



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:27 PM BST

PDB ID : 5BQZ
Title : Crystal structure of hemagglutinin of A/Chicken/Guangdong/S1311/2010 (H6N6) in complex with human-like receptor LSTc
Authors : Ni, F.; Kondrashkina, E.; Wang, Q.
Deposited on : 2015-05-29
Resolution : 2.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

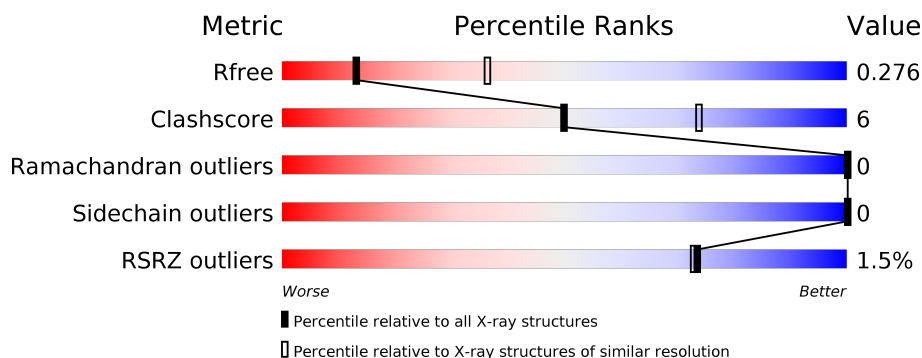
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

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




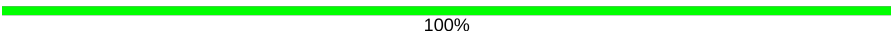


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	323	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>15%</div> </div> </div>
1	C	323	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>19%</div> </div> </div>
1	E	323	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>
2	B	191	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>11%</div> </div> </div>
2	D	191	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>9%</div> </div> </div>
2	F	191	<div> <div></div> <div> <div></div> <div>77%</div> <div>11%</div> <div>12%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	4	
4	H	2	
4	J	2	
5	I	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	SIA	G	4	X	-	-	-
6	NAG	E	401	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11950 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HEMAGGLUTININ HA1 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2548	1608	449	479	12			
1	C	323	Total	C	N	O	S	0	0	0
			2548	1608	449	479	12			
1	E	323	Total	C	N	O	S	0	0	0
			2548	1608	449	479	12			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1366	849	241	269	7			
2	D	173	Total	C	N	O	S	0	0	0
			1381	858	244	272	7			
2	F	169	Total	C	N	O	S	0	0	0
			1361	846	240	268	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	186	GLY	-	expression tag	UNP A0A067YZV9
B	187	ALA	-	expression tag	UNP A0A067YZV9
B	188	LEU	-	expression tag	UNP A0A067YZV9
B	189	VAL	-	expression tag	UNP A0A067YZV9
B	190	PRO	-	expression tag	UNP A0A067YZV9
B	191	ARG	-	expression tag	UNP A0A067YZV9
D	186	GLY	-	expression tag	UNP A0A067YZV9
D	187	ALA	-	expression tag	UNP A0A067YZV9
D	188	LEU	-	expression tag	UNP A0A067YZV9
D	189	VAL	-	expression tag	UNP A0A067YZV9
D	190	PRO	-	expression tag	UNP A0A067YZV9
D	191	ARG	-	expression tag	UNP A0A067YZV9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	186	GLY	-	expression tag	UNP A0A067YZV9
F	187	ALA	-	expression tag	UNP A0A067YZV9
F	188	LEU	-	expression tag	UNP A0A067YZV9
F	189	VAL	-	expression tag	UNP A0A067YZV9
F	190	PRO	-	expression tag	UNP A0A067YZV9
F	191	ARG	-	expression tag	UNP A0A067YZV9

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



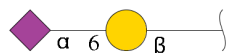
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	4	Total	C	N	O	0	0	0
			57	31	2	24			

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



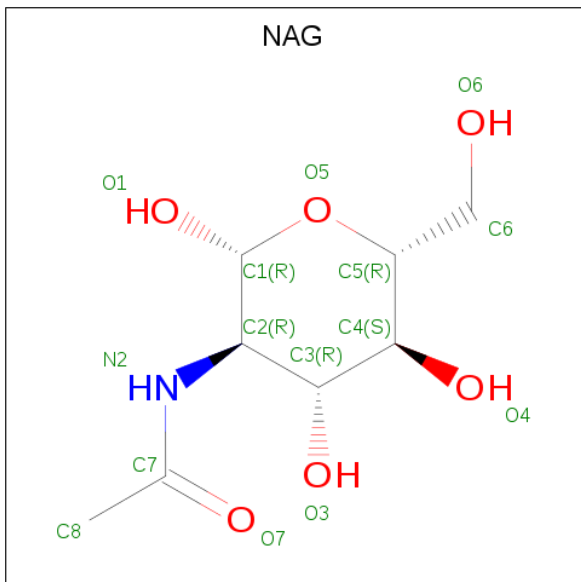
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			27	15	2	10			

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	2	Total	C	N	O	0	0	0
			31	17	1	13			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

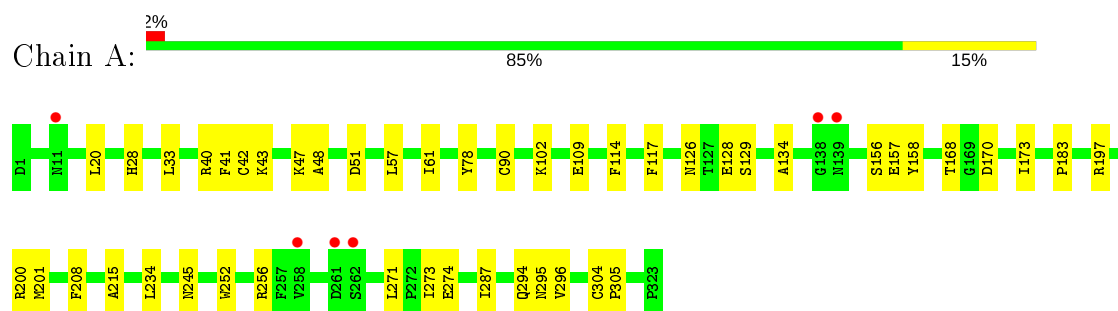


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			13	8	1	4		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		

