



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:06 AM UTC

PDB ID : 1NHC / pdb_00001nhc
Title : Structural insights into the processivity of endopolygalacturonase I from *Aspergillus niger*
Authors : van Pouderoyen, G.; Snijder, H.J.; Benen, J.A.; Dijkstra, B.W.
Deposited on : 2002-12-19
Resolution : 1.70 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

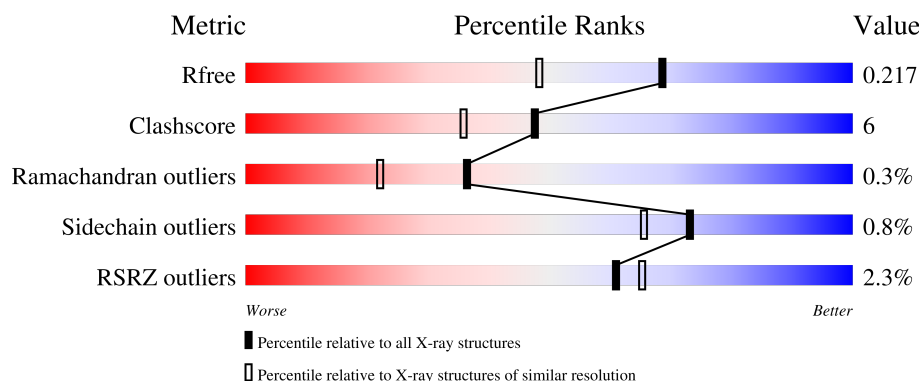
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	336	3% 90% 10%
1	B	336	4% 88% 12%
1	C	336	% 91% 9%
1	D	336	2% 88% 11%
1	E	336	% 90% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	336	 3% 90% 9%
2	G	2	 100%
3	H	6	 17% 83%
4	I	3	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	I	3	X	-	-	-
7	GOL	B	405	-	-	X	-
7	GOL	D	405	-	-	X	-
7	GOL	E	408	-	-	X	-
7	GOL	F	405	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 16429 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 Polygalacturonase I.

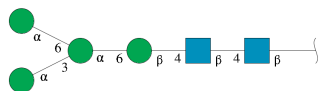
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	B	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	C	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	D	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	E	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	F	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			

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



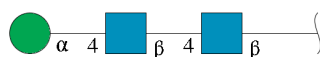
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



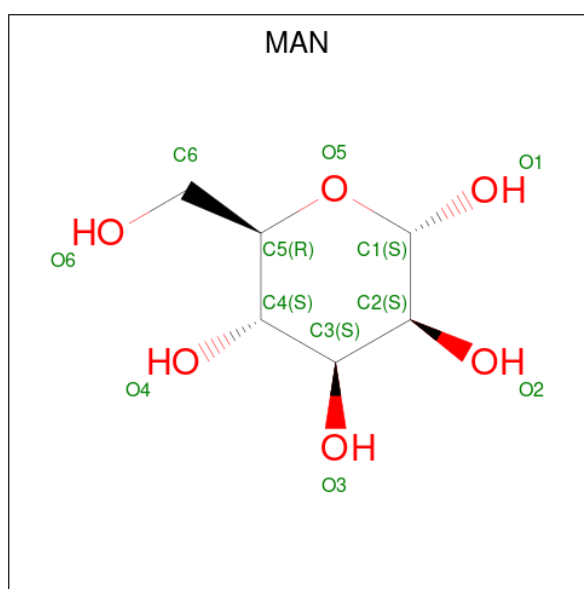
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



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

- Molecule 5 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		
5	E	1	Total	C	O	0	0
			11	6	5		
5	E	1	Total	C	O	0	0
			11	6	5		
5	F	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

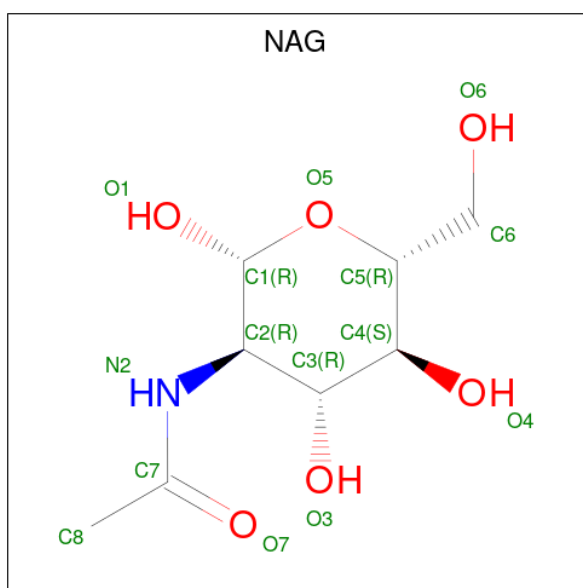
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0
7	F	1	Total C O 6 3 3	0	0

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



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	236	Total O 236 236	0	0

Continued on next page...

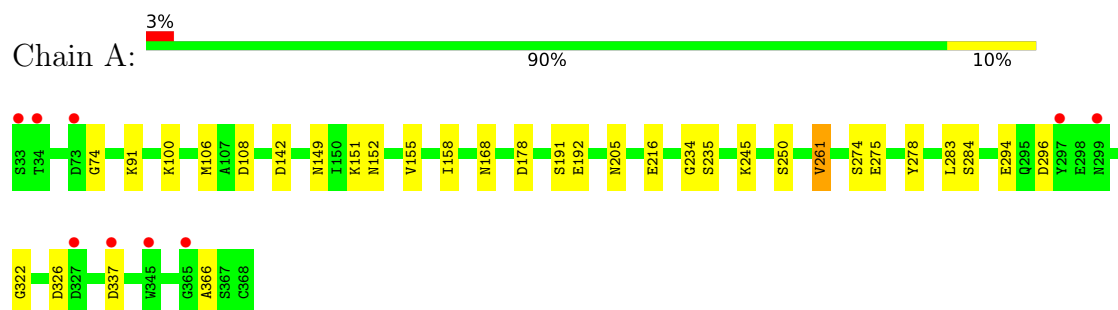
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	162	Total 162	O 162	0	0
9	C	258	Total 258	O 258	0	0
9	D	211	Total 211	O 211	0	0
9	E	252	Total 252	O 252	0	0
9	F	234	Total 234	O 234	0	0

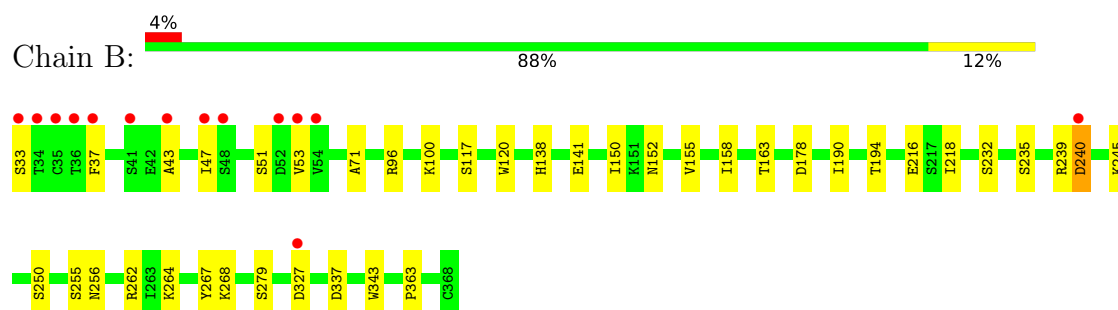
3 Residue-property plots [i](#)

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.

