



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:02 AM UTC

PDB ID : 5E2Y / pdb_00005e2y
Title : Crystal structure of H5 hemagglutinin Q226L mutant from the influenza virus A/duck/Egypt/10185SS/2010 (H5N1)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2015-10-01
Resolution : 2.60 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

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Mol	Chain	Length	Quality of chain
2	F	180	9% 76% 19%
3	G	3	33% 67%
3	I	3	33% 67%
4	H	4	75% 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12273 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	323	Total	C	N	O	S	0	0	0
			2558	1611	443	490	14			
1	C	323	Total	C	N	O	S	0	0	0
			2558	1611	443	490	14			
1	E	323	Total	C	N	O	S	0	0	0
			2558	1611	443	490	14			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP G8IPF0
A	8	ASP	-	expression tag	UNP G8IPF0
A	9	PRO	-	expression tag	UNP G8IPF0
A	10	GLY	-	expression tag	UNP G8IPF0
A	226	LEU	GLN	engineered mutation	UNP G8IPF0
C	7	ALA	-	expression tag	UNP G8IPF0
C	8	ASP	-	expression tag	UNP G8IPF0
C	9	PRO	-	expression tag	UNP G8IPF0
C	10	GLY	-	expression tag	UNP G8IPF0
C	226	LEU	GLN	engineered mutation	UNP G8IPF0
E	7	ALA	-	expression tag	UNP G8IPF0
E	8	ASP	-	expression tag	UNP G8IPF0
E	9	PRO	-	expression tag	UNP G8IPF0
E	10	GLY	-	expression tag	UNP G8IPF0
E	226	LEU	GLN	engineered mutation	UNP G8IPF0

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1418	880	248	282	8			

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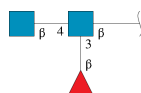
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	175	Total	C	N	O	S	0	0	0
			1418	880	248	282	8			
2	F	175	Total	C	N	O	S	0	0	0
			1418	880	248	282	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP G8IPF0
B	176	ARG	-	expression tag	UNP G8IPF0
B	177	LEU	-	expression tag	UNP G8IPF0
B	178	VAL	-	expression tag	UNP G8IPF0
B	179	PRO	-	expression tag	UNP G8IPF0
B	180	ARG	-	expression tag	UNP G8IPF0
D	1	GLY	-	expression tag	UNP G8IPF0
D	176	ARG	-	expression tag	UNP G8IPF0
D	177	LEU	-	expression tag	UNP G8IPF0
D	178	VAL	-	expression tag	UNP G8IPF0
D	179	PRO	-	expression tag	UNP G8IPF0
D	180	ARG	-	expression tag	UNP G8IPF0
F	1	GLY	-	expression tag	UNP G8IPF0
F	176	ARG	-	expression tag	UNP G8IPF0
F	177	LEU	-	expression tag	UNP G8IPF0
F	178	VAL	-	expression tag	UNP G8IPF0
F	179	PRO	-	expression tag	UNP G8IPF0
F	180	ARG	-	expression tag	UNP G8IPF0

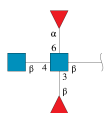
- Molecule 3 is an oligosaccharide called beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O		0	0	0
			38	22	2	14				
3	I	3	Total	C	N	O		0	0	0
			38	22	2	14				

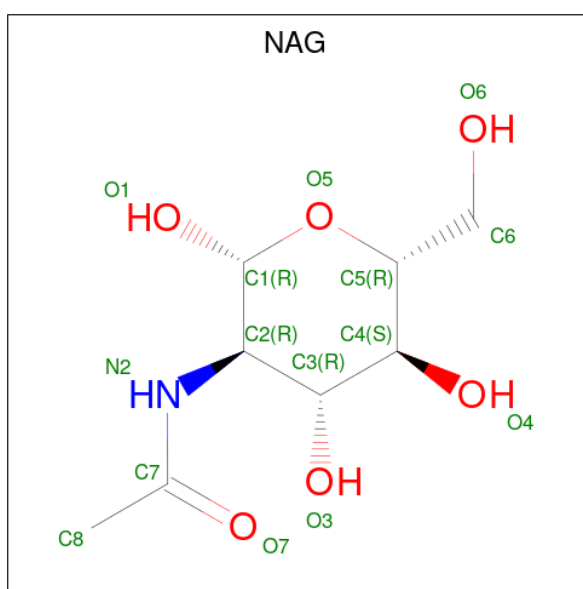
- Molecule 4 is an oligosaccharide called beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyra

nose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			48	28	2	18			

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		
6	B	5	Total	O	0	0
			5	5		

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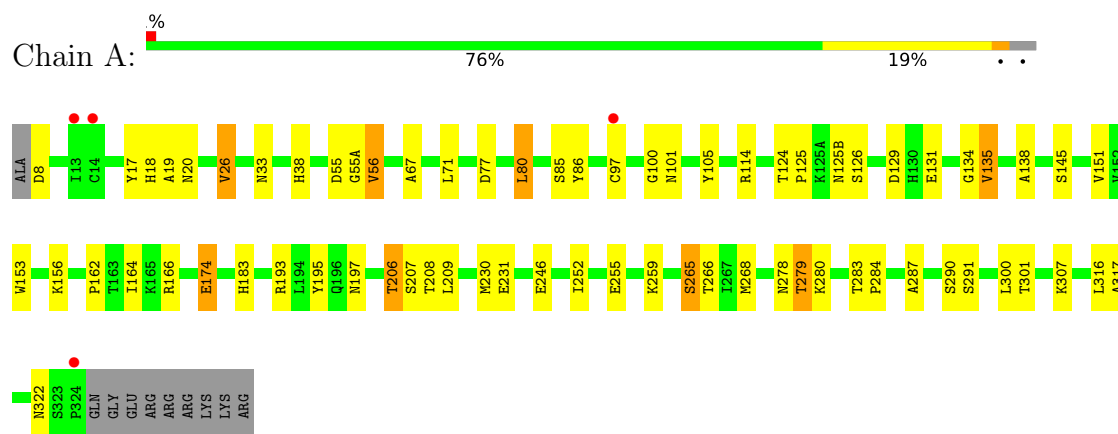
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	56	Total 56	O 56	0	0
6	D	9	Total 9	O 9	0	0
6	E	52	Total 52	O 52	0	0
6	F	10	Total 10	O 10	0	0

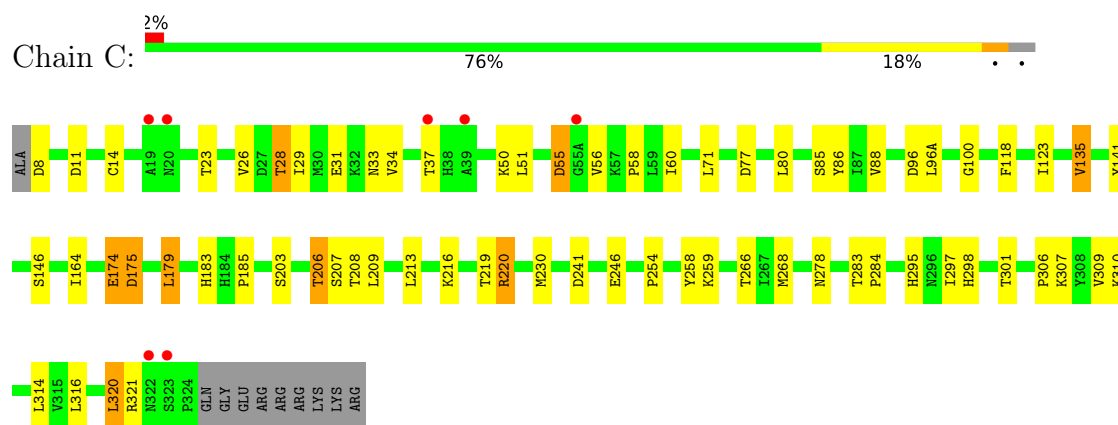
3 Residue-property plots [i](#)

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.

