



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:05 PM UTC

PDB ID : 4CYV / pdb_00004cyv
Title : Structure of the A_mallard_Sweden_51_2002 H10 Avian Haemmagglutinin
Authors : Vachieri, S.G.; Xiong, X.; Collins, P.J.; Walker, P.A.; Martin, S.R.; Haire, L.F.; McCauley, J.W.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2014-04-15
Resolution : 2.30 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

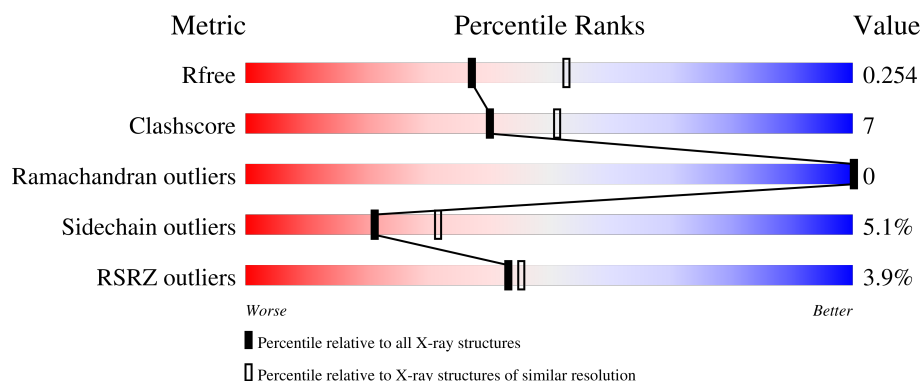
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	324	3% 79% 17% ..
1	C	324	% 87% 10% ..
1	E	324	3% 81% 15% ..
2	B	172	9% 86% 12% .
2	D	172	5% 92% 7% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	172	
3	G	5	
3	I	5	
3	K	5	
4	H	3	
5	J	2	

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
3	MAN	K	5	X	-	-	-
5	NAG	J	2	X	-	-	-
6	NAG	A	401	X	-	-	-
6	NAG	A	420	X	-	-	-
6	NAG	C	420	X	-	-	-
6	NAG	E	420	X	-	-	-
7	EDO	E	1328	-	-	X	-
7	EDO	F	1176	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12135 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.

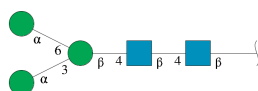
- Molecule 1 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	1	0
			2427	1501	436	474	16			
1	C	319	Total	C	N	O	S	0	0	0
			2430	1504	437	473	16			
1	E	319	Total	C	N	O	S	0	0	0
			2426	1501	436	473	16			

- Molecule 2 is a protein called HEMAGGLUTININ.

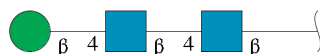
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1384	855	239	282	8			
2	D	172	Total	C	N	O	S	0	0	0
			1377	851	240	278	8			
2	F	172	Total	C	N	O	S	0	0	0
			1380	851	239	282	8			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	K	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



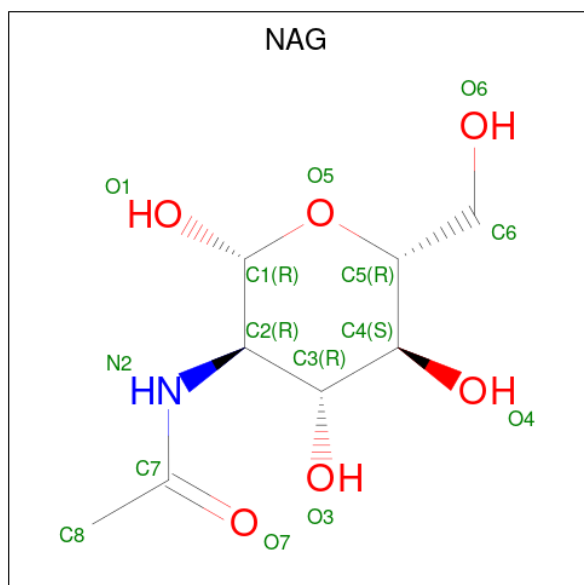
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



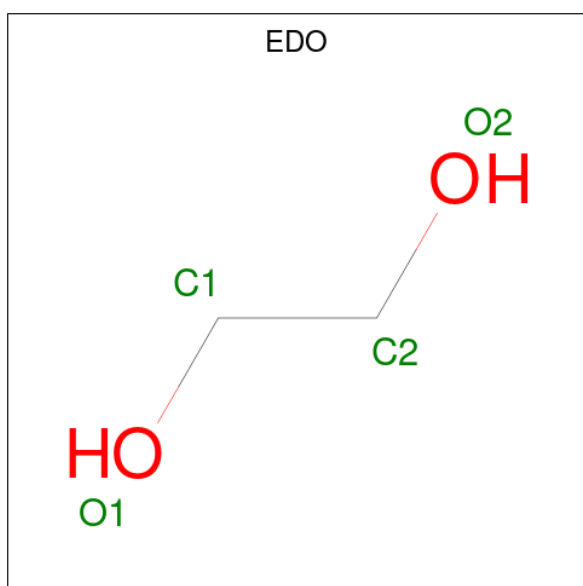
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

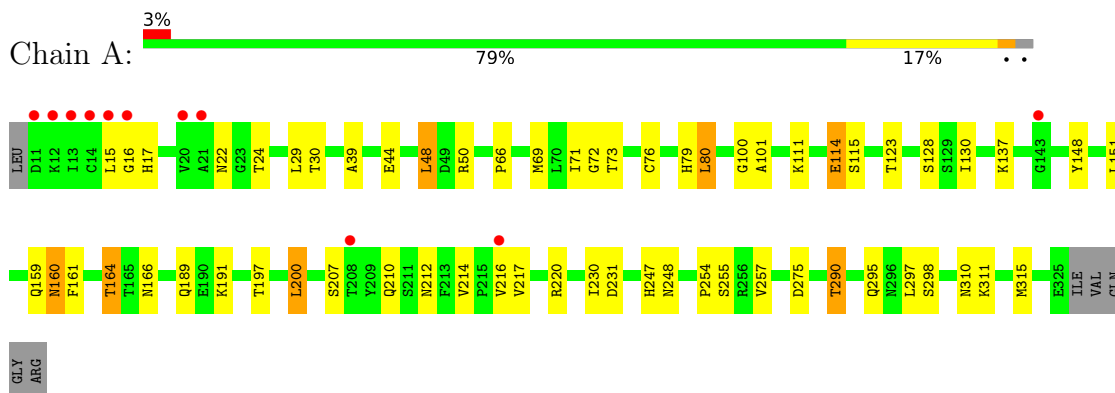
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	69	Total O 69 69	0	0
8	B	43	Total O 43 43	0	0
8	C	98	Total O 98 98	0	0
8	D	27	Total O 27 27	0	0
8	E	52	Total O 52 52	0	0
8	F	16	Total O 16 16	0	0

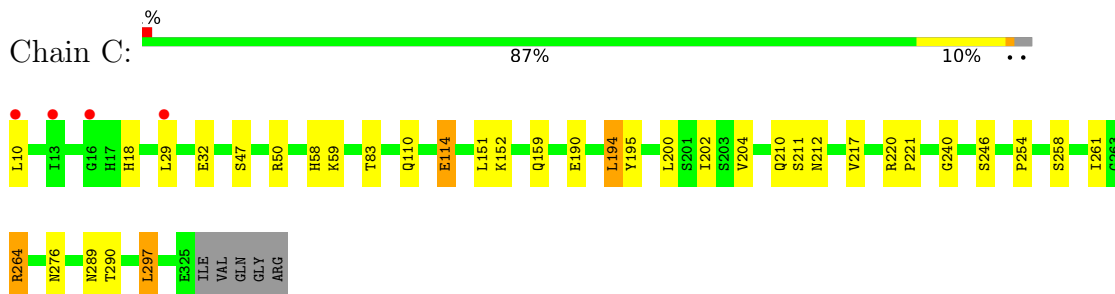
3 Residue-property plots [i](#)

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.

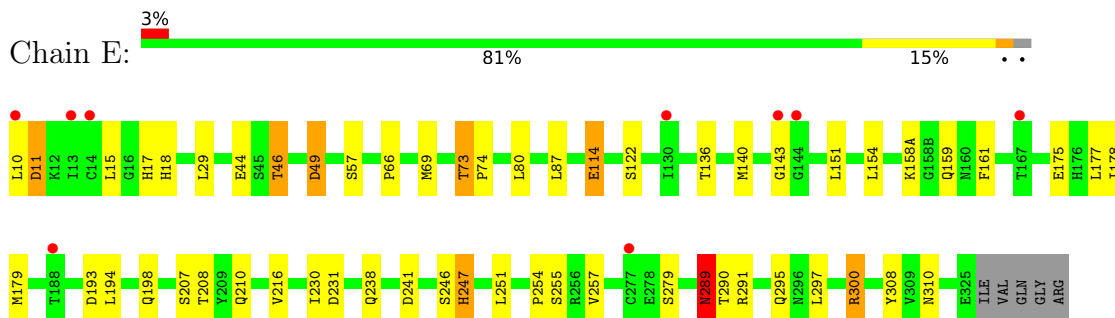
• Molecule 1: HEMAGGLUTININ



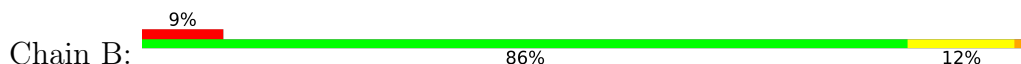
• Molecule 1: HEMAGGLUTININ

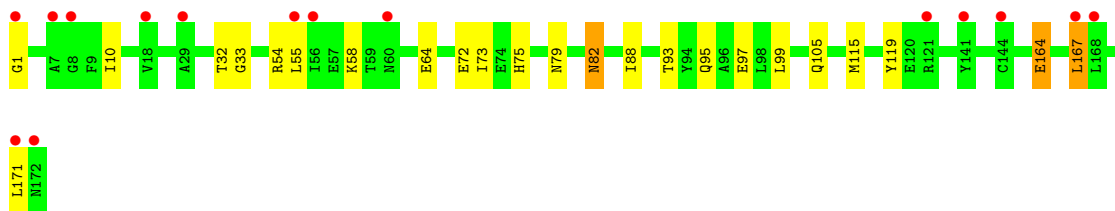


• Molecule 1: HEMAGGLUTININ

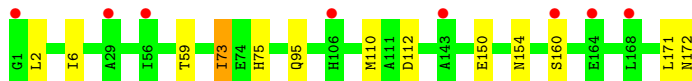


• Molecule 2: HEMAGGLUTININ

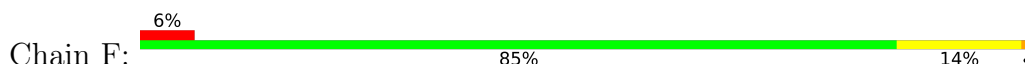




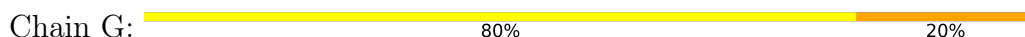
● Molecule 2: HEMAGGLUTININ



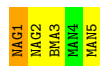
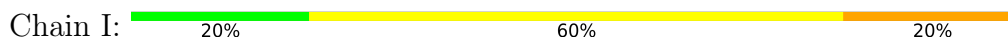
● Molecule 2: HEMAGGLUTININ