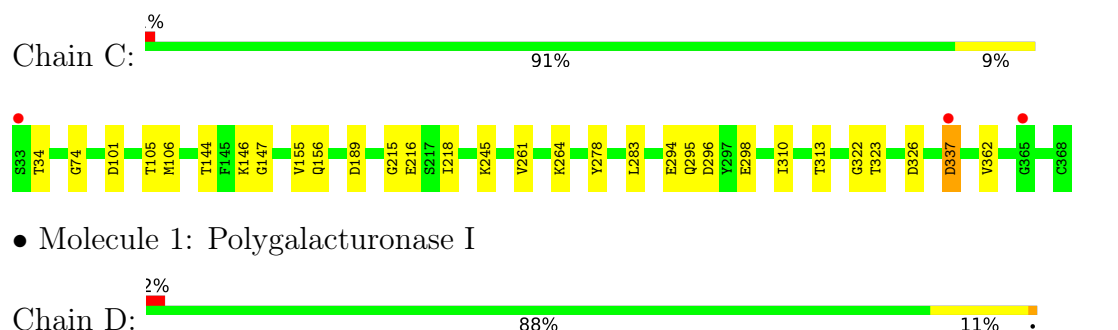
• Molecule 1: Polygalacturonase I



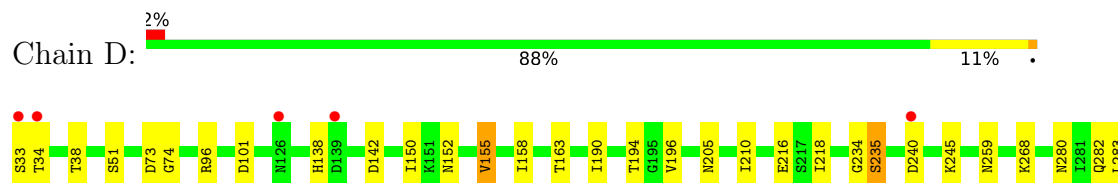
• Molecule 1: Polygalacturonase I



• Molecule 1: Polygalacturonase I

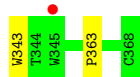
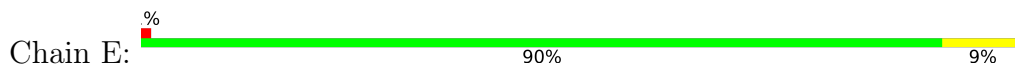


• Molecule 1: Polygalacturonase I

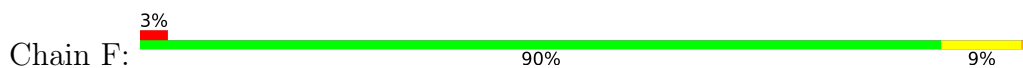




- Molecule 1: Polygalacturonase I



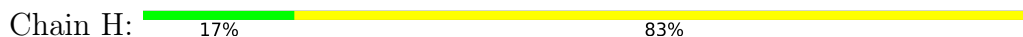
- Molecule 1: Polygalacturonase I



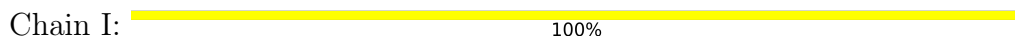
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.01Å 84.13Å 96.03Å 114.32° 98.00° 89.75°	Depositor
Resolution (Å)	35.81 – 1.70 35.81 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.81-1.70) 97.5 (35.81-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.209 0.185 , 0.217	Depositor DCC
R_{free} test set	10409 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.055 for -h,k,-k-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16429	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, SO4, NAG, GOL

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	0.91	2/2482 (0.1%)	1.09	7/3374 (0.2%)
1	B	0.85	1/2482 (0.0%)	1.06	2/3374 (0.1%)
1	C	0.92	0/2482	1.10	4/3374 (0.1%)
1	D	0.90	0/2482	1.09	4/3374 (0.1%)
1	E	0.91	1/2482 (0.0%)	1.04	3/3374 (0.1%)
1	F	0.92	1/2482 (0.0%)	1.05	4/3374 (0.1%)
All	All	0.90	5/14892 (0.0%)	1.07	24/20244 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	VAL	CA-CB	7.63	1.63	1.54
1	E	106	MET	SD-CE	-7.17	1.61	1.79
1	F	261	VAL	CA-CB	5.28	1.60	1.54
1	B	337	ASP	N-CA	-5.16	1.39	1.46
1	A	158	ILE	CA-CB	-5.11	1.47	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	34	THR	N-CA-C	7.90	120.92	108.67
1	A	326	ASP	N-CA-C	6.99	119.79	111.33
1	D	152	ASN	N-CA-C	6.56	119.22	111.02
1	F	152	ASN	N-CA-C	6.04	118.57	111.02
1	E	266	ILE	N-CA-C	5.94	117.14	108.58
1	C	34	THR	N-CA-C	5.81	123.17	110.80
1	B	232	SER	N-CA-C	5.73	118.74	109.40
1	A	168	ASN	N-CA-C	5.57	118.56	109.59
1	B	152	ASN	N-CA-C	5.56	117.97	111.02
1	E	47	ILE	N-CA-C	5.47	116.20	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	232	SER	N-CA-C	5.45	117.84	109.07
1	C	326	ASP	N-CA-C	5.45	117.97	111.71
1	F	168	ASN	N-CA-C	5.41	118.30	109.59
1	A	250	SER	N-CA-C	5.34	117.18	109.07
1	D	326	ASP	N-CA-C	5.32	117.76	111.33
1	A	366	ALA	N-CA-C	5.30	116.70	109.18
1	C	313	THR	N-CA-C	5.28	117.71	109.52
1	A	91	LYS	N-CA-C	5.25	119.68	113.28
1	F	250	SER	N-CA-C	5.24	117.04	109.07
1	A	152	ASN	N-CA-C	5.22	117.55	111.02
1	E	205	ASN	N-CA-C	5.11	115.28	108.23
1	C	323	THR	N-CA-C	5.08	117.68	109.40
1	A	205	ASN	N-CA-C	5.08	115.24	108.23
1	D	205	ASN	N-CA-C	5.07	114.73	108.19

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	2444	0	2273	20	2
1	B	2444	0	2273	36	2
1	C	2444	0	2273	15	2
1	D	2444	0	2273	32	1
1	E	2444	0	2273	27	1
1	F	2444	0	2274	29	1
2	G	28	0	25	2	0
3	H	72	0	61	1	0
4	I	39	0	34	0	0
5	A	22	0	20	0	0
5	B	22	0	20	0	0
5	C	22	0	20	0	0
5	D	22	0	20	0	0
5	E	22	0	20	0	0
5	F	11	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	10	0	0	0	0
6	B	10	0	0	0	0
6	C	20	0	0	0	0
6	D	10	0	0	0	0
6	E	20	0	0	0	0
6	F	10	0	0	0	0
7	A	6	0	8	1	0
7	B	6	0	8	6	0
7	D	6	0	8	6	1
7	E	6	0	8	8	0
7	F	6	0	8	5	0
8	C	14	0	13	0	0
8	E	14	0	13	0	0
8	F	14	0	13	4	0
9	A	236	0	0	9	1
9	B	162	0	0	3	0
9	C	258	0	0	4	0
9	D	211	0	0	8	0
9	E	252	0	0	6	1
9	F	234	0	0	4	0
All	All	16429	0	13948	163	6

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 6.