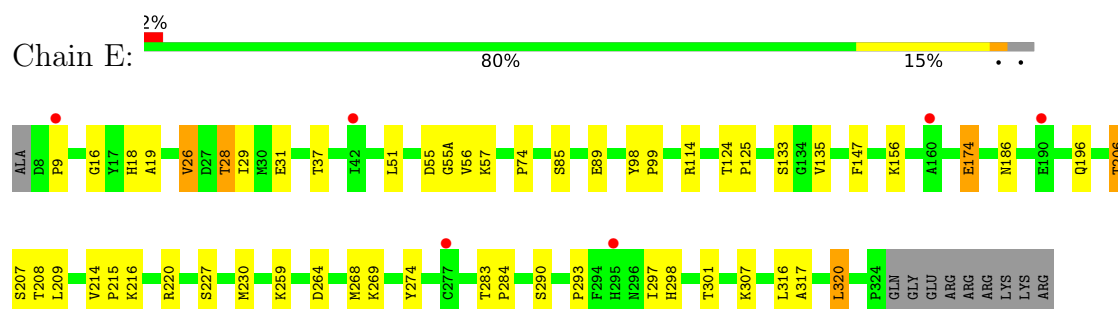
• Molecule 1: Hemagglutinin



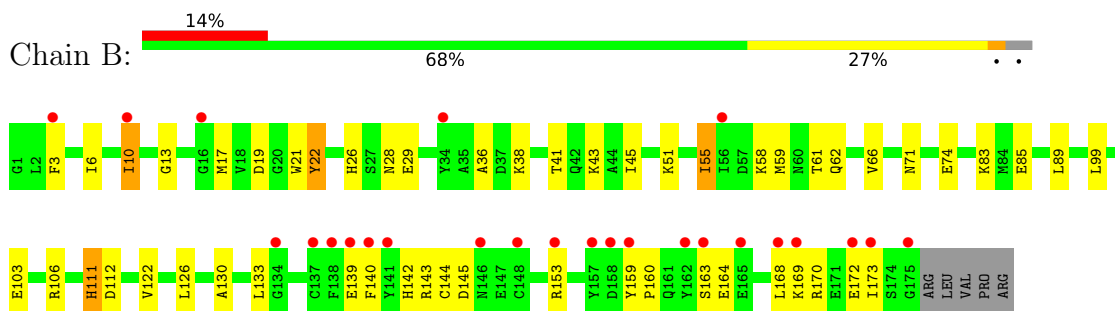
• Molecule 1: Hemagglutinin



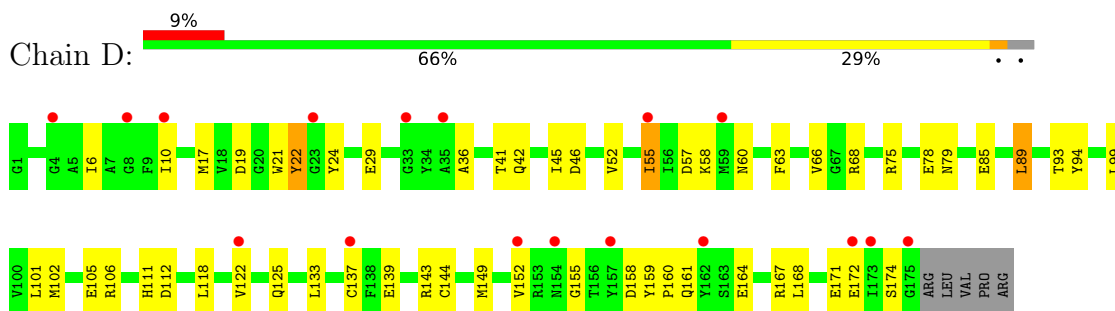
• Molecule 1: Hemagglutinin



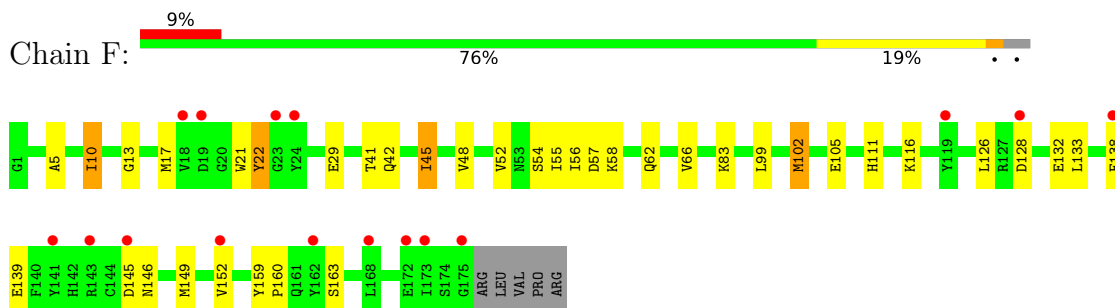
- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



- Molecule 3: beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain H:



MAG1
FUL2
MAG3
FUC4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.80Å 235.77Å 71.52Å 90.00° 114.37° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.9 (50.00-2.60) 87.2 (50.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.196 , 0.236 0.200 , 0.240	Depositor DCC
R_{free} test set	2922 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12273	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: NAG, FUC, FUL

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	0.66	0/2619	0.94	4/3559 (0.1%)
1	C	0.65	0/2619	0.96	5/3559 (0.1%)
1	E	0.63	0/2619	0.92	0/3559
2	B	0.53	0/1445	0.84	2/1942 (0.1%)
2	D	0.49	0/1445	0.81	0/1942
2	F	0.50	0/1445	0.80	0/1942
All	All	0.60	0/12192	0.90	11/16503 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	ASP	CA-C-N	7.27	128.93	119.84
1	C	8	ASP	C-N-CA	7.27	128.93	119.84
1	C	141	TYR	CA-C-N	-6.05	114.16	122.87
1	C	141	TYR	C-N-CA	-6.05	114.16	122.87
2	B	142	HIS	N-CA-C	5.83	115.94	108.24
1	A	265	SER	N-CA-C	-5.73	100.64	108.38
1	C	55	ASP	CB-CA-C	-5.72	109.97	116.54
1	A	56	VAL	N-CA-C	5.53	116.27	108.36
2	B	111	HIS	N-CA-C	5.42	116.99	111.14
1	A	8	ASP	CA-C-N	5.26	125.56	119.93
1	A	8	ASP	C-N-CA	5.26	125.56	119.93

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	2558	0	2493	44	0
1	C	2558	0	2493	42	0
1	E	2558	0	2493	39	0
2	B	1418	0	1322	43	0
2	D	1418	0	1322	43	0
2	F	1418	0	1322	27	0
3	G	38	0	34	0	0
3	I	38	0	34	0	0
4	H	48	0	43	1	0
5	A	14	0	13	1	0
5	C	14	0	13	1	0
5	E	14	0	13	0	0
6	A	47	0	0	1	0
6	B	5	0	0	0	0
6	C	56	0	0	1	0
6	D	9	0	0	0	0
6	E	52	0	0	0	0
6	F	10	0	0	0	0
All	All	12273	0	11595	210	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 9.

