



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:36 AM UTC

PDB ID : 6TVR / pdb_00006tvr
Title : Crystal structure of the haemagglutinin mutant (Gln226Leu) from an H10N7 seal influenza virus isolated in Germany
Authors : Zhang, J.; Xiong, X.; Purkiss, A.; Walker, P.; Gamblin, S.; Skehel, J.J.
Deposited on : 2020-01-10
Resolution : 2.63 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

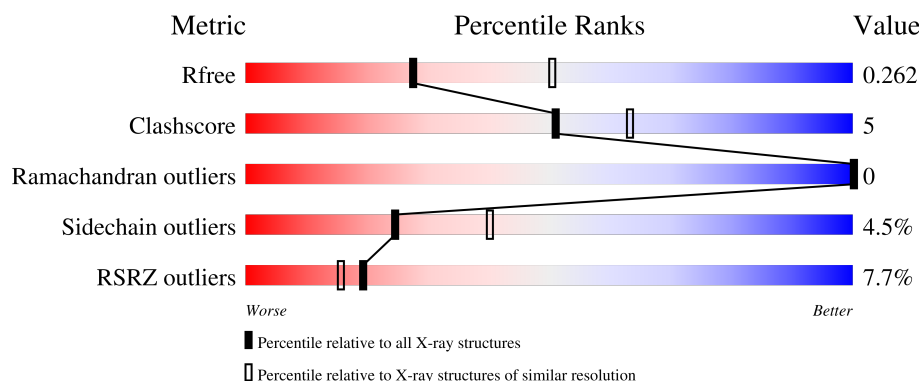
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	3% 90% 8% .
1	C	325	6% 89% 9% ..
1	E	325	11% 81% 17% .
1	G	325	23% 81% 16% ..
1	I	325	19% 80% 18% .

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Mol	Chain	Length	Quality of chain
1	K	325	2% 90% 7% ..
2	B	177	% 86% 11% .
2	D	177	% 86% 11% ..
2	F	177	5% 82% 15% .
2	H	177	% 86% 10% ..
2	J	177	% 86% 11% .
2	L	177	% 88% 10% .
3	M	2	50% 50%
3	N	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23416 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 HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2450	1521	443	470	16			
1	C	320	Total	C	N	O	S	0	0	0
			2442	1515	442	469	16			
1	E	320	Total	C	N	O	S	0	0	0
			2442	1515	442	469	16			
1	G	319	Total	C	N	O	S	0	0	0
			2434	1511	441	466	16			
1	I	319	Total	C	N	O	S	0	0	0
			2435	1512	440	467	16			
1	K	320	Total	C	N	O	S	0	0	0
			2442	1515	442	469	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASP	-	expression tag	UNP A0A0A7HR51
A	2	PRO	-	expression tag	UNP A0A0A7HR51
C	1	ASP	-	expression tag	UNP A0A0A7HR51
C	2	PRO	-	expression tag	UNP A0A0A7HR51
E	1	ASP	-	expression tag	UNP A0A0A7HR51
E	2	PRO	-	expression tag	UNP A0A0A7HR51
G	0	ASP	-	expression tag	UNP A0A0A7HR51
G	1	PRO	-	expression tag	UNP A0A0A7HR51
I	1	ASP	-	expression tag	UNP A0A0A7HR51
I	2	PRO	-	expression tag	UNP A0A0A7HR51
K	1	ASP	-	expression tag	UNP A0A0A7HR51
K	2	PRO	-	expression tag	UNP A0A0A7HR51

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			
2	D	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			
2	F	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			
2	H	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			
2	J	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			
2	L	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	LYS	-	expression tag	UNP A0A0A7HR51
D	177	LYS	-	expression tag	UNP A0A0A7HR51
F	177	LYS	-	expression tag	UNP A0A0A7HR51
H	177	LYS	-	expression tag	UNP A0A0A7HR51
J	177	LYS	-	expression tag	UNP A0A0A7HR51
L	177	LYS	-	expression tag	UNP A0A0A7HR51

- 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	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

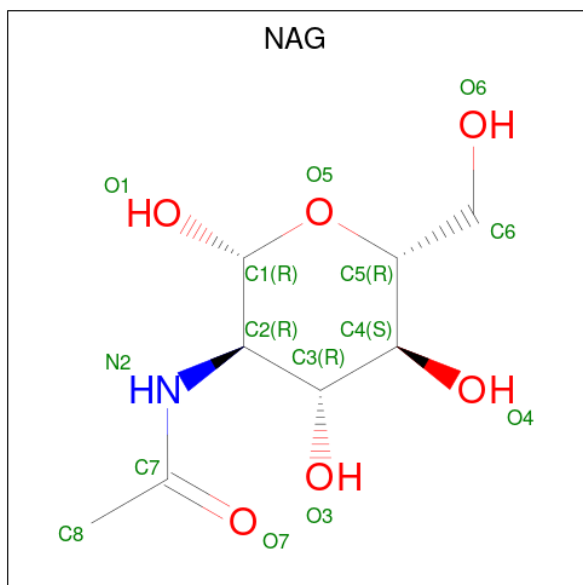
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	D	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Ca	0	0
			1	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	K	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	42	Total	O	0	0
			42	42		
7	B	37	Total	O	0	0
			37	37		
7	C	26	Total	O	0	0
			26	26		
7	D	34	Total	O	0	0
			34	34		
7	E	16	Total	O	0	0
			16	16		
7	F	17	Total	O	0	0
			17	17		
7	G	22	Total	O	0	0
			22	22		
7	H	30	Total	O	0	0
			30	30		
7	I	17	Total	O	0	0
			17	17		
7	J	18	Total	O	0	0
			18	18		
7	K	51	Total	O	0	0
			51	51		

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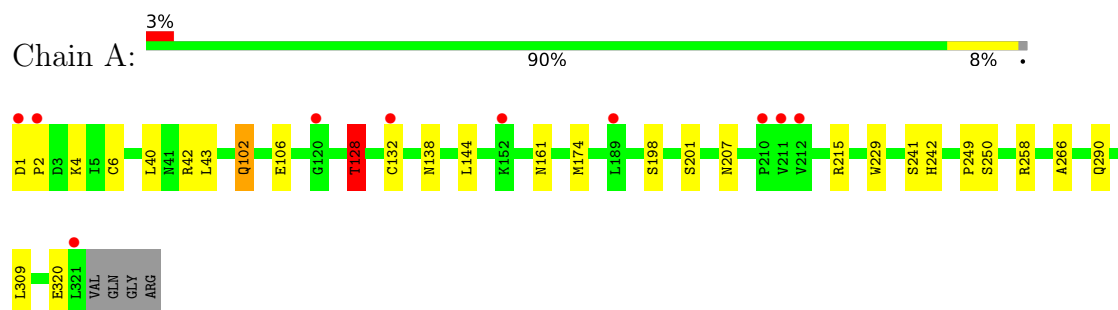
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	29	Total	O	0	0
			29	29		

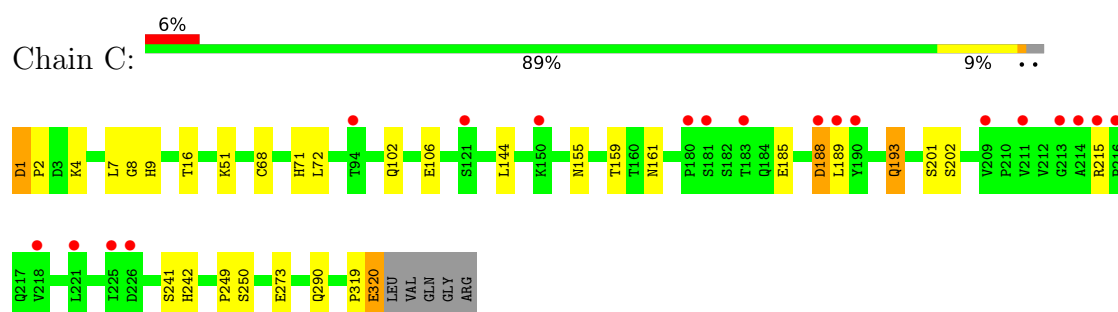
3 Residue-property plots [i](#)

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.

