



## Full wwPDB EM Validation Report ⓘ

Jul 13, 2025 – 12:08 AM JST

PDB ID : 9JQ6 / pdb\_00009jq6  
EMDB ID : EMD-61724  
Title : Cryo-EM structure of BTN2A1 in complex with antagonist antibody TH002  
Authors : Zhang, M.; Wang, Y.Q.; Xiao, J.Y.  
Deposited on : 2024-09-27  
Resolution : 3.34 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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>.

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

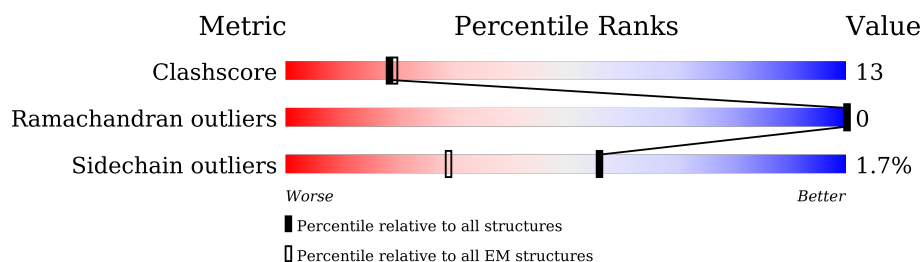
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.34 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	E	532	30% 10% 60%
1	F	532	34% 7% 60%
2	H	231	76% 18% 5%
2	J	231	68% 26% . .
3	I	218	68% 29% ..
3	K	218	72% 26% .
4	A	2	100%
4	B	2	50% 50%
4	C	2	100%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10236 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Butyrophilin subfamily 2 member A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	215	Total	C	N	O	S	0	0
			1691	1067	296	317	11		
1	F	215	Total	C	N	O	S	0	0
			1691	1067	296	317	11		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	500	GLY	-	expression tag	UNP Q7KYR7
E	501	GLY	-	expression tag	UNP Q7KYR7
E	502	GLY	-	expression tag	UNP Q7KYR7
E	503	GLY	-	expression tag	UNP Q7KYR7
E	504	SER	-	expression tag	UNP Q7KYR7
E	505	TRP	-	expression tag	UNP Q7KYR7
E	506	SER	-	expression tag	UNP Q7KYR7
E	507	HIS	-	expression tag	UNP Q7KYR7
E	508	PRO	-	expression tag	UNP Q7KYR7
E	509	GLN	-	expression tag	UNP Q7KYR7
E	510	PHE	-	expression tag	UNP Q7KYR7
E	511	GLU	-	expression tag	UNP Q7KYR7
E	512	LYS	-	expression tag	UNP Q7KYR7
E	513	GLY	-	expression tag	UNP Q7KYR7
E	514	GLY	-	expression tag	UNP Q7KYR7
E	515	GLY	-	expression tag	UNP Q7KYR7
E	516	SER	-	expression tag	UNP Q7KYR7
E	517	GLY	-	expression tag	UNP Q7KYR7
E	518	GLY	-	expression tag	UNP Q7KYR7
E	519	GLY	-	expression tag	UNP Q7KYR7
E	520	SER	-	expression tag	UNP Q7KYR7
E	521	GLY	-	expression tag	UNP Q7KYR7
E	522	GLY	-	expression tag	UNP Q7KYR7
E	523	SER	-	expression tag	UNP Q7KYR7
E	524	ALA	-	expression tag	UNP Q7KYR7
E	525	TRP	-	expression tag	UNP Q7KYR7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	526	SER	-	expression tag	UNP Q7KYR7
E	527	HIS	-	expression tag	UNP Q7KYR7
E	528	PRO	-	expression tag	UNP Q7KYR7
E	529	GLN	-	expression tag	UNP Q7KYR7
E	530	PHE	-	expression tag	UNP Q7KYR7
E	531	GLU	-	expression tag	UNP Q7KYR7
E	532	LYS	-	expression tag	UNP Q7KYR7
F	500	GLY	-	expression tag	UNP Q7KYR7
F	501	GLY	-	expression tag	UNP Q7KYR7
F	502	GLY	-	expression tag	UNP Q7KYR7
F	503	GLY	-	expression tag	UNP Q7KYR7
F	504	SER	-	expression tag	UNP Q7KYR7
F	505	TRP	-	expression tag	UNP Q7KYR7
F	506	SER	-	expression tag	UNP Q7KYR7
F	507	HIS	-	expression tag	UNP Q7KYR7
F	508	PRO	-	expression tag	UNP Q7KYR7
F	509	GLN	-	expression tag	UNP Q7KYR7
F	510	PHE	-	expression tag	UNP Q7KYR7
F	511	GLU	-	expression tag	UNP Q7KYR7
F	512	LYS	-	expression tag	UNP Q7KYR7
F	513	GLY	-	expression tag	UNP Q7KYR7
F	514	GLY	-	expression tag	UNP Q7KYR7
F	515	GLY	-	expression tag	UNP Q7KYR7
F	516	SER	-	expression tag	UNP Q7KYR7
F	517	GLY	-	expression tag	UNP Q7KYR7
F	518	GLY	-	expression tag	UNP Q7KYR7
F	519	GLY	-	expression tag	UNP Q7KYR7
F	520	SER	-	expression tag	UNP Q7KYR7
F	521	GLY	-	expression tag	UNP Q7KYR7
F	522	GLY	-	expression tag	UNP Q7KYR7
F	523	SER	-	expression tag	UNP Q7KYR7
F	524	ALA	-	expression tag	UNP Q7KYR7
F	525	TRP	-	expression tag	UNP Q7KYR7
F	526	SER	-	expression tag	UNP Q7KYR7
F	527	HIS	-	expression tag	UNP Q7KYR7
F	528	PRO	-	expression tag	UNP Q7KYR7
F	529	GLN	-	expression tag	UNP Q7KYR7
F	530	PHE	-	expression tag	UNP Q7KYR7
F	531	GLU	-	expression tag	UNP Q7KYR7
F	532	LYS	-	expression tag	UNP Q7KYR7

- Molecule 2 is a protein called BTN2A1 antagonist antibody TH002-Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	219	Total	C	N	O	S	0	0
			1670	1059	280	323	8		
2	J	221	Total	C	N	O	S	0	0
			1684	1067	282	327	8		

- Molecule 3 is a protein called BTN2A1 antagonist antibody TH002-Fab light chain.