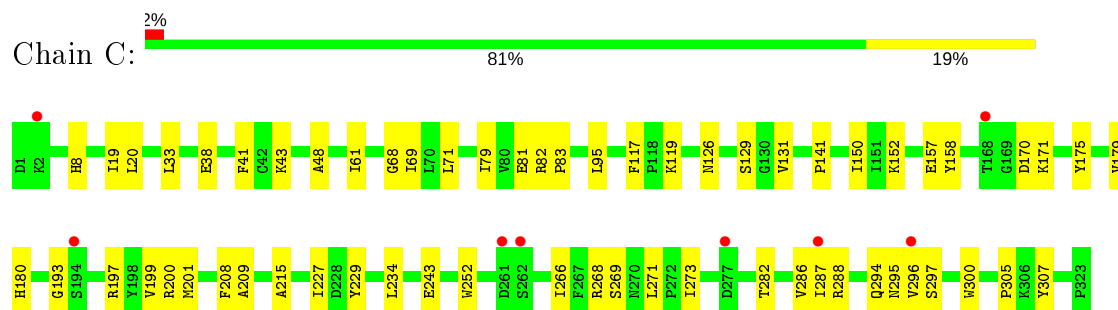
3 Residue-property plots [i](#)

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

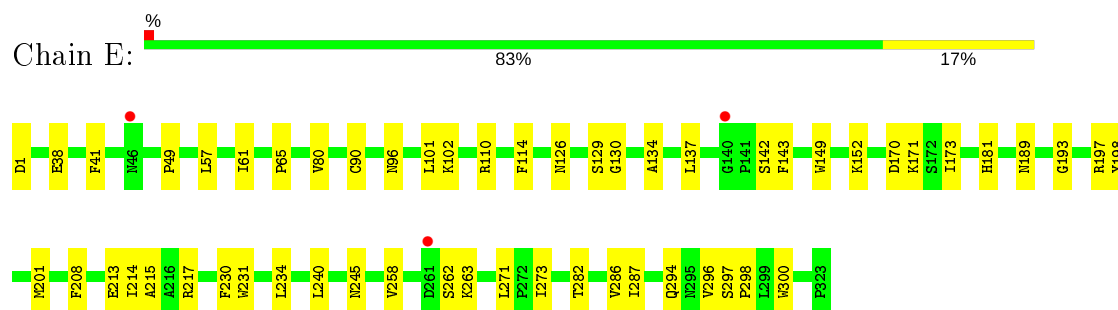
• Molecule 1: HEMAGGLUTININ HA1 CHAIN



• Molecule 1: HEMAGGLUTININ HA1 CHAIN

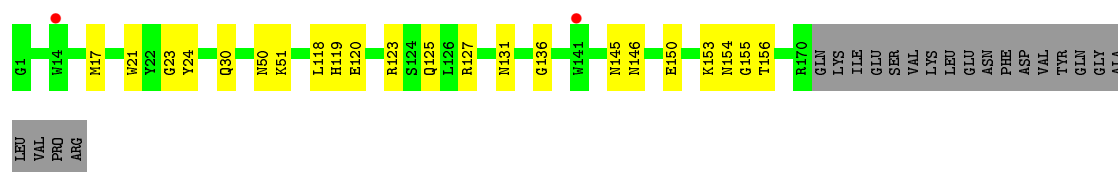


• Molecule 1: HEMAGGLUTININ HA1 CHAIN

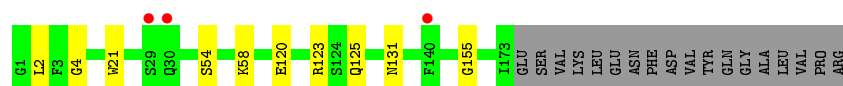
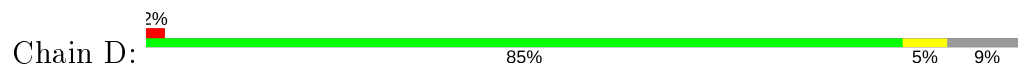


• Molecule 2: Hemagglutinin

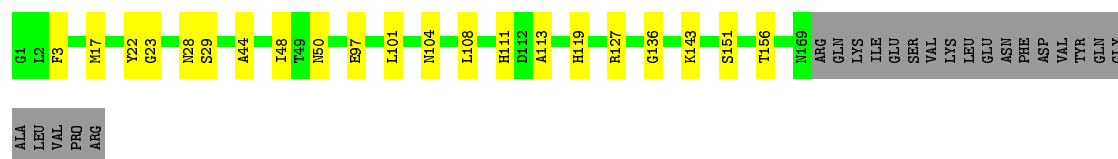




- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



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



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



- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.62Å 138.63Å 199.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.94 – 2.89 47.94 – 2.89	Depositor EDS
% Data completeness (in resolution range)	90.4 (47.94-2.89) 90.4 (47.94-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.274 0.232 , 0.276	Depositor DCC
R_{free} test set	1986 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11950	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: SIA, GAL, 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	0.26	0/2608	0.47	0/3541
1	C	0.29	0/2608	0.50	0/3541
1	E	0.26	0/2608	0.49	0/3541
2	B	0.24	0/1394	0.42	0/1878
2	D	0.23	0/1409	0.41	0/1899
2	F	0.24	0/1389	0.43	0/1871
All	All	0.26	0/12016	0.47	0/16271

