



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2026 – 05:30 PM JST

PDB ID : 9XA0 / pdb_00009xa0
Title : Structure of the Omicron KP.3.1.1 variant Spike N-terminal domain(NTD)in complex with the C1717 Fab and S2L20 Fab
Authors : Zhou, J.J.; Gao, G.F.
Deposited on : 2025-10-22
Resolution : 3.51 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:

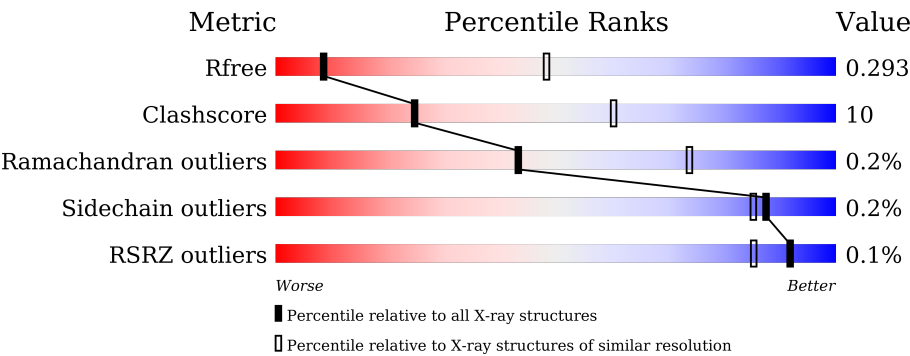
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.51 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.



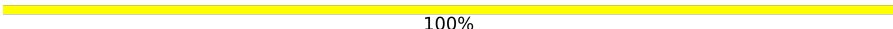
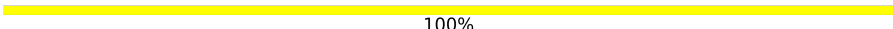
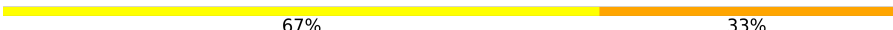
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	C	297	70%23%6%
2	D	233	73%23%5%
3	E	217	82%18%
4	A	235	73%22%6%
5	B	215	77%22%
6	F	2	50%50%

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Mol	Chain	Length	Quality of chain
6	H	2	 50% 50%
7	G	5	 60% 40%
8	I	2	 100%
9	J	3	 100%
9	K	3	 67% 33%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9057 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	280	Total	C	N	O	S	0	0	0
			2247	1452	365	421	9			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	17	MET	-	insertion	UNP P0DTC2
C	18	PRO	-	insertion	UNP P0DTC2
C	19	LEU	-	insertion	UNP P0DTC2
C	20	PHE	-	insertion	UNP P0DTC2
C	23	ILE	THR	variant	UNP P0DTC2
C	25	THR	ARG	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	28	SER	ALA	variant	UNP P0DTC2
C	?	-	SER	deletion	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	125	PHE	VAL	conflict	UNP P0DTC2
C	140	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	154	SER	PHE	conflict	UNP P0DTC2
C	155	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	208	ILE	LEU	variant	UNP P0DTC2
C	209	GLY	VAL	variant	UNP P0DTC2
C	212	PHE	LEU	conflict	UNP P0DTC2
C	241	ASN	HIS	conflict	UNP P0DTC2
C	260	ASP	ALA	conflict	UNP P0DTC2
C	302	HIS	-	expression tag	UNP P0DTC2
C	303	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	304	HIS	-	expression tag	UNP P0DTC2
C	305	HIS	-	expression tag	UNP P0DTC2
C	306	HIS	-	expression tag	UNP P0DTC2
C	307	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called C1717 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	222	Total	C	N	O	S	0	0	0
			1658	1049	279	324	6			

- Molecule 3 is a protein called C1717 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	215	Total	C	N	O	S	0	0	0
			1587	982	271	329	5			

- Molecule 4 is a protein called S2L20 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	222	Total	C	N	O	S	0	0	0
			1677	1059	284	328	6			

- Molecule 5 is a protein called S2L20 light chain.

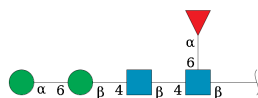
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	214	Total	C	N	O	S	0	0	0
			1658	1042	274	335	7			

- Molecule 6 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
6	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



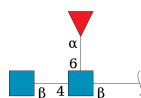
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 8 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



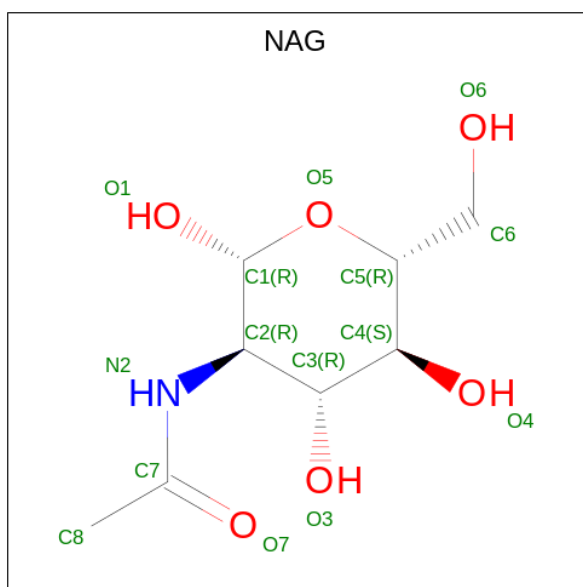
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
9	K	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

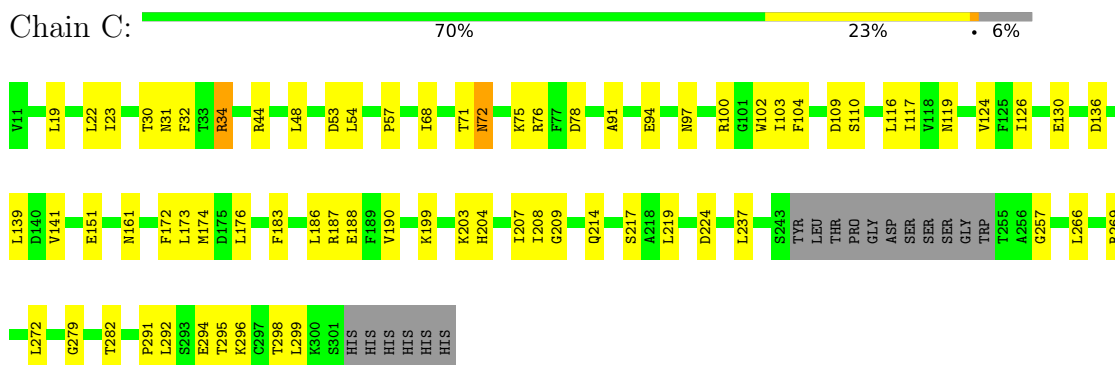


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	N	O	0	0
			14	8	1	5		

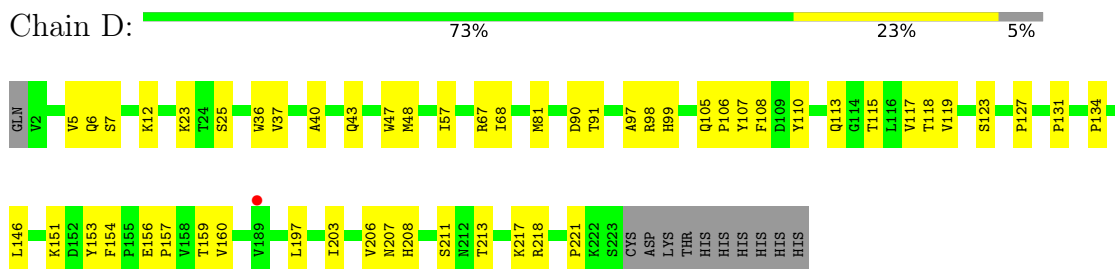
3 Residue-property plots

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.