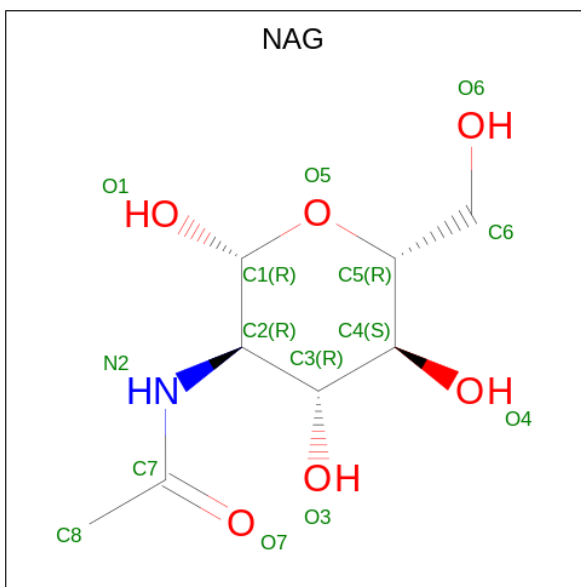
Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	216	Total	C	N	O	S	0	0
			1659	1032	279	343	5		
3	K	216	Total	C	N	O	S	0	0
			1659	1032	279	343	5		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



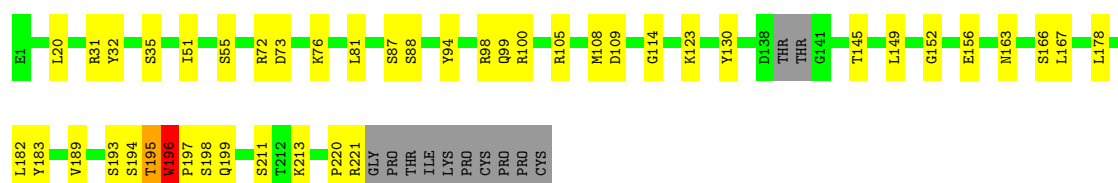
Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	



PRO	ARG	GLN	SER	GLU	ALA	PHE	SER	GLY	VAL	PRO	VAL	ARG	PRO	PHE	PHE	ARG	LEU	GLY	CYS	GLU	ASP	SER	PRO	ILE	PHE	GLN	PHE	GLY	GLU	LYS
PRO	GLN	PHE	GLU	GLY	LYS	PHE	GLY	GLY	GLY	SER	SER	GLY	GLY	GLY	GLY	GLY	SER	SER	ALA	TRP	SER	HIS	PRO	PRO	PHE	GLN	PHE	GLY	GLU	LYS

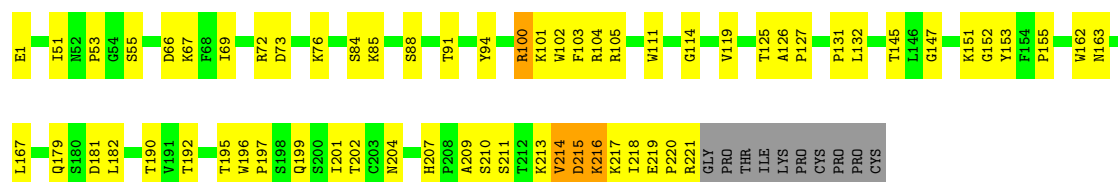
• Molecule 2: BTN2A1 antagonist antibody TH002-Fab heavy chain

Chain H:  76% 18% 5%



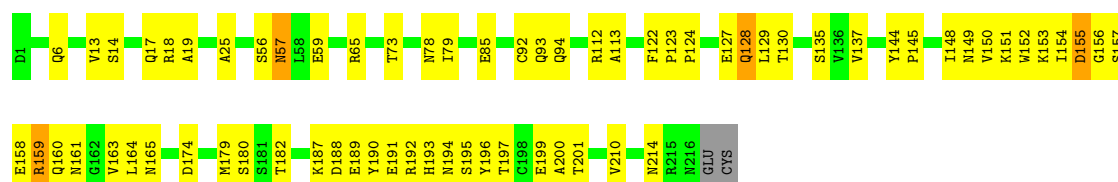
• Molecule 2: BTN2A1 antagonist antibody TH002-Fab heavy chain

Chain J:  68% 26% 6%



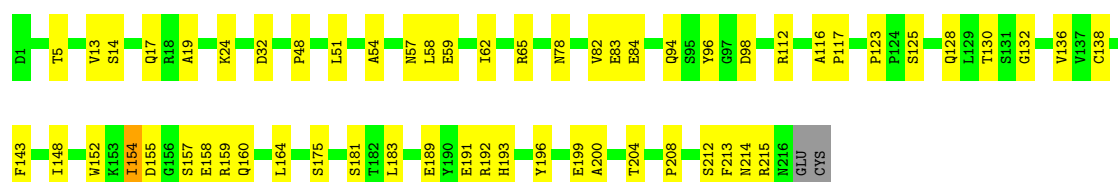
• Molecule 3: BTN2A1 antagonist antibody TH002-Fab light chain

Chain I:  68% 29% 3%



• Molecule 3: BTN2A1 antagonist antibody TH002-Fab light chain

Chain K:  72% 26% 2%



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

Chain A:  100%





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

Chain B:  50% 50%



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

Chain C:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	247369	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60.0	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 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	E	0.27	0/1728	0.51	4/2338 (0.2%)
1	F	0.18	0/1728	0.38	0/2338
2	H	0.27	0/1712	0.51	2/2330 (0.1%)
2	J	0.30	0/1727	0.56	0/2353
3	I	0.24	0/1699	0.47	1/2313 (0.0%)
3	K	0.19	0/1699	0.43	1/2313 (0.0%)
All	All	0.25	0/10293	0.48	8/13985 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	130	THR	N-CA-C	-9.41	100.98	111.14
1	E	155	GLY	N-CA-C	7.03	121.10	113.58
2	H	195	THR	N-CA-C	-6.04	105.77	113.02
2	H	196	TRP	N-CA-C	-5.59	105.14	112.75
1	E	156	GLY	N-CA-C	5.53	119.61	112.54
3	I	155	ASP	N-CA-C	-5.43	103.90	111.39
1	E	152	ASP	CA-C-N	-5.43	114.08	119.56
1	E	152	ASP	C-N-CA	-5.43	114.08	119.56

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	E	1691	0	1670	34	0
1	F	1691	0	1670	24	0
2	H	1670	0	1646	34	0
2	J	1684	0	1661	58	0
3	I	1659	0	1569	77	0
3	K	1659	0	1569	42	0
4	A	28	0	25	0	0
4	B	28	0	25	1	0
4	C	28	0	25	0	0
5	E	42	0	39	0	0
5	F	56	0	52	2	0
All	All	10236	0	9951	258	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 13.

