



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 12:11 PM EDT

PDB ID : 8TXT
Title : Crystal structure of 05.GC.w13.02 Fab in complex with H5 HA from A/Viet Nam/1203/2004(H5N1)
Authors : Lin, T.H.; Moore, N.; Wilson, I.A.
Deposited on : 2023-08-24
Resolution : 3.19 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

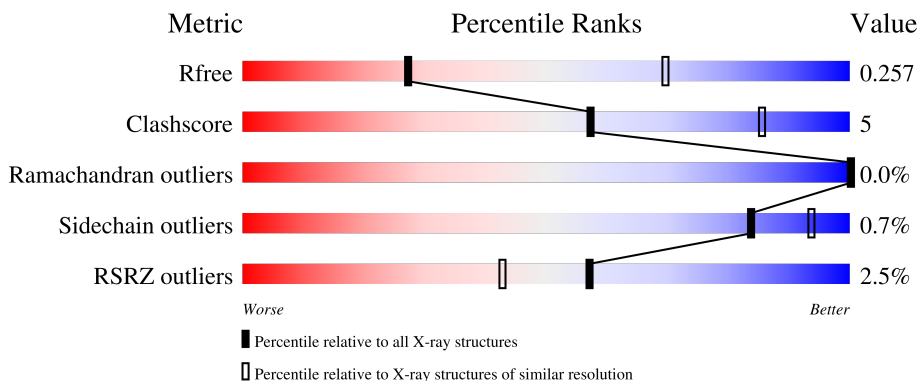
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	334	89% 8% .
1	C	334	84% 13% .
1	E	334	82% 15% .
2	B	177	91% 8% ..
2	D	177	93% 7% .

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Mol	Chain	Length	Quality of chain
2	F	177	 6% 89% 10%
3	G	225	 % 88% 10%
3	H	225	 2% 83% 16%
3	J	225	 4% 82% 18%
4	I	214	 % 86% 13%
4	K	214	 3% 81% 19%
4	L	214	 % 83% 16%
5	M	3	 100%
5	Q	3	 100%
6	N	2	 50% 50%
6	O	2	 50% 50%
6	P	2	 100%
6	R	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BMA	Q	3	-	-	-	X
6	NAG	O	2	-	-	-	X
6	NAG	R	2	-	-	-	X
7	NAG	F	201	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 22149 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
			Total	C	N	O	S			
1	A	324	Total 2579	C 1629	N 446	O 489	S 15	0	2	0
1	C	324	Total 2579	C 1629	N 446	O 489	S 15	0	2	0
1	E	324	Total 2579	C 1629	N 446	O 489	S 15	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q5EP31
A	8	ASP	-	expression tag	UNP Q5EP31
A	9	PRO	-	expression tag	UNP Q5EP31
A	10	GLY	-	expression tag	UNP Q5EP31
C	7	ALA	-	expression tag	UNP Q5EP31
C	8	ASP	-	expression tag	UNP Q5EP31
C	9	PRO	-	expression tag	UNP Q5EP31
C	10	GLY	-	expression tag	UNP Q5EP31
E	7	ALA	-	expression tag	UNP Q5EP31
E	8	ASP	-	expression tag	UNP Q5EP31
E	9	PRO	-	expression tag	UNP Q5EP31
E	10	GLY	-	expression tag	UNP Q5EP31

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	176	Total 1427	C 888	N 247	O 284	S 8	0	1	0
2	D	176	Total 1427	C 888	N 247	O 284	S 8	5	1	0
2	F	176	Total 1427	C 888	N 247	O 284	S 8	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A6B7HQ27
B	176	GLY	-	expression tag	UNP A0A6B7HQ27
B	177	ARG	-	expression tag	UNP A0A6B7HQ27
D	175	SER	-	expression tag	UNP A0A6B7HQ27
D	176	GLY	-	expression tag	UNP A0A6B7HQ27
D	177	ARG	-	expression tag	UNP A0A6B7HQ27
F	175	SER	-	expression tag	UNP A0A6B7HQ27
F	176	GLY	-	expression tag	UNP A0A6B7HQ27
F	177	ARG	-	expression tag	UNP A0A6B7HQ27

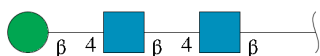
- Molecule 3 is a protein called GC_W13B_B, Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	223	Total	C	N	O	S	0	0	0
			1643	1041	275	319	8			
3	G	224	Total	C	N	O	S	0	0	0
			1649	1044	276	320	9			
3	J	224	Total	C	N	O	S	0	0	0
			1649	1044	276	320	9			

- Molecule 4 is a protein called GC_w13_B, Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	0	0
			1634	1019	278	332	5			
4	I	213	Total	C	N	O	S	0	0	0
			1634	1019	278	332	5			
4	K	213	Total	C	N	O	S	0	0	0
			1634	1019	278	332	5			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

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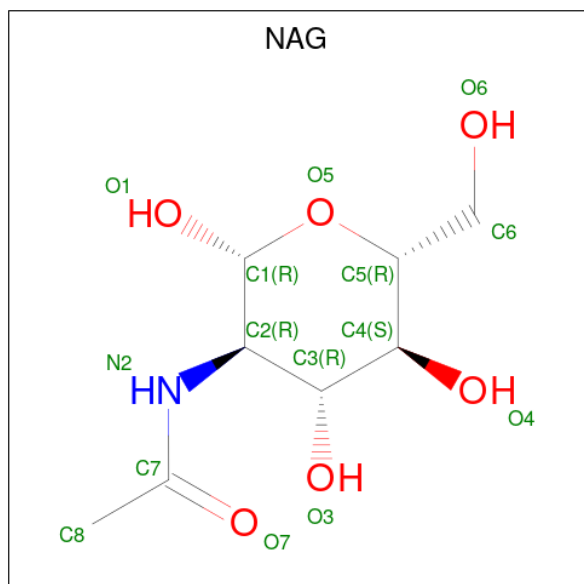
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	Q	3	39	22	2	15	0	0	0

- 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
			Total	C	N	O			
6	N	2	28	16	2	10	0	0	0
6	O	2	28	16	2	10	0	0	0
6	P	2	28	16	2	10	0	0	0
6	R	2	28	16	2	10	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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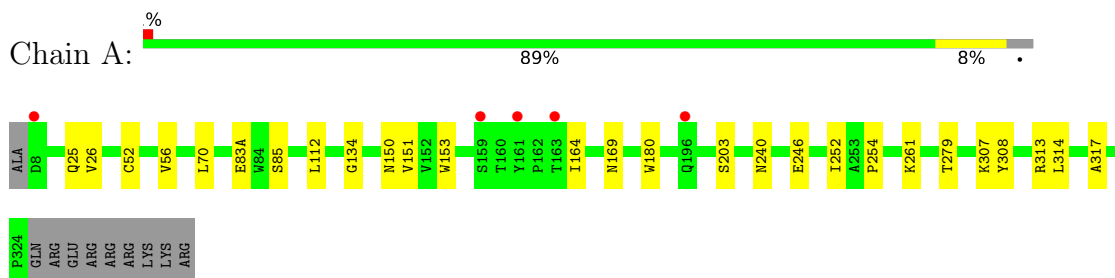
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 14	C 8	N 1	O 5	0	0
7	C	1	Total 14	C 8	N 1	O 5	0	0
7	E	1	Total 14	C 8	N 1	O 5	0	0
7	F	1	Total 14	C 8	N 1	O 5	0	0
7	L	1	Total 14	C 8	N 1	O 5	0	0
7	I	1	Total 14	C 8	N 1	O 5	0	0

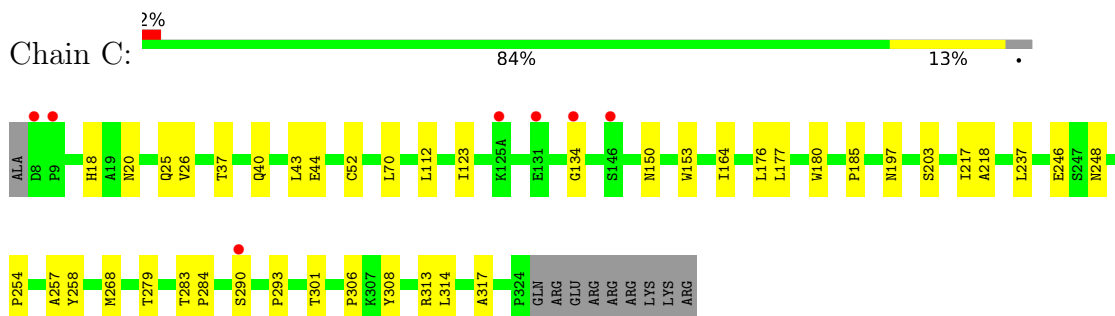
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

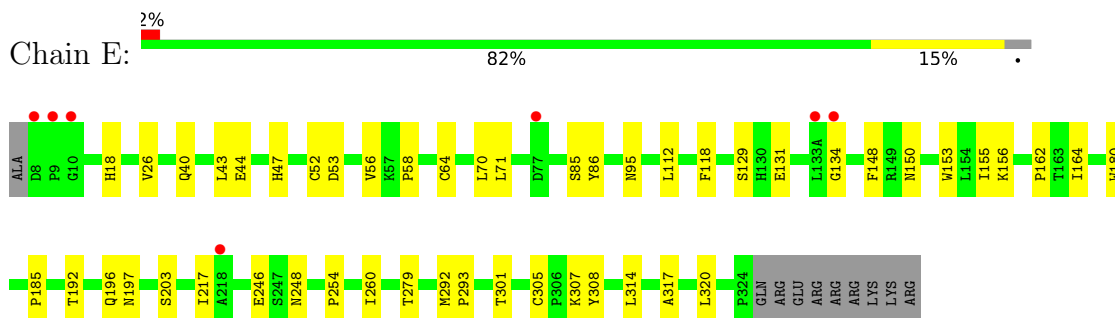
- Molecule 1: Hemagglutinin



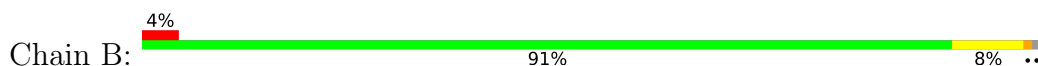
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin

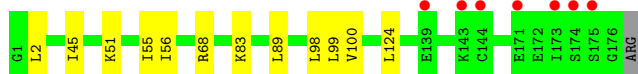
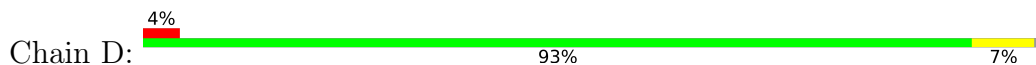


- Molecule 2: Hemagglutinin

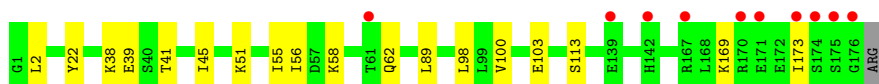
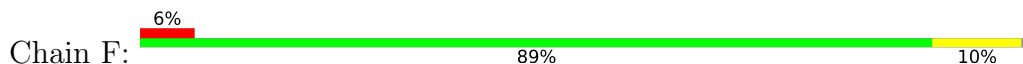




