



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:22 PM UTC

PDB ID : 5Y2L / pdb_00005y2l
Title : Crystal structure of a group 2 HA binding antibody AF4H1K1 Fab in complex with the 1968 H3N2 pandemic (H3-AC/68) hemagglutinin
Authors : Xiao, H.; Qi, J.; Gao, F.G.
Deposited on : 2017-07-26
Resolution : 2.90 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:

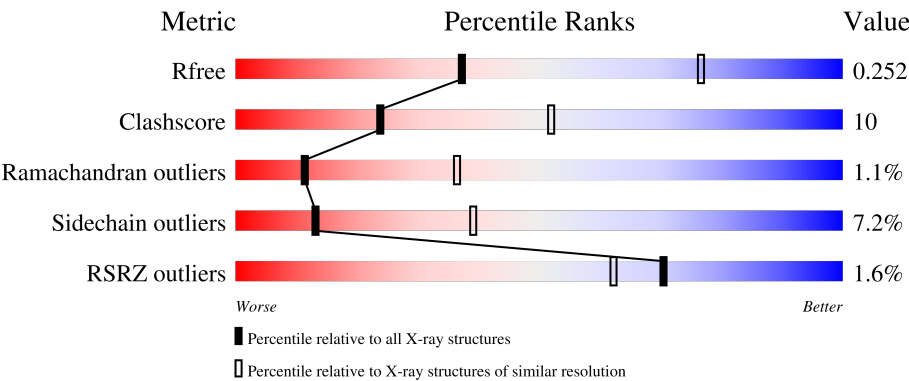
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	329	% 77% 18% • •
2	B	176	2% 59% 25% 7% • 7%
3	I	233	2% 70% 22% • •
4	J	220	% 71% 19% 6% •
5	C	2	50% 50%

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Mol	Chain	Length	Quality of chain
5	D	2	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7189 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	317	Total	C	N	O	S	0	0	0
			2446	1532	429	472	13			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	163	Total	C	N	O	S	0	0	0
			1335	823	236	270	6			

- Molecule 3 is a protein called a group 2 HA binding antibody AF4H1K1 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	224	Total	C	N	O	S	0	0	0
			1694	1077	286	325	6			

- Molecule 4 is a protein called a group 2 HA binding antibody AF4H1K1 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	212	Total	C	N	O	S	0	0	0
			1630	1018	278	329	5			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



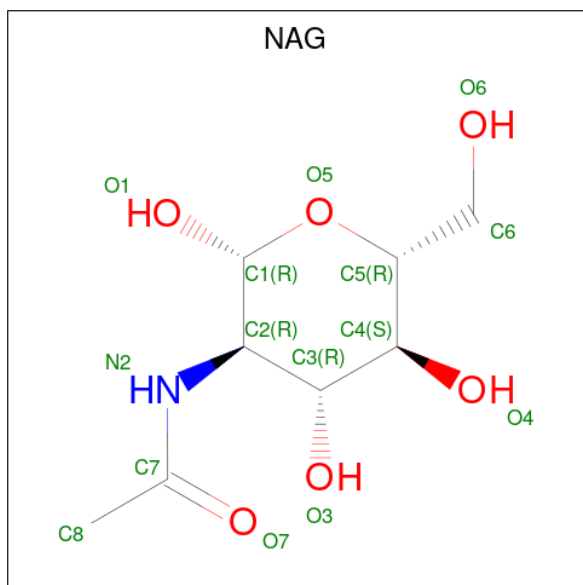
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

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

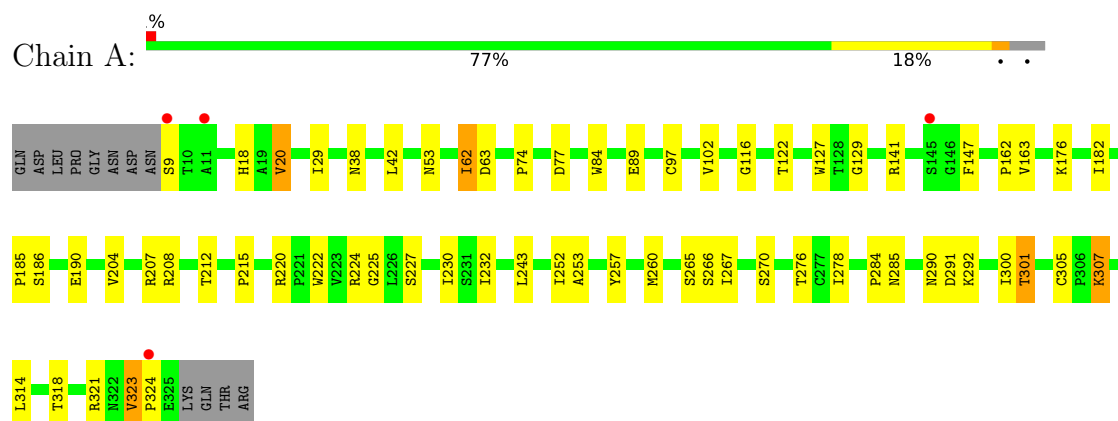


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

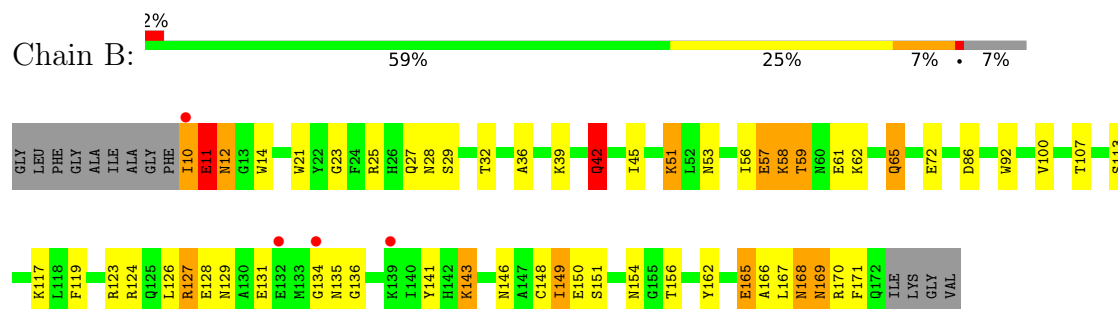
3 Residue-property plots [i](#)

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.