All (258) 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:H:195:THR:HA	2:H:198:SER:HB2	1.47	0.96
3:I:157:SER:HB3	3:I:159:ARG:HH11	1.31	0.92
3:I:159:ARG:HA	3:I:159:ARG:CZ	2.04	0.87
2:H:196:TRP:CZ2	2:H:220:PRO:HA	2.11	0.86
2:H:196:TRP:HZ2	2:H:220:PRO:HA	1.44	0.81
3:I:158:GLU:HB3	3:I:161:ASN:HB2	1.62	0.80
2:J:162:TRP:HB3	2:J:167:LEU:HD12	1.64	0.78
1:E:126:ARG:HG3	1:E:136:GLU:HG3	1.66	0.76
2:J:197:PRO:HG2	2:J:199:GLN:HB2	1.66	0.76
3:I:6:GLN:NE2	3:I:92:CYS:SG	2.58	0.74
3:K:214:ASN:OD1	3:K:215:ARG:N	2.21	0.74
2:H:195:THR:HA	2:H:198:SER:CB	2.19	0.72
3:I:197:THR:CG2	3:I:210:VAL:CG1	2.69	0.71
2:J:216:LYS:HZ2	2:J:216:LYS:HB3	1.54	0.71
3:I:157:SER:HB3	3:I:159:ARG:NH1	2.06	0.70
3:K:65:ARG:NH1	3:K:83:GLU:OE1	2.27	0.68
3:I:199:GLU:N	3:I:199:GLU:OE1	2.27	0.68
2:J:1:GLU:OE1	2:J:1:GLU:N	2.21	0.67
2:J:126:ALA:HB1	2:J:127:PRO:HD2	1.77	0.67
2:J:207:HIS:HD2	2:J:210:SER:H	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:167:LEU:HD23	2:H:189:VAL:HG21	1.77	0.66
3:I:151:LYS:HB2	3:I:159:ARG:NH1	2.11	0.66
2:H:195:THR:O	2:H:199:GLN:HG2	1.94	0.66
3:K:199:GLU:OE2	3:K:199:GLU:N	2.29	0.66
3:I:153:LYS:HA	3:I:157:SER:HA	1.77	0.66
3:I:154:ILE:HB	3:I:158:GLU:OE1	1.95	0.65
3:K:152:TRP:HB2	3:K:183:LEU:HD13	1.78	0.65
1:F:18:ASN:HB3	1:F:85:HIS:HA	1.79	0.65
1:E:31:ALA:HA	1:E:34:MET:HG3	1.79	0.65
3:I:57:ASN:N	3:I:57:ASN:HD22	1.94	0.64
1:F:1:GLN:H1	2:H:32:TYR:HE1	1.44	0.63
2:J:217:LYS:HZ2	2:J:221:ARG:HH12	1.45	0.63
3:K:183:LEU:H	3:K:183:LEU:HD23	1.64	0.62
1:F:59:GLU:N	1:F:59:GLU:OE1	2.31	0.62
1:E:62:GLU:HA	1:E:65:ARG:HG3	1.80	0.62
1:F:3:ILE:HG23	2:H:31:ARG:HG2	1.82	0.62
3:K:84:GLU:OE2	3:K:84:GLU:N	2.24	0.61
3:I:19:ALA:HB3	3:I:79:ILE:HB	1.82	0.61
3:I:112:ARG:NH1	3:I:113:ALA:O	2.33	0.61
2:J:207:HIS:CD2	2:J:210:SER:H	2.18	0.61
3:I:159:ARG:HA	3:I:159:ARG:NH2	2.16	0.60
2:J:66:ASP:OD1	2:J:67:LYS:N	2.34	0.60
1:E:149:VAL:HG13	1:E:157:VAL:HG13	1.82	0.60
3:K:138:CYS:SG	3:K:181:SER:OG	2.60	0.60
1:F:34:MET:HG2	1:F:101:GLU:HB2	1.84	0.60
3:I:149:ASN:HB2	3:I:201:THR:HG22	1.82	0.60
3:I:199:GLU:HB3	3:I:210:VAL:HG13	1.82	0.59
2:H:94:TYR:O	2:H:114:GLY:HA2	2.02	0.59
2:J:217:LYS:NZ	2:J:221:ARG:HH12	2.00	0.59
1:F:49:VAL:HG21	1:F:59:GLU:HB2	1.85	0.58
3:K:58:LEU:HD11	3:K:62:ILE:HB	1.84	0.58
2:J:155:PRO:HB2	2:J:207:HIS:CE1	2.38	0.58
3:I:197:THR:HG23	3:I:210:VAL:HG12	1.86	0.57
5:F:601:NAG:H3	5:F:601:NAG:H83	1.86	0.57
2:J:127:PRO:HA	2:J:152:GLY:O	2.03	0.57
1:F:33:ASP:OD1	1:F:33:ASP:N	2.33	0.57
2:H:100:ARG:HH11	2:H:105:ARG:HG3	1.69	0.57
2:H:156:GLU:OE2	2:H:183:TYR:OH	2.20	0.57
1:E:106:ASP:HB2	2:J:102:TRP:HZ2	1.70	0.56
1:F:120:LYS:NZ	1:F:204:SER:OG	2.39	0.56
2:J:51:ILE:HD11	2:J:55:SER:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:57:ASN:HD22	3:K:57:ASN:N	2.02	0.56
2:J:104:ARG:HH22	3:K:32:ASP:HB3	1.69	0.56
3:I:165:ASN:HB2	3:I:179:MET:HE3	1.88	0.56
1:F:151:ARG:NH2	1:F:155:GLY:O	2.38	0.55
3:K:17:GLN:H	3:K:82:VAL:HG12	1.70	0.55
2:J:202:THR:HG23	2:J:216:LYS:O	2.06	0.55
3:I:159:ARG:HA	3:I:159:ARG:NE	2.18	0.55
3:I:157:SER:CB	3:I:159:ARG:HE	2.20	0.55
3:I:163:VAL:C	3:I:164:LEU:HD22	2.32	0.55
3:K:159:ARG:NE	3:K:159:ARG:HA	2.22	0.55
2:H:100:ARG:NH2	3:I:59:GLU:OE2	2.40	0.54
3:K:125:SER:N	3:K:128:GLN:OE1	2.39	0.54
3:I:151:LYS:NZ	3:I:199:GLU:OE2	2.22	0.54
2:J:88:SER:O	2:J:88:SER:OG	2.24	0.54
2:H:20:LEU:HD13	2:H:81:LEU:HD23	1.90	0.54
3:I:197:THR:CG2	3:I:210:VAL:HG12	2.38	0.53
3:K:158:GLU:HG2	3:K:160:GLN:H	1.74	0.53
3:K:123:PRO:HB3	3:K:213:PHE:CZ	2.43	0.53
2:H:87:SER:OG	2:H:88:SER:N	2.40	0.53
3:I:164:LEU:HB2	3:I:182:THR:HG22	1.91	0.53
3:I:153:LYS:HD2	3:I:157:SER:N	2.23	0.53
3:I:152:TRP:CE3	3:I:154:ILE:HD11	2.44	0.52
1:F:164:VAL:HG12	1:F:164:VAL:O	2.08	0.52
3:K:136:VAL:HG13	3:K:183:LEU:HG	1.91	0.52