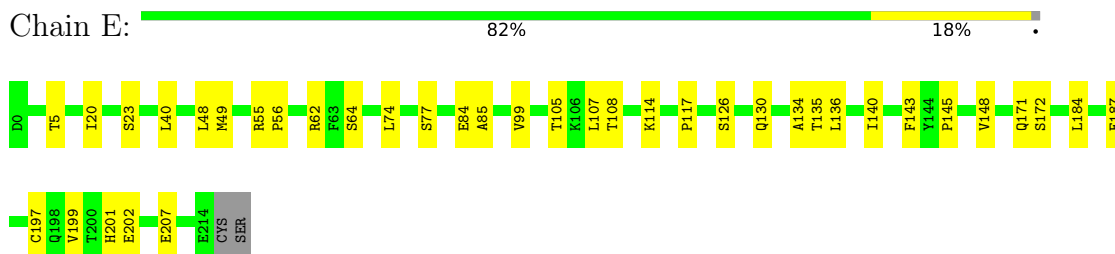
- Molecule 1: Spike glycoprotein



- Molecule 2: C1717 heavy chain

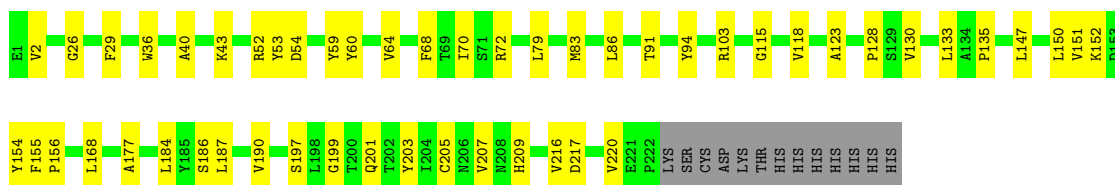


- Molecule 3: C1717 light chain

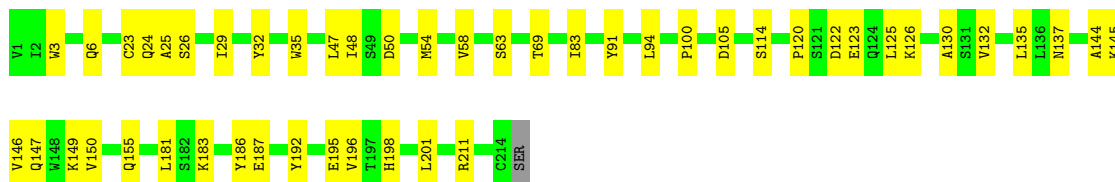
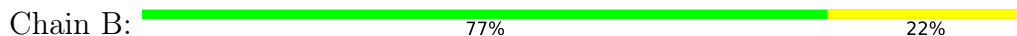


- Molecule 4: S2L20 heavy chain





- Molecule 5: S2L20 light chain



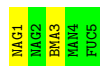
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



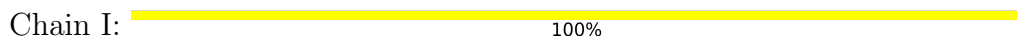
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1
MAG2
FUC3

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67%  33%

MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.30Å 122.66Å 151.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.08 – 3.51 36.08 – 3.51	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.08-3.51) 99.3 (36.08-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.211 , 0.292 0.211 , 0.293	Depositor DCC
R_{free} test set	778 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9057	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	C	0.14	0/2306	0.37	0/3133
2	D	0.13	0/1699	0.34	0/2318
3	E	0.12	0/1624	0.31	0/2217
4	A	0.13	0/1719	0.35	0/2338
5	B	0.12	0/1697	0.33	0/2306
All	All	0.13	0/9045	0.34	0/12312

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2247	0	2171	57	0
2	D	1658	0	1638	38	0
3	E	1587	0	1534	22	0
4	A	1677	0	1630	32	0
5	B	1658	0	1596	31	0
6	F	28	0	25	0	0
6	H	28	0	25	1	0
7	G	60	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	24	0	22	0	0
9	J	38	0	34	4	0
9	K	38	0	34	2	0
10	C	14	0	13	0	0
All	All	9057	0	8774	174	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 10.