All (210) 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:A:206:THR:HG22	1:A:208:THR:H	1.33	0.94
1:E:174:GLU:HG3	1:E:259:LYS:HB3	1.58	0.85
2:B:168:LEU:O	2:B:172:GLU:HG3	1.79	0.83
1:E:307:LYS:HE2	2:F:62:GLN:HB3	1.59	0.82
1:E:55:ASP:OD1	1:E:55(A):GLY:N	2.15	0.79
1:E:206:THR:HG22	1:E:208:THR:H	1.49	0.78
1:A:307:LYS:HE2	2:B:62:GLN:HB3	1.65	0.76
1:A:174:GLU:HG3	1:A:259:LYS:HB3	1.68	0.75
1:C:55:ASP:O	1:C:278:ASN:ND2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:LYS:HE3	2:D:89:LEU:HD21	1.70	0.73
1:E:28:THR:HG22	1:E:31:GLU:H	1.55	0.72
2:B:169:LYS:HD2	2:B:172:GLU:OE1	1.89	0.71
1:C:206:THR:HG22	1:C:208:THR:H	1.54	0.71
1:C:310:LYS:HG3	2:D:89:LEU:HD11	1.71	0.71
2:D:75:ARG:NH1	2:D:78:GLU:OE1	2.23	0.71
1:A:268:MET:HE3	1:A:284:PRO:HA	1.73	0.70
2:B:133:LEU:HD11	2:B:139:GLU:HG2	1.74	0.69
1:A:283:THR:HG22	1:A:301:THR:HG22	1.76	0.67
2:D:171:GLU:HA	2:D:174:SER:HB2	1.76	0.67
1:E:89:GLU:OE1	1:E:269:LYS:NZ	2.27	0.66
2:F:5:ALA:HB2	2:F:116:LYS:HB2	1.77	0.66
1:A:206:THR:HB	1:A:209:LEU:HB3	1.77	0.66
2:D:168:LEU:O	2:D:172:GLU:HG3	1.95	0.66
2:B:59:MET:HE2	2:D:94:TYR:CE2	2.31	0.66
1:C:206:THR:HB	1:C:209:LEU:HB3	1.78	0.65
1:C:11:ASP:OD2	2:D:144:CYS:N	2.24	0.65
1:C:268:MET:HE3	1:C:284:PRO:HA	1.80	0.64
2:B:169:LYS:CD	2:B:172:GLU:OE1	2.45	0.63
2:D:106:ARG:NH2	2:F:105:GLU:HG2	2.13	0.63
1:E:268:MET:HE3	1:E:284:PRO:HA	1.80	0.62
1:C:295:HIS:CD2	1:C:306:PRO:HG2	2.34	0.62
1:E:293:PRO:HG3	2:F:56:ILE:HG12	1.80	0.62
1:A:77:ASP:HA	1:A:80:LEU:HD13	1.82	0.61
1:C:123:ILE:HD11	1:C:254:PRO:HB2	1.81	0.61
1:A:135:VAL:HG13	1:A:145:SER:HB3	1.84	0.60
2:B:106:ARG:NH2	2:D:105:GLU:HG2	2.17	0.60
1:C:175:ASP:N	1:C:175:ASP:OD1	2.34	0.60
2:F:133:LEU:HD11	2:F:139:GLU:HB2	1.84	0.59
2:F:145:ASP:CG	2:F:146:ASN:H	2.11	0.59
1:C:283:THR:HG22	1:C:301:THR:HG22	1.85	0.59
1:E:55:ASP:CG	1:E:55(A):GLY:H	2.11	0.57
1:C:28:THR:HG22	1:C:31:GLU:H	1.70	0.57
2:B:29:GLU:OE2	2:B:143:ARG:NH1	2.38	0.57
1:E:56:VAL:HB	1:E:85:SER:HB3	1.87	0.57
1:E:283:THR:HG22	1:E:301:THR:HG22	1.87	0.57
1:A:166:ARG:NH2	6:A:1102:HOH:O	2.28	0.57
1:E:186:ASN:HD21	1:E:227:SER:C	2.13	0.57
2:B:170:ARG:O	2:B:173:ILE:HG13	2.05	0.56
2:B:26:HIS:HD2	2:B:153:ARG:NH2	2.04	0.56
2:D:55:ILE:HD11	2:D:99:LEU:HG	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:THR:HB	1:E:209:LEU:HB3	1.86	0.56
1:A:156:LYS:NZ	1:A:193:ARG:O	2.39	0.56
1:A:26:VAL:HG11	1:A:317:ALA:HB2	1.88	0.55
1:E:29:ILE:HD11	2:F:102:MET:HA	1.87	0.55
1:E:98:TYR:CD1	1:E:99:PRO:HD2	2.42	0.55
1:C:58:PRO:HG2	1:C:60:ILE:HD11	1.88	0.54
2:D:6:ILE:HD13	2:D:112:ASP:HA	1.88	0.54
2:D:17:MET:HE1	2:D:22:TYR:C	2.33	0.54
1:E:283:THR:HG21	1:E:297:ILE:HD11	1.90	0.54
1:A:100:GLY:HA3	1:A:230:MET:O	2.08	0.54
2:B:21:TRP:H	2:B:41:THR:HG21	1.73	0.53
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.90	0.52
2:D:63:PHE:HZ	2:D:85:GLU:HG2	1.75	0.52
2:B:130:ALA:HA	2:B:140:PHE:HA	1.91	0.52
1:C:297:ILE:HG13	1:C:298:HIS:N	2.25	0.52
1:A:279:THR:HG21	1:A:287:ALA:HB1	1.91	0.52
1:C:316:LEU:HD23	2:D:52:VAL:HG22	1.92	0.52
2:B:28:ASN:ND2	2:B:144:CYS:O	2.37	0.52
2:D:57:ASP:O	2:D:60:ASN:ND2	2.42	0.52
1:A:284:PRO:HD3	1:A:300:LEU:O	2.10	0.52
2:B:26:HIS:HD2	2:B:153:ARG:HH22	1.57	0.51
2:F:17:MET:HE1	2:F:22:TYR:C	2.35	0.51
2:D:19:ASP:HB3	2:D:36:ALA:HB2	1.91	0.51
1:E:320:LEU:HB3	2:F:111:HIS:CG	2.45	0.51
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.92	0.50
1:C:71:LEU:HD23	1:C:179:LEU:HD23	1.93	0.50
2:D:63:PHE:CZ	2:D:85:GLU:HG2	2.46	0.50
1:A:38:HIS:CD2	2:B:21:TRP:HE1	2.29	0.50
2:D:29:GLU:OE2	2:D:143:ARG:NH1	2.44	0.50
1:E:9:PRO:HA	2:F:139:GLU:OE2	2.11	0.49
2:F:160:PRO:HA	2:F:163:SER:HB2	1.94	0.49
1:A:164:ILE:O	1:A:246:GLU:HA	2.11	0.49
1:C:295:HIS:HD2	1:C:306:PRO:HG2	1.77	0.49
2:B:55:ILE:HG13	2:B:99:LEU:HD23	1.93	0.49
2:D:58:LYS:HA	2:D:58:LYS:HD3	1.61	0.49
1:E:316:LEU:HD13	2:F:52:VAL:HG22	1.95	0.49
1:A:56:VAL:HB	1:A:85:SER:HB3	1.95	0.49
1:C:174:GLU:HG3	1:C:259:LYS:HB3	1.95	0.48
2:D:164:GLU:OE1	2:D:167:ARG:NH2	2.42	0.48
1:A:124:THR:HG22	1:A:255:GLU:HA	1.95	0.48
1:E:297:ILE:HG13	1:E:298:HIS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:VAL:HB	1:A:252:ILE:HG22	1.94	0.48
1:C:309:VAL:HG13	2:D:93:THR:HA	1.95	0.48
2:D:42:GLN:NE2	2:D:46:ASP:OD1	2.47	0.48
1:E:18:HIS:ND1	1:E:19:ALA:N	2.61	0.48
1:A:97:CYS:HB2	1:A:138:ALA:O	2.13	0.48
2:F:132:GLU:HG2	2:F:138:PHE:HE1	1.79	0.47
1:A:20:ASN:H	1:A:322:ASN:HD21	1.62	0.47
2:B:85:GLU:O	2:B:89:LEU:HG	2.15	0.47
1:E:114:ARG:NH1	1:E:264:ASP:OD1	2.48	0.47
1:A:195:TYR:O	1:A:197:ASN:N	2.46	0.47
2:F:55:ILE:HG23	2:F:99:LEU:HD23	1.96	0.47
1:C:96:ASP:CG	1:C:96(A):LEU:H	2.22	0.47
1:C:310:LYS:HE3	2:D:89:LEU:CD2	2.44	0.47
2:D:21:TRP:CZ3	2:D:111:HIS:HE1	2.32	0.47
1:E:19:ALA:HB2	2:F:13:GLY:HA3	1.97	0.47
2:B:51:LYS:O	2:B:55:ILE:HG22	2.14	0.47
1:C:216:LYS:O	1:C:220:ARG:NH2	2.47	0.46
2:B:106:ARG:HH22	2:D:105:GLU:HG2	1.79	0.46
2:B:140:PHE:CE2	2:B:144:CYS:HB2	2.50	0.46
1:C:283:THR:HG21	1:C:297:ILE:HD11	1.97	0.46
1:C:58:PRO:HB3	1:C:86:TYR:CE1	2.50	0.46