3:I:127:GLU:O	3:I:130:THR:OG1	2.27	0.52
3:I:158:GLU:OE1	3:I:158:GLU:N	2.43	0.52
2:H:193:SER:O	2:H:194:SER:C	2.52	0.52
3:I:152:TRP:O	3:I:157:SER:HA	2.11	0.51
3:K:154:ILE:HG23	3:K:155:ASP:H	1.74	0.51
2:J:125:THR:O	2:J:153:TYR:HA	2.10	0.51
2:J:91:THR:HG22	2:J:119:VAL:HB	1.92	0.51
2:J:201:ILE:HB	2:J:218:ILE:HD11	1.92	0.51
3:I:19:ALA:O	3:I:78:ASN:HA	2.11	0.51
3:I:150:VAL:HG12	3:I:200:ALA:HB2	1.92	0.51
3:I:159:ARG:O	3:I:160:GLN:HG3	2.11	0.51
3:I:57:ASN:N	3:I:57:ASN:ND2	2.58	0.51
2:H:194:SER:O	2:H:197:PRO:HD2	2.11	0.50
2:H:163:ASN:HB2	2:H:166:SER:HB3	1.94	0.50
2:J:201:ILE:O	2:J:218:ILE:HG12	2.12	0.50
3:K:19:ALA:O	3:K:78:ASN:HA	2.11	0.50
1:E:201:LYS:HB2	4:B:1:NAG:H83	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:153:LYS:HA	3:I:157:SER:CA	2.42	0.50
3:K:128:GLN:O	3:K:132:GLY:N	2.45	0.49
3:I:155:ASP:OD2	3:I:193:HIS:HB3	2.11	0.49
3:I:157:SER:HB3	3:I:159:ARG:HE	1.78	0.49
2:J:147:GLY:HA2	2:J:162:TRP:CH2	2.47	0.49
2:H:35:SER:OG	2:H:99:GLN:OE1	2.27	0.49
3:I:85:GLU:H	3:I:85:GLU:CD	2.19	0.49
3:I:151:LYS:HB2	3:I:159:ARG:CZ	2.43	0.49
3:I:197:THR:HG21	3:I:210:VAL:CG1	2.43	0.49
2:H:221:ARG:HH22	3:I:123:PRO:HG2	1.78	0.49
1:F:194:ASN:HB2	5:F:604:NAG:O5	2.13	0.49
3:I:153:LYS:HZ2	3:I:156:GLY:H	1.61	0.48
3:I:25:ALA:HB3	3:I:73:THR:HG23	1.94	0.48
1:E:31:ALA:HB3	1:E:75:ILE:O	2.12	0.48
1:E:123:ILE:HD11	1:E:191:CYS:HB2	1.94	0.48
1:F:21:LEU:O	1:F:81:ALA:HA	2.13	0.48
2:H:32:TYR:HE2	2:H:98:ARG:CZ	2.26	0.48
3:K:5:THR:HG23	3:K:24:LYS:HB3	1.96	0.48
3:I:56:SER:C	3:I:57:ASN:HD22	2.21	0.47
3:I:129:LEU:HD12	3:I:187:LYS:HD3	1.96	0.47
3:K:191:GLU:HB3	3:K:215:ARG:HH12	1.79	0.47
3:I:154:ILE:HB	3:I:158:GLU:CD	2.40	0.47
2:H:152:GLY:HA2	2:H:182:LEU:HD22	1.96	0.47
2:H:178:LEU:HD12	2:H:182:LEU:O	2.14	0.47
1:E:190:SER:HA	1:E:204:SER:O	2.14	0.47
3:K:189:GLU:OE2	3:K:192:ARG:NE	2.48	0.47
1:E:99:PHE:O	1:E:105:TYR:HA	2.15	0.47
2:J:210:SER:O	2:J:211:SER:C	2.57	0.47
1:E:153:PRO:CD	1:E:186:VAL:HG23	2.45	0.47
2:J:132:LEU:HD12	2:J:132:LEU:H	1.79	0.47
3:K:117:PRO:HB3	3:K:143:PHE:HB3	1.96	0.47
3:K:143:PHE:CG	3:K:148:ILE:HD11	2.50	0.47
1:E:54:ARG:HH12	1:E:56:ARG:NH2	2.13	0.47
2:H:213:LYS:HA	2:H:213:LYS:HD3	1.76	0.47
3:K:51:LEU:HD22	3:K:62:ILE:HG21	1.96	0.47
3:I:153:LYS:NZ	3:I:156:GLY:H	2.13	0.46
3:I:158:GLU:O	3:I:160:GLN:N	2.48	0.46
2:J:152:GLY:HA2	2:J:182:LEU:CD1	2.45	0.46
2:J:67:LYS:HB2	2:J:84:SER:O	2.15	0.46
2:H:145:THR:O	3:I:122:PHE:HZ	1.98	0.46
3:I:155:ASP:CG	3:I:193:HIS:HB3	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:MET:HG3	1:E:167:PRO:HD2	1.98	0.46
2:J:53:PRO:HA	2:J:72:ARG:NH1	2.31	0.46
3:I:144:TYR:CD1	3:I:145:PRO:HA	2.51	0.46
3:I:154:ILE:O	3:I:155:ASP:C	2.58	0.46
1:F:126:ARG:HG3	1:F:136:GLU:HG3	1.98	0.45
1:F:126:ARG:HB2	1:F:134:ARG:HG2	1.97	0.45
3:I:148:ILE:HD12	3:I:148:ILE:HA	1.82	0.45
2:H:195:THR:CA	2:H:198:SER:HB2	2.32	0.45
3:I:152:TRP:CZ3	3:I:154:ILE:HD11	2.51	0.45
3:K:94:GLN:HG2	3:K:96:TYR:H	1.80	0.45
1:E:151:ARG:NH1	1:E:151:ARG:HB3	2.32	0.45
2:J:179:GLN:HG2	3:K:164:LEU:HD21	1.98	0.45
2:J:202:THR:HG21	2:J:215:ASP:HB3	1.99	0.45
2:J:131:PRO:HG3	2:J:216:LYS:HB3	1.98	0.45
3:K:57:ASN:N	3:K:57:ASN:ND2	2.65	0.45
1:E:1:GLN:CD	1:E:1:GLN:N	2.75	0.45
1:E:94:THR:HG23	1:E:109:ILE:HG23	1.99	0.45
1:F:61:MET:HE3	1:F:61:MET:HB2	1.86	0.45
2:J:100:ARG:NH2	3:K:59:GLU:OE1	2.49	0.45
1:F:1:GLN:O	1:F:27:PRO:HG2	2.17	0.45
3:I:189:GLU:HA	3:I:192:ARG:HD2	1.99	0.45
3:I:195:SER:HA	3:I:214:ASN:HB2	1.98	0.45
1:E:11:ILE:HB	1:E:112:LEU:HD12	1.99	0.45
3:I:194:ASN:O	3:I:214:ASN:HB2	2.17	0.45
3:I:17:GLN:OE1	3:I:17:GLN:HA	2.16	0.45
2:J:152:GLY:HA2	2:J:182:LEU:HD12	1.98	0.45
3:I:122:PHE:HB2	3:I:137:VAL:HG23	1.98	0.44
3:I:85:GLU:OE1	3:I:85:GLU:N	2.37	0.44
3:I:93:GLN:HG2	3:I:94:GLN:N	2.33	0.44
3:I:158:GLU:O	3:I:159:ARG:C	2.59	0.44
