



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:26 AM UTC

PDB ID : 4XQO / pdb_00004xqo
Title : Crystal structure of hemagglutinin from Jiangxi-Donghu (2013) H10N8 influenza virus in complex with 6'-SLN
Authors : Tzarum, N.; Zhang, H.; Zhu, X.; Wilson, I.A.
Deposited on : 2015-01-19
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

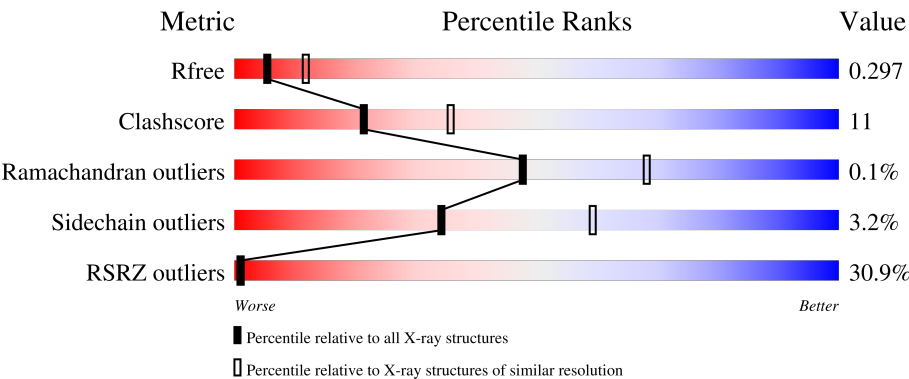
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	326	19% 78% 18% ..
1	C	326	26% 70% 25% ..
1	E	326	21% 73% 23% ..
2	B	181	35% 60% 33% 7%
2	D	181	41% 63% 28% 7%

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Mol	Chain	Length	Quality of chain
2	F	181	50% 66% 22% 8%
3	G	2	100%
3	J	2	50% 50%
4	H	3	33% 33% 33%
5	I	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11538 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	316	Total	C	N	O	S	0	0	0
			2424	1499	447	461	17			
1	C	315	Total	C	N	O	S	0	0	0
			2411	1491	445	458	17			
1	E	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	-	expression tag	UNP A0A059T4A1
A	9	ASP	-	expression tag	UNP A0A059T4A1
A	10	PRO	-	expression tag	UNP A0A059T4A1
C	8	ALA	-	expression tag	UNP A0A059T4A1
C	9	ASP	-	expression tag	UNP A0A059T4A1
C	10	PRO	-	expression tag	UNP A0A059T4A1
E	8	ALA	-	expression tag	UNP A0A059T4A1
E	9	ASP	-	expression tag	UNP A0A059T4A1
E	10	PRO	-	expression tag	UNP A0A059T4A1

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1364	843	236	277	8			
2	D	168	Total	C	N	O	S	0	0	0
			1362	842	235	277	8			
2	F	166	Total	C	N	O	S	0	0	0
			1351	837	233	273	8			

There are 21 discrepancies between the modelled and reference sequences:

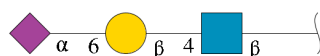
Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A059T4A1
B	176	GLY	-	expression tag	UNP A0A059T4A1
B	177	ARG	-	expression tag	UNP A0A059T4A1
B	178	LEU	-	expression tag	UNP A0A059T4A1
B	179	VAL	-	expression tag	UNP A0A059T4A1
B	180	PRO	-	expression tag	UNP A0A059T4A1
B	181	ARG	-	expression tag	UNP A0A059T4A1
D	175	SER	-	expression tag	UNP A0A059T4A1
D	176	GLY	-	expression tag	UNP A0A059T4A1
D	177	ARG	-	expression tag	UNP A0A059T4A1
D	178	LEU	-	expression tag	UNP A0A059T4A1
D	179	VAL	-	expression tag	UNP A0A059T4A1
D	180	PRO	-	expression tag	UNP A0A059T4A1
D	181	ARG	-	expression tag	UNP A0A059T4A1
F	175	SER	-	expression tag	UNP A0A059T4A1
F	176	GLY	-	expression tag	UNP A0A059T4A1
F	177	ARG	-	expression tag	UNP A0A059T4A1
F	178	LEU	-	expression tag	UNP A0A059T4A1
F	179	VAL	-	expression tag	UNP A0A059T4A1
F	180	PRO	-	expression tag	UNP A0A059T4A1
F	181	ARG	-	expression tag	UNP A0A059T4A1

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



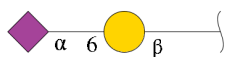
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



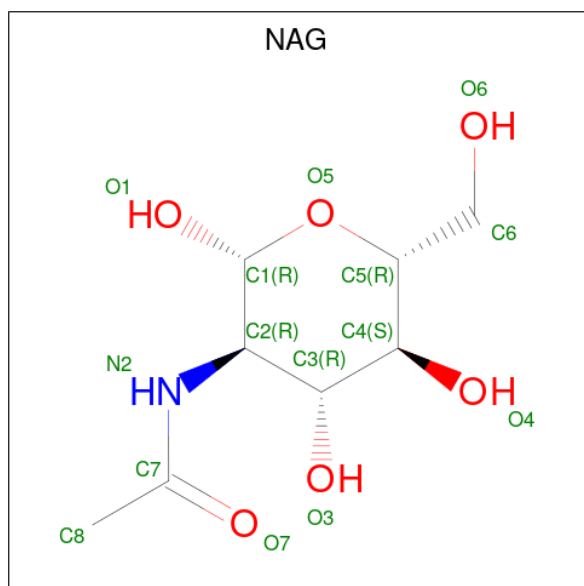
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			46	25	2	19			

- 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
			32	17	1	14			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		

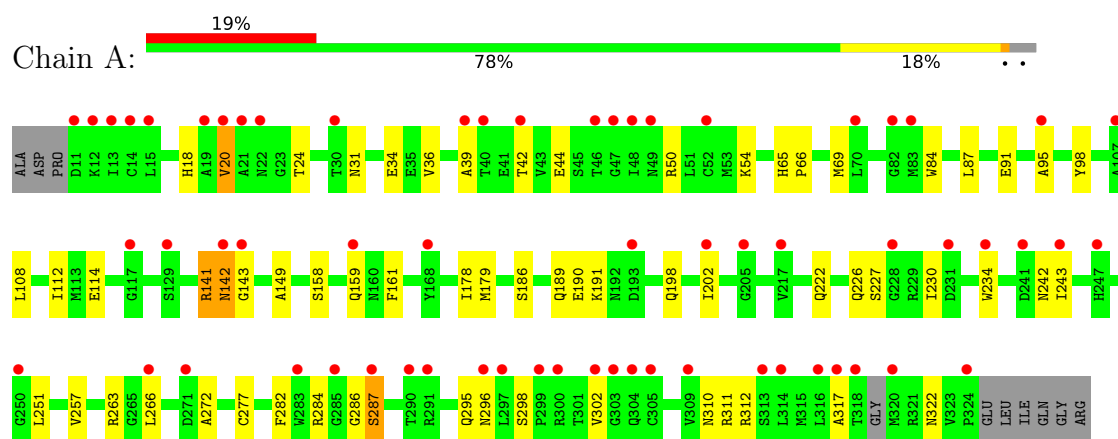
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total 12	O 12	0	0
7	B	4	Total 4	O 4	0	0
7	C	6	Total 6	O 6	0	0
7	D	1	Total 1	O 1	0	0
7	E	4	Total 4	O 4	0	0

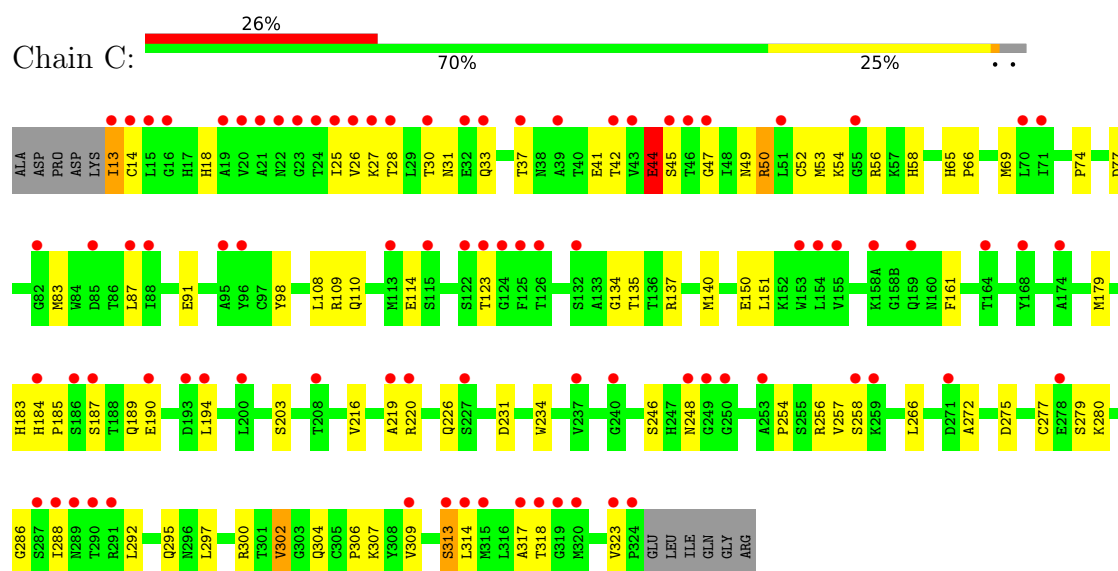
3 Residue-property plots [i](#)