All (163) 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:B:96:ARG:NH2	7:B:405:GOL:H12	1.23	1.46
1:B:96:ARG:NH2	7:B:405:GOL:C1	1.98	1.26
1:F:100:LYS:HG2	1:F:141:GLU:OE2	1.50	1.12
1:D:284:SER:HB3	1:F:282:GLN:HE22	1.18	1.06
1:A:261:VAL:HG22	9:A:686:HOH:O	1.55	1.04
1:E:80:GLU:CD	9:E:504:HOH:O	2.02	1.01
1:D:240:ASP:HB2	9:D:516:HOH:O	1.61	0.98
1:B:96:ARG:HH22	7:B:405:GOL:C1	1.69	0.96
1:C:105:THR:OG1	9:C:501:HOH:O	1.83	0.95
1:B:240:ASP:HB2	9:B:538:HOH:O	1.69	0.93
1:A:261:VAL:HA	9:A:686:HOH:O	1.70	0.91
1:F:44:SER:CB	9:F:501:HOH:O	2.04	0.91
1:A:74:GLY:O	9:A:501:HOH:O	1.89	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:LYS:CE	9:C:512:HOH:O	2.20	0.89
8:F:402:NAG:H3	8:F:402:NAG:H83	1.56	0.88
1:B:96:ARG:HH21	7:B:405:GOL:H12	0.82	0.83
1:D:138:HIS:ND1	7:D:405:GOL:H11	1.95	0.82
1:D:138:HIS:ND1	7:D:405:GOL:C1	2.43	0.82
1:B:216:GLU:OE2	1:B:245:LYS:HB3	1.81	0.81
1:F:100:LYS:CG	1:F:141:GLU:OE2	2.28	0.81
1:D:73:ASP:HB3	9:D:517:HOH:O	1.81	0.80
1:D:284:SER:HB3	1:F:282:GLN:NE2	1.94	0.80
1:F:96:ARG:NH2	7:F:405:GOL:H32	1.96	0.80
1:E:299:ASN:HA	3:H:5:MAN:H2	1.66	0.77
1:D:284:SER:CB	1:F:282:GLN:HE22	1.96	0.76
1:A:108:ASP:OD2	9:A:502:HOH:O	2.04	0.74
1:A:261:VAL:CA	9:A:686:HOH:O	2.32	0.73
1:F:44:SER:HB2	9:F:501:HOH:O	1.75	0.73
1:B:262:ARG:CZ	1:B:264:LYS:HE2	2.19	0.72
1:E:67:ASP:CG	7:E:408:GOL:H2	2.15	0.72
1:E:96:ARG:HE	7:E:408:GOL:C3	2.03	0.71
1:E:80:GLU:CG	9:E:504:HOH:O	2.36	0.70
1:A:100:LYS:HE3	1:A:142:ASP:OD2	1.91	0.70
1:B:33:SER:HB2	1:B:51:SER:H	1.56	0.70
1:B:96:ARG:HH21	7:B:405:GOL:C1	1.75	0.70
1:B:267:TYR:CE2	1:B:268:LYS:HD3	2.28	0.69
1:A:261:VAL:CG2	9:A:686:HOH:O	2.25	0.69
1:E:113:ASP:OD1	1:E:151:LYS:HE2	1.93	0.68
1:C:264:LYS:HE3	9:C:512:HOH:O	1.86	0.68
1:E:67:ASP:OD1	7:E:408:GOL:H2	1.94	0.67
1:D:96:ARG:NH2	7:D:405:GOL:O3	2.28	0.67
1:D:190:ILE:HD12	1:D:210:ILE:HD11	1.78	0.66
7:A:405:GOL:H12	9:A:505:HOH:O	1.94	0.65
1:D:38:THR:OG1	9:D:502:HOH:O	2.15	0.65
8:F:402:NAG:C1	8:F:402:NAG:H82	2.26	0.65
1:E:80:GLU:OE2	9:E:501:HOH:O	2.14	0.64
1:D:282:GLN:NE2	1:F:323:THR:HG23	2.13	0.63
1:F:100:LYS:HG2	1:F:141:GLU:CD	2.22	0.63
1:D:280:ASN:HB3	9:D:687:HOH:O	1.99	0.62
1:D:33:SER:HB2	1:D:51:SER:OG	2.00	0.62
1:E:96:ARG:HE	7:E:408:GOL:H32	1.65	0.61
1:A:151:LYS:HE3	9:A:703:HOH:O	2.01	0.61
1:E:96:ARG:NE	7:E:408:GOL:H32	2.17	0.60
1:D:196:VAL:HB	1:D:218:ILE:HD12	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:HIS:ND1	7:D:405:GOL:H12	2.17	0.59
1:F:256:ASN:OD1	9:F:502:HOH:O	2.16	0.59
1:B:100:LYS:HG2	1:B:141:GLU:OE1	2.03	0.58
1:D:73:ASP:OD2	9:D:503:HOH:O	2.17	0.58
8:F:402:NAG:C1	8:F:402:NAG:C8	2.76	0.58
2:G:1:NAG:H62	2:G:2:NAG:N2	2.20	0.57
1:E:80:GLU:HG3	9:E:504:HOH:O	2.03	0.56
1:B:240:ASP:CB	9:B:538:HOH:O	2.40	0.56
1:C:264:LYS:HE2	9:C:512:HOH:O	1.97	0.56
1:D:190:ILE:CD1	1:D:210:ILE:HD11	2.36	0.56
2:G:1:NAG:H62	2:G:2:NAG:HN2	1.71	0.55
1:E:96:ARG:NE	7:E:408:GOL:C3	2.70	0.54
1:D:196:VAL:HB	1:D:218:ILE:CD1	2.38	0.54
1:B:47:ILE:CD1	1:B:53:VAL:HG21	2.37	0.53
1:A:261:VAL:HG13	1:A:278:TYR:CE2	2.44	0.52
1:F:96:ARG:HH21	7:F:405:GOL:H32	1.74	0.52
1:B:343:TRP:CD2	1:B:363:PRO:HG2	2.45	0.52
1:B:47:ILE:HD12	1:B:53:VAL:HG21	1.92	0.51
1:B:267:TYR:CZ	1:B:268:LYS:HD3	2.46	0.51
1:C:215:GLY:HA3	1:C:218:ILE:HD11	1.93	0.51
1:A:261:VAL:CB	9:A:686:HOH:O	2.56	0.50
1:A:245:LYS:NZ	1:A:275:GLU:OE1	2.42	0.50
1:E:79:PHE:HB2	1:E:106:MET:HG2	1.93	0.50
1:B:267:TYR:CZ	1:B:268:LYS:NZ	2.80	0.49
7:F:405:GOL:H12	9:F:512:HOH:O	2.12	0.49
1:C:261:VAL:HG13	1:C:278:TYR:CZ	2.48	0.49
1:B:150:ILE:CD1	1:B:158:ILE:HD11	2.42	0.48
1:C:106:MET:HG3	1:C:147:GLY:O	2.12	0.48
1:D:234:GLY:HA2	1:D:235:SER:C	2.39	0.48
1:E:261:VAL:HG13	1:E:278:TYR:CZ	2.49	0.48
1:D:282:GLN:NE2	1:F:323:THR:CG2	2.76	0.48
1:B:262:ARG:CZ	1:B:264:LYS:CE	2.90	0.48
1:E:216:GLU:HA	1:E:245:LYS:O	2.14	0.48
1:C:144:THR:HG22	1:C:146:LYS:HG2	1.96	0.48
1:D:245:LYS:NZ	9:D:514:HOH:O	2.47	0.47
1:E:264:LYS:HD2	1:E:297:TYR:CZ	2.48	0.47
1:A:234:GLY:HA2	1:A:235:SER:C	2.40	0.47
1:B:47:ILE:HG13	1:B:71:ALA:HA	1.96	0.47
1:C:295:GLN:NE2	1:C:310:ILE:O	2.47	0.47
1:B:216:GLU:OE2	1:B:245:LYS:CB	2.59	0.47
1:D:138:HIS:CE1	7:D:405:GOL:H11	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:LYS:HG2	1:F:141:GLU:CG	2.45	0.47
7:D:405:GOL:O1	9:D:501:HOH:O	1.97	0.47
1:B:267:TYR:CD2	1:B:268:LYS:HD3	2.50	0.47
1:D:101:ASP:HA	1:D:142:ASP:O	2.15	0.47
1:D:283:LEU:O	1:D:322:GLY:HA3	2.15	0.46
1:A:261:VAL:HG13	1:A:278:TYR:CZ	2.50	0.46
1:B:216:GLU:HA	1:B:245:LYS:O	2.15	0.46
1:B:194:THR:HA	1:B:216:GLU:O	2.15	0.46
1:E:146:LYS:NZ	1:E:168:ASN:HD22	2.13	0.46
1:B:262:ARG:NH1	1:B:264:LYS:HE2	2.31	0.46
1:D:74:GLY:HA2	1:D:101:ASP:O	2.16	0.46
1:A:106:MET:HE2	1:A:149:ASN:HB3	1.96	0.46
8:F:402:NAG:H3	8:F:402:NAG:C8	2.35	0.46
1:F:100:LYS:HG2	1:F:141:GLU:HG2	1.98	0.45
1:A:191:SER:O	1:A:192:GLU:C	2.57	0.45
1:C:283:LEU:O	1:C:322:GLY:HA3	2.15	0.45
1:B:37:PHE:CD1	1:B:43:ALA:HA	2.51	0.45
1:B:138:HIS:ND1	7:B:405:GOL:O1	2.03	0.44
1:F:96:ARG:NH2	7:F:405:GOL:C3	2.75	0.44
1:F:264:LYS:HD2	1:F:297:TYR:CZ	2.52	0.44
1:C:74:GLY:HA2	1:C:101:ASP:O	2.18	0.44
1:C:156:GLN:HG2	1:C:189:ASP:OD2	2.18	0.44
1:D:216:GLU:HA	1:D:245:LYS:O	2.17	0.44
1:B:163:THR:HA	1:B:194:THR:O	2.18	0.44
1:F:96:ARG:HH21	7:F:405:GOL:H12	1.83	0.43
1:D:150:ILE:CD1	1:D:158:ILE:HD11	2.48	0.43
1:D:268:LYS:NZ	9:D:515:HOH:O	2.50	0.43
1:F:234:GLY:HA2	1:F:235:SER:C	2.43	0.43
1:A:283:LEU:O	1:A:322:GLY:HA3	2.19	0.43
1:B:190:ILE:HG21	1:B:218:ILE:HD13	2.00	0.43
1:C:294:GLU:OE1	1:C:296:ASP:OD2	2.37	0.42
1:E:343:TRP:CD2	1:E:363:PRO:HG2	2.54	0.42
1:A:294:GLU:OE1	1:A:296:ASP:OD2	2.38	0.42
1:B:117:SER:HA	1:B:120:TRP:CE3	2.54	0.42
1:E:248:THR:HG22	9:E:523:HOH:O	2.19	0.42
1:F:106:MET:HE2	1:F:149:ASN:HB3	2.02	0.42
1:C:216:GLU:HA	1:C:245:LYS:O	2.18	0.42
1:D:234:GLY:CA	1:D:235:SER:C	2.92	0.42
1:E:156:GLN:HG2	1:E:189:ASP:OD2	2.20	0.42
1:F:141:GLU:CD	1:F:141:GLU:N	2.77	0.42
1:A:245:LYS:HA	1:A:274:SER:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:LEU:O	1:E:322:GLY:HA3	2.19	0.42
1:B:96:ARG:NH1	1:B:96:ARG:HG3	2.35	0.42
1:D:259:ASN:HA	1:D:289:TYR:O	2.19	0.42
1:E:261:VAL:HG13	1:E:278:TYR:CE1	2.55	0.42
1:D:295:GLN:NE2	1:D:310:ILE:O	2.53	0.41
1:A:234:GLY:CA	1:A:235:SER:C	2.93	0.41
1:E:262:ARG:HA	1:E:292:VAL:O	2.20	0.41
1:F:74:GLY:HA2	1:F:101:ASP:O	2.20	0.41
1:F:343:TRP:CD2	1:F:363:PRO:HG2	2.54	0.41
1:F:274:SER:HA	1:F:313:THR:O	2.20	0.41
1:B:216:GLU:CD	1:B:245:LYS:HB3	2.43	0.41
1:E:96:ARG:HD2	7:E:408:GOL:H31	2.02	0.41
1:F:261:VAL:HG13	1:F:278:TYR:CZ	2.55	0.41
1:F:264:LYS:HE3	1:F:264:LYS:HB2	1.81	0.41
1:B:235:SER:O	1:B:239:ARG:NH2	2.48	0.41
1:C:261:VAL:HG13	1:C:278:TYR:CE2	2.56	0.41
1:D:163:THR:HA	1:D:194:THR:O	2.21	0.41
1:E:67:ASP:OD1	7:E:408:GOL:C2	2.65	0.41
1:E:144:THR:HG22	1:E:146:LYS:HG3	2.02	0.41
1:A:216:GLU:HA	1:A:245:LYS:O	2.21	0.41
1:F:267:TYR:CE2	1:F:268:LYS:HG3	2.55	0.41
1:B:250:SER:HA	1:B:279:SER:O	2.20	0.40
1:E:245:LYS:NZ	9:E:522:HOH:O	2.54	0.40
1:B:240:ASP:HB2	9:B:505:HOH:O	2.21	0.40
1:F:264:LYS:HD2	1:F:297:TYR:CE1	2.56	0.40
1:B:255:SER:O	1:B:256:ASN:C	2.65	0.40
1:F:191:SER:O	1:F:192:GLU:C	2.65	0.40

