH	2.18	0.43
1:G:116:ILE:HD13	1:G:116:ILE:HG21	1.66	0.43
1:I:6:GLY:O	2:J:23:GLY:N	2.44	0.43
1:K:136:CYS:O	1:K:143:SER:HB3	2.18	0.43
1:A:1:ASP:OD1	2:B:144:CYS:N	2.41	0.43
1:C:123:TRP:CZ2	1:C:250:VAL:HG11	2.53	0.43
2:J:91:ILE:HD12	2:J:91:ILE:HG21	1.58	0.43
1:C:138:HIS:O	1:C:140:GLY:N	2.47	0.43
1:G:57:ILE:O	1:G:61:ILE:HG13	2.19	0.43
1:K:61:ILE:HD12	1:K:62:LEU:N	2.34	0.43
1:I:87:ASN:HD22	3:O:1:NAG:C7	2.31	0.43
2:H:125:GLN:HG2	2:H:157:TYR:HB3	2.01	0.42
1:K:5:ILE:O	2:L:10:ILE:HD13	2.18	0.42
1:A:99:GLU:HA	1:A:102:ARG:HG3	2.01	0.42
1:C:166:ILE:CD1	1:K:109:SER:HB3	2.49	0.42
1:E:166:ILE:H	1:E:166:ILE:HG13	1.65	0.42
1:K:132:VAL:HG13	1:K:142:LYS:HB3	2.01	0.42
2:B:91:ILE:HD12	2:B:91:ILE:HG21	1.35	0.42
1:C:110:SER:OG	1:C:171:LYS:HE3	2.20	0.42
1:K:79:ILE:HB	1:K:265:ILE:HG13	2.02	0.42
1:C:87:ASN:ND2	3:M:1:NAG:O7	2.42	0.42
2:F:9:PHE:O	2:F:135:ASN:HA	2.19	0.42
1:G:1:ASP:HB2	2:H:27:GLN:O	2.19	0.42
1:K:62:LEU:O	1:K:147:ASN:HB2	2.19	0.42
2:L:9:PHE:O	2:L:135:ASN:HA	2.19	0.42
1:A:61:ILE:H	1:A:61:ILE:HG13	1.68	0.42
2:B:87:GLY:HA3	2:F:88:PHE:CZ	2.55	0.42
1:G:166:ILE:H	1:G:166:ILE:HG13	1.65	0.42
1:A:104:GLN:HG2	1:A:259:ARG:NH1	2.33	0.42
2:L:84:ILE:HG12	2:L:85:ASP:N	2.35	0.42
1:G:132:VAL:HG13	1:G:142:LYS:HB3	2.01	0.42
1:K:5:ILE:HG13	2:L:119:TYR:CA	2.33	0.42
1:E:132:VAL:HG13	1:E:142:LYS:HB3	2.02	0.42
2:H:91:ILE:HG23	2:H:91:ILE:HD13	1.43	0.41
1:I:81:GLU:O	1:I:267:ILE:HA	2.19	0.41
1:A:132:VAL:CG2	1:A:143:SER:HA	2.48	0.41
1:G:137:PRO:HD2	4:N:1:NAG:H83	2.01	0.41
1:A:-2:ASP:CB	1:A:-1:PRO:HD3	2.50	0.41
1:A:107:SER:HB2	1:A:263:SER:CB	2.51	0.41
1:C:81:GLU:O	1:C:267:ILE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:LEU:C	1:G:161:LEU:HD23	2.39	0.41
2:H:71:ASN:OD1	2:H:72:HIS:N	2.54	0.41
1:I:318:LEU:CD2	2:J:21:TRP:CD1	3.03	0.41
2:F:75:LYS:HE2	2:F:75:LYS:HB2	1.86	0.41
2:L:119:TYR:CE1	2:L:136:GLY:HA2	2.55	0.41
1:A:266:ILE:HG21	1:A:266:ILE:HD13	1.81	0.41
2:B:91:ILE:HG23	2:B:91:ILE:HD13	1.37	0.41
1:K:5:ILE:N	2:L:136:GLY:O	2.45	0.41
1:C:137:PRO:HD2	3:M:1:NAG:H83	2.02	0.41
2:D:84:ILE:HD11	2:F:83:LYS:CE	2.37	0.41
2:H:119:TYR:CE1	2:H:136:GLY:HA2	2.56	0.41
1:K:104:GLN:HG2	1:K:259:ARG:HH12	1.86	0.41
1:C:166:ILE:HD11	1:K:109:SER:HB3	2.02	0.41
1:A:137:PRO:HD2	5:A:328:NAG:H83	2.02	0.41
2:D:119:TYR:CE1	2:D:136:GLY:HA2	2.55	0.41
1:C:98:TYR:O	1:C:102:ARG:HG2	2.21	0.41
1:I:116:ILE:HD13	1:I:116:ILE:HG21	1.78	0.41
1:I:306:TYR:CD2	2:J:89:LEU:HD13	2.56	0.41
2:J:58:LYS:HD3	2:J:58:LYS:HA	1.90	0.41
2:B:62:GLN:NE2	2:D:89:LEU:HD23	2.36	0.41
1:C:237:GLY:HA2	1:K:45:ARG:O	2.20	0.41
1:A:103:GLU:O	1:A:106:SER:HB2	2.21	0.40
1:G:299:THR:HB	1:G:303:CYS:SG	2.61	0.40
1:C:172:GLU:OE2	1:C:259:ARG:NE	2.38	0.40
1:C:305:LYS:HG3	2:D:92:TRP:CE2	2.56	0.40
2:F:133:ILE:O	2:F:133:ILE:CG2	2.70	0.40
1:I:110:SER:OG	1:I:171:LYS:HE3	2.22	0.40
2:D:88:PHE:CE2	2:F:87:GLY:HA3	2.56	0.40
1:E:57:ILE:O	1:E:61:ILE:HG13	2.21	0.40
1:I:6:GLY:O	2:J:22:TYR:HA	2.22	0.40
2:L:58:LYS:HD3	2:L:58:LYS:HA	1.89	0.40
2:D:71:ASN:OD1	2:D:72:HIS:N	2.55	0.40
2:D:91:ILE:HD12	2:D:91:ILE:HG21	1.47	0.40
1:E:43:LYS:HG2	1:E:48:ALA:HA	2.03	0.40
1:E:153:LYS:HE2	1:E:190:SER:O	2.21	0.40
1:G:164:SER:OG	1:G:241:THR:HG22	2.22	0.40
2:J:125:GLN:HG2	2:J:157:TYR:HB3	2.03	0.40
2:F:84:ILE:HG12	2:F:85:ASP:N	2.37	0.40
2:J:125:GLN:OE1	2:J:155:GLY:HA2	2.21	0.40

All (4) 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)
2:B:143:LYS:CE	1:G:224:GLU:OE1[1_466]	1.91	0.29
1:A:168:ASP:O	1:K:273:HIS:CE1[1_655]	1.98	0.22
2:B:169:ASN:OD1	1:G:222:ASP:OD2[1_466]	2.13	0.07
2:B:164:GLU:OE1	1:E:120:THR:O[1_556]	2.19	0.01

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	323/331 (98%)	305 (94%)	16 (5%)	2 (1%)	25	56
1	C	321/331 (97%)	303 (94%)	16 (5%)	2 (1%)	25	56
1	E	321/331 (97%)	303 (94%)	16 (5%)	2 (1%)	25	56
1	G	320/331 (97%)	303 (95%)	16 (5%)	1 (0%)	41	72
1	I	320/331 (97%)	299 (93%)	19 (6%)	2 (1%)	25	56
1	K	319/331 (96%)	300 (94%)	18 (6%)	1 (0%)	41	72
2	B	167/181 (92%)	163 (98%)	4 (2%)	0	100	100
2	D	169/181 (93%)	163 (96%)	6 (4%)	0	100	100
2	F	169/181 (93%)	164 (97%)	5 (3%)	0	100	100
2	H	168/181 (93%)	164 (98%)	4 (2%)	0	100	100
2	J	168/181 (93%)	162 (96%)	6 (4%)	0	100	100
2	L	169/181 (93%)	162 (96%)	7 (4%)	0	100	100
All	All	2934/3072 (96%)	2791 (95%)	133 (4%)	10 (0%)	41	72