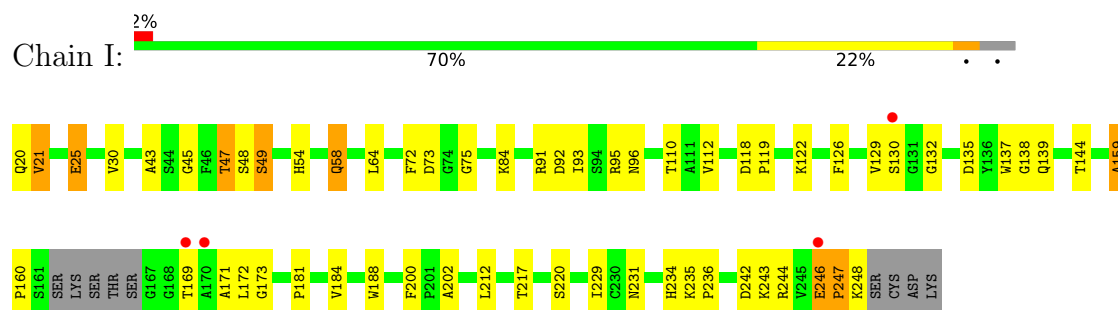
• Molecule 1: Hemagglutinin



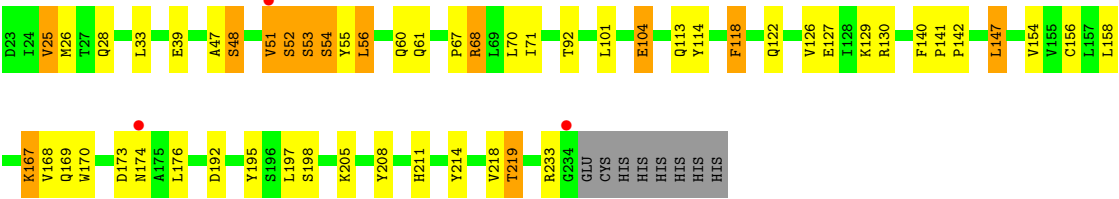
• Molecule 2: Hemagglutinin



• Molecule 3: a group 2 HA binding antibody AF4H1K1 Fab heavy chain



• Molecule 4: a group 2 HA binding antibody AF4H1K1 Fab light chain



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	157.48Å 157.48Å 355.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.33 – 2.90 47.33 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.33-2.90) 99.8 (47.33-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.212 , 0.244 0.222 , 0.252	Depositor DCC
R_{free} test set	1888 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.710	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7189	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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

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	0.47	0/2502	0.82	0/3410
2	B	0.70	3/1357 (0.2%)	1.04	7/1825 (0.4%)
3	I	0.52	0/1739	0.87	6/2372 (0.3%)
4	J	0.53	0/1665	0.86	1/2258 (0.0%)
All	All	0.54	3/7263 (0.0%)	0.88	14/9865 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	165	GLU	C-O	-8.45	1.14	1.24
2	B	65	GLN	CA-C	-6.29	1.50	1.53
2	B	169	ASN	CA-C	-5.16	1.45	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	11	GLU	N-CA-CB	-13.08	88.39	110.49
2	B	136	GLY	N-CA-C	-9.53	101.73	115.64
3	I	235	LYS	CA-C-N	-7.77	111.64	119.56
3	I	235	LYS	C-N-CA	-7.77	111.64	119.56
2	B	42	GLN	CA-CB-CG	6.24	126.59	114.10
4	J	54	SER	N-CA-C	-6.16	105.34	112.86
3	I	246	GLU	CA-C-N	6.14	127.51	119.84
3	I	246	GLU	C-N-CA	6.14	127.51	119.84
2	B	65	GLN	CB-CA-C	-5.92	107.82	116.53
2	B	167	LEU	CA-C-N	5.88	128.97	120.79
2	B	167	LEU	C-N-CA	5.88	128.97	120.79
3	I	159	ALA	CA-C-N	5.60	125.80	120.31
3	I	159	ALA	C-N-CA	5.60	125.80	120.31
2	B	134	GLY	N-CA-C	-5.52	107.40	115.63