All (6) 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:B:178:ASP:OD2	1:C:337:ASP:OD2[1_646]	1.79	0.41
9:A:687:HOH:O	9:E:725:HOH:O[1_554]	1.94	0.26
1:F:100:LYS:CE	7:D:405:GOL:O2[1_455]	1.97	0.23
1:A:337:ASP:OD2	1:E:178:ASP:OD2[1_554]	2.11	0.09
1:B:327:ASP:OD2	1:C:298:GLU:OE2[1_646]	2.17	0.03
1:A:178:ASP:OD2	1:D:337:ASP:OD2[1_454]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/336 (99%)	313 (94%)	20 (6%)	1 (0%)	36	22
1	B	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	36	22
1	C	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	36	22
1	D	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	36	22
1	E	334/336 (99%)	313 (94%)	20 (6%)	1 (0%)	36	22
1	F	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	36	22
All	All	2004/2016 (99%)	1886 (94%)	112 (6%)	6 (0%)	36	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	155	VAL
1	A	155	VAL
1	B	155	VAL
1	D	155	VAL
1	C	155	VAL
1	E	155	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/278 (100%)	277 (100%)	1 (0%)	84	80
1	B	278/278 (100%)	277 (100%)	1 (0%)	84	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	278/278 (100%)	276 (99%)	2 (1%)	76	69
1	D	278/278 (100%)	273 (98%)	5 (2%)	51	36
1	E	278/278 (100%)	277 (100%)	1 (0%)	84	80
1	F	278/278 (100%)	274 (99%)	4 (1%)	59	46
All	All	1668/1668 (100%)	1654 (99%)	14 (1%)	73	65

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	284	SER
1	B	240	ASP
1	C	337	ASP
1	C	362	VAL
1	D	155	VAL
1	D	235	SER
1	D	284	SER
1	D	292	VAL
1	D	351	SER
1	E	70	ASP
1	F	151	LYS
1	F	155	VAL
1	F	292	VAL
1	F	351	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	161	GLN
1	A	180	ASN
1	B	213	ASN
1	B	282	GLN
1	C	126	ASN
1	C	168	ASN
1	C	180	ASN
1	C	213	ASN
1	C	299	ASN
1	D	168	ASN
1	D	282	GLN
1	E	168	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	180	ASN
1	E	183	HIS
1	F	168	ASN
1	F	180	ASN
1	F	282	GLN
1	F	299	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

11 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	G	1	1,2	14,14,15	0.62	0	17,19,21	2.12	4 (23%)
2	NAG	G	2	2	14,14,15	0.57	0	17,19,21	2.68	5 (29%)
3	NAG	H	1	1,3	14,14,15	0.50	0	17,19,21	1.06	2 (11%)
3	NAG	H	2	3	14,14,15	0.58	0	17,19,21	2.65	2 (11%)
3	BMA	H	3	3	11,11,12	0.88	1 (9%)	15,15,17	1.82	4 (26%)
3	MAN	H	4	3	11,11,12	0.65	0	15,15,17	1.25	2 (13%)
3	MAN	H	5	3	11,11,12	0.67	0	15,15,17	0.82	0
3	MAN	H	6	3	11,11,12	0.65	0	15,15,17	0.57	0
4	NAG	I	1	1,4	14,14,15	0.65	0	17,19,21	1.14	3 (17%)
4	NAG	I	2	4	14,14,15	0.56	0	17,19,21	2.57	4 (23%)
4	MAN	I	3	4	11,11,12	0.67	0	15,15,17	2.47	3 (20%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	3	BMA	O5-C1	-2.34	1.39	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	C1-O5-C5	7.22	121.87	112.19
3	H	2	NAG	C1-O5-C5	7.16	121.78	112.19
4	I	3	MAN	C1-O5-C5	7.04	121.62	112.19
3	H	2	NAG	O5-C1-C2	7.00	122.12	111.29
2	G	2	NAG	C1-O5-C5	6.66	121.12	112.19
2	G	2	NAG	O5-C1-C2	6.28	121.01	111.29
4	I	2	NAG	O5-C1-C2	5.73	120.15	111.29
2	G	1	NAG	O4-C4-C3	-5.00	98.58	110.38
4	I	3	MAN	O5-C1-C2	4.67	121.94	110.79
3	H	3	BMA	C1-O5-C5	4.44	118.14	112.19
2	G	1	NAG	O5-C5-C6	-3.50	100.84	107.66
4	I	2	NAG	O4-C4-C3	-3.42	102.31	110.38
2	G	1	NAG	O4-C4-C5	3.37	117.61	109.32
2	G	2	NAG	C2-N2-C7	-3.30	118.47	122.90
3	H	3	BMA	O5-C1-C2	2.86	117.62	110.79
2	G	1	NAG	C1-O5-C5	2.86	116.02	112.19
3	H	3	BMA	O5-C5-C6	-2.74	102.33	107.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	BMA	C1-C2-C3	2.69	113.56	109.64
3	H	1	NAG	C2-N2-C7	-2.53	119.50	122.90
4	I	3	MAN	C2-C3-C4	-2.51	106.44	110.86
4	I	2	NAG	C3-C4-C5	2.50	114.77	110.23
2	G	2	NAG	C4-C3-C2	-2.50	107.36	111.02
3	H	1	NAG	O4-C4-C3	-2.42	104.67	110.38
3	H	4	MAN	O3-C3-C4	-2.36	104.80	110.38
2	G	2	NAG	C1-C2-N2	2.33	114.10	110.43
4	I	1	NAG	O4-C4-C3	-2.22	105.15	110.38
4	I	1	NAG	O5-C1-C2	-2.19	107.90	111.29
4	I	1	NAG	C2-N2-C7	-2.17	119.99	122.90
3	H	4	MAN	O3-C3-C2	2.08	114.30	110.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	I	3	MAN	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	4	MAN	C4-C5-C6-O6
3	H	4	MAN	O5-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
4	I	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	H	5	MAN	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
3	H	6	MAN	C4-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	H	6	MAN	O5-C5-C6-O6
4	I	1	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