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



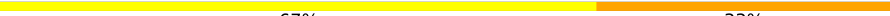
● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

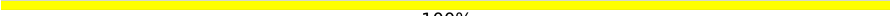


● Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  67% 33%

MAG1
MAG2
BGA3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.61Å 227.99Å 68.72Å 90.00° 110.32° 90.00°	Depositor
Resolution (Å)	113.99 – 2.30 113.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (113.99-2.30) 98.4 (113.99-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.214 , 0.252 0.217 , 0.254	Depositor DCC
R_{free} test set	4237 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12135	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, EDO, 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	0.83	4/2479 (0.2%)	0.92	4/3361 (0.1%)
1	C	0.94	6/2479 (0.2%)	1.01	8/3361 (0.2%)
1	E	0.81	6/2475 (0.2%)	0.96	7/3357 (0.2%)
2	B	0.70	0/1409	0.91	2/1902 (0.1%)
2	D	0.76	0/1402	0.91	2/1892 (0.1%)
2	F	0.77	0/1405	0.90	1/1897 (0.1%)
All	All	0.82	16/11649 (0.1%)	0.94	24/15770 (0.2%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	114	GLU	CD-OE2	9.70	1.43	1.25
1	A	114	GLU	CD-OE2	8.74	1.42	1.25
1	C	114	GLU	CA-CB	8.12	1.66	1.53
1	C	114	GLU	CA-C	7.36	1.62	1.52
1	E	114	GLU	CD-OE2	6.79	1.38	1.25
1	A	114	GLU	CA-C	6.71	1.61	1.52
1	E	114	GLU	CA-C	6.50	1.61	1.52
1	E	114	GLU	N-CA	6.43	1.54	1.46
1	A	114	GLU	N-CA	5.89	1.53	1.46
1	A	114	GLU	CA-CB	5.89	1.63	1.53
1	C	59	LYS	C-O	5.89	1.30	1.24
1	E	114	GLU	CB-CG	5.80	1.69	1.52
1	E	114	GLU	CA-CB	5.63	1.62	1.53
1	C	114	GLU	N-CA	5.60	1.53	1.46
1	C	114	GLU	CB-CG	5.42	1.68	1.52
1	E	289	ASN	CA-C	-5.12	1.46	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	GLU	N-CA-C	-12.86	97.68	113.50
1	E	114	GLU	N-CA-C	-11.93	98.44	113.23
1	E	114	GLU	CA-CB-CG	9.54	133.19	114.10
1	C	114	GLU	CA-CB-CG	8.89	131.87	114.10
1	A	114	GLU	N-CA-C	-8.84	102.62	113.50
1	E	290	THR	N-CA-C	-7.27	97.27	108.76
1	C	114	GLU	CG-CD-OE1	-6.94	102.43	118.40
1	E	230	ILE	CB-CA-C	-6.33	103.20	110.73
1	A	114	GLU	CA-CB-CG	6.26	126.61	114.10
1	E	114	GLU	CG-CD-OE1	-6.08	104.42	118.40
2	F	23	GLY	N-CA-C	5.96	118.62	110.69
1	A	115	SER	N-CA-C	5.65	118.18	110.55
1	E	114	GLU	CG-CD-OE2	5.61	131.31	118.40
1	C	289	ASN	CB-CA-C	-5.46	103.73	111.76
2	D	75	HIS	N-CA-C	5.45	116.90	111.07
1	E	247	HIS	N-CA-C	5.38	116.70	108.52
2	D	2	LEU	N-CA-C	5.37	116.82	111.07
1	C	114	GLU	CG-CD-OE2	5.36	130.73	118.40
1	A	114	GLU	CG-CD-OE1	-5.23	106.38	118.40
2	B	82	ASN	CA-CB-CG	5.12	117.72	112.60
1	C	261	ILE	CB-CA-C	-5.07	103.06	110.62
2	B	82	ASN	CB-CG-ND2	5.07	124.00	116.40
1	C	290	THR	N-CA-C	-5.05	101.61	109.24
1	C	297	LEU	N-CA-C	5.01	116.55	111.14

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	2427	0	2360	50	0
1	C	2430	0	2367	17	1
1	E	2426	0	2356	38	1
2	B	1384	0	1276	33	0
2	D	1377	0	1270	9	0
2	F	1380	0	1266	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	61	0	50	3	0
3	I	61	0	52	1	0
3	K	61	0	52	2	0
4	H	39	0	34	4	0
5	J	28	0	25	0	0
6	A	28	0	26	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
6	D	14	0	13	1	0
6	E	14	0	13	0	0
7	A	12	0	18	2	0
7	B	12	0	18	1	0
7	C	16	0	24	2	0
7	D	4	0	6	0	0
7	E	12	0	18	7	0
7	F	16	0	24	8	0
8	A	69	0	0	1	0
8	B	43	0	0	4	0
8	C	98	0	0	1	0
8	D	27	0	0	0	0
8	E	52	0	0	3	0
8	F	16	0	0	0	0
All	All	12135	0	11294	153	1

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 7.