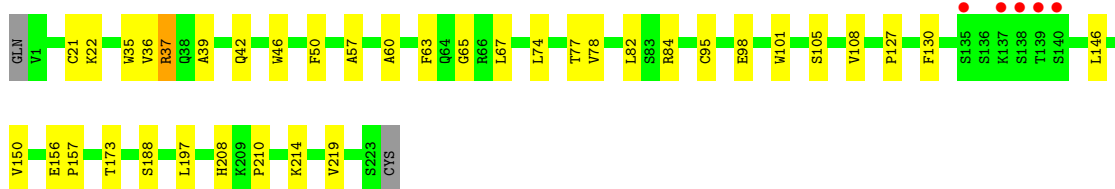
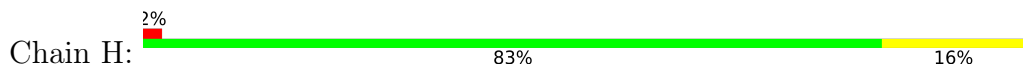
- Molecule 2: Hemagglutinin



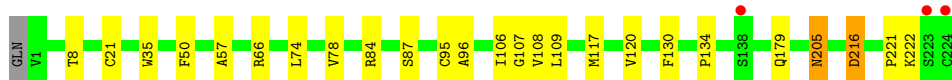
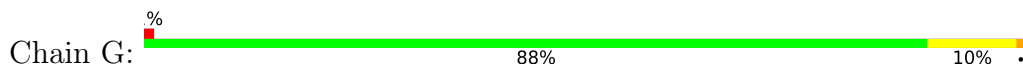
- Molecule 2: Hemagglutinin



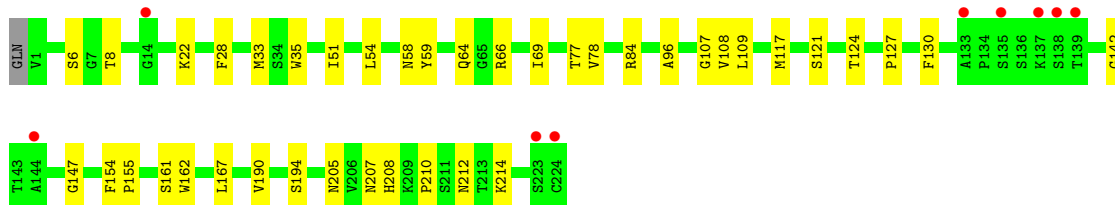
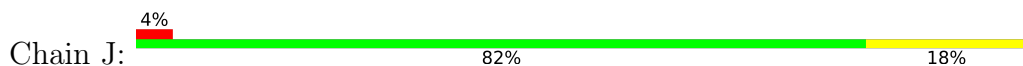
- Molecule 3: GC_W13B_B, Fab heavy chain



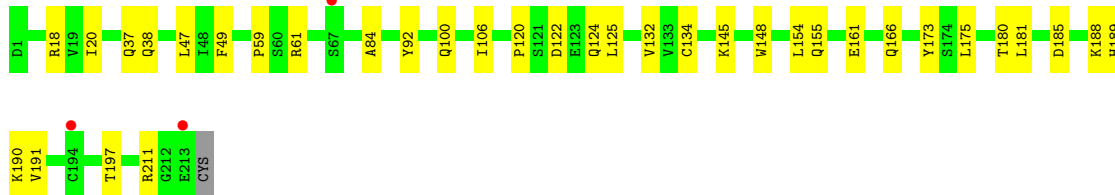
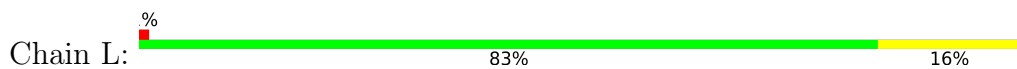
- Molecule 3: GC_W13B_B, Fab heavy chain



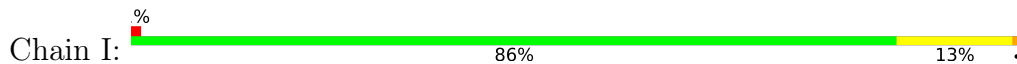
- Molecule 3: GC_W13B_B, Fab heavy chain



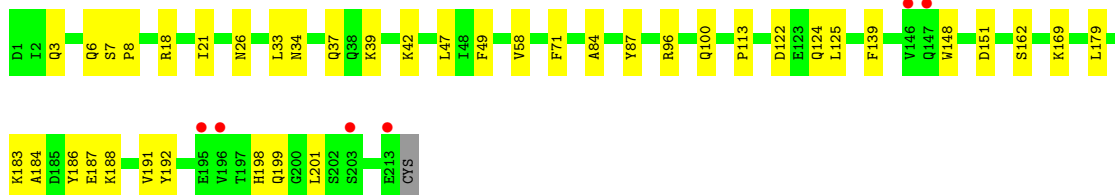
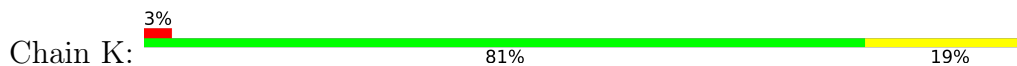
- Molecule 4: GC_w13_B, Fab light chain



- Molecule 4: GC_w13_B, Fab light chain



- Molecule 4: GC_w13_B, Fab light chain



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



- Molecule 5: beta-D-mannopyranose-(1-4)-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 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2

4 Data and refinement statistics i

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	159.46Å 232.60Å 233.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.12 – 3.19 47.12 – 3.19	Depositor EDS
% Data completeness (in resolution range)	79.1 (47.12-3.19) 79.1 (47.12-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.217 , 0.258 0.217 , 0.257	Depositor DCC
R_{free} test set	2892 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtrriage
Anisotropy	0.313	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.018 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	22149	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: BMA, 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	0.24	0/2648	0.47	0/3596
1	C	0.24	0/2648	0.47	0/3596
1	E	0.24	0/2648	0.48	0/3596
2	B	0.24	0/1457	0.45	0/1958
2	D	0.24	0/1457	0.45	0/1958
2	F	0.24	0/1457	0.45	0/1958
3	G	0.26	0/1686	0.48	0/2294
3	H	0.26	0/1680	0.50	0/2286
3	J	0.25	0/1686	0.49	0/2294
4	I	0.25	0/1668	0.48	0/2265
4	K	0.25	0/1668	0.48	0/2265
4	L	0.25	0/1668	0.48	0/2265
All	All	0.25	0/22371	0.47	0/30331

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	A	2579	0	2524	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2579	0	2525	28	0
1	E	2579	0	2525	36	0
2	B	1427	0	1337	12	0
2	D	1427	0	1337	12	0
2	F	1427	0	1337	14	0
3	G	1649	0	1654	18	0
3	H	1643	0	1649	24	0
3	J	1649	0	1654	24	0
4	I	1634	0	1585	21	0
4	K	1634	0	1584	25	0
4	L	1634	0	1584	20	0
5	M	39	0	34	0	0
5	Q	39	0	34	0	0
6	N	28	0	25	2	0
6	O	28	0	25	1	0
6	P	28	0	25	0	0
6	R	28	0	25	0	0
7	A	28	0	26	1	0
7	C	14	0	13	0	0
7	E	14	0	13	1	0
7	F	14	0	13	0	0
7	I	14	0	13	0	0
7	L	14	0	13	0	0
All	All	22149	0	21554	213	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 5.