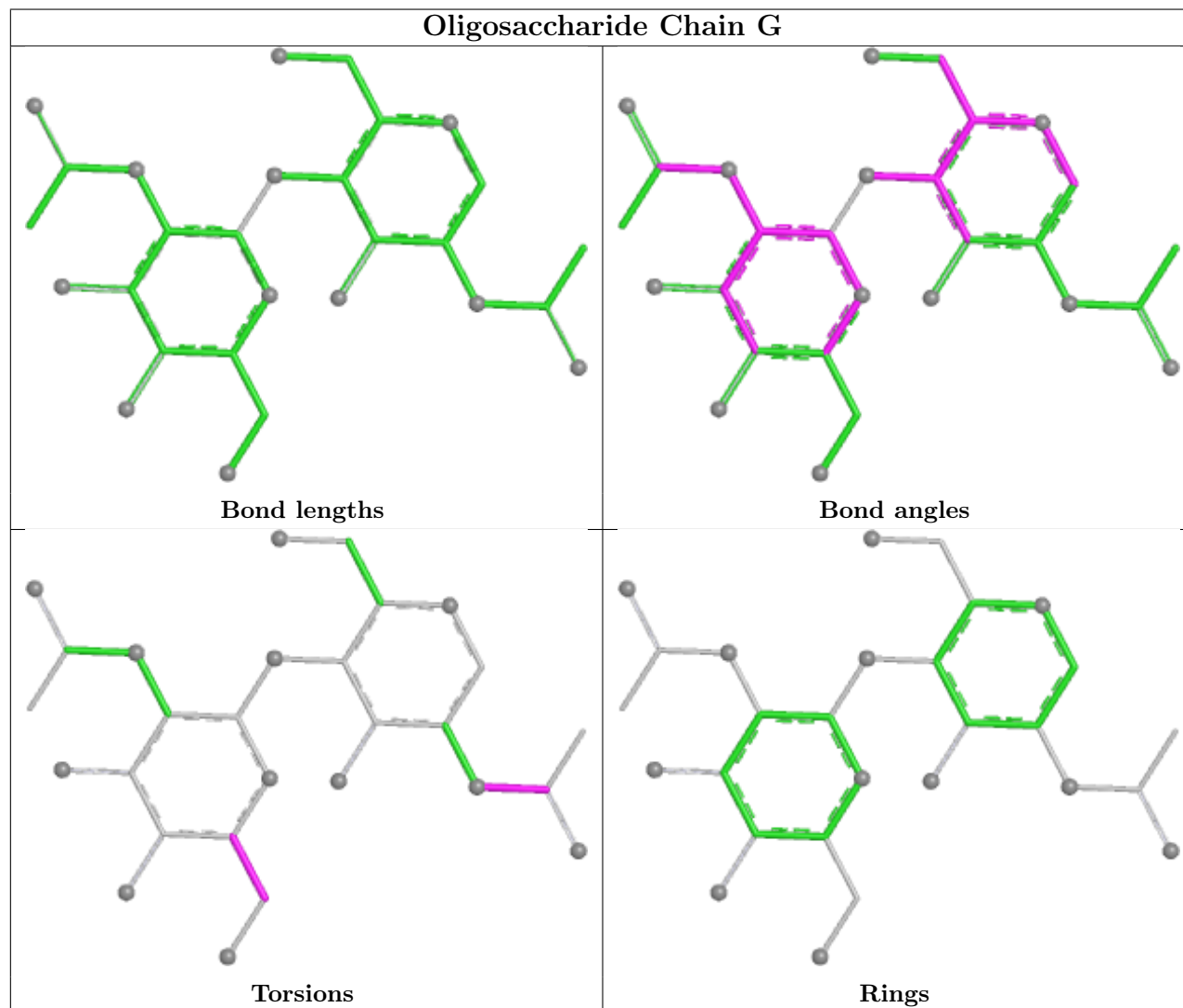
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	2	0

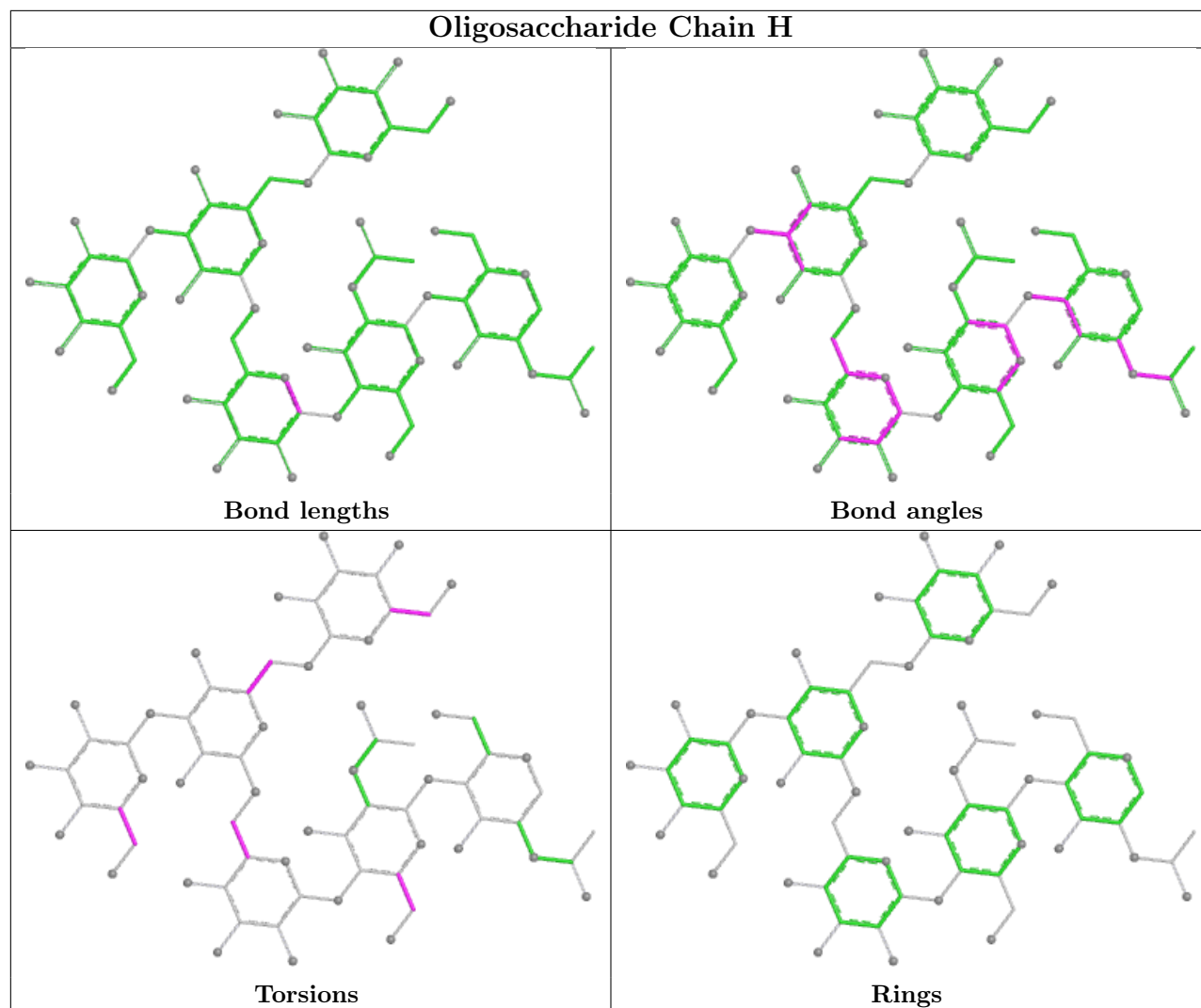
Continued on next page...