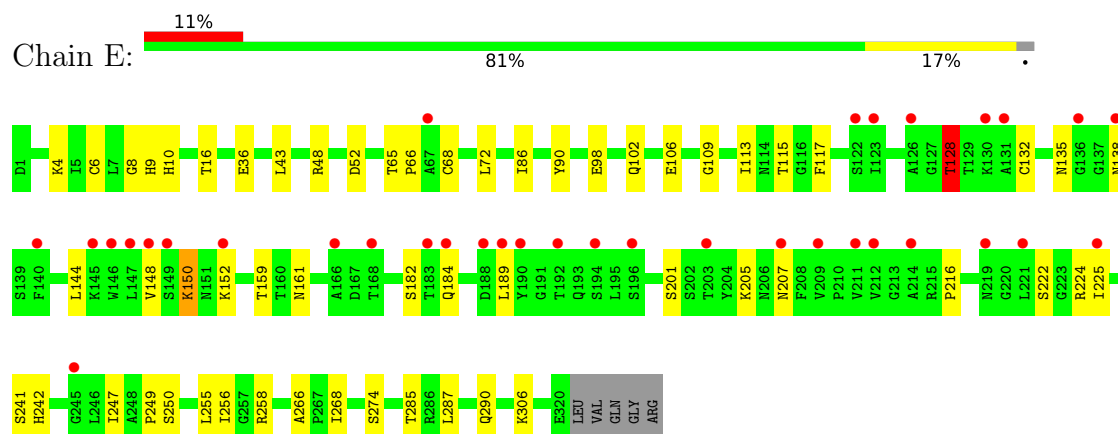
• Molecule 1: Hemagglutinin HA1



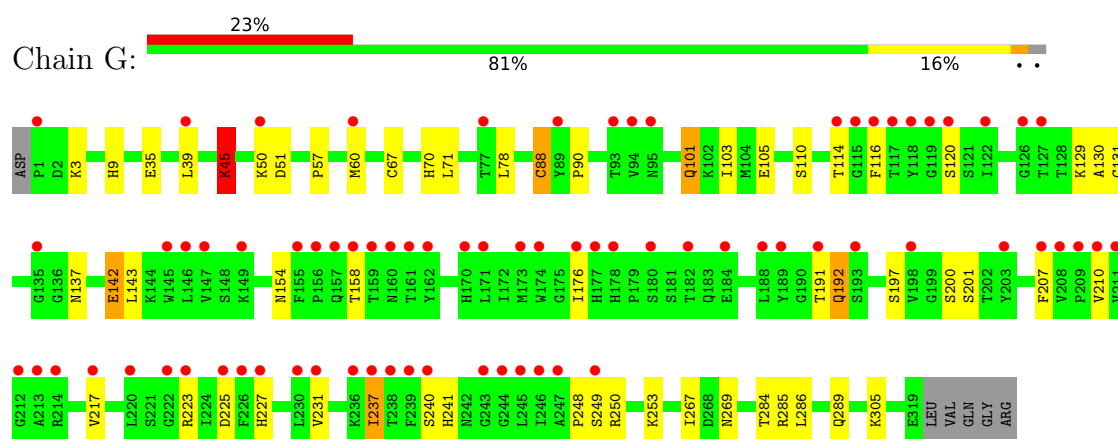
• Molecule 1: Hemagglutinin HA1



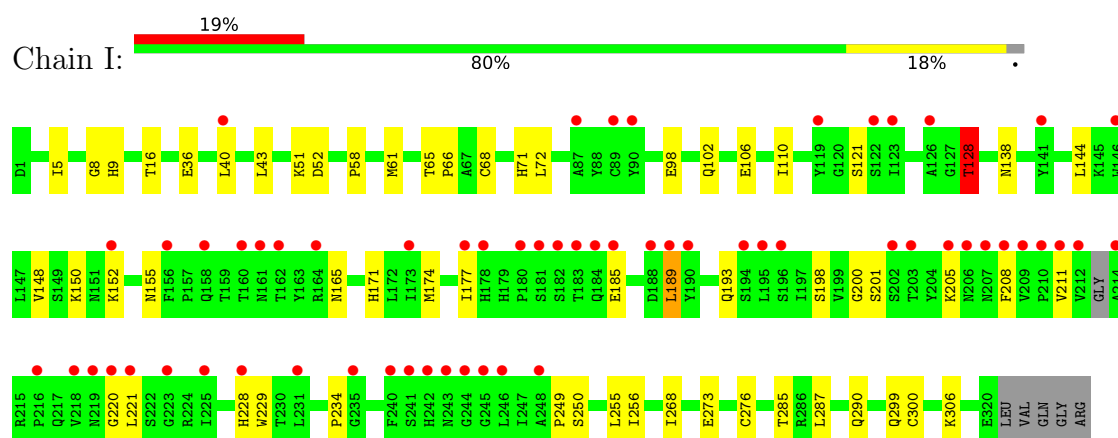
• Molecule 1: Hemagglutinin HA1



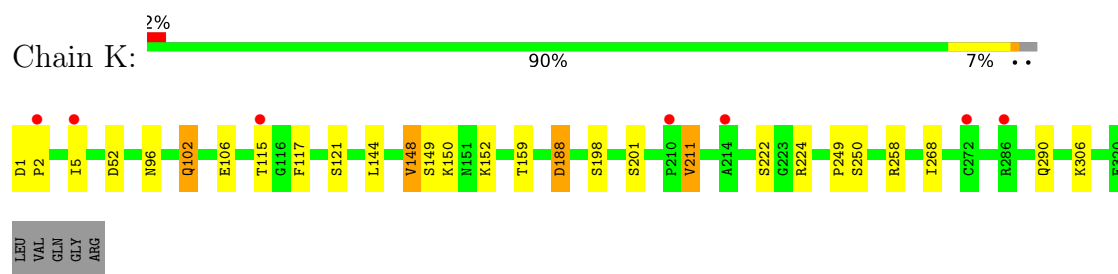
• Molecule 1: Hemagglutinin HA1



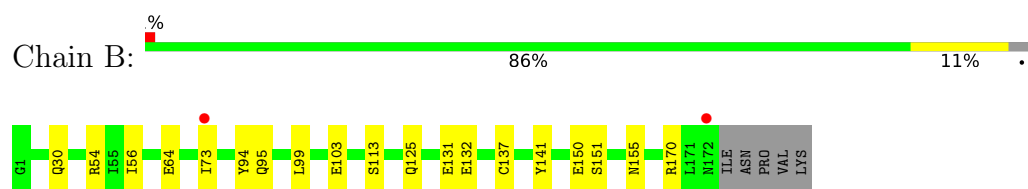
• Molecule 1: Hemagglutinin HA1



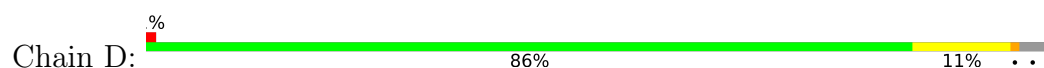
• Molecule 1: Hemagglutinin HA1



• Molecule 2: Hemagglutinin HA2

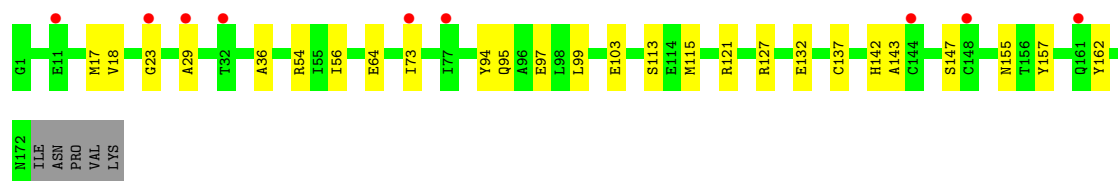
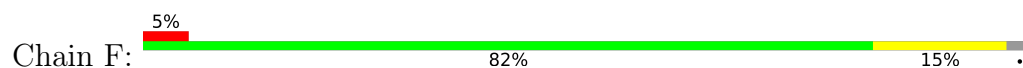


• Molecule 2: Hemagglutinin HA2

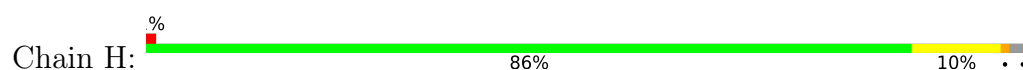




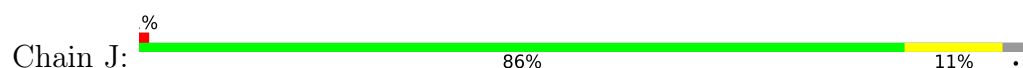
• Molecule 2: Hemagglutinin HA2



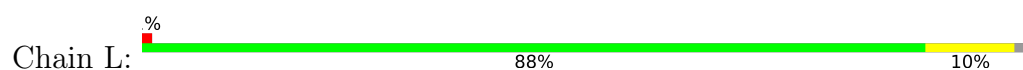
• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2