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 HA1 chain

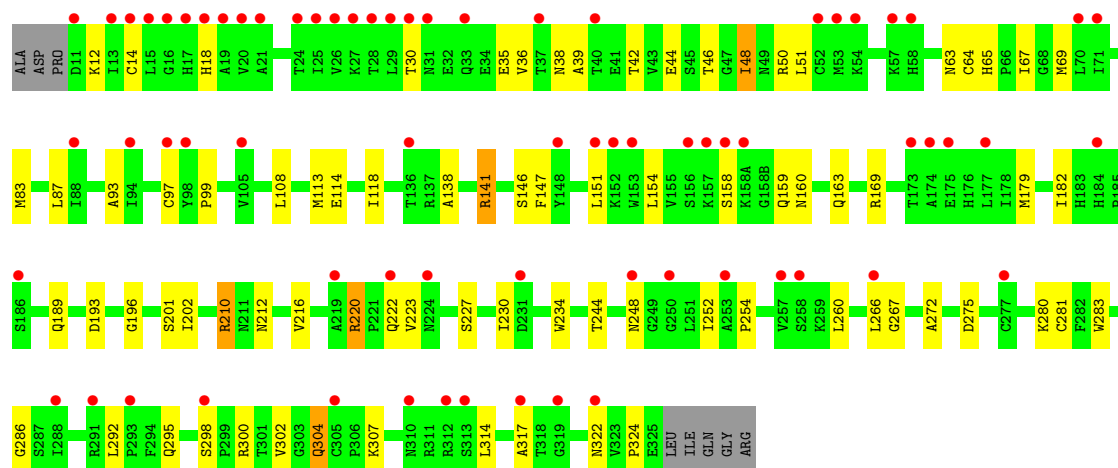


- Molecule 1: Hemagglutinin HA1 chain

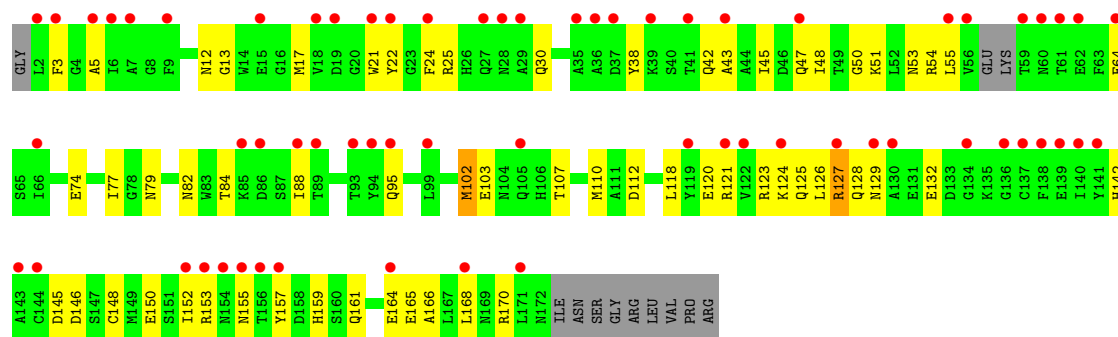


- Molecule 1: Hemagglutinin HA1 chain

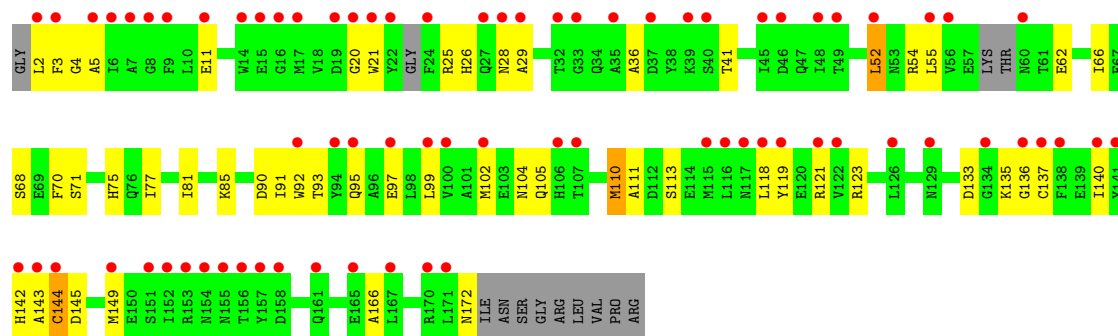
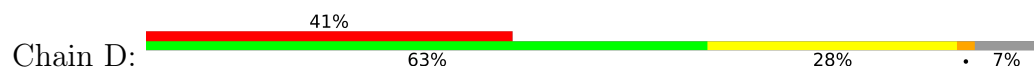




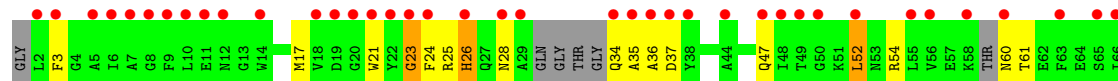
• Molecule 2: Hemagglutinin HA2 chain

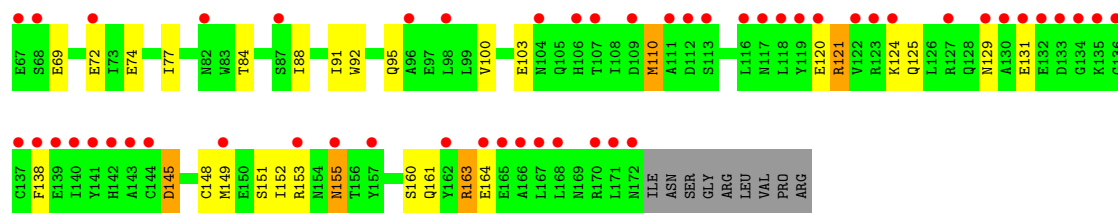


• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain





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

Chain G: 100%



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

Chain J: 50% 50%



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

Chain H: 33% 33% 33%



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

Chain I: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.07Å 245.42Å 71.30Å 90.00° 112.46° 90.00°	Depositor
Resolution (Å)	46.17 – 2.85 46.17 – 2.85	Depositor EDS
% Data completeness (in resolution range)	88.3 (46.17-2.85) 83.3 (46.17-2.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.259 , 0.291 0.279 , 0.297	Depositor DCC
R_{free} test set	2125 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 20.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	11538	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: 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	0.29	0/2472	0.78	1/3348 (0.0%)
1	C	0.29	0/2460	0.80	8/3334 (0.2%)
1	E	0.29	0/2486	0.79	2/3368 (0.1%)
2	B	0.30	0/1388	0.80	2/1873 (0.1%)
2	D	0.31	0/1385	0.81	2/1867 (0.1%)
2	F	0.31	0/1374	0.83	4/1851 (0.2%)
All	All	0.30	0/11565	0.80	19/15641 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	ASN	N-CA-C	-6.56	100.81	110.52
2	D	4	GLY	N-CA-C	6.38	120.94	112.77
2	F	153	ARG	N-CA-C	6.23	118.15	111.36
1	C	44	GLU	N-CA-C	-5.88	101.49	110.14
2	D	5	ALA	N-CA-C	5.60	117.24	111.03
1	C	184	HIS	CA-C-N	5.54	125.45	119.85
1	C	184	HIS	C-N-CA	5.54	125.45	119.85
1	C	313	SER	N-CA-C	5.43	116.66	108.46
2	F	52	LEU	N-CA-C	-5.25	105.64	111.36
1	E	220	ARG	CA-C-N	5.23	125.23	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	220	ARG	C-N-CA	5.23	125.23	119.89
1	C	292	LEU	CA-C-N	5.20	125.00	119.28
1	C	292	LEU	C-N-CA	5.20	125.00	119.28
2	F	23	GLY	N-CA-C	5.17	118.67	110.96
2	F	26	HIS	N-CA-C	5.17	116.92	108.55
2	B	5	ALA	N-CA-C	5.16	116.75	111.03
1	C	272	ALA	CA-C-N	5.04	124.97	119.78
1	C	272	ALA	C-N-CA	5.04	124.97	119.78
2	B	127	ARG	CB-CA-C	-5.02	110.81	116.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	155	ASN	Peptide

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	2424	0	2375	38	0
1	C	2411	0	2363	67	0
1	E	2437	0	2386	54	0
2	B	1364	0	1259	45	0
2	D	1362	0	1254	44	0
2	F	1351	0	1249	35	0
3	G	28	0	25	1	0
3	J	28	0	25	1	0
4	H	46	0	40	2	0
5	I	32	0	27	4	0
6	A	14	0	13	0	0
6	C	14	0	13	0	0
7	A	12	0	0	3	0
7	B	4	0	0	1	0
7	C	6	0	0	0	0
7	D	1	0	0	0	0
7	E	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11538	0	11029	246	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 11.