All (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:ILE:HG21	7:F:1176:EDO:O1	1.72	0.88
2:B:10:ILE:HD13	2:B:115:MET:HE3	1.56	0.85
1:A:16:GLY:C	2:B:115:MET:HE1	2.04	0.81
2:F:56:ILE:HG22	2:F:56:ILE:O	1.82	0.78
1:E:158(A):LYS:O	1:E:193:ASP:O	2.06	0.74
2:F:14:TRP:CE2	7:F:1176:EDO:H21	2.23	0.73
2:F:102:MET:SD	7:F:1175:EDO:O2	2.47	0.73
1:E:291:ARG:HB3	2:F:56:ILE:HG21	1.69	0.72
4:H:1:NAG:H83	4:H:1:NAG:H3	1.71	0.71
1:A:114:GLU:OE2	3:K:1:NAG:O7	2.11	0.68
1:A:44:GLU:OE1	1:A:290:THR:CG2	2.41	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ARG:HG3	1:C:264:ARG:HH11	1.60	0.67
1:A:66:PRO:O	1:A:69:MET:HG2	1.94	0.66
8:E:2046:HOH:O	2:F:59:THR:HG21	1.95	0.65
2:F:10:ILE:CG2	7:F:1176:EDO:O1	2.44	0.65
1:A:295:GLN:HE21	1:A:297:LEU:H	1.45	0.65
1:A:295:GLN:HE22	1:A:298:SER:H	1.42	0.64
8:E:2046:HOH:O	2:F:59:THR:CG2	2.44	0.64
1:A:16:GLY:CA	2:B:115:MET:HE1	2.28	0.64
1:A:311:LYS:HE3	2:B:97:GLU:CD	2.23	0.64
2:F:13:GLY:HA2	7:F:1176:EDO:O2	1.98	0.63
2:F:14:TRP:CD2	7:F:1176:EDO:H21	2.35	0.61
2:D:73:ILE:N	2:D:73:ILE:HD13	2.14	0.61
1:E:291:ARG:HB3	2:F:56:ILE:CG2	2.31	0.61
1:E:44:GLU:OE2	1:E:46:THR:HB	2.02	0.60
1:E:300:ARG:NH1	2:F:67:GLU:OE1	2.34	0.60
4:H:1:NAG:H3	4:H:1:NAG:C8	2.32	0.59
1:A:17:HIS:HD2	2:B:115:MET:HE2	1.68	0.59
1:C:264:ARG:HH11	1:C:264:ARG:CG	2.15	0.59
1:A:76:CYS:O	1:A:80:LEU:HD13	2.03	0.58
1:A:111:LYS:NZ	8:A:2031:HOH:O	2.33	0.57
1:E:175:GLU:OE1	1:E:238:GLN:NE2	2.38	0.57
2:B:82:ASN:OD1	3:G:1:NAG:C2	2.47	0.57
1:A:257:VAL:HA	7:A:1328:EDO:H11	1.85	0.56
1:C:58:HIS:HE1	1:C:276:ASN:HD21	1.52	0.56
1:A:100:GLY:HA3	1:A:230:ILE:O	2.05	0.56
1:A:295:GLN:HE21	1:A:297:LEU:N	2.03	0.56
1:A:295:GLN:NE2	1:A:298:SER:H	2.02	0.56
1:E:154:LEU:HB2	7:E:1328:EDO:H21	1.87	0.56
2:F:102:MET:SD	7:F:1175:EDO:C2	2.94	0.55
1:C:18:HIS:HE1	8:C:2004:HOH:O	1.90	0.54
1:E:291:ARG:O	2:F:56:ILE:HG23	2.07	0.54
1:E:73:THR:HG22	1:E:74:PRO:HD2	1.90	0.54
1:A:69:MET:HB2	1:A:79:HIS:O	2.08	0.54
2:B:10:ILE:CD1	2:B:115:MET:HE3	2.34	0.54
1:E:231:ASP:OD1	1:E:231:ASP:O	2.26	0.53
1:C:204:VAL:O	1:C:210:GLN:HA	2.09	0.52
1:E:295:GLN:OE1	1:E:297:LEU:N	2.43	0.52
2:F:115:MET:HE3	2:F:115:MET:HA	1.91	0.52
1:E:247:HIS:ND1	7:E:1328:EDO:O1	2.40	0.52
1:A:123:THR:CG2	1:A:255:SER:HA	2.40	0.51
1:A:151:LEU:HD23	1:A:254:PRO:HA	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:2005:HOH:O	2:F:95:GLN:HG3	2.10	0.51
1:A:17:HIS:CD2	2:B:115:MET:HE2	2.46	0.51
1:A:123:THR:HG21	1:A:254:PRO:O	2.11	0.51
1:A:161:PHE:HB3	1:A:248:ASN:O	2.10	0.51
1:A:160:ASN:HD21	1:A:197:THR:HG22	1.75	0.51
1:A:216:VAL:HG22	1:C:212:ASN:HB2	1.92	0.51
1:A:44:GLU:OE1	1:A:290:THR:HG23	2.09	0.50
2:F:38:TYR:CE1	2:F:42:GLN:HG3	2.46	0.50
1:E:279:SER:CB	1:E:289:ASN:OD1	2.60	0.50
1:E:15:LEU:CD1	2:F:119:TYR:HA	2.42	0.49
1:E:208:THR:O	1:E:208:THR:CG2	2.59	0.49
1:A:44:GLU:HB2	1:A:290:THR:HG21	1.94	0.49
1:A:15:LEU:CD1	2:B:119:TYR:HA	2.42	0.49
2:B:95:GLN:HE22	2:F:95:GLN:NE2	2.11	0.49
2:D:150:GLU:HB3	6:D:211:NAG:H61	1.95	0.49
1:A:212:ASN:CG	1:E:216:VAL:HG21	2.38	0.49
1:A:24:THR:HG21	1:A:315:MET:HE2	1.95	0.48
1:A:16:GLY:HA2	2:B:115:MET:HE1	1.95	0.48
1:C:47:SER:HB2	1:C:297:LEU:HD22	1.94	0.48
2:B:93:THR:O	2:B:97:GLU:HG3	2.13	0.48
2:D:150:GLU:O	2:D:154:ASN:HB2	2.14	0.48
1:E:11:ASP:OD1	1:E:11:ASP:N	2.45	0.48
1:A:210:GLN:HE21	1:E:231:ASP:HB3	1.78	0.47
1:C:220:ARG:HB2	1:C:221:PRO:CD	2.44	0.47
1:C:240:GLY:O	4:H:1:NAG:H82	2.14	0.47
1:E:15:LEU:HD21	2:F:24:PHE:CE1	2.49	0.47
1:E:154:LEU:HB2	7:E:1328:EDO:C2	2.44	0.47
2:B:82:ASN:OD1	3:G:1:NAG:H2	2.12	0.47
1:E:208:THR:O	1:E:208:THR:HG22	2.14	0.47
2:B:82:ASN:OD1	8:B:2020:HOH:O	2.20	0.47
1:A:22:ASN:HD22	1:A:22:ASN:N	2.12	0.47
1:E:140:MET:SD	1:E:143:GLY:O	2.73	0.47
2:B:1:GLY:N	8:B:2001:HOH:O	2.45	0.46
2:B:32:THR:HG22	2:B:33:GLY:N	2.31	0.46
2:B:164:GLU:N	2:B:164:GLU:CD	2.73	0.46
1:C:110:GLN:O	7:C:1329:EDO:H22	2.14	0.46
1:A:166:ASN:HD22	1:A:247:HIS:HE1	1.62	0.46
1:C:258:SER:OG	7:C:1328:EDO:O1	2.27	0.46
1:E:69:MET:HE1	1:E:87:LEU:HD21	1.96	0.46
1:A:130:ILE:HD11	1:A:164:THR:HG21	1.96	0.46
2:B:55:LEU:HD21	2:B:99:LEU:HD21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:LEU:C	1:E:177:LEU:HD23	2.41	0.46
1:A:123:THR:HG22	1:A:255:SER:HA	1.98	0.46
3:K:1:NAG:O4	3:K:2:NAG:H61	2.15	0.46
1:A:48:LEU:HD23	1:A:50:ARG:CZ	2.46	0.46
1:E:73:THR:HG22	1:E:74:PRO:CD	2.46	0.46
1:A:39:ALA:HB3	1:A:315:MET:HE3	1.97	0.46
2:B:95:GLN:NE2	2:F:95:GLN:HE21	2.13	0.46
1:E:251:LEU:HB3	7:E:1328:EDO:O1	2.16	0.46
2:B:164:GLU:CD	2:B:164:GLU:H	2.24	0.45
2:B:73:ILE:HD12	2:B:73:ILE:N	2.32	0.45
2:B:75:HIS:HE1	1:C:114:GLU:OE1	1.99	0.45
2:D:6:ILE:HD12	2:D:112:ASP:HA	1.97	0.45
1:C:190:GLU:O	1:C:194:LEU:HD22	2.15	0.45
1:E:179:MET:HB2	7:E:1326:EDO:H12	1.98	0.45
2:B:10:ILE:HD13	2:B:115:MET:CE	2.39	0.45
1:C:240:GLY:O	4:H:1:NAG:C8	2.64	0.45
1:E:17:HIS:HA	8:E:2002:HOH:O	2.16	0.45
1:E:295:GLN:O	1:E:308:TYR:HA	2.17	0.45
2:F:73:ILE:HD12	2:F:73:ILE:N	2.32	0.45
2:B:1:GLY:CA	8:B:2001:HOH:O	2.65	0.44
2:B:79:ASN:OD1	3:G:1:NAG:C8	2.65	0.44
1:A:189:GLN:OE1	1:A:189:GLN:N	2.44	0.44
2:B:95:GLN:NE2	2:D:95:GLN:NE2	2.65	0.44
1:A:72:GLY:HA2	1:A:80:LEU:HD11	1.99	0.44
1:E:178:ILE:HG13	1:E:257:VAL:HG12	1.99	0.44
2:F:17:MET:HE2	2:F:34:GLN:CG	2.48	0.44
2:F:52:LEU:O	2:F:56:ILE:HD12	2.18	0.44
2:B:88:ILE:HG21	7:B:1175:EDO:H22	1.99	0.44
1:E:114:GLU:OE2	3:I:1:NAG:O7	2.35	0.44
1:A:160:ASN:N	1:A:160:ASN:HD22	2.17	0.43
1:A:212:ASN:ND2	1:E:216:VAL:HG21	2.33	0.43
1:A:166:ASN:ND2	1:A:247:HIS:HE1	2.16	0.43
1:A:44:GLU:OE1	1:A:290:THR:HG21	2.18	0.43
1:A:30:THR:HG22	2:B:105:GLN:HE22	1.83	0.43
2:D:171:LEU:O	2:D:172:ASN:C	2.62	0.43
2:D:110:MET:C	2:D:110:MET:SD	3.02	0.43
1:C:220:ARG:HB2	1:C:221:PRO:HD2	2.00	0.42
1:A:114:GLU:OE2	2:B:64:GLU:OE2	2.37	0.42
2:F:171:LEU:O	2:F:172:ASN:CB	2.67	0.42
2:B:95:GLN:NE2	2:D:95:GLN:HE21	2.18	0.42
2:B:95:GLN:NE2	2:F:95:GLN:NE2	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ALA:N	1:A:231[A]:ASP:OD1	2.53	0.42
2:B:167:LEU:O	2:B:171:LEU:HD13	2.20	0.41
1:E:66:PRO:HA	1:E:69:MET:HE2	2.01	0.41
1:E:247:HIS:CG	7:E:1328:EDO:O1	2.73	0.41
1:A:50:ARG:NH1	1:A:275:ASP:OD2	2.53	0.41
1:A:257:VAL:CA	7:A:1328:EDO:H11	2.50	0.41
1:C:151:LEU:HD23	1:C:254:PRO:HA	2.02	0.41
1:A:200:LEU:O	1:A:214:VAL:HG13	2.20	0.41
1:A:71:ILE:O	1:A:148:TYR:HB3	2.20	0.41
1:E:151:LEU:HD23	1:E:254:PRO:HA	2.03	0.41
2:F:73:ILE:HD12	2:F:73:ILE:H	1.86	0.41
2:F:102:MET:SD	7:F:1175:EDO:H22	2.60	0.41
2:B:95:GLN:HE21	2:D:95:GLN:HE21	1.69	0.41
1:C:194:LEU:HD21	1:C:195:TYR:CE2	2.56	0.41
1:E:207:SER:HB3	1:E:241:ASP:OD1	2.21	0.41
1:E:161:PHE:CZ	7:E:1328:EDO:H21	2.56	0.40
1:A:166:ASN:HD22	1:A:247:HIS:CE1	2.39	0.40
1:E:231:ASP:OD1	1:E:231:ASP:C	2.65	0.40
2:F:56:ILE:O	2:F:56:ILE:CG2	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:THR:OG1	1:E:49:ASP:OD2[1_655]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	317/324 (98%)	304 (96%)	13 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	317/324 (98%)	306 (96%)	11 (4%)	0	100	100
1	E	317/324 (98%)	299 (94%)	18 (6%)	0	100	100
2	B	170/172 (99%)	159 (94%)	11 (6%)	0	100	100
2	D	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	F	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
All	All	1461/1488 (98%)	1395 (96%)	66 (4%)	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	270/275 (98%)	254 (94%)	16 (6%)	18	26
1	C	270/275 (98%)	257 (95%)	13 (5%)	23	35
1	E	269/275 (98%)	249 (93%)	20 (7%)	13	17
2	B	145/146 (99%)	140 (97%)	5 (3%)	32	49
2	D	143/146 (98%)	140 (98%)	3 (2%)	47	66
2	F	144/146 (99%)	138 (96%)	6 (4%)	26	40
All	All	1241/1263 (98%)	1178 (95%)	63 (5%)	21	32

