



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 05:22 PM UTC

PDB ID : 3BIW / pdb_00003biw
Title : Crystal structure of the Neuroligin-1/Neurexin-1beta synaptic adhesion complex
Authors : Arac, D.; Boucard, A.A.; Ozkan, E.; Strop, P.; Newell, E.; Sudhof, T.C.; Brunger, A.T.
Deposited on : 2007-12-01
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

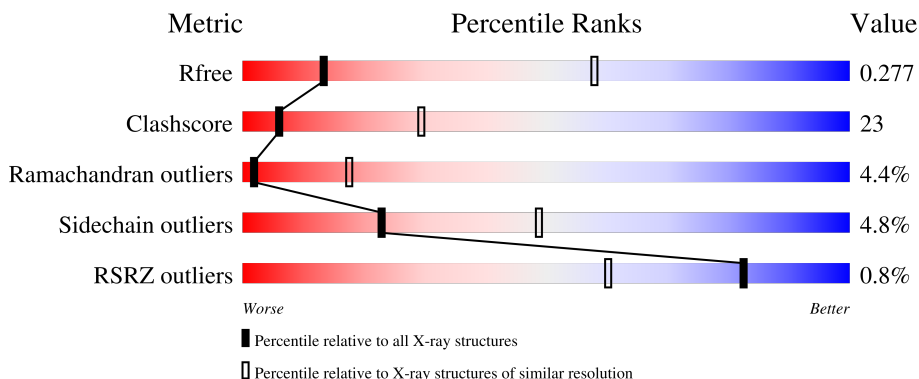
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



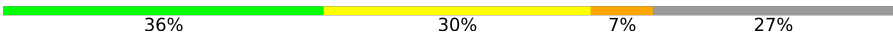
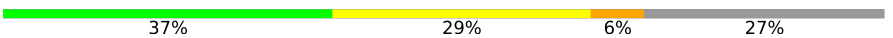
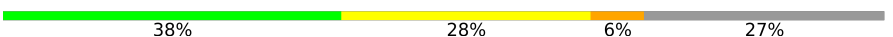
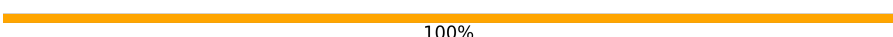
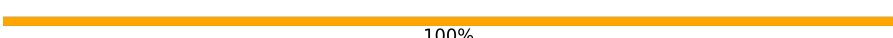
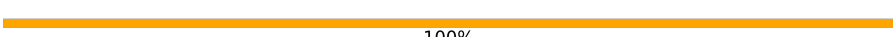
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	574	51% 35% 6% 7%
1	B	574	51% 36% 6% 7%
1	C	574	51% 36% 6% 7%
1	D	574	50% 37% 6% 7%
2	E	243	37% 30% 6% 27%

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Mol	Chain	Length	Quality of chain
2	F	243	
2	G	243	
2	H	243	
3	I	2	
3	J	2	
3	K	2	

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
3	NAG	I	1	-	-	X	-
3	NAG	J	1	-	-	X	-
3	NAG	K	1	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22438 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 Neuroligin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4186	2690	697	783	16			
1	B	533	Total	C	N	O	S	0	0	0
			4186	2690	697	783	16			
1	C	533	Total	C	N	O	S	0	0	0
			4186	2690	697	783	16			
1	D	533	Total	C	N	O	S	0	0	0
			4186	2690	697	783	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ALA	-	expression tag	UNP Q62765
A	44	ASP	-	expression tag	UNP Q62765
A	45	PRO	-	expression tag	UNP Q62765
A	639	HIS	-	expression tag	UNP Q62765
A	640	HIS	-	expression tag	UNP Q62765
A	641	HIS	-	expression tag	UNP Q62765
A	642	HIS	-	expression tag	UNP Q62765
A	643	HIS	-	expression tag	UNP Q62765
A	644	HIS	-	expression tag	UNP Q62765
B	43	ALA	-	expression tag	UNP Q62765
B	44	ASP	-	expression tag	UNP Q62765
B	45	PRO	-	expression tag	UNP Q62765
B	639	HIS	-	expression tag	UNP Q62765
B	640	HIS	-	expression tag	UNP Q62765
B	641	HIS	-	expression tag	UNP Q62765
B	642	HIS	-	expression tag	UNP Q62765
B	643	HIS	-	expression tag	UNP Q62765
B	644	HIS	-	expression tag	UNP Q62765
C	43	ALA	-	expression tag	UNP Q62765
C	44	ASP	-	expression tag	UNP Q62765
C	45	PRO	-	expression tag	UNP Q62765

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Chain	Residue	Modelled	Actual	Comment	Reference
C	639	HIS	-	expression tag	UNP Q62765
C	640	HIS	-	expression tag	UNP Q62765
C	641	HIS	-	expression tag	UNP Q62765
C	642	HIS	-	expression tag	UNP Q62765
C	643	HIS	-	expression tag	UNP Q62765
C	644	HIS	-	expression tag	UNP Q62765
D	43	ALA	-	expression tag	UNP Q62765
D	44	ASP	-	expression tag	UNP Q62765
D	45	PRO	-	expression tag	UNP Q62765
D	639	HIS	-	expression tag	UNP Q62765
D	640	HIS	-	expression tag	UNP Q62765
D	641	HIS	-	expression tag	UNP Q62765
D	642	HIS	-	expression tag	UNP Q62765
D	643	HIS	-	expression tag	UNP Q62765
D	644	HIS	-	expression tag	UNP Q62765

- Molecule 2 is a protein called Neurexin-1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			
2	F	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			
2	G	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			
2	H	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	33	GLY	-	expression tag	UNP Q63373
E	34	SER	-	expression tag	UNP Q63373
E	35	PRO	-	expression tag	UNP Q63373
E	36	GLY	-	expression tag	UNP Q63373
E	37	ILE	-	expression tag	UNP Q63373
E	38	SER	-	expression tag	UNP Q63373
E	39	GLY	-	expression tag	UNP Q63373
E	40	GLY	-	expression tag	UNP Q63373
E	41	GLY	-	expression tag	UNP Q63373
E	42	GLY	-	expression tag	UNP Q63373
E	43	GLY	-	expression tag	UNP Q63373