1:A:125:PRO:HG2	1:A:126:SER:HB3	1.97	0.46
2:B:51:LYS:HD3	2:B:103:GLU:HB3	1.98	0.46
2:D:17:MET:HE3	2:D:36:ALA:HA	1.98	0.46
1:A:101:ASN:OD1	1:A:231:GLU:HG3	2.16	0.46
1:A:33:ASN:HD21	5:A:1001:NAG:C1	2.28	0.46
1:E:26:VAL:HG11	1:E:317:ALA:HB2	1.98	0.46
1:C:56:VAL:HB	1:C:85:SER:HB3	1.97	0.45
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.99	0.45
2:B:17:MET:HE1	2:B:22:TYR:C	2.41	0.45
1:E:156:LYS:HE3	1:E:196:GLN:OE1	2.17	0.45
2:F:42:GLN:OE1	2:F:45:ILE:HD11	2.17	0.45
1:A:17:TYR:CZ	2:B:6:ILE:HG23	2.52	0.45
2:B:19:ASP:OD2	2:B:38:LYS:NZ	2.44	0.45
2:F:128:ASP:OD1	2:F:159:TYR:OH	2.30	0.45
2:B:38:LYS:HA	2:B:41:THR:OG1	2.17	0.45
1:E:216:LYS:O	1:E:220:ARG:NH2	2.48	0.45
1:A:18:HIS:N	2:B:21:TRP:O	2.45	0.44
1:A:55:ASP:HB3	1:A:55(A):GLY:H	1.63	0.44
2:D:125:GLN:OE1	2:D:155:GLY:HA2	2.17	0.44
1:E:16:GLY:HA2	2:F:10:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:O	2:B:172:GLU:N	2.50	0.44
2:D:41:THR:O	2:D:45:ILE:HG12	2.18	0.44
2:F:54:SER:HA	2:F:57:ASP:OD2	2.17	0.44
1:A:67:ALA:HB2	1:A:105:TYR:CE1	2.53	0.44
1:A:114:ARG:HH22	2:D:79:ASN:ND2	2.14	0.44
2:B:22:TYR:OH	2:B:111:HIS:ND1	2.37	0.44
1:E:16:GLY:HA2	2:F:10:ILE:CD1	2.48	0.44
2:F:21:TRP:HB2	2:F:41:THR:HG22	2.00	0.44
2:D:118:LEU:HD12	2:D:118:LEU:HA	1.77	0.44
1:E:74:PRO:HG3	1:E:147:PHE:O	2.17	0.44
2:B:160:PRO:HA	2:B:163:SER:HB3	2.00	0.43
1:E:133:SER:O	1:E:135:VAL:HG13	2.18	0.43
2:B:159:TYR:HB3	2:B:160:PRO:HD3	2.00	0.43
2:D:158:ASP:CG	2:D:161:GLN:HB2	2.43	0.43
1:C:29:ILE:HD11	2:D:102:MET:HA	2.00	0.43
1:C:164:ILE:O	1:C:246:GLU:HA	2.18	0.43
1:E:37:THR:HG23	1:E:320:LEU:O	2.18	0.43
2:B:59:MET:HE2	2:D:94:TYR:CZ	2.54	0.43
1:C:51:LEU:HD13	1:C:88:VAL:HG21	1.99	0.43
1:E:55:ASP:CG	1:E:55(A):GLY:N	2.71	0.43
1:A:125:PRO:HB2	1:A:125(B):ASN:OD1	2.18	0.43
1:A:279:THR:HG22	1:A:280:LYS:H	1.84	0.43
2:D:149:MET:O	2:D:152:VAL:HG12	2.19	0.43
2:B:10:ILE:O	2:B:10:ILE:HG12	2.17	0.43
2:D:29:GLU:OE1	2:D:29:GLU:N	2.51	0.43
1:C:50:LYS:HB3	1:C:50:LYS:HE2	1.56	0.42
1:C:100:GLY:HA3	1:C:230:MET:O	2.18	0.42
1:E:114:ARG:HE	1:E:114:ARG:HB3	1.60	0.42
1:A:20:ASN:OD1	1:A:322:ASN:ND2	2.53	0.42
1:C:37:THR:HG23	1:C:320:LEU:O	2.19	0.42
1:A:252:ILE:HD12	1:A:252:ILE:N	2.35	0.42
1:C:206:THR:HG21	6:C:1113:HOH:O	2.19	0.42
2:B:26:HIS:CD2	2:B:153:ARG:HH22	2.36	0.42
1:A:135:VAL:HG13	1:A:145:SER:CB	2.50	0.42
2:F:21:TRP:H	2:F:41:THR:HG21	1.84	0.42
2:F:29:GLU:OE1	2:F:29:GLU:N	2.51	0.42
1:A:290:SER:OG	1:A:291:SER:N	2.53	0.42
1:C:14:CYS:O	2:D:24:TYR:HA	2.19	0.42
1:C:206:THR:HG23	1:C:241:ASP:OD2	2.20	0.42
2:D:17:MET:HE1	2:D:22:TYR:O	2.20	0.42
2:D:158:ASP:OD1	2:D:160:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:HIS:O	1:C:185:PRO:HD3	2.19	0.42
1:C:307:LYS:N	1:C:307:LYS:HD2	2.34	0.42
2:B:17:MET:HE3	2:B:36:ALA:HA	2.01	0.41
1:A:206:THR:CG2	1:A:207:SER:N	2.82	0.41
2:B:83:LYS:HA	2:B:83:LYS:HD3	1.89	0.41
2:B:71:ASN:N	2:B:74:GLU:OE1	2.42	0.41
1:C:206:THR:CG2	1:C:207:SER:N	2.83	0.41
4:H:2:FUL:H61	4:H:3:NAG:H2	2.03	0.41
1:E:57:LYS:HE3	1:E:274:TYR:CE2	2.55	0.41
1:E:206:THR:CG2	1:E:207:SER:N	2.83	0.41
2:B:169:LYS:HD3	2:B:172:GLU:OE1	2.20	0.41
1:E:156:LYS:CD	1:E:196:GLN:HB2	2.51	0.41
2:D:68:ARG:HH22	2:F:83:LYS:HG3	1.84	0.41
2:D:158:ASP:HB3	2:D:161:GLN:OE1	2.20	0.41
1:E:98:TYR:CD1	1:E:230:MET:HG2	2.54	0.41
1:A:55:ASP:O	1:A:278:ASN:OD1	2.38	0.41
2:B:3:PHE:HB2	2:B:112:ASP:OD2	2.21	0.41
1:C:31:GLU:OE2	1:C:321:ARG:NH1	2.39	0.41
1:C:33:ASN:HD21	5:C:1001:NAG:C1	2.34	0.41
1:C:118:PHE:CD1	1:C:258:TYR:HB3	2.56	0.41
2:F:145:ASP:O	2:F:149:MET:HG2	2.21	0.41
2:F:149:MET:O	2:F:152:VAL:HG12	2.21	0.41
1:A:129:ASP:HB3	1:A:162:PRO:HG2	2.03	0.41
2:B:43:LYS:HE2	2:B:43:LYS:HB3	1.90	0.41
2:B:145:ASP:OD1	2:B:145:ASP:N	2.53	0.41
1:C:77:ASP:HA	1:C:80:LEU:HG	2.03	0.41
1:C:135:VAL:HG22	1:C:146:SER:HA	2.01	0.41
1:E:124:THR:HA	1:E:125:PRO:HD2	1.87	0.41
2:B:21:TRP:H	2:B:41:THR:CG2	2.34	0.41
1:E:214:VAL:HA	1:E:215:PRO:HD3	1.95	0.40
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.81	0.40
1:A:86:TYR:HA	1:A:265:SER:HB2	2.04	0.40
2:B:21:TRP:HB2	2:B:41:THR:HG22	2.03	0.40
2:D:133:LEU:HD11	2:D:139:GLU:HB2	2.03	0.40
1:A:19:ALA:HB2	2:B:13:GLY:HA3	2.03	0.40
2:D:143:ARG:HD3	2:D:143:ARG:HA	1.90	0.40
2:F:58:LYS:HD3	2:F:58:LYS:HA	1.79	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	321/333 (96%)	303 (94%)	18 (6%)	0	100	100
1	C	321/333 (96%)	305 (95%)	16 (5%)	0	100	100
1	E	321/333 (96%)	303 (94%)	18 (6%)	0	100	100
2	B	173/180 (96%)	162 (94%)	11 (6%)	0	100	100
2	D	173/180 (96%)	161 (93%)	12 (7%)	0	100	100
2	F	173/180 (96%)	162 (94%)	11 (6%)	0	100	100
All	All	1482/1539 (96%)	1396 (94%)	86 (6%)	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	290/298 (97%)	281 (97%)	9 (3%)	35	63
1	C	290/298 (97%)	274 (94%)	16 (6%)	19	41
1	E	290/298 (97%)	283 (98%)	7 (2%)	43	70
2	B	149/154 (97%)	139 (93%)	10 (7%)	15	33
2	D	149/154 (97%)	141 (95%)	8 (5%)	20	42
2	F	149/154 (97%)	142 (95%)	7 (5%)	23	48
All	All	1317/1356 (97%)	1260 (96%)	57 (4%)	26	51