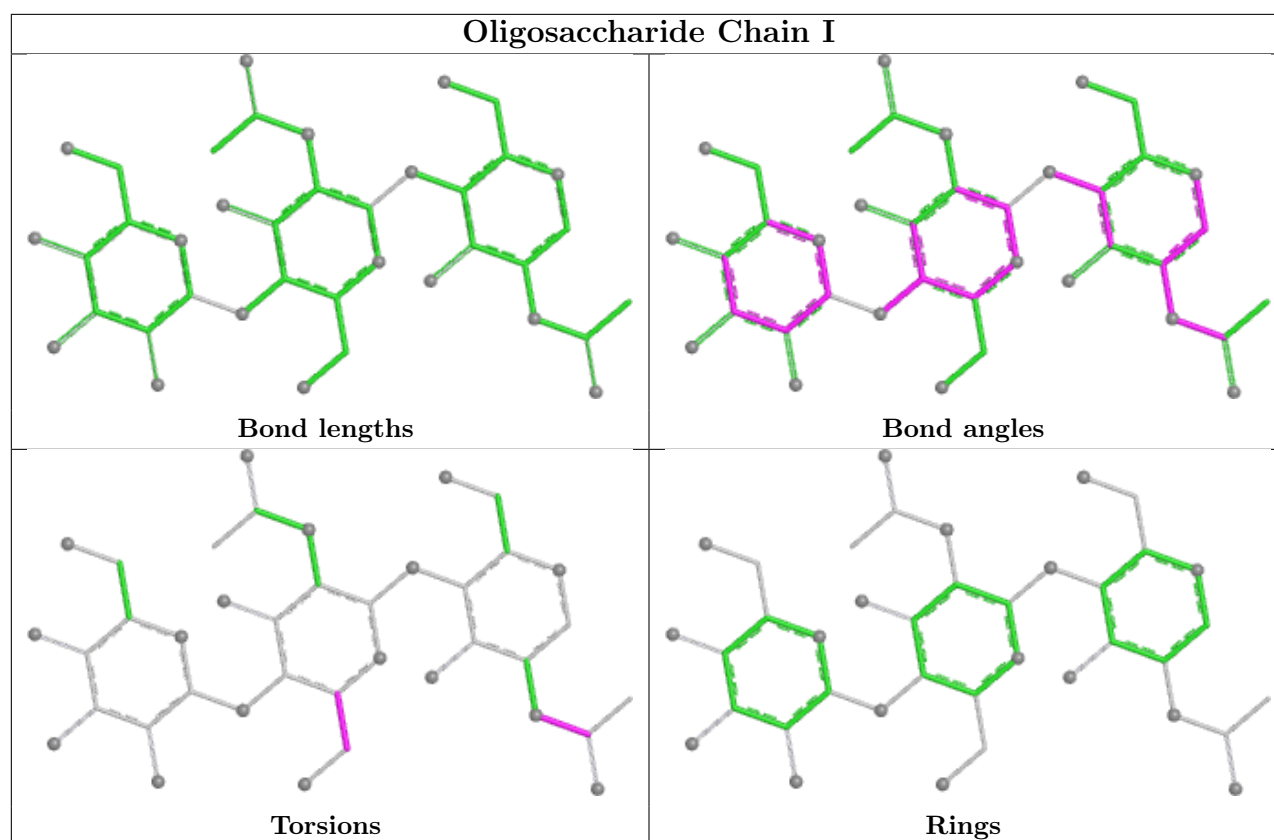
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	5	MAN	1	0
2	G	2	NAG	2	0

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







5.6 Ligand geometry [i](#)

35 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	$\# Z > 2$
6	SO4	F	404	-	4,4,4	0.77	0	6,6,6	0.72	0
8	NAG	F	402	1	14,14,15	1.13	3 (21%)	17,19,21	2.18	6 (35%)
6	SO4	E	404	-	4,4,4	0.27	0	6,6,6	0.42	0
6	SO4	C	406	-	4,4,4	0.34	0	6,6,6	0.61	0
6	SO4	A	403	-	4,4,4	0.26	0	6,6,6	0.74	0
5	MAN	A	402	1	11,11,12	0.64	0	15,15,17	0.95	1 (6%)
6	SO4	E	407	-	4,4,4	0.16	0	6,6,6	0.49	0
7	GOL	B	405	-	5,5,5	0.37	0	5,5,5	0.80	0
6	SO4	A	404	-	4,4,4	0.42	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	F	405	-	5,5,5	0.49	0	5,5,5	0.36	0
7	GOL	D	405	-	5,5,5	0.59	0	5,5,5	2.64	3 (60%)
5	MAN	D	401	1	11,11,12	0.79	1 (9%)	15,15,17	0.83	0
6	SO4	D	404	-	4,4,4	0.43	0	6,6,6	0.47	0
5	MAN	E	402	1	11,11,12	0.58	0	15,15,17	1.26	1 (6%)
6	SO4	B	404	-	4,4,4	0.48	0	6,6,6	0.36	0
5	MAN	B	401	1	11,11,12	0.85	1 (9%)	15,15,17	0.88	0
6	SO4	F	403	-	4,4,4	0.43	0	6,6,6	0.42	0
5	MAN	E	401	1	11,11,12	0.57	0	15,15,17	0.94	0
5	MAN	C	402	1	11,11,12	0.92	1 (9%)	15,15,17	0.89	0
8	NAG	E	403	1	14,14,15	0.67	0	17,19,21	0.97	0
6	SO4	C	407	-	4,4,4	0.36	0	6,6,6	0.54	0
6	SO4	E	406	-	4,4,4	0.73	0	6,6,6	0.43	0
5	MAN	D	402	1	11,11,12	0.92	2 (18%)	15,15,17	0.76	0
6	SO4	B	403	-	4,4,4	0.32	0	6,6,6	0.25	0
6	SO4	C	404	-	4,4,4	0.26	0	6,6,6	0.66	0
8	NAG	C	403	1	14,14,15	0.50	0	17,19,21	0.73	0
5	MAN	B	402	1	11,11,12	0.70	0	15,15,17	1.06	1 (6%)
6	SO4	D	403	-	4,4,4	0.19	0	6,6,6	0.60	0
7	GOL	E	408	-	5,5,5	0.19	0	5,5,5	0.72	0
6	SO4	E	405	-	4,4,4	0.44	0	6,6,6	0.64	0
7	GOL	A	405	-	5,5,5	0.42	0	5,5,5	0.44	0
5	MAN	A	401	1	11,11,12	0.90	1 (9%)	15,15,17	1.20	1 (6%)
6	SO4	C	405	-	4,4,4	0.45	0	6,6,6	0.46	0
5	MAN	C	401	1	11,11,12	0.73	0	15,15,17	1.13	1 (6%)
5	MAN	F	401	1	11,11,12	0.76	0	15,15,17	0.93	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
8	NAG	F	402	1	-	4/6/23/26	0/1/1/1
5	MAN	A	402	1	-	0/2/19/22	0/1/1/1
7	GOL	B	405	-	-	0/4/4/4	-
7	GOL	F	405	-	-	1/4/4/4	-
7	GOL	D	405	-	-	2/4/4/4	-
5	MAN	D	401	1	-	2/2/19/22	0/1/1/1
5	MAN	E	402	1	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	B	401	1	-	2/2/19/22	0/1/1/1
5	MAN	E	401	1	-	0/2/19/22	0/1/1/1
5	MAN	C	402	1	-	2/2/19/22	0/1/1/1
8	NAG	E	403	1	-	2/6/23/26	0/1/1/1
5	MAN	D	402	1	-	0/2/19/22	0/1/1/1
8	NAG	C	403	1	-	0/6/23/26	0/1/1/1
5	MAN	B	402	1	-	2/2/19/22	0/1/1/1
7	GOL	E	408	-	-	2/4/4/4	-
7	GOL	A	405	-	-	4/4/4/4	-
5	MAN	A	401	1	-	2/2/19/22	0/1/1/1
5	MAN	C	401	1	-	2/2/19/22	0/1/1/1
5	MAN	F	401	1	-	1/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	MAN	O5-C1	-2.25	1.39	1.43
8	F	402	NAG	O5-C1	-2.23	1.39	1.43
5	D	401	MAN	O5-C1	-2.23	1.39	1.43
5	C	402	MAN	O5-C1	-2.16	1.40	1.43
8	F	402	NAG	C3-C2	2.15	1.57	1.52
5	D	402	MAN	O2-C2	-2.07	1.39	1.43
5	B	401	MAN	O5-C1	-2.06	1.40	1.43
8	F	402	NAG	C2-N2	-2.06	1.42	1.46
5	D	402	MAN	O5-C1	-2.03	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	402	NAG	C2-N2-C7	-5.59	115.41	122.90
7	D	405	GOL	C3-C2-C1	4.46	128.16	111.80
8	F	402	NAG	C8-C7-N2	3.36	121.69	116.12
8	F	402	NAG	O7-C7-C8	-2.93	116.84	122.05
5	C	401	MAN	C1-C2-C3	2.83	113.77	109.64
7	D	405	GOL	O2-C2-C1	-2.80	97.57	109.18
5	A	401	MAN	C1-C2-C3	2.77	113.68	109.64
8	F	402	NAG	O5-C1-C2	-2.70	107.11	111.29
8	F	402	NAG	O3-C3-C2	2.57	114.74	109.40
5	E	402	MAN	O5-C5-C6	2.50	112.53	107.66
5	B	402	MAN	C1-C2-C3	2.33	113.03	109.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	MAN	C2-C3-C4	-2.28	106.86	110.86
8	F	402	NAG	O3-C3-C4	-2.15	105.31	110.38
7	D	405	GOL	O3-C3-C2	2.03	119.51	110.38