All (246) 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:44:GLU:OE1	1:C:45:SER:N	2.11	0.80
2:B:125:GLN:HE21	2:B:157:TYR:HB3	1.48	0.78
1:A:226:GLN:NE2	4:H:3:SIA:O1A	2.17	0.77
1:E:63:ASN:OD1	7:E:701:HOH:O	2.03	0.76
1:C:69:MET:HE1	1:C:87:LEU:HD21	1.67	0.76
1:C:30:THR:HG22	2:D:105:GLN:HE22	1.51	0.74
1:A:226:GLN:NE2	4:H:3:SIA:O8	2.22	0.72
2:B:47:GLN:HB2	2:B:110:MET:HE2	1.72	0.72
2:D:95:GLN:HE21	2:F:95:GLN:HE22	1.36	0.72
2:B:150:GLU:HG2	2:B:153:ARG:HD2	1.72	0.71
1:E:48:ILE:H	1:E:48:ILE:HD12	1.56	0.71
1:A:20:VAL:H	1:A:322:ASN:HD21	1.39	0.71
1:A:284:ARG:NH2	7:A:502:HOH:O	2.20	0.71
1:C:231:ASP:OD2	1:E:210:ARG:NH2	2.22	0.69
2:D:77:ILE:HD13	2:F:77:ILE:HD11	1.74	0.69
1:C:226:GLN:HE22	5:I:1:GAL:H62	1.60	0.66
1:E:50:ARG:NH2	1:E:275:ASP:OD2	2.28	0.66
1:E:51:LEU:HG	1:E:272:ALA:HB3	1.77	0.66
1:A:186:SER:OG	1:A:190:GLU:OE1	2.14	0.66
2:B:120:GLU:OE1	2:B:123:ARG:NH2	2.29	0.66
1:A:296:ASN:HD21	1:A:312:ARG:HA	1.61	0.65
1:A:295:GLN:NE2	1:A:298:SER:H	1.94	0.65
1:C:179:MET:HG2	1:C:234:TRP:HB3	1.79	0.64
2:B:132:GLU:OE1	2:D:123:ARG:NH1	2.31	0.63
1:E:69:MET:HE1	1:E:87:LEU:HD21	1.81	0.63
2:F:145:ASP:OD2	2:F:145:ASP:N	2.23	0.63
2:F:121:ARG:HH11	2:F:155:ASN:HD21	1.47	0.63
1:C:42:THR:HG22	2:D:55:LEU:HD21	1.81	0.62
2:F:23:GLY:HA2	2:F:36:ALA:HA	1.82	0.61
2:B:150:GLU:HA	2:B:153:ARG:HB2	1.82	0.61
1:A:310:ASN:O	1:A:311:ARG:NH1	2.34	0.61
1:E:36:VAL:HG11	1:E:317:ALA:HB1	1.83	0.61
1:A:158:SER:HB2	1:A:159:GLN:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:CYS:O	2:B:152:ILE:HD12	2.00	0.61
1:C:18:HIS:CD2	2:D:21:TRP:HA	2.36	0.60
1:E:169:ARG:NH1	3:J:1:NAG:O6	2.35	0.60
1:E:99:PRO:HB3	1:E:223:VAL:HB	1.84	0.59
2:D:142:HIS:ND1	2:D:142:HIS:O	2.34	0.59
2:F:54:ARG:NH2	2:F:103:GLU:OE2	2.34	0.59
1:A:295:GLN:HE21	1:A:298:SER:H	1.48	0.59
1:E:182:ILE:HD12	1:E:202:ILE:HD13	1.84	0.58
1:C:66:PRO:HA	1:C:69:MET:HE3	1.84	0.58
1:C:307:LYS:HG3	2:D:92:TRP:CE2	2.37	0.58
1:A:42:THR:HG22	2:B:55:LEU:HD21	1.85	0.58
1:C:187:SER:OG	1:C:189:GLN:O	2.19	0.58
1:C:203:SER:OG	1:C:246:SER:OG	2.22	0.58
2:D:142:HIS:HD2	2:D:166:ALA:HB2	1.68	0.58
1:C:18:HIS:CE1	1:C:37:THR:HG21	2.39	0.57
1:C:18:HIS:HD2	2:D:21:TRP:HA	1.68	0.57
1:A:202:ILE:HG12	1:A:251:LEU:HB2	1.87	0.57
1:C:110:GLN:O	1:C:114:GLU:HG3	2.05	0.57
1:C:13:ILE:HG22	2:D:140:ILE:HD11	1.87	0.56
2:B:30:GLN:OE1	2:B:30:GLN:N	2.38	0.56
2:D:21:TRP:H	2:D:41:THR:HG21	1.70	0.56
1:C:50:ARG:NH1	1:C:275:ASP:OD2	2.38	0.56
1:E:266:LEU:HD11	1:E:302:VAL:HG12	1.88	0.56
2:D:26:HIS:HB2	2:D:149:MET:HE3	1.87	0.55
2:D:119:TYR:HE2	2:D:136:GLY:HA2	1.71	0.55
1:E:158:SER:H	1:E:159:GLN:HE21	1.54	0.55
1:A:161:PHE:O	1:A:198:GLN:NE2	2.36	0.55
1:C:288:ILE:HG12	1:C:297:LEU:HD12	1.89	0.55
2:B:123:ARG:HG2	2:B:123:ARG:HH11	1.71	0.55
1:E:67:ILE:HD12	1:E:108:LEU:HD23	1.89	0.55
1:A:18:HIS:CD2	2:B:21:TRP:HA	2.42	0.55
1:C:41:GLU:HG3	1:C:42:THR:H	1.71	0.55
1:E:179:MET:HG2	1:E:234:TRP:HB3	1.89	0.55
1:C:50:ARG:HG3	1:C:50:ARG:HH21	1.71	0.54
2:F:24:PHE:HE1	2:F:37:ASP:HB2	1.73	0.54
1:C:295:GLN:HG2	1:C:306:PRO:HG2	1.89	0.54
1:E:141:ARG:NH1	1:E:147:PHE:O	2.31	0.54
2:B:127:ARG:HD3	2:B:159:HIS:CD2	2.43	0.54
1:E:272:ALA:HB2	1:E:286:GLY:H	1.71	0.54
1:C:52:CYS:HB2	1:C:279:SER:HB2	1.90	0.54
1:A:189:GLN:NE2	7:A:504:HOH:O	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:O	1:A:287:SER:OG	2.25	0.53
1:C:108:LEU:HD22	1:C:234:TRP:CD1	2.44	0.53
2:D:143:ALA:O	2:D:144:CYS:HB2	2.08	0.53
2:D:145:ASP:OD1	2:D:145:ASP:N	2.40	0.53
1:E:35:GLU:HG2	1:E:322:ASN:HB3	1.90	0.53
1:C:41:GLU:HG3	1:C:42:THR:N	2.24	0.53
2:D:21:TRP:H	2:D:41:THR:CG2	2.21	0.53
2:D:54:ARG:HH12	2:D:99:LEU:HD11	1.74	0.53
1:E:283:TRP:CE3	1:E:298:SER:HB2	2.45	0.52
2:B:24:PHE:CD2	2:B:153:ARG:HG2	2.45	0.52
1:C:280:LYS:HB2	1:C:304:GLN:HB2	1.91	0.52
1:C:91:GLU:HA	2:D:70:PHE:CG	2.44	0.52
1:E:295:GLN:NE2	1:E:298:SER:H	2.08	0.52
1:E:113:MET:HB3	1:E:267:GLY:HA3	1.90	0.52
2:B:118:LEU:HD11	2:B:121:ARG:HH21	1.75	0.51
1:E:158:SER:O	1:E:159:GLN:HG2	2.10	0.51
1:C:309:VAL:HG23	2:D:93:THR:HA	1.92	0.51
1:A:263:ARG:O	7:A:501:HOH:O	2.19	0.51
2:B:102:MET:HG3	2:B:103:GLU:N	2.26	0.51
2:F:24:PHE:N	2:F:35:ALA:O	2.36	0.51
1:E:222:GLN:HG2	1:E:227:SER:OG	2.11	0.50
1:C:26:VAL:HG21	1:C:317:ALA:HB2	1.94	0.50
1:A:272:ALA:HB2	1:A:286:GLY:H	1.75	0.50
1:E:38:ASN:OD1	1:E:39:ALA:N	2.45	0.50
1:E:314:LEU:HD22	2:F:100:VAL:HG21	1.92	0.50
1:C:14:CYS:N	2:D:25:ARG:O	2.41	0.50
2:B:79:ASN:HA	2:B:82:ASN:HB2	1.95	0.49
1:E:44:GLU:OE2	1:E:46:THR:N	2.32	0.49
1:A:141:ARG:NH2	1:A:149:ALA:HB2	2.27	0.49
2:B:95:GLN:HE21	2:F:95:GLN:NE2	2.11	0.49
1:C:216:VAL:HG11	1:E:212:ASN:HB2	1.94	0.49
2:B:165:GLU:O	2:B:168:LEU:HG	2.13	0.49
1:C:313:SER:O	1:C:314:LEU:HD23	2.13	0.49
2:D:28:ASN:CG	2:D:29:ALA:H	2.20	0.49
2:F:120:GLU:OE1	2:F:124:LYS:NZ	2.36	0.49
1:C:18:HIS:HE1	1:C:37:THR:HG21	1.77	0.48
1:E:304:GLN:NE2	2:F:60:ASN:O	2.44	0.48
1:A:282:PHE:CD2	1:A:287:SER:HB3	2.49	0.48
2:D:2:LEU:HD23	2:F:110:MET:HA	1.95	0.48
2:F:129:ASN:HD21	2:F:163:ARG:HA	1.78	0.48
2:B:129:ASN:HB3	2:B:142:HIS:HD2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:GLU:HG2	2:D:135:LYS:HE3	1.96	0.48
2:B:145:ASP:OD1	2:B:146:ASP:N	2.47	0.48
1:C:49:ASN:HA	1:C:286:GLY:HA3	1.96	0.48
1:C:300:ARG:HG2	2:D:85:LYS:NZ	2.28	0.48
2:B:74:GLU:HB3	2:B:77:ILE:HG22	1.94	0.48
2:B:125:GLN:NE2	2:B:155:ASN:HA	2.29	0.48
1:E:160:ASN:HA	1:E:196:GLY:HA3	1.95	0.48
1:A:54:LYS:HB3	1:A:277:CYS:O	2.14	0.48
1:C:28:THR:N	1:C:31:ASN:O	2.46	0.48
1:C:123:THR:HG22	1:C:257:VAL:HG23	1.96	0.48
2:B:12:ASN:OD1	2:B:13:GLY:N	2.47	0.48
2:F:26:HIS:HB2	2:F:149:MET:HE1	1.95	0.48
2:B:126:LEU:HD21	2:B:152:ILE:HG12	1.95	0.47
2:D:119:TYR:CE2	2:D:136:GLY:HA2	2.48	0.47
1:E:230:ILE:HD13	1:E:252:ILE:HG13	1.96	0.47
1:A:24:THR:HG21	1:A:39:ALA:HB3	1.96	0.47
1:E:281:CYS:HB2	1:E:304:GLN:O	2.15	0.47
1:A:179:MET:HG2	1:A:234:TRP:HB3	1.95	0.47
1:C:98:TYR:CE2	1:C:226:GLN:HG2	2.50	0.47
1:C:49:ASN:O	1:C:50:ARG:HG2	2.15	0.47
2:B:64:GLU:OE2	7:B:201:HOH:O	2.21	0.46
1:C:49:ASN:C	1:C:50:ARG:HG2	2.40	0.46
2:D:95:GLN:HE21	2:F:95:GLN:NE2	2.09	0.46
1:E:14:CYS:N	2:F:25:ARG:O	2.36	0.46
1:C:108:LEU:HD13	1:C:234:TRP:CD2	2.50	0.46
1:E:12:LYS:HB2	2:F:138:PHE:O	2.15	0.46
2:F:17:MET:HE3	2:F:17:MET:HB2	1.75	0.46
2:B:128:GLN:OE1	2:B:170:ARG:NH1	2.43	0.46
1:E:151:LEU:HD23	1:E:254:PRO:HA	1.98	0.46
1:C:135:THR:O	5:I:2:SIA:H4	2.15	0.46
1:C:219:ALA:HB3	1:E:244:THR:HG21	1.98	0.46
2:D:3:PHE:CE2	2:D:113:SER:HB2	2.50	0.46
2:B:38:TYR:CZ	2:B:42:GLN:HG3	2.50	0.46
1:C:50:ARG:HG3	1:C:50:ARG:NH2	2.29	0.46
1:A:31:ASN:ND2	1:A:34:GLU:OE2	2.48	0.46
1:C:109:ARG:HG2	1:C:109:ARG:HH11	1.81	0.46
1:E:18:HIS:ND1	2:F:21:TRP:HA	2.30	0.46
2:F:52:LEU:HD23	2:F:52:LEU:HA	1.80	0.46
1:E:163:GLN:NE2	1:E:248:ASN:OD1	2.48	0.46
1:A:178:ILE:HG13	1:A:257:VAL:HG12	1.98	0.46
1:A:178:ILE:HG21	1:A:243:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:HIS:CG	1:C:66:PRO:HD2	2.51	0.46
2:D:118:LEU:HA	2:D:121:ARG:HG2	1.98	0.46
1:E:42:THR:HA	1:E:292:LEU:HD22	1.98	0.46
1:C:47:GLY:H	1:C:297:LEU:HD11	1.81	0.45
1:C:266:LEU:HD11	1:C:302:VAL:HG13	1.97	0.45
2:D:28:ASN:OD1	2:D:29:ALA:N	2.49	0.45
1:E:300:ARG:NE	2:F:69:GLU:OE2	2.30	0.45
2:B:3:PHE:HB2	2:B:112:ASP:CG	2.41	0.45
1:E:65:HIS:CE1	1:E:67:ILE:HG12	2.52	0.45
2:D:75:HIS:NE2	1:E:114:GLU:OE1	2.47	0.45
1:C:74:PRO:HA	1:C:77:ASP:OD1	2.17	0.45
1:A:191:LYS:NZ	1:A:198:GLN:O	2.42	0.45
2:D:68:SER:OG	2:D:71:SER:OG	2.26	0.45
2:B:166:ALA:O	2:B:170:ARG:N	2.49	0.45
1:E:65:HIS:ND1	1:E:67:ILE:HG12	2.32	0.45
1:E:48:ILE:HD12	1:E:48:ILE:N	2.30	0.44
2:D:66:ILE:HD11	2:D:85:LYS:HD3	1.99	0.44
2:F:17:MET:HE1	2:F:23:GLY:HA3	1.99	0.44
1:C:27:LYS:O	2:D:104:ASN:ND2	2.32	0.44
1:A:98:TYR:CE1	1:A:230:ILE:HG13	2.52	0.44
2:D:2:LEU:HD22	2:F:3:PHE:HE2	1.83	0.44
1:A:20:VAL:N	1:A:322:ASN:HD21	2.10	0.44
1:C:25:ILE:HG21	1:C:33:GLN:OE1	2.18	0.44
2:B:17:MET:HE1	2:B:22:TYR:C	2.42	0.43
2:B:48:ILE:HD11	2:B:107:THR:HG23	2.00	0.43
2:B:51:LYS:HZ2	2:B:107:THR:HG1	1.60	0.43
2:D:20:GLY:HA3	2:D:36:ALA:HB1	1.99	0.43
1:C:54:LYS:C	1:C:56:ARG:H	2.27	0.43
2:F:160:SER:HA	2:F:163:ARG:HE	1.83	0.43
1:E:83:MET:HE3	1:E:83:MET:HB3	1.93	0.43
2:D:77:ILE:O	2:D:81:ILE:HG13	2.19	0.43
1:E:307:LYS:HG3	2:F:92:TRP:CE2	2.54	0.43
2:D:133:ASP:OD2	2:D:137:CYS:HB2	2.19	0.43
1:E:118:ILE:HG12	1:E:260:LEU:HD23	2.00	0.43
2:D:91:ILE:HD13	2:F:91:ILE:HG21	2.01	0.43
2:B:50:GLY:HA3	1:E:30:THR:O	2.19	0.42
1:E:64:CYS:C	1:E:93:ALA:HB1	2.44	0.42
2:B:84:THR:O	2:B:88:ILE:HG12	2.18	0.42
2:B:142:HIS:HB3	2:B:166:ALA:HB2	2.02	0.42
1:C:109:ARG:HG2	1:C:109:ARG:NH1	2.34	0.42
2:B:121:ARG:HA	2:B:124:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:GLU:HA	2:D:70:PHE:CD2	2.54	0.42
1:C:150:GLU:OE1	1:C:256:ARG:NE	2.51	0.42
1:C:151:LEU:HD23	1:C:254:PRO:HA	2.01	0.42
2:D:90:ASP:OD1	2:F:61:THR:OG1	2.37	0.42
1:A:65:HIS:HB3	1:A:95:ALA:HB2	2.01	0.42
1:A:84:TRP:NE1	1:A:87:LEU:HB2	2.34	0.42
1:C:53:MET:HE2	1:C:58:HIS:HB3	2.01	0.42
2:F:149:MET:HA	2:F:152:ILE:HG13	1.99	0.42
1:C:314:LEU:HD21	2:D:97:GLU:OE2	2.19	0.42
2:F:25:ARG:NE	2:F:34:GLN:OE1	2.53	0.42
2:B:123:ARG:HG2	2:B:123:ARG:NH1	2.34	0.42
1:A:266:LEU:HD11	1:A:302:VAL:HG12	2.02	0.42
2:B:123:ARG:HD3	2:B:132:GLU:OE2	2.20	0.42
1:C:194:LEU:HD11	5:I:2:SIA:O7	2.20	0.42
1:C:52:CYS:HB3	1:C:277:CYS:O	2.20	0.42
1:C:318:THR:HG22	2:D:52:LEU:HD21	2.01	0.42
1:E:48:ILE:H	1:E:48:ILE:CD1	2.30	0.42
2:B:54:ARG:HH11	2:B:54:ARG:HG3	1.84	0.41
3:G:1:NAG:H61	3:G:2:NAG:N2	2.35	0.41
1:A:142:ASN:O	1:A:143:GLY:C	2.62	0.41
1:A:222:GLN:HG2	1:A:227:SER:HB2	2.02	0.41
1:E:314:LEU:HD23	1:E:314:LEU:HA	1.90	0.41
2:B:51:LYS:NZ	2:B:103:GLU:O	2.54	0.41
1:C:183:HIS:O	1:C:185:PRO:HD3	2.19	0.41
1:A:114:GLU:HB3	1:A:263:ARG:NH1	2.36	0.41
1:E:216:VAL:O	1:E:220:ARG:NH2	2.53	0.41
2:B:53:ASN:HD22	2:B:53:ASN:HA	1.71	0.41
2:B:54:ARG:HG3	2:B:54:ARG:NH1	2.36	0.41
1:E:201:SER:C	1:E:202:ILE:HG13	2.46	0.41
2:B:129:ASN:HB3	2:B:142:HIS:CD2	2.56	0.41
1:C:50:ARG:N	1:C:286:GLY:HA2	2.36	0.41
1:C:108:LEU:HD12	1:C:108:LEU:HA	1.89	0.41
2:F:125:GLN:HE22	2:F:155:ASN:HA	1.85	0.41
1:E:146:SER:OG	1:E:147:PHE:N	2.52	0.41
1:E:189:GLN:HG2	1:E:193:ASP:OD2	2.21	0.41
1:C:134:GLY:HA3	5:I:2:SIA:H113	2.02	0.40
2:D:110:MET:HG3	2:D:111:ALA:N	2.36	0.40
1:A:36:VAL:HG11	1:A:317:ALA:HB1	2.04	0.40
1:A:108:LEU:O	1:A:112:ILE:HG13	2.21	0.40
1:E:97:CYS:HB2	1:E:138:ALA:O	2.21	0.40
2:F:47:GLN:HB2	2:F:110:MET:HE1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLN:HG3	1:C:190:GLU:N	2.36	0.40
2:F:148:CYS:O	2:F:151:SER:HB2	2.20	0.40
1:A:66:PRO:HA	1:A:69:MET:HE2	2.01	0.40
1:C:161:PHE:HB3	1:C:248:ASN:O	2.21	0.40
2:F:84:THR:O	2:F:88:ILE:HG12	2.20	0.40
2:B:43:ALA:O	2:B:47:GLN:HG3	2.22	0.40
2:B:128:GLN:NE2	2:F:131:GLU:OE2	2.55	0.40
1:C:137:ARG:HB2	1:C:140:MET:HE3	2.04	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	312/326 (96%)	302 (97%)	10 (3%)	0	100	100
1	C	313/326 (96%)	295 (94%)	18 (6%)	0	100	100
1	E	316/326 (97%)	305 (96%)	10 (3%)	1 (0%)	36	54
2	B	165/181 (91%)	161 (98%)	4 (2%)	0	100	100
2	D	162/181 (90%)	149 (92%)	12 (7%)	1 (1%)	21	38
2	F	160/181 (88%)	157 (98%)	3 (2%)	0	100	100
All	All	1428/1521 (94%)	1369 (96%)	57 (4%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	144	CYS
1	E	324	PRO