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	48	LEU
1	A	73	THR
1	A	80	LEU
1	A	128	SER
1	A	137	LYS
1	A	159	GLN
1	A	160	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	164	THR
1	A	191	LYS
1	A	200	LEU
1	A	207	SER
1	A	217	VAL
1	A	220	ARG
1	A	290	THR
1	A	310	ASN
2	B	54	ARG
2	B	58	LYS
2	B	72	GLU
2	B	164	GLU
2	B	167	LEU
1	C	10	LEU
1	C	29	LEU
1	C	32	GLU
1	C	50	ARG
1	C	152	LYS
1	C	159	GLN
1	C	194	LEU
1	C	200	LEU
1	C	202	ILE
1	C	211	SER
1	C	217	VAL
1	C	246	SER
1	C	264	ARG
2	D	59	THR
2	D	73	ILE
2	D	160	SER
1	E	10	LEU
1	E	11	ASP
1	E	18	HIS
1	E	29	LEU
1	E	46	THR
1	E	49	ASP
1	E	57	SER
1	E	73	THR
1	E	80	LEU
1	E	122	SER
1	E	136	THR
1	E	159	GLN
1	E	194	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	198	GLN
1	E	210	GLN
1	E	246	SER
1	E	255	SER
1	E	289	ASN
1	E	300	ARG
1	E	310	ASN
2	F	54	ARG
2	F	59	THR
2	F	113	SER
2	F	135	LYS
2	F	156	THR
2	F	164	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	18	HIS
1	A	22	ASN
1	A	160	ASN
1	A	166	ASN
1	A	183	HIS
1	A	212	ASN
1	A	224	ASN
1	A	247	HIS
1	A	295	GLN
1	A	304	GLN
2	B	12	ASN
2	B	47	GLN
2	B	75	HIS
2	B	95	GLN
2	B	105	GLN
2	B	106	HIS
2	B	117	ASN
1	C	58	HIS
1	C	212	ASN
1	C	222	GLN
1	C	276	ASN
2	D	95	GLN
2	D	105	GLN
1	E	18	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	159	GLN
1	E	160	ASN
1	E	210	GLN
2	F	105	GLN
2	F	159	HIS
2	F	161	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 ⓘ

20 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	G	1	3,2	14,14,15	1.95	3 (21%)	17,19,21	5.12	8 (47%)
3	NAG	G	2	3	14,14,15	0.92	1 (7%)	17,19,21	1.52	4 (23%)
3	BMA	G	3	3	11,11,12	0.80	0	15,15,17	1.97	3 (20%)
3	MAN	G	4	3	11,11,12	0.58	0	15,15,17	1.09	1 (6%)
3	MAN	G	5	3	11,11,12	0.66	0	15,15,17	1.39	2 (13%)
4	NAG	H	1	4,1	14,14,15	0.53	0	17,19,21	1.40	4 (23%)
4	NAG	H	2	4	14,14,15	0.76	0	17,19,21	1.41	3 (17%)
4	BMA	H	3	4	11,11,12	0.56	0	15,15,17	2.28	3 (20%)
3	NAG	I	1	3,2	14,14,15	0.73	0	17,19,21	1.75	6 (35%)
3	NAG	I	2	3	14,14,15	0.54	0	17,19,21	1.16	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	I	3	3	11,11,12	0.65	0	15,15,17	2.19	2 (13%)
3	MAN	I	4	3	11,11,12	0.44	0	15,15,17	0.97	0
3	MAN	I	5	3	11,11,12	0.62	0	15,15,17	1.52	3 (20%)
5	NAG	J	1	1,5	14,14,15	0.52	0	17,19,21	1.60	3 (17%)
5	NAG	J	2	5	14,14,15	0.55	0	17,19,21	1.68	4 (23%)
3	NAG	K	1	3,2	14,14,15	0.65	0	17,19,21	1.75	5 (29%)
3	NAG	K	2	3	14,14,15	0.76	0	17,19,21	1.54	3 (17%)
3	BMA	K	3	3	11,11,12	0.65	0	15,15,17	1.56	2 (13%)
3	MAN	K	4	3	11,11,12	0.54	0	15,15,17	1.35	2 (13%)
3	MAN	K	5	3	11,11,12	0.72	0	15,15,17	2.05	4 (26%)

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	G	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	MAN	G	5	3	-	0/2/19/22	1/1/1/1
4	NAG	H	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	1/2/19/22	0/1/1/1
3	NAG	I	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1
3	MAN	I	5	3	-	0/2/19/22	1/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	K	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	1/2/19/22	0/1/1/1
3	MAN	K	4	3	-	0/2/19/22	1/1/1/1
3	MAN	K	5	3	1/1/4/5	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	C1-C2	5.89	1.60	1.52
3	G	1	NAG	C8-C7	3.13	1.57	1.50
3	G	1	NAG	C3-C2	2.47	1.57	1.52
3	G	2	NAG	O5-C1	-2.26	1.39	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	O5-C1-C2	-12.09	92.59	111.29
3	G	1	NAG	C1-C2-N2	8.69	124.13	110.43
3	G	1	NAG	C8-C7-N2	7.85	129.14	116.12
4	H	3	BMA	C1-O5-C5	7.57	122.33	112.19
3	G	1	NAG	O7-C7-N2	-7.38	108.94	121.98
3	I	3	BMA	C1-O5-C5	7.37	122.06	112.19
3	G	1	NAG	C1-O5-C5	6.17	120.45	112.19
3	G	3	BMA	O3-C3-C4	5.55	123.46	110.38
3	G	1	NAG	C2-N2-C7	5.28	129.98	122.90
3	G	1	NAG	C3-C4-C5	-4.64	101.81	110.23
3	K	5	MAN	C3-C4-C5	4.63	118.63	110.23
3	K	5	MAN	C1-O5-C5	4.08	117.65	112.19
5	J	1	NAG	C4-C3-C2	-3.96	105.21	111.02
5	J	2	NAG	C4-C3-C2	-3.80	105.44	111.02
3	K	4	MAN	C1-O5-C5	3.69	117.13	112.19
3	G	1	NAG	O3-C3-C2	3.66	117.00	109.40
3	K	1	NAG	C1-O5-C5	3.47	116.84	112.19
3	I	5	MAN	C1-O5-C5	3.40	116.74	112.19
3	G	2	NAG	C1-O5-C5	3.40	116.74	112.19
3	K	2	NAG	C2-N2-C7	-3.33	118.44	122.90
4	H	2	NAG	C4-C3-C2	3.24	115.77	111.02
3	K	3	BMA	O5-C5-C6	-3.18	101.48	107.66
3	K	5	MAN	O5-C5-C4	3.13	118.44	110.83
3	K	5	MAN	O5-C1-C2	3.11	118.20	110.79
3	G	3	BMA	C3-C4-C5	-3.11	104.60	110.23
3	K	2	NAG	C1-O5-C5	3.08	116.31	112.19
5	J	2	NAG	C1-C2-N2	3.05	115.25	110.43
3	K	1	NAG	C3-C4-C5	-2.93	104.92	110.23
3	K	1	NAG	O7-C7-N2	2.91	127.11	121.98
3	I	1	NAG	C6-C5-C4	2.87	120.08	113.02
3	K	1	NAG	O5-C1-C2	-2.78	106.99	111.29
5	J	1	NAG	O4-C4-C5	2.77	116.15	109.32
3	G	5	MAN	C3-C4-C5	-2.77	105.21	110.23
3	I	1	NAG	C3-C4-C5	-2.76	105.23	110.23
4	H	2	NAG	O5-C1-C2	-2.75	107.03	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	O7-C7-C8	-2.69	117.27	122.05
3	K	3	BMA	C1-O5-C5	2.66	115.75	112.19
3	G	2	NAG	C3-C4-C5	2.62	114.98	110.23
4	H	1	NAG	C1-O5-C5	2.59	115.66	112.19
5	J	2	NAG	C8-C7-N2	2.54	120.33	116.12
4	H	1	NAG	O5-C1-C2	-2.48	107.45	111.29
3	I	2	NAG	O5-C1-C2	-2.48	107.46	111.29
3	I	1	NAG	C2-N2-C7	2.46	126.19	122.90
3	G	2	NAG	C6-C5-C4	-2.46	106.98	113.02
3	K	1	NAG	C8-C7-N2	-2.44	112.07	116.12
3	K	4	MAN	C1-C2-C3	2.44	113.19	109.64
3	I	5	MAN	C3-C4-C5	-2.43	105.82	110.23
4	H	2	NAG	O4-C4-C5	2.40	115.24	109.32
3	I	1	NAG	O7-C7-N2	2.35	126.13	121.98
3	G	4	MAN	O4-C4-C3	-2.34	104.85	110.38
3	I	1	NAG	O4-C4-C3	-2.33	104.87	110.38
5	J	1	NAG	C1-O5-C5	2.31	115.29	112.19
5	J	2	NAG	O7-C7-C8	-2.30	117.95	122.05
4	H	3	BMA	C2-C3-C4	-2.22	106.95	110.86
4	H	3	BMA	C1-C2-C3	2.21	112.87	109.64
3	G	5	MAN	C1-O5-C5	2.20	115.14	112.19
3	I	3	BMA	C2-C3-C4	-2.20	107.00	110.86
3	I	5	MAN	O5-C5-C6	2.16	111.86	107.66
3	G	2	NAG	O4-C4-C3	-2.11	105.41	110.38
3	I	1	NAG	C1-O5-C5	2.03	114.91	112.19
4	H	1	NAG	C8-C7-N2	2.02	119.47	116.12
3	K	2	NAG	O4-C4-C3	-2.02	105.62	110.38
3	G	3	BMA	O2-C2-C3	2.01	114.31	110.15

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	K	5	MAN	C1
5	J	2	NAG	C1

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	J	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	G	4	MAN	C4-C5-C6-O6
3	K	5	MAN	O5-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
3	G	3	BMA	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
4	H	1	NAG	C3-C2-N2-C7
3	I	3	BMA	C4-C5-C6-O6