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	80	LEU
1	A	131	GLU
1	A	135	VAL
1	A	174	GLU
1	A	206	THR
1	A	266	THR
1	A	279	THR
1	A	316	LEU
2	B	10	ILE
2	B	22	TYR
2	B	45	ILE
2	B	55	ILE
2	B	58	LYS
2	B	61	THR
2	B	66	VAL
2	B	122	VAL
2	B	126	LEU
2	B	164	GLU
1	C	23	THR
1	C	26	VAL
1	C	28	THR
1	C	34	VAL
1	C	135	VAL
1	C	174	GLU
1	C	175	ASP
1	C	179	LEU
1	C	203	SER
1	C	206	THR
1	C	213	LEU
1	C	219	THR
1	C	220	ARG
1	C	266	THR
1	C	314	LEU
1	C	320	LEU
2	D	10	ILE
2	D	22	TYR
2	D	55	ILE
2	D	66	VAL
2	D	89	LEU
2	D	101	LEU
2	D	122	VAL

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Mol	Chain	Res	Type
2	D	137	CYS
1	E	26	VAL
1	E	28	THR
1	E	51	LEU
1	E	174	GLU
1	E	206	THR
1	E	290	SER
1	E	320	LEU
2	F	10	ILE
2	F	22	TYR
2	F	45	ILE
2	F	48	VAL
2	F	66	VAL
2	F	102	MET
2	F	126	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	81	ASN
1	A	110	HIS
1	A	116	ASN
1	A	159	ASN
1	A	196	GLN
1	A	197	ASN
1	A	322	ASN
2	B	15	GLN
2	B	26	HIS
2	B	142	HIS
1	C	33	ASN
1	C	122	GLN
1	C	159	ASN
1	C	172	ASN
1	C	196	GLN
1	C	278	ASN
1	E	33	ASN
1	E	159	ASN
1	E	172	ASN
1	E	186	ASN
1	E	211	GLN
1	E	240	ASN

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Mol	Chain	Res	Type
2	F	15	GLN
2	F	26	HIS

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	NAG	G	1	3,1	14,14,15	0.77	1 (7%)	17,19,21	0.97	1 (5%)
3	FUL	G	2	3	10,10,11	1.20	1 (10%)	14,14,16	0.64	0
3	NAG	G	3	3	14,14,15	0.33	0	17,19,21	0.40	0
4	NAG	H	1	1,4	14,14,15	0.76	1 (7%)	17,19,21	1.07	1 (5%)
4	FUL	H	2	4	10,10,11	1.19	1 (10%)	14,14,16	0.81	0
4	NAG	H	3	4	14,14,15	0.53	0	17,19,21	0.55	0
4	FUC	H	4	4	10,10,11	1.68	3 (30%)	14,14,16	1.53	3 (21%)
3	NAG	I	1	3,1	14,14,15	0.86	1 (7%)	17,19,21	1.03	1 (5%)
3	FUL	I	2	3	10,10,11	1.36	1 (10%)	14,14,16	0.85	0
3	NAG	I	3	3	14,14,15	0.29	0	17,19,21	0.34	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	NAG	G	1	3,1	-	1/6/23/26	0/1/1/1
3	FUL	G	2	3	-	-	0/1/1/1
3	NAG	G	3	3	-	0/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	FUL	H	2	4	-	-	0/1/1/1
4	NAG	H	3	4	-	2/6/23/26	0/1/1/1
4	FUC	H	4	4	-	-	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	FUL	I	2	3	-	-	0/1/1/1
3	NAG	I	3	3	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	O5-C1	-3.15	1.38	1.43
3	I	2	FUL	C4-C3	3.05	1.60	1.52
4	H	4	FUC	C4-C5	2.83	1.59	1.52
3	G	1	NAG	O5-C1	-2.73	1.39	1.43
4	H	4	FUC	O5-C5	2.66	1.48	1.43
4	H	1	NAG	O5-C1	-2.53	1.39	1.43
4	H	4	FUC	C6-C5	2.41	1.57	1.51
4	H	2	FUL	C4-C3	2.17	1.58	1.52
3	G	2	FUL	C4-C3	2.08	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	4	FUC	C6-C5-C4	2.88	118.35	113.08
4	H	4	FUC	O2-C2-C1	2.84	115.72	109.22
4	H	4	FUC	C2-C3-C4	-2.82	105.91	110.86
4	H	1	NAG	C4-C3-C2	2.15	114.17	111.02
3	G	1	NAG	C3-C4-C5	2.12	114.08	110.23
3	I	1	NAG	C3-C4-C5	2.08	114.01	110.23

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	3	NAG	C4-C5-C6-O6
4	H	3	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6

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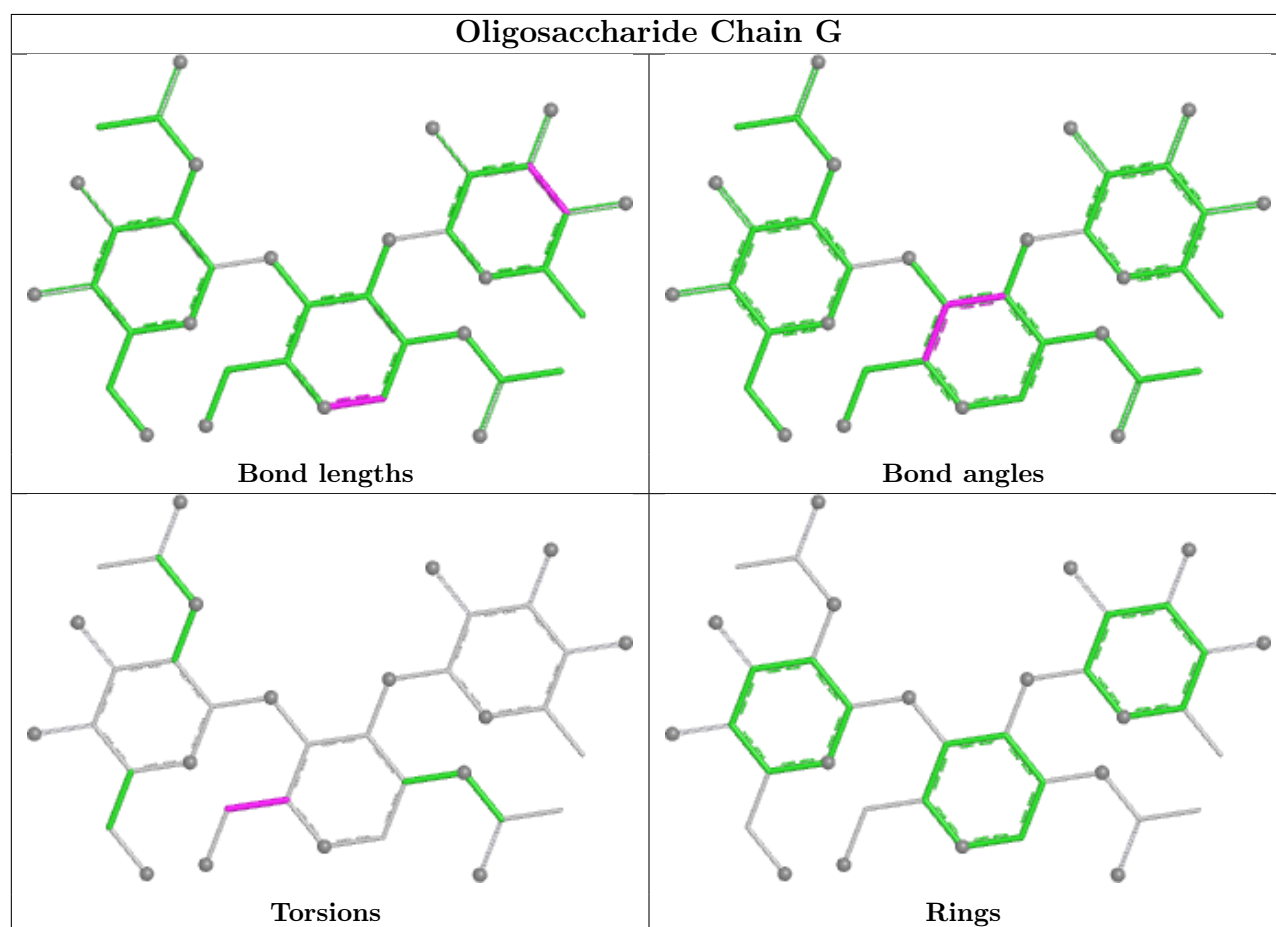
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	O5-C5-C6-O6
3	I	3	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	I	3	NAG	O5-C5-C6-O6