2:J:192:THR:HG22	2:J:195:THR:H	1.83	0.44
3:K:191:GLU:HB2	3:K:215:ARG:HH22	1.81	0.44
2:J:196:TRP:HZ2	2:J:220:PRO:HG3	1.83	0.44
2:J:217:LYS:HD3	2:J:219:GLU:HG3	2.00	0.44
1:F:135:LEU:HB2	1:F:179:VAL:HG12	1.99	0.43
2:J:101:LYS:O	2:J:102:TRP:HB2	2.18	0.43
2:J:213:LYS:O	2:J:214:VAL:HG13	2.18	0.43
1:E:168:ASP:OD1	1:E:172:LEU:N	2.52	0.43
1:E:181:ILE:HG12	1:E:189:MET:HE3	1.99	0.43
3:I:165:ASN:N	3:I:165:ASN:OD1	2.49	0.43
3:I:187:LYS:NZ	3:I:191:GLU:HB2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:163:ASN:HB2	2:J:167:LEU:HG	2.00	0.43
1:E:21:LEU:O	1:E:81:ALA:HA	2.19	0.43
3:K:155:ASP:HB2	3:K:193:HIS:CE1	2.53	0.43
2:H:221:ARG:NH2	3:I:123:PRO:HG2	2.34	0.43
3:I:13:VAL:HG12	3:I:14:SER:O	2.18	0.43
3:I:158:GLU:C	3:I:160:GLN:N	2.73	0.43
2:J:145:THR:HG22	2:J:190:THR:HB	2.00	0.43
2:H:211:SER:HB3	2:H:213:LYS:NZ	2.33	0.43
2:J:216:LYS:HZ2	2:J:216:LYS:CB	2.29	0.43
3:K:13:VAL:HG12	3:K:14:SER:O	2.19	0.43
3:I:128:GLN:C	3:I:128:GLN:HE21	2.27	0.43
3:K:157:SER:H	3:K:159:ARG:HH22	1.66	0.43
2:J:73:ASP:OD2	2:J:76:LYS:HE2	2.19	0.43
1:F:151:ARG:HB2	1:F:190:SER:OG	2.18	0.42
2:J:69:ILE:HD13	2:J:69:ILE:HA	1.91	0.42
3:K:112:ARG:HD3	3:K:175:SER:O	2.19	0.42
2:H:98:ARG:NH2	2:H:109:ASP:OD2	2.52	0.42
2:J:151:LYS:HZ1	2:J:182:LEU:HD12	1.84	0.42
2:J:105:ARG:HG3	3:K:54:ALA:HB2	2.00	0.42
2:J:103:PHE:O	2:J:104:ARG:HB2	2.19	0.42
1:E:184:LYS:O	1:E:187:ARG:NH2	2.53	0.42
1:E:50:TYR:CE1	1:E:53:GLY:HA2	2.55	0.42
1:E:148:THR:OG1	1:E:163:GLU:OE2	2.35	0.42
3:I:65:ARG:H	3:I:65:ARG:HG2	1.68	0.42
2:H:51:ILE:HD11	2:H:55:SER:HA	2.02	0.42
3:I:188:ASP:O	3:I:192:ARG:HG3	2.20	0.42
2:J:151:LYS:NZ	2:J:182:LEU:HD12	2.35	0.42
1:F:184:LYS:O	1:F:187:ARG:NH1	2.52	0.42
3:I:154:ILE:HD13	3:I:197:THR:H	1.85	0.42
2:J:111:TRP:CE3	3:K:48:PRO:HD2	2.55	0.42
2:J:131:PRO:CG	2:J:216:LYS:HB3	2.49	0.42
3:K:84:GLU:H	3:K:84:GLU:CD	2.23	0.42
3:I:174:ASP:OD1	3:I:174:ASP:N	2.50	0.41
2:J:94:TYR:O	2:J:114:GLY:HA2	2.20	0.41
2:J:162:TRP:CE3	2:J:201:ILE:HG21	2.54	0.41
3:K:200:ALA:O	3:K:208:PRO:HA	2.20	0.41
1:E:20:THR:HA	1:E:82:LEU:O	2.20	0.41
2:H:123:LYS:HD3	2:H:123:LYS:HA	1.85	0.41
2:J:217:LYS:HD2	2:J:217:LYS:C	2.44	0.41
1:E:153:PRO:HG2	1:E:154:TYR:CD1	2.55	0.41
1:F:29:LYS:HE3	1:F:29:LYS:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:PHE:CZ	1:F:70:PHE:HB2	2.56	0.41
3:K:196:TYR:O	3:K:212:SER:HA	2.21	0.41
1:E:153:PRO:HD3	1:E:186:VAL:HG23	2.02	0.41
2:H:73:ASP:OD1	2:H:76:LYS:HG3	2.20	0.41
2:J:147:GLY:HA2	2:J:162:TRP:CZ2	2.55	0.41
1:E:194:ASN:OD1	1:E:194:ASN:N	2.53	0.41
2:H:98:ARG:O	2:H:108:MET:HA	2.20	0.41
3:I:124:PRO:HG3	3:I:135:SER:O	2.21	0.41
1:E:37:ARG:NH1	1:E:43:PHE:O	2.53	0.41
1:E:137:CYS:HB3	1:E:177:THR:HG23	2.03	0.41
1:F:49:VAL:HG12	1:F:49:VAL:O	2.21	0.41
2:J:126:ALA:HB1	2:J:127:PRO:CD	2.49	0.41
2:J:155:PRO:HG2	2:J:209:ALA:HB3	2.03	0.41
1:E:62:GLU:OE1	1:E:62:GLU:N	2.39	0.41
1:E:192:SER:HB2	1:E:201:LYS:HD2	2.03	0.41
3:I:18:ARG:HA	3:I:18:ARG:HE	1.85	0.41
3:I:157:SER:HB2	3:I:159:ARG:HE	1.83	0.41
3:I:190:TYR:O	3:I:196:TYR:OH	2.35	0.41
2:J:85:LYS:O	2:J:85:LYS:HG3	2.21	0.41
2:J:181:ASP:OD1	2:J:181:ASP:N	2.54	0.41
3:K:98:ASP:N	3:K:98:ASP:OD1	2.50	0.41
1:E:184:LYS:NZ	1:E:210:GLU:OE2	2.49	0.41
3:I:197:THR:HG21	3:I:210:VAL:HG11	2.02	0.41
1:E:35:GLU:HG3	1:E:51:LYS:HE3	2.03	0.40
1:F:42:GLN:NE2	1:F:45:PRO:HD2	2.36	0.40
2:H:109:ASP:OD1	2:H:109:ASP:N	2.38	0.40
2:J:201:ILE:HD12	2:J:201:ILE:H	1.87	0.40
1:E:86:ASN:HD22	1:E:86:ASN:HA	1.57	0.40
3:K:116:ALA:HB2	3:K:204:THR:HG21	2.02	0.40
3:K:123:PRO:HB3	3:K:213:PHE:CE2	2.56	0.40
2:J:201:ILE:HD12	2:J:201:ILE:N	2.36	0.40
1:F:14:THR:OG1	1:F:17:GLU:HB3	2.21	0.40
2:H:130:TYR:HB2	2:H:149:LEU:HB3	2.02	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 PDB entries followed by that with respect to all EM entries.