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Chain	Residue	Modelled	Actual	Comment	Reference
E	44	ILE	-	expression tag	UNP Q63373
E	45	LEU	-	expression tag	UNP Q63373
E	46	GLU	-	expression tag	UNP Q63373
E	300	HIS	-	expression tag	UNP Q63373
E	301	HIS	-	expression tag	UNP Q63373
E	302	HIS	-	expression tag	UNP Q63373
E	303	HIS	-	expression tag	UNP Q63373
E	304	HIS	-	expression tag	UNP Q63373
E	305	HIS	-	expression tag	UNP Q63373
F	33	GLY	-	expression tag	UNP Q63373
F	34	SER	-	expression tag	UNP Q63373
F	35	PRO	-	expression tag	UNP Q63373
F	36	GLY	-	expression tag	UNP Q63373
F	37	ILE	-	expression tag	UNP Q63373
F	38	SER	-	expression tag	UNP Q63373
F	39	GLY	-	expression tag	UNP Q63373
F	40	GLY	-	expression tag	UNP Q63373
F	41	GLY	-	expression tag	UNP Q63373
F	42	GLY	-	expression tag	UNP Q63373
F	43	GLY	-	expression tag	UNP Q63373
F	44	ILE	-	expression tag	UNP Q63373
F	45	LEU	-	expression tag	UNP Q63373
F	46	GLU	-	expression tag	UNP Q63373
F	300	HIS	-	expression tag	UNP Q63373
F	301	HIS	-	expression tag	UNP Q63373
F	302	HIS	-	expression tag	UNP Q63373
F	303	HIS	-	expression tag	UNP Q63373
F	304	HIS	-	expression tag	UNP Q63373
F	305	HIS	-	expression tag	UNP Q63373
G	33	GLY	-	expression tag	UNP Q63373
G	34	SER	-	expression tag	UNP Q63373
G	35	PRO	-	expression tag	UNP Q63373
G	36	GLY	-	expression tag	UNP Q63373
G	37	ILE	-	expression tag	UNP Q63373
G	38	SER	-	expression tag	UNP Q63373
G	39	GLY	-	expression tag	UNP Q63373
G	40	GLY	-	expression tag	UNP Q63373
G	41	GLY	-	expression tag	UNP Q63373
G	42	GLY	-	expression tag	UNP Q63373
G	43	GLY	-	expression tag	UNP Q63373
G	44	ILE	-	expression tag	UNP Q63373
G	45	LEU	-	expression tag	UNP Q63373

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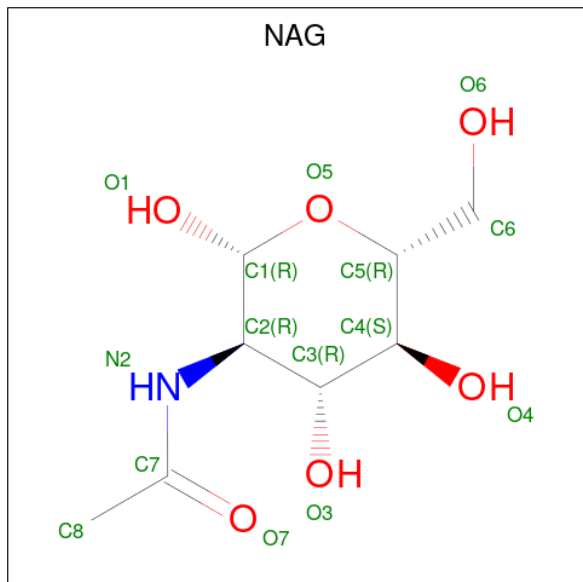
Chain	Residue	Modelled	Actual	Comment	Reference
G	46	GLU	-	expression tag	UNP Q63373
G	300	HIS	-	expression tag	UNP Q63373
G	301	HIS	-	expression tag	UNP Q63373
G	302	HIS	-	expression tag	UNP Q63373
G	303	HIS	-	expression tag	UNP Q63373
G	304	HIS	-	expression tag	UNP Q63373
G	305	HIS	-	expression tag	UNP Q63373
H	33	GLY	-	expression tag	UNP Q63373
H	34	SER	-	expression tag	UNP Q63373
H	35	PRO	-	expression tag	UNP Q63373
H	36	GLY	-	expression tag	UNP Q63373
H	37	ILE	-	expression tag	UNP Q63373
H	38	SER	-	expression tag	UNP Q63373
H	39	GLY	-	expression tag	UNP Q63373
H	40	GLY	-	expression tag	UNP Q63373
H	41	GLY	-	expression tag	UNP Q63373
H	42	GLY	-	expression tag	UNP Q63373
H	43	GLY	-	expression tag	UNP Q63373
H	44	ILE	-	expression tag	UNP Q63373
H	45	LEU	-	expression tag	UNP Q63373
H	46	GLU	-	expression tag	UNP Q63373
H	300	HIS	-	expression tag	UNP Q63373
H	301	HIS	-	expression tag	UNP Q63373
H	302	HIS	-	expression tag	UNP Q63373
H	303	HIS	-	expression tag	UNP Q63373
H	304	HIS	-	expression tag	UNP Q63373
H	305	HIS	-	expression tag	UNP Q63373

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

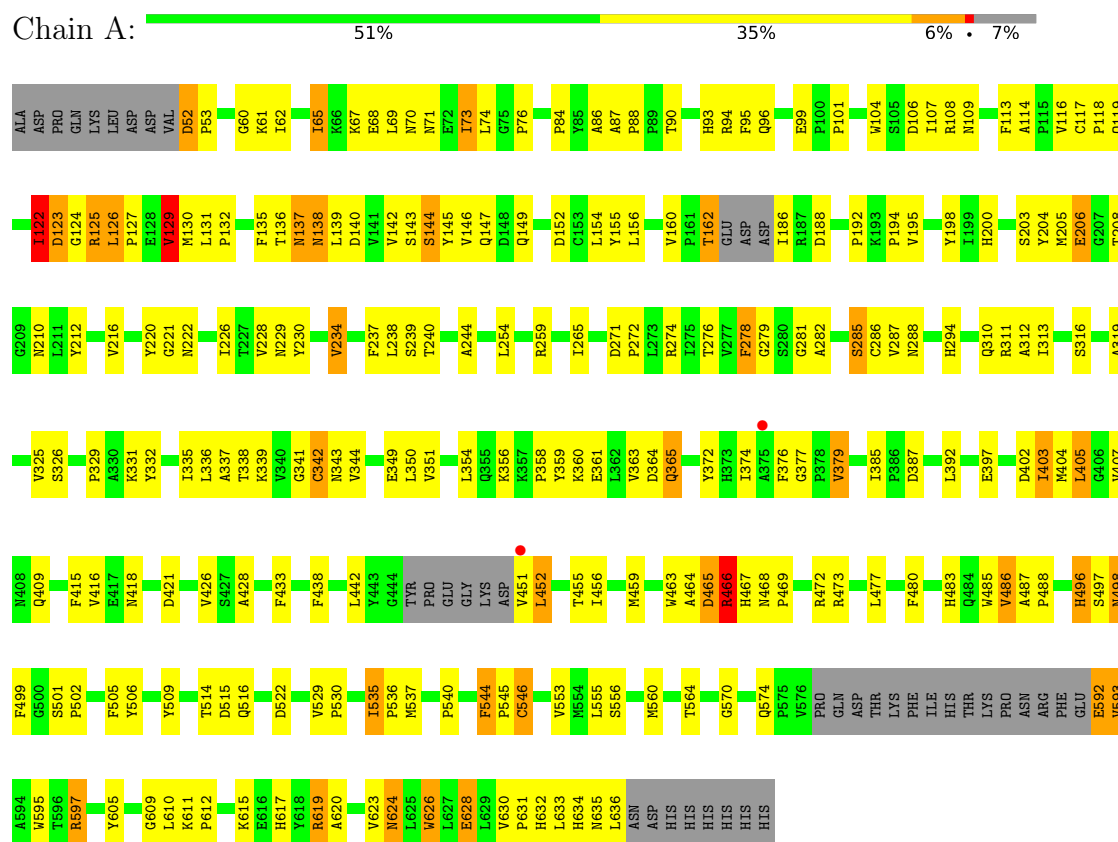
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	2	Total 2	Ca 2	0	0
5	F	2	Total 2	Ca 2	0	0
5	G	2	Total 2	Ca 2	0	0