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	ALA
1	G	261	ALA
1	I	261	ALA
1	K	261	ALA

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Mol	Chain	Res	Type
1	C	261	ALA
1	E	261	ALA
1	A	275	CYS
1	C	275	CYS
1	E	275	CYS
1	I	275	CYS

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	284/289 (98%)	254 (89%)	30 (11%)	6	20
1	C	282/289 (98%)	254 (90%)	28 (10%)	8	23
1	E	282/289 (98%)	249 (88%)	33 (12%)	5	16
1	G	282/289 (98%)	251 (89%)	31 (11%)	6	19
1	I	281/289 (97%)	250 (89%)	31 (11%)	6	19
1	K	281/289 (97%)	249 (89%)	32 (11%)	5	18
2	B	146/156 (94%)	128 (88%)	18 (12%)	4	15
2	D	148/156 (95%)	131 (88%)	17 (12%)	5	17
2	F	148/156 (95%)	133 (90%)	15 (10%)	7	22
2	H	147/156 (94%)	129 (88%)	18 (12%)	5	15
2	J	147/156 (94%)	131 (89%)	16 (11%)	6	19
2	L	148/156 (95%)	132 (89%)	16 (11%)	6	19
All	All	2576/2670 (96%)	2291 (89%)	285 (11%)	6	19

All (285) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	45	ARG
1	A	47	VAL
1	A	68	GLU

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Mol	Chain	Res	Type
1	A	72	THR
1	A	75	SER
1	A	86	ASP
1	A	95	PHE
1	A	102	ARG
1	A	103	GLU
1	A	106	SER
1	A	116	ILE
1	A	132	VAL
1	A	152	VAL
1	A	157	SER
1	A	166	ILE
1	A	173	VAL
1	A	175	VAL
1	A	179	ILE
1	A	189	GLN
1	A	216	ILE
1	A	239	LYS
1	A	250	VAL
1	A	259	ARG
1	A	260	ASN
1	A	266	ILE
1	A	272	VAL
1	A	309	SER
1	A	314	LEU
1	A	318	LEU
2	B	22	TYR
2	B	26	HIS
2	B	38	LEU
2	B	45	ILE
2	B	60	ASN
2	B	64	THR
2	B	69	GLU
2	B	71	ASN
2	B	75	LYS
2	B	80	LEU
2	B	84	ILE
2	B	91	ILE
2	B	103	GLU
2	B	105	GLU
2	B	108	LEU
2	B	121	LYS

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Mol	Chain	Res	Type
2	B	124	SER
2	B	125	GLN
1	C	3	LEU
1	C	45	ARG
1	C	47	VAL
1	C	68	GLU
1	C	72	THR
1	C	75	SER
1	C	84	SER
1	C	86	ASP
1	C	102	ARG
1	C	106	SER
1	C	116	ILE
1	C	132	VAL
1	C	157	SER
1	C	166	ILE
1	C	175	VAL
1	C	179	ILE
1	C	183	SER
1	C	189	GLN
1	C	216	ILE
1	C	239	LYS
1	C	250	VAL
1	C	259	ARG
1	C	260	ASN
1	C	266	ILE
1	C	272	VAL
1	C	309	SER
1	C	314	LEU
1	C	318	LEU
2	D	22	TYR
2	D	26	HIS
2	D	38	LEU
2	D	45	ILE
2	D	64	THR
2	D	69	GLU
2	D	71	ASN
2	D	75	LYS
2	D	80	LEU
2	D	84	ILE
2	D	91	ILE
2	D	103	GLU

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Mol	Chain	Res	Type
2	D	105	GLU
2	D	121	LYS
2	D	124	SER
2	D	131	LYS
2	D	167	LYS
1	E	1	ASP
1	E	3	LEU
1	E	45	ARG
1	E	47	VAL
1	E	68	GLU
1	E	72	THR
1	E	75	SER
1	E	84	SER
1	E	86	ASP
1	E	95	PHE
1	E	102	ARG
1	E	103	GLU
1	E	106	SER
1	E	116	ILE
1	E	132	VAL
1	E	152	VAL
1	E	157	SER
1	E	161	LEU
1	E	166	ILE
1	E	173	VAL
1	E	175	VAL
1	E	179	ILE
1	E	183	SER
1	E	189	GLN
1	E	216	ILE
1	E	250	VAL
1	E	259	ARG
1	E	260	ASN
1	E	266	ILE
1	E	272	VAL
1	E	309	SER
1	E	314	LEU
1	E	318	LEU
2	F	22	TYR
2	F	26	HIS
2	F	38	LEU
2	F	45	ILE

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Mol	Chain	Res	Type
2	F	64	THR
2	F	71	ASN
2	F	75	LYS
2	F	80	LEU
2	F	84	ILE
2	F	91	ILE
2	F	103	GLU
2	F	105	GLU
2	F	121	LYS
2	F	131	LYS
2	F	167	LYS
1	G	3	LEU
1	G	45	ARG
1	G	47	VAL
1	G	61	ILE
1	G	68	GLU
1	G	72	THR
1	G	75	SER
1	G	84	SER
1	G	86	ASP
1	G	102	ARG
1	G	103	GLU
1	G	106	SER
1	G	116	ILE
1	G	132	VAL
1	G	152	VAL
1	G	157	SER
1	G	161	LEU
1	G	166	ILE
1	G	175	VAL
1	G	179	ILE
1	G	189	GLN
1	G	216	ILE
1	G	249	VAL
1	G	250	VAL
1	G	259	ARG
1	G	260	ASN
1	G	266	ILE
1	G	272	VAL
1	G	309	SER
1	G	314	LEU
1	G	318	LEU

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Mol	Chain	Res	Type
2	H	26	HIS
2	H	38	LEU
2	H	45	ILE
2	H	60	ASN
2	H	64	THR
2	H	69	GLU
2	H	71	ASN
2	H	75	LYS
2	H	80	LEU
2	H	84	ILE
2	H	91	ILE
2	H	103	GLU
2	H	105	GLU
2	H	121	LYS
2	H	125	GLN
2	H	131	LYS
2	H	143	LYS
2	H	167	LYS
1	I	3	LEU
1	I	29	SER
1	I	45	ARG
1	I	47	VAL
1	I	68	GLU
1	I	72	THR
1	I	75	SER
1	I	86	ASP
1	I	102	ARG
1	I	103	GLU
1	I	105	LEU
1	I	106	SER
1	I	116	ILE
1	I	132	VAL
1	I	152	VAL
1	I	157	SER
1	I	161	LEU
1	I	166	ILE
1	I	175	VAL
1	I	179	ILE
1	I	189	GLN
1	I	216	ILE
1	I	249	VAL
1	I	250	VAL

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Mol	Chain	Res	Type
1	I	259	ARG
1	I	260	ASN
1	I	266	ILE
1	I	272	VAL
1	I	309	SER
1	I	314	LEU
1	I	318	LEU
2	J	26	HIS
2	J	38	LEU
2	J	45	ILE
2	J	64	THR
2	J	69	GLU
2	J	71	ASN
2	J	80	LEU
2	J	84	ILE
2	J	91	ILE
2	J	103	GLU
2	J	105	GLU
2	J	108	LEU
2	J	121	LYS
2	J	125	GLN
2	J	143	LYS
2	J	167	LYS
1	K	3	LEU
1	K	29	SER
1	K	45	ARG
1	K	47	VAL
1	K	68	GLU
1	K	72	THR
1	K	75	SER
1	K	84	SER
1	K	86	ASP
1	K	102	ARG
1	K	103	GLU
1	K	106	SER
1	K	116	ILE
1	K	132	VAL
1	K	157	SER
1	K	161	LEU
1	K	166	ILE
1	K	173	VAL
1	K	175	VAL