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	E	213/532 (40%)	201 (94%)	12 (6%)	0	100	100
1	F	213/532 (40%)	202 (95%)	11 (5%)	0	100	100
2	H	215/231 (93%)	201 (94%)	14 (6%)	0	100	100
2	J	219/231 (95%)	200 (91%)	19 (9%)	0	100	100
3	I	214/218 (98%)	196 (92%)	18 (8%)	0	100	100
3	K	214/218 (98%)	195 (91%)	19 (9%)	0	100	100
All	All	1288/1962 (66%)	1195 (93%)	93 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	E	186/463 (40%)	182 (98%)	4 (2%)	47	70
1	F	186/463 (40%)	183 (98%)	3 (2%)	58	75
2	H	188/199 (94%)	186 (99%)	2 (1%)	70	82
2	J	190/199 (96%)	185 (97%)	5 (3%)	41	66
3	I	187/189 (99%)	183 (98%)	4 (2%)	48	70
3	K	187/189 (99%)	186 (100%)	1 (0%)	86	91
All	All	1124/1702 (66%)	1105 (98%)	19 (2%)	56	75

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	86	ASN
1	E	152	ASP
1	E	154	TYR
1	E	194	ASN
1	F	85	HIS
1	F	147	LEU
1	F	177	THR
2	H	72	ARG
2	H	196	TRP
3	I	57	ASN
3	I	128	GLN
3	I	159	ARG
3	I	180	SER
2	J	100	ARG
2	J	204	ASN
2	J	214	VAL
2	J	215	ASP
2	J	216	LYS
3	K	154	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	90	GLN
1	F	200	GLN
2	H	199	GLN
3	I	128	GLN
3	I	161	ASN
2	J	99	GLN
2	J	172	HIS
3	K	57	ASN
3	K	78	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