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2548	0	2506	32	0
1	C	2548	0	2505	43	0
1	E	2548	0	2506	35	0
2	B	1366	0	1273	18	0
2	D	1381	0	1280	7	0
2	F	1361	0	1271	12	0
3	G	57	0	49	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	28	0	25	0	0
4	J	27	0	22	0	0
5	I	31	0	26	0	0
6	A	14	0	13	1	0
6	C	27	0	23	0	0
6	E	14	0	13	1	0
All	All	11950	0	11512	136	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (136) 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:C:294:GLN:NE2	1:C:297:SER:O	2.14	0.81
1:E:126:ASN:ND2	1:E:129:SER:OG	2.17	0.78
1:C:200:ARG:NH1	1:E:214:ILE:O	2.15	0.78
1:C:200:ARG:HD3	1:E:215:ALA:HA	1.67	0.77
1:E:170:ASP:OD2	1:E:171:LYS:NZ	2.19	0.76
1:C:201:MET:HB2	1:C:208:PHE:HB3	1.69	0.74
1:E:57:LEU:HD23	1:E:102:LYS:HG2	1.69	0.74
1:C:193:GLY:HA3	1:C:197:ARG:HH21	1.52	0.73
1:E:294:GLN:NE2	1:E:297:SER:O	2.21	0.72
1:C:282:THR:HG22	1:C:300:TRP:HB3	1.73	0.70
1:A:57:LEU:HD23	1:A:102:LYS:HG2	1.72	0.70
1:C:152:LYS:HD2	1:C:157:GLU:HA	1.72	0.69
1:E:152:LYS:NZ	1:E:189:ASN:O	2.20	0.69
1:C:294:GLN:HB3	1:C:305:PRO:HG2	1.76	0.67
1:C:180:HIS:HA	1:C:227:ILE:HG22	1.76	0.66
2:B:125:GLN:HE22	2:B:155:GLY:HA2	1.60	0.65
1:C:126:ASN:ND2	1:C:129:SER:OG	2.28	0.64
2:B:120:GLU:OE2	2:B:123:ARG:NH2	2.29	0.64
1:E:193:GLY:HA3	1:E:197:ARG:HH21	1.62	0.63
1:A:33:LEU:HD21	1:A:295:ASN:ND2	2.13	0.63
1:C:170:ASP:OD2	1:C:171:LYS:NZ	2.31	0.62
1:A:33:LEU:HD21	1:A:295:ASN:HD22	1.64	0.61
1:C:170:ASP:N	1:C:170:ASP:OD1	2.32	0.61
1:E:201:MET:HB2	1:E:208:PHE:HB3	1.83	0.60
1:A:201:MET:HB2	1:A:208:PHE:HB3	1.84	0.60
1:E:170:ASP:N	1:E:170:ASP:OD1	2.36	0.59
2:B:127:ARG:NH2	2:D:131:ASN:OD1	2.35	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:ASN:OD1	2:F:127:ARG:NH2	2.34	0.58
1:A:173:ILE:HB	1:A:234:LEU:HB3	1.86	0.58
2:D:2:LEU:HG	2:D:4:GLY:H	1.68	0.58
2:B:30:GLN:NE2	2:B:146:ASN:H	2.03	0.57
1:A:200:ARG:HD3	1:C:215:ALA:HB2	1.87	0.57
6:E:401:NAG:H3	6:E:401:NAG:H83	1.86	0.57
1:C:82:ARG:NH1	1:C:269:SER:O	2.36	0.56
2:B:119:HIS:CD2	2:B:136:GLY:HA2	2.40	0.56
1:A:294:GLN:HE22	1:A:304:CYS:HB3	1.71	0.56
1:E:282:THR:HG22	1:E:300:TRP:HB3	1.87	0.56
1:A:42:CYS:O	1:A:78:TYR:OH	2.18	0.55
1:C:33:LEU:HD21	1:C:295:ASN:HB2	1.87	0.55
1:A:117:PHE:O	1:A:252:TRP:HD1	1.90	0.55
1:A:170:ASP:OD1	1:A:170:ASP:N	2.39	0.55
1:A:51:ASP:HB2	1:A:273:ILE:HD12	1.89	0.55
1:C:209:ALA:HB3	1:E:213:GLU:HB3	1.89	0.54
1:A:168:THR:HG22	6:A:401:NAG:H2	1.90	0.54
1:A:197:ARG:NH1	1:A:245:ASN:O	2.41	0.54
1:A:126:ASN:ND2	1:A:129:SER:OG	2.39	0.54
1:A:156:SER:OG	1:A:157:GLU:N	2.40	0.54
1:A:41:PHE:CE2	1:A:271:LEU:HB2	2.44	0.53
2:D:125:GLN:HE22	2:D:155:GLY:C	2.11	0.53
2:B:30:GLN:HE22	2:B:146:ASN:H	1.56	0.53
2:F:29:SER:H	2:F:143:LYS:HZ1	1.56	0.52
1:E:80:VAL:HG21	1:E:273:ILE:HD11	1.91	0.52
1:E:198:TYR:N	1:E:245:ASN:OD1	2.32	0.52
1:C:43:LYS:HG2	1:C:48:ALA:HA	1.91	0.52
1:E:65:PRO:HB3	1:E:137:LEU:HD12	1.91	0.51
1:E:262:SER:OG	1:E:263:LYS:N	2.41	0.51
1:C:175:TYR:HE2	1:C:234:LEU:HB2	1.74	0.51
1:C:193:GLY:HA3	1:C:197:ARG:NH2	2.23	0.50
1:E:96:ASN:HD22	1:E:230:PHE:HE1	1.58	0.50
1:E:181:HIS:O	1:E:217:ARG:NH2	2.44	0.50
2:F:17:MET:SD	2:F:23:GLY:HA3	2.51	0.50
1:C:150:ILE:HG22	1:C:158:TYR:HE1	1.77	0.49
1:E:49:PRO:HG2	1:E:273:ILE:HD13	1.95	0.49
1:C:79:ILE:HB	1:C:266:ILE:HG12	1.95	0.48
1:A:47:LYS:NZ	1:A:109:GLU:OE2	2.45	0.48
1:E:173:ILE:HB	1:E:234:LEU:HB3	1.95	0.48
1:A:294:GLN:NE2	1:A:304:CYS:HB3	2.28	0.48
2:B:154:ASN:HB3	2:B:156:THR:HG22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:HB2	1:C:286:VAL:HB	1.96	0.47
1:E:130:GLY:HA3	1:E:149:TRP:HB3	1.96	0.47
1:A:40:ARG:NH1	1:A:274:GLU:OE1	2.47	0.47
1:A:157:GLU:HG2	1:A:158:TYR:N	2.29	0.47
1:C:179:VAL:HG12	1:C:199:VAL:HG21	1.96	0.47
1:E:110:ARG:O	1:E:258:VAL:HG12	2.13	0.47
1:A:20:LEU:C	2:F:50:ASN:HD22	2.17	0.47
1:E:114:PHE:CZ	1:E:173:ILE:HD12	2.50	0.47
1:A:157:GLU:HG2	1:A:158:TYR:H	1.79	0.46
1:A:294:GLN:HE21	1:A:305:PRO:HG2	1.80	0.46
1:C:82:ARG:HA	1:C:83:PRO:HD3	1.85	0.46
2:D:120:GLU:OE2	2:D:123:ARG:NH2	2.48	0.46
1:E:142:SER:OG	1:E:143:PHE:N	2.47	0.46
1:C:200:ARG:HB2	1:C:243:GLU:HB3	1.97	0.46
2:B:125:GLN:HE22	2:B:155:GLY:CA	2.27	0.46
1:C:95:LEU:HA	1:C:229:TYR:HB2	1.97	0.46
1:E:41:PHE:CE2	1:E:271:LEU:HB2	2.51	0.45
1:C:131:VAL:HG22	1:C:141:PRO:HB2	1.98	0.45
1:C:175:TYR:CE2	1:C:234:LEU:HB2	2.51	0.45
1:C:69:ILE:H	1:C:69:ILE:HD12	1.82	0.45
2:F:97:GLU:O	2:F:101:LEU:HD13	2.17	0.45
2:B:17:MET:SD	2:B:23:GLY:HA3	2.57	0.45
2:B:24:TYR:OH	2:B:118:LEU:HD11	2.17	0.45
1:E:90:CYS:HB2	1:E:134:ALA:O	2.17	0.45
1:C:294:GLN:HG2	1:C:307:TYR:HA	1.99	0.45
1:C:41:PHE:HB2	1:C:273:ILE:HG12	1.98	0.44
1:C:117:PHE:O	1:C:252:TRP:HD1	2.01	0.44
2:D:54:SER:O	2:D:58:LYS:HG2	2.18	0.43
1:E:101:LEU:HB2	1:E:231:TRP:CE2	2.53	0.43
1:E:297:SER:HA	1:E:298:PRO:HD3	1.89	0.43
1:C:287:ILE:HD11	1:C:296:VAL:CG2	2.48	0.43
1:C:68:GLY:HA2	1:C:71:LEU:HG	2.00	0.43
2:F:44:ALA:O	2:F:48:ILE:HG12	2.18	0.43
1:C:199:VAL:O	1:C:209:ALA:HA	2.18	0.43
2:F:3:PHE:CE2	2:F:113:ALA:HB2	2.53	0.43
1:C:61:ILE:H	1:C:61:ILE:HG13	1.59	0.42
2:F:151:SER:O	2:F:156:THR:N	2.50	0.42
1:E:38:GLU:HB2	1:E:286:VAL:HB	2.01	0.42
1:E:61:ILE:H	1:E:61:ILE:HG13	1.69	0.42
1:A:43:LYS:HG2	1:A:48:ALA:HA	2.01	0.42
1:C:41:PHE:CE2	1:C:271:LEU:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ILE:HD11	1:A:296:VAL:CG2	2.50	0.42
1:E:1:ASP:OD1	2:F:28:ASN:HA	2.20	0.42
2:B:50:ASN:HD22	1:C:20:LEU:C	2.22	0.41
1:A:287:ILE:HD11	1:A:296:VAL:HG21	2.01	0.41
2:B:146:ASN:O	2:B:150:GLU:HG2	2.20	0.41
2:B:51:LYS:HG3	1:C:19:ILE:HG13	2.03	0.41
1:A:128:GLU:N	1:A:128:GLU:OE1	2.53	0.41
1:A:183:PRO:HA	1:A:215:ALA:O	2.19	0.41
1:A:61:ILE:H	1:A:61:ILE:HG13	1.66	0.41
1:C:8:HIS:HB2	2:D:21:TRP:HA	2.03	0.41
1:E:201:MET:HE3	1:E:240:LEU:HD11	2.03	0.41
1:A:28:HIS:CE1	2:B:21:TRP:HE1	2.39	0.41
2:D:125:GLN:NE2	2:D:155:GLY:O	2.52	0.41
1:C:81:GLU:O	1:C:268:ARG:HA	2.20	0.41
1:E:193:GLY:HA3	1:E:197:ARG:NH2	2.32	0.41
1:E:65:PRO:HB3	1:E:137:LEU:HB2	2.03	0.41
1:A:114:PHE:CE2	1:A:256:ARG:HG3	2.55	0.41
2:B:24:TYR:CD2	2:B:153:LYS:HG2	2.56	0.41
2:B:30:GLN:NE2	2:B:145:ASN:HB2	2.36	0.41
2:B:30:GLN:HE22	2:B:145:ASN:HB2	1.86	0.41
1:E:287:ILE:HD11	1:E:296:VAL:CG2	2.51	0.41
1:C:38:GLU:CD	1:C:288:ARG:HE	2.24	0.41
2:F:104:ASN:O	2:F:108:LEU:HD13	2.21	0.40
2:F:119:HIS:CD2	2:F:136:GLY:HA2	2.56	0.40
1:A:90:CYS:HB2	1:A:134:ALA:O	2.22	0.40
1:C:119:LYS:HE3	1:C:252:TRP:CZ2	2.56	0.40
2:F:22:TYR:OH	2:F:111:HIS:ND1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/323 (99%)	306 (95%)	15 (5%)	0	100	100
1	C	321/323 (99%)	308 (96%)	13 (4%)	0	100	100
1	E	321/323 (99%)	307 (96%)	14 (4%)	0	100	100
2	B	168/191 (88%)	165 (98%)	3 (2%)	0	100	100
2	D	171/191 (90%)	168 (98%)	3 (2%)	0	100	100
2	F	167/191 (87%)	164 (98%)	3 (2%)	0	100	100
All	All	1469/1542 (95%)	1418 (96%)	51 (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	280/280 (100%)	280 (100%)	0	100	100
1	C	280/280 (100%)	280 (100%)	0	100	100
1	E	280/280 (100%)	280 (100%)	0	100	100
2	B	144/164 (88%)	144 (100%)	0	100	100
2	D	144/164 (88%)	144 (100%)	0	100	100
2	F	144/164 (88%)	144 (100%)	0	100	100
All	All	1272/1332 (96%)	1272 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	ASN
1	A	294	GLN
1	A	295	ASN
2	B	30	GLN
2	B	68	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	125	GLN
2	B	142	HIS
1	C	188	GLN
1	C	247	ASN
1	C	259	ASN
2	D	79	ASN
2	D	125	GLN
1	E	126	ASN
1	E	259	ASN
2	F	50	ASN
2	F	125	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 ⓘ