All (213) 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)
4:K:6:GLN:O	4:K:100:GLN:NE2	2.24	0.71
4:K:6:GLN:HE22	4:K:87:TYR:HA	1.56	0.71
1:A:25:GLN:O	1:A:313:ARG:NH2	2.26	0.67
3:J:108:VAL:HG11	4:K:49:PHE:HB2	1.76	0.67
3:H:101:TRP:HA	6:O:1:NAG:H83	1.77	0.67
3:G:8:THR:HG23	3:G:117:MET:HB3	1.76	0.67
1:E:44:GLU:HG3	1:E:292:MET:HB2	1.77	0.66
3:H:65:GLY:O	3:H:84:ARG:NH2	2.29	0.66
4:L:190:LYS:HD3	4:L:191:VAL:HG23	1.77	0.65
1:E:40:GLN:HE21	3:H:74:LEU:HD11	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:120:PRO:HD3	4:L:132:VAL:HG22	1.80	0.63
3:H:156:GLU:HG2	3:H:157:PRO:HA	1.82	0.62
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.82	0.62
2:D:45:ILE:HG21	3:G:106:ILE:HD12	1.83	0.60
1:C:40:GLN:HE22	3:G:74:LEU:HD21	1.67	0.59
1:E:47:HIS:HA	7:E:401:NAG:H81	1.84	0.59
1:E:129:SER:HB3	1:E:162:PRO:HG2	1.84	0.59
1:C:180:TRP:HB3	1:C:254:PRO:HG3	1.85	0.58
4:I:142:ARG:O	4:I:142:ARG:NH1	2.30	0.58
4:I:37:GLN:HB2	4:I:47:LEU:HD11	1.84	0.57
1:E:293:PRO:HG3	2:F:56:ILE:HD13	1.85	0.57
2:B:156:THR:HG21	6:N:1:NAG:H83	1.86	0.57
4:K:7:SER:HB2	4:K:8:PRO:HD3	1.86	0.57
3:H:37:ARG:HH21	3:H:63:PHE:HE1	1.53	0.56
4:I:29:ILE:HG22	4:I:32:TYR:HB2	1.87	0.56
4:K:37:GLN:HB2	4:K:47:LEU:HD11	1.87	0.56
4:I:29:ILE:HG23	4:I:92:TYR:HB2	1.88	0.56
1:E:197:ASN:ND2	1:E:248:ASN:O	2.37	0.56
2:B:113:SER:OG	2:F:2:LEU:O	2.20	0.56
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.86	0.56
1:E:293:PRO:HB3	2:F:56:ILE:HG23	1.88	0.56
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.88	0.55
3:J:167:LEU:HD21	3:J:190:VAL:HG21	1.88	0.55
3:J:8:THR:HG23	3:J:117:MET:HB3	1.88	0.55
1:E:307:LYS:HD2	2:F:62:GLN:HB3	1.87	0.55
1:C:40:GLN:HE21	3:G:74:LEU:HD11	1.72	0.54
6:N:1:NAG:O7	6:N:1:NAG:O3	2.24	0.54
2:D:98:LEU:HD13	2:F:58:LYS:HE3	1.90	0.54
1:A:26:VAL:HG21	1:A:317:ALA:HB2	1.90	0.54
1:E:156:LYS:HD2	1:E:196:GLN:HB2	1.89	0.54
4:L:189:HIS:O	4:L:211:ARG:NE	2.39	0.54
3:G:66:ARG:HG3	3:G:84:ARG:HH21	1.73	0.53
1:E:185:PRO:HG2	1:E:217:ILE:HG12	1.91	0.53
4:K:39:LYS:HD2	4:K:84:ALA:HB2	1.90	0.53
3:H:36:VAL:HG22	3:H:46:TRP:HA	1.91	0.53
3:H:146:LEU:HD13	3:H:219:VAL:HG11	1.90	0.53
3:H:67:LEU:HD13	3:H:82:LEU:HD13	1.91	0.53
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.90	0.52
3:J:59:TYR:HE1	3:J:69:ILE:HG13	1.74	0.52
1:C:197:ASN:ND2	1:C:248:ASN:O	2.41	0.52
4:I:38:GLN:HG3	4:I:44:PRO:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:GLN:O	1:C:313:ARG:NH2	2.38	0.52
1:C:314:LEU:HD22	2:D:100:VAL:HG21	1.92	0.52
4:K:184:ALA:O	4:K:188:LYS:HG2	2.10	0.52
3:J:22:LYS:HG3	3:J:77:THR:HG23	1.92	0.52
3:J:207:ASN:HD21	3:J:214:LYS:HE2	1.74	0.52
3:J:51:ILE:HD12	3:J:54:LEU:HD12	1.92	0.51
3:J:208:HIS:CD2	3:J:210:PRO:HD2	2.45	0.51
1:C:26:VAL:HG21	1:C:317:ALA:HB2	1.93	0.51
3:H:208:HIS:CD2	3:H:210:PRO:HD2	2.45	0.51
2:B:79:ASN:OD1	2:D:68:ARG:NH1	2.44	0.51
1:C:40:GLN:NE2	3:G:74:LEU:HD21	2.25	0.51
4:L:18:ARG:HH21	4:L:20:ILE:HD11	1.75	0.51
1:C:177:LEU:HB3	1:C:258:TYR:HB2	1.93	0.51
4:I:187:GLU:HA	4:I:211:ARG:HD3	1.94	0.50
3:H:108:VAL:HG21	4:L:49:PHE:HB3	1.94	0.50
3:J:33:MET:HG3	3:J:78:VAL:HG11	1.93	0.50
4:K:47:LEU:HA	4:K:58:VAL:HG21	1.94	0.50
4:K:151:ASP:HA	4:K:191:VAL:HB	1.94	0.50
1:E:64:CYS:HA	1:E:95:ASN:HB2	1.94	0.50
1:E:43:LEU:HB2	1:E:314:LEU:HB2	1.92	0.50
1:C:44:GLU:HG2	1:C:290:SER:HB2	1.94	0.49
2:F:55:ILE:HD11	2:F:103:GLU:HG3	1.93	0.49
1:C:293:PRO:HG3	2:D:56:ILE:HG12	1.94	0.49
3:H:22:LYS:HG2	3:H:77:THR:HG23	1.94	0.49
4:I:33:LEU:HD13	4:I:71:PHE:CD1	2.47	0.49
4:K:113:PRO:HD3	4:K:198:HIS:ND1	2.27	0.49
1:E:308:TYR:HD2	2:F:89:LEU:HD22	1.78	0.49
1:E:26:VAL:HG11	1:E:317:ALA:HB2	1.95	0.49
3:J:130:PHE:CD2	4:K:124:GLN:HB2	2.48	0.49
2:F:38:LYS:HD3	4:L:92:TYR:CE2	2.48	0.48
1:E:180:TRP:HB3	1:E:254:PRO:HG3	1.95	0.48
1:A:314:LEU:HD22	2:B:100:VAL:HG21	1.96	0.48
4:L:106:ILE:HB	4:L:166:GLN:HE22	1.79	0.48
3:H:127:PRO:HB3	3:H:150:VAL:HG13	1.94	0.48
3:J:59:TYR:HB2	3:J:64:GLN:HG3	1.96	0.48
2:B:59:MET:O	2:B:61:THR:N	2.47	0.48
1:C:176:LEU:HB3	1:C:237:LEU:HB3	1.94	0.48
4:L:161:GLU:HB3	4:L:175:LEU:HD11	1.94	0.48
1:E:131:GLU:HB3	1:E:155:ILE:HB	1.96	0.47
3:G:35:TRP:CZ3	3:G:95:CYS:HB3	2.49	0.47
4:I:6:GLN:O	4:I:100:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:108:VAL:HG11	4:I:49:PHE:CB	2.44	0.47
1:A:70:LEU:O	1:A:150:ASN:ND2	2.45	0.47
2:D:2:LEU:O	2:F:113:SER:OG	2.27	0.47
3:J:66:ARG:HG3	3:J:84:ARG:NH2	2.30	0.47
1:E:40:GLN:NE2	3:H:74:LEU:HD21	2.28	0.47
3:H:21:CYS:HB3	3:H:78:VAL:HG23	1.97	0.47
1:A:180:TRP:HB3	1:A:254:PRO:HG3	1.95	0.47
1:E:156:LYS:NZ	1:E:192:THR:O	2.39	0.47
2:B:58:LYS:HE3	2:F:98:LEU:HB2	1.97	0.47
3:G:134:PRO:HD2	3:G:221:PRO:HA	1.95	0.47
4:L:134:CYS:HB2	4:L:148:TRP:CZ2	2.50	0.46
1:A:169:ASN:HD21	7:A:401:NAG:C1	2.28	0.46
2:B:134:GLY:HA2	2:D:124:LEU:HD22	1.98	0.46
3:H:173:THR:HG23	3:H:188:SER:HB2	1.97	0.46
3:J:59:TYR:CE1	3:J:69:ILE:HG13	2.50	0.46
4:K:33:LEU:HD13	4:K:71:PHE:CG	2.51	0.46
1:E:52:CYS:HB2	1:E:279:THR:HG22	1.98	0.46
3:G:87:SER:HA	3:G:120:VAL:HB	1.97	0.46
3:J:142:GLY:HA2	3:J:194:SER:HB2	1.98	0.46
1:A:56:VAL:HB	1:A:85:SER:HB3	1.97	0.46
2:D:55:ILE:HG23	2:D:99:LEU:HD23	1.99	0.46
3:J:96:ALA:HB1	3:J:109:LEU:HB3	1.98	0.46
4:I:148:TRP:CG	4:I:179:LEU:HD13	2.51	0.45
2:F:41:THR:O	2:F:45:ILE:HG13	2.16	0.45
2:F:51:LYS:HB2	2:F:51:LYS:HE2	1.82	0.45
4:I:134:CYS:HB2	4:I:148:TRP:CZ2	2.52	0.45
3:J:35:TRP:HD1	3:J:69:ILE:HD13	1.81	0.45
4:K:183:LYS:O	4:K:187:GLU:HG2	2.16	0.45
1:E:70:LEU:O	1:E:150:ASN:ND2	2.48	0.45
1:E:164:ILE:O	1:E:246:GLU:HA	2.17	0.45
1:E:18:HIS:O	1:E:320:LEU:HD11	2.17	0.44
1:E:44:GLU:OE2	1:E:292:MET:N	2.50	0.44
1:C:70:LEU:O	1:C:150:ASN:ND2	2.46	0.44
2:F:169:LYS:HE2	2:F:173:ILE:HD11	2.00	0.44
4:L:59:PRO:HB2	4:L:61:ARG:HG2	1.98	0.44
4:L:185:ASP:HA	4:L:188:LYS:NZ	2.32	0.44
1:E:314:LEU:HD22	2:F:100:VAL:HG21	1.99	0.44
3:H:98:GLU:HB3	3:H:105:SER:O	2.18	0.44
4:L:145:LYS:HB2	4:L:197:THR:HB	2.00	0.44
3:G:108:VAL:HG11	4:I:49:PHE:HB3	2.00	0.44
3:J:124:THR:HG22	3:J:155:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:O	1:A:246:GLU:HA	2.18	0.44
3:H:39:ALA:HB3	3:H:42:GLN:HB2	1.98	0.44
3:G:96:ALA:HB1	3:G:109:LEU:HB3	2.00	0.44
4:L:38:GLN:O	4:L:84:ALA:HB1	2.18	0.44
1:A:52:CYS:HB2	1:A:279:THR:HG22	1.99	0.44
1:C:52:CYS:HB2	1:C:279:THR:HG22	1.99	0.44
1:A:151:VAL:HB	1:A:252:ILE:HG22	2.00	0.44
3:H:130:PHE:CG	4:L:124:GLN:HB2	2.53	0.44
4:I:186:TYR:HA	4:I:192:TYR:OH	2.18	0.44
3:J:127:PRO:HD3	3:J:208:HIS:ND1	2.32	0.44
3:G:205:ASN:ND2	3:G:216:ASP:OD2	2.46	0.44
3:J:147:GLY:HA2	3:J:162:TRP:CZ2	2.53	0.44
1:C:290:SER:OG	1:C:306:PRO:HG2	2.18	0.43
3:J:121:SER:HB3	3:J:154:PHE:CE2	2.53	0.43
4:K:8:PRO:HG2	4:K:21:ILE:HA	2.00	0.43
4:L:154:LEU:HD12	4:L:155:GLN:H	1.83	0.43
2:B:55:ILE:HD11	2:B:103:GLU:HG3	2.00	0.43
2:B:56:ILE:CG2	3:J:28:PHE:HB2	2.48	0.43
4:L:166:GLN:HG3	4:L:173:TYR:CZ	2.53	0.43
4:I:150:VAL:HG22	4:I:192:TYR:CD2	2.53	0.43
1:E:56:VAL:HB	1:E:85:SER:HB3	2.00	0.43
3:G:21:CYS:HB3	3:G:78:VAL:HG23	2.01	0.43
3:J:108:VAL:HG12	4:K:34:ASN:CG	2.39	0.43
1:C:20:ASN:ND2	1:C:37:THR:O	2.52	0.43
1:C:203[A]:SER:OG	1:C:246:GLU:HB3	2.19	0.43
1:C:218:ALA:HB2	1:E:203[B]:SER:HB3	2.01	0.42
4:I:190:LYS:HD3	4:I:191:VAL:HG23	2.01	0.42
4:K:122:ASP:HA	4:K:125:LEU:HB2	1.99	0.42
1:E:58:PRO:HB3	1:E:86:TYR:CE1	2.54	0.42
1:C:43:LEU:HB2	1:C:314:LEU:HB2	2.01	0.42
1:E:118:PHE:HE1	1:E:260:ILE:HG12	1.83	0.42
1:A:308:TYR:O	2:B:62:GLN:NE2	2.52	0.42
4:L:180:THR:O	4:L:181:LEU:HD23	2.20	0.42
4:I:201:LEU:HD13	4:I:205:VAL:HB	2.00	0.42
3:J:107:GLY:HA2	4:K:96:ARG:NH1	2.35	0.42
1:A:83(A):GLU:OE2	1:A:261:LYS:NZ	2.36	0.42
1:C:18:HIS:NE2	1:C:20:ASN:HB3	2.35	0.42
2:D:98:LEU:HD12	2:D:98:LEU:HA	1.84	0.42
1:E:40:GLN:HE22	3:H:74:LEU:HD21	1.85	0.42
1:E:112:LEU:HA	1:E:112:LEU:HD23	1.81	0.42
3:H:50:PHE:HD1	3:H:57:ALA:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.82	0.42
1:C:268:MET:HG3	1:C:284:PRO:HG3	2.02	0.42
3:G:130:PHE:HB3	4:I:121:SER:OG	2.19	0.42
4:K:18:ARG:HG3	4:K:18:ARG:HH11	1.85	0.42
4:K:148:TRP:CG	4:K:179:LEU:HD13	2.54	0.42
1:A:307:LYS:HD2	2:B:62:GLN:HB3	2.00	0.42
2:B:22:TYR:OH	2:B:111:HIS:ND1	2.38	0.42
4:K:42:LYS:HD3	4:K:42:LYS:HA	1.89	0.42
1:E:53:ASP:HA	1:E:58:PRO:HD3	2.01	0.42
1:C:164:ILE:O	1:C:246:GLU:HA	2.19	0.41
3:H:60:ALA:HB3	3:H:63:PHE:HD2	1.84	0.41
3:G:179:GLN:HA	4:I:160:GLN:HE22	1.85	0.41
3:H:82:LEU:HD12	3:H:82:LEU:HA	1.89	0.41
3:G:50:PHE:HD1	3:G:57:ALA:HB2	1.85	0.41
4:K:139:PHE:HB2	4:K:198:HIS:CE1	2.56	0.41
1:C:112:LEU:HD23	1:C:112:LEU:HA	1.86	0.41
1:C:283:THR:HG22	1:C:301:THR:HG22	2.03	0.41
2:D:83:LYS:HD3	2:D:83:LYS:HA	1.87	0.41
1:E:314:LEU:HD23	1:E:314:LEU:HA	1.87	0.41
1:A:203[A]:SER:OG	1:A:246:GLU:HB3	2.20	0.41
1:E:26:VAL:HG21	1:E:317:ALA:HB2	2.01	0.41
2:D:51:LYS:HB2	2:D:51:LYS:HE2	1.90	0.41
3:H:35:TRP:CZ3	3:H:95:CYS:HB3	2.56	0.41
4:K:198:HIS:CD2	4:K:199:GLN:H	2.39	0.41
1:E:71:LEU:O	1:E:148:PHE:HB3	2.21	0.41
3:J:161:SER:HB3	3:J:205:ASN:HB2	2.02	0.41
4:K:3:GLN:HB3	4:K:26:ASN:HB2	2.02	0.41
1:E:301:THR:HB	1:E:305:CYS:SG	2.61	0.41
3:H:197:LEU:HD23	3:H:197:LEU:HA	1.91	0.41
4:I:32:TYR:HB3	4:I:91:ASN:HB2	2.02	0.41
4:K:186:TYR:HA	4:K:192:TYR:OH	2.20	0.41
4:I:38:GLN:O	4:I:84:ALA:HB1	2.21	0.40
1:C:123:ILE:HD13	1:C:257:ALA:HB2	2.03	0.40
4:L:100:GLN:H	4:L:100:GLN:HG2	1.60	0.40
1:C:308:TYR:HD2	2:D:89:LEU:HD22	1.86	0.40
4:L:122:ASP:HA	4:L:125:LEU:HB2	2.03	0.40
1:C:185:PRO:HG2	1:C:217:ILE:HG12	2.03	0.40
4:K:113:PRO:HD2	4:K:201:LEU:HG	2.03	0.40
3:G:107:GLY:O	4:I:91:ASN:ND2	2.54	0.40