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



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



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.35Å 214.10Å 157.16Å 90.00° 102.06° 90.00°	Depositor
Resolution (Å)	72.33 – 2.63 72.33 – 2.63	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.33-2.63) 100.0 (72.33-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.241 , 0.264 0.239 , 0.262	Depositor DCC
R_{free} test set	6486 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23416	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6327e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EDO, CA, 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	1.02	0/2500	1.33	1/3388 (0.0%)
1	C	1.04	0/2492	1.34	1/3377 (0.0%)
1	E	1.03	0/2492	1.34	1/3377 (0.0%)
1	G	1.03	0/2484	1.35	1/3365 (0.0%)
1	I	1.04	0/2484	1.34	1/3365 (0.0%)
1	K	1.02	0/2492	1.33	0/3377
2	B	0.98	0/1408	1.50	2/1900 (0.1%)
2	D	0.97	0/1408	1.51	4/1900 (0.2%)
2	F	0.99	0/1408	1.51	4/1900 (0.2%)
2	H	0.97	0/1408	1.52	2/1900 (0.1%)
2	J	0.99	0/1408	1.50	4/1900 (0.2%)
2	L	0.98	0/1408	1.51	2/1900 (0.1%)
All	All	1.01	0/23392	1.40	23/31649 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	128	THR	CA-CB-OG1	-5.88	100.78	109.60
1	A	128	THR	CA-CB-OG1	-5.69	101.06	109.60
2	J	132	GLU	CA-C-N	5.67	127.88	120.28
2	J	132	GLU	C-N-CA	5.67	127.88	120.28
1	I	128	THR	CA-CB-OG1	-5.66	101.11	109.60
2	F	132	GLU	CA-C-N	5.65	127.85	120.28
2	F	132	GLU	C-N-CA	5.65	127.85	120.28
2	B	132	GLU	CA-C-N	5.57	127.74	120.28
2	B	132	GLU	C-N-CA	5.57	127.74	120.28
2	L	132	GLU	CA-C-N	5.48	127.62	120.28
2	L	132	GLU	C-N-CA	5.48	127.62	120.28
2	H	132	GLU	CA-C-N	5.37	127.47	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	132	GLU	C-N-CA	5.37	127.47	120.28
1	G	45	LYS	CA-C-O	-5.33	115.23	120.82
2	D	29	ALA	CA-C-N	5.24	127.83	120.28
2	D	29	ALA	C-N-CA	5.24	127.83	120.28
1	C	188	ASP	CA-CB-CG	5.22	117.82	112.60
2	F	29	ALA	CA-C-N	5.11	127.64	120.28
2	F	29	ALA	C-N-CA	5.11	127.64	120.28
2	D	132	GLU	CA-C-N	5.09	127.51	120.29
2	D	132	GLU	C-N-CA	5.09	127.51	120.29
2	J	29	ALA	CA-C-N	5.07	127.58	120.28
2	J	29	ALA	C-N-CA	5.07	127.58	120.28