10 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	GAL	G	1	3	12,12,12	0.65	0	17,17,17	0.73	0
3	NAG	G	2	3	14,14,15	0.29	0	17,19,21	0.46	0
3	GAL	G	3	3	11,11,12	0.60	0	15,15,17	1.23	1 (6%)
3	SIA	G	4	3	17,20,21	1.23	3 (17%)	21,28,31	1.29	4 (19%)
4	NAG	H	1	2,4	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	H	2	4	14,14,15	0.29	0	17,19,21	0.56	0
5	GAL	I	1	5	11,11,12	0.61	0	15,15,17	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SIA	I	2	5	17,20,21	1.17	3 (17%)	21,28,31	1.23	3 (14%)
4	NAG	J	1	2,4	13,13,15	0.79	1 (7%)	14,17,21	0.82	0
4	NAG	J	2	4	14,14,15	0.34	0	17,19,21	0.46	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
3	GAL	G	1	3	-	0/2/22/22	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	GAL	G	3	3	-	0/2/19/22	0/1/1/1
3	SIA	G	4	3	1/1/8/9	8/14/34/38	0/1/1/1
4	NAG	H	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	3/6/23/26	0/1/1/1
5	GAL	I	1	5	-	0/2/19/22	0/1/1/1
5	SIA	I	2	5	-	4/14/34/38	0/1/1/1
4	NAG	J	1	2,4	-	2/5/22/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	NAG	C1-C2	2.44	1.56	1.52
3	G	4	SIA	C10-N5	2.42	1.42	1.34
5	I	2	SIA	C10-N5	2.32	1.42	1.34
3	G	4	SIA	C4-C5	-2.30	1.51	1.53
5	I	2	SIA	C5-N5	-2.13	1.42	1.45
3	G	4	SIA	C5-N5	-2.06	1.42	1.45
5	I	2	SIA	C4-C5	-2.05	1.51	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2	SIA	O6-C2-C3	-3.15	104.36	109.87
3	G	3	GAL	C1-O5-C5	2.68	115.82	112.19
3	G	4	SIA	C3-C4-C5	-2.66	108.24	111.46
5	I	2	SIA	C11-C10-N5	2.59	120.48	116.10
3	G	4	SIA	O6-C2-C3	-2.46	105.56	109.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4	SIA	C11-C10-N5	2.43	120.21	116.10
3	G	4	SIA	C9-C8-C7	-2.09	107.89	112.41
5	I	2	SIA	C9-C8-C7	-2.05	107.98	112.41