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	268/275 (98%)	262 (98%)	6 (2%)	45	69
1	C	266/275 (97%)	258 (97%)	8 (3%)	36	61
1	E	269/275 (98%)	263 (98%)	6 (2%)	45	69
2	B	144/154 (94%)	139 (96%)	5 (4%)	32	57
2	D	144/154 (94%)	139 (96%)	5 (4%)	32	57
2	F	143/154 (93%)	134 (94%)	9 (6%)	16	34
All	All	1234/1287 (96%)	1195 (97%)	39 (3%)	34	59

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	44	GLU
1	A	91	GLU
1	A	141	ARG
1	A	242	ASN
1	A	287	SER
2	B	25	ARG
2	B	45	ILE
2	B	102	MET
2	B	161	GLN
2	B	164	GLU
1	C	13	ILE
1	C	44	GLU
1	C	50	ARG
1	C	83	MET
1	C	220	ARG
1	C	258	SER
1	C	302	VAL
1	C	323	VAL
2	D	52	LEU
2	D	62	GLU
2	D	102	MET

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Mol	Chain	Res	Type
2	D	110	MET
2	D	172	ASN
1	E	48	ILE
1	E	141	ARG
1	E	154	LEU
1	E	210	ARG
1	E	280	LYS
1	E	304	GLN
2	F	28	ASN
2	F	72	GLU
2	F	74	GLU
2	F	110	MET
2	F	121	ARG
2	F	145	ASP
2	F	161	GLN
2	F	163	ARG
2	F	164	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	18	HIS
1	A	49	ASN
1	A	238	GLN
1	A	276	ASN
1	A	295	GLN
1	A	296	ASN
1	A	310	ASN
1	A	322	ASN
2	B	28	ASN
2	B	53	ASN
2	B	95	GLN
2	B	125	GLN
2	B	129	ASN
2	B	142	HIS
2	B	154	ASN
1	C	18	HIS
1	C	110	GLN
1	C	192	ASN
1	C	226	GLN
1	C	269	GLN

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Mol	Chain	Res	Type
2	D	12	ASN
2	D	53	ASN
2	D	60	ASN
2	D	76	GLN
2	D	95	GLN
2	D	105	GLN
2	D	117	ASN
2	D	154	ASN
1	E	22	ASN
1	E	159	GLN
1	E	198	GLN
1	E	212	ASN
1	E	226	GLN
1	E	295	GLN
2	F	28	ASN
2	F	42	GLN
2	F	60	ASN
2	F	117	ASN
2	F	125	GLN
2	F	129	ASN
2	F	155	ASN
2	F	161	GLN
2	F	169	ASN
2	F	172	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