There are no symmetry-related clashes.

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	324/334 (97%)	319 (98%)	5 (2%)	0	100	100
1	C	324/334 (97%)	316 (98%)	8 (2%)	0	100	100
1	E	324/334 (97%)	316 (98%)	8 (2%)	0	100	100
2	B	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
2	D	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
2	F	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
3	G	222/225 (99%)	217 (98%)	5 (2%)	0	100	100
3	H	221/225 (98%)	214 (97%)	7 (3%)	0	100	100
3	J	222/225 (99%)	219 (99%)	3 (1%)	0	100	100
4	I	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
4	K	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
4	L	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
All	All	2795/2850 (98%)	2726 (98%)	68 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	ASN

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	A	293/300 (98%)	292 (100%)	1 (0%)	92	96
1	C	293/300 (98%)	293 (100%)	0	100	100
1	E	293/300 (98%)	293 (100%)	0	100	100
2	B	151/151 (100%)	150 (99%)	1 (1%)	84	94
2	D	151/151 (100%)	151 (100%)	0	100	100
2	F	151/151 (100%)	149 (99%)	2 (1%)	69	87
3	G	185/186 (100%)	182 (98%)	3 (2%)	62	84
3	H	184/186 (99%)	182 (99%)	2 (1%)	73	88
3	J	185/186 (100%)	182 (98%)	3 (2%)	62	84
4	I	186/187 (100%)	184 (99%)	2 (1%)	73	88
4	K	186/187 (100%)	184 (99%)	2 (1%)	73	88
4	L	186/187 (100%)	186 (100%)	0	100	100
All	All	2444/2472 (99%)	2428 (99%)	16 (1%)	84	94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
2	B	59	MET
2	F	22	TYR
2	F	39	GLU
3	H	37	ARG
3	H	214	LYS
3	G	205	ASN
3	G	216	ASP
3	G	222	LYS
4	I	33	LEU
4	I	142	ARG
3	J	6	SER
3	J	58	ASN
3	J	212	ASN
4	K	162	SER
4	K	169	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	40	GLN

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Mol	Chain	Res	Type
1	E	40	GLN
4	K	6	GLN
4	K	100	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

14 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	M	1	1,5	14,14,15	0.19	0	17,19,21	0.56	0
5	NAG	M	2	5	14,14,15	0.21	0	17,19,21	0.38	0
5	BMA	M	3	5	11,11,12	0.64	0	15,15,17	0.71	0
6	NAG	N	1	2,6	14,14,15	0.35	0	17,19,21	1.09	2 (11%)
6	NAG	N	2	6	14,14,15	0.46	0	17,19,21	0.78	0
6	NAG	O	1	1,6	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	O	2	6	14,14,15	0.27	0	17,19,21	0.39	0
6	NAG	P	1	2,6	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	P	2	6	14,14,15	0.29	0	17,19,21	0.46	0
5	NAG	Q	1	1,5	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	Q	2	5	14,14,15	0.22	0	17,19,21	0.36	0
5	BMA	Q	3	5	11,11,12	0.62	0	15,15,17	0.77	0
6	NAG	R	1	4,6	14,14,15	0.25	0	17,19,21	0.48	0
6	NAG	R	2	6	14,14,15	0.32	0	17,19,21	0.46	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	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	3/6/23/26	0/1/1/1
6	NAG	O	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	O	2	6	-	1/6/23/26	0/1/1/1
6	NAG	P	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
5	NAG	Q	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	2/2/19/22	0/1/1/1
6	NAG	R	1	4,6	-	1/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	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(°)
6	N	1	NAG	O4-C4-C3	-2.65	104.21	110.35
6	N	1	NAG	O4-C4-C5	2.09	114.48	109.30

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	1	NAG	C1-C2-N2-C7
6	N	2	NAG	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
6	O	1	NAG	C8-C7-N2-C2
6	O	1	NAG	O7-C7-N2-C2
6	R	2	NAG	O5-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6

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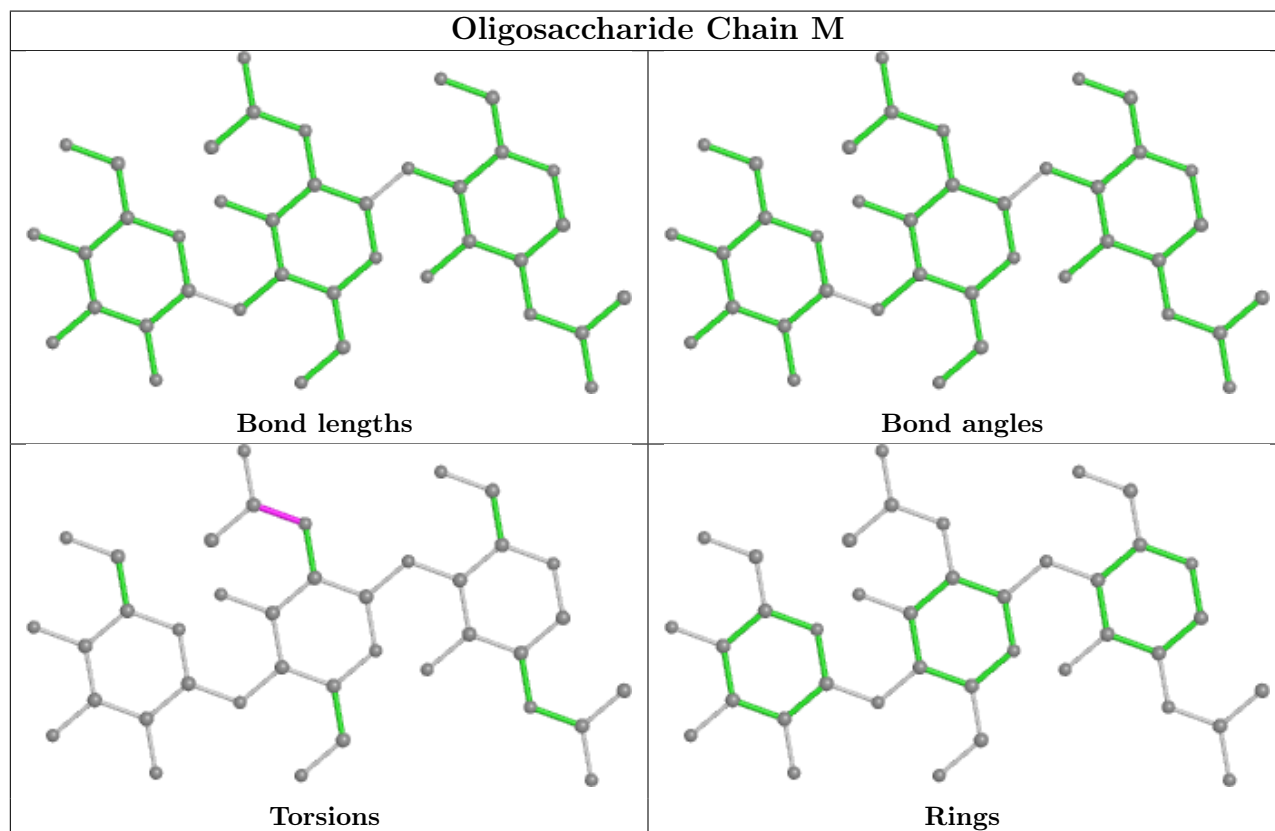
Mol	Chain	Res	Type	Atoms
6	N	2	NAG	C1-C2-N2-C7
6	O	1	NAG	C4-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
5	Q	3	BMA	O5-C5-C6-O6
5	Q	3	BMA	C4-C5-C6-O6
6	N	1	NAG	C3-C2-N2-C7
6	P	2	NAG	C4-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6