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	405	GOL	O1-C1-C2-O2
7	A	405	GOL	O1-C1-C2-C3
7	A	405	GOL	C1-C2-C3-O3
7	E	408	GOL	C1-C2-C3-O3
5	B	402	MAN	O5-C5-C6-O6
5	A	401	MAN	O5-C5-C6-O6
5	E	402	MAN	O5-C5-C6-O6
5	B	402	MAN	C4-C5-C6-O6
5	E	402	MAN	C4-C5-C6-O6
5	D	401	MAN	O5-C5-C6-O6
5	A	401	MAN	C4-C5-C6-O6
5	B	401	MAN	O5-C5-C6-O6
8	F	402	NAG	C8-C7-N2-C2
8	F	402	NAG	O7-C7-N2-C2
7	E	408	GOL	O2-C2-C3-O3
5	C	401	MAN	O5-C5-C6-O6
5	C	402	MAN	O5-C5-C6-O6
5	D	401	MAN	C4-C5-C6-O6
5	C	402	MAN	C4-C5-C6-O6
5	B	401	MAN	C4-C5-C6-O6
7	A	405	GOL	O2-C2-C3-O3
8	E	403	NAG	C8-C7-N2-C2
7	D	405	GOL	O2-C2-C3-O3
8	E	403	NAG	O7-C7-N2-C2
5	C	401	MAN	C4-C5-C6-O6
7	D	405	GOL	C1-C2-C3-O3
7	F	405	GOL	O2-C2-C3-O3
8	F	402	NAG	C3-C2-N2-C7
8	F	402	NAG	C1-C2-N2-C7
5	F	401	MAN	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	402	NAG	4	0
7	B	405	GOL	6	0
7	F	405	GOL	5	0
7	D	405	GOL	6	1
7	E	408	GOL	8	0
7	A	405	GOL	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	336/336 (100%)	0.10	9 (2%) 56 60	14, 22, 34, 50	0
1	B	336/336 (100%)	0.36	14 (4%) 40 45	15, 25, 42, 66	0
1	C	336/336 (100%)	-0.06	3 (0%) 81 83	13, 21, 33, 54	0
1	D	336/336 (100%)	0.09	6 (1%) 67 72	15, 22, 34, 52	0
1	E	336/336 (100%)	-0.01	3 (0%) 81 83	13, 21, 33, 63	0
1	F	336/336 (100%)	0.11	11 (3%) 49 53	14, 22, 35, 60	0
All	All	2016/2016 (100%)	0.10	46 (2%) 61 65	13, 22, 35, 66	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	34	THR	6.0
1	E	33	SER	5.5
1	F	33	SER	5.0
1	B	33	SER	4.2
1	E	34	THR	4.2
1	C	33	SER	3.7
1	F	100	LYS	3.6
1	D	327	ASP	3.4
1	C	337	ASP	3.1
1	B	34	THR	3.1
1	B	35	CYS	3.0
1	F	297	TYR	3.0
1	D	33	SER	2.9
1	D	34	THR	2.7
1	A	33	SER	2.7
1	A	299	ASN	2.6
1	B	54	VAL	2.6
1	F	139	ASP	2.5
1	B	41	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	126	ASN	2.5
1	D	139	ASP	2.5
1	B	47	ILE	2.5
1	A	297	TYR	2.3
1	A	345	TRP	2.3
1	C	365	GLY	2.3
1	B	327	ASP	2.3
1	A	34	THR	2.3
1	B	37	PHE	2.3
1	F	300	GLY	2.3
1	B	52	ASP	2.2
1	B	240	ASP	2.2
1	E	345	TRP	2.2
1	A	365	GLY	2.2
1	B	36	THR	2.2
1	B	53	VAL	2.1
1	F	299	ASN	2.1
1	B	48	SER	2.1
1	D	240	ASP	2.1
1	F	73	ASP	2.1
1	F	365	GLY	2.1
1	A	327	ASP	2.1
1	F	101	ASP	2.1
1	A	337	ASP	2.0
1	F	240	ASP	2.0
1	A	73	ASP	2.0
1	B	43	ALA	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.

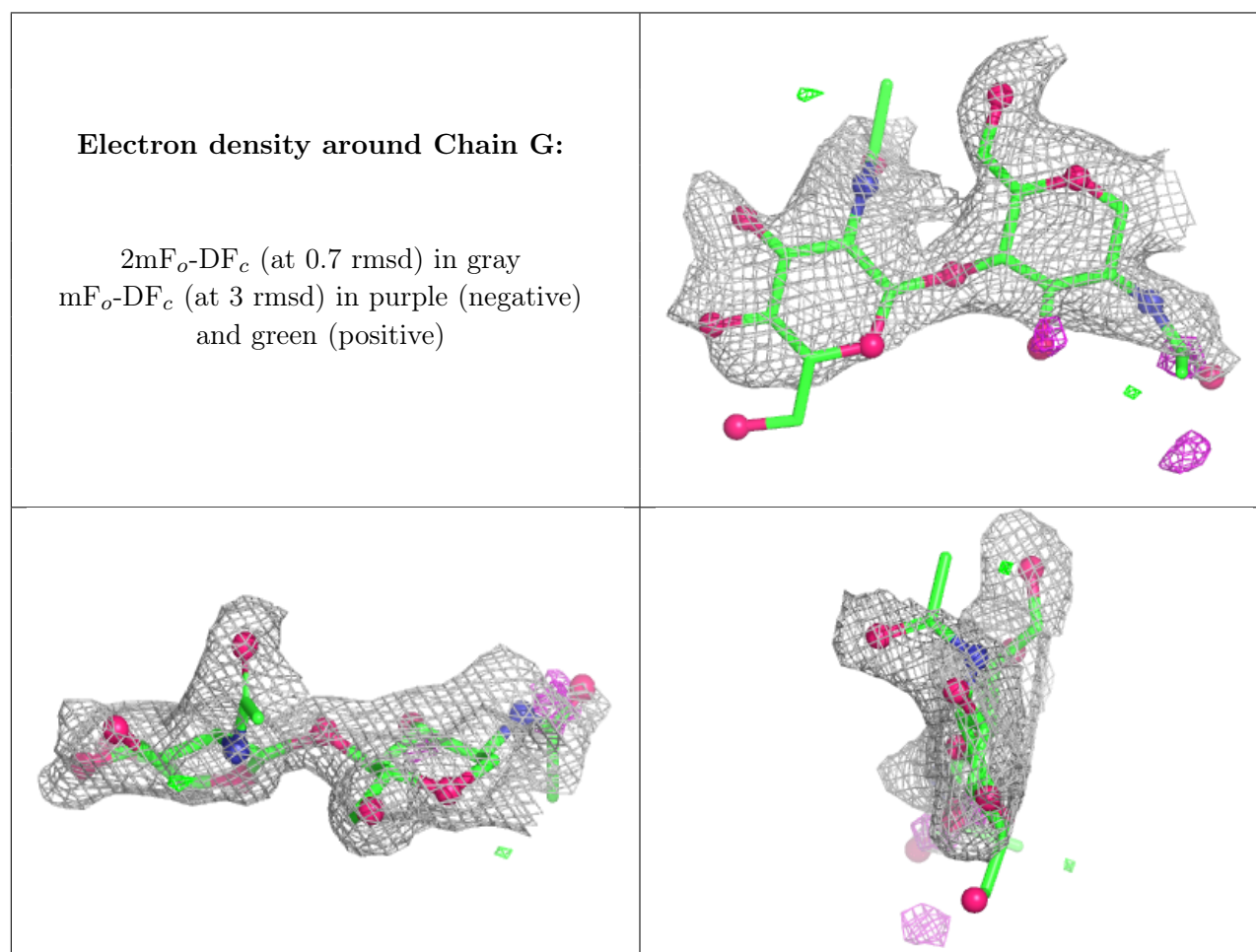
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	H	6	11/12	0.35	0.19	69,70,71,71	0

Continued on next page...

Continued from previous page...