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	4	SIA	C2

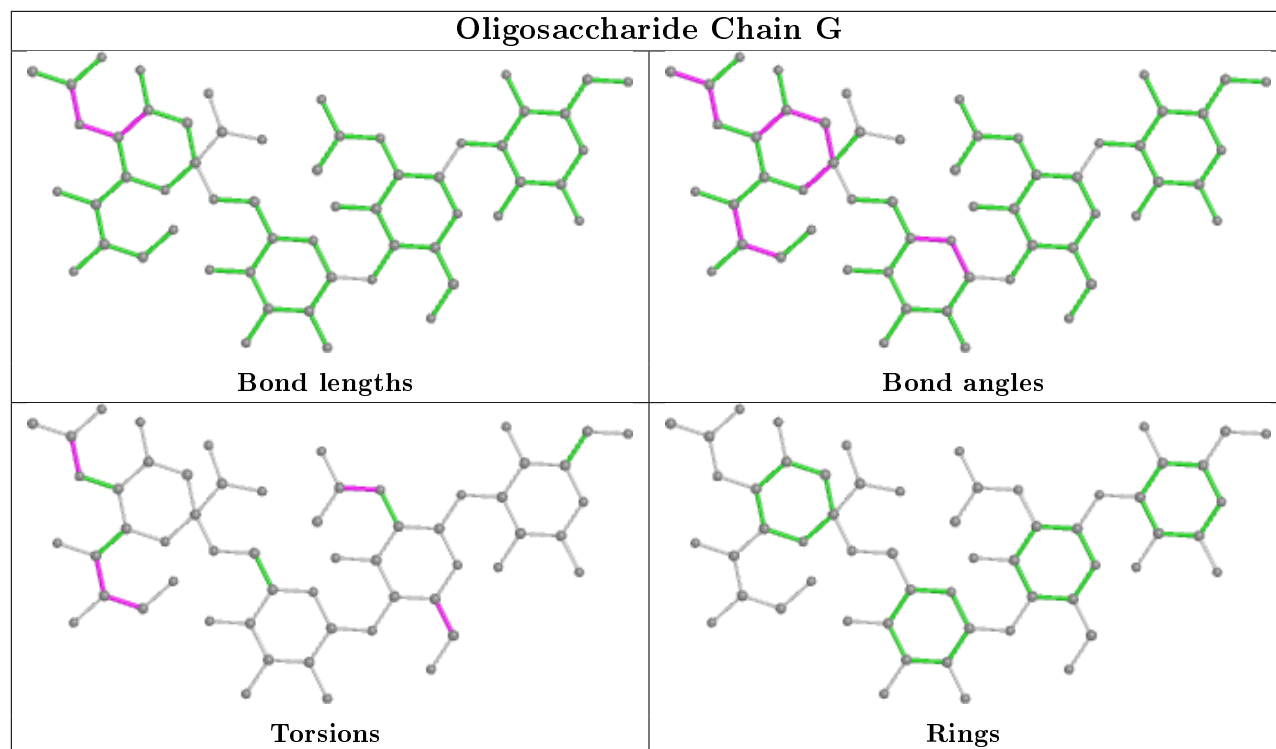
All (22) torsion outliers are listed below:

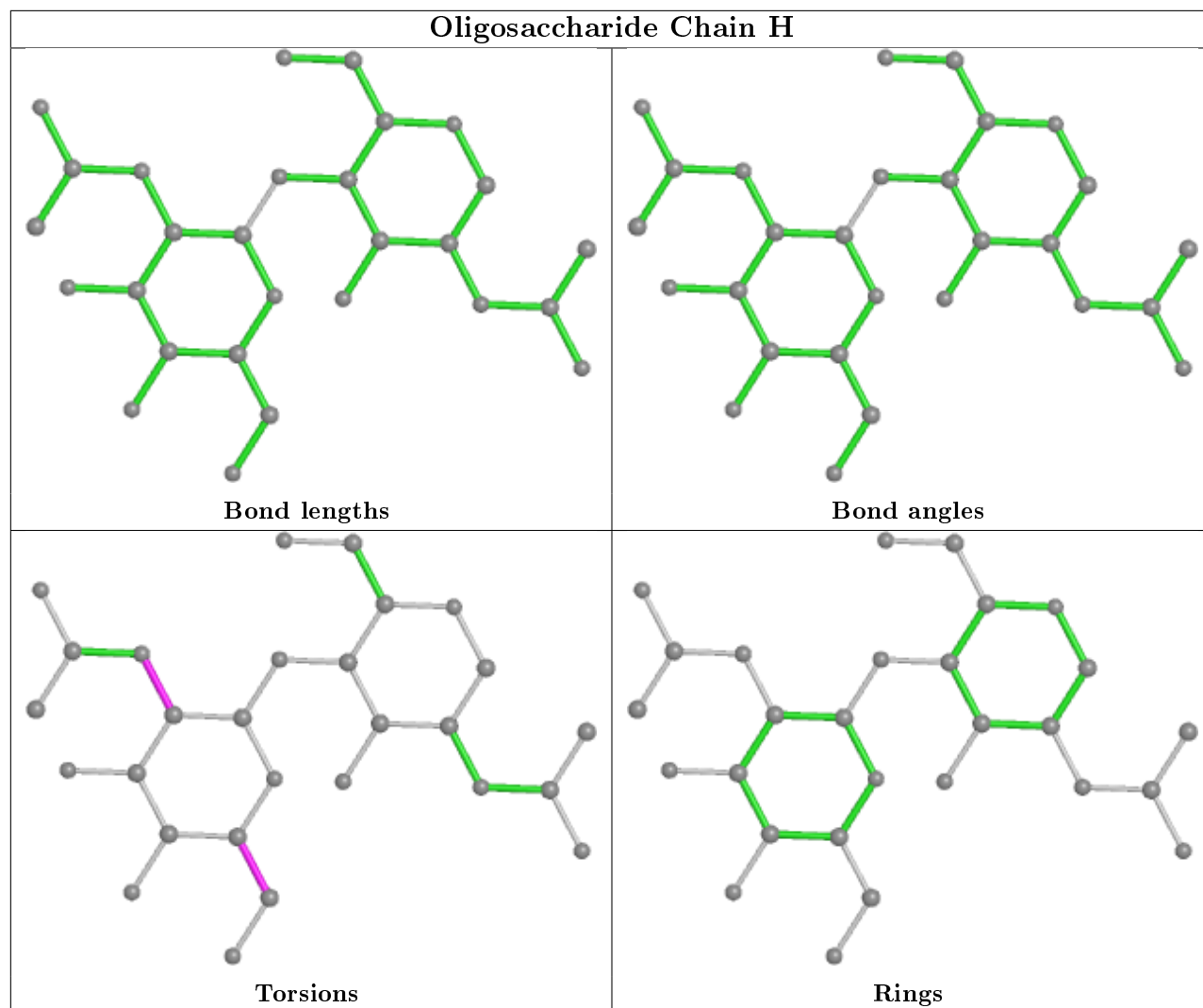
Mol	Chain	Res	Type	Atoms
3	G	4	SIA	C6-C7-C8-C9
3	G	4	SIA	O7-C7-C8-C9
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
3	G	4	SIA	O7-C7-C8-O8
3	G	4	SIA	C6-C7-C8-O8
4	J	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
5	I	2	SIA	C11-C10-N5-C5
5	I	2	SIA	O10-C10-N5-C5
3	G	4	SIA	C11-C10-N5-C5
3	G	4	SIA	O10-C10-N5-C5
4	J	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
5	I	2	SIA	O8-C8-C9-O9
3	G	4	SIA	O8-C8-C9-O9
5	I	2	SIA	C7-C8-C9-O9
3	G	4	SIA	C7-C8-C9-O9
4	H	2	NAG	C3-C2-N2-C7