9 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	0.73	1 (7%)	17,19,21	0.89	1 (5%)
3	NAG	G	2	3	14,14,15	0.45	0	17,19,21	0.92	1 (5%)
4	NAG	H	1	4	15,15,15	0.47	0	21,21,21	1.47	4 (19%)
4	GAL	H	2	4	11,11,12	0.44	0	15,15,17	0.81	0
4	SIA	H	3	4	20,20,21	0.57	0	21,28,31	1.38	4 (19%)
5	GAL	I	1	5	12,12,12	1.12	1 (8%)	17,17,17	0.90	1 (5%)
5	SIA	I	2	5	20,20,21	0.55	0	21,28,31	1.34	5 (23%)
3	NAG	J	1	3,1	14,14,15	0.72	1 (7%)	17,19,21	0.98	1 (5%)
3	NAG	J	2	3	14,14,15	0.32	0	17,19,21	0.77	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	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
4	NAG	H	1	4	-	1/6/26/26	0/1/1/1
4	GAL	H	2	4	-	0/2/19/22	0/1/1/1
4	SIA	H	3	4	-	0/18/34/38	0/1/1/1
5	GAL	I	1	5	-	0/2/22/22	0/1/1/1
5	SIA	I	2	5	-	0/18/34/38	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1	GAL	O1-C1	-3.75	1.27	1.39
3	J	1	NAG	O5-C1	-2.35	1.39	1.43
3	G	1	NAG	O5-C1	-2.30	1.39	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	3	SIA	O6-C2-C1	3.42	114.17	107.72
4	H	1	NAG	C1-C2-N2	-3.39	106.80	110.73
4	H	1	NAG	C4-C3-C2	3.33	115.25	110.40
5	I	2	SIA	C4-C5-N5	-3.20	104.13	110.44
3	J	1	NAG	C1-C2-N2	-2.75	106.10	110.43
4	H	1	NAG	C3-C4-C5	2.72	115.16	110.23
4	H	1	NAG	C3-C2-N2	-2.65	105.73	110.62
4	H	3	SIA	C4-C5-N5	-2.65	105.22	110.44
3	G	2	NAG	C2-N2-C7	-2.57	119.46	122.90
5	I	2	SIA	O1B-C1-C2	2.51	119.24	112.71
5	I	1	GAL	O5-C1-C2	-2.43	106.03	110.30
5	I	2	SIA	O6-C2-C1	2.38	112.21	107.72
4	H	3	SIA	O1B-C1-C2	2.28	118.63	112.71
4	H	3	SIA	C6-C5-N5	-2.10	107.56	110.91
5	I	2	SIA	O1A-C1-C2	-2.08	118.35	122.85
3	G	1	NAG	C1-C2-N2	-2.05	107.20	110.43
5	I	2	SIA	C6-C5-N5	-2.02	107.68	110.91

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
4	H	1	NAG	C1-C2-N2-C7
3	G	2	NAG	O7-C7-N2-C2

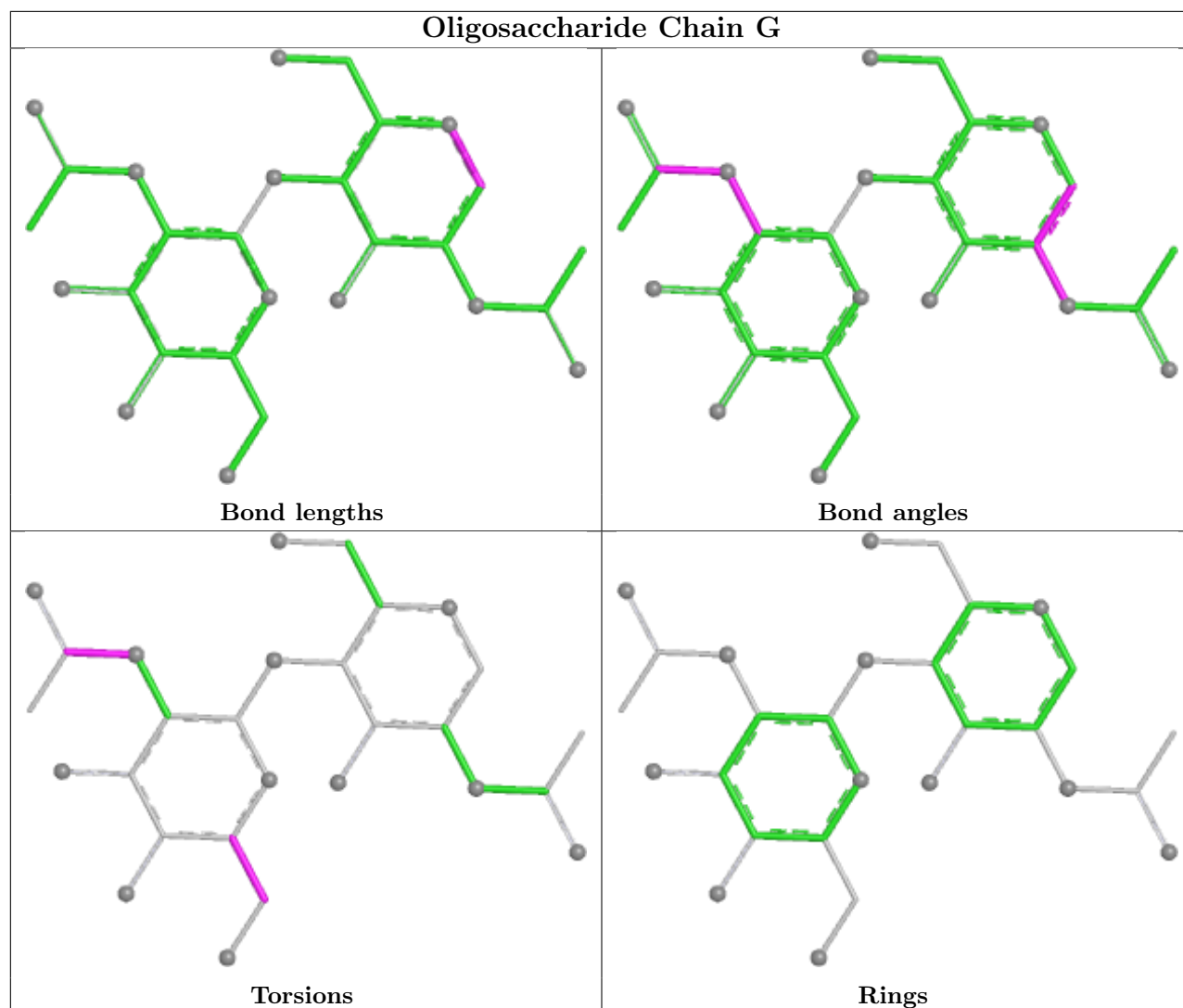
There are no ring outliers.

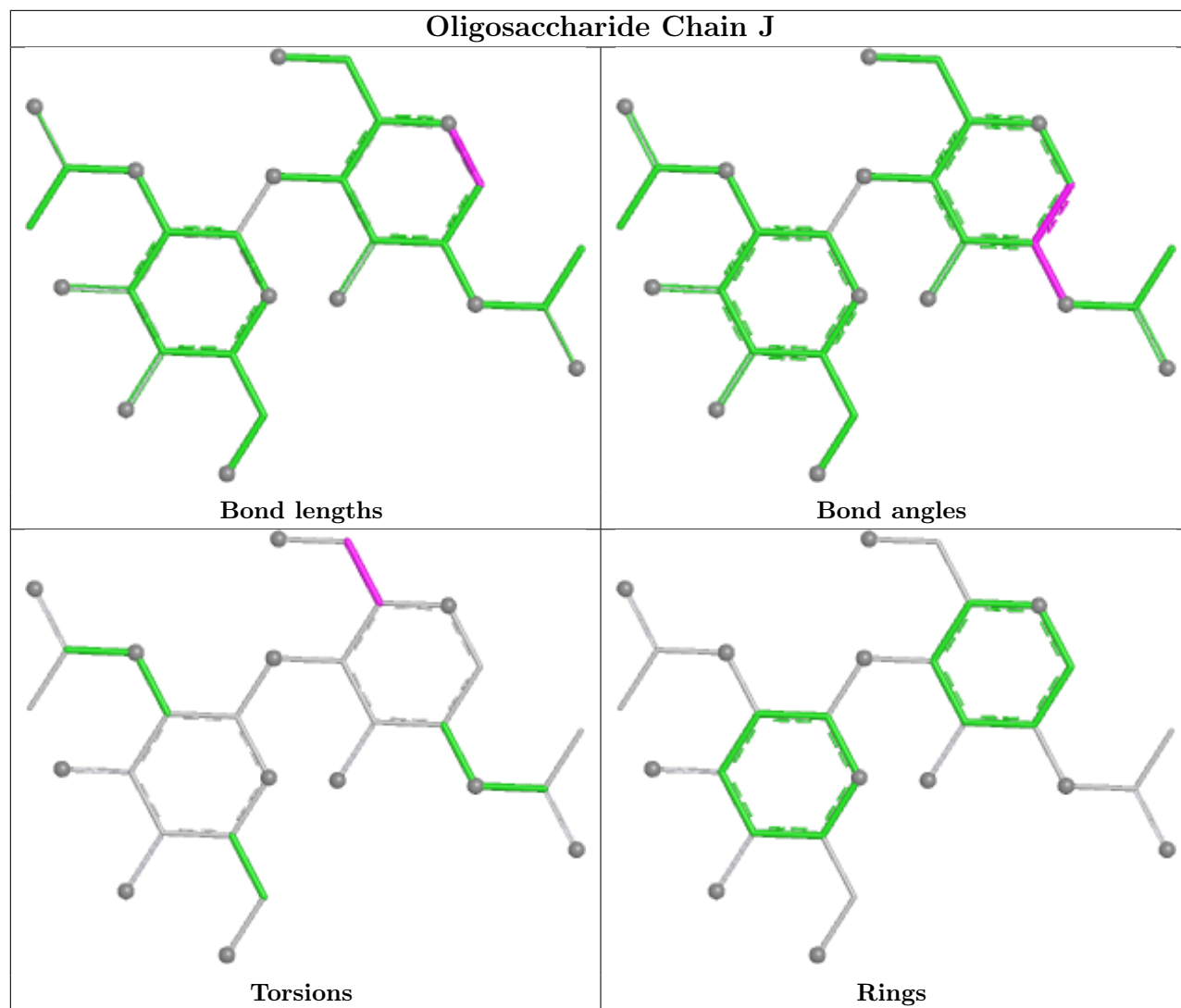
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0
4	H	3	SIA	2	0
5	I	2	SIA	3	0
3	J	1	NAG	1	0
5	I	1	GAL	1	0
3	G	1	NAG	1	0