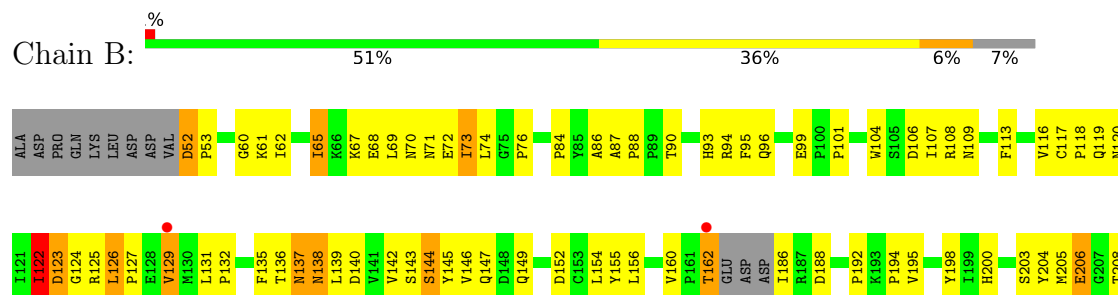
3 Residue-property plots

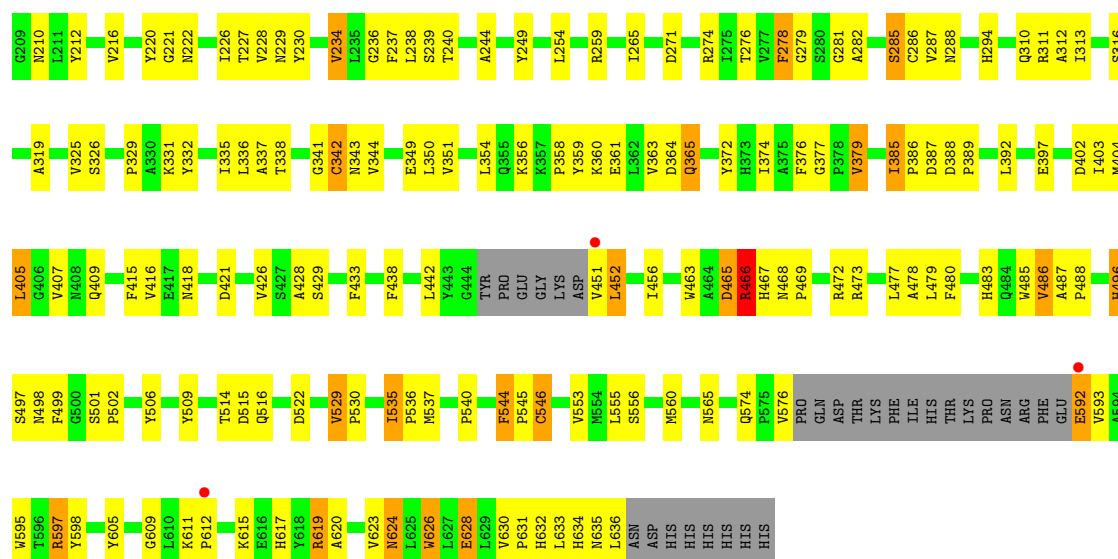
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Neuroligin-1