All (174) 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:D:6:GLN:H	2:D:113:GLN:HE22	1.30	0.78
1:C:174:MET:HG3	1:C:187:ARG:HB3	1.68	0.75
5:B:35:TRP:HB2	5:B:48:ILE:HG12	1.68	0.75
1:C:103:ILE:HG22	1:C:116:LEU:HD13	1.70	0.74
1:C:72:ASN:HD22	1:C:72:ASN:H	1.38	0.69
1:C:76:ARG:NH1	1:C:136:ASP:OD1	2.27	0.68
2:D:40:ALA:HB3	2:D:43:GLN:HB2	1.77	0.67
2:D:127:PRO:HD2	2:D:213:THR:HG21	1.78	0.64
4:A:94:TYR:O	4:A:115:GLY:HA2	1.98	0.64
3:E:108:THR:HG21	3:E:145:PRO:HB3	1.80	0.63
1:C:190:VAL:HG23	1:C:219:LEU:HD22	1.79	0.63
3:E:134:ALA:HB3	3:E:184:LEU:O	1.97	0.63
2:D:134:PRO:HB3	2:D:146:LEU:HD23	1.81	0.61
2:D:5:VAL:HG23	2:D:23:LYS:HB3	1.81	0.60
4:A:155:PHE:HB2	4:A:184:LEU:HD22	1.81	0.60
1:C:109:ASP:OD1	1:C:110:SER:N	2.34	0.60
2:D:127:PRO:HB3	2:D:153:TYR:HB3	1.83	0.59
2:D:91:THR:HG23	2:D:118:THR:HA	1.85	0.58
1:C:68:ILE:HD12	1:C:257:GLY:HA3	1.84	0.58
5:B:192:TYR:HE1	5:B:211:ARG:HB2	1.68	0.58
1:C:282:THR:O	2:D:105:GLN:NE2	2.38	0.57
1:C:141:VAL:HG22	1:C:151:GLU:HB3	1.86	0.56
4:A:207:VAL:HB	4:A:216:VAL:HG23	1.87	0.56
5:B:144:ALA:HB2	5:B:198:HIS:HD2	1.71	0.56
3:E:136:LEU:HD13	3:E:184:LEU:HD12	1.88	0.55
1:C:174:MET:HB3	1:C:204:HIS:HD2	1.71	0.55
5:B:3:TRP:H	5:B:26:SER:HB2	1.70	0.55
1:C:183:PHE:HZ	1:C:209:GLY:H	1.53	0.55
1:C:117:ILE:HG23	1:C:126:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:GLU:HG2	2:D:157:PRO:HA	1.89	0.54
2:D:37:VAL:HG22	2:D:47:TRP:HA	1.89	0.54
5:B:123:GLU:OE1	5:B:123:GLU:N	2.39	0.54
1:C:119:ASN:OD1	1:C:124:VAL:HG23	2.08	0.54
2:D:151:LYS:HE3	3:E:135:THR:OG1	2.08	0.53
1:C:94:GLU:O	1:C:176:LEU:HD11	2.07	0.53
3:E:148:VAL:HG12	3:E:201:HIS:HB2	1.89	0.53
4:A:103:ARG:HH21	6:H:1:NAG:H62	1.73	0.53
2:D:48:MET:HE2	2:D:68:ILE:HD12	1.89	0.53
2:D:99:HIS:NE2	2:D:106:PRO:HA	2.23	0.53
4:A:150:LEU:HG	4:A:152:LYS:HG3	1.90	0.53
3:E:187:GLU:OE1	3:E:187:GLU:N	2.41	0.53
4:A:83:MET:HE3	4:A:86:LEU:HD11	1.91	0.53
1:C:48:LEU:HB3	1:C:272:LEU:HD11	1.90	0.52
2:D:208:HIS:ND1	2:D:211:SER:OG	2.41	0.52
5:B:130:ALA:HB3	5:B:181:LEU:HG	1.90	0.52
3:E:5:THR:HB	3:E:23:SER:HB2	1.92	0.52
2:D:134:PRO:HD3	2:D:146:LEU:HD22	1.93	0.51
1:C:30:THR:HG22	1:C:30:THR:O	2.10	0.51
5:B:24:GLN:HA	5:B:69:THR:O	2.11	0.51
5:B:6:GLN:HG3	5:B:100:PRO:HD2	1.92	0.51
1:C:295:THR:O	1:C:299:LEU:HG	2.11	0.51
3:E:126:SER:O	3:E:130:GLN:HG2	2.11	0.50
4:A:91:THR:HA	4:A:118:VAL:O	2.11	0.50
1:C:119:ASN:ND2	1:C:172:PHE:HB2	2.27	0.50
2:D:91:THR:HA	2:D:117:VAL:O	2.11	0.50
4:A:59:TYR:CE1	5:B:94:LEU:HD13	2.46	0.50
1:C:72:ASN:HD22	1:C:72:ASN:N	2.04	0.50
5:B:122:ASP:O	5:B:126:LYS:HG2	2.12	0.49
5:B:198:HIS:HB3	5:B:201:LEU:HG	1.94	0.49
1:C:22:LEU:O	1:C:75:LYS:NZ	2.45	0.49
9:K:1:NAG:H4	9:K:3:FUC:H5	1.94	0.49
1:C:44:ARG:O	1:C:279:GLY:HA2	2.12	0.49
1:C:97:ASN:HD21	1:C:173:LEU:HD13	1.78	0.49
1:C:190:VAL:HG13	1:C:266:LEU:HD11	1.94	0.49
3:E:117:PRO:HA	3:E:143:PHE:HB3	1.94	0.48
5:B:114:SER:HB2	5:B:137:ASN:HB3	1.96	0.48
2:D:123:SER:HA	2:D:154:PHE:CD1	2.49	0.48
5:B:186:TYR:O	5:B:192:TYR:OH	2.31	0.48
5:B:120:PRO:HD3	5:B:132:VAL:HG22	1.96	0.48
2:D:134:PRO:HG3	2:D:146:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.47	0.47
3:E:49:MET:HE2	3:E:55:ARG:HB2	1.95	0.47
1:C:174:MET:CG	1:C:187:ARG:HB3	2.41	0.47
4:A:64:VAL:HB	4:A:68:PHE:CG	2.50	0.47
1:C:91:ALA:HA	1:C:187:ARG:O	2.15	0.47
4:A:147:LEU:HB2	4:A:220:VAL:HG11	1.96	0.47
2:D:131:PRO:HD3	2:D:217:LYS:HE2	1.96	0.47
3:E:40:LEU:HG	3:E:85:ALA:HB2	1.96	0.47
5:B:183:LYS:O	5:B:187:GLU:HG2	2.15	0.47
1:C:23:ILE:HG13	1:C:75:LYS:HE3	1.97	0.47
1:C:100:ARG:NH1	1:C:151:GLU:OE1	2.47	0.47
1:C:116:LEU:HD11	1:C:237:LEU:HD13	1.96	0.47
4:A:199:GLY:C	4:A:201:GLN:H	2.23	0.47
1:C:183:PHE:CE1	1:C:208:ILE:HA	2.50	0.47
2:D:197:LEU:HD22	2:D:221:PRO:HG3	1.96	0.47
1:C:32:PHE:H	9:J:1:NAG:C8	2.29	0.46
1:C:130:GLU:HB2	1:C:161:ASN:O	2.15	0.46
3:E:197:CYS:O	3:E:207:GLU:HA	2.15	0.46
4:A:130:VAL:HG11	4:A:216:VAL:HB	1.98	0.46
4:A:147:LEU:HD21	4:A:203:TYR:HD2	1.81	0.46
5:B:146:VAL:HG22	5:B:196:VAL:HG22	1.96	0.46
1:C:102:TRP:HB2	1:C:104:PHE:CE1	2.51	0.46
1:C:174:MET:SD	1:C:204:HIS:HB2	2.56	0.46
4:A:52:ARG:O	4:A:72:ARG:NH1	2.41	0.45
1:C:117:ILE:HG12	1:C:126:ILE:HG23	1.97	0.45
1:C:183:PHE:HE1	1:C:208:ILE:HA	1.81	0.45
1:C:186:LEU:HB2	1:C:207:ILE:HD11	1.97	0.45
2:D:12:LYS:O	2:D:119:VAL:HA	2.17	0.45
5:B:144:ALA:HB2	5:B:198:HIS:CD2	2.49	0.45
5:B:54:MET:SD	5:B:63:SER:HA	2.57	0.45
4:A:135:PRO:HD3	4:A:147:LEU:HB3	1.99	0.45
1:C:203:LYS:HE2	1:C:217:SER:HB3	1.98	0.44
1:C:183:PHE:HZ	1:C:209:GLY:N	2.16	0.44
5:B:145:LYS:HA	5:B:145:LYS:HD2	1.78	0.44
1:C:34:ARG:HE	1:C:188:GLU:CD	2.26	0.44
1:C:57:PRO:HG3	1:C:269:ARG:NE	2.33	0.44
2:D:6:GLN:N	2:D:113:GLN:HE22	2.05	0.44
1:C:75:LYS:HZ1	1:C:78:ASP:CG	2.24	0.44
1:C:176:LEU:HD12	1:C:187:ARG:NH2	2.33	0.44
3:E:84:GLU:HG3	3:E:107:LEU:O	2.17	0.44
2:D:67:ARG:HH22	2:D:90:ASP:CG	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:47:LEU:O	5:B:58:VAL:HG21	2.18	0.44
1:C:296:LYS:NZ	2:D:107:TYR:OH	2.47	0.43
1:C:31:ASN:CG	9:J:1:NAG:H82	2.43	0.43
1:C:183:PHE:H	1:C:183:PHE:HD1	1.65	0.43
4:A:29:PHE:O	4:A:72:ARG:NH2	2.51	0.43
1:C:292:LEU:O	1:C:296:LYS:HG3	2.17	0.43
4:A:205:CYS:O	4:A:217:ASP:HA	2.17	0.43
3:E:201:HIS:CE1	3:E:202:GLU:HG2	2.53	0.43
4:A:197:SER:O	4:A:201:GLN:NE2	2.36	0.43
1:C:214:GLN:HE22	9:J:1:NAG:H83	1.82	0.43
2:D:7:SER:O	2:D:115:THR:OG1	2.35	0.43
4:A:177:ALA:HA	4:A:187:LEU:HB3	2.00	0.43
4:A:190:VAL:HG11	5:B:135:LEU:HD22	2.00	0.43
1:C:291:PRO:O	1:C:295:THR:HG23	2.18	0.43
1:C:139:LEU:HB2	1:C:237:LEU:HD21	2.00	0.43
2:D:36:TRP:CD1	2:D:81:MET:HB2	2.54	0.43
4:A:128:PRO:HB3	4:A:154:TYR:HB3	2.01	0.43
5:B:25:ALA:HB2	5:B:29:ILE:HD11	2.01	0.43
5:B:3:TRP:H	5:B:26:SER:CB	2.32	0.42
2:D:6:GLN:H	2:D:113:GLN:NE2	2.09	0.42
5:B:149:LYS:NZ	5:B:195:GLU:HB2	2.34	0.42
1:C:53:ASP:OD1	1:C:54:LEU:N	2.37	0.42
5:B:145:LYS:HG3	5:B:147:GLN:HG3	2.02	0.42
1:C:71:THR:HG22	9:K:1:NAG:H82	2.02	0.42
2:D:47:TRP:CG	3:E:99:VAL:HB	2.55	0.42
5:B:83:ILE:HG23	5:B:105:ASP:HA	2.01	0.42
1:C:203:LYS:HB2	1:C:219:LEU:HG	2.02	0.42
2:D:23:LYS:NZ	2:D:25:SER:O	2.51	0.42
1:C:199:LYS:HG2	1:C:224:ASP:OD1	2.20	0.41
4:A:40:ALA:HB3	4:A:43:LYS:HG3	2.01	0.41
5:B:125:LEU:HD22	5:B:183:LYS:HG3	2.02	0.41
2:D:160:VAL:HG22	2:D:206:VAL:HG22	2.02	0.41
3:E:20:ILE:HG12	3:E:105:THR:HG21	2.01	0.41
1:C:292:LEU:HG	1:C:296:LYS:HD2	2.02	0.41
5:B:29:ILE:HG22	5:B:32:TYR:H	1.85	0.41
3:E:140:ILE:HG12	3:E:199:VAL:HG21	2.02	0.41
3:E:64:SER:O	3:E:74:LEU:HD12	2.21	0.41
4:A:168:LEU:HD23	4:A:168:LEU:HA	1.94	0.41
2:D:217:LYS:HA	2:D:217:LYS:HD2	1.87	0.41
3:E:62:ARG:HB3	3:E:77:SER:O	2.21	0.41
4:A:103:ARG:HD3	5:B:32:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD13	1:C:19:LEU:HA	1.88	0.41
2:D:48:MET:HE2	2:D:48:MET:HB3	1.98	0.41
1:C:294:GLU:O	1:C:298:THR:HG23	2.20	0.41
2:D:159:THR:OG1	2:D:207:ASN:HB3	2.20	0.41
4:A:123:ALA:HB3	4:A:155:PHE:CD1	2.56	0.41
4:A:151:VAL:O	4:A:186:SER:HA	2.21	0.41
5:B:150:VAL:HB	5:B:155:GLN:NE2	2.36	0.41
3:E:171:GLN:HG3	3:E:172:SER:H	1.85	0.41
4:A:156:PRO:HB2	4:A:209:HIS:CE1	2.55	0.41
4:A:2:VAL:HA	4:A:26:GLY:HA3	2.03	0.40
4:A:53:TYR:CG	4:A:54:ASP:N	2.89	0.40
5:B:50:ASP:OD1	5:B:91:TYR:OH	2.36	0.40
2:D:57:ILE:HG21	9:J:1:NAG:O7	2.21	0.40
3:E:48:LEU:O	3:E:56:PRO:HD2	2.22	0.40
4:A:36:TRP:HE1	4:A:79:LEU:HG	1.87	0.40
4:A:60:TYR:CZ	4:A:70:ILE:HG22	2.56	0.40
4:A:133:LEU:HD21	4:A:150:LEU:HB2	2.03	0.40
2:D:98:ARG:HE	2:D:110:TYR:HB2	1.86	0.40
1:C:23:ILE:HG22	1:C:68:ILE:HG23	2.04	0.40
2:D:97:ALA:HB1	2:D:108:PHE:HB3	2.02	0.40
2:D:203:ILE:HG12	2:D:218:ARG:HA	2.04	0.40
3:E:140:ILE:HG12	3:E:199:VAL:HG11	2.03	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	C	276/297 (93%)	260 (94%)	15 (5%)	1 (0%)	30	62
2	D	220/233 (94%)	209 (95%)	11 (5%)	0	100	100
3	E	213/217 (98%)	200 (94%)	12 (6%)	1 (0%)	24	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	220/235 (94%)	209 (95%)	11 (5%)	0	100	100
5	B	212/215 (99%)	198 (93%)	14 (7%)	0	100	100
All	All	1141/1197 (95%)	1076 (94%)	63 (6%)	2 (0%)	43	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	ARG
3	E	114	LYS