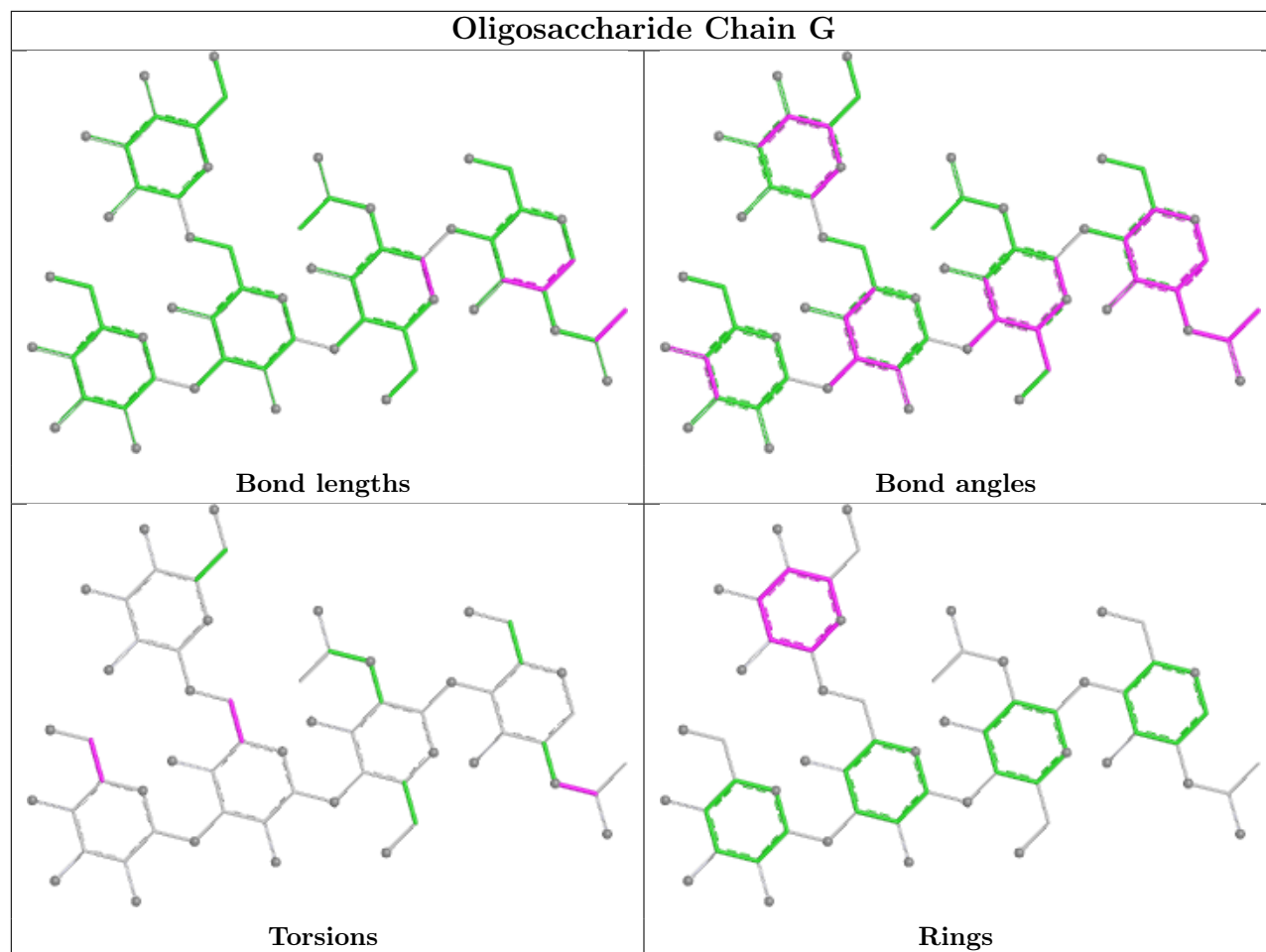
All (3) ring outliers are listed below:

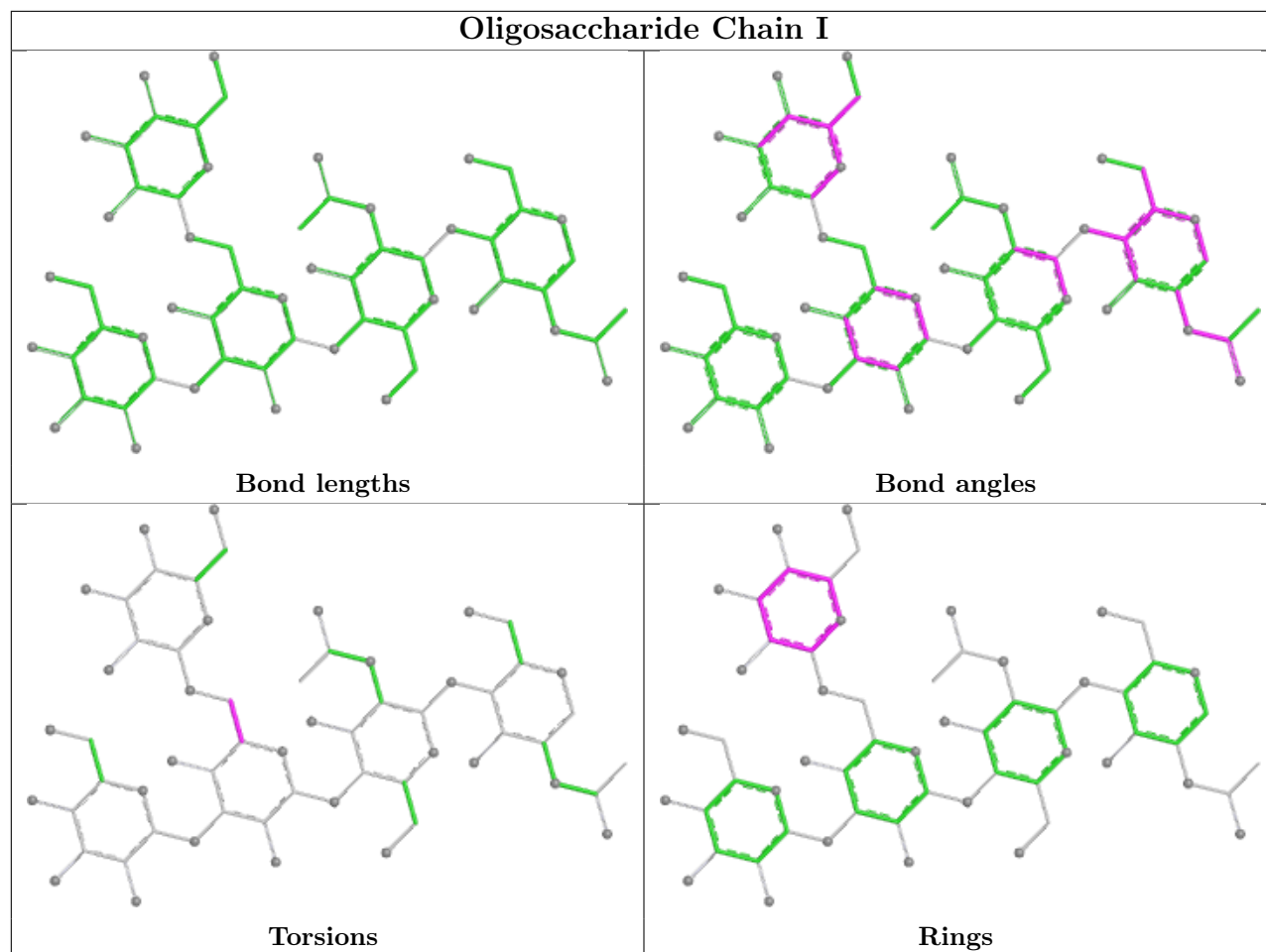
Mol	Chain	Res	Type	Atoms
3	K	4	MAN	C1-C2-C3-C4-C5-O5
3	I	5	MAN	C1-C2-C3-C4-C5-O5
3	G	5	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 10 short contacts:

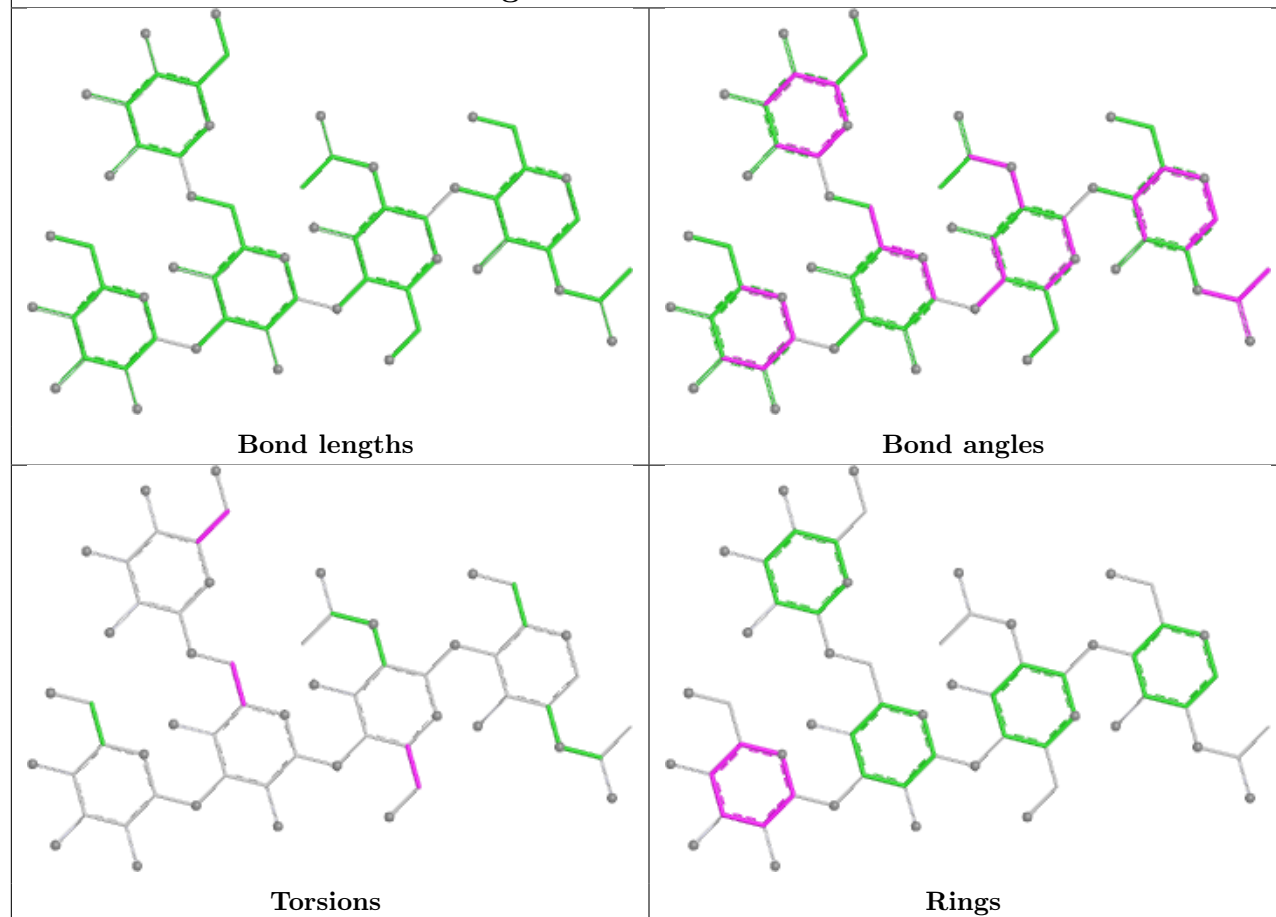
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	3	0
4	H	1	NAG	4	0
3	K	1	NAG	2	0
3	I	1	NAG	1	0
3	K	2	NAG	1	0