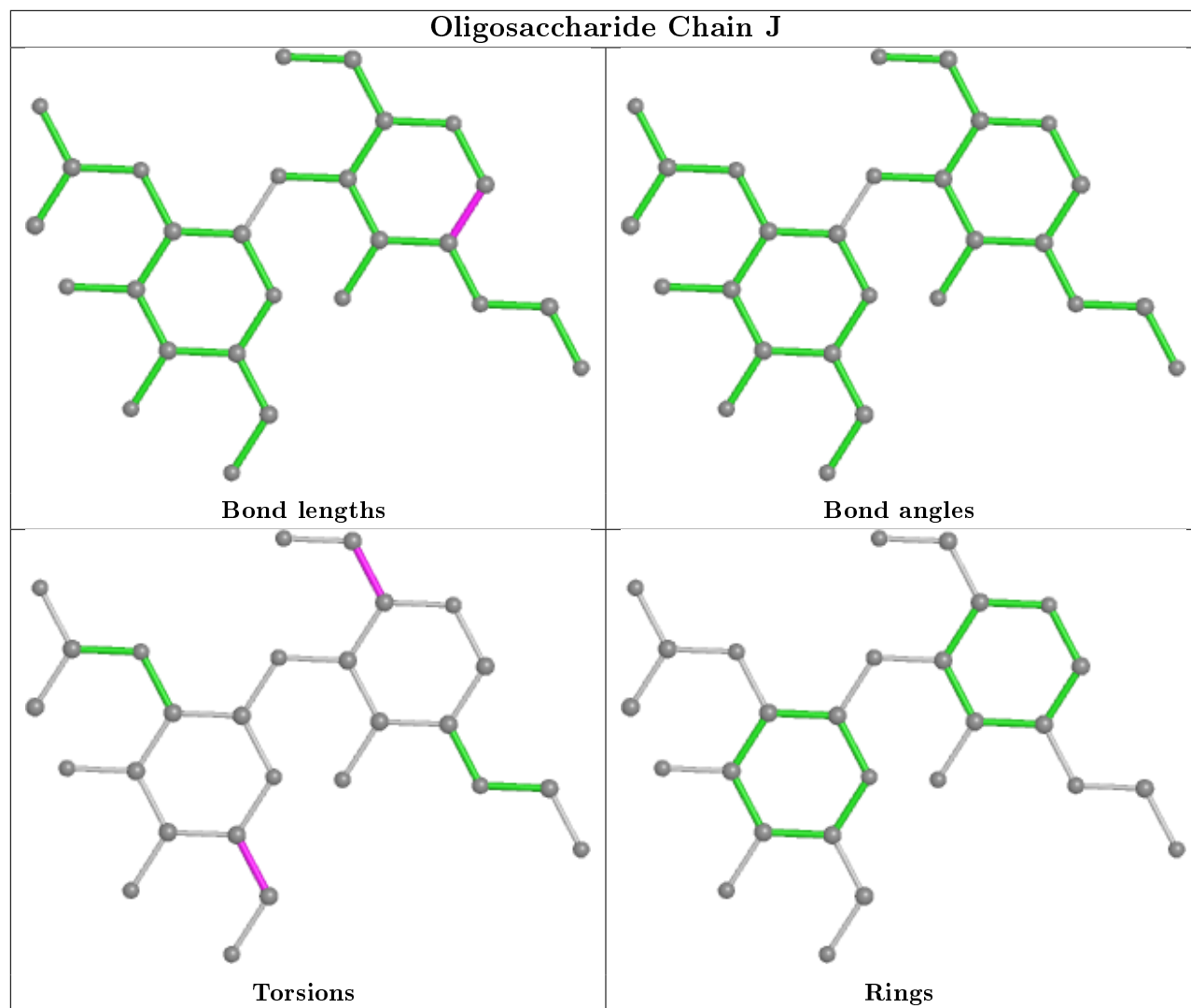
There are no ring outliers.