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	2450	0	2410	17	0
1	C	2442	0	2399	20	0
1	E	2442	0	2399	46	0
1	G	2434	0	2395	42	0
1	I	2435	0	2390	48	0
1	K	2442	0	2399	15	0
2	B	1383	0	1282	10	0
2	D	1383	0	1282	16	0
2	F	1383	0	1282	25	0
2	H	1383	0	1282	9	0
2	J	1383	0	1282	18	0
2	L	1383	0	1282	11	0
3	M	28	0	25	1	0
3	N	28	0	25	0	0
4	A	1	0	0	0	0
4	D	2	0	0	0	0
4	G	1	0	0	0	0
5	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	14	0	13	0	0
5	H	14	0	13	0	0
5	I	14	0	13	0	0
5	J	14	0	13	0	0
6	K	4	0	6	0	0
7	A	42	0	0	0	0
7	B	37	0	0	0	0
7	C	26	0	0	0	0
7	D	34	0	0	0	0
7	E	16	0	0	0	0
7	F	17	0	0	1	0
7	G	22	0	0	1	0
7	H	30	0	0	1	0
7	I	17	0	0	0	0
7	J	18	0	0	0	0
7	K	51	0	0	1	0
7	L	29	0	0	0	0
All	All	23416	0	22205	233	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (233) 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:E:90:TYR:CE1	1:E:225:ILE:HD13	1.81	1.16
2:F:17:MET:HE1	2:F:23:GLY:HA3	1.42	0.97
1:E:90:TYR:CD1	1:E:225:ILE:HD13	2.01	0.96
1:I:276:CYS:SG	1:I:299:GLN:O	2.31	0.89
1:C:8:GLY:C	2:D:115:MET:HE1	1.99	0.87
1:E:90:TYR:CE1	1:E:225:ILE:CD1	2.58	0.85
1:E:207:ASN:HB2	1:K:211:VAL:HG21	1.59	0.82
1:I:285:THR:HG22	1:I:287:LEU:H	1.45	0.82
1:I:8:GLY:C	2:J:115:MET:HE1	2.06	0.81
1:G:88:CYS:SG	1:G:131:CYS:N	2.54	0.81
1:G:176:ILE:HD13	1:G:207:PHE:HB3	1.62	0.81
1:E:285:THR:HG22	1:E:287:LEU:H	1.44	0.81
1:I:177:ILE:HD13	1:I:208:PHE:HB3	1.63	0.80
1:G:284:THR:HG22	1:G:286:LEU:H	1.46	0.79
1:C:9:HIS:HB3	2:D:115:MET:HE2	1.65	0.78
1:I:276:CYS:SG	1:I:299:GLN:C	2.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:HIS:HB3	2:J:115:MET:HE2	1.63	0.78
1:C:155:ASN:HD21	1:C:193:GLN:HB3	1.51	0.75
1:E:8:GLY:C	2:F:115:MET:HE1	2.14	0.73
2:F:17:MET:CE	2:F:36:ALA:HA	2.18	0.73
1:G:88:CYS:SG	1:G:130:ALA:C	2.72	0.73
1:E:9:HIS:HB3	2:F:115:MET:HE2	1.70	0.73
1:A:128:THR:CG2	1:A:138:ASN:HB3	2.20	0.71
1:I:128:THR:CG2	1:I:138:ASN:HB3	2.19	0.70
1:I:148:VAL:HG23	1:I:189:LEU:HG	1.73	0.70
1:E:9:HIS:HB3	2:F:115:MET:CE	2.22	0.70
1:G:231:VAL:HG22	1:G:237:ILE:CD1	2.22	0.69
1:C:9:HIS:HB3	2:D:115:MET:CE	2.22	0.69
1:I:9:HIS:HB3	2:J:115:MET:CE	2.21	0.69
1:E:225:ILE:HG23	1:E:247:ILE:HD12	1.75	0.69
1:E:128:THR:CG2	1:E:138:ASN:HB3	2.23	0.69
1:G:176:ILE:HD12	1:G:227:HIS:CE1	2.28	0.68
1:I:58:PRO:O	1:I:61:MET:HG2	1.93	0.68
1:E:43:LEU:HD13	1:E:266:ALA:O	1.94	0.68
1:K:115:THR:HG21	1:K:249:PRO:O	1.94	0.67
1:G:57:PRO:O	1:G:60:MET:HG2	1.94	0.67
1:E:115:THR:HG21	1:E:249:PRO:O	1.96	0.66
1:G:176:ILE:HD11	1:G:207:PHE:CG	2.31	0.66
1:A:43:LEU:HD23	1:A:266:ALA:O	1.96	0.66
1:I:177:ILE:HD12	1:I:228:HIS:CE1	2.31	0.66
1:G:60:MET:HE2	1:G:103:ILE:HG21	1.78	0.65
1:G:114:THR:HG21	1:G:248:PRO:O	1.96	0.65
1:I:5:ILE:HB	2:J:149:MET:HE1	1.79	0.64
1:I:177:ILE:HD11	1:I:208:PHE:CG	2.32	0.64
2:D:95:GLN:NE2	2:F:95:GLN:OE1	2.31	0.64
1:G:231:VAL:HG22	1:G:237:ILE:HD11	1.78	0.64
2:J:26:HIS:HB3	2:J:149:MET:HE2	1.78	0.64
2:F:142:HIS:HE1	2:F:157:TYR:OH	1.79	0.63
1:K:115:THR:HG23	1:K:117:PHE:H	1.63	0.63
1:A:258:ARG:NH2	2:B:64:GLU:OE1	2.32	0.63
1:G:154:ASN:CG	1:G:192:GLN:HG3	2.23	0.62
1:E:115:THR:HG23	1:E:117:PHE:H	1.63	0.62
2:F:17:MET:HE1	2:F:36:ALA:HA	1.81	0.62
2:B:131:GLU:OE2	2:B:170:ARG:HD2	2.00	0.62
1:I:148:VAL:CG2	1:I:189:LEU:HG	2.30	0.61
1:E:43:LEU:CD1	1:E:266:ALA:HB3	2.31	0.61
2:H:125:GLN:CD	2:H:155:ASN:HD22	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:LYS:HD3	1:K:224:ARG:HG3	1.84	0.60
2:F:127:ARG:NH2	2:L:139:GLU:OE1	2.24	0.60
1:G:114:THR:HG23	1:G:116:PHE:H	1.64	0.60
2:L:56:ILE:HG22	2:L:56:ILE:O	2.02	0.60
2:F:56:ILE:O	2:F:56:ILE:HG22	2.02	0.59
2:F:18:VAL:HG12	2:F:18:VAL:O	2.01	0.59
1:G:50:LYS:HE2	1:G:70:HIS:CE1	2.37	0.59
2:F:143:ALA:N	7:F:301:HOH:O	2.33	0.59
1:I:52:ASP:OD2	1:I:268:ILE:HD11	2.03	0.59
1:K:258:ARG:NH2	2:L:64:GLU:OE1	2.36	0.59
1:G:60:MET:HE2	1:G:103:ILE:CG2	2.33	0.59
1:K:96:ASN:ND2	7:K:501:HOH:O	2.37	0.58
1:E:225:ILE:HG13	1:E:247:ILE:HD11	1.85	0.57
1:E:207:ASN:HB2	1:K:211:VAL:CG2	2.31	0.57
1:E:161:ASN:HD22	1:E:242:HIS:HE1	1.52	0.57
2:L:51:LYS:HE3	2:L:103:GLU:OE1	2.04	0.57
2:F:99:LEU:HD22	2:L:94:TYR:OH	2.04	0.57
2:H:56:ILE:HG22	2:H:56:ILE:O	2.03	0.57
2:B:94:TYR:OH	2:J:99:LEU:HD22	2.05	0.57
1:E:225:ILE:CG2	1:E:247:ILE:HD12	2.35	0.56
2:B:56:ILE:HG22	2:B:56:ILE:O	2.04	0.56
1:G:35:GLU:HG2	1:G:284:THR:OG1	2.06	0.56
1:G:200:SER:HB2	1:G:237:ILE:HG12	1.87	0.56
1:I:8:GLY:O	2:J:115:MET:HE1	2.05	0.56
2:D:56:ILE:O	2:D:56:ILE:HG22	2.04	0.56
1:G:284:THR:CG2	1:G:286:LEU:HG	2.35	0.56
2:J:56:ILE:HG22	2:J:56:ILE:O	2.06	0.56
1:A:43:LEU:CD2	1:A:266:ALA:HB3	2.35	0.56
2:J:26:HIS:CB	2:J:149:MET:HE2	2.36	0.56
1:I:220:GLY:C	1:I:221:LEU:HD22	2.31	0.56
1:I:36:GLU:HG2	1:I:285:THR:OG1	2.06	0.55
1:C:161:ASN:HD22	1:C:242:HIS:HE1	1.53	0.55
1:E:306:LYS:HE3	2:F:97:GLU:OE1	2.07	0.55
1:G:176:ILE:HD13	1:G:207:PHE:CB	2.36	0.55
1:G:176:ILE:CD1	1:G:207:PHE:CG	2.90	0.55
1:A:161:ASN:HD22	1:A:242:HIS:HE1	1.52	0.55
1:I:155:ASN:ND2	1:I:193:GLN:HB3	2.22	0.54
1:E:36:GLU:HG2	1:E:285:THR:OG1	2.06	0.54
2:H:99:LEU:HD22	2:J:94:TYR:OH	2.08	0.54
1:I:177:ILE:CD1	1:I:208:PHE:CG	2.91	0.54
1:I:285:THR:CG2	1:I:287:LEU:HG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:ARG:HG3	7:H:308:HOH:O	2.09	0.53
1:G:101:GLN:O	1:G:105:GLU:HG3	2.09	0.53
1:C:8:GLY:O	2:D:115:MET:HE1	2.09	0.53
1:E:258:ARG:NH2	2:F:64:GLU:OE2	2.42	0.53
1:G:50:LYS:HE2	1:G:70:HIS:ND1	2.24	0.53
1:A:102:GLN:O	1:A:106:GLU:HG3	2.09	0.53
1:I:177:ILE:HD13	1:I:208:PHE:CB	2.37	0.53
1:G:110:SER:OG	1:G:253:LYS:HB3	2.09	0.52
1:C:201:SER:C	1:E:216:PRO:HD2	2.35	0.52
1:E:285:THR:CG2	1:E:287:LEU:HG	2.40	0.52
1:G:154:ASN:OD1	1:G:192:GLN:HG3	2.10	0.52
1:I:306:LYS:HE3	2:J:97:GLU:OE2	2.09	0.52
1:C:51:LYS:HE3	1:C:71:HIS:ND1	2.25	0.51
1:A:43:LEU:HD22	1:A:266:ALA:HB3	1.92	0.51
1:K:102:GLN:O	1:K:106:GLU:HG3	2.11	0.51
1:I:51:LYS:HE3	1:I:71:HIS:ND1	2.25	0.51
1:C:319:PRO:O	1:C:320:GLU:HB2	2.11	0.50
1:G:60:MET:HE1	1:G:78:LEU:HD21	1.94	0.50
2:D:99:LEU:HD22	2:F:94:TYR:OH	2.11	0.50
2:F:142:HIS:CE1	2:F:157:TYR:OH	2.63	0.50
1:E:224:ARG:C	1:E:225:ILE:HD12	2.36	0.50
1:G:142:GLU:HG3	1:G:250:ARG:HB2	1.94	0.49
1:E:148:VAL:HG21	1:E:189:LEU:HD22	1.93	0.49
1:I:61:MET:HE3	1:I:71:HIS:O	2.12	0.49
1:I:155:ASN:HD21	1:I:193:GLN:HB3	1.78	0.49
1:A:161:ASN:ND2	1:A:242:HIS:HE1	2.11	0.49
2:B:54:ARG:NH2	2:B:103:GLU:OE2	2.43	0.49
2:F:99:LEU:HD22	2:L:94:TYR:HH	1.76	0.49
1:I:220:GLY:O	1:I:221:LEU:HD22	2.12	0.49
2:L:54:ARG:NH2	2:L:103:GLU:OE2	2.42	0.49
1:G:158:THR:HG23	1:G:241:HIS:NE2	2.27	0.49
1:I:61:MET:HE2	1:I:110:ILE:HD12	1.95	0.49
1:K:152:LYS:HE3	1:K:188:ASP:OD1	2.12	0.49
2:B:125:GLN:HE22	2:B:155:ASN:HA	1.78	0.48
1:K:148:VAL:HG12	1:K:149:SER:O	2.13	0.48
1:E:102:GLN:O	1:E:106:GLU:HG3	2.13	0.48
2:J:125:GLN:HE22	2:J:155:ASN:HA	1.78	0.48
2:L:51:LYS:HE2	2:L:107:THR:OG1	2.14	0.48
2:D:164:GLU:O	2:D:168:LEU:HD23	2.13	0.47
1:E:8:GLY:O	2:F:115:MET:HE1	2.13	0.47
1:I:5:ILE:HD13	2:J:152:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:GLN:HG2	2:J:95:GLN:HE21	1.78	0.47
1:I:121:SER:O	1:I:150:LYS:HE2	2.15	0.47
2:J:148:CYS:O	2:J:151:SER:OG	2.28	0.47
2:D:54:ARG:NH2	2:D:103:GLU:OE2	2.42	0.47
1:G:129:LYS:HD3	1:G:137:ASN:HD21	1.80	0.47
1:I:68:CYS:O	1:I:72:LEU:CD1	2.63	0.47
1:E:43:LEU:HD12	1:E:266:ALA:HB3	1.97	0.46
1:E:48:ARG:NH1	1:E:274:SER:O	2.48	0.46
1:G:67:CYS:O	1:G:71:LEU:CD1	2.63	0.46
1:C:68:CYS:O	1:C:72:LEU:CD1	2.64	0.46
1:A:1:ASP:N	1:A:2:PRO:CD	2.78	0.46
2:D:94:TYR:OH	2:L:99:LEU:HD22	2.16	0.46
1:G:39:LEU:HD12	1:G:39:LEU:N	2.31	0.46
2:H:54:ARG:NH2	2:H:103:GLU:OE1	2.44	0.46
1:E:68:CYS:O	1:E:72:LEU:HD13	2.16	0.46
2:H:164:GLU:O	2:H:168:LEU:HD23	2.15	0.46
1:I:177:ILE:HD11	1:I:208:PHE:CD1	2.51	0.46
1:G:45:LYS:HG3	1:G:269:ASN:O	2.15	0.46
1:I:102:GLN:O	1:I:106:GLU:HG3	2.16	0.46
1:I:68:CYS:O	1:I:72:LEU:HD13	2.16	0.46
1:C:201:SER:OG	1:C:202:SER:N	2.48	0.45
1:E:150:LYS:O	1:E:150:LYS:HD3	2.16	0.45
1:I:144:LEU:HD23	1:I:249:PRO:HA	1.99	0.45
1:C:144:LEU:HD23	1:C:249:PRO:HA	1.98	0.45
1:E:43:LEU:HD11	1:E:266:ALA:HB3	1.99	0.45
3:M:2:NAG:H3	3:M:2:NAG:H83	1.99	0.45
2:B:99:LEU:HD22	2:H:94:TYR:OH	2.16	0.45
1:E:68:CYS:O	1:E:72:LEU:CD1	2.65	0.45
1:K:1:ASP:N	1:K:2:PRO:CD	2.78	0.45
1:C:161:ASN:ND2	1:C:242:HIS:HE1	2.14	0.45
1:E:52:ASP:HB2	1:E:268:ILE:HD11	1.97	0.45
1:G:200:SER:OG	1:G:201:SER:N	2.49	0.45
1:K:52:ASP:HB2	1:K:268:ILE:HD11	1.99	0.45
2:F:18:VAL:O	2:F:18:VAL:CG1	2.65	0.45
1:C:1:ASP:N	1:C:2:PRO:CD	2.80	0.45
1:C:9:HIS:N	2:D:115:MET:HE1	2.31	0.45
1:E:6:CYS:HA	2:F:137:CYS:HA	1.99	0.44
2:L:2:LEU:HD22	2:L:109:ASP:CG	2.42	0.44
1:A:144:LEU:HD23	1:A:249:PRO:HA	1.98	0.44
1:C:9:HIS:HA	2:D:21:TRP:O	2.17	0.44
1:C:102:GLN:O	1:C:106:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:LEU:HD23	1:E:249:PRO:HA	1.98	0.44
1:G:143:LEU:HD23	1:G:248:PRO:HA	1.98	0.44
1:G:3:LYS:HG2	2:H:137:CYS:SG	2.58	0.44
1:I:165:ASN:OD1	1:I:171:HIS:CG	2.71	0.44
2:F:17:MET:CE	2:F:36:ALA:CA	2.93	0.44
1:K:144:LEU:HD23	1:K:249:PRO:HA	1.98	0.44
1:I:165:ASN:HD22	1:I:234:PRO:HA	1.81	0.44
2:D:148:CYS:O	2:D:151:SER:OG	2.27	0.43
1:E:65:THR:HG22	1:E:66:PRO:HD2	1.99	0.43
1:I:5:ILE:HD12	2:J:149:MET:CE	2.48	0.43
1:E:207:ASN:CB	1:K:211:VAL:HG21	2.38	0.43
2:J:54:ARG:NH2	2:J:103:GLU:OE2	2.43	0.43
1:E:161:ASN:ND2	1:E:242:HIS:HE1	2.14	0.43
1:K:121:SER:O	1:K:150:LYS:HE2	2.18	0.43
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.87	0.43
2:B:141:TYR:CG	2:B:170:ARG:HG2	2.53	0.43
2:F:121:ARG:NH1	2:F:155:ASN:OD1	2.52	0.43
2:F:54:ARG:NH2	2:F:103:GLU:OE2	2.43	0.43
2:F:142:HIS:ND1	2:F:162:TYR:HB3	2.34	0.43
1:G:176:ILE:HD11	1:G:207:PHE:CD1	2.54	0.43
1:E:109:GLY:C	1:E:256:ILE:HD12	2.44	0.43
1:C:4:LYS:HG2	2:D:137:CYS:SG	2.59	0.42
1:C:68:CYS:O	1:C:72:LEU:HD13	2.19	0.42
1:I:36:GLU:HB2	1:I:285:THR:HG21	2.01	0.42
1:G:51:ASP:HB2	1:G:267:ILE:HD11	2.01	0.42
1:I:276:CYS:SG	1:I:300:CYS:N	2.84	0.42
1:E:36:GLU:HB2	1:E:285:THR:HG21	2.02	0.42
1:C:7:LEU:CD2	2:D:118:LEU:HG	2.50	0.42
1:I:177:ILE:CD1	1:I:208:PHE:CD1	3.03	0.42
1:I:40:LEU:N	1:I:40:LEU:HD12	2.35	0.42
1:A:6:CYS:HA	2:B:137:CYS:HA	2.02	0.41
1:E:225:ILE:CG1	1:E:247:ILE:HD11	2.48	0.41
1:I:36:GLU:OE1	1:I:285:THR:CG2	2.68	0.41
1:A:207:ASN:CG	1:G:210:VAL:HG11	2.45	0.41
1:A:215:ARG:HB3	1:I:200:GLY:HA3	2.01	0.41
1:E:36:GLU:OE1	1:E:285:THR:CG2	2.69	0.41
1:E:182:SER:HB2	1:E:184:GLN:HG2	2.02	0.41
2:L:148:CYS:O	2:L:151:SER:OG	2.27	0.41
1:G:35:GLU:HB2	1:G:284:THR:HG21	2.01	0.41
1:G:67:CYS:O	1:G:71:LEU:HD13	2.21	0.41
2:H:148:CYS:O	2:H:151:SER:OG	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD12	1:A:40:LEU:N	2.36	0.41
1:G:90:PRO:HB3	1:G:217:VAL:HB	2.02	0.41
2:D:2:LEU:HD23	2:D:2:LEU:HA	1.93	0.41
1:E:128:THR:CG2	1:E:138:ASN:CB	2.98	0.41
1:G:35:GLU:OE1	1:G:284:THR:CG2	2.69	0.41
1:A:128:THR:HG23	1:A:138:ASN:HB3	2.01	0.40
1:I:65:THR:HG22	1:I:66:PRO:HD2	2.03	0.40
1:A:174:MET:HG2	1:A:229:TRP:HB3	2.03	0.40
1:I:9:HIS:HD2	2:J:115:MET:HE3	1.86	0.40
1:I:177:ILE:HD12	1:I:228:HIS:HE1	1.84	0.40
1:G:101:GLN:HB2	7:G:514:HOH:O	2.20	0.40
1:I:174:MET:HG2	1:I:229:TRP:HB3	2.03	0.40