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	2446	0	2393	33	0
2	B	1335	0	1246	51	1
3	I	1694	0	1644	36	0
4	J	1630	0	1581	37	0
5	C	28	0	25	2	0
5	D	28	0	25	0	0
6	A	28	0	26	1	0
All	All	7189	0	6940	142	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:LYS:HG2	2:B:59:THR:H	1.29	0.94
3:I:58:GLN:HG3	3:I:64:LEU:HD23	1.54	0.90
2:B:42:GLN:HA	2:B:42:GLN:HE21	1.36	0.88
4:J:51:VAL:HG23	4:J:52:SER:H	1.37	0.88
1:A:18:HIS:HD2	2:B:21:TRP:HA	1.37	0.88
2:B:168:ASN:OD1	2:B:169:ASN:ND2	2.07	0.87
4:J:52:SER:O	4:J:53:SER:OG	1.94	0.84
2:B:39:LYS:HD2	2:B:39:LYS:H	1.40	0.84
1:A:77:ASP:OD2	1:A:141:ARG:NH1	2.10	0.83
2:B:28:ASN:ND2	2:B:146:ASN:OD1	2.16	0.79
1:A:185:PRO:HB3	1:A:190:GLU:HG2	1.68	0.76
3:I:229:ILE:HG12	3:I:244:ARG:HG3	1.67	0.75
4:J:211:HIS:O	4:J:233:ARG:NH2	2.20	0.74
2:B:58:LYS:CG	2:B:59:THR:H	2.02	0.71
1:A:285:ASN:HD22	6:A:606:NAG:H83	1.56	0.70
4:J:51:VAL:HG23	4:J:52:SER:N	2.03	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:GLU:O	2:B:58:LYS:O	2.10	0.68
1:A:9:SER:N	2:B:143:LYS:HZ3	1.92	0.68
4:J:60:GLN:NE2	4:J:68:ARG:HE	1.91	0.67
4:J:26:MET:HE3	4:J:113:GLN:HB3	1.78	0.66
1:A:18:HIS:CD2	2:B:21:TRP:HA	2.26	0.65
3:I:30:VAL:HG21	3:I:181:PRO:HG3	1.78	0.65
4:J:25:VAL:H	4:J:48:SER:HB3	1.61	0.65
2:B:42:GLN:HA	2:B:42:GLN:NE2	2.10	0.65
2:B:126:LEU:O	2:B:127:ARG:C	2.40	0.65
1:A:129:GLY:HA3	1:A:162:PRO:HG3	1.79	0.65
2:B:119:PHE:HE2	2:B:123:ARG:HH21	1.44	0.64
2:B:12:ASN:N	2:B:12:ASN:OD1	2.31	0.63
2:B:42:GLN:NE2	3:I:129:VAL:HG13	2.14	0.63
4:J:54:SER:O	4:J:56:LEU:N	2.32	0.63
3:I:75:GLY:HA2	5:C:2:NAG:H82	1.81	0.62
1:A:74:PRO:HA	1:A:141:ARG:HH12	1.64	0.62
2:B:56:ILE:O	2:B:58:LYS:N	2.33	0.62
3:I:160:PRO:HG3	3:I:172:LEU:HB3	1.83	0.61
2:B:58:LYS:HG2	2:B:59:THR:N	2.10	0.60
2:B:39:LYS:HD2	2:B:39:LYS:N	2.15	0.60
3:I:58:GLN:OE1	4:J:61:GLN:NE2	2.27	0.60
1:A:53:ASN:HD21	1:A:276:THR:HG23	1.66	0.60
3:I:25:GLU:OE1	3:I:139:GLN:N	2.35	0.59
4:J:53:SER:O	4:J:54:SER:HB2	2.03	0.59
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.37	0.59
1:A:89:GLU:HG3	1:A:267:ILE:HD11	1.85	0.58
3:I:202:ALA:HB2	3:I:212:LEU:HD23	1.85	0.58
4:J:26:MET:HE2	4:J:113:GLN:HG2	1.87	0.57
1:A:323:VAL:CG2	2:B:12:ASN:HA	2.35	0.57
2:B:168:ASN:OD1	2:B:169:ASN:N	2.37	0.57
4:J:118:PHE:N	4:J:118:PHE:CD2	2.73	0.56
2:B:128:GLU:HB3	2:B:170:ARG:HH12	1.71	0.56
3:I:25:GLU:OE1	3:I:138:GLY:HA3	2.06	0.56
2:B:61:GLU:O	2:B:62:LYS:HG2	2.05	0.55
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.70	0.55
2:B:10:ILE:HD13	2:B:10:ILE:N	2.21	0.55
3:I:169:THR:HA	3:I:220:SER:HB2	1.89	0.55
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.89	0.55
4:J:51:VAL:CG2	4:J:52:SER:H	2.13	0.54
4:J:169:GLN:HG2	4:J:176:LEU:HD11	1.88	0.54
3:I:49:SER:O	3:I:72:PHE:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:60:GLN:HB2	4:J:70:LEU:HD11	1.89	0.54
2:B:11:GLU:OE2	2:B:11:GLU:HA	2.08	0.54
3:I:184:VAL:HG12	3:I:234:HIS:HB2	1.90	0.54
3:I:119:PRO:HD3	3:I:135:ASP:HB2	1.89	0.53
1:A:307:LYS:HE2	2:B:92:TRP:CZ2	2.43	0.53
2:B:128:GLU:O	2:B:170:ARG:NH1	2.40	0.53
2:B:61:GLU:C	2:B:62:LYS:HG2	2.34	0.52
4:J:168:VAL:HG12	4:J:218:VAL:HG22	1.91	0.52
1:A:182:ILE:HD11	1:A:215:PRO:HD3	1.92	0.52
1:A:220:ARG:O	1:A:227:SER:HB2	2.09	0.52
3:I:91:ARG:HG2	3:I:92:ASP:N	2.25	0.52
4:J:51:VAL:O	4:J:52:SER:HB2	2.10	0.51