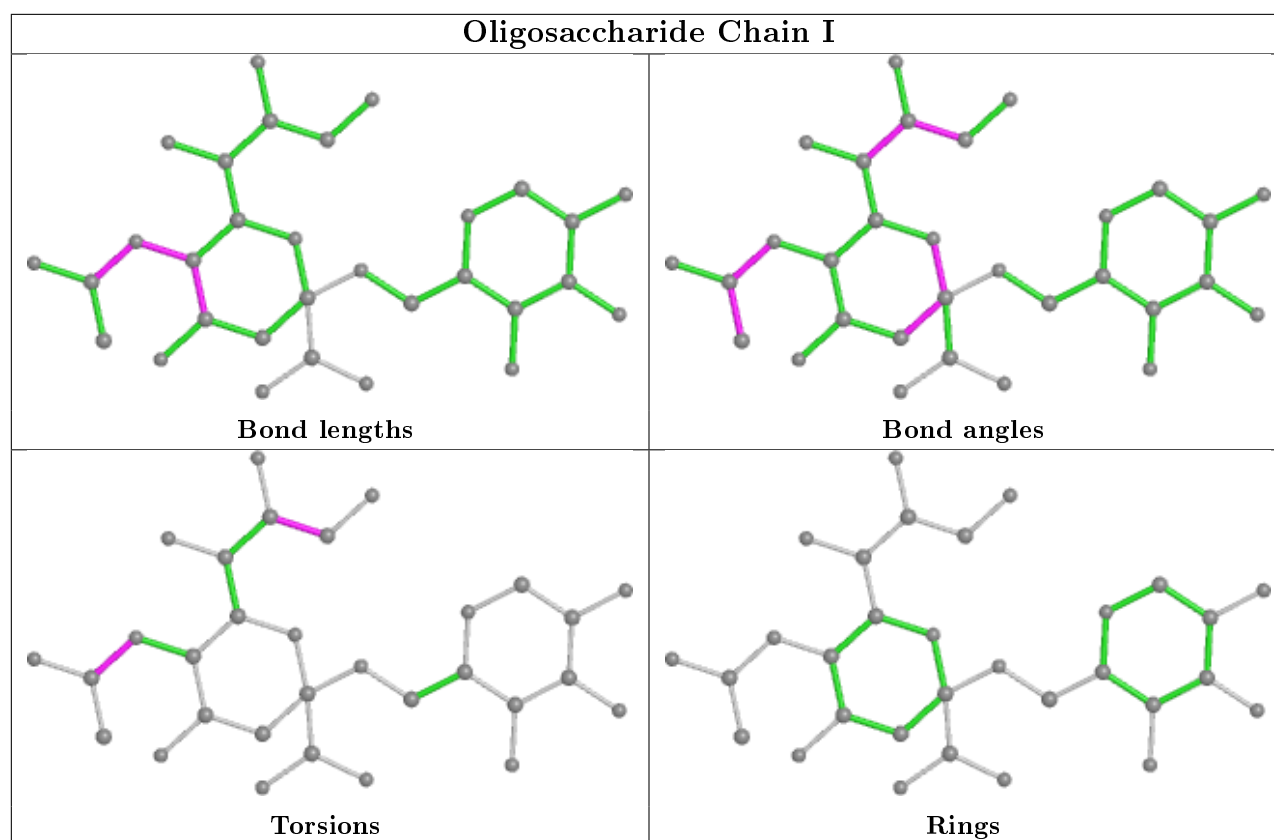
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	E	401	1	14,14,15	0.44	0	17,19,21	1.24	1 (5%)
6	NAG	C	402	1	13,13,15	0.32	0	16,18,21	0.36	0
6	NAG	C	401	1	14,14,15	0.40	0	17,19,21	0.87	1 (5%)
6	NAG	A	401	1	14,14,15	0.38	0	17,19,21	0.35	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
6	NAG	E	401	1	-	5/6/23/26	0/1/1/1
6	NAG	C	402	1	-	0/4/21/26	0/1/1/1
6	NAG	C	401	1	-	3/6/23/26	0/1/1/1
6	NAG	A	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	401	NAG	C2-N2-C7	4.26	128.98	122.90
6	C	401	NAG	C1-O5-C5	2.40	115.45	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	401	NAG	C4-C5-C6-O6
6	C	401	NAG	O5-C5-C6-O6
6	E	401	NAG	O5-C5-C6-O6
6	C	401	NAG	C4-C5-C6-O6
6	E	401	NAG	C8-C7-N2-C2
6	E	401	NAG	O7-C7-N2-C2
6	A	401	NAG	O5-C5-C6-O6
6	A	401	NAG	C4-C5-C6-O6
6	C	401	NAG	C1-C2-N2-C7
6	E	401	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	401	NAG	1	0
6	A	401	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	323/323 (100%)	0.03	6 (1%) 66 65	28, 41, 56, 84	0
1	C	323/323 (100%)	0.23	8 (2%) 57 55	27, 41, 58, 78	0
1	E	323/323 (100%)	0.19	3 (0%) 84 84	29, 45, 61, 77	0
2	B	170/191 (89%)	0.16	2 (1%) 79 79	27, 39, 68, 79	0
2	D	173/191 (90%)	0.07	3 (1%) 70 69	26, 42, 59, 70	0
2	F	169/191 (88%)	-0.08	0 100 100	27, 39, 53, 74	0
All	All	1481/1542 (96%)	0.12	22 (1%) 73 73	26, 42, 61, 84	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	46	ASN	3.3
2	D	29	SER	3.0
1	A	11	ASN	2.9
1	E	140	GLY	2.9
1	A	261	ASP	2.7
1	C	168	THR	2.6
1	A	138	GLY	2.6
1	A	262	SER	2.5
1	C	262	SER	2.5
1	C	296	VAL	2.5
1	A	139	ASN	2.4
1	C	261	ASP	2.3
1	C	194	SER	2.3
2	B	14	TRP	2.3
2	D	140	PHE	2.3
1	E	261	ASP	2.2
2	B	141	TRP	2.2
1	C	2	LYS	2.1
1	C	287	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	277	ASP	2.1
2	D	30	GLN	2.0
1	A	258	VAL	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](#)

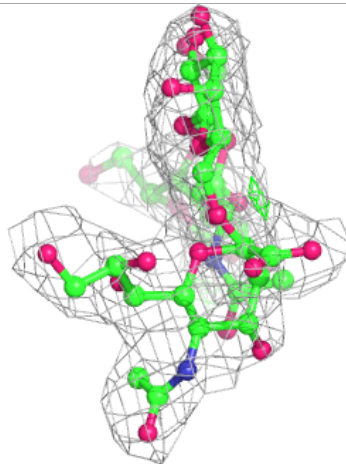
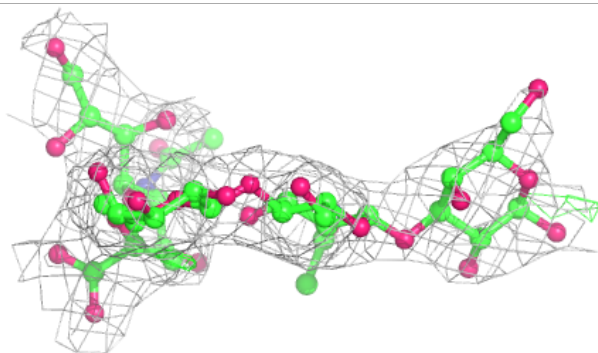
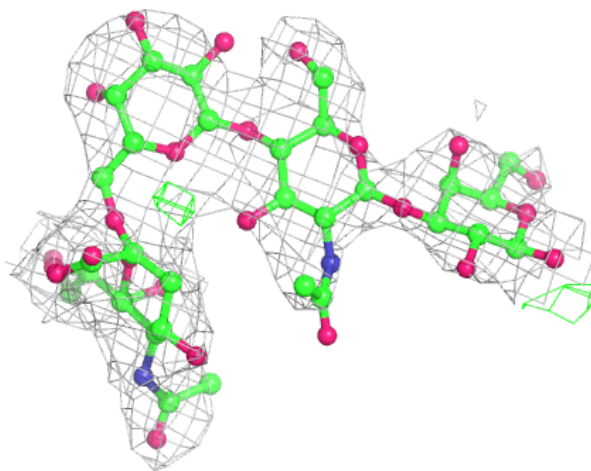
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	J	1	13/15	0.70	0.36	64,70,73,76	0
4	NAG	H	2	14/15	0.73	0.25	57,65,70,70	0
3	GAL	G	1	12/12	0.76	0.29	56,65,73,73	0
4	NAG	J	2	14/15	0.81	0.27	63,67,69,69	0
5	GAL	I	1	11/12	0.83	0.33	54,65,72,80	0
4	NAG	H	1	14/15	0.83	0.23	56,62,66,68	0
3	NAG	G	2	14/15	0.86	0.26	62,66,78,83	0
5	SIA	I	2	20/21	0.91	0.21	46,53,55,58	0
3	GAL	G	3	11/12	0.92	0.16	51,54,63,71	0
3	SIA	G	4	20/21	0.93	0.17	40,47,52,54	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.