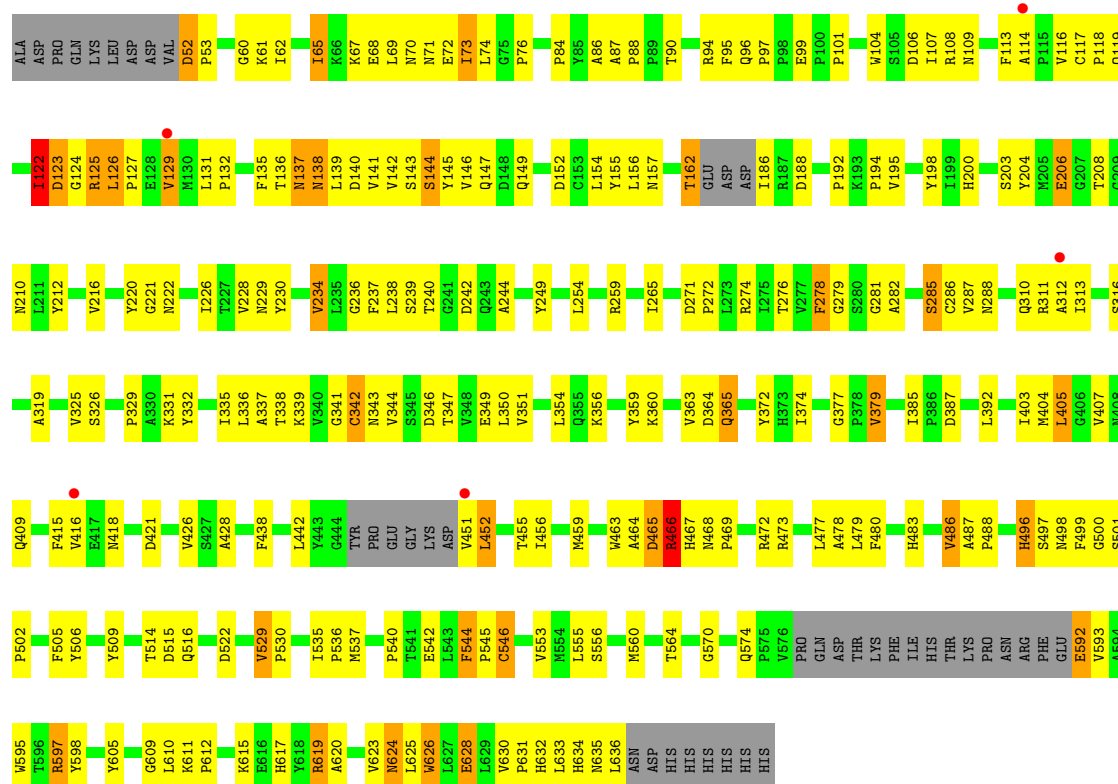


• Molecule 1: Neuroligin-1

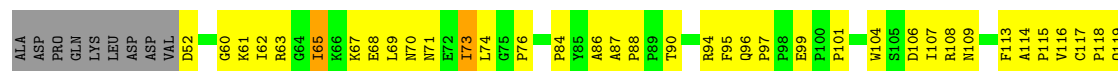


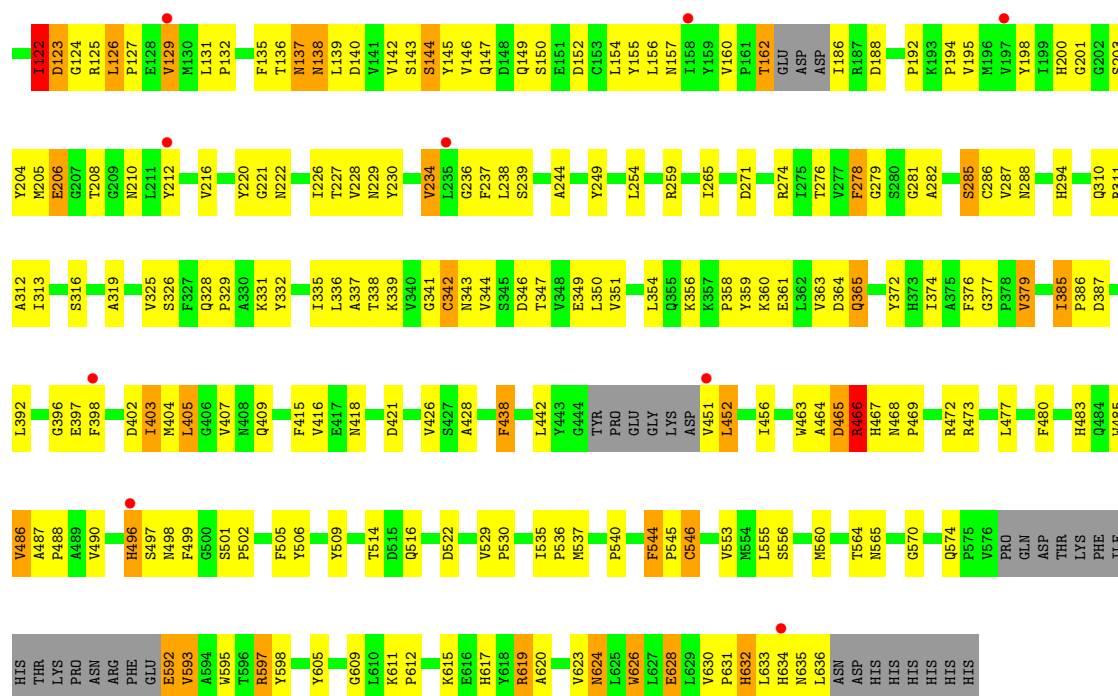


• Molecule 1: Neuroligin-1

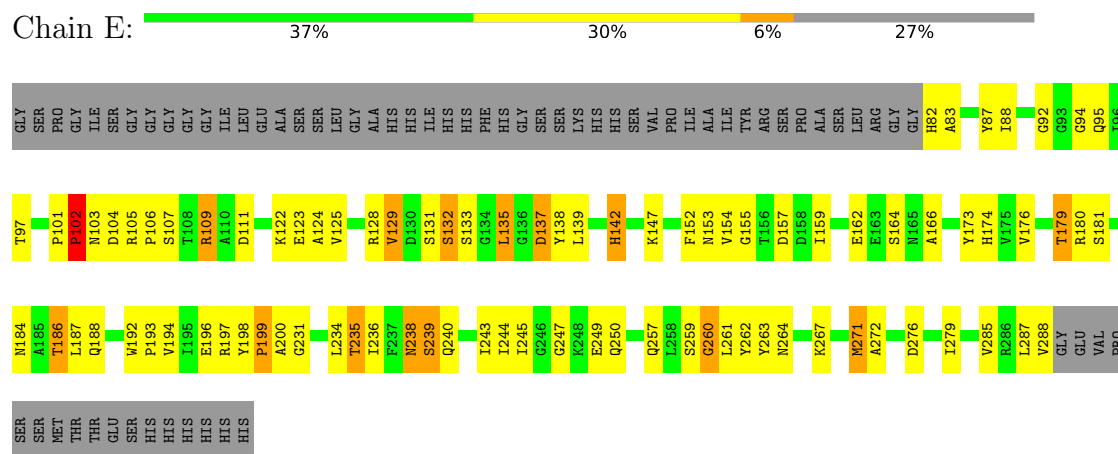


• Molecule 1: Neuroligin-1

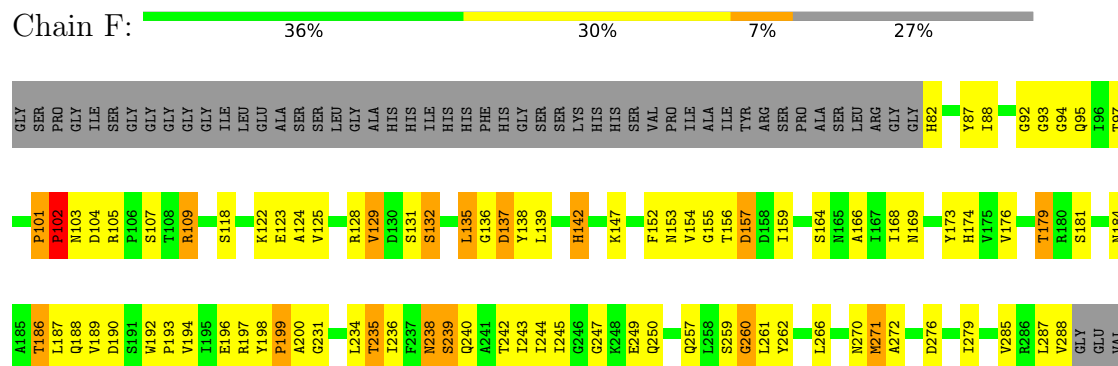




• Molecule 2: Neurexin-1-beta

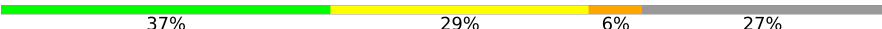


• Molecule 2: Neurexin-1-beta



PRO
SER
SER
MET
THR
THR
GLU
SER
HIS
HIS
HIS
HIS
HIS

• Molecule 2: Neurexin-1-beta

Chain G:  37% 29% 6% 27%

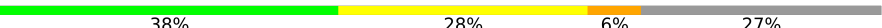
GLY
SER
PRO
GLY
ILE
SER
GLY
GLY
GLY
GLY
ILE
LEU
GLU
ALA
SER
SER
LEU
GLY
ALA
HIS
HIS
HIS
HIS
HIS
HIS
PHE
HIS
GLY
D137
SER
SER
LYS
HIS
HIS
SER
VAL
PRO
TLE
ALA
TLE
TYR
ARG
SER
PRO
ALA
SER
LEU
ARG
GLY
GLY
H82
H83
I88
G92
G93
G94
Q95
I96
T97

P101
P102
N103
D104
R105
P106
S107
T108
R109
A110
D111
K122
E123
A124
V125
R128
V129
D130
S131
S132
S133
G134
L135
G136
D137
Y138
L139
H142
K147
F152
N153
V154
G155
T156
D157
D158
I159
E162
E163
S164
N165
A166
T167
I168
Y173
H174
V175
V176
T179
R180
I186
S181

N184
A185
T186
L187
Q188
W192
V193
T194
H195
E196
R197
Y198
A200
G231
L234
T235
I236
F237
N238
S239
Q240
A241
T242
I243
I244
I245
G246
G247
K248
E249
Q250
Q257
L258
S259
G260
Y263
D157
N264
K267
V268
L269
N270
N271
A272
D276
I279
V285
K286
L287
V288
GLU

VAL
PRO
SER
SER
MET
THR
THR
GLU
SER
SER
HIS
HIS
HIS
HIS
HIS

• Molecule 2: Neurexin-1-beta

Chain H:  38% 28% 6% 27%

GLY
SER
PRO
GLY
ILE
SER
GLY
GLY
GLY
GLY
ILE
LEU
GLU
ALA
SER
SER
LEU
GLY
ALA
HIS
HIS
HIS
HIS
HIS
HIS
PHE
HIS
GLY
D137
SER
SER
LYS
HIS
HIS
SER
VAL
PRO
TLE
ALA
TLE
TYR
ARG
SER
PRO
ALA
SER
LEU
ARG
GLY
GLY
H82
Y87
I88
G92
G93
G94
Q95
I96
T97

P101
P102
N103
D104
R105
P106
S107
T108
R109
A110
D111
E123
A124
V125
R128
V129
D130
S131
S132
S133
G134
L135
G136
D137
Y138
L139
H142
K147
F152
N153
V154
G155
T156
D157
I159
S164
R165
A166
I167
I168
Y173
H174
V175
V176
T179
R180
S181
T186
L187