1:A:97:CYS:O	1:A:224:ARG:NH1	2.44	0.51
1:A:20:VAL:HG11	5:C:1:NAG:C8	2.41	0.50
1:A:42:LEU:HD12	2:B:100:VAL:HG12	1.92	0.50
1:A:314:LEU:HB3	2:B:100:VAL:HG11	1.93	0.49
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.47	0.49
1:A:230:ILE:HD12	1:A:252:ILE:HG13	1.93	0.49
3:I:73:ASP:HB3	3:I:75:GLY:H	1.75	0.49
2:B:165:GLU:O	2:B:168:ASN:OD1	2.29	0.49
2:B:113:SER:O	2:B:117:LYS:HG2	2.12	0.49
1:A:266:SER:OG	1:A:267:ILE:N	2.46	0.49
4:J:147:LEU:O	4:J:205:LYS:HD2	2.13	0.49
2:B:10:ILE:HG22	2:B:11:GLU:N	2.28	0.48
1:A:290:ASN:OD1	3:I:47:THR:OG1	2.29	0.48
3:I:231:ASN:ND2	3:I:242:ASP:OD1	2.38	0.48
1:A:204:VAL:HG13	1:A:243:LEU:HD11	1.96	0.48
3:I:92:ASP:O	3:I:93:ILE:C	2.55	0.48
4:J:158:LEU:HB2	4:J:197:LEU:HB3	1.96	0.48
2:B:170:ARG:HB3	2:B:171:PHE:CD1	2.48	0.48
1:A:301:THR:HG23	1:A:305:CYS:SG	2.54	0.47
4:J:173:ASP:OD2	4:J:211:HIS:HB3	2.14	0.47
3:I:21:VAL:HA	3:I:45:GLY:HA3	1.97	0.47
2:B:14:TRP:HB3	2:B:25:ARG:NH2	2.30	0.47
4:J:60:GLN:HE22	4:J:68:ARG:HE	1.61	0.46
2:B:10:ILE:HG22	2:B:11:GLU:H	1.80	0.46
3:I:43:ALA:O	3:I:96:ASN:ND2	2.49	0.46
3:I:173:GLY:HA2	3:I:188:TRP:CH2	2.51	0.46
4:J:26:MET:HE1	4:J:47:ALA:HB2	1.97	0.45
2:B:168:ASN:CG	2:B:169:ASN:N	2.73	0.45
3:I:159:ALA:HA	3:I:160:PRO:HD3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:NH2	1:A:147:PHE:O	2.49	0.45
2:B:128:GLU:HB3	2:B:170:ARG:NH1	2.32	0.45
4:J:130:ARG:HD2	4:J:192:ASP:O	2.16	0.45
3:I:126:PHE:HB2	3:I:129:VAL:HG23	1.99	0.45
1:A:127:TRP:CZ2	1:A:253:ALA:HB1	2.52	0.44
2:B:45:ILE:HG21	3:I:129:VAL:HG11	2.00	0.44
4:J:104:GLU:H	4:J:104:GLU:HG3	1.60	0.44
4:J:142:PRO:HD3	4:J:154:VAL:HG22	1.99	0.44
4:J:28:GLN:O	4:J:122:GLN:NE2	2.49	0.44
2:B:124:ARG:HH11	2:B:124:ARG:CG	2.31	0.44
3:I:132:GLY:HA2	4:J:114:TYR:CD1	2.53	0.44
4:J:156:CYS:HB2	4:J:170:TRP:CH2	2.52	0.44
2:B:53:ASN:OD1	3:I:122:LYS:HG3	2.17	0.44
4:J:208:TYR:O	4:J:214:TYR:OH	2.35	0.44
2:B:131:GLU:OE2	2:B:170:ARG:HG2	2.18	0.44
2:B:170:ARG:HB3	2:B:171:PHE:HD1	1.83	0.43
1:A:291:ASP:OD1	1:A:292:LYS:HG3	2.17	0.43
4:J:147:LEU:H	4:J:147:LEU:HD12	1.82	0.43
2:B:141:TYR:CG	2:B:170:ARG:HG3	2.54	0.43
3:I:73:ASP:HB3	3:I:75:GLY:N	2.34	0.43
3:I:171:ALA:HB2	3:I:217:THR:HG22	2.00	0.43
1:A:62:ILE:HG22	1:A:63:ASP:N	2.34	0.43
2:B:51:LYS:HE3	2:B:107:THR:OG1	2.19	0.42
2:B:162:TYR:O	2:B:166:ALA:N	2.38	0.42
3:I:137:TRP:CZ3	4:J:67:PRO:HG2	2.55	0.42
4:J:167:LYS:HB3	4:J:219:THR:HG23	2.02	0.42
1:A:38:ASN:C	1:A:318:THR:HG22	2.44	0.42
3:I:110:THR:HG23	3:I:144:THR:HA	2.01	0.42
2:B:148:CYS:O	2:B:151:SER:OG	2.32	0.42
3:I:54:HIS:CD2	3:I:118:ASP:HB2	2.55	0.42
1:A:270:SER:HB2	1:A:284:PRO:HA	2.02	0.41
4:J:26:MET:CE	4:J:113:GLN:HB3	2.47	0.41
4:J:39:GLU:O	4:J:101:LEU:HB2	2.20	0.41
1:A:176:LYS:HE2	1:A:257:TYR:CE1	2.56	0.41
3:I:246:GLU:O	3:I:247:PRO:O	2.38	0.41
4:J:140:PHE:HA	4:J:141:PRO:HD2	1.91	0.41
2:B:23:GLY:HA3	2:B:36:ALA:HA	2.03	0.41
2:B:149:ILE:HD12	2:B:150:GLU:N	2.36	0.41
3:I:234:HIS:CD2	3:I:236:PRO:HD2	2.56	0.41
4:J:127:GLU:OE2	4:J:195:TYR:OH	2.30	0.41
3:I:129:VAL:HG12	3:I:130:SER:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ASN:O	2:B:156:THR:HG23	2.21	0.40
2:B:27:GLN:HG3	2:B:32:THR:HG22	2.03	0.40
3:I:200:PHE:CE2	4:J:198:SER:HB2	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:LYS:NZ	2:B:86:ASP:OD2[3_655]	1.47	0.73