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Mol	Chain	Res	Type
1	K	179	ILE
1	K	183	SER
1	K	189	GLN
1	K	216	ILE
1	K	239	LYS
1	K	249	VAL
1	K	250	VAL
1	K	259	ARG
1	K	266	ILE
1	K	272	VAL
1	K	309	SER
1	K	314	LEU
1	K	318	LEU
2	L	26	HIS
2	L	38	LEU
2	L	45	ILE
2	L	64	THR
2	L	69	GLU
2	L	71	ASN
2	L	80	LEU
2	L	84	ILE
2	L	91	ILE
2	L	103	GLU
2	L	105	GLU
2	L	121	LYS
2	L	124	SER
2	L	131	LYS
2	L	171	GLU
2	L	172	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

11 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	3,1	14,14,15	0.77	0	17,19,21	2.00	3 (17%)
3	NAG	M	2	3	14,14,15	0.91	1 (7%)	17,19,21	2.05	7 (41%)
4	NAG	N	1	4,1	14,14,15	0.81	0	17,19,21	1.68	4 (23%)
4	NAG	N	2	4	14,14,15	0.77	0	17,19,21	2.07	5 (29%)
4	MAN	N	3	4	11,11,12	0.89	0	15,15,17	2.85	7 (46%)
3	NAG	O	1	3,1	14,14,15	0.55	0	17,19,21	2.21	5 (29%)
3	NAG	O	2	3	14,14,15	1.02	1 (7%)	17,19,21	1.51	4 (23%)
3	NAG	P	1	3,1	14,14,15	1.10	1 (7%)	17,19,21	2.36	5 (29%)
3	NAG	P	2	3	14,14,15	0.63	0	17,19,21	1.30	4 (23%)
3	NAG	Q	1	3,1	14,14,15	1.74	2 (14%)	17,19,21	1.82	4 (23%)
3	NAG	Q	2	3	14,14,15	0.99	1 (7%)	17,19,21	2.05	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
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	MAN	N	3	4	1/1/4/5	2/2/19/22	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	2	3	-	1/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	1	NAG	C1-C2	5.10	1.60	1.52
3	P	1	NAG	C1-C2	3.80	1.58	1.52
3	O	2	NAG	C1-C2	2.56	1.56	1.52
3	Q	2	NAG	C1-C2	2.18	1.55	1.52
3	M	2	NAG	C1-C2	2.14	1.55	1.52
3	Q	1	NAG	C3-C2	2.09	1.56	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1	NAG	O5-C1-C2	-6.00	101.81	111.29
3	O	1	NAG	C1-O5-C5	5.92	120.22	112.19
4	N	3	MAN	C1-O5-C5	5.43	119.56	112.19
3	P	1	NAG	C1-O5-C5	5.05	119.03	112.19
4	N	2	NAG	C1-O5-C5	4.90	118.83	112.19
3	Q	2	NAG	C2-N2-C7	4.57	129.41	122.90
3	P	1	NAG	O5-C1-C2	-4.55	104.11	111.29
3	Q	2	NAG	C4-C3-C2	4.35	117.39	111.02
4	N	3	MAN	O5-C5-C6	4.29	113.93	107.20
4	N	3	MAN	C3-C4-C5	-4.20	102.74	110.24
4	N	2	NAG	C4-C3-C2	4.12	117.05	111.02
3	M	2	NAG	C4-C3-C2	4.11	117.04	111.02
3	P	1	NAG	O4-C4-C3	-4.06	100.97	110.35
3	Q	1	NAG	C1-O5-C5	4.04	117.67	112.19
3	O	1	NAG	O5-C1-C2	-4.00	104.97	111.29
3	P	1	NAG	C1-C2-N2	3.98	117.28	110.49
3	M	2	NAG	C1-C2-N2	-3.85	103.90	110.49
4	N	3	MAN	C2-C3-C4	-3.66	104.56	110.89
3	Q	1	NAG	C4-C3-C2	3.40	116.00	111.02
4	N	1	NAG	C3-C4-C5	-3.32	104.31	110.24
3	O	2	NAG	C4-C3-C2	3.31	115.87	111.02
4	N	1	NAG	O5-C5-C6	3.27	112.33	107.20
4	N	3	MAN	O4-C4-C5	3.15	117.12	109.30
3	O	2	NAG	C1-C2-N2	-3.06	105.26	110.49
4	N	1	NAG	O5-C1-C2	-3.03	106.51	111.29
3	M	1	NAG	O5-C5-C6	3.02	111.94	107.20
3	Q	2	NAG	C3-C4-C5	3.01	115.61	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	2	NAG	O5-C5-C4	3.00	118.12	110.83
3	M	2	NAG	O4-C4-C5	2.79	116.21	109.30
3	M	1	NAG	C2-N2-C7	-2.75	118.98	122.90
3	M	2	NAG	C6-C5-C4	2.66	119.22	113.00
3	M	2	NAG	O5-C5-C6	2.61	111.30	107.20
3	Q	1	NAG	C8-C7-N2	2.60	120.50	116.10
4	N	3	MAN	O5-C1-C2	2.57	114.75	110.77
4	N	3	MAN	C6-C5-C4	2.55	118.97	113.00
4	N	2	NAG	C3-C4-C5	2.53	114.76	110.24
3	P	2	NAG	C1-C2-N2	-2.47	106.27	110.49
3	Q	2	NAG	C1-O5-C5	2.46	115.53	112.19
3	P	1	NAG	C4-C3-C2	2.36	114.48	111.02
3	Q	1	NAG	O4-C4-C3	2.29	115.64	110.35
3	O	1	NAG	O3-C3-C2	-2.29	104.73	109.47
3	P	2	NAG	C2-N2-C7	2.26	126.12	122.90
3	M	2	NAG	O5-C5-C4	-2.18	105.52	110.83
4	N	2	NAG	O4-C4-C5	-2.17	103.90	109.30
3	O	1	NAG	C6-C5-C4	-2.16	107.94	113.00
3	M	2	NAG	C1-O5-C5	-2.10	109.34	112.19
3	O	2	NAG	O4-C4-C5	2.09	114.49	109.30
3	P	2	NAG	O7-C7-N2	2.07	125.75	121.95
3	O	2	NAG	O3-C3-C2	2.07	113.74	109.47
3	P	2	NAG	O5-C5-C6	2.05	110.42	107.20
4	N	1	NAG	C6-C5-C4	2.04	117.78	113.00
3	O	1	NAG	O4-C4-C5	2.01	114.29	109.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	N	3	MAN	C1

All (8) torsion outliers are listed below:

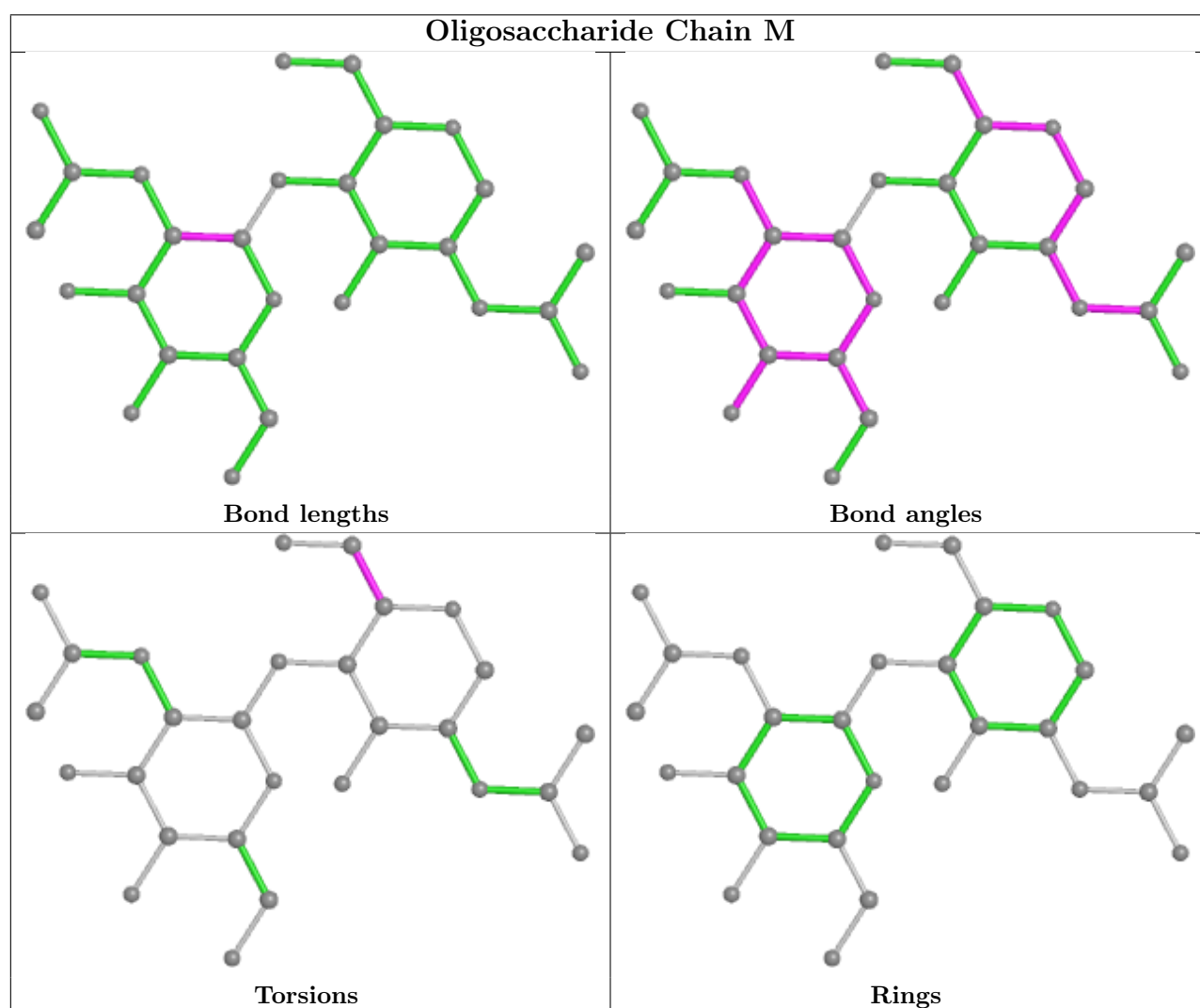
Mol	Chain	Res	Type	Atoms
4	N	3	MAN	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
4	N	3	MAN	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	C1-C2-N2-C7
4	N	1	NAG	C4-C5-C6-O6

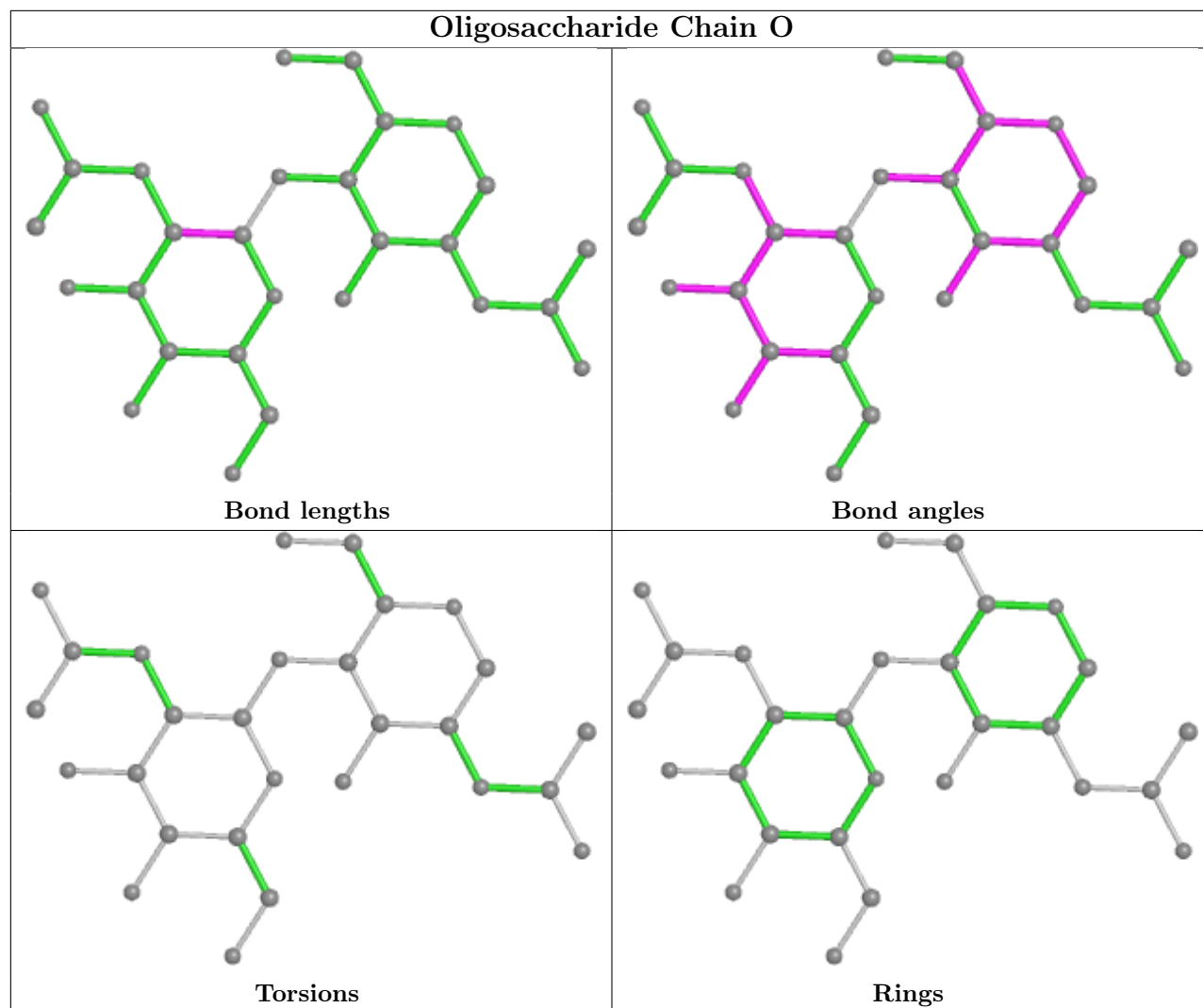
There are no ring outliers.