6 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
4	NAG	A	1	1,4	14,14,15	0.19	0	17,19,21	0.48	0
4	NAG	A	2	4	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	B	1	1,4	14,14,15	0.76	1 (7%)	17,19,21	1.00	1 (5%)
4	NAG	B	2	4	14,14,15	0.19	0	17,19,21	0.49	0
4	NAG	C	1	1,4	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	C	2	4	14,14,15	0.20	0	17,19,21	0.42	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
4	NAG	A	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	NAG	B	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1
4	NAG	C	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	NAG	C1-C2	2.54	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	NAG	C1-O5-C5	3.39	116.79	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

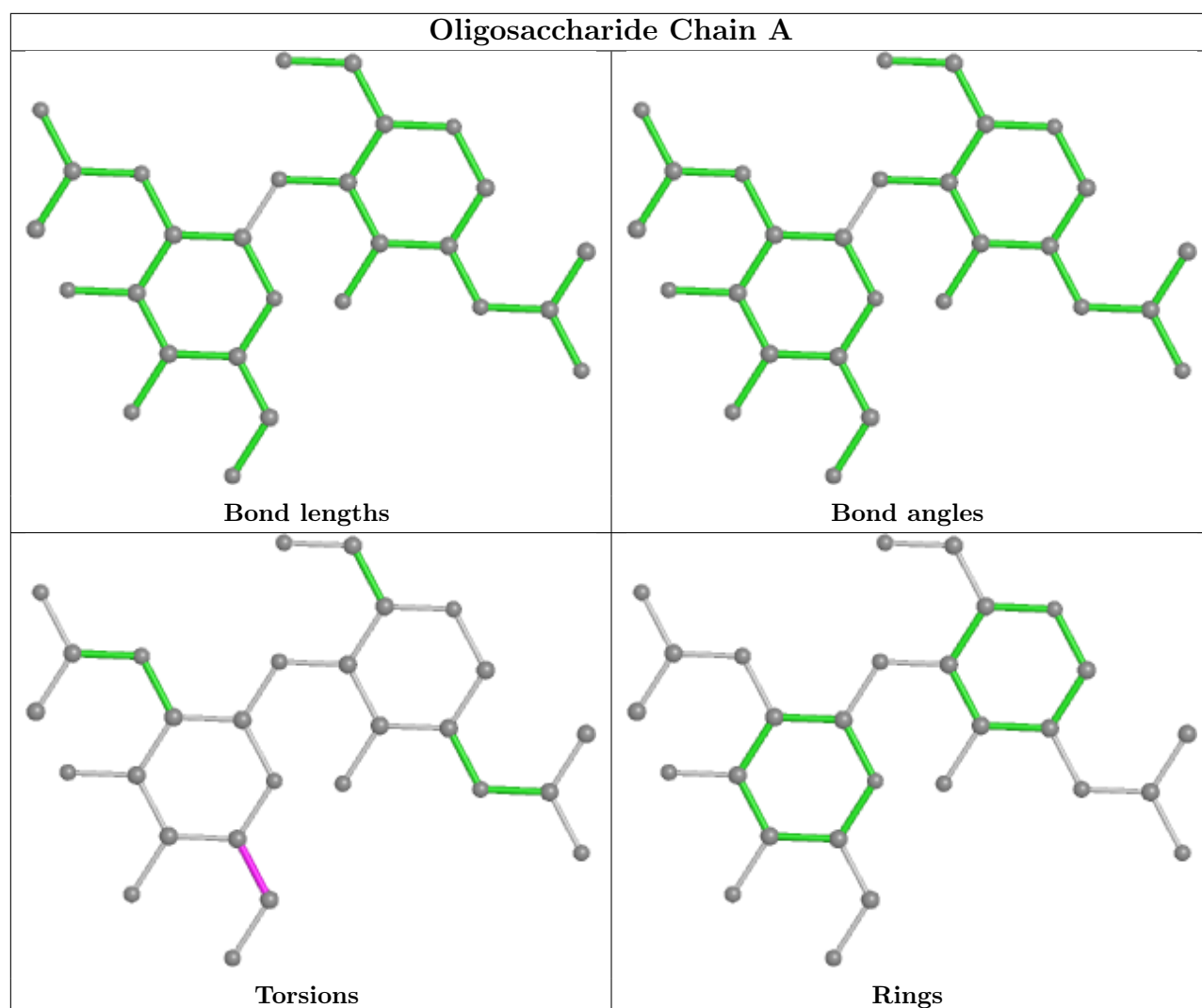
Mol	Chain	Res	Type	Atoms
4	A	2	NAG	O5-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6
4	C	1	NAG	C8-C7-N2-C2
4	C	1	NAG	O7-C7-N2-C2
4	B	2	NAG	O5-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
4	B	1	NAG	C3-C2-N2-C7
4	B	2	NAG	C3-C2-N2-C7

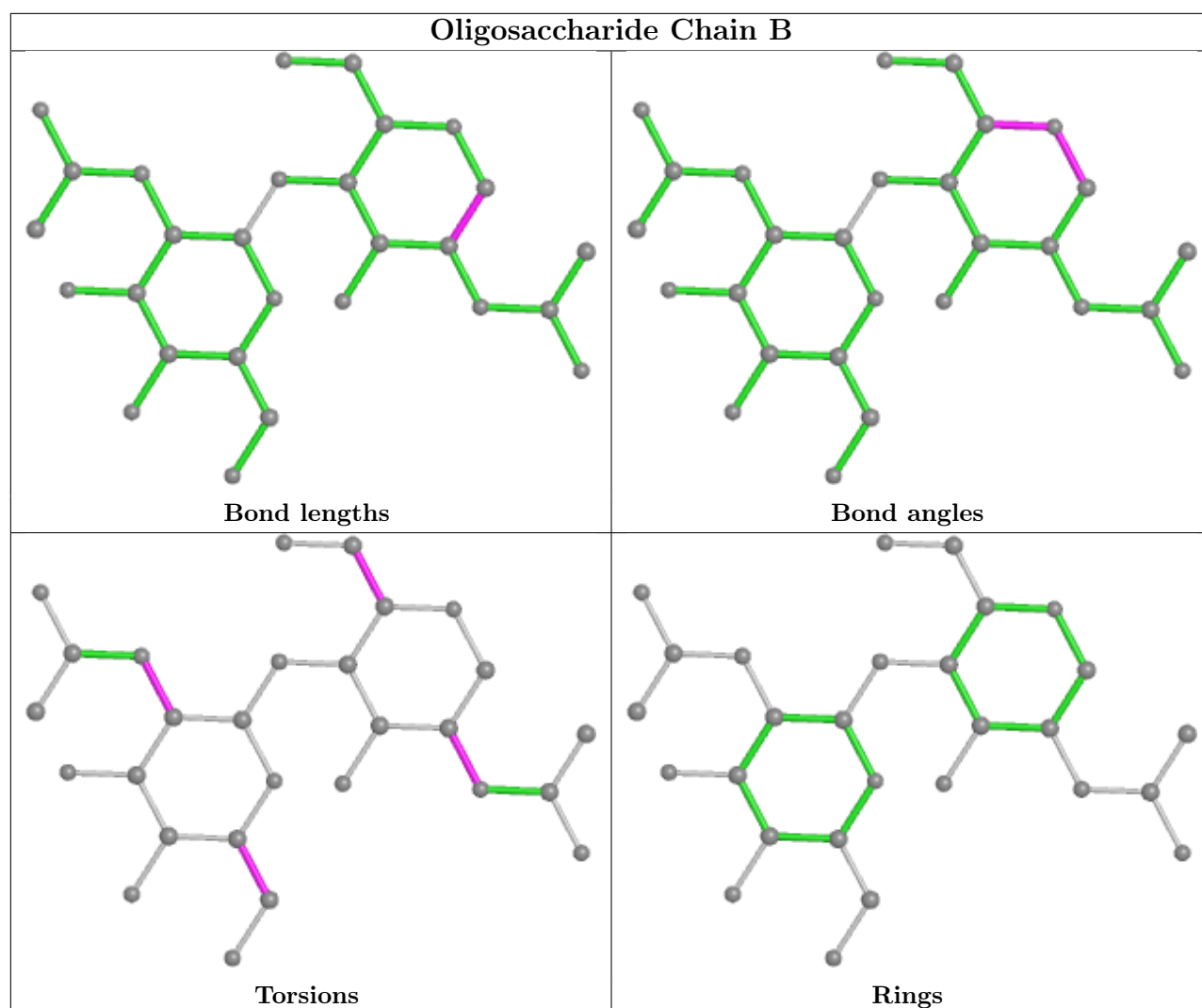
There are no ring outliers.