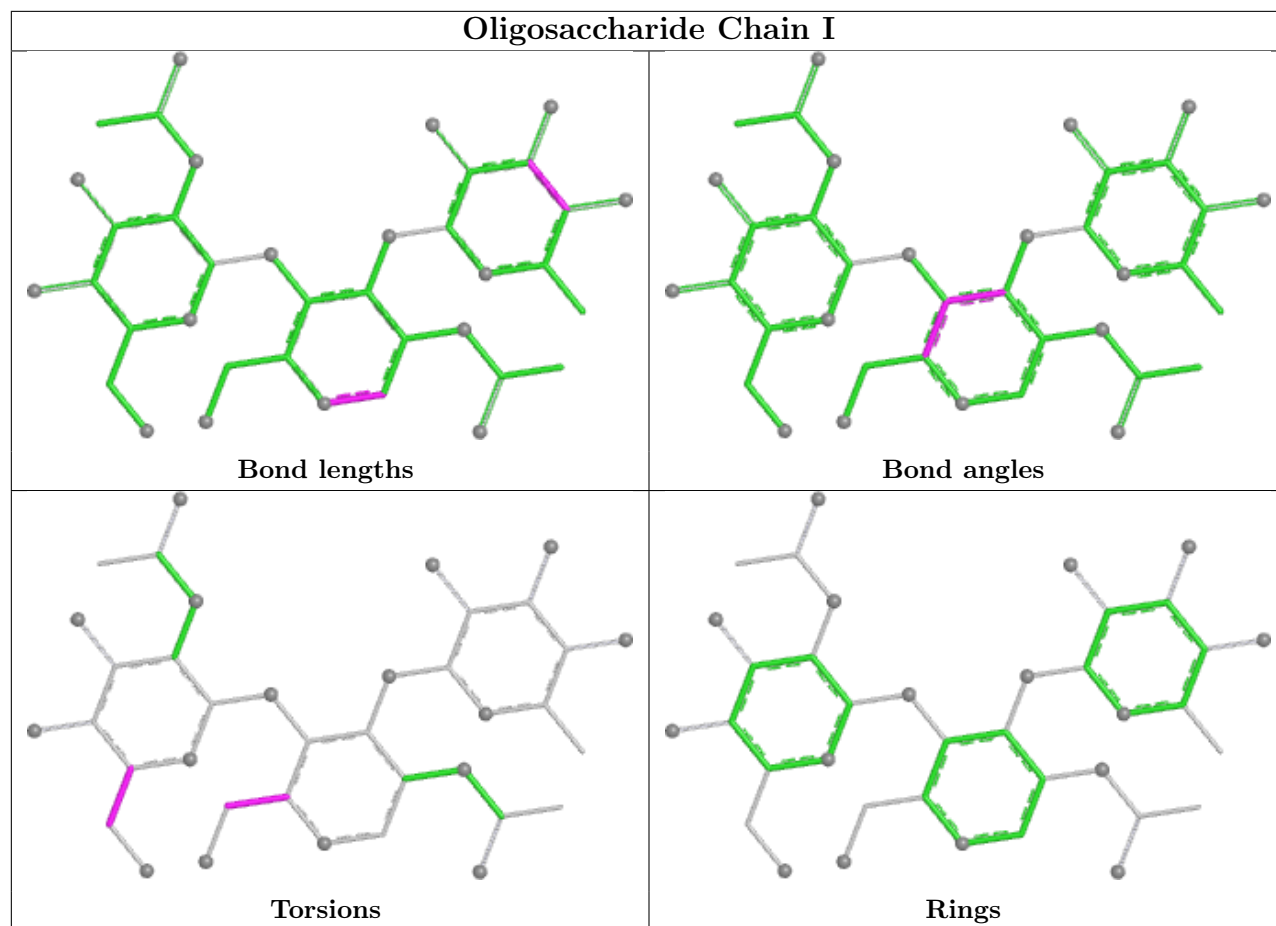
There are no ring outliers.

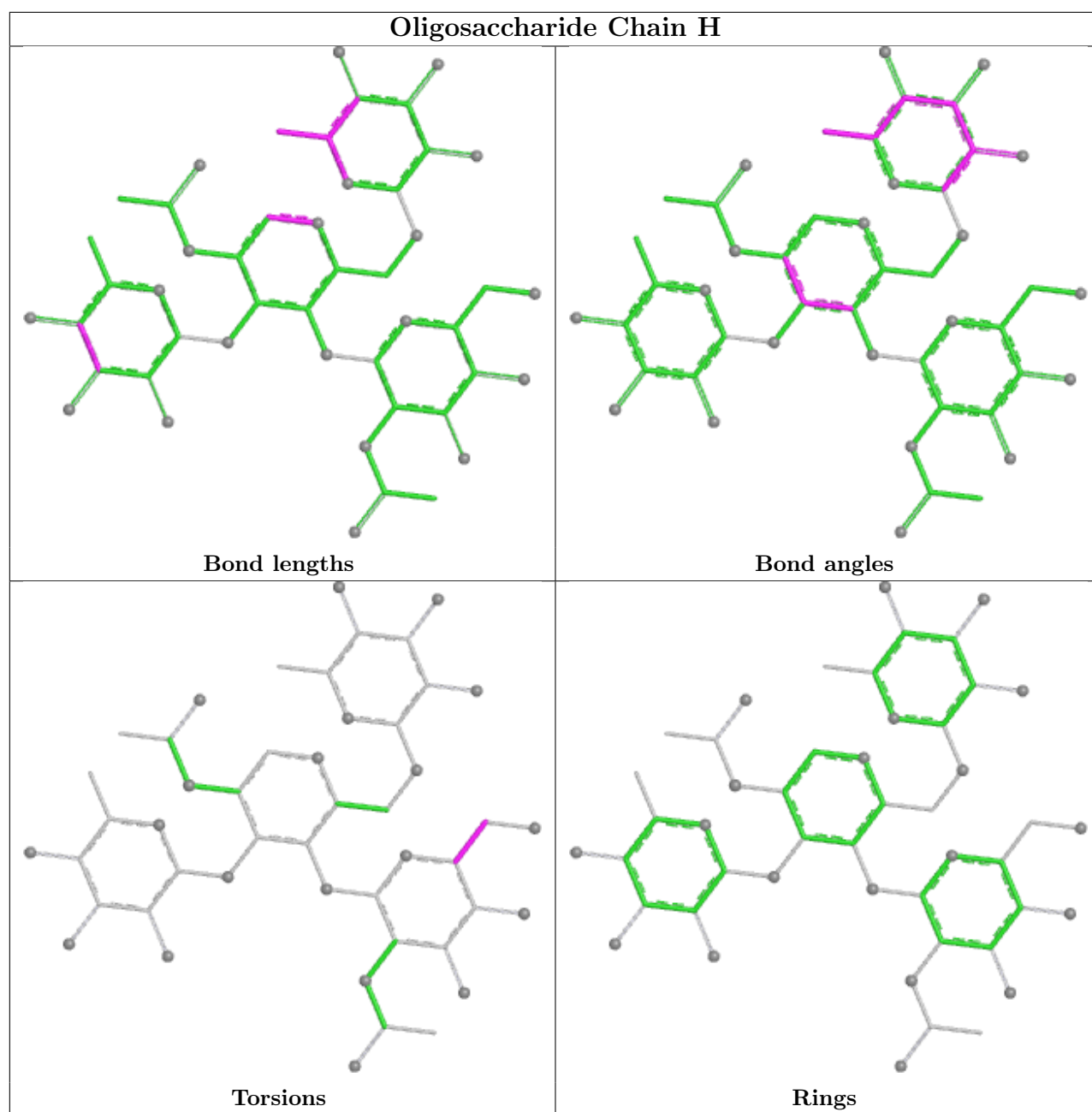
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	3	NAG	1	0
4	H	2	FUL	1	0