There are no symmetry-related clashes.

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	319/325 (98%)	310 (97%)	9 (3%)	0	100	100
1	C	318/325 (98%)	309 (97%)	9 (3%)	0	100	100
1	E	318/325 (98%)	309 (97%)	9 (3%)	0	100	100
1	G	317/325 (98%)	309 (98%)	8 (2%)	0	100	100
1	I	315/325 (97%)	306 (97%)	9 (3%)	0	100	100
1	K	318/325 (98%)	310 (98%)	8 (2%)	0	100	100
2	B	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	D	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	F	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	H	170/177 (96%)	165 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	L	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
All	All	2925/3012 (97%)	2843 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	271/275 (98%)	260 (96%)	11 (4%)	27	44
1	C	270/275 (98%)	257 (95%)	13 (5%)	23	37
1	E	270/275 (98%)	252 (93%)	18 (7%)	15	24
1	G	269/275 (98%)	252 (94%)	17 (6%)	16	27
1	I	269/275 (98%)	253 (94%)	16 (6%)	18	29
1	K	270/275 (98%)	258 (96%)	12 (4%)	25	41
2	B	145/151 (96%)	140 (97%)	5 (3%)	32	52
2	D	145/151 (96%)	141 (97%)	4 (3%)	38	58
2	F	145/151 (96%)	142 (98%)	3 (2%)	47	67
2	H	145/151 (96%)	138 (95%)	7 (5%)	23	37
2	J	145/151 (96%)	142 (98%)	3 (2%)	47	67
2	L	145/151 (96%)	142 (98%)	3 (2%)	47	67
All	All	2489/2556 (97%)	2377 (96%)	112 (4%)	24	40

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	42	ARG
1	A	102	GLN
1	A	128	THR

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Mol	Chain	Res	Type
1	A	132	CYS
1	A	198	SER
1	A	201	SER
1	A	241	SER
1	A	250	SER
1	A	290	GLN
1	A	320	GLU
2	B	30	GLN
2	B	73	ILE
2	B	113	SER
2	B	150	GLU
2	B	151	SER
1	C	1	ASP
1	C	16	THR
1	C	159	THR
1	C	185	GLU
1	C	188	ASP
1	C	189	LEU
1	C	193	GLN
1	C	215	ARG
1	C	241	SER
1	C	250	SER
1	C	273	GLU
1	C	290	GLN
1	C	320	GLU
2	D	73	ILE
2	D	113	SER
2	D	137	CYS
2	D	147	SER
1	E	4	LYS
1	E	10	HIS
1	E	16	THR
1	E	86	ILE
1	E	98	GLU
1	E	113	ILE
1	E	128	THR
1	E	132	CYS
1	E	135	ASN
1	E	150	LYS
1	E	152	LYS
1	E	159	THR
1	E	201	SER

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Mol	Chain	Res	Type
1	E	222	SER
1	E	241	SER
1	E	250	SER
1	E	255	LEU
1	E	290	GLN
2	F	73	ILE
2	F	113	SER
2	F	147	SER
1	G	9	HIS
1	G	45	LYS
1	G	88	CYS
1	G	101	GLN
1	G	120	SER
1	G	142	GLU
1	G	191	THR
1	G	192	GLN
1	G	197	SER
1	G	223	ARG
1	G	225	ASP
1	G	237	ILE
1	G	240	SER
1	G	249	SER
1	G	285	ARG
1	G	289	GLN
1	G	305	LYS
2	H	58	LYS
2	H	73	ILE
2	H	95	GLN
2	H	113	SER
2	H	127	ARG
2	H	137	CYS
2	H	147	SER
1	I	16	THR
1	I	43	LEU
1	I	98	GLU
1	I	128	THR
1	I	152	LYS
1	I	185	GLU
1	I	189	LEU
1	I	198	SER
1	I	201	SER
1	I	205	LYS

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Mol	Chain	Res	Type
1	I	211	VAL
1	I	250	SER
1	I	255	LEU
1	I	256	ILE
1	I	273	GLU
1	I	290	GLN
2	J	30	GLN
2	J	73	ILE
2	J	113	SER
1	K	5	ILE
1	K	102	GLN
1	K	148	VAL
1	K	159	THR
1	K	188	ASP
1	K	198	SER
1	K	201	SER
1	K	211	VAL
1	K	222	SER
1	K	250	SER
1	K	290	GLN
1	K	306	LYS
2	L	30	GLN
2	L	73	ILE
2	L	113	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	154	GLN
1	A	161	ASN
1	A	193	GLN
1	A	242	HIS
2	B	12	ASN
2	B	27	GLN
2	B	30	GLN
2	B	47	GLN
2	B	76	GLN
2	B	95	GLN
2	B	105	GLN
1	C	50	HIS
1	C	84	ASN