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/329 (96%)	295 (94%)	18 (6%)	2 (1%)	21	51
2	B	161/176 (92%)	145 (90%)	13 (8%)	3 (2%)	6	23
3	I	220/233 (94%)	200 (91%)	19 (9%)	1 (0%)	24	54
4	J	210/220 (96%)	193 (92%)	13 (6%)	4 (2%)	6	23
All	All	906/958 (95%)	833 (92%)	63 (7%)	10 (1%)	11	36

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	57	GLU
2	B	58	LYS
2	B	127	ARG
3	I	247	PRO
4	J	51	VAL
4	J	52	SER
4	J	53	SER

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Mol	Chain	Res	Type
4	J	55	TYR
1	A	62	ILE
1	A	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	279/290 (96%)	263 (94%)	16 (6%)	18	49
2	B	142/150 (95%)	128 (90%)	14 (10%)	7	24
3	I	187/196 (95%)	175 (94%)	12 (6%)	16	44
4	J	184/192 (96%)	169 (92%)	15 (8%)	10	32
All	All	792/828 (96%)	735 (93%)	57 (7%)	13	39

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

Mol	Chain	Res	Type
1	A	20	VAL
1	A	29	ILE
1	A	122	THR
1	A	163	VAL
1	A	186	SER
1	A	207	ARG
1	A	208	ARG
1	A	212	THR
1	A	260	MET
1	A	265	SER
1	A	278	ILE
1	A	300	ILE
1	A	301	THR
1	A	307	LYS
1	A	321	ARG
1	A	323	VAL
2	B	10	ILE
2	B	11	GLU

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Mol	Chain	Res	Type
2	B	12	ASN
2	B	29	SER
2	B	42	GLN
2	B	51	LYS
2	B	59	THR
2	B	65	GLN
2	B	72	GLU
2	B	129	ASN
2	B	135	ASN
2	B	143	LYS
2	B	149	ILE
2	B	168	ASN
3	I	20	GLN
3	I	21	VAL
3	I	25	GLU
3	I	47	THR
3	I	48	SER
3	I	49	SER
3	I	58	GLN
3	I	84	LYS
3	I	95	ARG
3	I	112	VAL
3	I	243	LYS
3	I	248	LYS
4	J	25	VAL
4	J	33	LEU
4	J	48	SER
4	J	56	LEU
4	J	68	ARG
4	J	71	ILE
4	J	92	THR
4	J	104	GLU
4	J	118	PHE
4	J	126	VAL
4	J	129	LYS
4	J	147	LEU
4	J	167	LYS
4	J	174	ASN
4	J	219	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	211	GLN
1	A	216	ASN
1	A	296	ASN
2	B	42	GLN
2	B	47	GLN
2	B	60	ASN
2	B	135	ASN
2	B	169	ASN
3	I	54	HIS
4	J	49	GLN
4	J	60	GLN
4	J	182	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 ⓘ

4 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	$\# Z > 2$
5	NAG	C	1	5,1	14,14,15	0.33	0	17,19,21	0.64	0
5	NAG	C	2	5	14,14,15	1.00	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	D	1	5,1	14,14,15	0.52	0	17,19,21	0.94	1 (5%)
5	NAG	D	2	5	14,14,15	0.81	0	17,19,21	0.75	1 (5%)

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	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	1/6/23/26	0/1/1/1
5	NAG	D	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	D	2	5	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2	NAG	O5-C1	3.29	1.49	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1	NAG	C1-O5-C5	2.85	116.01	112.19
5	C	2	NAG	C1-O5-C5	2.68	115.78	112.19
5	D	2	NAG	C2-N2-C7	2.09	125.70	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