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







5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1001	-	14,14,15	0.27	0	17,19,21	0.41	0
5	NAG	A	1001	-	14,14,15	0.34	0	17,19,21	0.49	0
5	NAG	E	1001	-	14,14,15	0.29	0	17,19,21	0.55	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
5	NAG	C	1001	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1001	-	-	1/6/23/26	0/1/1/1
5	NAG	E	1001	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1001	NAG	C4-C5-C6-O6
5	E	1001	NAG	O5-C5-C6-O6
5	A	1001	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1001	NAG	1	0
5	A	1001	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/333 (96%)	-0.10	4 (1%) 76 73	19, 41, 84, 147	0
1	C	323/333 (96%)	-0.03	7 (2%) 62 57	22, 43, 79, 117	0
1	E	323/333 (96%)	-0.01	6 (1%) 66 61	22, 43, 81, 124	0
2	B	175/180 (97%)	1.00	25 (14%) 6 5	23, 92, 137, 142	0
2	D	175/180 (97%)	0.81	17 (9%) 13 10	24, 81, 109, 127	0
2	F	175/180 (97%)	0.78	16 (9%) 15 11	25, 82, 108, 129	0
All	All	1494/1539 (97%)	0.27	75 (5%) 34 28	19, 51, 112, 147	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	CYS	5.4
2	B	172	GLU	5.1
1	A	13	ILE	4.8
2	F	172	GLU	4.8
2	D	172	GLU	4.5
2	B	137	CYS	4.1
2	B	173	ILE	3.9
2	D	162	TYR	3.8
2	F	145	ASP	3.8
2	B	157	TYR	3.7
1	C	323	SER	3.7
2	B	159	TYR	3.5
2	D	173	ILE	3.5
2	B	139	GLU	3.4
2	F	175	GLY	3.4
2	B	138	PHE	3.4
2	B	56	ILE	3.2
2	B	175	GLY	3.1
2	D	8	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	9	PRO	3.0
2	F	23	GLY	3.0
1	C	19	ALA	3.0
1	A	97	CYS	2.9
2	B	162	TYR	2.9
2	B	168	LEU	2.9
2	B	141	TYR	2.8
1	C	55(A)	GLY	2.8
2	D	35	ALA	2.8
2	F	119	TYR	2.8
1	C	322	ASN	2.7
1	E	190	GLU	2.7
2	B	153	ARG	2.7
2	D	175	GLY	2.7
2	D	152	VAL	2.7
2	B	169	LYS	2.7
2	F	128	ASP	2.5
2	B	34	TYR	2.5
2	D	23	GLY	2.5
2	B	134	GLY	2.5
2	F	138	PHE	2.4
2	B	148	CYS	2.4
2	B	140	PHE	2.4
2	B	10	ILE	2.4
2	F	18	VAL	2.3
2	F	143	ARG	2.3
2	D	4	GLY	2.3
1	E	42	ILE	2.3
2	D	55	ILE	2.3
2	B	3	PHE	2.3
2	B	165	GLU	2.2
1	E	277	CYS	2.2
2	F	162	TYR	2.2
1	A	324	PRO	2.2
1	E	295	HIS	2.2
2	D	154	ASN	2.2
2	F	168	LEU	2.2
2	F	19	ASP	2.2
2	D	33	GLY	2.1
2	B	163	SER	2.1
2	D	59	MET	2.1
2	B	16	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	37	THR	2.1
2	B	146	ASN	2.1
2	F	173	ILE	2.1
2	B	158	ASP	2.0
1	C	39	ALA	2.0
1	E	160	ALA	2.0
2	D	137	CYS	2.0
2	D	157	TYR	2.0
2	F	24	TYR	2.0
2	F	152	VAL	2.0
1	C	20	ASN	2.0
2	D	10	ILE	2.0
2	D	122	VAL	2.0
2	F	141	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

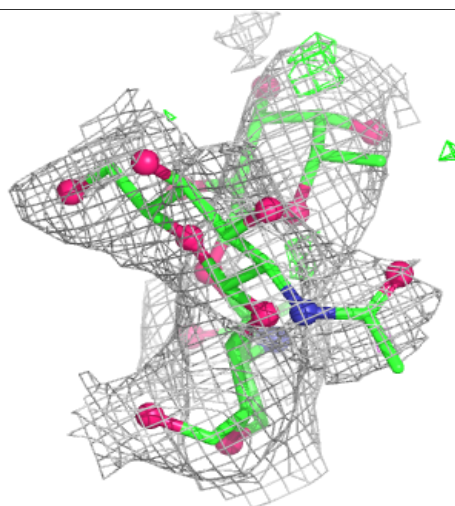
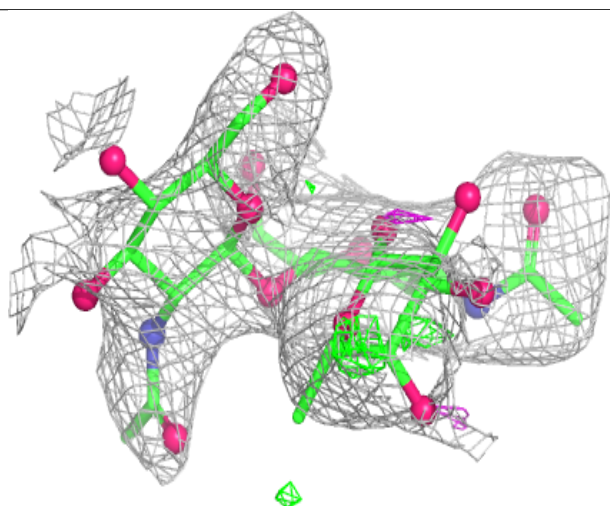
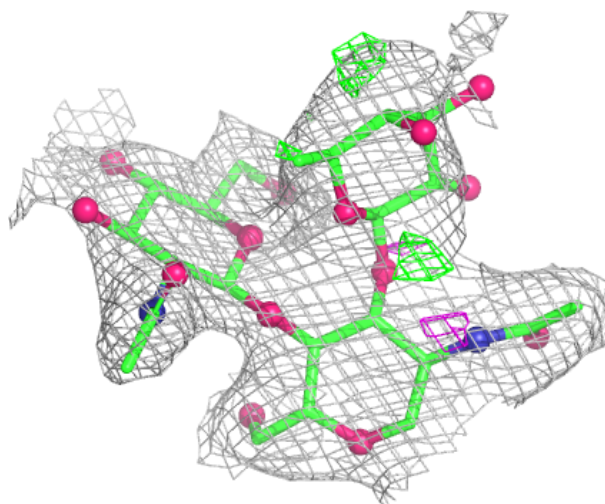
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FUC	H	4	10/11	0.51	0.15	58,74,84,90	0
4	NAG	H	3	14/15	0.66	0.15	74,85,93,102	0
3	FUL	I	2	10/11	0.66	0.19	70,81,89,96	0
3	FUL	G	2	10/11	0.68	0.18	68,82,93,93	0
4	FUL	H	2	10/11	0.72	0.23	75,81,92,92	0
3	NAG	I	3	14/15	0.75	0.13	74,91,100,101	0
3	NAG	G	3	14/15	0.80	0.11	70,78,86,86	0
4	NAG	H	1	14/15	0.86	0.11	51,67,79,83	0
3	NAG	I	1	14/15	0.86	0.13	51,61,79,81	0
3	NAG	G	1	14/15	0.90	0.08	38,56,75,77	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.