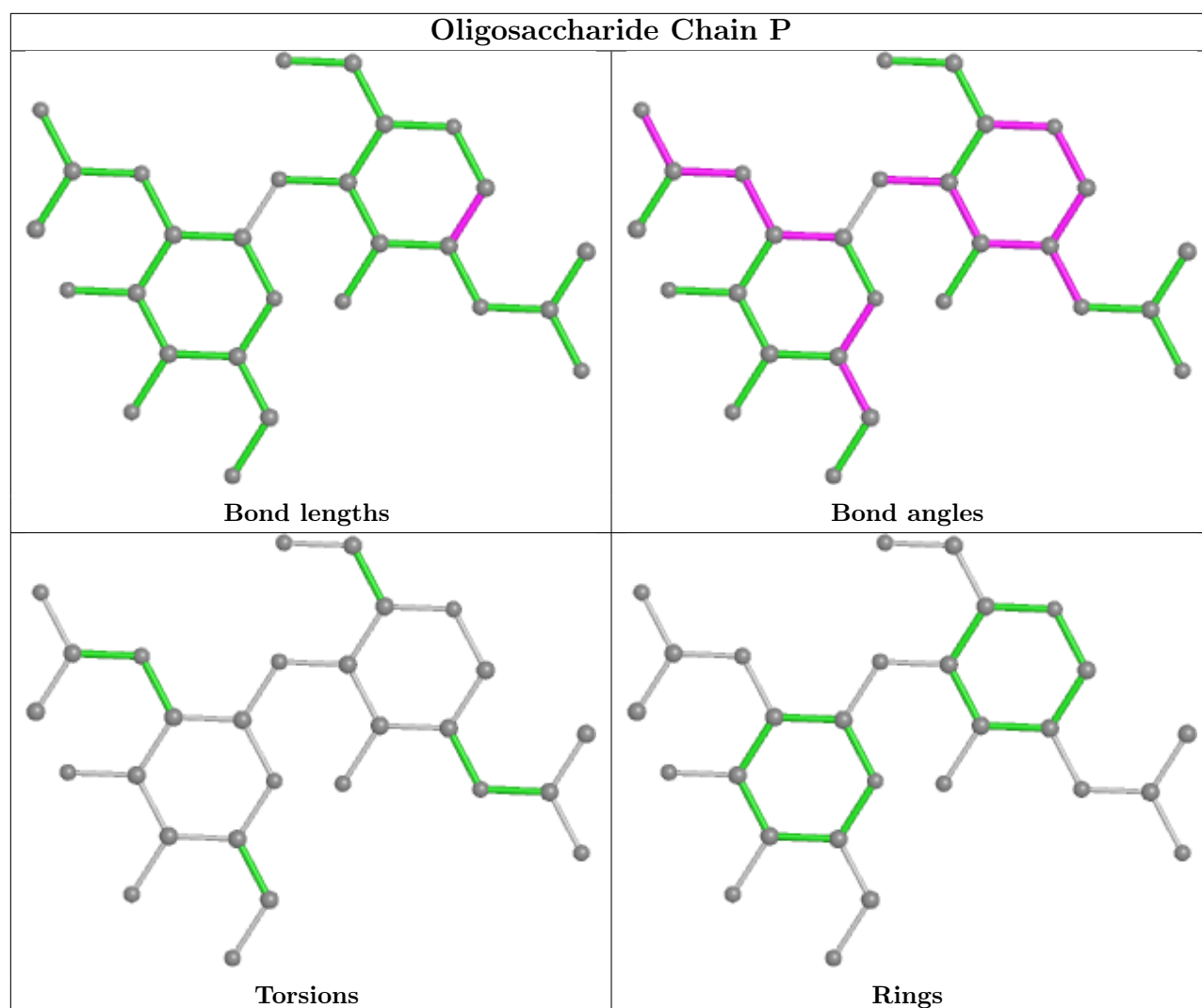
5 monomers are involved in 6 short contacts:

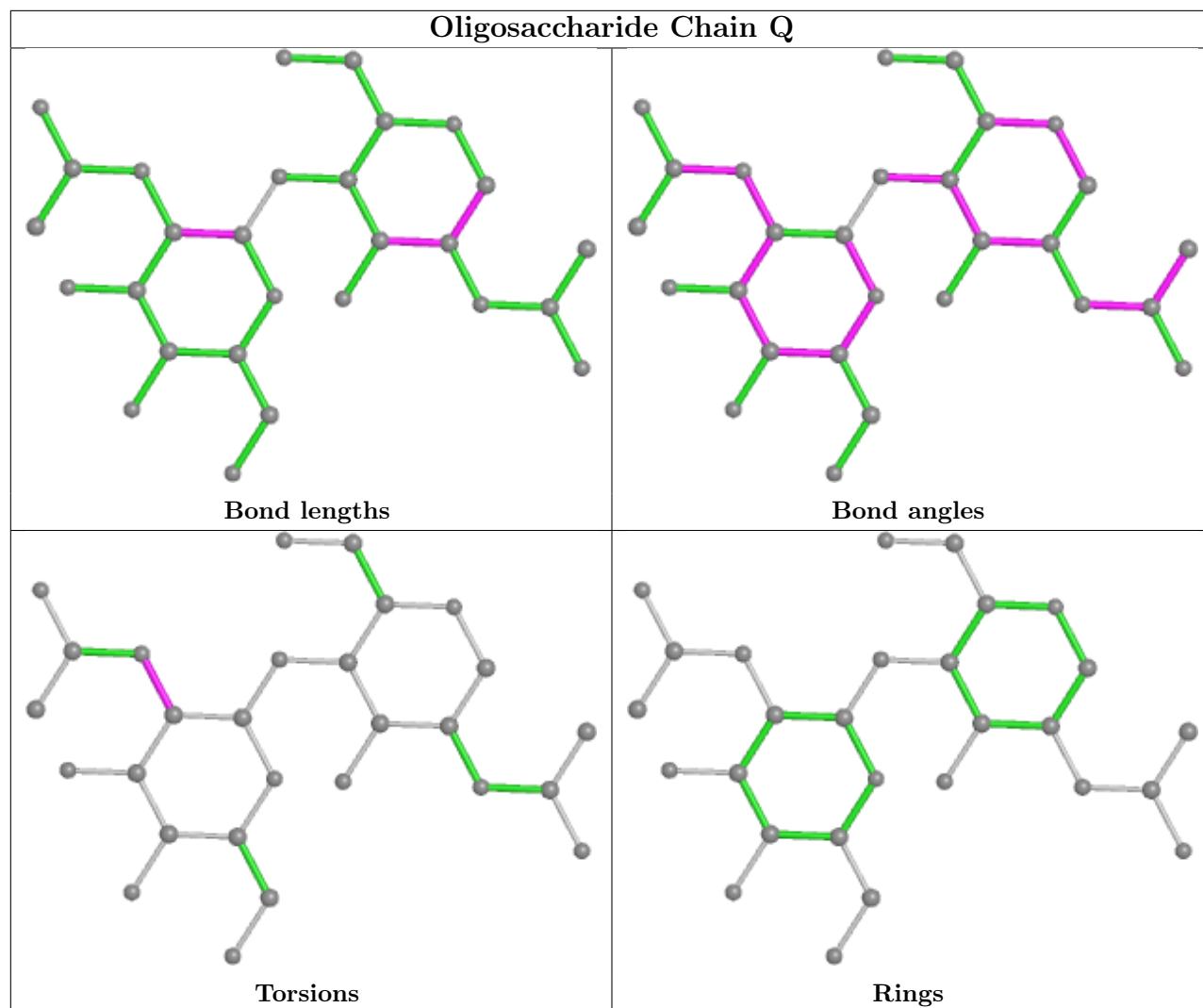
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	2	0
4	N	1	NAG	1	0
3	O	2	NAG	1	0
3	P	1	NAG	1	0
3	O	1	NAG	2	0