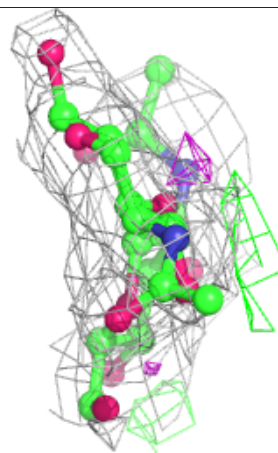
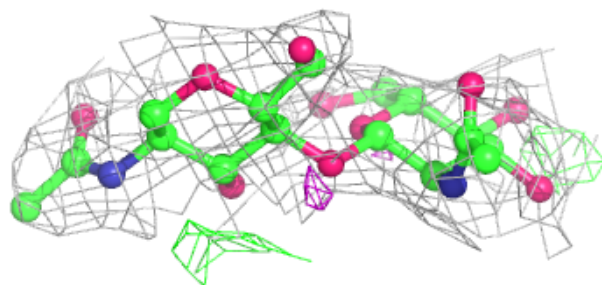
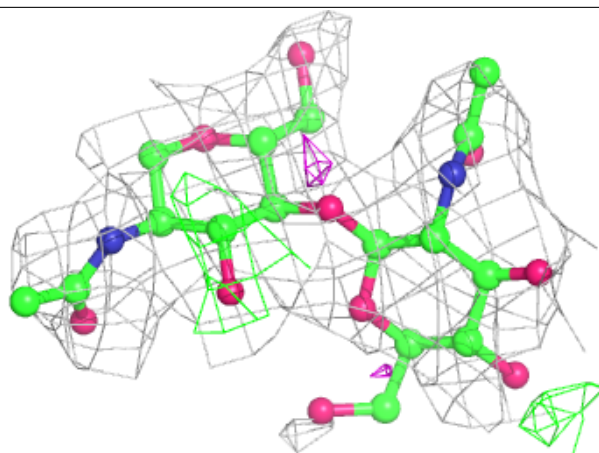
Electron density around Chain G:

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



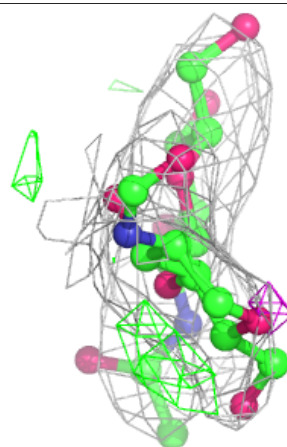
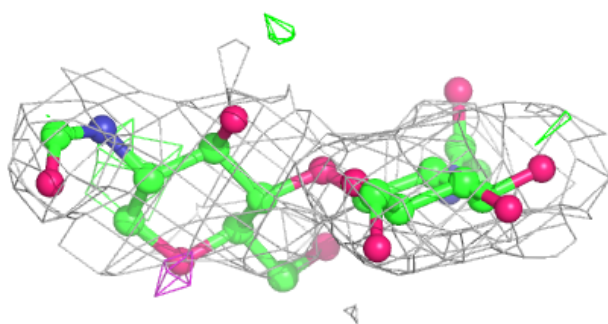
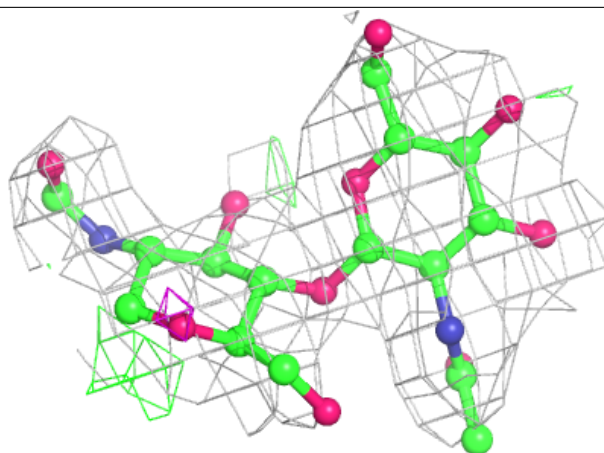
Electron density around Chain H:

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

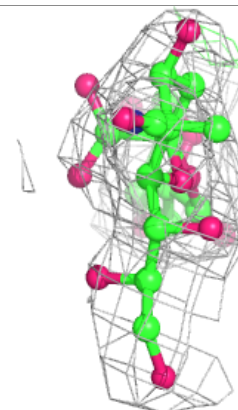
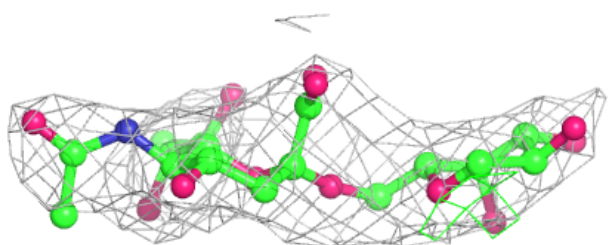
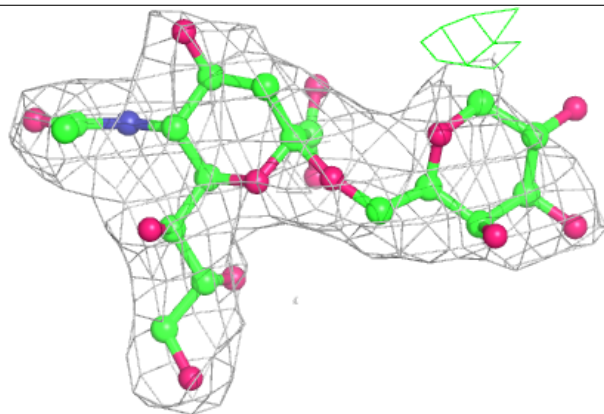


Electron density around Chain J:

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

**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)



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	E	401	14/15	0.78	0.43	63,77,86,87	0
6	NAG	A	401	14/15	0.78	0.36	59,65,70,75	0
6	NAG	C	401	14/15	0.79	0.30	65,70,78,82	0
6	NAG	C	402	13/15	0.86	0.40	52,60,66,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.