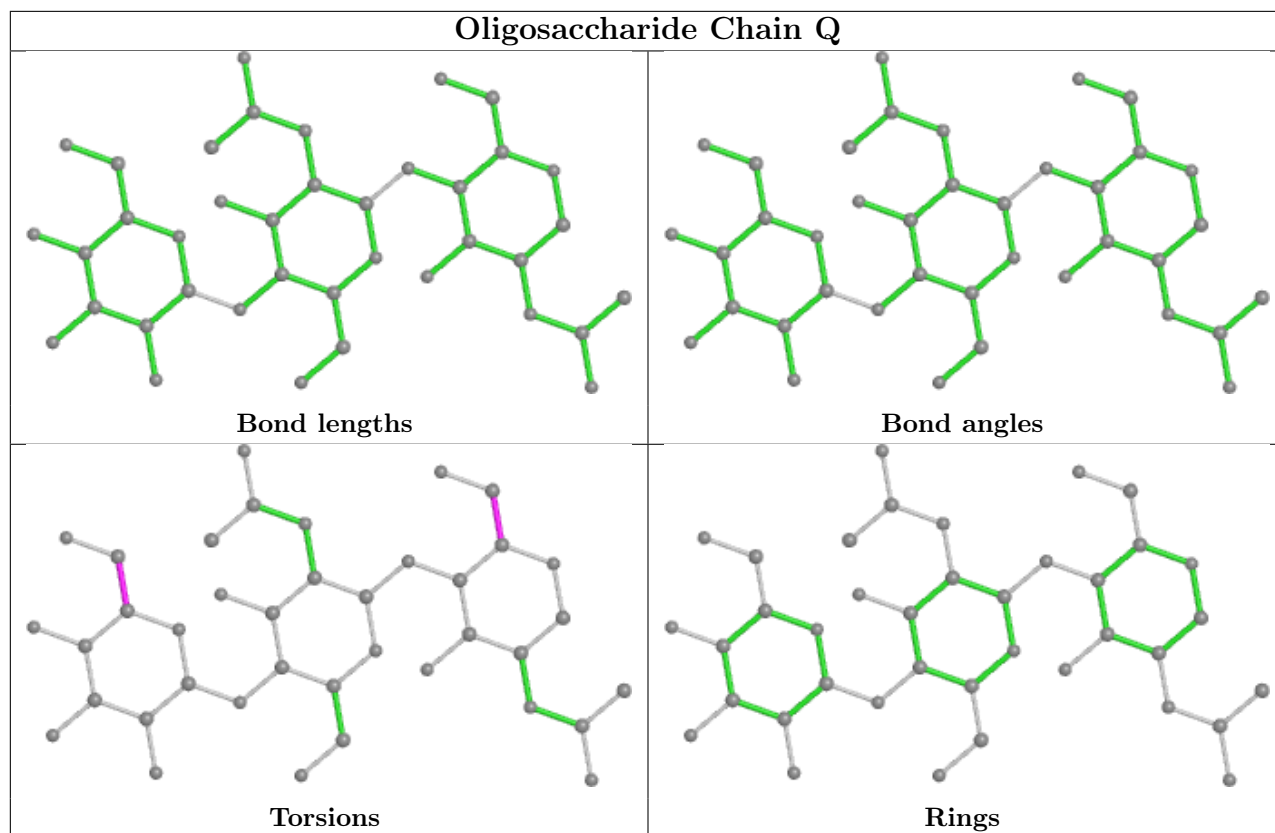
There are no ring outliers.

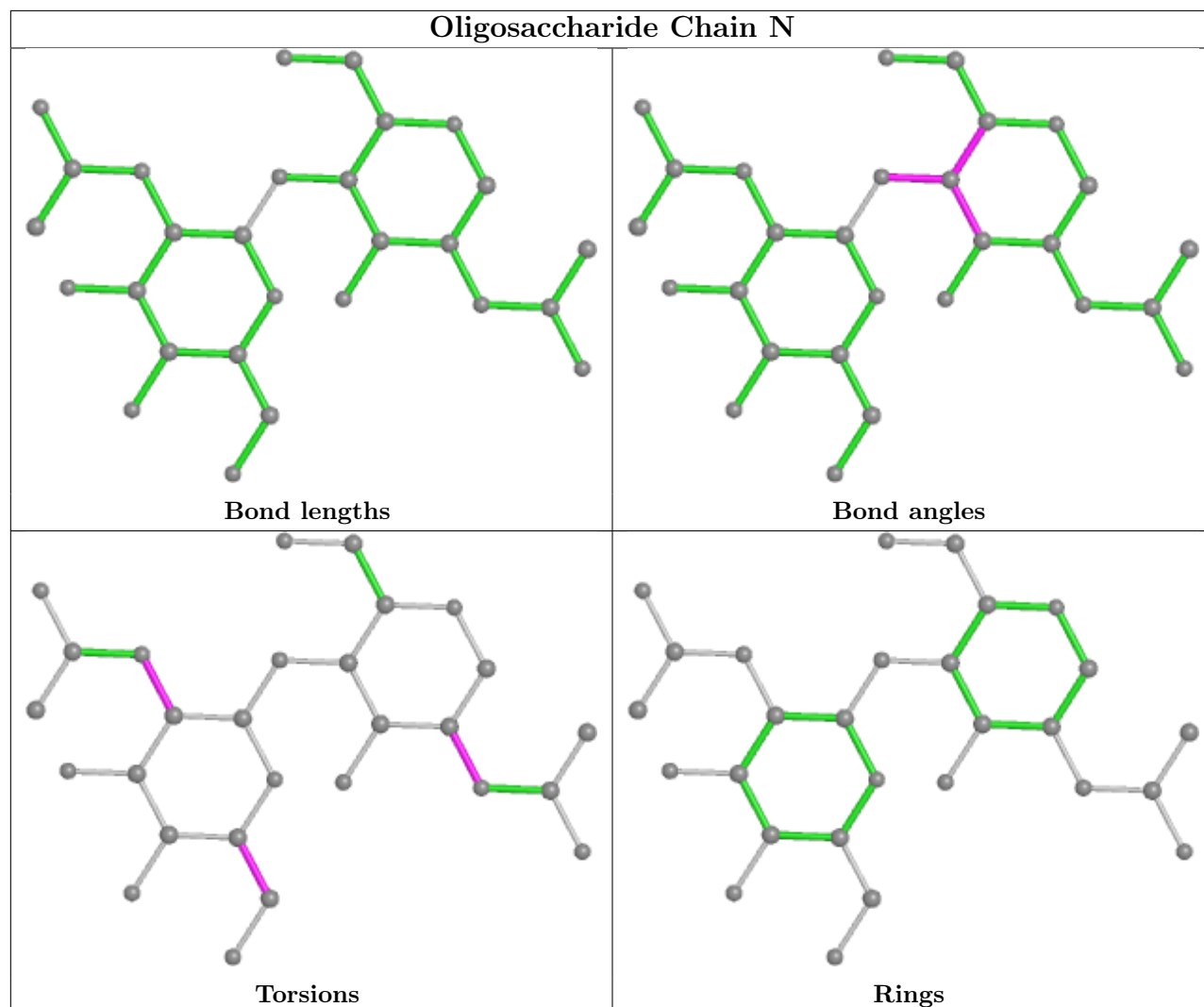
2 monomers are involved in 3 short contacts:

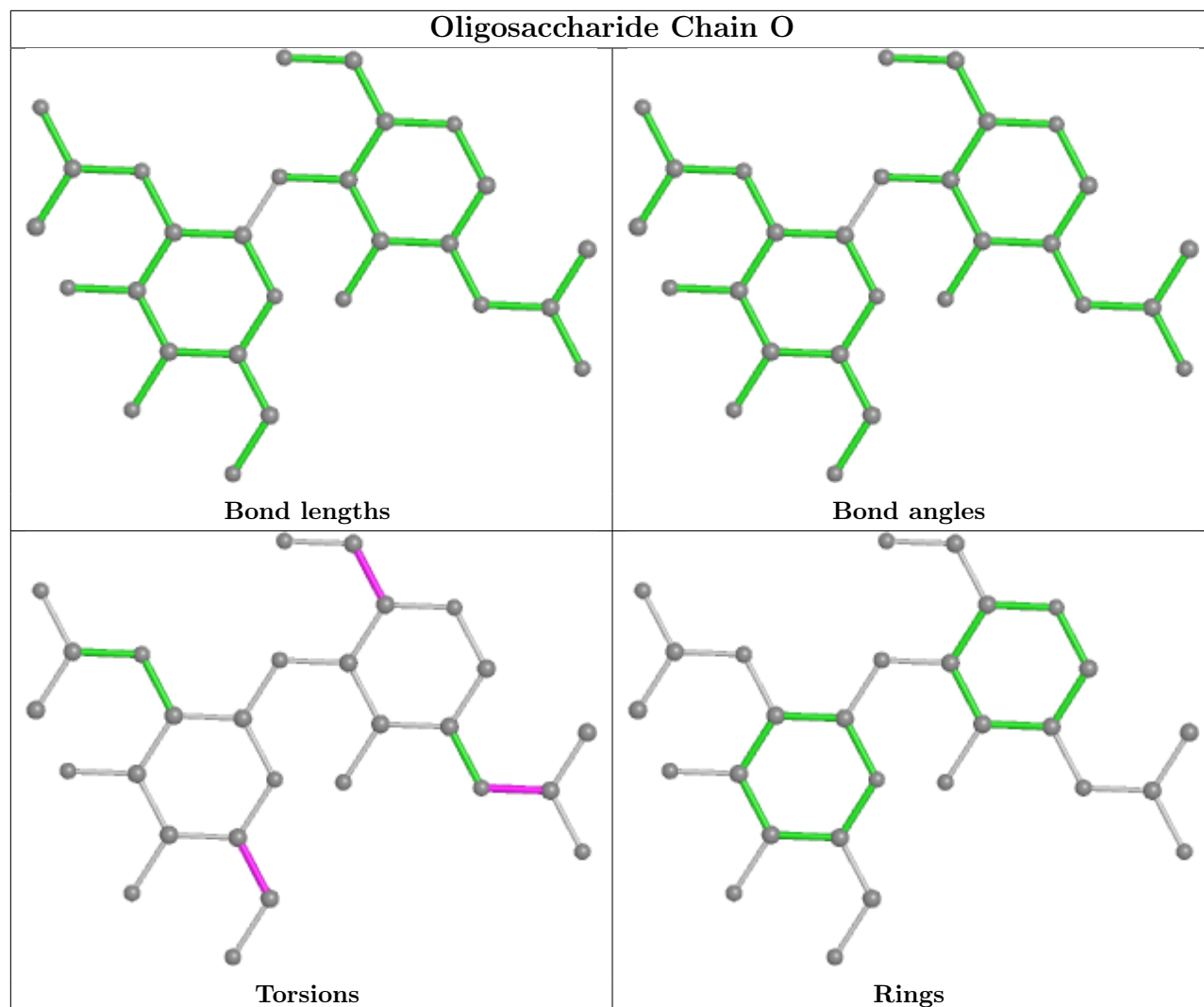
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	1	NAG	2	0
6	O	1	NAG	1	0