5.3.2 Protein sidechains [i](#)

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	C	253/268 (94%)	252 (100%)	1 (0%)	84	82
2	D	187/198 (94%)	187 (100%)	0	100	100
3	E	180/182 (99%)	180 (100%)	0	100	100
4	A	185/198 (93%)	185 (100%)	0	100	100
5	B	190/191 (100%)	189 (100%)	1 (0%)	81	81
All	All	995/1037 (96%)	993 (100%)	2 (0%)	87	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	72	ASN
5	B	23	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	143	HIS
1	C	235	GLN

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Mol	Chain	Res	Type
2	D	39	GLN
2	D	179	GLN
3	E	32	ASN
4	A	82	GLN
5	B	124	GLN
5	B	137	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

17 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	$\# Z > 2$
6	NAG	F	1	1,6	14,14,15	0.73	0	17,19,21	2.51	6 (35%)
6	NAG	F	2	6	14,14,15	0.71	0	17,19,21	0.95	0
7	NAG	G	1	1,7	14,14,15	0.71	0	17,19,21	0.95	2 (11%)
7	NAG	G	2	7	14,14,15	0.67	0	17,19,21	1.06	0
7	BMA	G	3	7	11,11,12	0.97	0	15,15,17	2.49	5 (33%)
7	MAN	G	4	7	11,11,12	0.76	0	15,15,17	0.99	0
7	FUC	G	5	7	10,10,11	0.76	0	14,14,16	1.03	0
6	NAG	H	1	1,6	14,14,15	0.67	0	17,19,21	2.59	5 (29%)
6	NAG	H	2	6	14,14,15	0.78	0	17,19,21	1.02	1 (5%)
8	NAG	I	1	1,8	14,14,15	0.65	0	17,19,21	1.09	1 (5%)
8	FUC	I	2	8	10,10,11	0.75	0	14,14,16	1.18	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	J	1	1,9	14,14,15	0.47	0	17,19,21	0.67	0
9	NAG	J	2	9	14,14,15	0.34	0	17,19,21	1.38	5 (29%)
9	FUC	J	3	9	10,10,11	0.35	0	14,14,16	1.19	1 (7%)
9	NAG	K	1	1,9	14,14,15	0.81	0	17,19,21	1.61	4 (23%)
9	NAG	K	2	9	14,14,15	0.73	0	17,19,21	1.06	1 (5%)
9	FUC	K	3	9	10,10,11	0.82	0	14,14,16	0.97	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	F	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
7	NAG	G	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	3/6/23/26	0/1/1/1
7	BMA	G	3	7	-	1/2/19/22	0/1/1/1
7	MAN	G	4	7	-	2/2/19/22	0/1/1/1
7	FUC	G	5	7	-	-	0/1/1/1
6	NAG	H	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1
8	NAG	I	1	1,8	-	2/6/23/26	0/1/1/1
8	FUC	I	2	8	-	-	0/1/1/1
9	NAG	J	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	J	2	9	-	3/6/23/26	0/1/1/1
9	FUC	J	3	9	-	-	0/1/1/1
9	NAG	K	1	1,9	-	3/6/23/26	0/1/1/1
9	NAG	K	2	9	-	0/6/23/26	0/1/1/1
9	FUC	K	3	9	-	-	0/1/1/1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1	NAG	C2-N2-C7	8.18	134.54	122.90
6	H	1	NAG	C1-O5-C5	7.04	121.73	112.19
7	G	3	BMA	C1-O5-C5	6.36	120.81	112.19
6	H	1	NAG	O4-C4-C5	4.46	120.38	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1	NAG	C4-C3-C2	-4.39	104.58	111.02
9	K	1	NAG	C1-O5-C5	-4.19	106.51	112.19
7	G	3	BMA	C3-C4-C5	3.83	117.07	110.24
7	G	3	BMA	C2-C3-C4	3.72	117.33	110.89
6	F	1	NAG	C4-C3-C2	-3.23	106.28	111.02
9	J	2	NAG	C1-O5-C5	3.05	116.33	112.19
6	H	1	NAG	O5-C5-C6	-2.96	102.56	107.20
9	K	2	NAG	O5-C1-C2	-2.77	106.91	111.29
8	I	1	NAG	C1-O5-C5	2.76	115.93	112.19
9	K	1	NAG	C3-C4-C5	2.75	115.14	110.24
9	J	3	FUC	C1-C2-C3	2.72	113.00	109.67
9	K	1	NAG	O5-C1-C2	-2.54	107.28	111.29
7	G	3	BMA	O4-C4-C3	-2.52	104.53	110.35
6	F	1	NAG	C1-O5-C5	2.45	115.51	112.19
9	J	2	NAG	C2-N2-C7	-2.37	119.53	122.90
9	K	1	NAG	C2-N2-C7	2.34	126.23	122.90
9	J	2	NAG	C3-C4-C5	2.32	114.37	110.24
6	F	1	NAG	C8-C7-N2	2.32	120.02	116.10
6	H	2	NAG	C2-N2-C7	2.29	126.17	122.90
8	I	2	FUC	C1-O5-C5	2.27	117.93	112.78
9	J	2	NAG	O5-C1-C2	2.21	114.78	111.29
7	G	3	BMA	O3-C3-C2	-2.15	105.87	109.99
6	F	1	NAG	C1-C2-N2	2.08	114.03	110.49
9	J	2	NAG	O5-C5-C6	2.07	110.45	107.20
7	G	1	NAG	C2-N2-C7	2.05	125.83	122.90
7	G	1	NAG	O4-C4-C3	-2.05	105.61	110.35
6	H	1	NAG	C3-C4-C5	-2.02	106.64	110.24
6	F	1	NAG	O4-C4-C5	2.01	114.29	109.30

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	1	NAG	C8-C7-N2-C2
9	J	1	NAG	O7-C7-N2-C2
9	J	2	NAG	C8-C7-N2-C2
9	J	2	NAG	O7-C7-N2-C2
9	K	1	NAG	C4-C5-C6-O6
9	J	1	NAG	O5-C5-C6-O6
9	K	1	NAG	O5-C5-C6-O6
7	G	4	MAN	O5-C5-C6-O6
9	J	1	NAG	C4-C5-C6-O6

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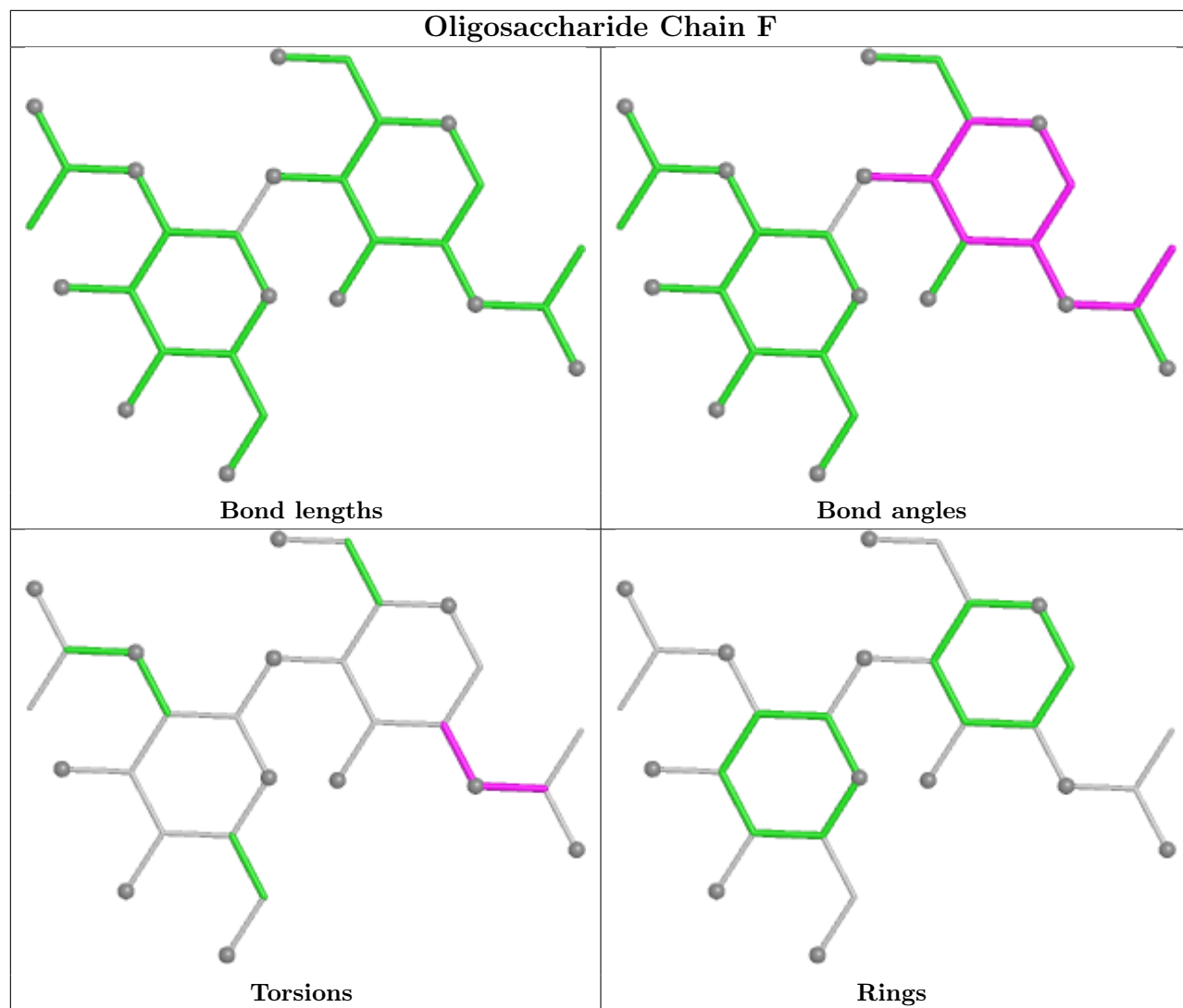
Mol	Chain	Res	Type	Atoms
6	F	1	NAG	C8-C7-N2-C2
6	F	1	NAG	O7-C7-N2-C2
7	G	1	NAG	C8-C7-N2-C2
7	G	1	NAG	O7-C7-N2-C2
7	G	2	NAG	C8-C7-N2-C2
7	G	2	NAG	O7-C7-N2-C2
8	I	1	NAG	C8-C7-N2-C2
8	I	1	NAG	O7-C7-N2-C2
7	G	4	MAN	C4-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
9	J	2	NAG	O5-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
9	K	1	NAG	C1-C2-N2-C7
7	G	3	BMA	O5-C5-C6-O6
6	F	1	NAG	C3-C2-N2-C7