Q188
V189
S191
W192
P193
V194
I195
E196
R197
Y198
P199
A200
G231
Q232
Q233
L234
T235
I236
F237
N238
S239
Q240
A241
T242
I243
I244
I245
G246
G247
K248
E249
Q250
Q257
L258
S259
G260
Y263
L269
N270
M271
A272
E274
N275
D276
I279
V285
K286
L287
V288
GLY
GLU
VAL
PRO

SER
SER
MET
THR
THR
GLU
SER
SER
HIS
HIS
HIS
HIS
HIS
HIS

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.83Å 148.80Å 123.60Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	45.90 – 3.50 45.90 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.9 (45.90-3.50) 94.8 (45.90-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.246 , 0.276 0.248 , 0.277	Depositor DCC
R_{free} test set	2737 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	97.9	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22438	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.58	1/4302 (0.0%)	1.03	29/5872 (0.5%)
1	B	0.58	1/4302 (0.0%)	1.04	24/5872 (0.4%)
1	C	0.55	1/4302 (0.0%)	1.02	24/5872 (0.4%)
1	D	0.45	1/4302 (0.0%)	1.00	31/5872 (0.5%)
2	E	0.56	1/1385 (0.1%)	1.04	12/1877 (0.6%)
2	F	0.63	1/1385 (0.1%)	1.06	13/1877 (0.7%)
2	G	0.60	1/1385 (0.1%)	1.06	12/1877 (0.6%)
2	H	0.43	1/1385 (0.1%)	1.00	8/1877 (0.4%)
All	All	0.55	8/22748 (0.0%)	1.03	153/30996 (0.5%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	142	HIS	ND1-CE1	5.60	1.38	1.32
2	F	142	HIS	ND1-CE1	5.42	1.38	1.32
2	G	142	HIS	ND1-CE1	5.40	1.38	1.32
1	D	632	HIS	ND1-CE1	5.31	1.37	1.32
2	H	142	HIS	ND1-CE1	5.26	1.37	1.32

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	452	LEU	N-CA-C	-12.05	96.87	111.69
1	A	452	LEU	N-CA-C	-11.74	97.24	111.69
1	B	452	LEU	N-CA-C	-11.70	97.31	111.69
1	C	452	LEU	N-CA-C	-11.68	97.52	112.23
2	G	236	ILE	N-CA-C	10.31	123.11	108.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4186	0	4046	187	0
1	B	4186	0	4046	191	0
1	C	4186	0	4046	188	0
1	D	4186	0	4045	190	0
2	E	1359	0	1345	61	1
2	F	1359	0	1345	68	0
2	G	1359	0	1345	61	0
2	H	1359	0	1347	68	0
3	I	28	0	25	7	0
3	J	28	0	25	7	0
3	K	28	0	25	7	0
4	A	42	0	39	3	0
4	B	42	0	39	3	0
4	C	42	0	39	3	0
4	D	42	0	39	2	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
All	All	22438	0	21796	1006	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 1006 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:G:147:LYS:HD3	2:G:164:SER:HA	1.48	0.95
2:E:147:LYS:HD3	2:E:164:SER:HA	1.47	0.93
2:F:147:LYS:HD3	2:F:164:SER:HA	1.51	0.92
2:H:147:LYS:HD3	2:H:164:SER:HA	1.50	0.90
1:D:426:VAL:HG23	1:D:473:ARG:HB2	1.62	0.80

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:TRP:NE1	2:E:192:TRP:NE1[2_556]	1.74	0.46

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	525/574 (92%)	441 (84%)	62 (12%)	22 (4%)	2	19
1	B	525/574 (92%)	441 (84%)	63 (12%)	21 (4%)	2	19
1	C	525/574 (92%)	441 (84%)	63 (12%)	21 (4%)	2	19
1	D	525/574 (92%)	441 (84%)	63 (12%)	21 (4%)	2	19
2	E	175/243 (72%)	143 (82%)	23 (13%)	9 (5%)	1	15
2	F	175/243 (72%)	143 (82%)	22 (13%)	10 (6%)	1	13
2	G	175/243 (72%)	142 (81%)	23 (13%)	10 (6%)	1	13
2	H	175/243 (72%)	143 (82%)	22 (13%)	10 (6%)	1	13
All	All	2800/3268 (86%)	2335 (83%)	341 (12%)	124 (4%)	2	17

5 of 124 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ASP
1	A	124	GLY
1	A	138	ASN
1	A	343	ASN
1	A	465	ASP

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	455/494 (92%)	434 (95%)	21 (5%)	24	50
1	B	455/494 (92%)	435 (96%)	20 (4%)	25	51
1	C	455/494 (92%)	434 (95%)	21 (5%)	24	50
1	D	455/494 (92%)	434 (95%)	21 (5%)	24	50
2	E	143/193 (74%)	134 (94%)	9 (6%)	16	42
2	F	143/193 (74%)	135 (94%)	8 (6%)	19	46
2	G	143/193 (74%)	135 (94%)	8 (6%)	19	46
2	H	143/193 (74%)	136 (95%)	7 (5%)	22	48
All	All	2392/2748 (87%)	2277 (95%)	115 (5%)	23	49

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	555	LEU
2	H	157	ASP
1	D	338	THR
2	H	129	VAL
2	F	271	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	188	GLN
2	H	250	GLN
2	H	252	GLN
2	H	188	GLN
1	D	525	HIS

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
3	NAG	I	1	3,2	14,14,15	1.23	1 (7%)	17,19,21	0.84	0
3	NAG	I	2	3	14,14,15	0.95	1 (7%)	17,19,21	0.66	0
3	NAG	J	1	3,2	14,14,15	1.27	1 (7%)	17,19,21	0.93	1 (5%)
3	NAG	J	2	3	14,14,15	1.01	1 (7%)	17,19,21	0.65	0
3	NAG	K	1	3,2	14,14,15	1.21	1 (7%)	17,19,21	0.92	0
3	NAG	K	2	3	14,14,15	1.08	1 (7%)	17,19,21	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	NAG	J	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	J	2	3	-	4/6/23/26	0/1/1/1
3	NAG	K	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	K	2	3	-	4/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	C1-C2	3.72	1.57	1.52
3	K	2	NAG	C1-C2	3.46	1.57	1.52
3	I	1	NAG	C1-C2	3.42	1.57	1.52
3	J	2	NAG	C1-C2	3.29	1.56	1.52
3	K	1	NAG	C1-C2	3.21	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	NAG	O7-C7-C8	-2.07	118.36	122.05