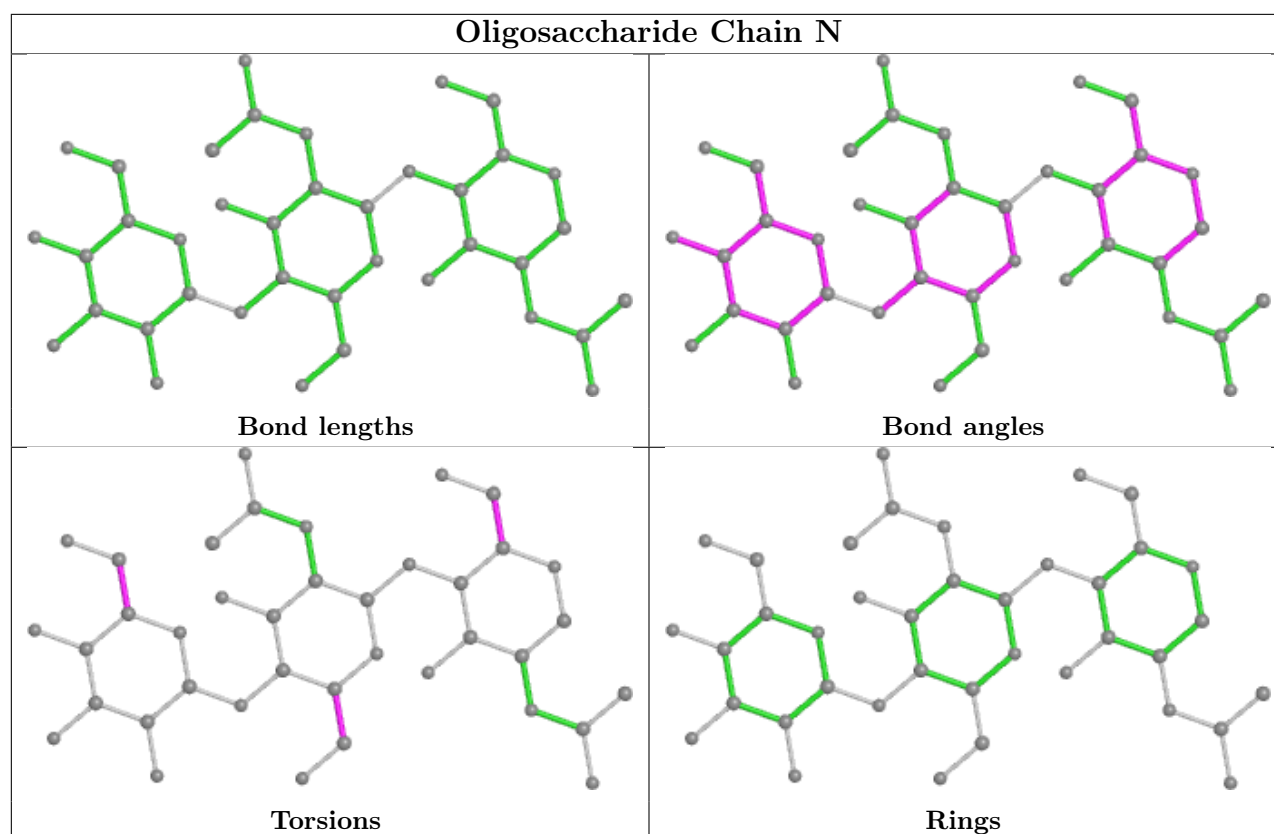
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
5	NAG	G	331	1	14,14,15	1.51	2 (14%)	17,19,21	2.32	7 (41%)
5	NAG	E	328	1	14,14,15	0.54	0	17,19,21	1.51	2 (11%)
5	NAG	A	328	1	14,14,15	0.86	1 (7%)	17,19,21	1.56	3 (17%)
5	NAG	G	332	1	14,14,15	0.98	1 (7%)	17,19,21	2.70	3 (17%)

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	E	328	1	-	2/6/23/26	0/1/1/1
5	NAG	G	331	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	A	328	1	-	2/6/23/26	0/1/1/1
5	NAG	G	332	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	331	NAG	C1-C2	4.46	1.59	1.52
5	G	332	NAG	C1-C2	2.42	1.56	1.52
5	G	331	NAG	C3-C2	2.35	1.57	1.52
5	A	328	NAG	C1-C2	2.09	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	332	NAG	C1-O5-C5	10.14	125.93	112.19
5	G	331	NAG	C1-O5-C5	6.51	121.01	112.19
5	A	328	NAG	C1-O5-C5	3.94	117.53	112.19
5	E	328	NAG	O5-C5-C6	3.92	113.35	107.20
5	G	331	NAG	C3-C4-C5	-3.15	104.63	110.24
5	E	328	NAG	C3-C4-C5	-2.92	105.04	110.24
5	A	328	NAG	C2-N2-C7	-2.81	118.91	122.90
5	G	331	NAG	O5-C1-C2	2.50	115.24	111.29
5	G	331	NAG	C1-C2-N2	2.49	114.74	110.49
5	G	331	NAG	O4-C4-C5	2.44	115.35	109.30
5	G	332	NAG	O5-C1-C2	2.27	114.88	111.29
5	A	328	NAG	O3-C3-C4	2.23	115.50	110.35
5	G	331	NAG	C4-C3-C2	2.22	114.27	111.02
5	G	331	NAG	O3-C3-C2	2.11	113.84	109.47
5	G	332	NAG	O4-C4-C3	2.08	115.16	110.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	331	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	328	NAG	C4-C5-C6-O6
5	A	328	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	E	328	NAG	C4-C5-C6-O6
5	E	328	NAG	O5-C5-C6-O6
5	G	331	NAG	O5-C5-C6-O6
5	G	331	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	328	NAG	1	0
5	A	328	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 ⓘ

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	325/331 (98%)	-0.13	9 (2%) 53 43	7, 20, 33, 49	0
1	C	323/331 (97%)	-0.27	3 (0%) 84 80	7, 20, 33, 49	0
1	E	323/331 (97%)	-0.07	14 (4%) 35 25	8, 20, 33, 48	0
1	G	322/331 (97%)	-0.21	9 (2%) 53 43	8, 20, 33, 49	0
1	I	322/331 (97%)	0.18	16 (4%) 28 19	8, 20, 33, 48	0
1	K	321/331 (96%)	-0.08	9 (2%) 53 43	8, 20, 33, 49	0
2	B	169/181 (93%)	0.07	3 (1%) 68 61	4, 31, 50, 69	1 (0%)
2	D	171/181 (94%)	-0.03	0 100 100	4, 32, 53, 69	0
2	F	171/181 (94%)	0.63	26 (15%) 2 1	4, 32, 50, 69	0
2	H	170/181 (93%)	0.13	7 (4%) 37 27	4, 32, 50, 69	0
2	J	170/181 (93%)	0.32	7 (4%) 37 27	4, 32, 50, 69	0
2	L	171/181 (94%)	0.67	26 (15%) 2 1	4, 32, 50, 69	0
All	All	2958/3072 (96%)	0.04	129 (4%) 34 24	4, 22, 44, 69	1 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	71	SER	8.1
1	G	71	SER	7.6
1	I	139	ALA	7.4
2	L	164	GLU	6.9
1	K	3	LEU	6.2
2	F	35	ALA	6.2
1	G	72	THR	6.2
2	F	29	GLU	5.9
2	F	32	SER	5.8
2	F	159	TYR	5.5
1	K	2	THR	5.0

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Mol	Chain	Res	Type	RSRZ
2	L	31	GLY	4.9
1	A	71	SER	4.6
1	E	11	ASN	4.5
2	L	148	CYS	4.5
1	G	70	LEU	4.5
2	F	38	LEU	4.5
1	A	70	LEU	4.4
2	L	141	TYR	4.4
2	F	33	GLY	4.3
2	L	139	GLU	4.3
2	L	159	TYR	4.2
2	H	128	ASN	4.2
1	A	69	SER	4.1
2	L	128	ASN	4.1
1	K	5	ILE	4.0
2	L	163	SER	4.0
1	I	72	THR	3.9
1	I	3	LEU	3.9
2	L	131	LYS	3.8
2	L	149	MET	3.8
2	B	168	LEU	3.8
1	E	36	LYS	3.7
2	L	27	GLN	3.7
2	H	19	ASP	3.7
2	F	34	TYR	3.7
2	L	162	TYR	3.6
2	F	147	THR	3.5
1	I	138	HIS	3.5
2	F	27	GLN	3.5
2	F	167	LYS	3.4
2	L	144	CYS	3.4
2	L	152	VAL	3.3
1	A	72	THR	3.3
2	F	128	ASN	3.3
2	L	133	ILE	3.2
1	E	71	SER	3.2
1	I	154	LYS	3.2
1	G	139	ALA	3.2
2	F	163	SER	3.2
1	I	140	GLY	3.2
1	A	274	ASP	3.1
2	L	140	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	275	CYS	3.1
1	G	2	THR	3.1
2	F	17	MET	3.1
1	A	275	CYS	3.1
1	K	68	GLU	3.1
2	H	164	GLU	3.1
1	I	321	VAL	3.0
2	F	152	VAL	3.0
1	E	274	ASP	3.0
1	K	69	SER	3.0
2	L	157	TYR	2.9
2	F	160	PRO	2.9
2	F	144	CYS	2.9
1	K	6	GLY	2.9
1	C	274	ASP	2.8
2	L	168	LEU	2.8
1	K	71	SER	2.8
2	J	168	LEU	2.8
2	L	142	HIS	2.7
1	G	4	CYS	2.7
1	E	1	ASP	2.7
2	F	145	ASP	2.7
1	A	45	ARG	2.7
2	F	18	VAL	2.7
2	F	143	LYS	2.7
1	K	4	CYS	2.6
1	I	70	LEU	2.6
1	E	3	LEU	2.6
1	E	46	GLY	2.6
1	I	68	GLU	2.6
2	L	32	SER	2.6
2	J	18	VAL	2.6
2	F	162	TYR	2.5
2	H	168	LEU	2.5
1	I	272	VAL	2.5
1	I	45	ARG	2.5
2	H	167	LYS	2.5
1	E	2	THR	2.5
1	K	70	LEU	2.5
2	L	14	TRP	2.4
1	I	54	LYS	2.4
2	F	16	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	J	164	GLU	2.4
1	C	72	THR	2.4
2	F	23	GLY	2.3
2	L	130	ALA	2.3
1	A	46	GLY	2.3
2	J	33	GLY	2.3
1	I	253	TYR	2.3
2	J	171	GLU	2.3
1	E	14	ASP	2.3
1	C	71	SER	2.3
1	G	73	ALA	2.3
2	B	169	ASN	2.3
2	L	138	PHE	2.3
1	I	275	CYS	2.2
1	E	13	THR	2.2
1	G	141	ALA	2.2
2	L	143	LYS	2.2
1	E	70	LEU	2.2
2	L	134	GLY	2.1
2	F	24	TYR	2.1
2	H	159	TYR	2.1
2	L	127	LYS	2.1
1	A	140	GLY	2.1
1	E	4	CYS	2.1
2	F	164	GLU	2.1
1	G	13	THR	2.1
2	J	154	ASN	2.1
2	B	29	GLU	2.0
1	E	9	ALA	2.0
2	F	20	GLY	2.0
2	F	150	GLU	2.0
2	H	141	TYR	2.0
1	I	277	THR	2.0
2	J	32	SER	2.0