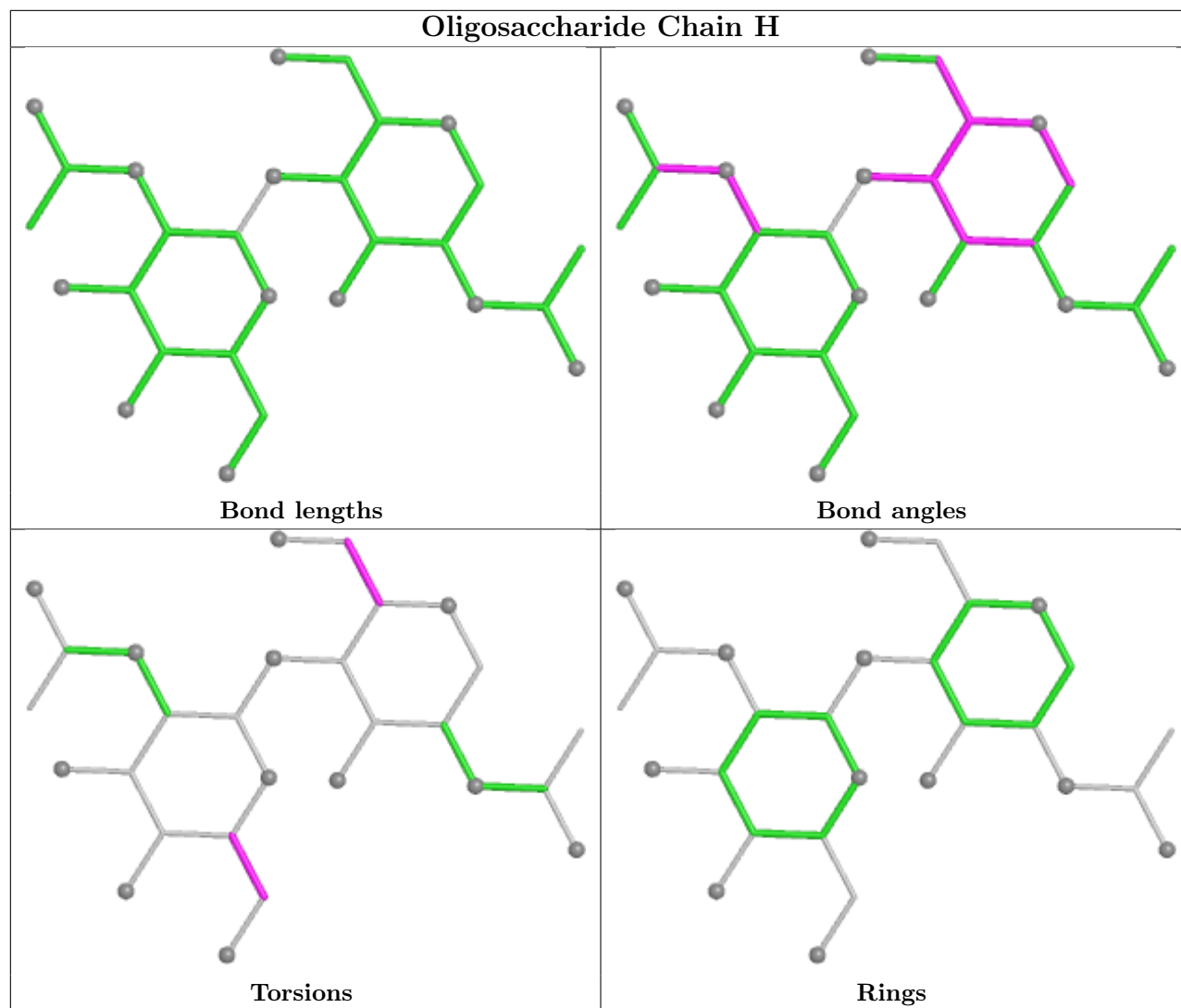
There are no ring outliers.

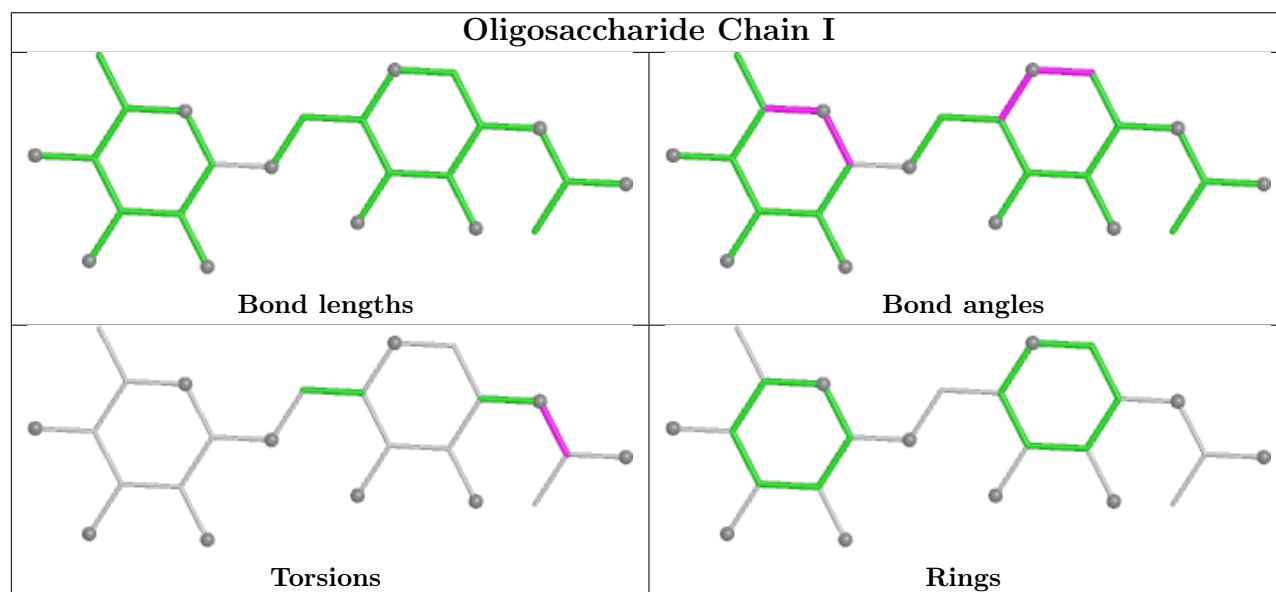
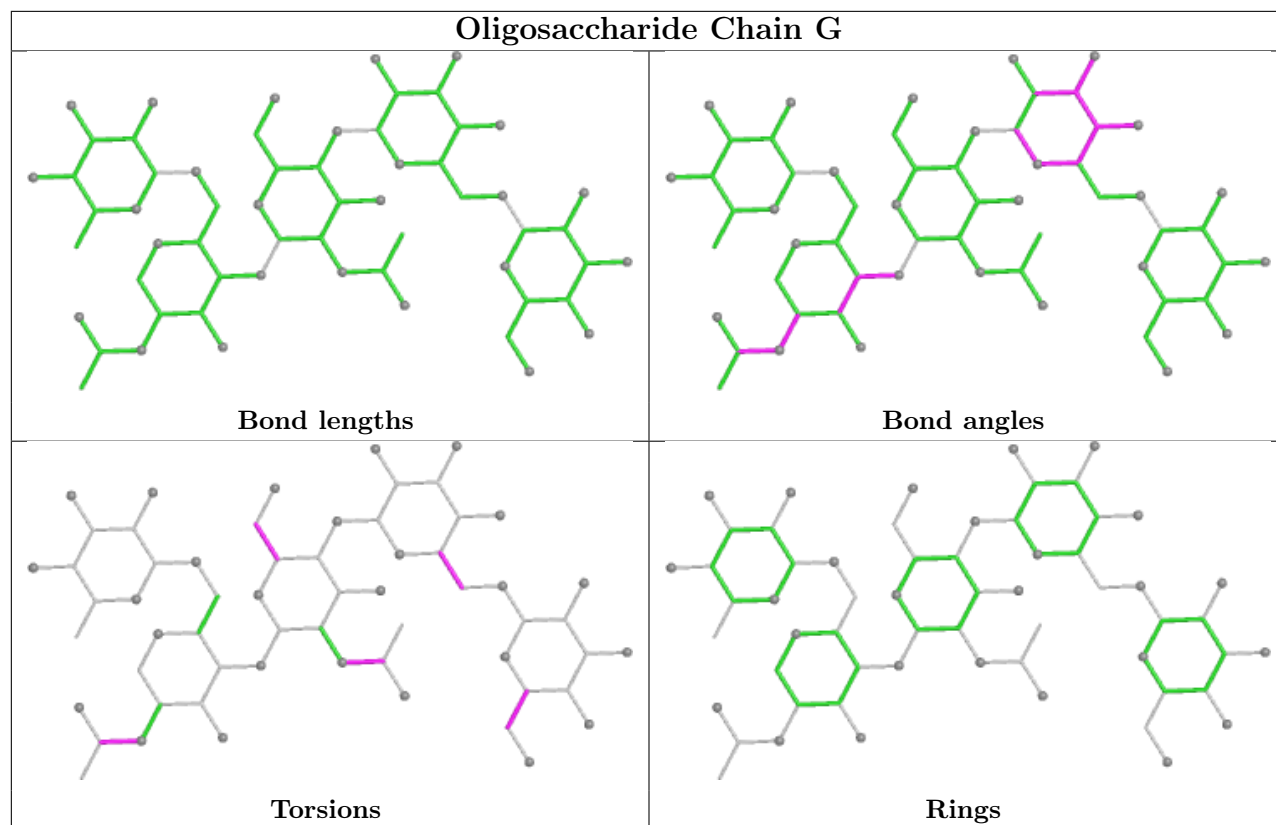
4 monomers are involved in 7 short contacts:

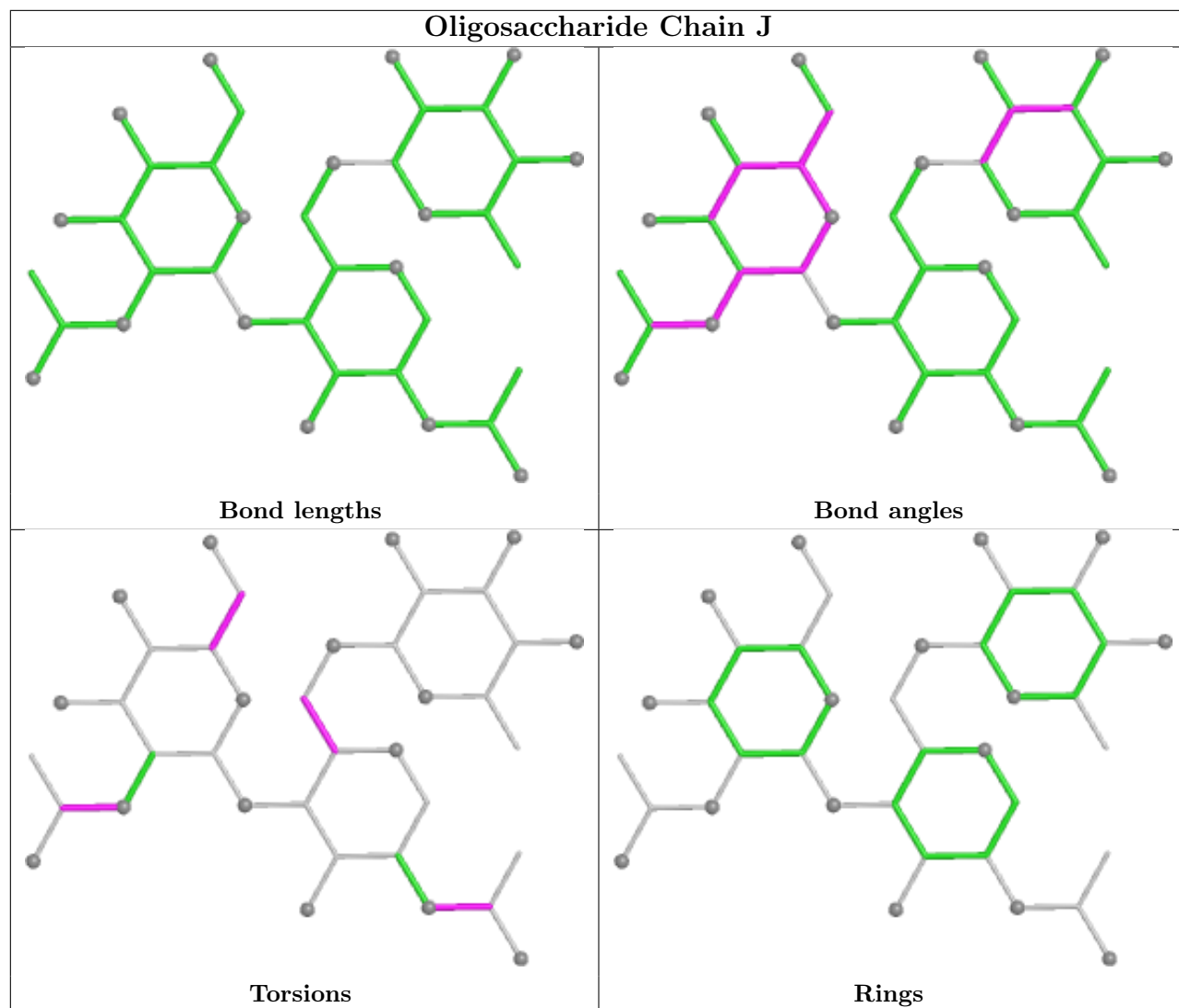
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	1	NAG	4	0
6	H	1	NAG	1	0
9	K	3	FUC	1	0
9	K	1	NAG	2	0

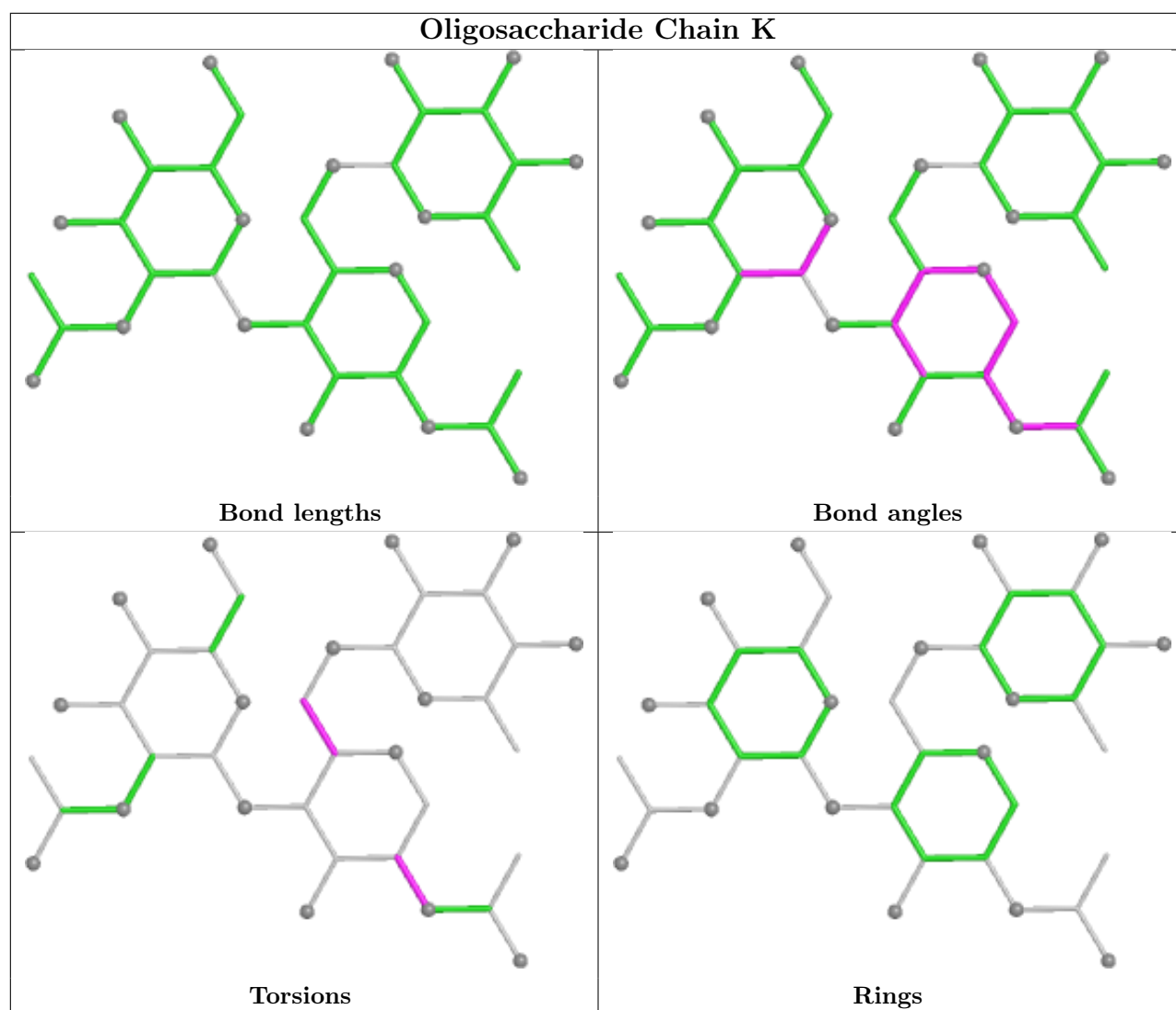
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
10	NAG	C	401	1	14,14,15	0.70	0	17,19,21	0.88	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
10	NAG	C	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 [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	C	280/297 (94%)	-0.03	0 100 100	53, 76, 139, 180	0
2	D	222/233 (95%)	-0.14	1 (0%) 87 67	46, 73, 122, 171	0
3	E	215/217 (99%)	-0.29	0 100 100	47, 64, 93, 157	0
4	A	222/235 (94%)	-0.13	0 100 100	51, 68, 104, 184	0
5	B	214/215 (99%)	-0.13	0 100 100	54, 78, 119, 153	0
All	All	1153/1197 (96%)	-0.14	1 (0%) 92 85	46, 71, 127, 184	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	189	VAL	2.1