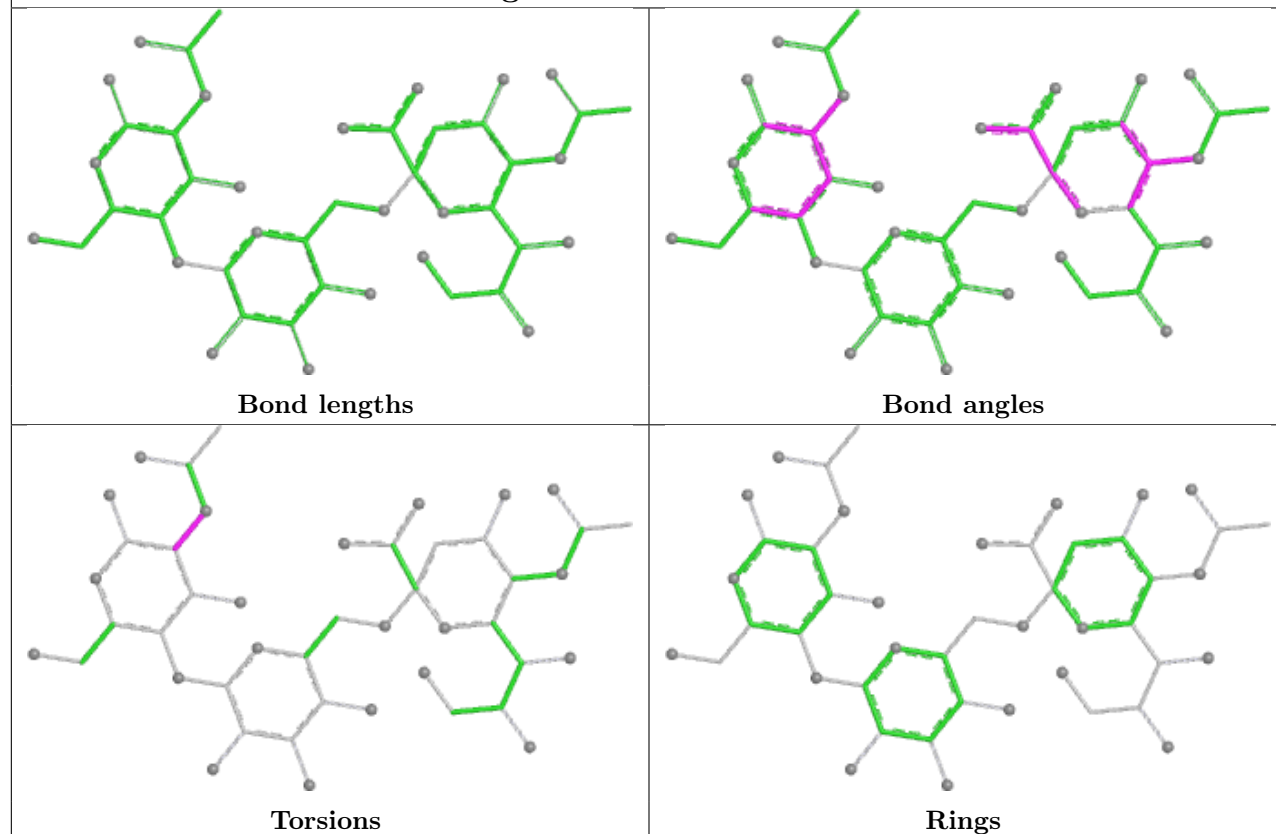
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

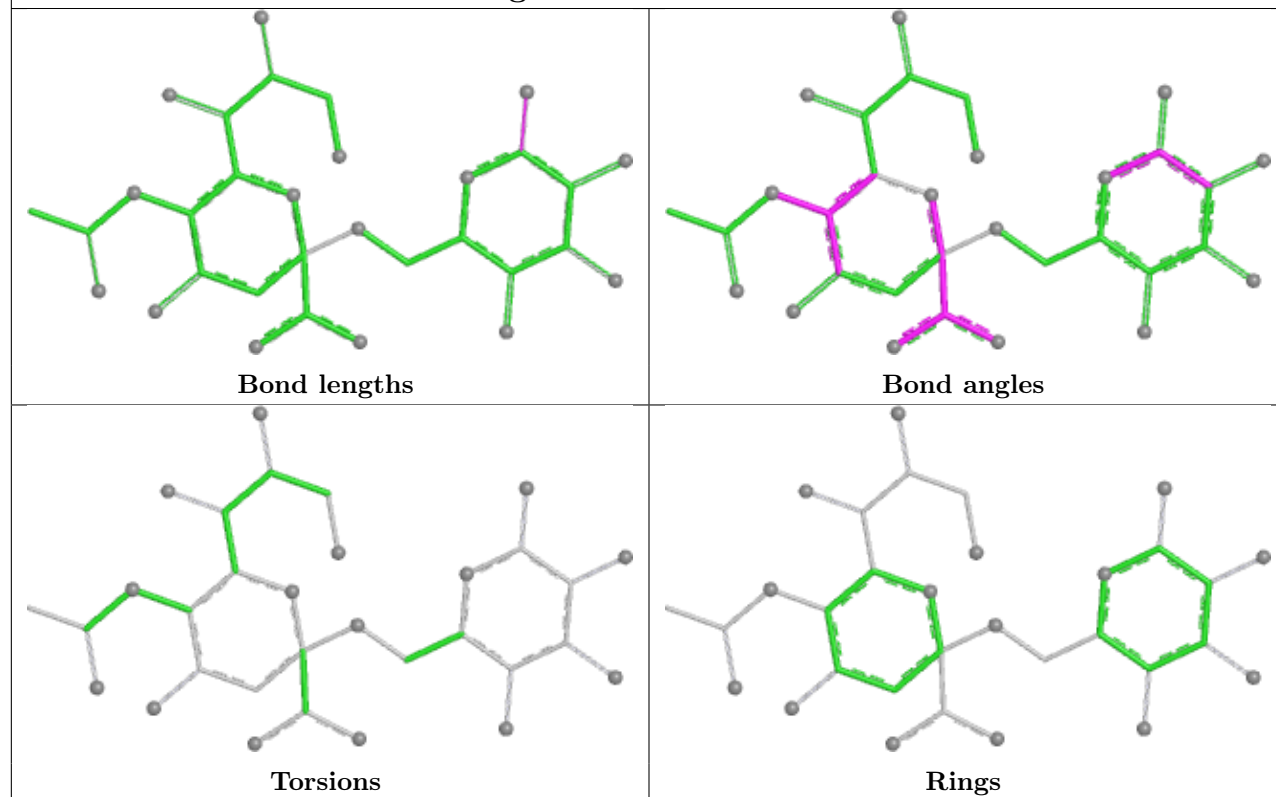




Oligosaccharide Chain H



Oligosaccharide Chain I



5.6 Ligand geometry

2 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	A	401	1	14,14,15	0.62	1 (7%)	17,19,21	0.58	0
6	NAG	C	501	1	14,14,15	0.76	1 (7%)	17,19,21	0.81	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	A	401	1	-	0/6/23/26	0/1/1/1
6	NAG	C	501	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	501	NAG	O5-C1	-2.31	1.39	1.43
6	A	401	NAG	O5-C1	-2.22	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	501	NAG	C4-C5-C6-O6
6	C	501	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	316/326 (96%)	1.36	63 (19%) 3 3	39, 53, 82, 99	0
1	C	315/326 (96%)	1.56	86 (27%) 1 1	40, 59, 87, 101	0
1	E	318/326 (97%)	1.44	70 (22%) 2 2	37, 60, 98, 113	0
2	B	169/181 (93%)	1.83	64 (37%) 1 0	45, 81, 100, 108	0
2	D	168/181 (92%)	2.00	75 (44%) 0 0	53, 83, 103, 112	0
2	F	166/181 (91%)	2.23	91 (54%) 0 0	42, 88, 108, 117	0
All	All	1452/1521 (95%)	1.65	449 (30%) 1 1	37, 65, 100, 117	0