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

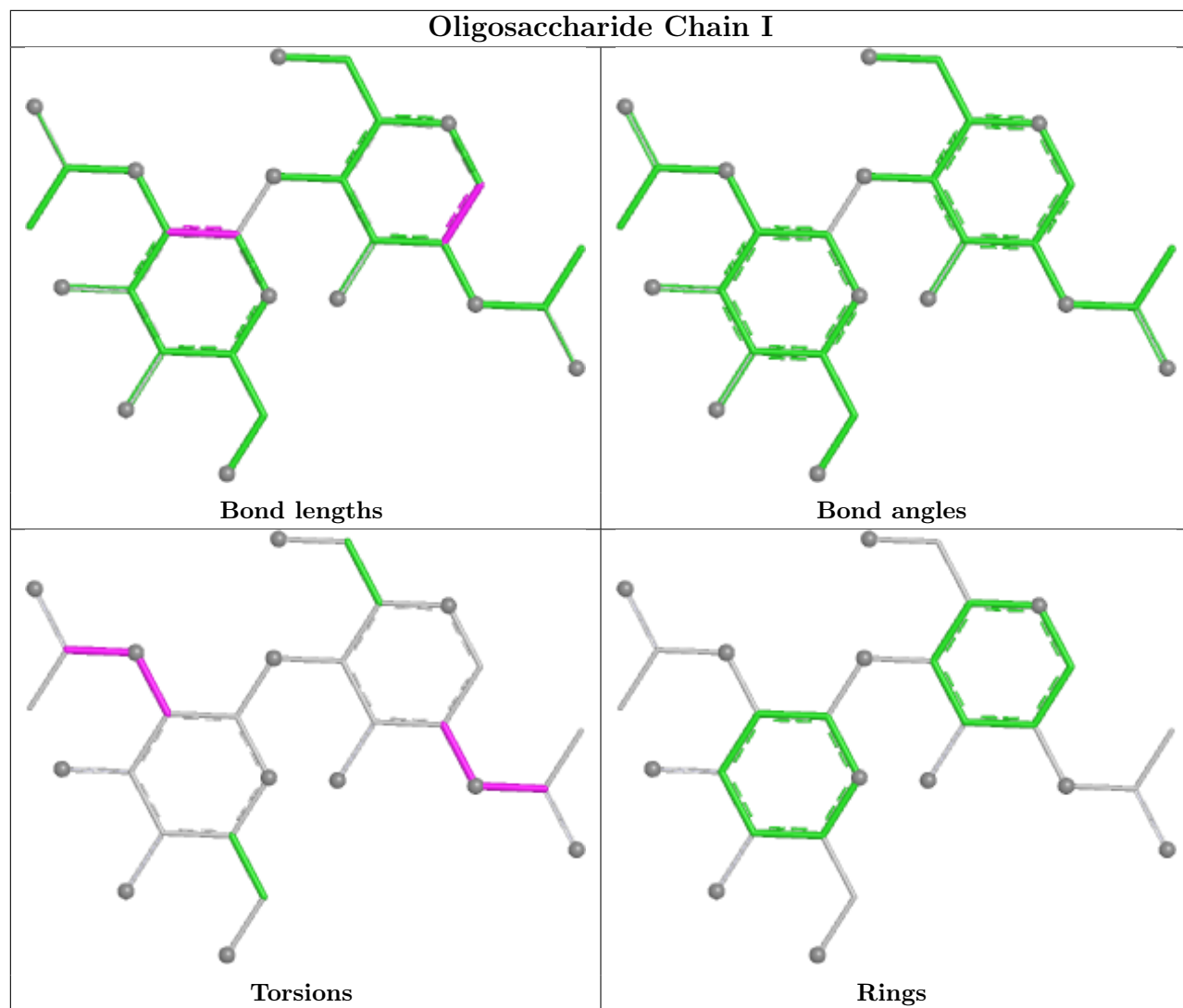
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C3-C2-N2-C7
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2

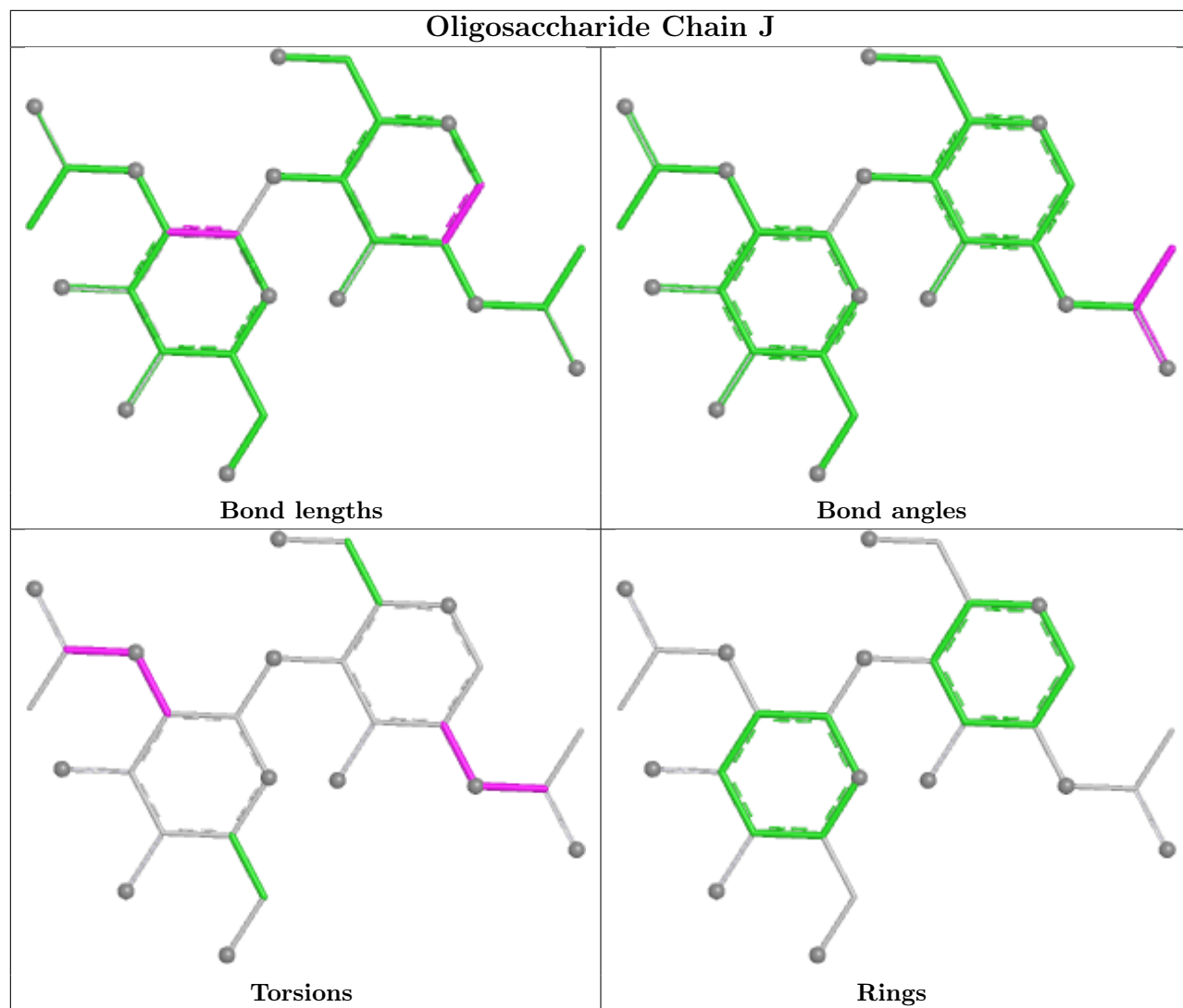
There are no ring outliers.