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.

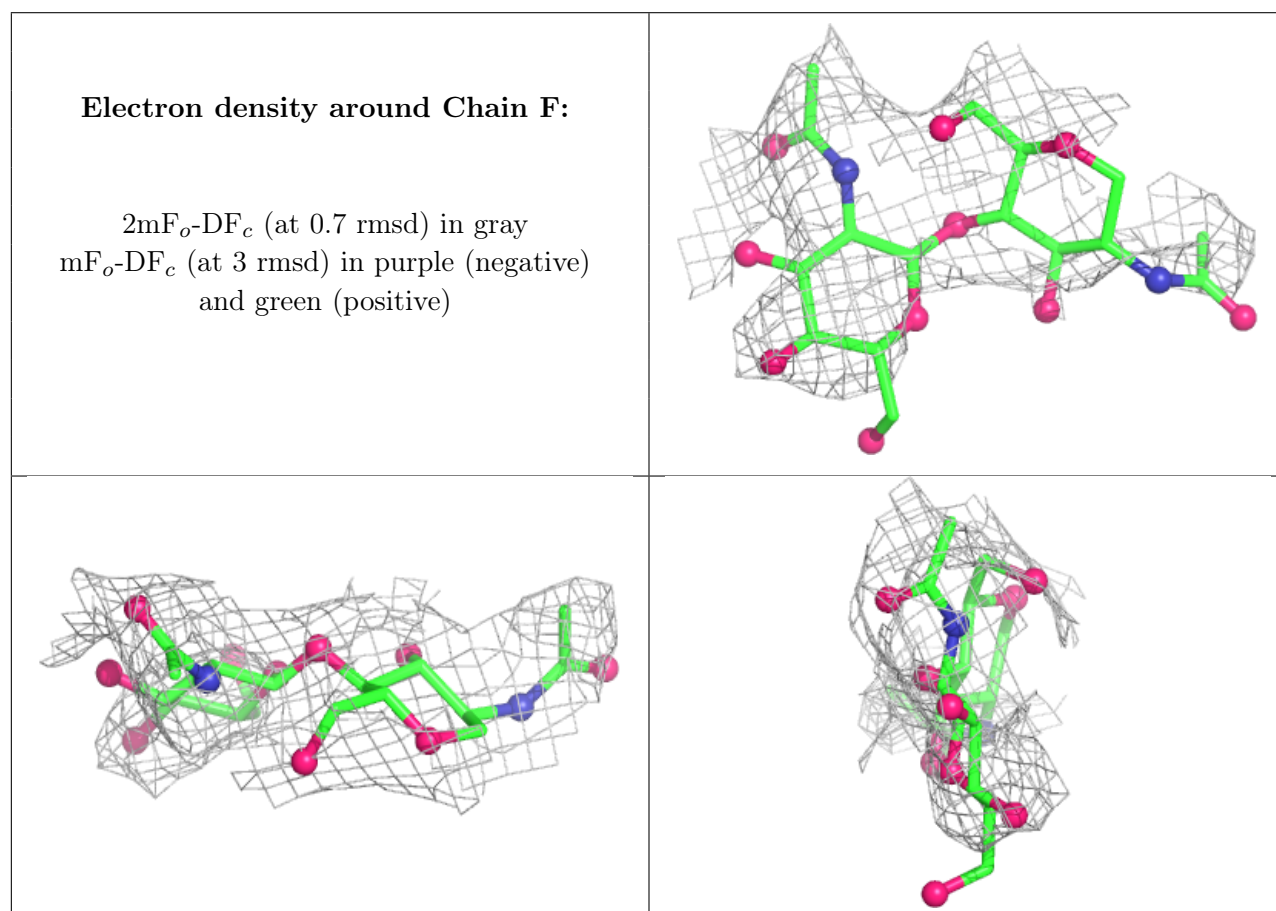
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	FUC	J	3	10/11	0.18	0.13	155,164,170,171	0
9	NAG	J	2	14/15	0.21	0.14	141,167,178,178	0
6	NAG	H	2	14/15	0.27	0.15	142,149,155,161	0
9	NAG	K	1	14/15	0.29	0.12	202,206,219,222	0

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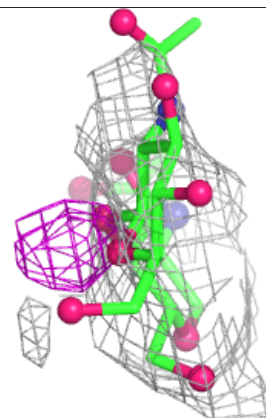
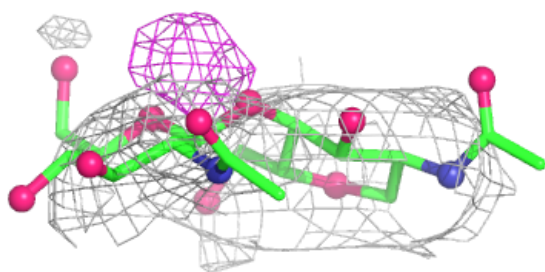
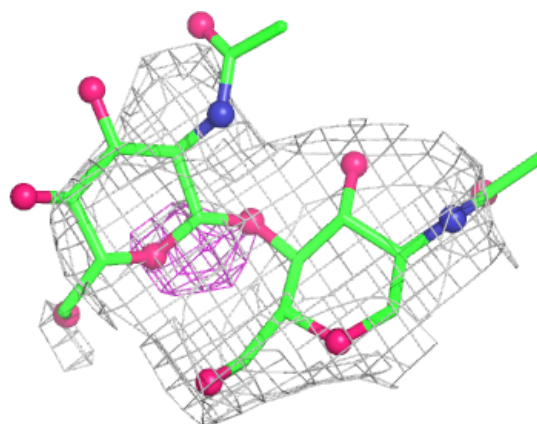
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	BMA	G	3	11/12	0.33	0.10	140,146,157,158	0
9	FUC	K	3	10/11	0.37	0.14	176,199,203,205	0
8	NAG	I	1	14/15	0.40	0.12	147,154,168,175	0
9	NAG	K	2	14/15	0.46	0.10	182,194,202,204	0
7	MAN	G	4	11/12	0.47	0.12	137,150,155,155	0
6	NAG	F	2	14/15	0.50	0.12	119,132,139,140	0
7	FUC	G	5	10/11	0.57	0.12	147,150,152,153	0
8	FUC	I	2	10/11	0.58	0.17	115,120,124,126	0
9	NAG	J	1	14/15	0.61	0.15	188,190,192,195	0
6	NAG	F	1	14/15	0.61	0.14	120,128,130,133	0
7	NAG	G	2	14/15	0.70	0.09	102,118,127,132	0
7	NAG	G	1	14/15	0.75	0.09	101,105,119,130	0
6	NAG	H	1	14/15	0.78	0.10	98,106,118,131	0