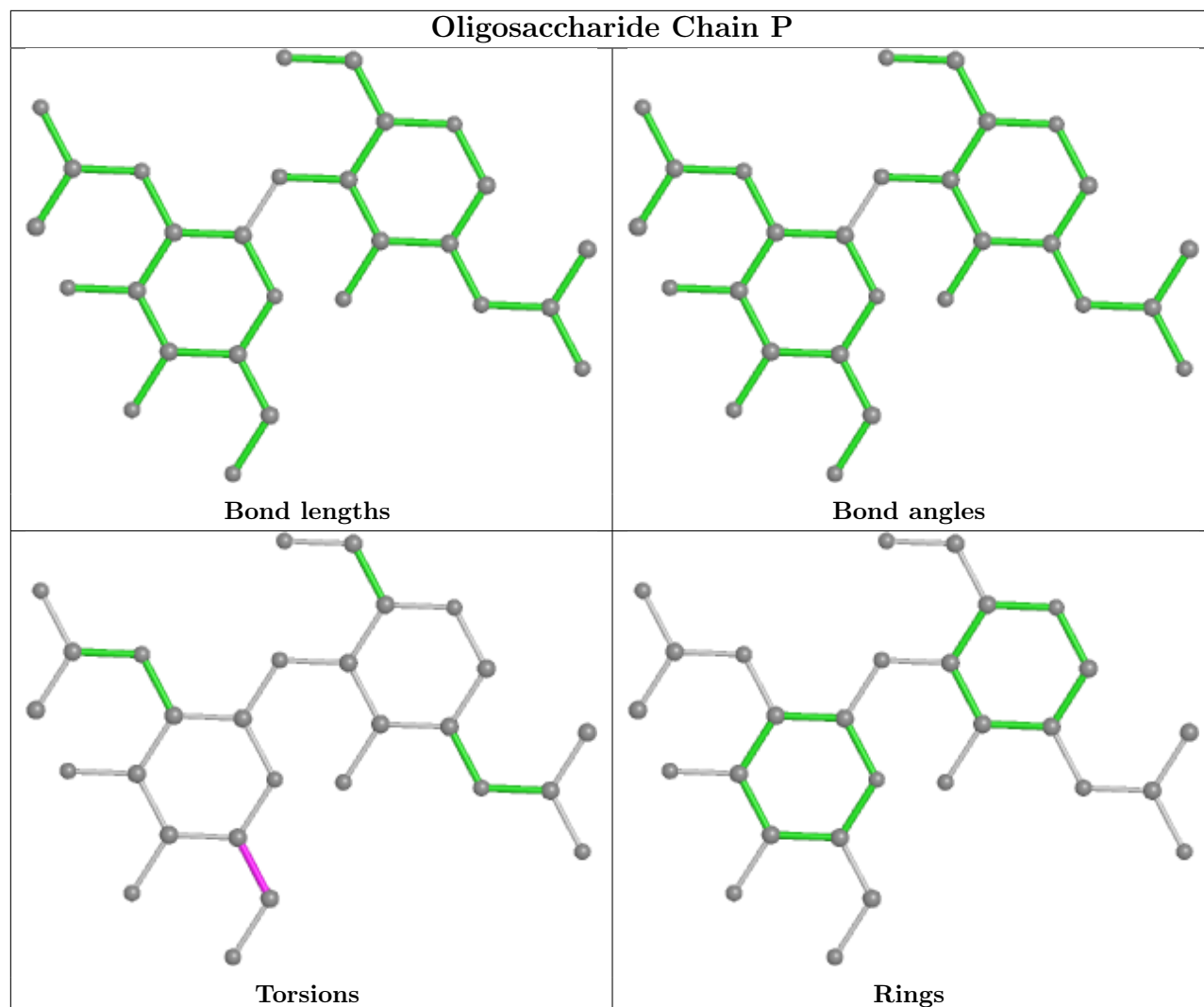
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

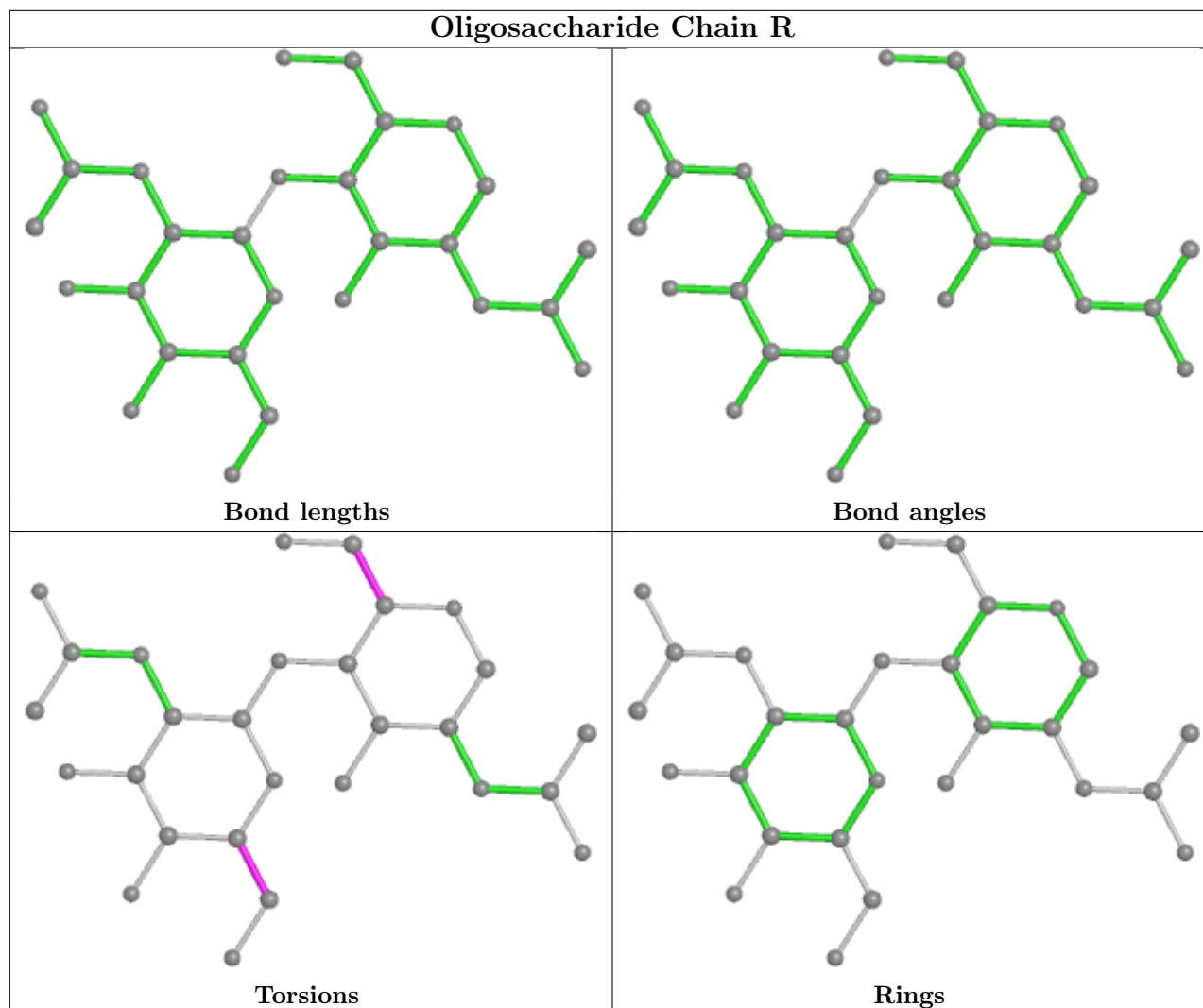












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
7	NAG	C	401	1	14,14,15	0.33	0	17,19,21	0.69	1 (5%)
7	NAG	F	201	2	14,14,15	0.26	0	17,19,21	0.66	0
7	NAG	E	401	1	14,14,15	0.32	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	402	1	14,14,15	1.65	1 (7%)	17,19,21	1.62	1 (5%)
7	NAG	A	401	1	14,14,15	1.89	2 (14%)	17,19,21	1.50	1 (5%)
7	NAG	L	301	4	14,14,15	0.35	0	17,19,21	0.49	0
7	NAG	I	301	-	14,14,15	0.30	0	17,19,21	0.45	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
7	NAG	C	401	1	-	0/6/23/26	0/1/1/1
7	NAG	F	201	2	-	1/6/23/26	0/1/1/1
7	NAG	E	401	1	-	4/6/23/26	0/1/1/1
7	NAG	A	402	1	-	4/6/23/26	0/1/1/1
7	NAG	A	401	1	-	2/6/23/26	0/1/1/1
7	NAG	L	301	4	-	0/6/23/26	0/1/1/1
7	NAG	I	301	-	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	402	NAG	O5-C1	5.85	1.53	1.43
7	A	401	NAG	O5-C1	5.53	1.52	1.43
7	A	401	NAG	C1-C2	4.24	1.58	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	402	NAG	C1-O5-C5	6.45	120.94	112.19
7	A	401	NAG	C1-O5-C5	5.74	119.96	112.19
7	C	401	NAG	C1-O5-C5	2.53	115.62	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	402	NAG	C4-C5-C6-O6
7	A	402	NAG	O5-C5-C6-O6
7	E	401	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	E	401	NAG	C4-C5-C6-O6
7	A	401	NAG	O5-C5-C6-O6
7	A	401	NAG	C4-C5-C6-O6
7	E	401	NAG	C1-C2-N2-C7
7	A	402	NAG	C1-C2-N2-C7
7	F	201	NAG	C3-C2-N2-C7
7	A	402	NAG	C3-C2-N2-C7
7	E	401	NAG	C3-C2-N2-C7
7	I	301	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
7	E	401	NAG	1	0
7	A	401	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	324/334 (97%)	0.09	5 (1%) 73 61	25, 68, 102, 134	0
1	C	324/334 (97%)	0.06	7 (2%) 62 48	21, 68, 102, 142	0
1	E	324/334 (97%)	0.01	7 (2%) 62 48	22, 70, 103, 152	0
2	B	176/177 (99%)	0.30	7 (3%) 38 25	23, 60, 116, 137	0
2	D	176/177 (99%)	0.34	7 (3%) 38 25	25, 59, 115, 172	0
2	F	176/177 (99%)	0.37	10 (5%) 23 13	26, 62, 119, 180	0
3	G	224/225 (99%)	-0.21	3 (1%) 77 65	23, 43, 77, 119	0
3	H	223/225 (99%)	-0.10	5 (2%) 62 48	25, 47, 99, 123	0
3	J	224/225 (99%)	0.11	9 (4%) 38 25	22, 56, 104, 146	0
4	I	213/214 (99%)	0.07	2 (0%) 84 75	31, 59, 84, 99	0
4	K	213/214 (99%)	0.12	6 (2%) 53 37	33, 58, 98, 125	0
4	L	213/214 (99%)	0.12	3 (1%) 75 63	28, 55, 80, 116	0
All	All	2810/2850 (98%)	0.09	71 (2%) 57 43	21, 58, 102, 180	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	8	ASP	11.3
2	D	174	SER	9.4
2	F	176	GLY	8.9
2	F	175	SER	8.3
2	F	174	SER	7.5
3	J	138	SER	6.9
2	D	175	SER	5.7
2	B	171	GLU	5.4
2	F	171	GLU	5.3
1	E	8	ASP	5.1
1	A	8	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
4	L	213	GLU	4.3
1	C	9	PRO	4.3
2	D	171	GLU	4.2
3	J	139	THR	4.0
4	K	146	VAL	3.8
2	F	173	ILE	3.5
3	J	137	LYS	3.5
3	G	224	CYS	3.4
1	C	134	GLY	3.3
2	F	170	ARG	3.2
1	E	133(A)	LEU	3.1
3	J	135	SER	3.0
3	J	133	ALA	3.0
2	B	175	SER	3.0
3	J	224	CYS	3.0
2	D	144	CYS	2.9
2	F	142	HIS	2.8
3	H	140	SER	2.8
2	F	139	GLU	2.7
3	H	135	SER	2.7
1	A	161	TYR	2.7
4	K	147	GLN	2.7
2	F	61	THR	2.6
1	E	9	PRO	2.6
1	E	134	GLY	2.6
4	K	213	GLU	2.6
1	C	146	SER	2.6
3	H	138	SER	2.6
2	B	173	ILE	2.6
3	J	144	ALA	2.6
2	B	142	HIS	2.6
4	K	195	GLU	2.6
2	B	144	CYS	2.5
3	G	138	SER	2.5
4	K	203	SER	2.5
2	B	167	ARG	2.5
2	D	173	ILE	2.4
3	J	223	SER	2.4
3	G	223	SER	2.4
4	I	213	GLU	2.4
3	H	139	THR	2.4
1	C	290	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	131	GLU	2.3
2	D	143	LYS	2.3
4	L	67	SER	2.3
2	F	167	ARG	2.3
1	C	125(A)	LYS	2.3
1	E	77	ASP	2.2
4	K	196	VAL	2.2
4	I	193	ALA	2.2
2	B	143	LYS	2.2
2	D	139	GLU	2.2
3	H	137	LYS	2.1
1	A	196	GLN	2.1
3	J	14	GLY	2.1
1	A	163	THR	2.1
1	A	159	SER	2.1
1	E	10	GLY	2.1
1	E	218	ALA	2.1
4	L	194	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