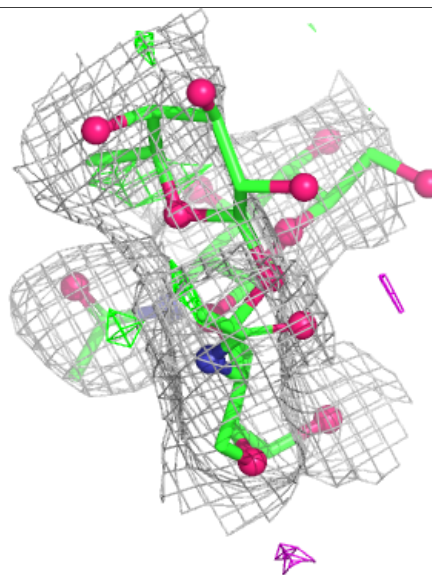
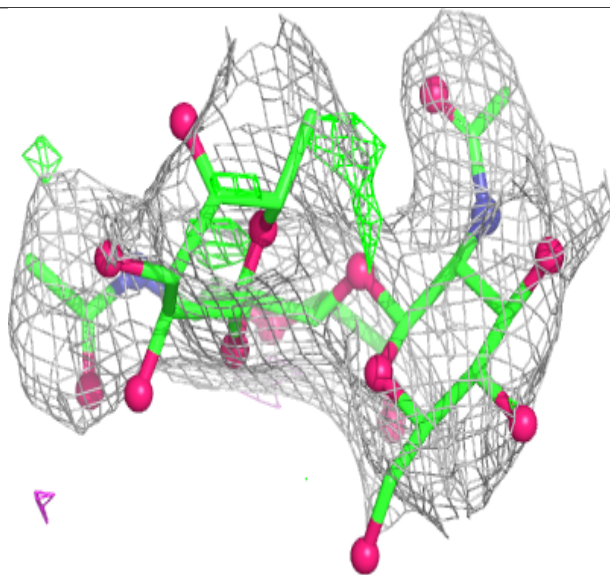
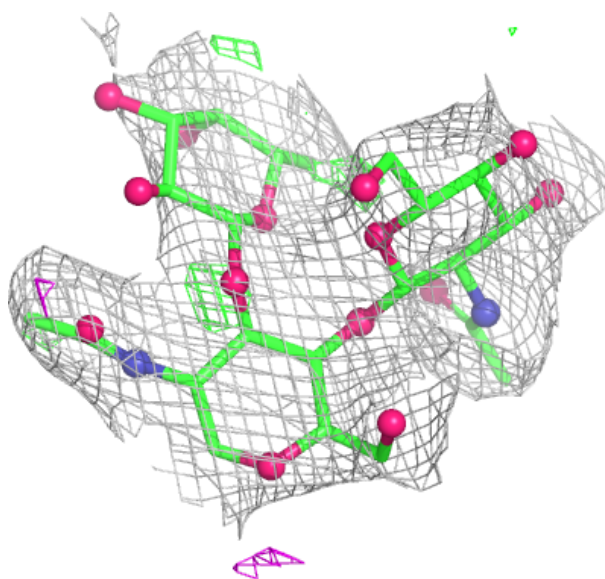
Electron density around Chain G:

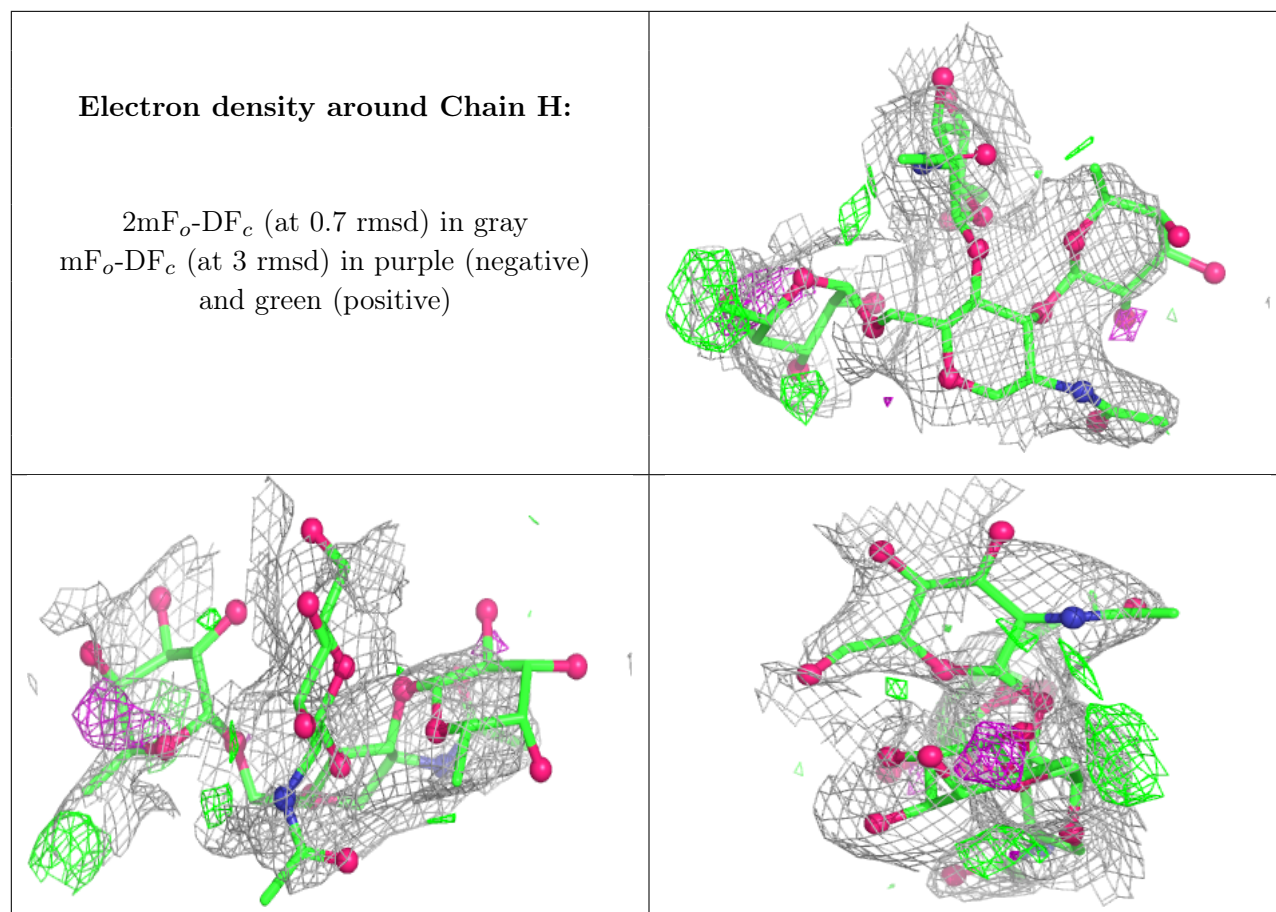
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
5	NAG	E	1001	14/15	0.62	0.14	99,109,116,120	0
5	NAG	C	1001	14/15	0.63	0.16	92,101,107,115	0
5	NAG	A	1001	14/15	0.81	0.12	91,98,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.