All (449) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	117	ASN	6.2
1	C	16	GLY	5.8
1	A	297	LEU	5.7
2	F	118	LEU	5.6
1	C	15	LEU	5.5
2	B	59	THR	5.4
2	F	170	ARG	5.4
1	E	15	LEU	5.2
2	B	56	VAL	5.1
1	E	319	GLY	4.9
2	F	164	GLU	4.8
1	A	48	ILE	4.7
2	F	7	ALA	4.7
1	A	202	ILE	4.7
1	A	40	THR	4.7
2	D	8	GLY	4.6
2	B	138	PHE	4.6
2	B	141	TYR	4.5
1	C	42	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	40	THR	4.5
2	D	136	GLY	4.5
1	A	47	GLY	4.4
2	F	136	GLY	4.4
2	F	131	GLU	4.3
1	A	143	GLY	4.3
2	D	138	PHE	4.3
2	D	24	PHE	4.2
2	F	2	LEU	4.2
2	F	23	GLY	4.2
1	E	14	CYS	4.1
2	F	141	TYR	4.1
2	F	134	GLY	4.1
2	D	16	GLY	4.1
1	C	70	LEU	4.1
2	D	2	LEU	4.0
2	B	143	ALA	4.0
1	C	26	VAL	4.0
2	B	43	ALA	4.0
2	F	87	SER	4.0
1	C	324	PRO	3.9
1	E	20	VAL	3.9
2	F	137	CYS	3.9
2	D	158	ASP	3.9
2	D	152	ILE	3.8
1	A	250	GLY	3.8
1	A	39	ALA	3.8
2	F	168	LEU	3.8
2	F	24	PHE	3.8
1	A	11	ASP	3.8
2	F	122	VAL	3.7
1	C	19	ALA	3.7
1	E	29	LEU	3.7
2	D	7	ALA	3.7
2	F	5	ALA	3.7
1	C	132	SER	3.7
2	F	47	GLN	3.7
1	E	98	TYR	3.7
2	F	119	TYR	3.7
2	B	55	LEU	3.6
2	D	119	TYR	3.6
1	E	313	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	22	TYR	3.6
2	B	61	THR	3.6
1	A	21	ALA	3.6
2	F	36	ALA	3.6
2	F	34	GLN	3.5
1	C	20	VAL	3.5
1	C	190	GLU	3.5
2	B	2	LEU	3.5
1	E	291	ARG	3.5
2	B	140	ILE	3.5
2	D	171	LEU	3.5
1	C	27	LYS	3.5
2	D	121	ARG	3.5
2	F	133	ASP	3.5
2	F	138	PHE	3.4
2	D	52	LEU	3.4
2	B	119	TYR	3.4
2	F	116	LEU	3.4
2	F	130	ALA	3.4
2	F	6	ILE	3.4
2	B	134	GLY	3.3
2	D	106	HIS	3.3
1	A	313	SER	3.3
2	F	65	SER	3.3
1	C	320	MET	3.3
1	A	95	ALA	3.3
1	E	277	CYS	3.3
1	E	312	ARG	3.3
2	F	29	ALA	3.3
1	A	20	VAL	3.2
1	A	303	GLY	3.2
2	D	21	TRP	3.2
2	F	172	ASN	3.2
2	F	123	ARG	3.2
1	C	323	VAL	3.2
2	D	149	MET	3.2
1	A	299	PRO	3.2
2	D	37	ASP	3.2
2	F	19	ASP	3.2
2	F	109	ASP	3.2
1	C	126	THR	3.2
1	C	193	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	290	THR	3.1
2	F	11	GLU	3.1
2	D	157	TYR	3.1
1	A	12	LYS	3.1
2	B	29	ALA	3.1
2	D	143	ALA	3.1
1	A	231	ASP	3.1
2	B	24	PHE	3.1
2	F	117	ASN	3.1
1	C	47	GLY	3.1
2	B	62	GLU	3.1
2	F	167	LEU	3.1
2	D	35	ALA	3.1
1	A	285	GLY	3.1
1	C	319	GLY	3.1
1	E	21	ALA	3.1
2	F	9	PHE	3.1
2	D	48	ILE	3.1
2	F	35	ALA	3.0
2	D	115	MET	3.0
1	C	289	ASN	3.0
2	F	58	LYS	3.0
2	F	96	ALA	3.0
2	F	143	ALA	3.0
1	C	315	MET	3.0
1	A	291	ARG	3.0
1	E	13	ILE	3.0
2	B	47	GLN	3.0
2	F	120	GLU	3.0
2	D	5	ALA	3.0
2	D	9	PHE	3.0
2	F	157	TYR	3.0
1	C	291	ARG	3.0
2	F	132	GLU	3.0
2	F	56	VAL	3.0
1	E	30	THR	3.0
2	F	44	ALA	3.0
2	D	3	PHE	3.0
2	F	171	LEU	2.9
1	A	159	GLN	2.9
2	B	127	ARG	2.9
2	F	28	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	137	CYS	2.9
2	D	156	THR	2.9
2	F	135	LYS	2.9
1	C	184	HIS	2.9
1	E	25	ILE	2.9
1	A	49	ASN	2.9
1	C	271	ASP	2.9
2	B	3	PHE	2.9
1	A	300	ARG	2.9
2	F	142	HIS	2.9
2	D	134	GLY	2.9
1	A	283	TRP	2.9
2	B	157	TYR	2.9
1	E	248	ASN	2.9
1	E	18	HIS	2.9
1	A	19	ALA	2.8
2	F	155	ASN	2.8
2	D	40	SER	2.8
2	D	140	ILE	2.8
1	A	228	GLY	2.8
2	B	164	GLU	2.8
2	D	15	GLU	2.8
2	D	100	VAL	2.8
1	C	22	ASN	2.8
1	A	290	THR	2.8
2	B	6	ILE	2.8
2	B	171	LEU	2.8
2	D	6	ILE	2.8
2	D	99	LEU	2.8
1	E	231	ASP	2.8
1	C	159	GLN	2.8
2	F	139	GLU	2.8
2	B	94	TYR	2.8
2	D	155	ASN	2.8
1	A	46	THR	2.8
1	C	250	GLY	2.8
1	C	309	VAL	2.7
2	D	14	TRP	2.7
1	A	82	GLY	2.7
2	F	18	VAL	2.7
1	E	266	LEU	2.7
1	E	317	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	288	ILE	2.7
2	B	66	ILE	2.7
2	B	168	LEU	2.7
2	D	116	LEU	2.7
1	E	224	ASN	2.7
1	A	318	THR	2.7
1	C	37	THR	2.7
2	B	27	GLN	2.7
2	D	97	GLU	2.7
2	B	21	TRP	2.7
1	C	249	GLY	2.7
2	B	93	THR	2.7
2	D	32	THR	2.7
2	D	95	GLN	2.7
1	E	94	ILE	2.7
2	F	140	ILE	2.7
1	A	42	THR	2.7
1	C	23	GLY	2.7
2	F	82	ASN	2.7
2	B	64	GLU	2.7
2	B	105	GLN	2.7
1	A	302	VAL	2.7
2	D	45	ILE	2.6
2	F	10	LEU	2.7
2	B	9	PHE	2.6
1	A	117	GLY	2.6
1	E	28	THR	2.6
1	E	11	ASP	2.6
2	D	19	ASP	2.6
1	A	317	ALA	2.6
2	F	68	SER	2.6
1	C	96	TYR	2.6
2	B	153	ARG	2.6
1	A	305	CYS	2.6
2	B	122	VAL	2.6
1	C	317	ALA	2.6
1	C	30	THR	2.6
2	D	126	LEU	2.6
1	C	21	ALA	2.6
1	C	174	ALA	2.6
1	E	158	SER	2.6
1	C	314	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	175	GLU	2.6
2	B	60	ASN	2.6
2	F	63	PHE	2.6
2	B	19	ASP	2.6
1	E	27	LYS	2.5
1	C	124	GLY	2.5
1	A	168	TYR	2.5
2	B	22	TYR	2.5
1	C	25	ILE	2.5
1	E	26	VAL	2.5
2	B	152	ILE	2.5
1	C	95	ALA	2.5
2	D	129	ASN	2.5
2	F	60	ASN	2.5
1	E	250	GLY	2.5
2	B	124	LYS	2.5
1	C	287	SER	2.5
1	E	186	SER	2.5
1	A	324	PRO	2.5
1	E	53	MET	2.5
2	F	52	LEU	2.5
1	A	13	ILE	2.5
2	F	20	GLY	2.5
1	E	24	THR	2.5
2	F	153	ARG	2.5
1	C	248	ASN	2.5
2	D	144	CYS	2.5
2	F	55	LEU	2.5
1	C	258	SER	2.5
1	C	33	GLN	2.5
1	E	253	ALA	2.5
2	D	161	GLN	2.5
2	B	41	THR	2.5
1	E	58	HIS	2.5
1	C	14	CYS	2.5
2	B	144	CYS	2.5
2	F	98	LEU	2.4
2	B	139	GLU	2.4
2	F	3	PHE	2.4
1	E	157	LYS	2.4
2	B	95	GLN	2.4
2	F	12	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	129	ASN	2.4
1	C	13	ILE	2.4
2	D	33	GLY	2.4
2	D	11	GLU	2.4
1	C	253	ALA	2.4
2	B	36	ALA	2.4
2	D	107	THR	2.4
1	A	15	LEU	2.4
1	A	296	ASN	2.4
1	E	88	ILE	2.4
1	C	82	GLY	2.4
2	D	46	ASP	2.4
1	C	115	SER	2.4
1	C	122	SER	2.4
1	E	174	ALA	2.4
2	B	5	ALA	2.4
2	B	35	ALA	2.4
2	F	111	ALA	2.4
2	D	27	GLN	2.4
2	F	22	TYR	2.4
1	E	17	HIS	2.4
1	E	31	ASN	2.4
1	A	309	VAL	2.4
1	E	305	CYS	2.4
2	B	130	ALA	2.4
1	A	287	SER	2.4
2	F	14	TRP	2.4
2	F	49	THR	2.4
1	E	70	LEU	2.4
2	D	55	LEU	2.4
1	E	71	ILE	2.4
2	B	154	ASN	2.3
2	B	136	GLY	2.3
2	F	67	GLU	2.3
1	E	258	SER	2.3
2	F	113	SER	2.3
1	C	46	THR	2.3
2	D	118	LEU	2.3
1	C	88	ILE	2.3
1	E	54	LYS	2.3
1	E	257	VAL	2.3
2	D	56	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	122	VAL	2.3
1	A	142	ASN	2.3
1	C	278	GLU	2.3
2	D	165	GLU	2.3
2	F	149	MET	2.3
1	C	200	LEU	2.3
1	C	28	THR	2.3
1	E	148	TYR	2.3
2	F	107	THR	2.3
2	B	121	ARG	2.3
1	C	155	VAL	2.3
2	D	20	GLY	2.3
1	E	184	HIS	2.3
2	F	50	GLY	2.3
2	D	60	ASN	2.3
1	C	39	ALA	2.3
1	A	304	GLN	2.3
1	E	97	CYS	2.3
1	E	158(A)	LYS	2.3
1	C	318	THR	2.3
2	D	49	THR	2.3
1	C	55	GLY	2.3
1	E	310	ASN	2.2
1	E	151	LEU	2.2
1	A	241	ASP	2.2
2	F	48	ILE	2.2
1	A	70	LEU	2.2
1	A	314	LEU	2.2
2	F	66	ILE	2.2
1	A	247	HIS	2.2
2	F	112	ASP	2.2
1	E	153	TRP	2.2
1	C	45	SER	2.2
2	D	17	MET	2.2
1	C	219	ALA	2.2
2	B	99	LEU	2.2
2	D	39	LYS	2.2
2	F	72	GLU	2.2
1	E	322	ASN	2.2
1	E	293	PRO	2.2
2	B	18	VAL	2.2
1	A	30	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	24	THR	2.2
2	B	89	THR	2.2
1	A	14	CYS	2.2
2	D	102	MET	2.2
1	C	187	SER	2.2
2	D	141	TYR	2.2
2	F	8	GLY	2.2
1	A	316	LEU	2.2
1	C	32	GLU	2.2
1	C	220	ARG	2.2
1	E	33	GLN	2.2
1	E	222	GLN	2.2
2	B	129	ASN	2.2
2	D	154	ASN	2.2
2	B	156	THR	2.2
1	A	129	SER	2.2
1	C	313	SER	2.2
1	A	107	ALA	2.2
1	E	19	ALA	2.2
2	D	142	HIS	2.1
1	C	123	THR	2.1
2	B	39	LYS	2.1
2	F	21	TRP	2.1
1	C	154	LEU	2.1
1	C	186	SER	2.1
2	F	26	HIS	2.1
2	F	106	HIS	2.1
1	A	83	MET	2.1
1	C	158(A)	LYS	2.1
1	E	57	LYS	2.1
1	E	152	LYS	2.1
2	B	86	ASP	2.1
1	A	205	GLY	2.1
1	C	208	THR	2.1
1	E	173	THR	2.1
2	D	167	LEU	2.1
1	A	234	TRP	2.1
2	D	170	ARG	2.1
2	F	166	ALA	2.1
1	E	52	CYS	2.1
1	E	298	SER	2.1
1	C	259	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	105	VAL	2.1
1	A	193	ASP	2.1
1	C	87	LEU	2.1
1	C	164	THR	2.1
2	D	29	ALA	2.1
2	B	15	GLU	2.1
1	E	156	SER	2.1
2	B	28	ASN	2.1
2	B	155	ASN	2.1
1	C	194	LEU	2.1
1	E	177	LEU	2.1
1	C	125	PHE	2.1
1	C	85	ASP	2.1
2	B	37	ASP	2.1
1	A	243	ILE	2.1
1	C	153	TRP	2.1
1	E	288	ILE	2.1
2	B	7	ALA	2.1
2	B	88	ILE	2.1
2	D	92	TRP	2.1
1	C	168	TYR	2.1
1	C	113	MET	2.0
1	C	227	SER	2.0
1	A	217	VAL	2.0
1	C	237	VAL	2.0
1	A	22	ASN	2.0
1	C	51	LEU	2.0
2	F	104	ASN	2.0
1	E	16	GLY	2.0
2	D	153	ARG	2.0
1	E	37	THR	2.0
1	A	271	ASP	2.0
2	F	165	GLU	2.0
2	B	85	LYS	2.0
2	F	162	TYR	2.0
2	D	151	SER	2.0
1	A	52	CYS	2.0
2	B	137	CYS	2.0
2	F	144	CYS	2.0
1	A	266	LEU	2.0
2	D	28	ASN	2.0
2	F	127	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	240	GLY	2.0
1	C	71	ILE	2.0
1	E	136	THR	2.0
1	E	219	ALA	2.0
2	F	37	ASP	2.0
2	F	124	LYS	2.0
1	A	320	MET	2.0
2	D	94	TYR	2.0
2	F	38	TYR	2.0
1	C	43	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](#)