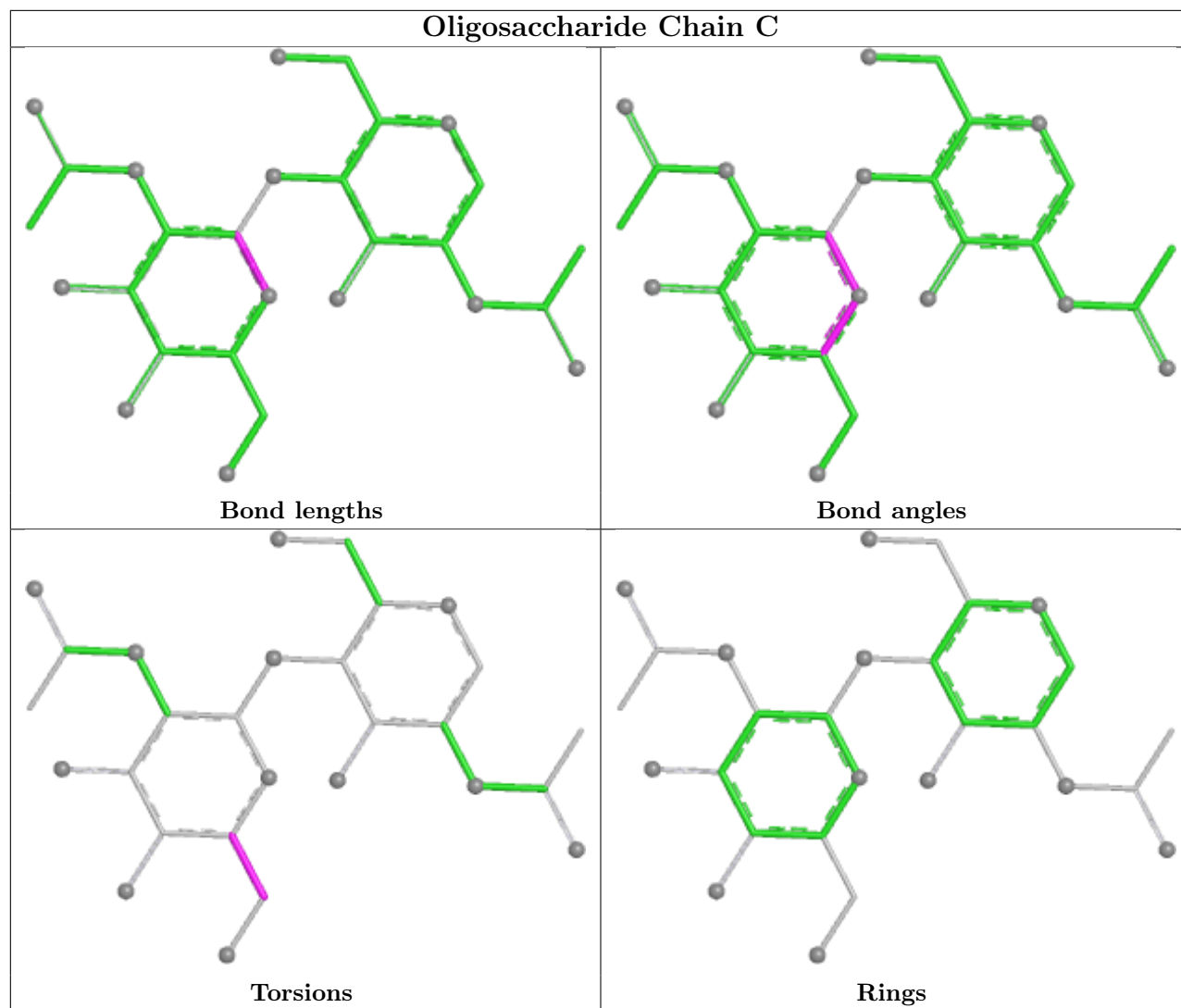
Mol	Chain	Res	Type	Atoms
5	D	1	NAG	O5-C5-C6-O6
5	D	1	NAG	C4-C5-C6-O6
5	D	2	NAG	C8-C7-N2-C2
5	D	2	NAG	O7-C7-N2-C2
5	C	2	NAG	O5-C5-C6-O6

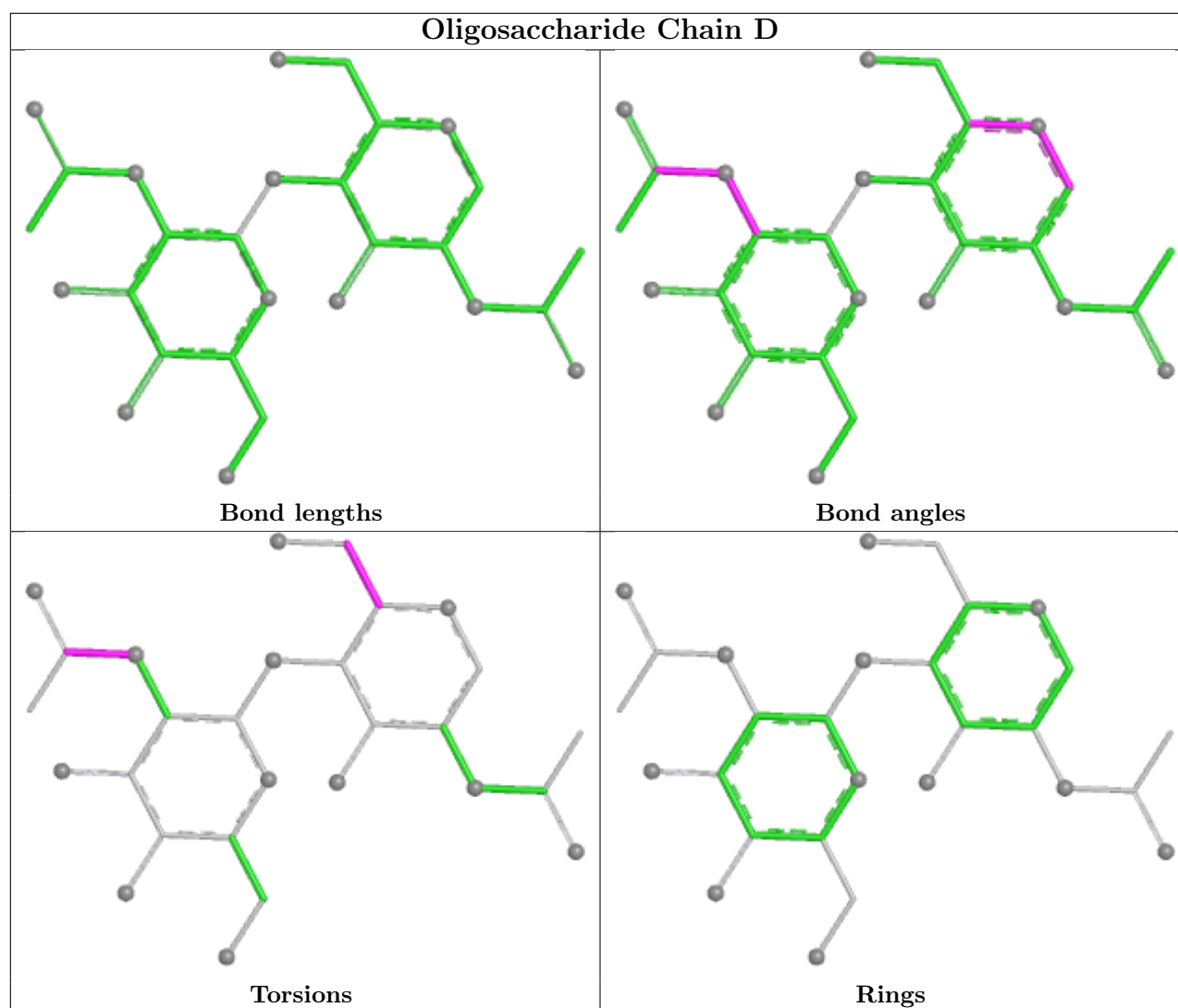
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	NAG	1	0
5	C	2	NAG	1	0