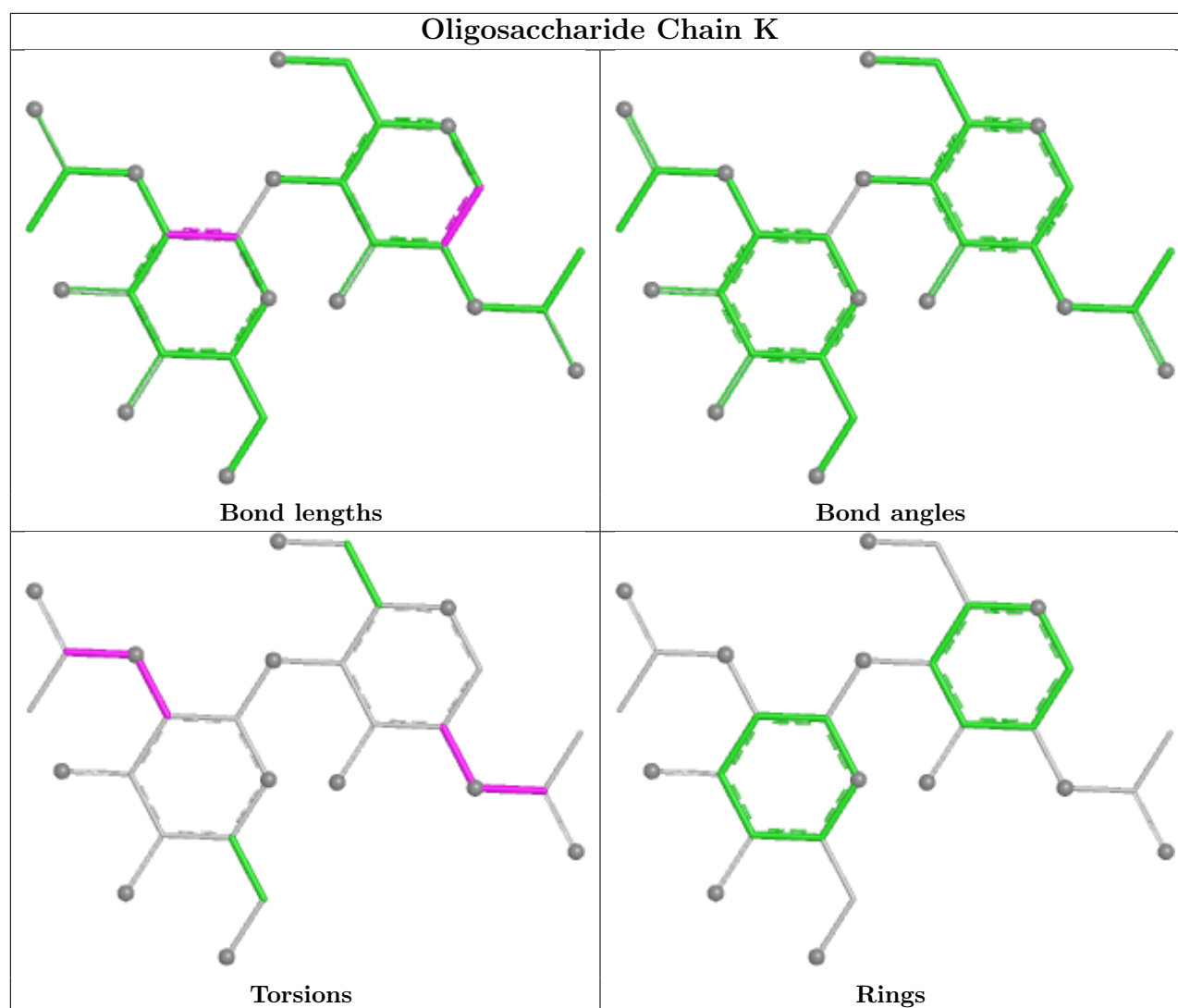
6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	7	0
3	K	1	NAG	7	0
3	I	2	NAG	4	0
3	K	2	NAG	4	0
3	J	1	NAG	7	0
3	J	2	NAG	4	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](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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	B	703	1	14,14,15	0.74	0	17,19,21	0.76	0
4	NAG	D	703	1	14,14,15	0.68	0	17,19,21	0.69	0
4	NAG	D	701	1	14,14,15	0.76	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	702	1	14,14,15	0.92	1 (7%)	17,19,21	0.89	1 (5%)
4	NAG	C	701	1	14,14,15	0.96	1 (7%)	17,19,21	0.61	0
4	NAG	D	702	1	14,14,15	0.80	1 (7%)	17,19,21	0.82	1 (5%)
4	NAG	C	702	1	14,14,15	0.90	1 (7%)	17,19,21	0.83	1 (5%)
4	NAG	A	702	1	14,14,15	1.07	1 (7%)	17,19,21	0.83	1 (5%)
4	NAG	A	701	1	14,14,15	1.04	1 (7%)	17,19,21	0.60	0
4	NAG	B	701	1	14,14,15	1.00	1 (7%)	17,19,21	0.60	0
4	NAG	A	703	1	14,14,15	0.81	0	17,19,21	0.75	0
4	NAG	C	703	1	14,14,15	0.79	0	17,19,21	0.76	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	B	703	1	-	5/6/23/26	0/1/1/1
4	NAG	D	703	1	-	3/6/23/26	0/1/1/1
4	NAG	D	701	1	-	5/6/23/26	0/1/1/1
4	NAG	B	702	1	-	4/6/23/26	0/1/1/1
4	NAG	C	701	1	-	4/6/23/26	0/1/1/1
4	NAG	D	702	1	-	4/6/23/26	0/1/1/1
4	NAG	C	702	1	-	4/6/23/26	0/1/1/1
4	NAG	A	702	1	-	4/6/23/26	0/1/1/1
4	NAG	A	701	1	-	4/6/23/26	0/1/1/1
4	NAG	B	701	1	-	4/6/23/26	0/1/1/1
4	NAG	A	703	1	-	5/6/23/26	0/1/1/1
4	NAG	C	703	1	-	5/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	NAG	C1-C2	3.09	1.56	1.52
4	B	701	NAG	C1-C2	2.94	1.56	1.52
4	C	701	NAG	C1-C2	2.87	1.56	1.52
4	A	702	NAG	C1-C2	2.46	1.55	1.52
4	C	702	NAG	C1-C2	2.33	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	702	NAG	C2-N2-C7	-2.35	119.75	122.90
4	C	702	NAG	C2-N2-C7	-2.34	119.77	122.90
4	D	702	NAG	C2-N2-C7	-2.18	119.98	122.90
4	A	702	NAG	C2-N2-C7	-2.17	119.99	122.90

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	NAG	C3-C2-N2-C7
4	A	701	NAG	C8-C7-N2-C2
4	A	701	NAG	O7-C7-N2-C2
4	A	702	NAG	C8-C7-N2-C2
4	A	702	NAG	O7-C7-N2-C2

There are no ring outliers.