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Mol	Chain	Res	Type
1	C	96	ASN
1	C	178	HIS
1	C	242	HIS
1	C	270	ASN
1	C	299	GLN
2	D	47	GLN
2	D	95	GLN
2	D	105	GLN
2	D	161	GLN
1	E	102	GLN
1	E	158	GLN
1	E	161	ASN
1	E	217	GLN
1	E	242	HIS
2	F	27	GLN
2	F	47	GLN
2	F	105	GLN
2	F	142	HIS
1	G	49	HIS
1	G	95	ASN
1	G	101	GLN
1	G	137	ASN
1	G	177	HIS
1	G	227	HIS
1	G	269	ASN
1	G	283	ASN
2	H	27	GLN
2	H	47	GLN
2	H	155	ASN
1	I	10	HIS
1	I	84	ASN
1	I	102	GLN
1	I	124	ASN
1	I	155	ASN
1	I	193	GLN
1	I	228	HIS
2	J	47	GLN
2	J	75	HIS
2	J	95	GLN
2	J	105	GLN
2	J	125	GLN
1	K	84	ASN

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Mol	Chain	Res	Type
1	K	96	ASN
1	K	154	GLN
1	K	161	ASN
1	K	193	GLN
1	K	242	HIS
2	L	30	GLN
2	L	47	GLN
2	L	95	GLN
2	L	105	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	M	1	2,4,3	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
3	NAG	M	2	3	14,14,15	0.40	0	17,19,21	1.86	2 (11%)
3	NAG	N	1	2,3	14,14,15	0.36	0	17,19,21	1.09	2 (11%)
3	NAG	N	2	3	14,14,15	0.49	0	17,19,21	1.05	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	2,4,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	3/6/23/26	0/1/1/1
3	NAG	N	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	2	NAG	C2-N2-C7	4.95	129.53	122.90
3	M	2	NAG	C8-C7-N2	3.41	121.78	116.12
3	M	1	NAG	C1-O5-C5	2.48	115.51	112.19
3	N	1	NAG	C4-C3-C2	2.22	114.28	111.02
3	N	2	NAG	C1-O5-C5	2.18	115.11	112.19
3	N	1	NAG	C2-N2-C7	2.05	125.65	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

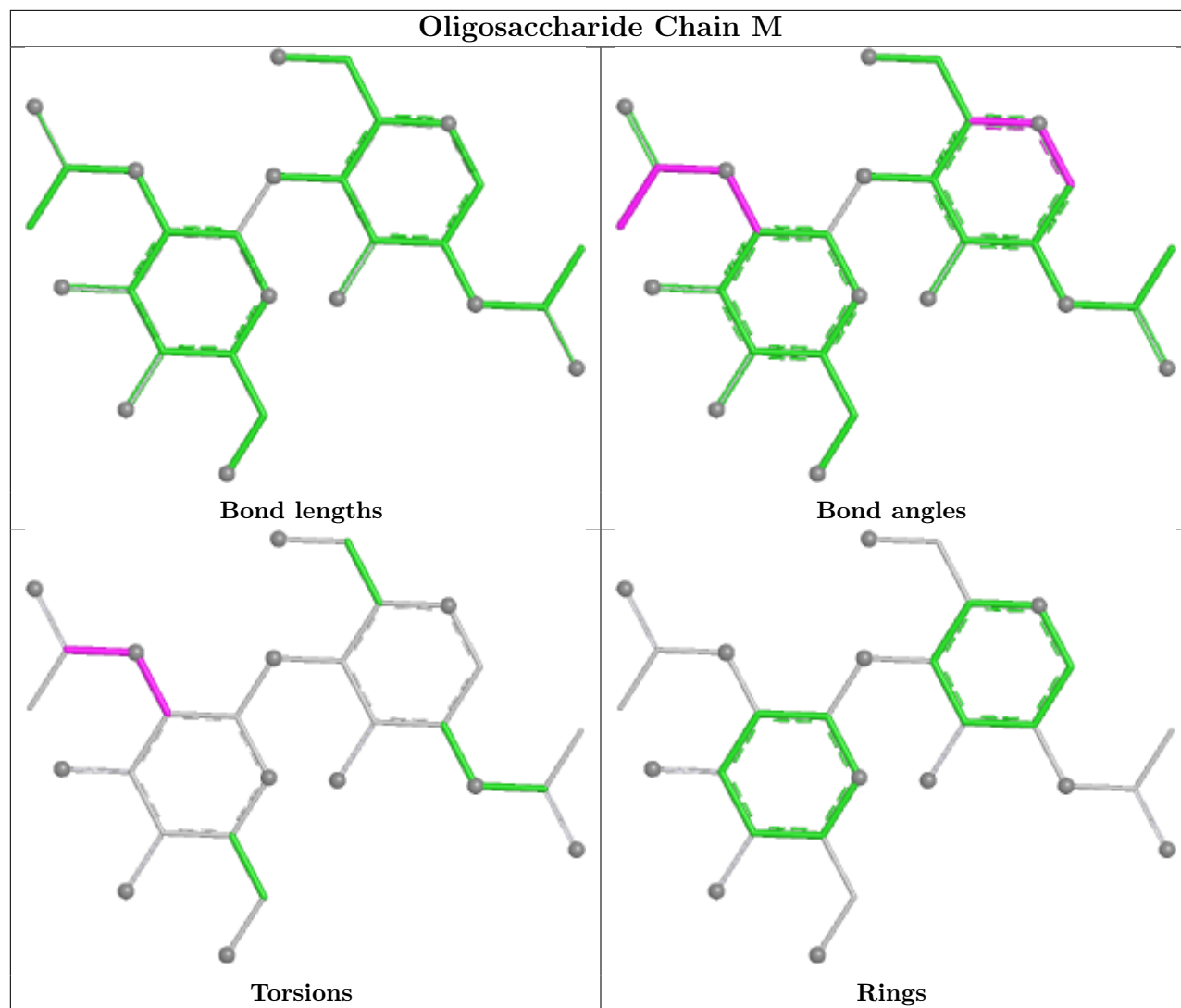
Mol	Chain	Res	Type	Atoms
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
3	N	1	NAG	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	M	2	NAG	C3-C2-N2-C7
3	N	2	NAG	C4-C5-C6-O6

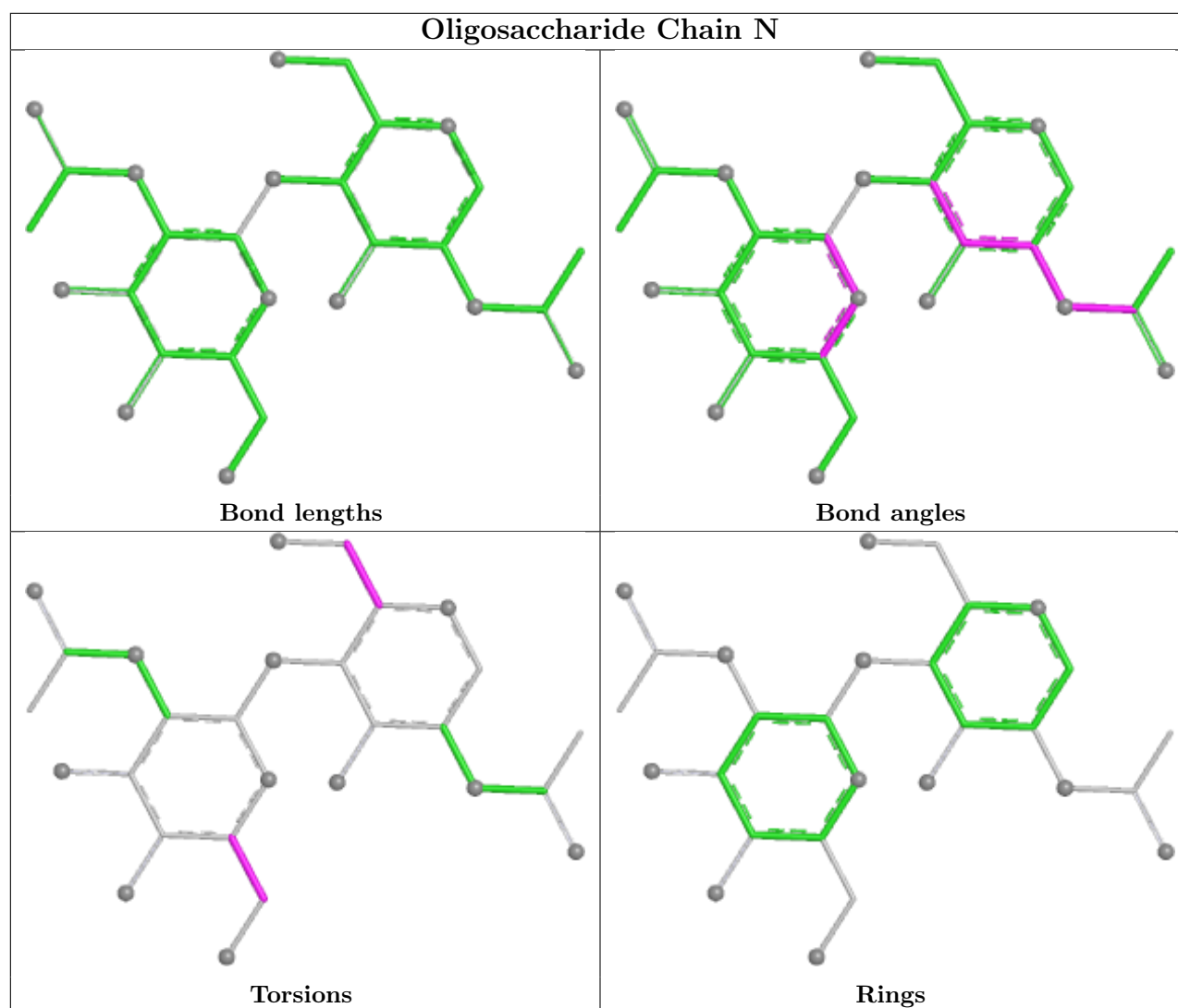
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	NAG	1	0