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





5.6 Ligand geometry [i](#)

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	606	1	14,14,15	0.63	0	17,19,21	0.53	0
6	NAG	A	603	1	14,14,15	0.31	0	17,19,21	0.60	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	606	1	-	4/6/23/26	0/1/1/1
6	NAG	A	603	1	-	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 (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	606	NAG	O5-C5-C6-O6
6	A	603	NAG	O5-C5-C6-O6
6	A	606	NAG	C4-C5-C6-O6
6	A	603	NAG	C4-C5-C6-O6
6	A	606	NAG	C8-C7-N2-C2
6	A	606	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	606	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	317/329 (96%)	-0.18	4 (1%) 75 67	55, 80, 108, 165	0
2	B	163/176 (92%)	0.02	4 (2%) 58 48	58, 92, 137, 189	0
3	I	224/233 (96%)	-0.07	4 (1%) 67 59	58, 82, 109, 153	0
4	J	212/220 (96%)	-0.03	3 (1%) 73 65	60, 83, 116, 149	0
All	All	916/958 (95%)	-0.08	15 (1%) 70 62	55, 83, 120, 189	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	10	ILE	5.7
3	I	130	SER	3.6
1	A	9	SER	3.2
3	I	169	THR	3.0
2	B	134	GLY	2.7
4	J	234	GLY	2.6
2	B	132	GLU	2.6
2	B	139	LYS	2.4
1	A	324	PRO	2.4
1	A	11	ALA	2.3
3	I	170	ALA	2.2
4	J	51	VAL	2.2
4	J	174	ASN	2.2
1	A	145	SER	2.0
3	I	246	GLU	2.0

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

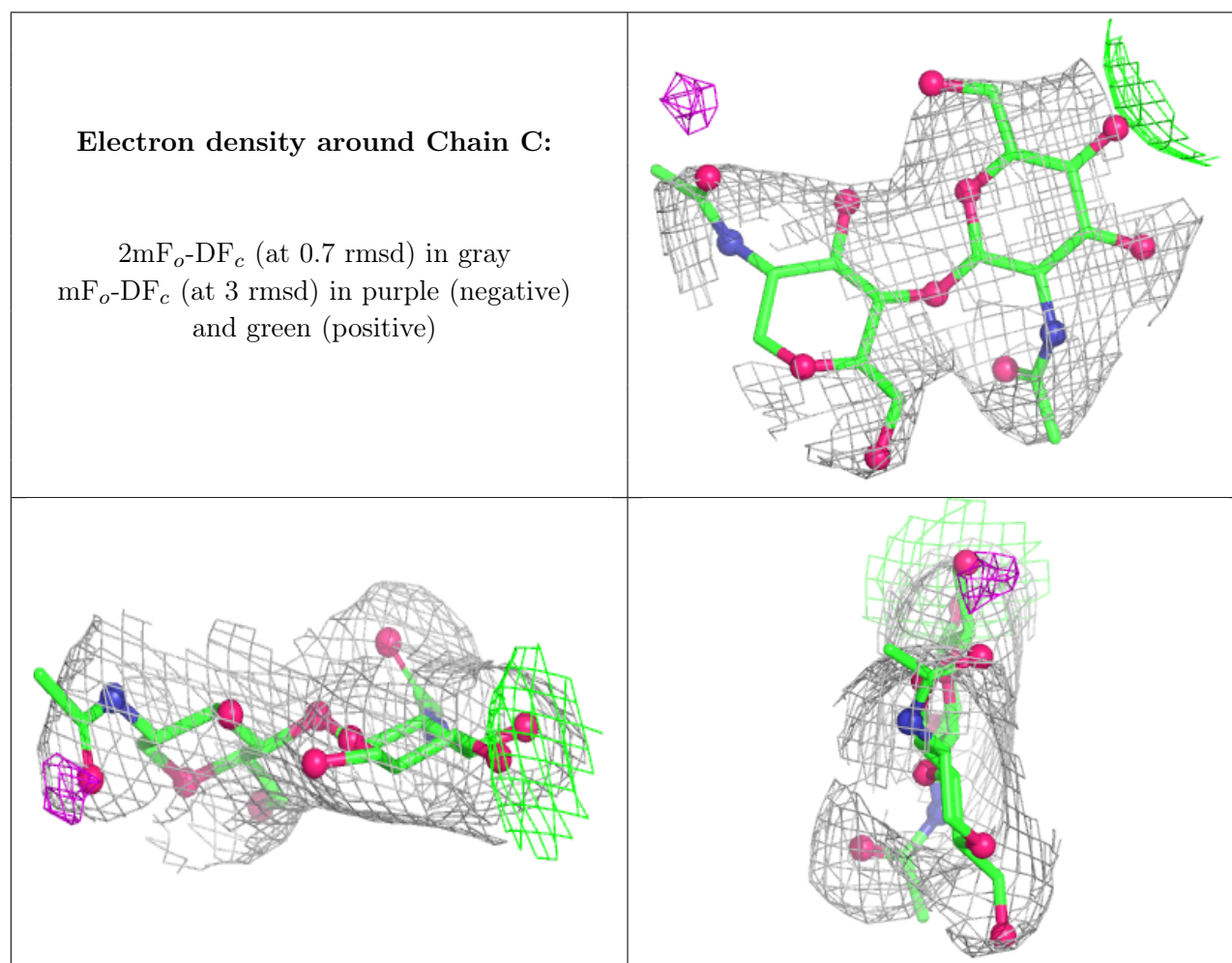
There are no non-standard protein/DNA/RNA residues in this entry.