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

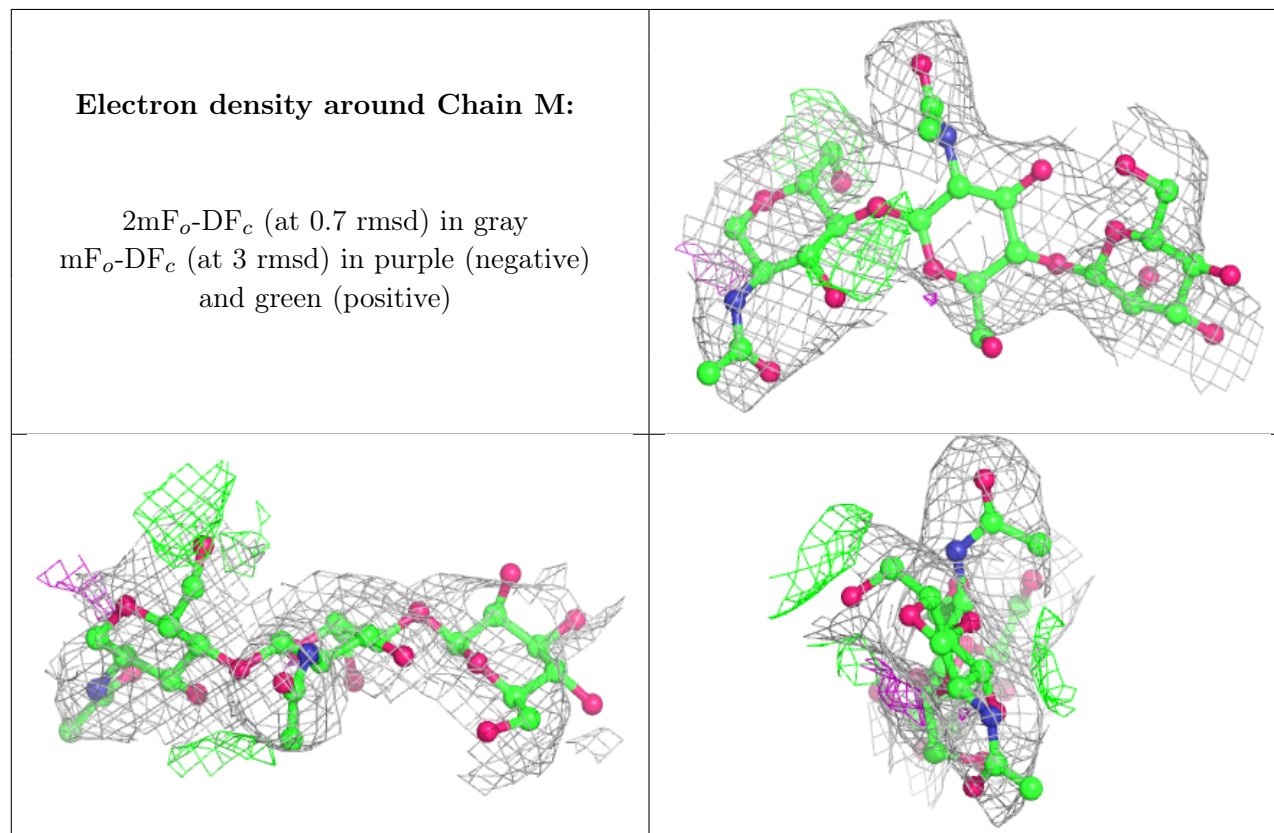
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	Q	3	11/12	0.49	0.43	107,131,141,142	0
5	BMA	M	3	11/12	0.56	0.32	81,112,119,122	0
6	NAG	N	2	14/15	0.62	0.31	61,121,129,129	0
6	NAG	R	2	14/15	0.65	0.43	82,142,155,157	0
6	NAG	R	1	14/15	0.73	0.30	83,96,120,133	0
6	NAG	O	2	14/15	0.73	0.45	86,111,122,127	0
5	NAG	Q	1	14/15	0.80	0.17	49,72,91,98	0
5	NAG	Q	2	14/15	0.81	0.31	51,98,126,134	0
6	NAG	P	2	14/15	0.81	0.33	85,106,113,119	0
6	NAG	N	1	14/15	0.85	0.21	82,93,105,106	0

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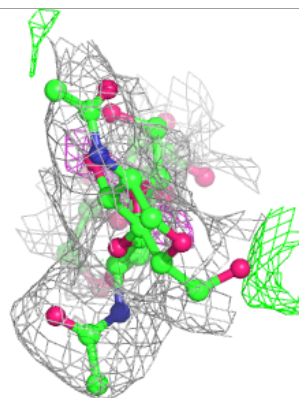
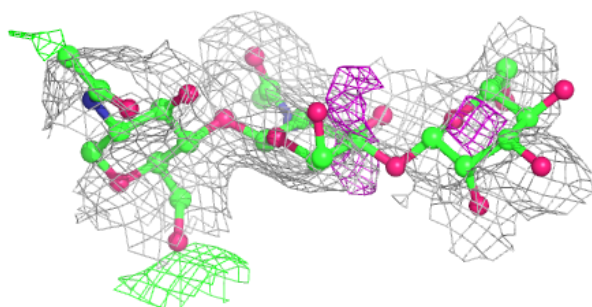
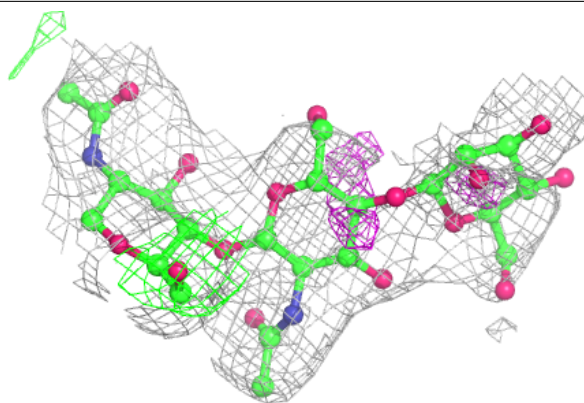
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	P	1	14/15	0.86	0.29	72,89,100,111	0
5	NAG	M	2	14/15	0.88	0.19	49,86,107,112	0
5	NAG	M	1	14/15	0.89	0.18	36,51,63,70	0
6	NAG	O	1	14/15	0.90	0.19	31,55,73,87	0

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.

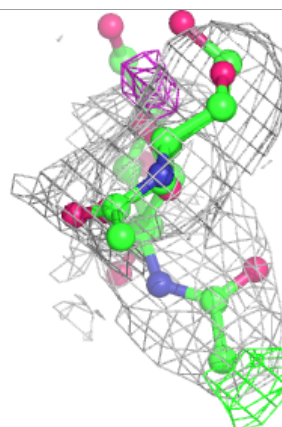
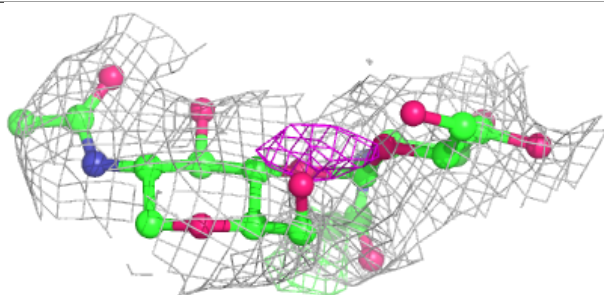
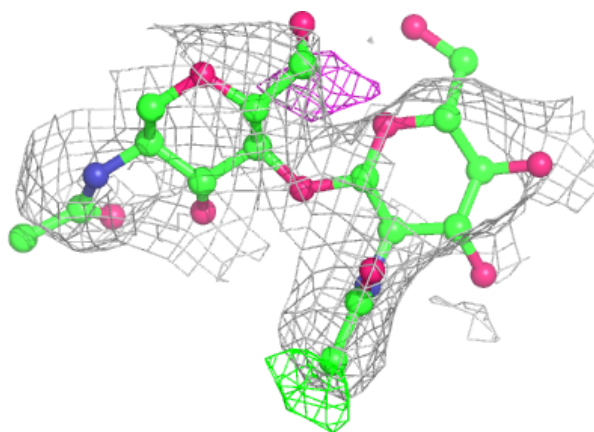