1 monomer is involved in 1 short contact:

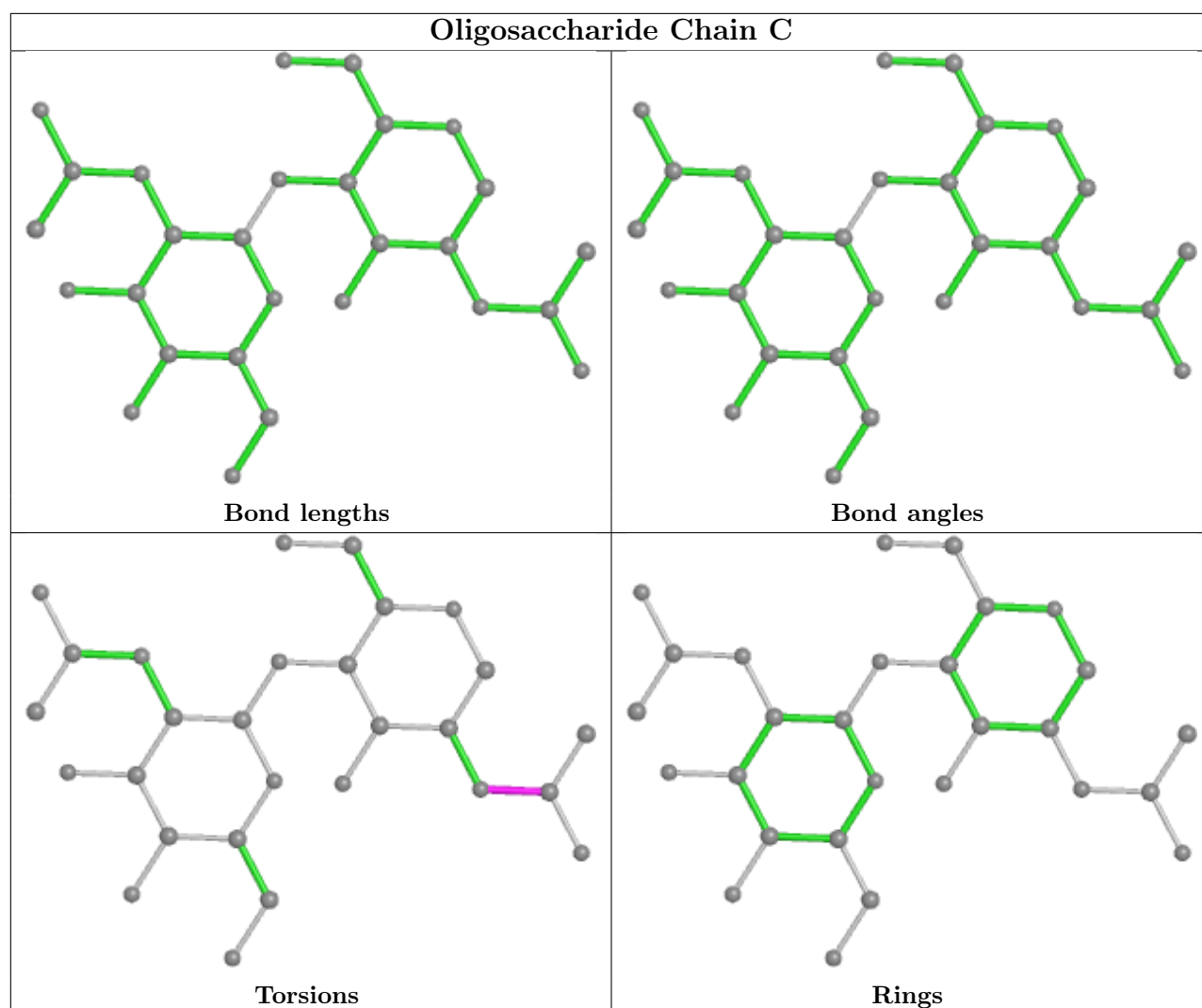
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	NAG	1	0

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









## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	E	601	1	14,14,15	0.28	0	17,19,21	0.55	0
5	NAG	F	603	1	14,14,15	0.27	0	17,19,21	0.38	0
5	NAG	E	603	1	14,14,15	0.29	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	F	601	1	14,14,15	0.47	0	17,19,21	1.27	2 (11%)
5	NAG	F	604	1	14,14,15	0.28	0	17,19,21	0.97	0
5	NAG	E	602	1	14,14,15	0.29	0	17,19,21	0.54	0
5	NAG	F	602	1	14,14,15	0.25	0	17,19,21	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	601	1	-	3/6/23/26	0/1/1/1
5	NAG	F	603	1	-	4/6/23/26	0/1/1/1
5	NAG	E	603	1	-	3/6/23/26	0/1/1/1
5	NAG	F	601	1	-	3/6/23/26	0/1/1/1
5	NAG	F	604	1	-	4/6/23/26	0/1/1/1
5	NAG	E	602	1	-	0/6/23/26	0/1/1/1
5	NAG	F	602	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	601	NAG	C2-N2-C7	4.29	129.02	122.90
5	F	601	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	601	NAG	C8-C7-N2-C2
5	E	601	NAG	O7-C7-N2-C2
5	F	604	NAG	C3-C2-N2-C7
5	F	604	NAG	C8-C7-N2-C2
5	F	604	NAG	O7-C7-N2-C2
5	F	602	NAG	O5-C5-C6-O6
5	F	603	NAG	O5-C5-C6-O6
5	F	602	NAG	C4-C5-C6-O6
5	E	601	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	F	603	NAG	C4-C5-C6-O6
5	F	601	NAG	C8-C7-N2-C2
5	F	601	NAG	O7-C7-N2-C2
5	F	603	NAG	C8-C7-N2-C2
5	F	603	NAG	O7-C7-N2-C2
5	E	603	NAG	O5-C5-C6-O6
5	F	604	NAG	C1-C2-N2-C7
5	F	602	NAG	C1-C2-N2-C7
5	E	603	NAG	C3-C2-N2-C7
5	F	601	NAG	C3-C2-N2-C7
5	E	603	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	601	NAG	1	0
5	F	604	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.