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

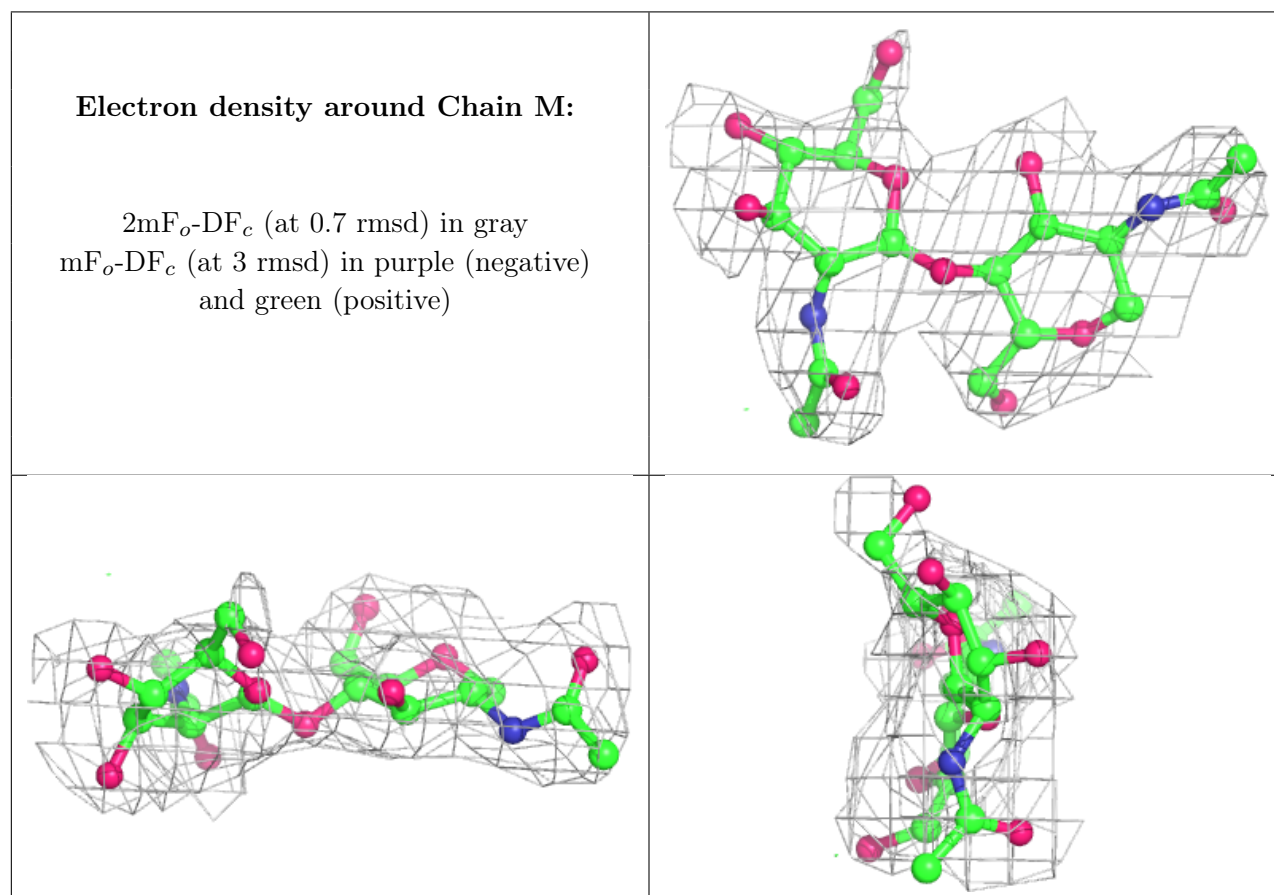
There are no non-standard protein/DNA/RNA residues in this entry.

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.

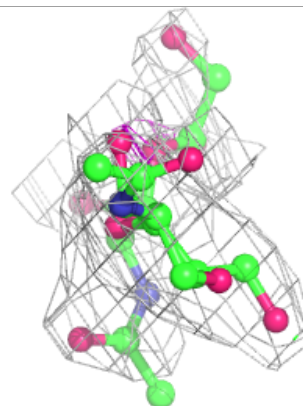
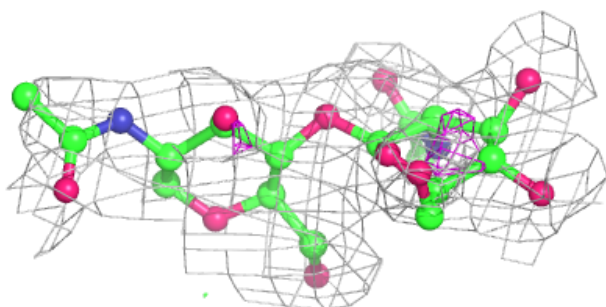
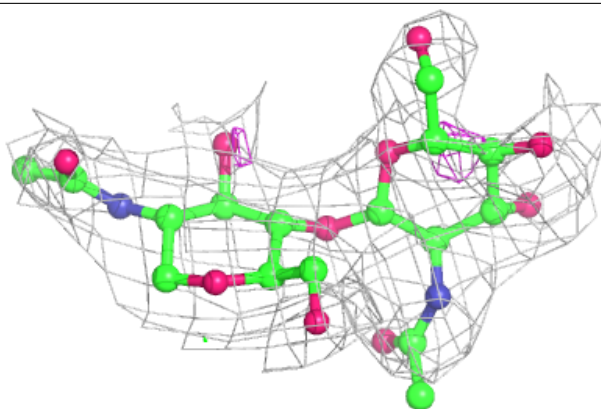
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	N	3	11/12	0.69	0.24	77,83,85,86	0
3	NAG	Q	2	14/15	0.73	0.31	81,84,88,88	0
3	NAG	Q	1	14/15	0.73	0.26	56,67,74,78	0
3	NAG	O	2	14/15	0.76	0.26	76,80,82,82	0
3	NAG	M	2	14/15	0.83	0.17	73,77,78,79	0
3	NAG	O	1	14/15	0.86	0.18	52,60,68,69	0
3	NAG	P	2	14/15	0.88	0.23	89,94,101,101	0
4	NAG	N	2	14/15	0.92	0.18	45,58,63,71	0
3	NAG	P	1	14/15	0.93	0.15	61,68,73,82	0
4	NAG	N	1	14/15	0.94	0.20	48,53,55,57	0
3	NAG	M	1	14/15	0.95	0.13	47,52,60,66	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.