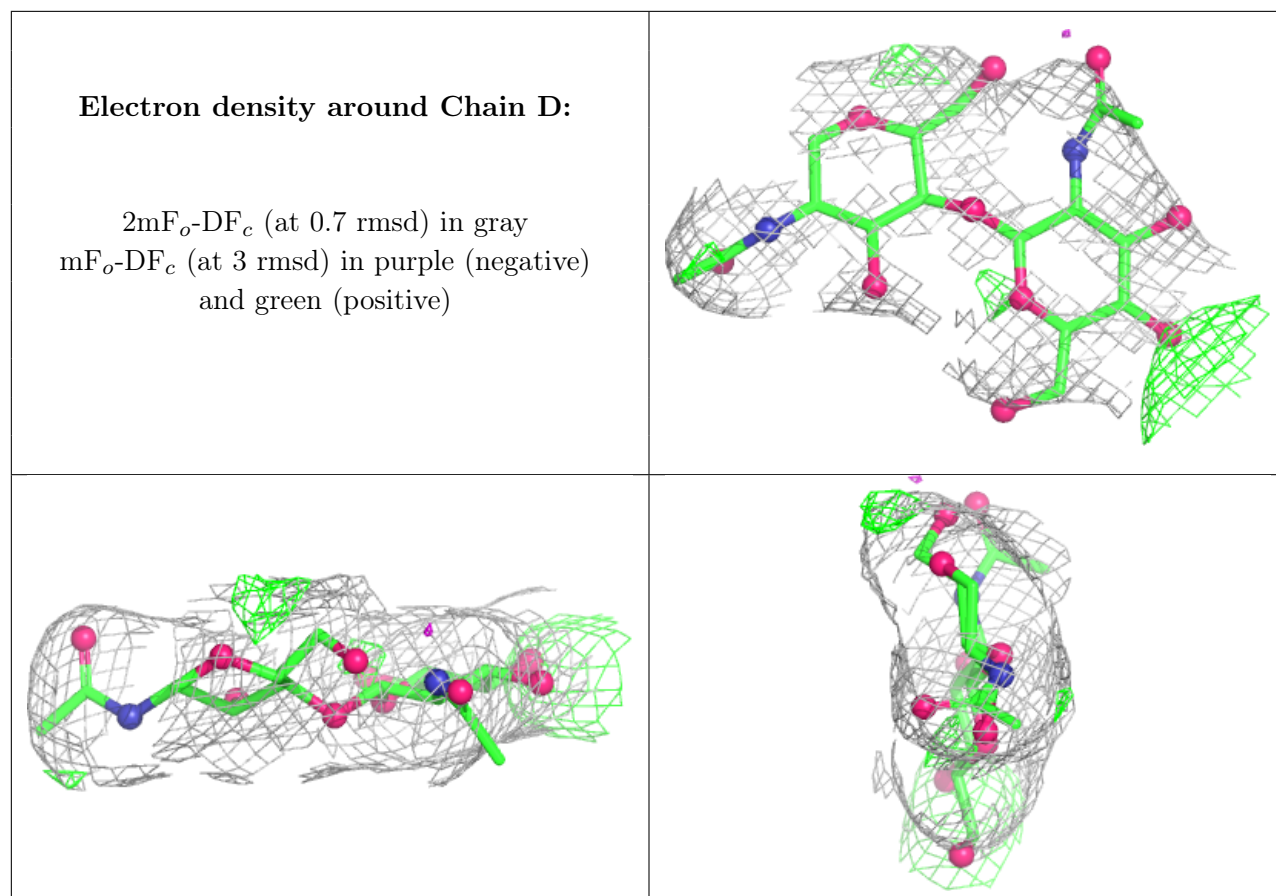
6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	C	1	14/15	-	-	87,95,106,110	0
5	NAG	C	2	14/15	-	-	77,93,98,99	0
5	NAG	D	1	14/15	-	-	81,87,99,105	0
5	NAG	D	2	14/15	-	-	107,112,121,130	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.





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	606	14/15	0.68	0.14	108,111,118,119	0
6	NAG	A	603	14/15	0.80	0.09	105,110,116,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.