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

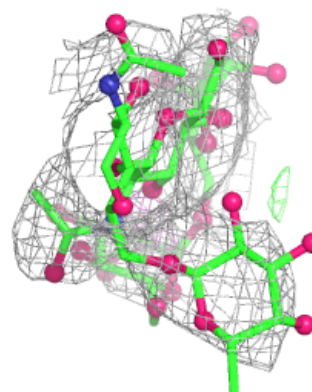
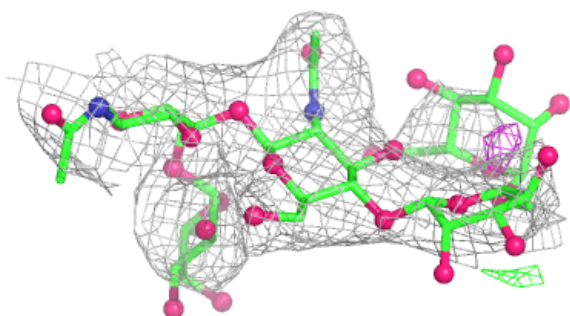
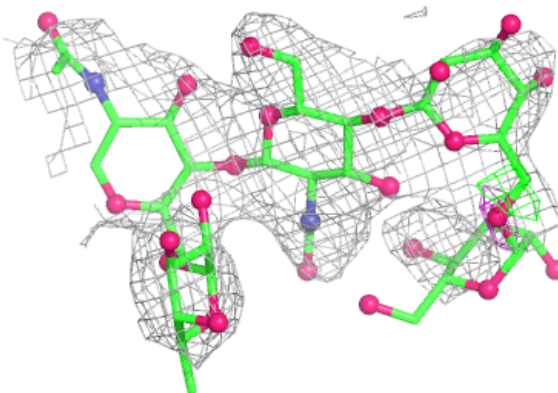


Electron density around Chain H:

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

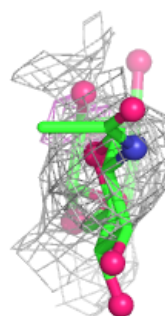
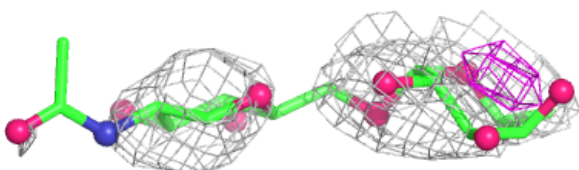
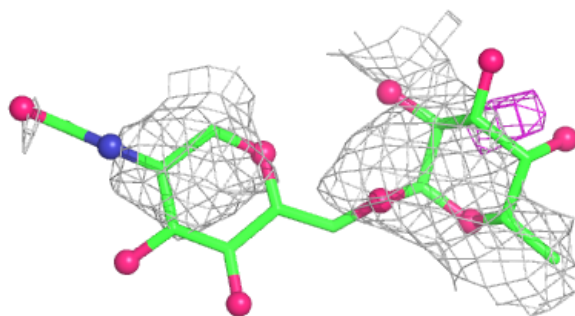
**Electron density around Chain G:**

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



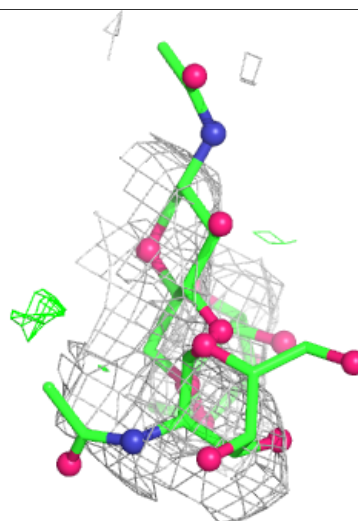
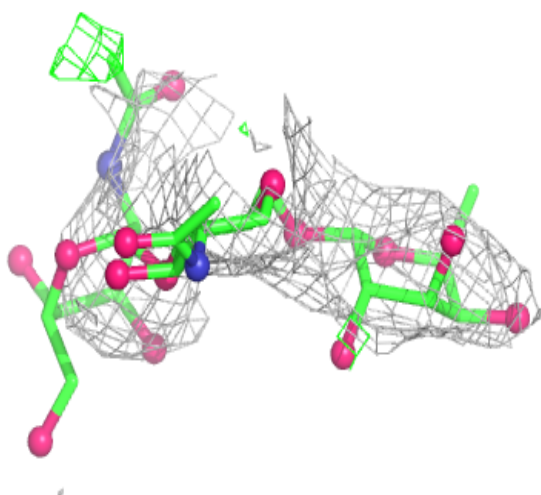
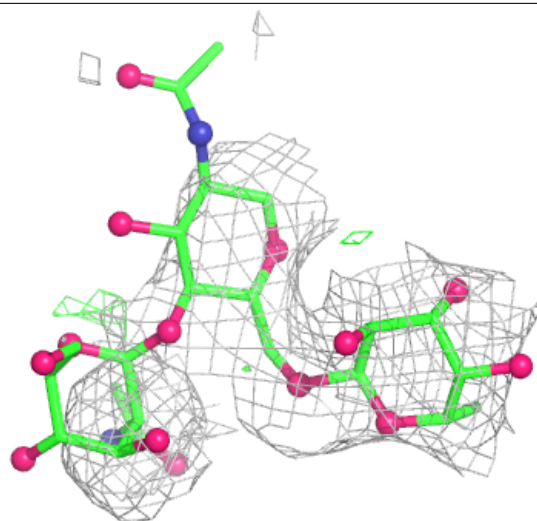
Electron density around Chain I:

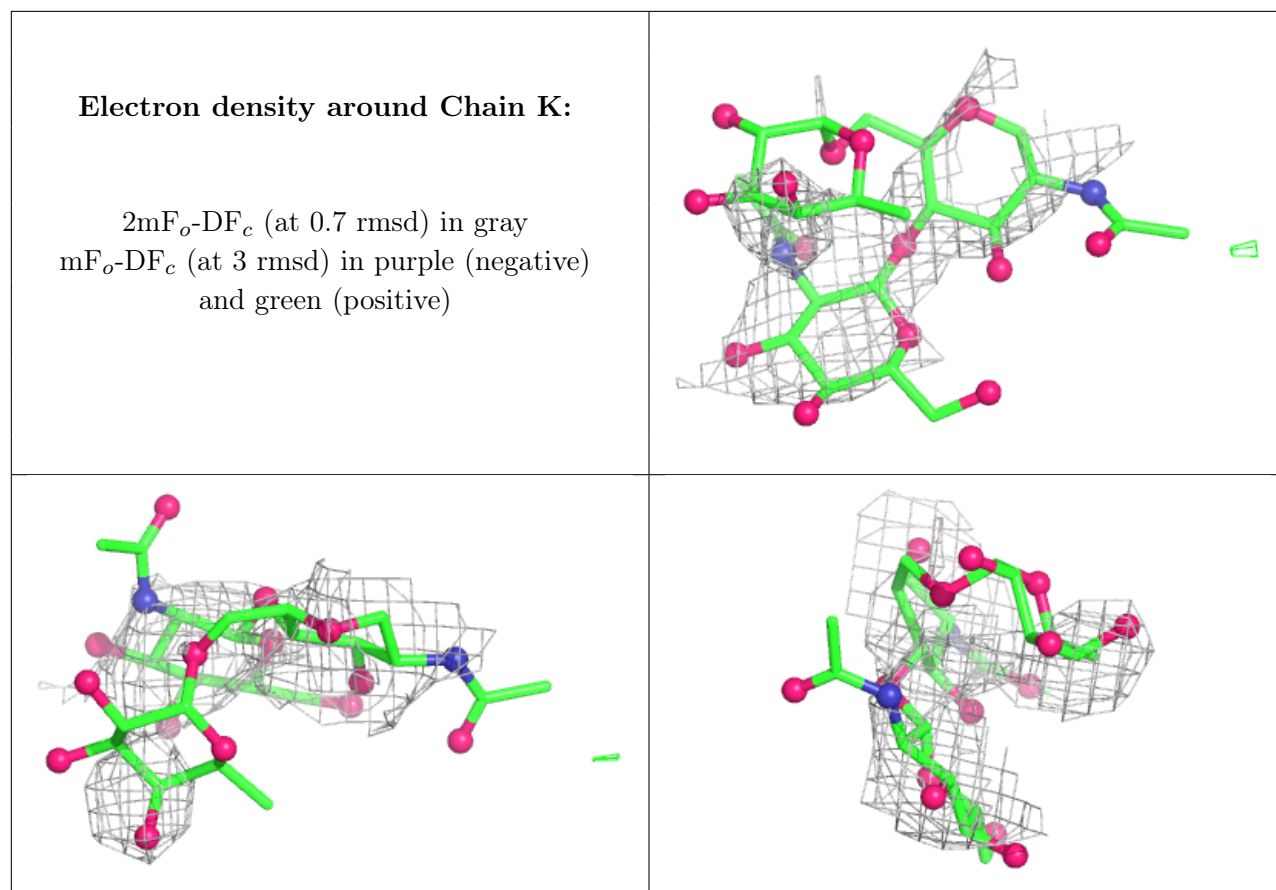
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
10	NAG	C	401	14/15	0.55	0.10	127,133,137,143	0

6.5 Other polymers [i](#)

There are no such residues in this entry.