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





5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	F	201	2,4	14,14,15	0.52	0	17,19,21	1.77	1 (5%)
5	NAG	I	401	1	14,14,15	0.67	0	17,19,21	2.06	7 (41%)
5	NAG	J	201	2,4	14,14,15	0.42	0	17,19,21	1.62	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	K	401	-	3,3,3	0.09	0	2,2,2	0.10	0
5	NAG	B	201	2	14,14,15	0.49	0	17,19,21	1.79	2 (11%)
5	NAG	H	201	2,4	14,14,15	0.79	0	17,19,21	1.38	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	F	201	2,4	-	0/6/23/26	0/1/1/1
5	NAG	I	401	1	-	3/6/23/26	0/1/1/1
5	NAG	J	201	2,4	-	1/6/23/26	0/1/1/1
6	EDO	K	401	-	-	1/1/1/1	-
5	NAG	B	201	2	-	1/6/23/26	0/1/1/1
5	NAG	H	201	2,4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	201	NAG	C1-O5-C5	6.59	121.02	112.19
5	J	201	NAG	C1-O5-C5	6.18	120.47	112.19
5	B	201	NAG	C1-O5-C5	6.15	120.43	112.19
5	H	201	NAG	C1-O5-C5	4.10	117.68	112.19
5	I	401	NAG	C2-N2-C7	3.78	127.97	122.90
5	I	401	NAG	O5-C1-C2	-3.72	105.53	111.29
5	I	401	NAG	C3-C4-C5	3.70	116.93	110.23
5	I	401	NAG	C1-O5-C5	2.83	115.98	112.19
5	B	201	NAG	O5-C1-C2	-2.76	107.02	111.29
5	I	401	NAG	C1-C2-N2	2.54	114.44	110.43
5	I	401	NAG	O5-C5-C4	2.16	116.07	110.83
5	I	401	NAG	C4-C3-C2	-2.03	108.05	111.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	401	NAG	C3-C2-N2-C7
5	I	401	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	H	201	NAG	O5-C5-C6-O6
5	I	401	NAG	O5-C5-C6-O6
5	H	201	NAG	C4-C5-C6-O6
5	B	201	NAG	O5-C5-C6-O6
6	K	401	EDO	O1-C1-C2-O2
5	J	201	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	321/325 (98%)	0.36	10 (3%) 51 45	44, 64, 98, 119	0
1	C	320/325 (98%)	0.52	19 (5%) 28 23	39, 73, 119, 142	0
1	E	320/325 (98%)	0.87	35 (10%) 10 8	56, 90, 143, 159	0
1	G	319/325 (98%)	1.17	76 (23%) 2 1	45, 92, 153, 185	0
1	I	319/325 (98%)	1.13	61 (19%) 3 2	52, 91, 160, 200	0
1	K	320/325 (98%)	0.25	7 (2%) 62 58	43, 60, 90, 115	0
2	B	172/177 (97%)	0.14	2 (1%) 76 73	41, 64, 94, 104	0
2	D	172/177 (97%)	-0.08	1 (0%) 85 83	37, 58, 75, 92	0
2	F	172/177 (97%)	0.49	9 (5%) 33 27	44, 73, 101, 118	0
2	H	172/177 (97%)	0.01	2 (1%) 76 73	39, 61, 81, 101	0
2	J	172/177 (97%)	0.28	2 (1%) 76 73	46, 69, 90, 108	0
2	L	172/177 (97%)	0.22	2 (1%) 76 73	44, 62, 85, 104	0
All	All	2951/3012 (97%)	0.53	226 (7%) 19 16	37, 71, 134, 200	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	213	ALA	5.9
1	G	145	TRP	5.6
1	G	159	THR	5.2
1	I	90	TYR	5.1
1	I	245	GLY	4.9
1	G	237	ILE	4.6
1	G	212	GLY	4.6
1	I	207	ASN	4.3
1	I	244	GLY	4.3
1	G	189	TYR	4.0
1	I	214	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	182	SER	3.9
1	I	190	TYR	3.9
1	E	184	GLN	3.9
1	I	164	ARG	3.9
1	I	141	TYR	3.9
1	G	244	GLY	3.8
1	I	181	SER	3.8
1	I	221	LEU	3.7
1	E	196	SER	3.7
1	G	225	ASP	3.7
2	J	73	ILE	3.7
1	A	321	LEU	3.7
1	I	240	PHE	3.7
1	G	243	GLY	3.6
1	G	210	VAL	3.6
1	G	214	ARG	3.6
1	G	188	LEU	3.6
1	G	146	LEU	3.6
1	G	245	LEU	3.6
1	G	222	GLY	3.5
1	I	208	PHE	3.5
1	G	211	VAL	3.4
1	I	218	VAL	3.4
1	C	214	ALA	3.4
1	E	192	THR	3.3
1	I	212	VAL	3.3
1	G	171	LEU	3.3
1	I	189	LEU	3.3
2	H	73	ILE	3.3
1	G	220	LEU	3.3
1	E	214	ALA	3.3
1	G	209	PRO	3.2
1	G	177	HIS	3.2
1	I	183	THR	3.2
1	I	203	THR	3.2
1	A	2	PRO	3.2
1	I	194	SER	3.2
1	G	162	TYR	3.2
1	G	147	VAL	3.1
1	G	118	TYR	3.1
1	G	160	ASN	3.1
1	I	211	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	157	GLN	3.1
1	C	213	GLY	3.1
1	I	205	LYS	3.1
1	C	183	THR	3.1
1	C	211	VAL	3.1
1	C	150	LYS	3.0
1	G	158	THR	3.0
1	E	146	TRP	3.0
1	E	207	ASN	3.0
1	E	245	GLY	3.0
1	E	67	ALA	2.9
1	G	207	PHE	2.9
1	G	217	VAL	2.9
1	I	225	ILE	2.9
1	G	119	GLY	2.9
1	E	190	TYR	2.9
1	G	176	ILE	2.9
1	E	183	THR	2.9
1	I	195	LEU	2.9
1	G	156	PRO	2.8
1	E	147	LEU	2.8
1	G	193	SER	2.8
1	I	243	ASN	2.8
1	G	239	PHE	2.8
1	I	160	THR	2.8
1	A	210	PRO	2.8
1	A	211	VAL	2.8
1	E	148	VAL	2.8
1	G	238	THR	2.8
1	G	226	PHE	2.8
1	I	156	PHE	2.8
1	I	185	GLU	2.8
1	K	272	CYS	2.7
1	I	196	SER	2.7
1	I	202	SER	2.7
1	I	219	ASN	2.7
2	B	172	ASN	2.7
1	I	184	GLN	2.7
1	C	216	PRO	2.7
1	G	236	LYS	2.7
2	F	73	ILE	2.7
1	C	218	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	116	PHE	2.7
1	G	182	THR	2.7
2	B	73	ILE	2.7
1	I	246	LEU	2.7
1	G	115	GLY	2.7
1	C	226	ASP	2.7
1	A	189	LEU	2.6
1	G	208	VAL	2.6
1	G	240	SER	2.6
1	A	132	CYS	2.6
1	G	178	HIS	2.6
1	G	77	THR	2.6
1	I	40	LEU	2.6
1	E	211	VAL	2.6
1	C	188	ASP	2.6
1	C	215	ARG	2.6
1	K	286	ARG	2.6
1	I	228	HIS	2.6
1	E	188	ASP	2.5
1	G	223	ARG	2.5
1	I	178	HIS	2.5
1	E	219	ASN	2.5
1	E	225	ILE	2.5
1	I	231	LEU	2.5
1	G	170	HIS	2.5
1	K	210	PRO	2.5
1	G	198	VAL	2.5
1	E	131	ALA	2.5
1	G	247	ALA	2.5
1	I	161	ASN	2.5
2	F	32	THR	2.5
1	E	152	LYS	2.5
2	D	137	CYS	2.5
1	I	177	ILE	2.4
1	G	149	LYS	2.4
1	E	126	ALA	2.4
1	E	123	ILE	2.4
2	F	148	CYS	2.4
1	G	126	GLY	2.4
1	I	210	PRO	2.4
1	G	203	TYR	2.4
1	G	155	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	168	THR	2.4
1	G	246	ILE	2.4
1	I	242	HIS	2.4
1	G	120	SER	2.4
1	I	122	SER	2.4
1	I	241	SER	2.4
1	G	173	MET	2.4
1	G	231	VAL	2.4
1	C	221	LEU	2.3
1	I	119	TYR	2.3
1	G	191	THR	2.3
1	C	121	SER	2.3
1	E	145	LYS	2.3
2	H	137	CYS	2.3
1	E	136	GLY	2.3
2	F	161	GLN	2.3
1	C	189	LEU	2.3
1	G	39	LEU	2.3
1	G	122	ILE	2.3
1	G	227	HIS	2.3
1	E	122	SER	2.3
1	I	180	PRO	2.3
2	F	144	CYS	2.3
1	E	189	LEU	2.3
1	I	162	THR	2.3
1	A	152	LYS	2.3
1	C	180	PRO	2.3
1	I	216	PRO	2.3
1	C	225	ILE	2.3
1	E	166	ALA	2.3
1	I	209	VAL	2.3
1	K	214	ALA	2.2
1	G	161	THR	2.2
1	K	2	PRO	2.2
2	F	23	GLY	2.2
2	F	29	ALA	2.2
2	F	77	ILE	2.2
1	E	203	THR	2.2
1	G	127	THR	2.2
1	I	206	ASN	2.2
1	C	181	SER	2.2
1	G	249	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	230	LEU	2.2
1	E	212	VAL	2.2
1	G	50	LYS	2.2
1	G	94	VAL	2.2
1	E	140	PHE	2.2
1	G	95	ASN	2.2
1	A	1	ASP	2.2
1	E	209	VAL	2.2
1	G	180	SER	2.2
1	E	130	LYS	2.1
1	I	173	ILE	2.1
1	K	5	ILE	2.1
1	K	115	THR	2.1
1	I	89	CYS	2.1
2	L	172	ASN	2.1
1	A	212	VAL	2.1
1	C	209	VAL	2.1
2	L	133	ASP	2.1
1	I	87	ALA	2.1
1	I	248	ALA	2.1
1	G	114	THR	2.1
1	I	152	LYS	2.1
1	G	1	PRO	2.1
1	I	158	GLN	2.1
1	E	138	ASN	2.1
1	I	188	ASP	2.1
1	E	194	SER	2.1
1	C	94	THR	2.1
2	J	156	THR	2.1
1	A	120	GLY	2.1
1	C	190	TYR	2.1
1	G	184	GLU	2.0
1	I	126	ALA	2.0
2	F	11	GLU	2.0
1	E	149	SER	2.0
1	I	146	TRP	2.0
1	G	93	THR	2.0
1	G	117	THR	2.0
1	G	60	MET	2.0
1	E	221	LEU	2.0
1	G	135	GLY	2.0
1	I	123	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	174	TRP	2.0
1	I	220	GLY	2.0
1	I	223	GLY	2.0
1	I	235	GLY	2.0
1	G	89	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