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

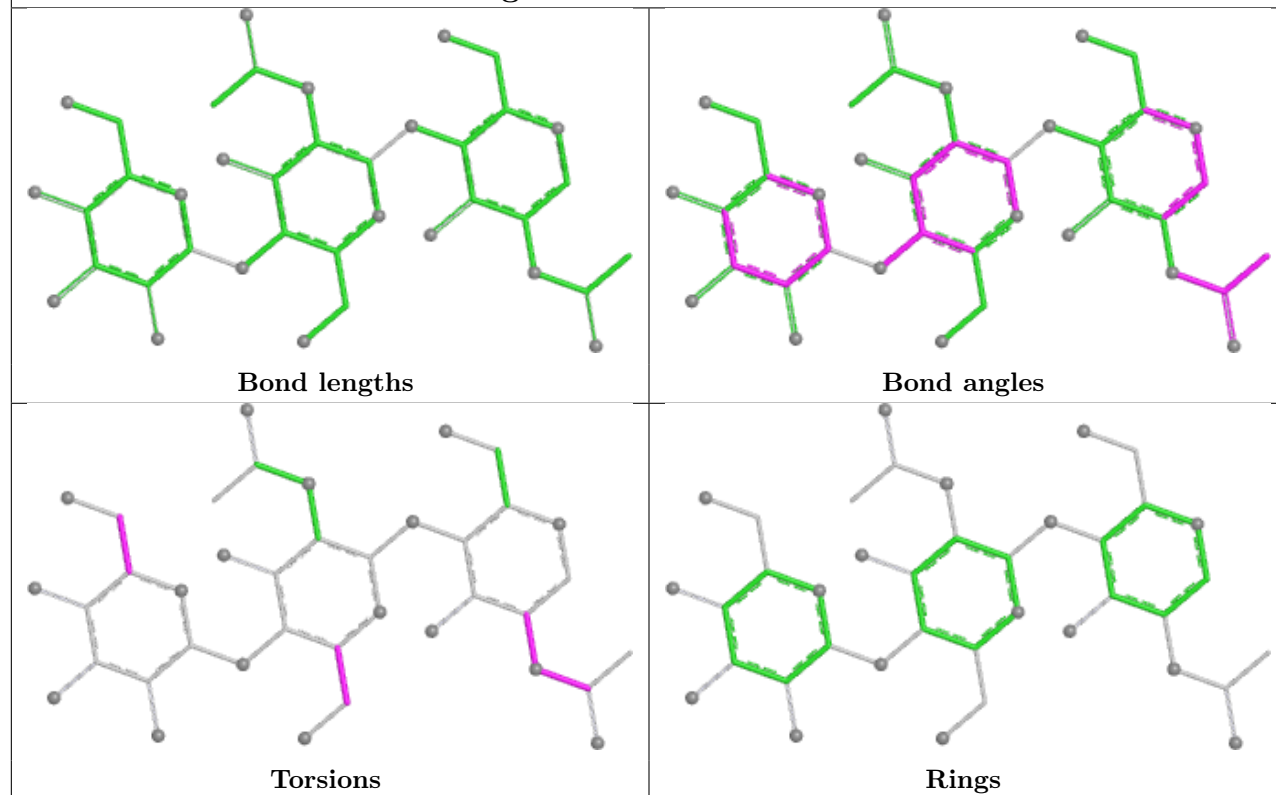


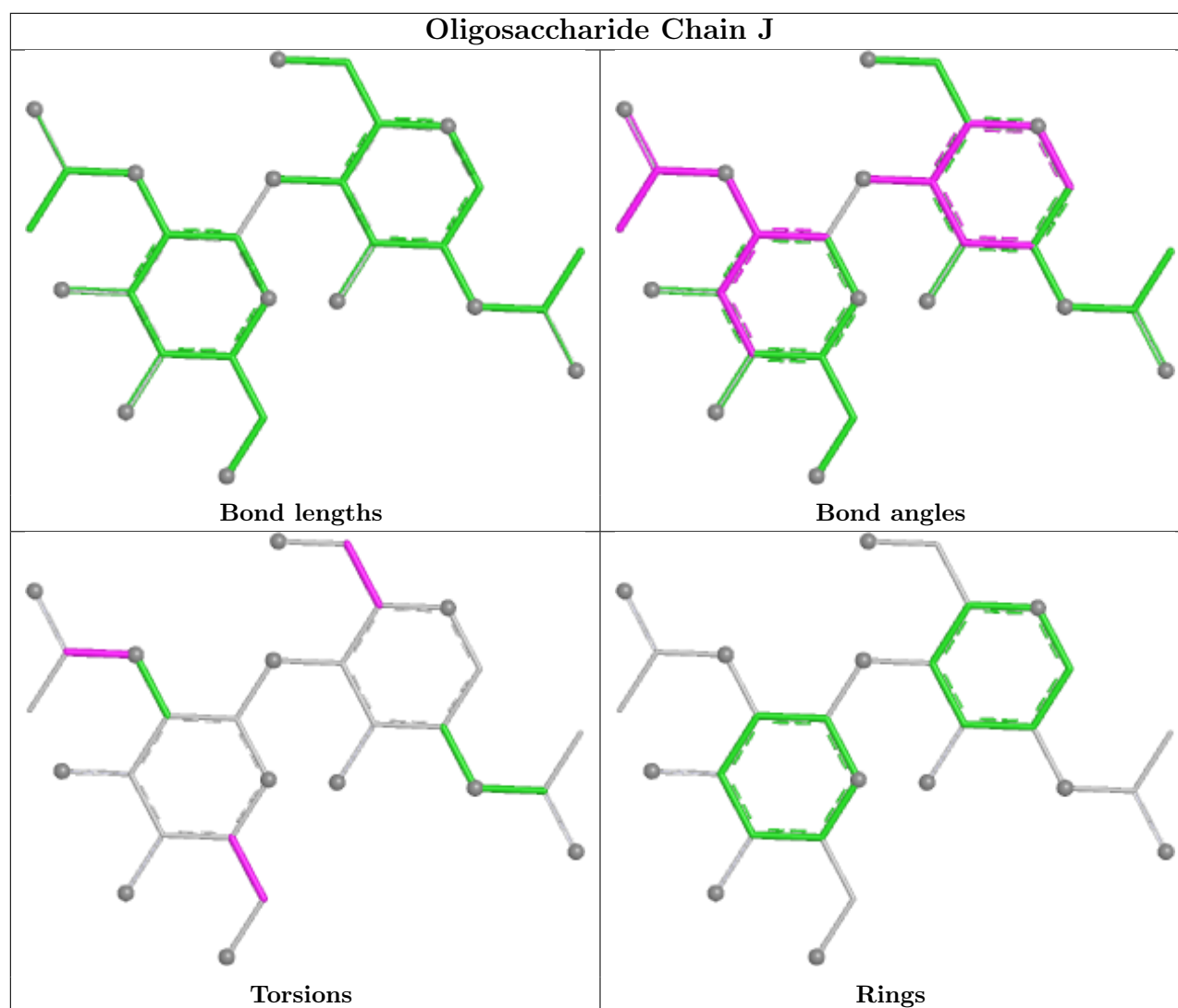


Oligosaccharide Chain K



Oligosaccharide Chain H





5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
7	EDO	F	1175	-	3,3,3	0.60	0	2,2,2	0.19	0
7	EDO	E	1327	-	3,3,3	0.58	0	2,2,2	0.09	0
7	EDO	E	1328	-	3,3,3	0.55	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	D	1173	-	3,3,3	0.53	0	2,2,2	0.35	0
7	EDO	F	1176	-	3,3,3	0.48	0	2,2,2	0.52	0
6	NAG	A	401	1	14,14,15	0.53	0	17,19,21	1.67	3 (17%)
6	NAG	E	420	1	14,14,15	0.54	0	17,19,21	1.81	3 (17%)
7	EDO	B	1175	-	3,3,3	0.37	0	2,2,2	0.55	0
6	NAG	C	420	1	14,14,15	0.59	0	17,19,21	2.63	4 (23%)
7	EDO	B	1173	-	3,3,3	0.58	0	2,2,2	0.20	0
7	EDO	A	1327	-	3,3,3	0.59	0	2,2,2	0.32	0
7	EDO	C	1327	-	3,3,3	0.40	0	2,2,2	0.37	0
7	EDO	E	1326	-	3,3,3	0.39	0	2,2,2	0.69	0
6	NAG	D	211	2	14,14,15	0.78	1 (7%)	17,19,21	1.36	2 (11%)
7	EDO	A	1328	-	3,3,3	0.67	0	2,2,2	0.29	0
7	EDO	F	1173	-	3,3,3	0.45	0	2,2,2	0.08	0
7	EDO	C	1328	-	3,3,3	0.61	0	2,2,2	0.20	0
7	EDO	C	1329	-	3,3,3	0.51	0	2,2,2	0.54	0
7	EDO	A	1326	-	3,3,3	0.59	0	2,2,2	0.32	0
6	NAG	A	420	1	14,14,15	0.56	0	17,19,21	1.87	3 (17%)
7	EDO	C	1326	-	3,3,3	0.57	0	2,2,2	0.50	0
7	EDO	B	1174	-	3,3,3	0.50	0	2,2,2	0.33	0
6	NAG	B	211	2	14,14,15	0.68	0	17,19,21	1.32	3 (17%)
7	EDO	F	1174	-	3,3,3	0.35	0	2,2,2	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	F	1175	-	-	1/1/1/1	-
7	EDO	E	1327	-	-	1/1/1/1	-
7	EDO	E	1328	-	-	1/1/1/1	-
7	EDO	D	1173	-	-	1/1/1/1	-
7	EDO	F	1176	-	-	1/1/1/1	-
6	NAG	A	401	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	E	420	1	1/1/5/7	4/6/23/26	0/1/1/1
7	EDO	B	1175	-	-	1/1/1/1	-
6	NAG	C	420	1	1/1/5/7	2/6/23/26	0/1/1/1
7	EDO	B	1173	-	-	1/1/1/1	-
7	EDO	A	1327	-	-	1/1/1/1	-
7	EDO	C	1327	-	-	1/1/1/1	-
7	EDO	E	1326	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	211	2	-	1/6/23/26	0/1/1/1
7	EDO	A	1328	-	-	1/1/1/1	-
7	EDO	F	1173	-	-	1/1/1/1	-
7	EDO	C	1328	-	-	1/1/1/1	-
7	EDO	C	1329	-	-	0/1/1/1	-
7	EDO	A	1326	-	-	1/1/1/1	-
6	NAG	A	420	1	1/1/5/7	2/6/23/26	0/1/1/1
7	EDO	C	1326	-	-	0/1/1/1	-
7	EDO	B	1174	-	-	1/1/1/1	-
6	NAG	B	211	2	-	0/6/23/26	0/1/1/1
7	EDO	F	1174	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	211	NAG	C1-C2	2.63	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	420	NAG	O5-C1-C2	-8.38	98.32	111.29
6	A	420	NAG	O5-C1-C2	-5.84	102.25	111.29
6	E	420	NAG	O5-C1-C2	-5.29	103.11	111.29
6	A	401	NAG	C1-O5-C5	5.15	119.09	112.19
6	C	420	NAG	C2-N2-C7	-4.05	117.47	122.90
6	D	211	NAG	C1-C2-N2	3.68	116.23	110.43
6	C	420	NAG	C4-C3-C2	3.67	116.40	111.02
6	A	420	NAG	C3-C4-C5	3.41	116.42	110.23
6	E	420	NAG	C1-C2-N2	3.11	115.33	110.43
6	B	211	NAG	C1-C2-N2	-3.01	105.69	110.43
6	A	401	NAG	C4-C3-C2	-2.48	107.38	111.02
6	C	420	NAG	C3-C4-C5	2.38	114.54	110.23
6	B	211	NAG	O5-C1-C2	-2.30	107.74	111.29
6	D	211	NAG	C1-O5-C5	2.20	115.14	112.19
6	E	420	NAG	C8-C7-N2	2.18	119.74	116.12
6	A	401	NAG	O5-C5-C6	2.17	111.88	107.66
6	B	211	NAG	O7-C7-C8	-2.15	118.22	122.05
6	A	420	NAG	O3-C3-C2	-2.09	105.06	109.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	401	NAG	C1
6	A	420	NAG	C1
6	C	420	NAG	C1
6	E	420	NAG	C1