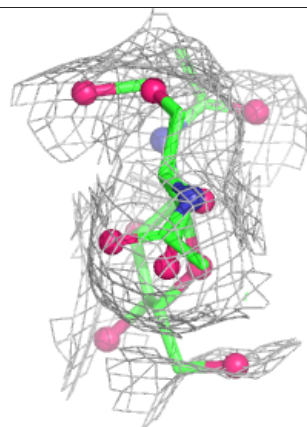
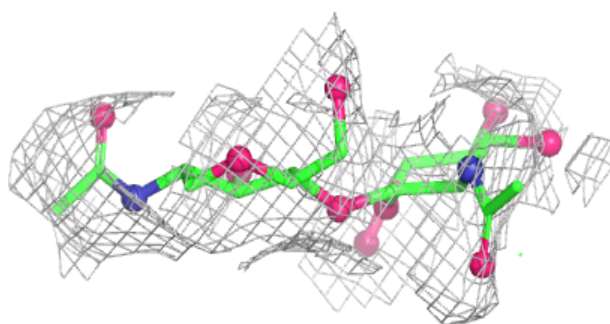
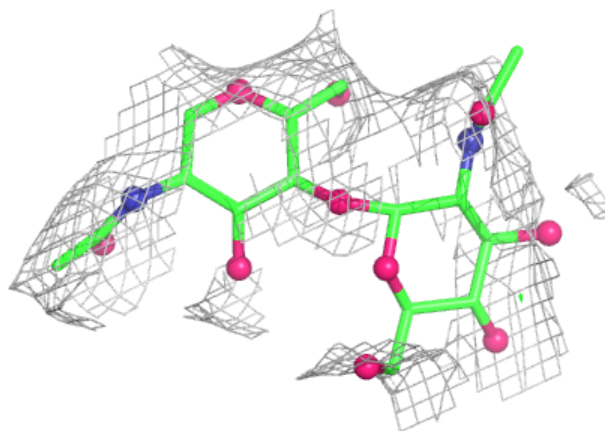
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	H	1	15/15	0.40	0.21	88,104,109,117	0
3	NAG	G	2	14/15	0.48	0.18	104,113,122,125	0
3	NAG	J	2	14/15	0.54	0.20	123,128,143,144	0
4	GAL	H	2	11/12	0.64	0.16	71,82,94,97	0
3	NAG	G	1	14/15	0.65	0.17	64,83,92,101	0
4	SIA	H	3	20/21	0.71	0.19	54,72,82,83	0
5	GAL	I	1	12/12	0.72	0.15	68,92,104,105	0
3	NAG	J	1	14/15	0.77	0.12	74,86,102,105	0
5	SIA	I	2	20/21	0.86	0.14	50,63,79,81	0

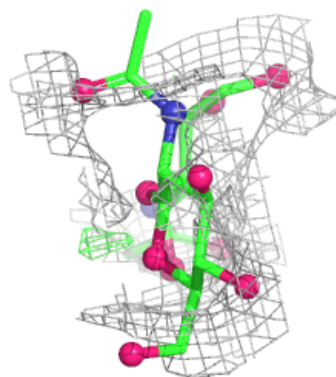
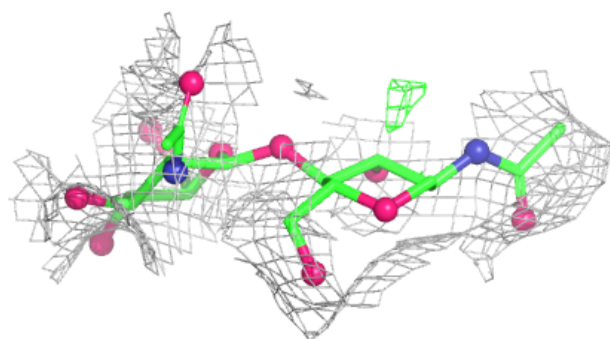
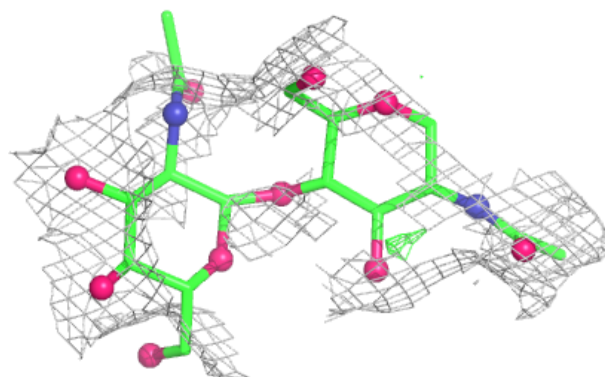
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

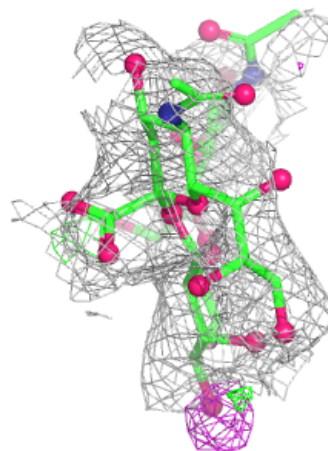
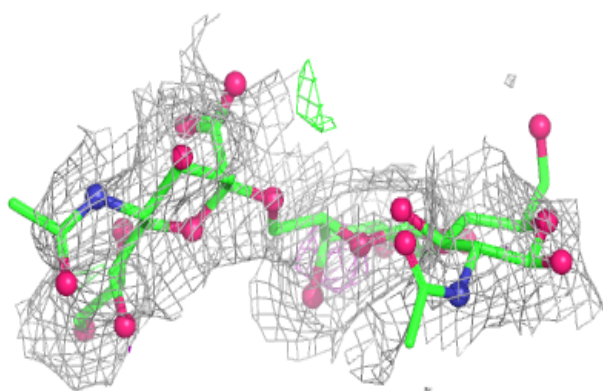
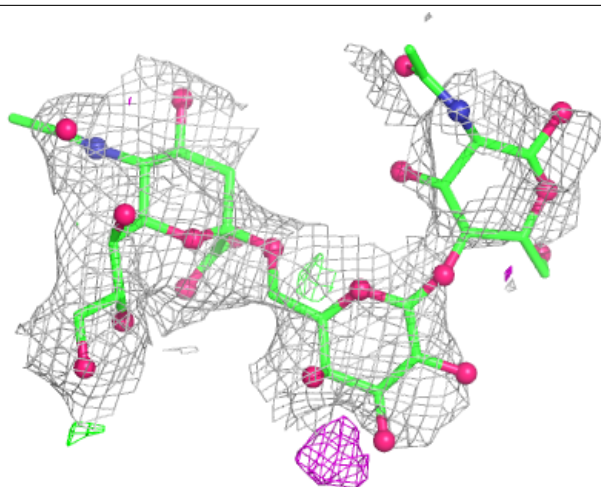
**Electron density around Chain J:**

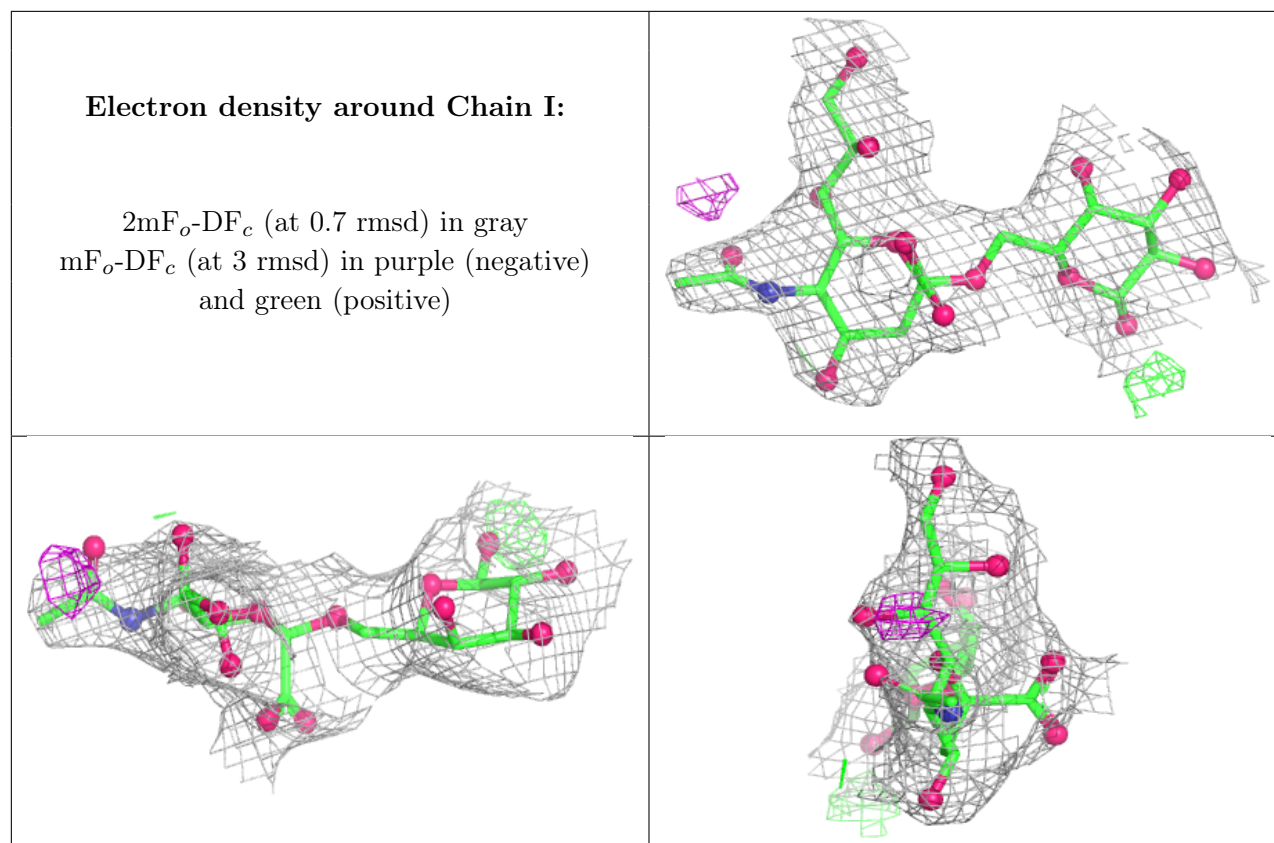
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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
6	NAG	A	401	14/15	0.69	0.18	86,98,107,112	0
6	NAG	C	501	14/15	0.71	0.22	61,80,94,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.