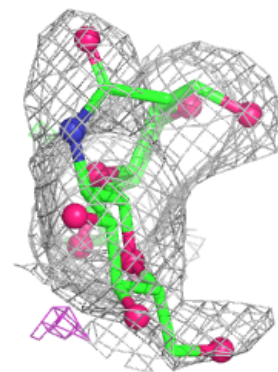
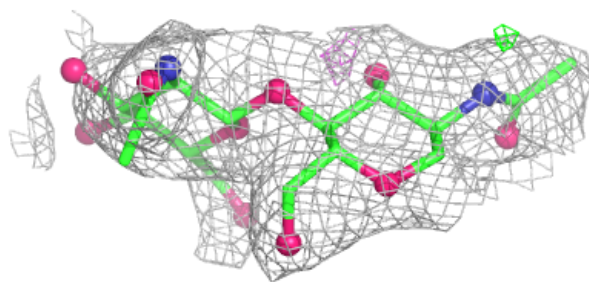
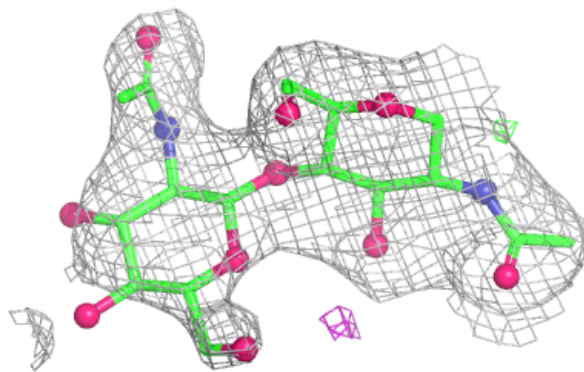
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

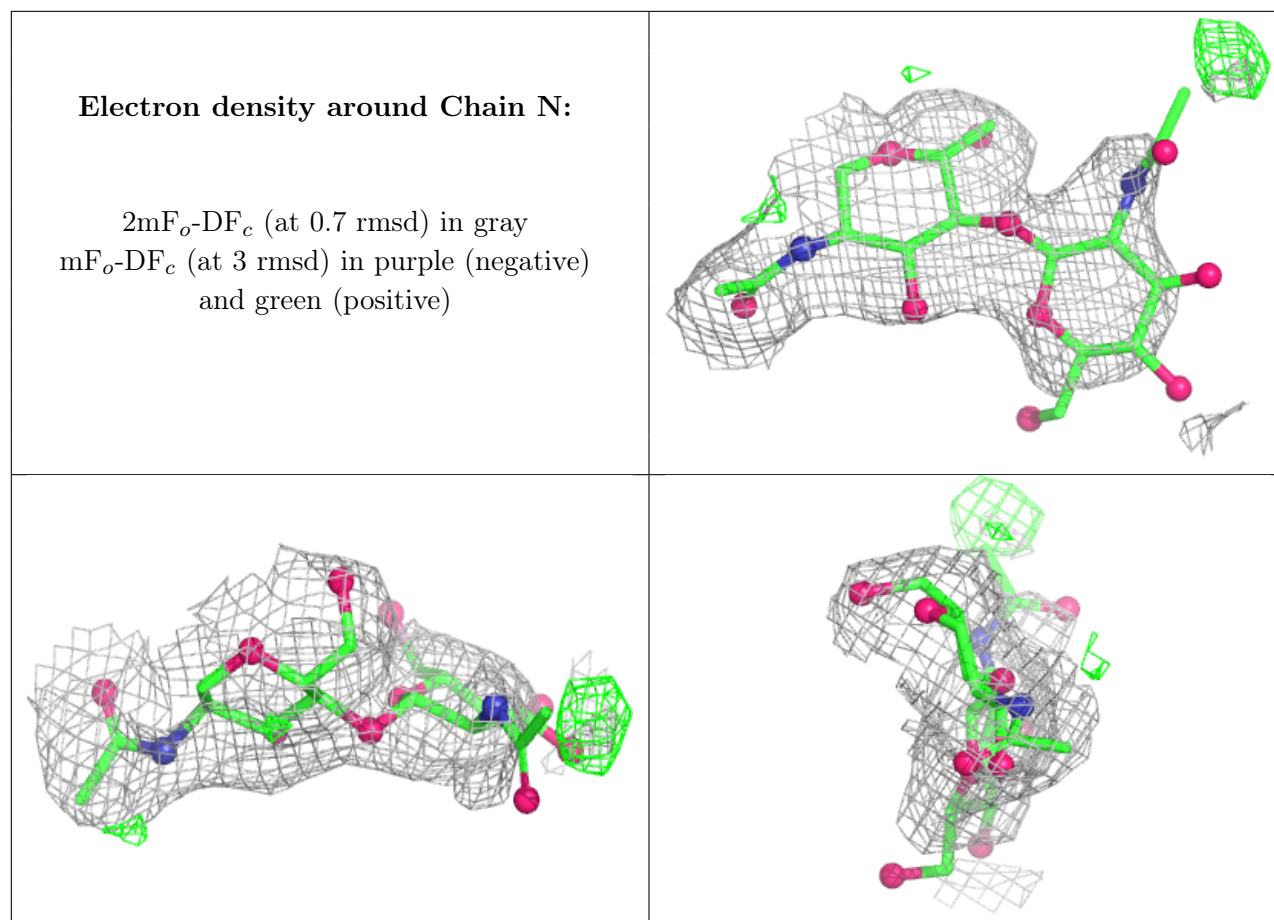
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	N	2	14/15	0.61	0.15	114,119,128,129	0
3	NAG	M	2	14/15	0.72	0.14	94,102,112,114	0
3	NAG	N	1	14/15	0.80	0.12	84,90,97,108	0
3	NAG	M	1	14/15	0.93	0.07	60,64,70,82	0

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 M:

$2mF_o-DF_c$ (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	I	401	14/15	0.47	0.16	110,127,132,133	0
5	NAG	J	201	14/15	0.72	0.14	96,103,107,107	0
5	NAG	F	201	14/15	0.80	0.12	91,98,101,105	0
5	NAG	B	201	14/15	0.83	0.11	76,85,91,100	0
4	CA	D	401	1/1	0.87	0.09	114,114,114,114	0
5	NAG	H	201	14/15	0.88	0.09	53,59,61,62	0
4	CA	G	401	1/1	0.92	0.08	105,105,105,105	0
6	EDO	K	401	4/4	0.93	0.13	62,65,66,70	0
4	CA	D	404	1/1	0.98	0.04	55,55,55,55	0
4	CA	A	401	1/1	0.99	0.04	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.