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	NAG	O5-C5-C6-O6
6	C	420	NAG	O5-C5-C6-O6
6	E	420	NAG	O5-C5-C6-O6
6	A	401	NAG	C4-C5-C6-O6
6	C	420	NAG	C4-C5-C6-O6
6	E	420	NAG	C4-C5-C6-O6
6	E	420	NAG	C8-C7-N2-C2
6	E	420	NAG	O7-C7-N2-C2
7	C	1327	EDO	O1-C1-C2-O2
6	A	420	NAG	C4-C5-C6-O6
7	C	1328	EDO	O1-C1-C2-O2
7	E	1327	EDO	O1-C1-C2-O2
7	F	1175	EDO	O1-C1-C2-O2
6	A	420	NAG	O5-C5-C6-O6
6	D	211	NAG	O5-C5-C6-O6
7	D	1173	EDO	O1-C1-C2-O2
7	E	1328	EDO	O1-C1-C2-O2
7	F	1176	EDO	O1-C1-C2-O2
7	B	1174	EDO	O1-C1-C2-O2
7	A	1326	EDO	O1-C1-C2-O2
7	A	1328	EDO	O1-C1-C2-O2
7	B	1173	EDO	O1-C1-C2-O2
7	A	1327	EDO	O1-C1-C2-O2
7	F	1173	EDO	O1-C1-C2-O2
7	F	1174	EDO	O1-C1-C2-O2
7	B	1175	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1175	EDO	3	0
7	E	1328	EDO	6	0
7	F	1176	EDO	5	0
7	B	1175	EDO	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	1326	EDO	1	0
6	D	211	NAG	1	0
7	A	1328	EDO	2	0
7	C	1328	EDO	1	0
7	C	1329	EDO	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	318/324 (98%)	0.27	11 (3%) 47 49	26, 51, 77, 149	1 (0%)
1	C	319/324 (98%)	0.04	4 (1%) 75 76	24, 42, 76, 140	0
1	E	319/324 (98%)	0.35	9 (2%) 55 57	33, 56, 88, 141	0
2	B	172/172 (100%)	0.82	15 (8%) 16 17	30, 66, 87, 91	0
2	D	172/172 (100%)	0.66	8 (4%) 36 38	30, 65, 94, 99	0
2	F	172/172 (100%)	0.69	11 (6%) 25 27	34, 71, 101, 108	0
All	All	1472/1488 (98%)	0.40	58 (3%) 43 45	24, 56, 91, 149	1 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1	GLY	4.7
2	D	1	GLY	4.3
1	C	10	LEU	4.3
1	E	10	LEU	4.3
1	A	16	GLY	4.1
1	A	11	ASP	4.0
1	A	13	ILE	3.9
1	A	15	LEU	3.8
1	E	144	GLY	3.3
1	A	21	ALA	3.3
1	A	14	CYS	3.3
1	C	13	ILE	3.2
2	B	29	ALA	3.2
1	A	208	THR	3.2
2	F	168	LEU	3.1
2	B	168	LEU	3.0
2	D	143	ALA	3.0
2	B	172	ASN	2.9
2	B	7	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	143	GLY	2.8
1	E	143	GLY	2.8
2	D	29	ALA	2.7
1	E	188	THR	2.6
2	F	29	ALA	2.6
2	D	106	HIS	2.5
2	F	18	VAL	2.5
2	F	164	GLU	2.5
1	A	216	VAL	2.5
2	D	168	LEU	2.5
2	F	171	LEU	2.5
1	C	16	GLY	2.5
1	C	29	LEU	2.4
2	B	8	GLY	2.4
1	E	14	CYS	2.4
2	F	172	ASN	2.4
1	E	130	ILE	2.4
2	B	56	ILE	2.4
2	F	58	LYS	2.3
2	B	167	LEU	2.3
2	B	171	LEU	2.3
1	E	13	ILE	2.3
1	A	12	LYS	2.3
2	B	144	CYS	2.2
2	F	106	HIS	2.2
2	B	55	LEU	2.2
2	B	1	GLY	2.2
2	D	160	SER	2.2
2	B	141	TYR	2.2
2	F	56	ILE	2.1
2	D	164	GLU	2.1
1	E	277	CYS	2.1
1	E	167	THR	2.1
2	B	121	ARG	2.1
1	A	20	VAL	2.1
2	F	35	ALA	2.1
2	D	56	ILE	2.1
2	B	18	VAL	2.1
2	B	60	ASN	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](#)

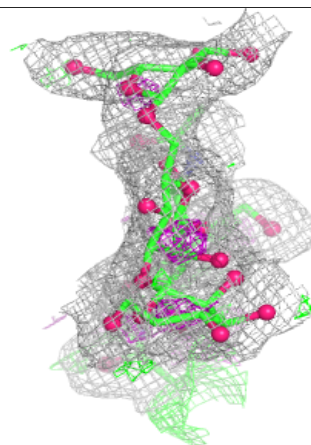
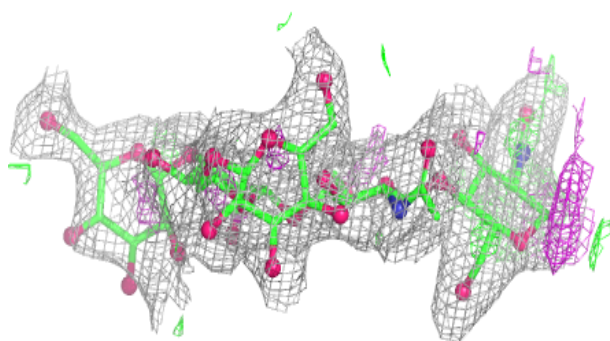
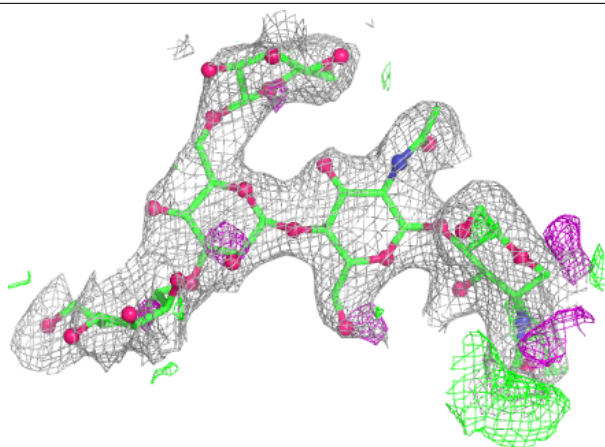
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	J	2	14/15	0.44	0.17	89,93,98,99	0
3	MAN	K	5	11/12	0.52	0.18	107,119,126,129	0
3	MAN	G	4	11/12	0.53	0.16	81,85,94,95	0
3	MAN	K	4	11/12	0.53	0.16	116,122,132,134	0
4	BMA	H	3	11/12	0.57	0.13	97,100,106,107	0
3	MAN	I	4	11/12	0.60	0.17	92,96,106,108	0
3	BMA	K	3	11/12	0.61	0.17	98,107,117,118	0
3	MAN	I	5	11/12	0.72	0.16	75,79,85,88	0
4	NAG	H	2	14/15	0.73	0.14	83,89,92,95	0
3	BMA	I	3	11/12	0.77	0.14	76,85,90,93	0
5	NAG	J	1	14/15	0.78	0.12	73,77,85,87	0
3	MAN	G	5	11/12	0.79	0.12	71,74,80,83	0
3	NAG	K	2	14/15	0.80	0.15	69,73,83,89	0
3	BMA	G	3	11/12	0.85	0.11	68,75,80,82	0
4	NAG	H	1	14/15	0.86	0.10	63,67,74,78	0
3	NAG	G	2	14/15	0.87	0.13	51,54,61,64	0
3	NAG	I	2	14/15	0.89	0.11	53,56,64,70	0
3	NAG	K	1	14/15	0.91	0.13	47,51,57,62	0
3	NAG	G	1	14/15	0.92	0.12	37,40,45,47	0
3	NAG	I	1	14/15	0.94	0.10	39,42,46,49	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.