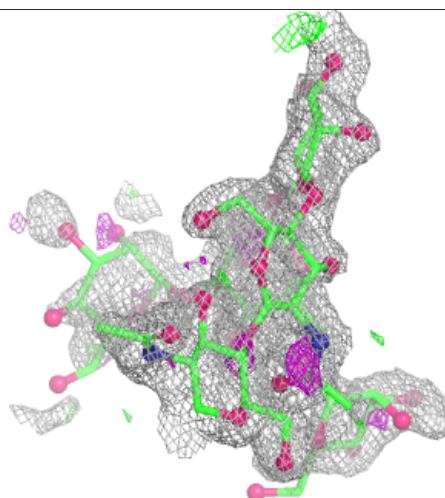
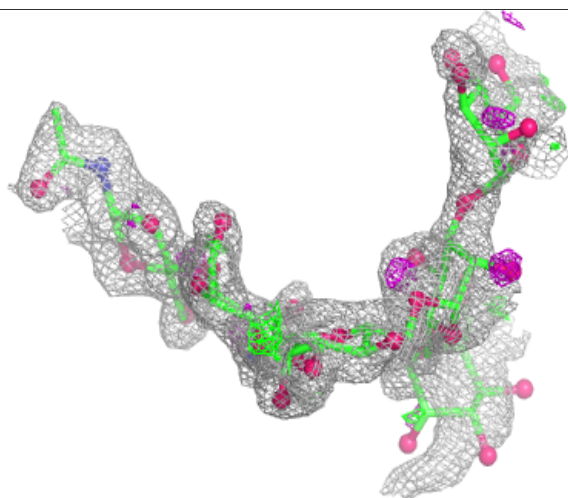
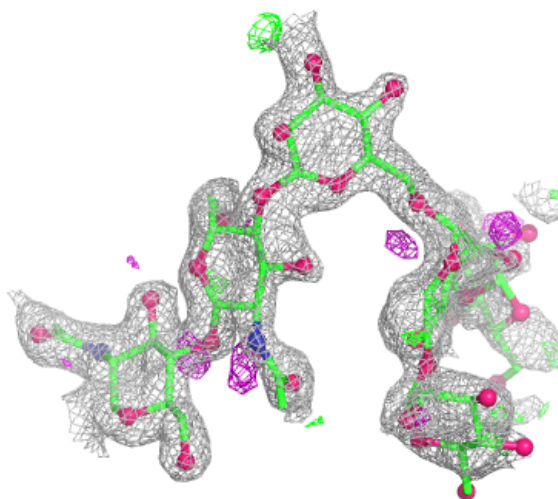
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	H	5	11/12	0.37	0.20	63,65,66,67	0
4	MAN	I	3	11/12	0.56	0.18	50,51,52,52	0
4	NAG	I	2	14/15	0.59	0.16	46,53,55,57	0
3	MAN	H	4	11/12	0.66	0.15	58,59,60,62	0
2	NAG	G	2	14/15	0.67	0.16	65,65,68,69	0
3	NAG	H	2	14/15	0.68	0.15	46,48,50,50	0
2	NAG	G	1	14/15	0.71	0.17	40,46,50,50	0
3	BMA	H	3	11/12	0.75	0.12	48,49,50,50	0
4	NAG	I	1	14/15	0.78	0.13	30,37,40,42	0
3	NAG	H	1	14/15	0.87	0.12	27,33,37,39	0

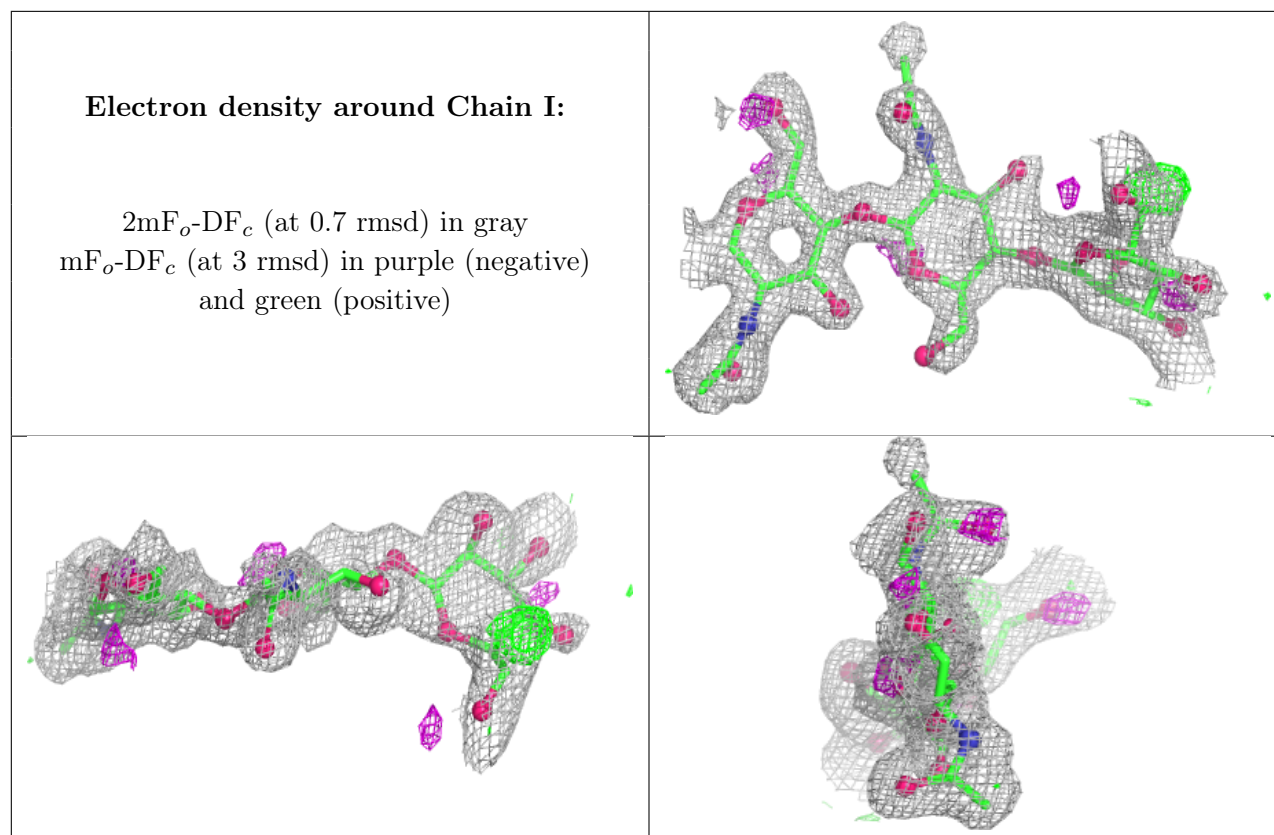
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain H:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
7	GOL	E	408	6/6	0.52	0.21	53,54,54,55	0
5	MAN	B	402	11/12	0.64	0.15	50,51,52,52	0
7	GOL	B	405	6/6	0.65	0.21	44,45,48,48	0
7	GOL	D	405	6/6	0.67	0.22	37,39,44,46	0
8	NAG	F	402	14/15	0.69	0.16	38,42,50,52	0
8	NAG	E	403	14/15	0.72	0.14	47,49,53,55	0
8	NAG	C	403	14/15	0.73	0.14	44,46,49,50	0
5	MAN	D	401	11/12	0.74	0.14	43,45,47,48	0
5	MAN	B	401	11/12	0.75	0.14	57,58,59,61	0
7	GOL	A	405	6/6	0.76	0.18	41,44,44,46	0
7	GOL	F	405	6/6	0.77	0.19	34,44,46,50	0
5	MAN	C	401	11/12	0.77	0.13	38,41,45,46	0
6	SO4	C	406	5/5	0.78	0.14	34,35,39,43	0
6	SO4	E	406	5/5	0.81	0.12	34,37,38,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	A	401	11/12	0.82	0.11	42,45,48,51	0
5	MAN	A	402	11/12	0.84	0.12	33,36,39,40	0
5	MAN	E	401	11/12	0.84	0.11	36,39,42,43	0
5	MAN	E	402	11/12	0.85	0.11	36,40,43,47	0
5	MAN	F	401	11/12	0.86	0.10	33,35,37,38	0
5	MAN	C	402	11/12	0.88	0.10	32,37,40,42	0
6	SO4	D	404	5/5	0.89	0.10	36,37,39,40	0
6	SO4	B	403	5/5	0.89	0.10	48,51,52,52	0
5	MAN	D	402	11/12	0.90	0.09	23,27,31,31	0
6	SO4	A	404	5/5	0.91	0.13	30,35,37,39	0
6	SO4	B	404	5/5	0.92	0.09	35,35,37,39	0
6	SO4	F	404	5/5	0.92	0.13	30,30,36,37	0
6	SO4	D	403	5/5	0.97	0.09	28,30,31,33	0
6	SO4	E	407	5/5	0.97	0.08	28,29,31,34	0
6	SO4	F	403	5/5	0.97	0.11	29,30,32,33	0
6	SO4	C	407	5/5	0.97	0.07	26,29,32,32	0
6	SO4	A	403	5/5	0.98	0.07	26,26,27,32	0
6	SO4	C	404	5/5	0.98	0.06	24,25,25,26	0
6	SO4	E	404	5/5	0.98	0.07	22,24,26,28	0
6	SO4	C	405	5/5	0.99	0.04	15,16,17,18	0
6	SO4	E	405	5/5	0.99	0.03	16,16,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.