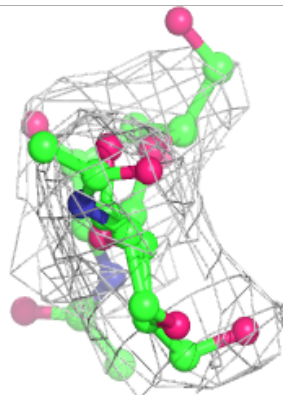
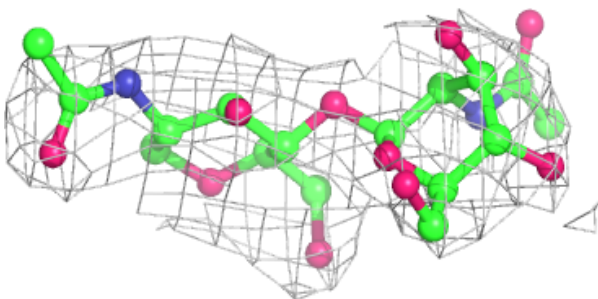
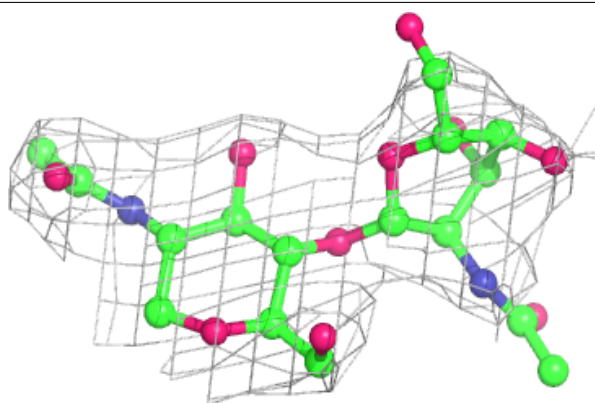


Electron density around Chain O:

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

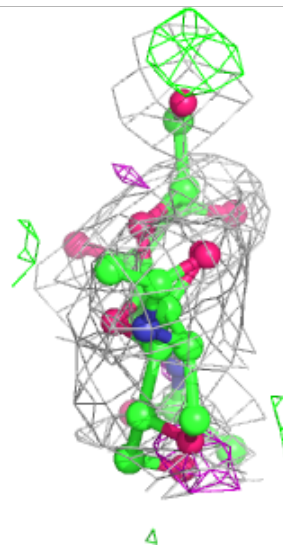
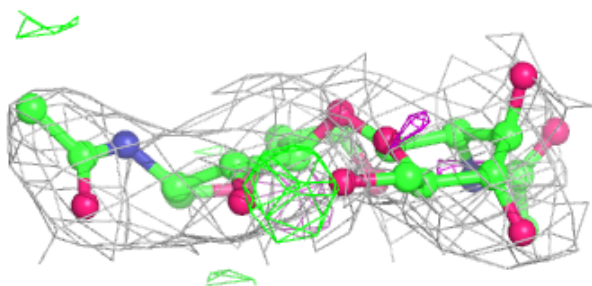
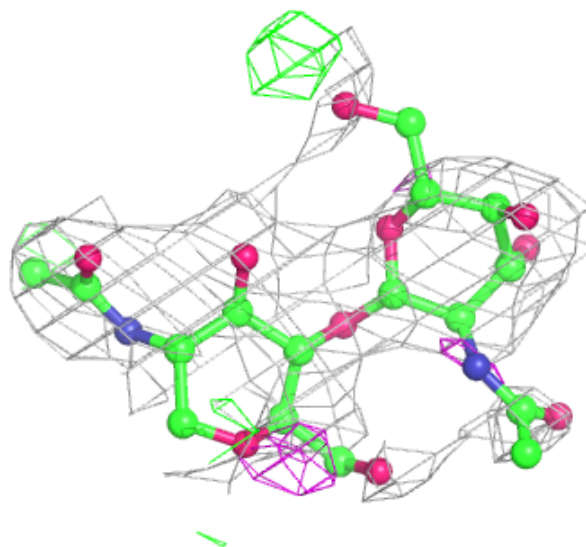
**Electron density around Chain P:**

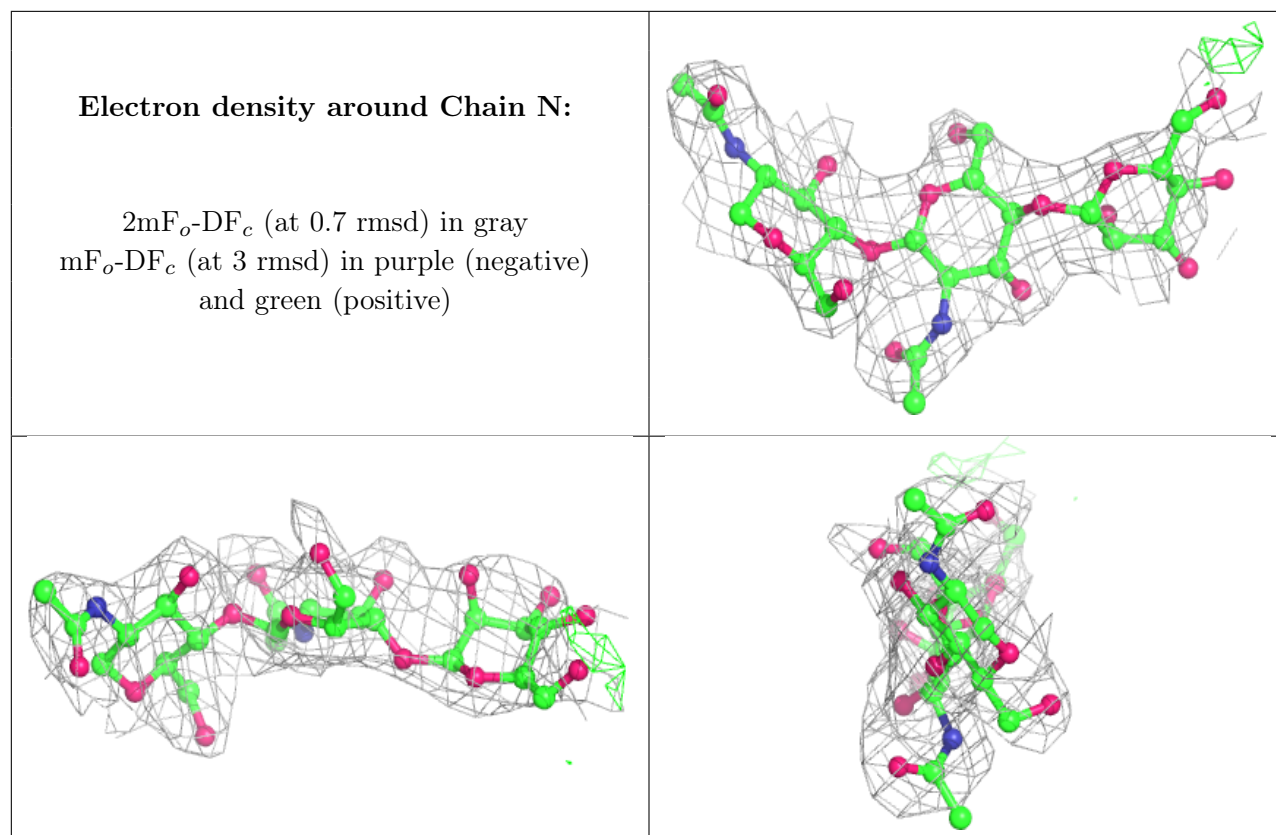
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain Q:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	G	331	14/15	0.63	0.27	59,72,74,76	0
5	NAG	G	332	14/15	0.73	0.21	64,74,80,81	0
5	NAG	A	328	14/15	0.90	0.17	49,55,59,59	0
5	NAG	E	328	14/15	0.95	0.19	46,51,53,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.