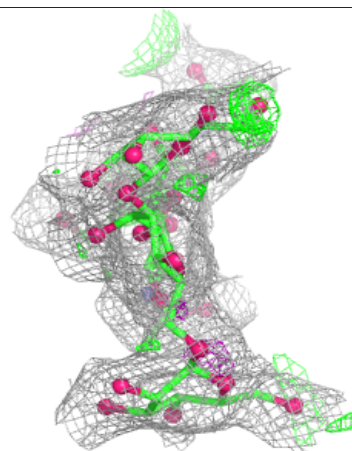
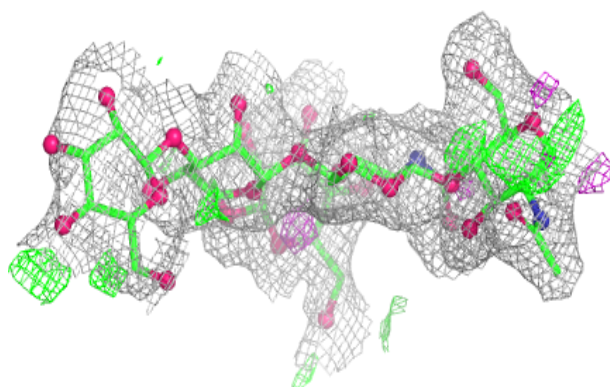
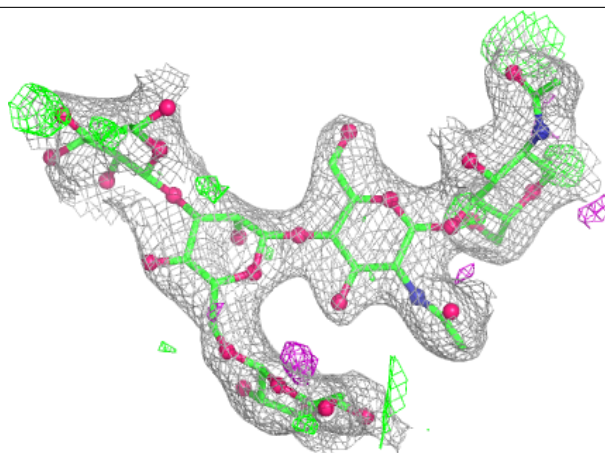
Electron density around Chain G:

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



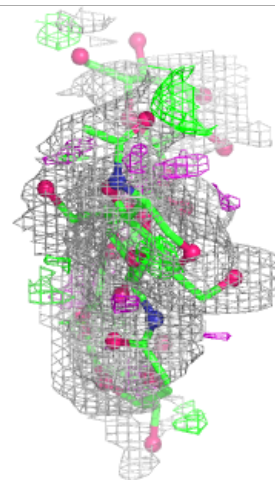
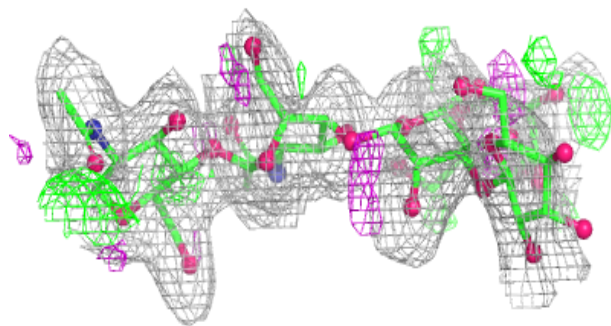
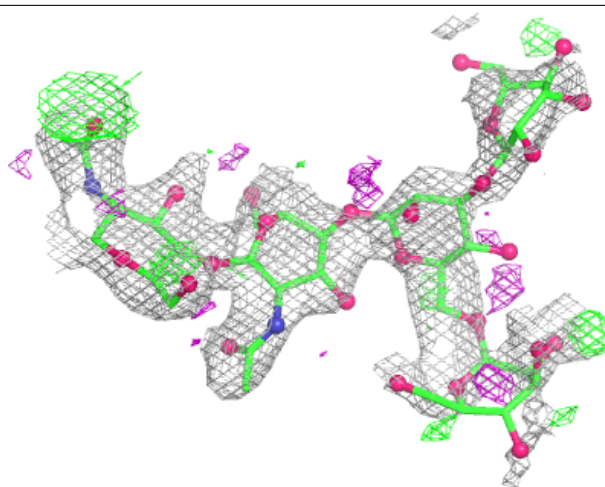
Electron density around Chain I:

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



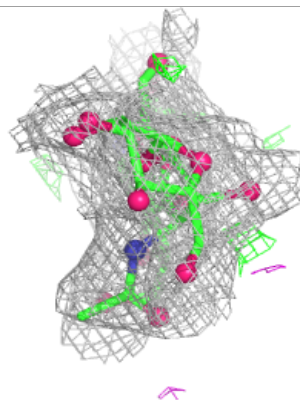
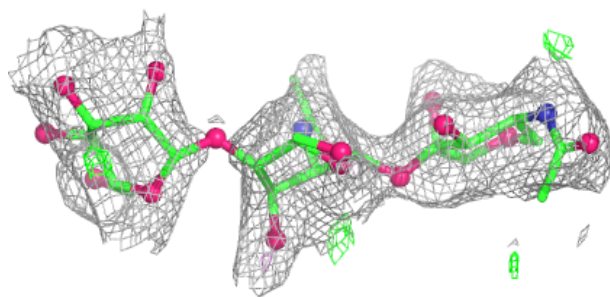
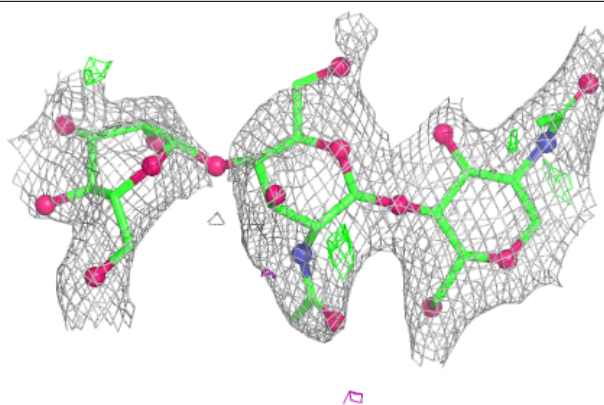
Electron density around Chain K:

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

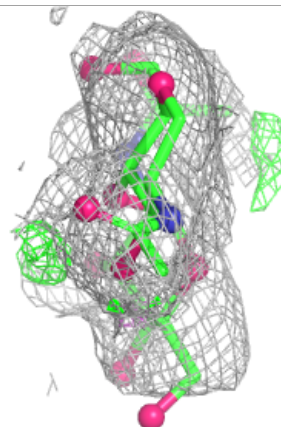
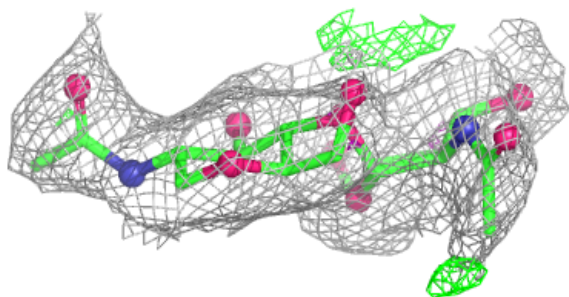
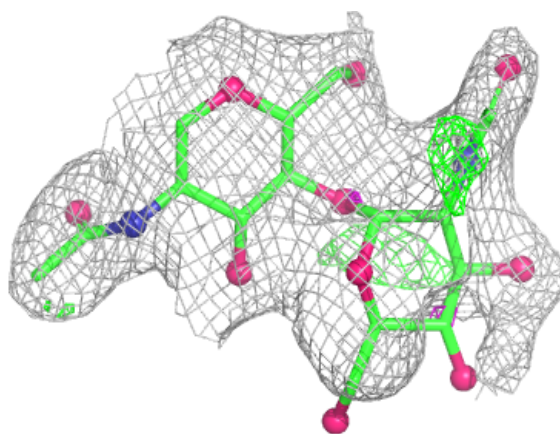


Electron density around Chain H:

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

**Electron density around Chain J:**

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



6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	D	211	14/15	0.35	0.17	94,100,105,106	0
6	NAG	B	211	14/15	0.59	0.17	93,100,103,105	0
6	NAG	C	420	14/15	0.59	0.16	61,67,72,73	0
6	NAG	A	420	14/15	0.59	0.18	72,78,84,84	0
7	EDO	F	1176	4/4	0.67	0.28	63,64,64,68	0
6	NAG	A	401	14/15	0.71	0.14	81,85,93,93	0
7	EDO	D	1173	4/4	0.74	0.18	50,52,56,58	0
6	NAG	E	420	14/15	0.76	0.13	68,74,79,79	0
7	EDO	F	1175	4/4	0.83	0.31	67,68,71,71	0
7	EDO	B	1175	4/4	0.86	0.39	40,44,45,45	0
7	EDO	E	1328	4/4	0.86	0.22	58,58,60,62	0
7	EDO	E	1327	4/4	0.87	0.33	53,55,55,56	0
7	EDO	C	1329	4/4	0.88	0.24	48,49,50,56	0
7	EDO	F	1173	4/4	0.89	0.15	41,42,43,48	0
7	EDO	F	1174	4/4	0.89	0.14	39,40,40,50	0
7	EDO	A	1327	4/4	0.89	0.15	49,52,54,57	0
7	EDO	C	1327	4/4	0.89	0.17	47,47,50,50	0
7	EDO	B	1174	4/4	0.90	0.15	43,45,45,46	0
7	EDO	E	1326	4/4	0.90	0.25	46,46,49,52	0
7	EDO	C	1328	4/4	0.92	0.22	39,48,50,51	0
7	EDO	A	1328	4/4	0.94	0.17	44,44,45,47	0
7	EDO	B	1173	4/4	0.95	0.24	34,34,38,39	0
7	EDO	C	1326	4/4	0.96	0.07	30,30,33,34	0
7	EDO	A	1326	4/4	0.96	0.09	30,32,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.