Electron density around Chain Q:

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

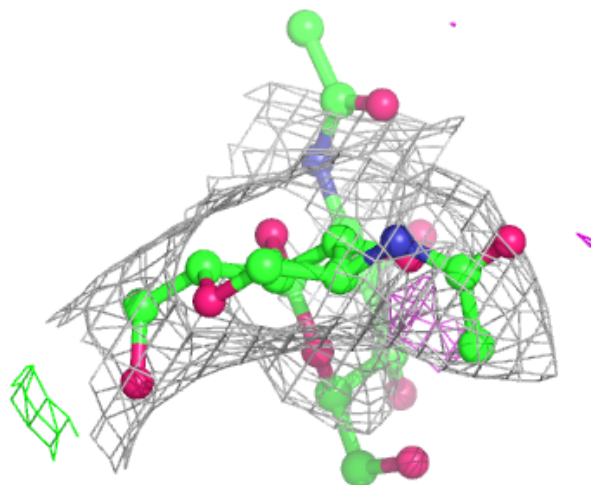
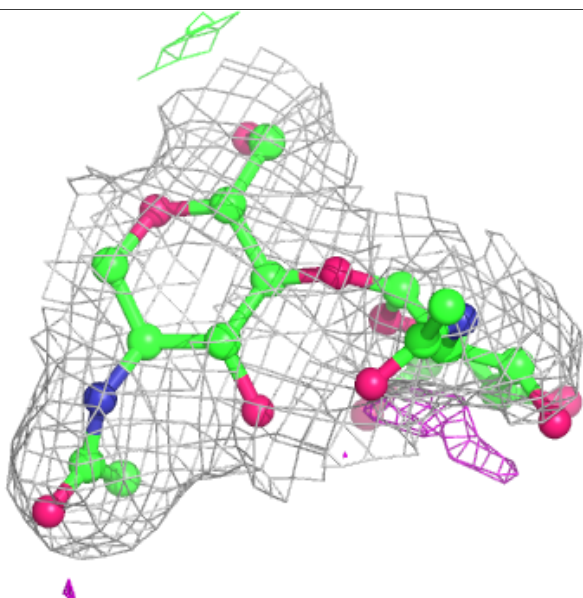
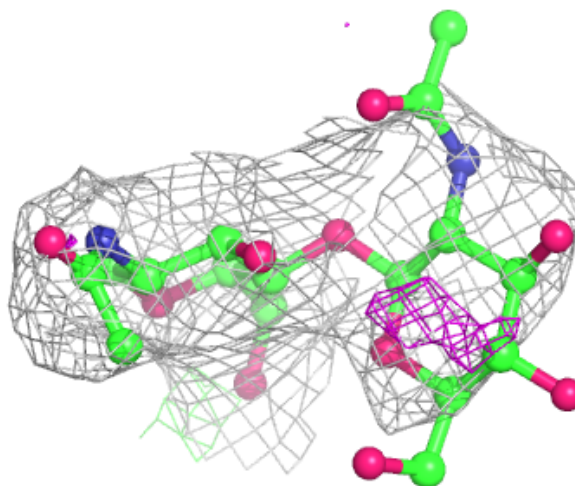
**Electron density around Chain N:**

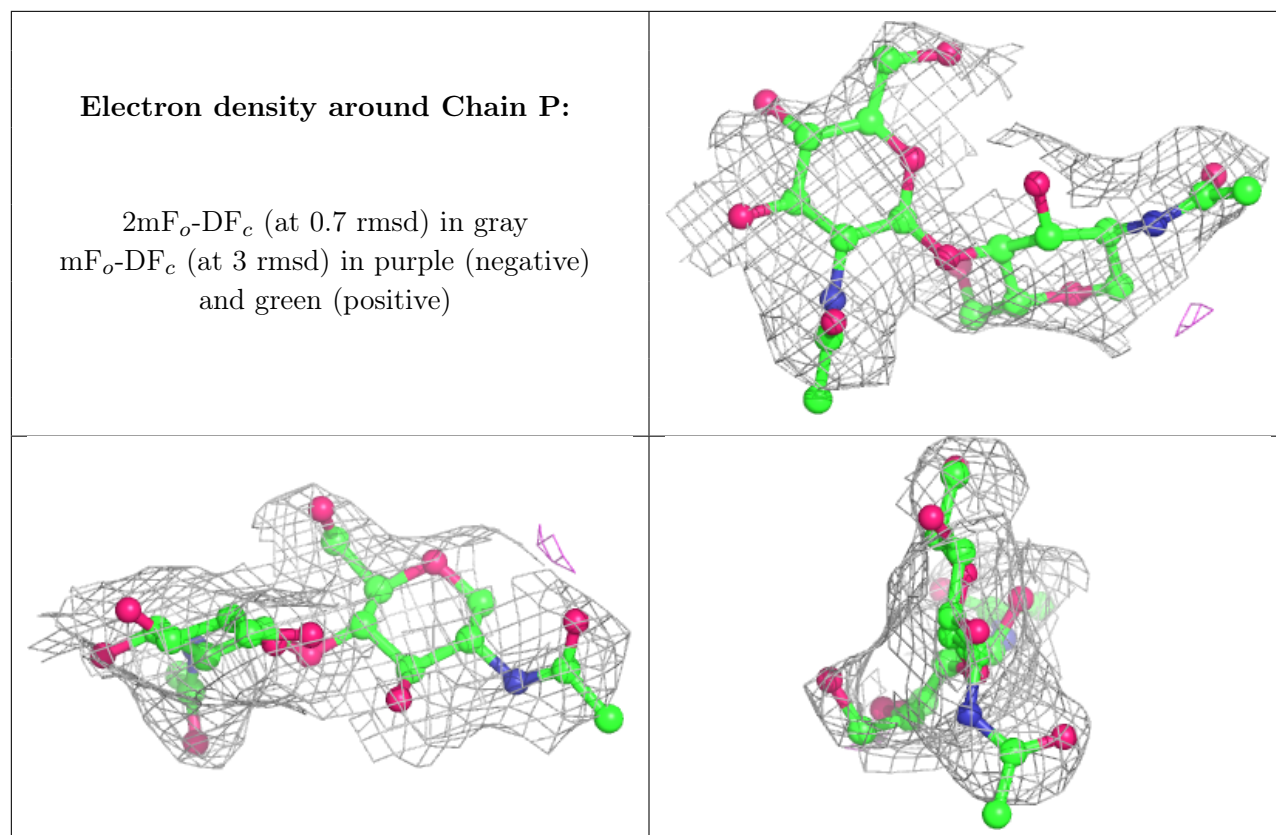
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

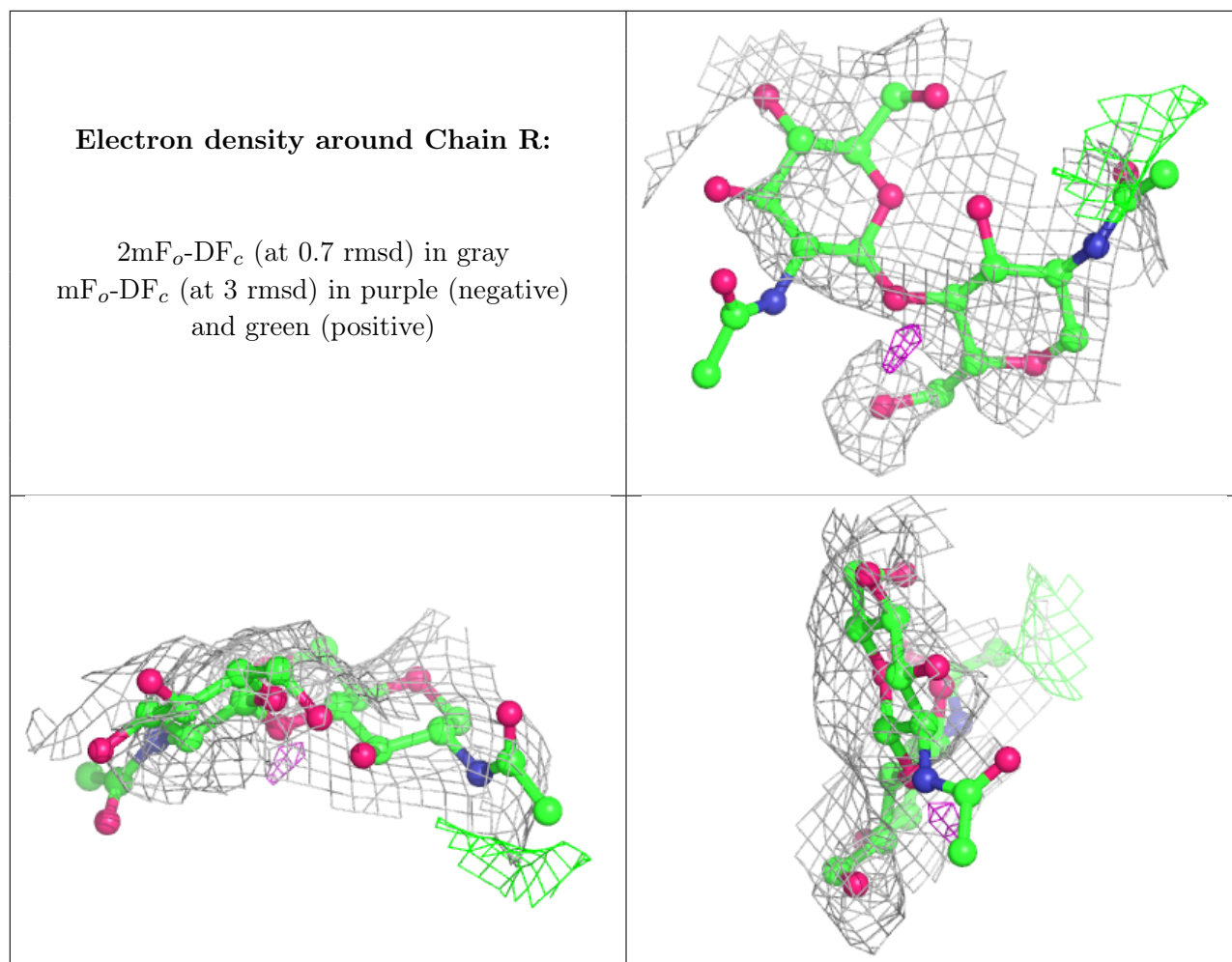


Electron density around Chain O:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
7	NAG	E	401	14/15	0.68	0.27	74,93,99,102	0
7	NAG	F	201	14/15	0.72	0.47	89,95,126,127	0
7	NAG	C	401	14/15	0.73	0.29	82,89,98,101	0
7	NAG	A	402	14/15	0.75	0.32	77,110,139,144	0
7	NAG	A	401	14/15	0.76	0.23	59,93,101,101	0
7	NAG	I	301	14/15	0.80	0.28	59,100,112,121	0
7	NAG	L	301	14/15	0.82	0.20	65,77,85,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.