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	703	NAG	1	0
4	D	701	NAG	1	0
4	B	702	NAG	1	0
4	C	701	NAG	1	0
4	D	702	NAG	1	0
4	C	702	NAG	1	0
4	A	702	NAG	1	0
4	A	701	NAG	1	0
4	B	701	NAG	1	0
4	A	703	NAG	1	0
4	C	703	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	533/574 (92%)	-0.19	2 (0%) 88 72	63, 100, 139, 162	0
1	B	533/574 (92%)	-0.17	5 (0%) 81 58	61, 96, 131, 178	0
1	C	533/574 (92%)	-0.03	5 (0%) 81 58	72, 115, 153, 180	0
1	D	533/574 (92%)	0.27	9 (1%) 69 43	75, 188, 282, 506	0
2	E	177/243 (72%)	-0.25	0 100 100	82, 120, 139, 154	0
2	F	177/243 (72%)	-0.27	0 100 100	77, 95, 110, 122	0
2	G	177/243 (72%)	-0.19	1 (0%) 85 65	78, 105, 130, 143	0
2	H	177/243 (72%)	0.06	1 (0%) 85 65	146, 268, 426, 538	0
All	All	2840/3268 (86%)	-0.06	23 (0%) 82 60	61, 112, 262, 538	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	451	VAL	4.7
1	C	451	VAL	3.9
1	D	129	VAL	3.7
1	A	451	VAL	3.5
2	H	263	TYR	3.1

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

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

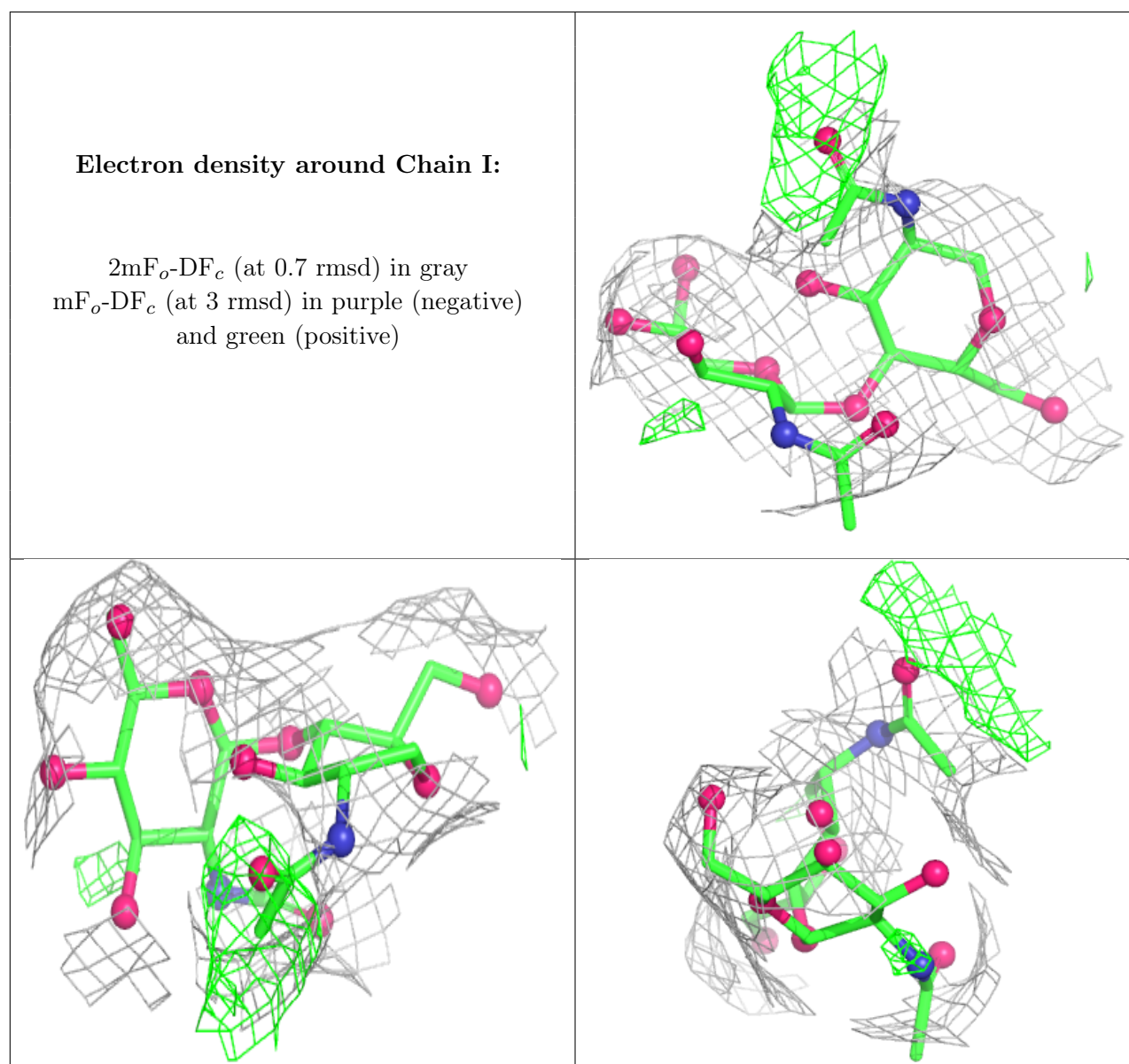
6.3 Carbohydrates [i](#)

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.

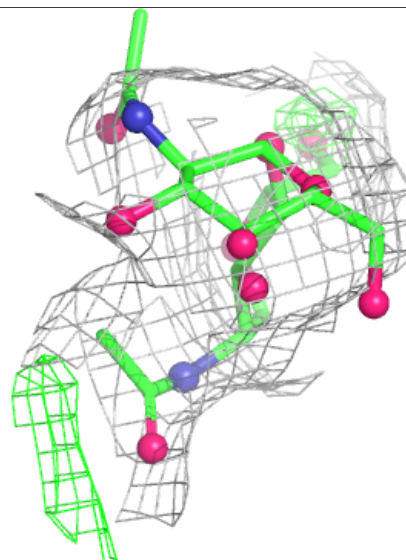
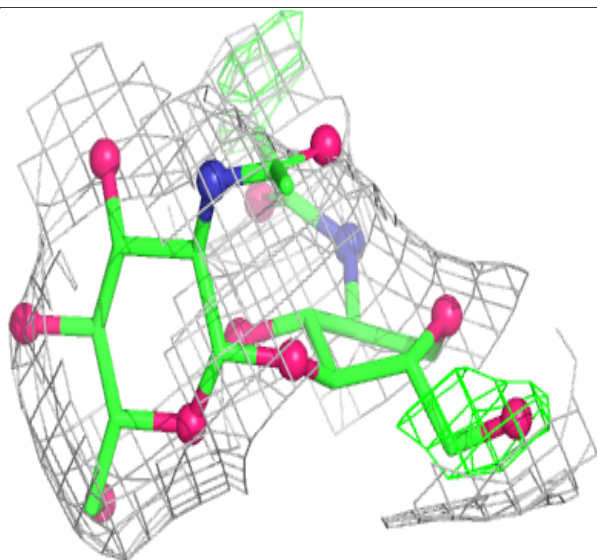
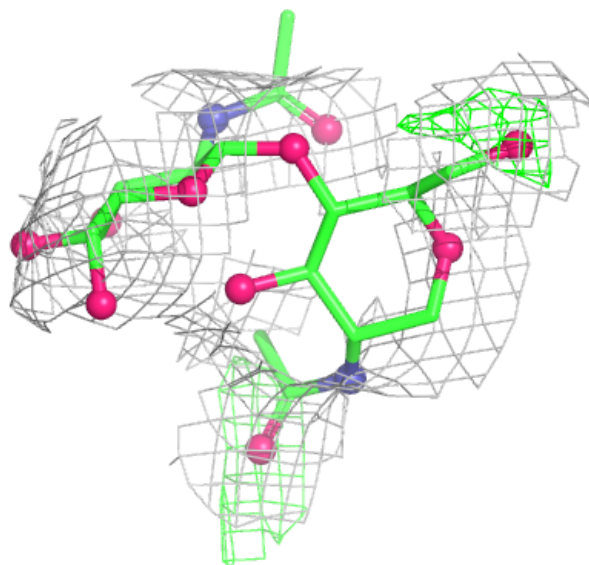
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	K	1	14/15	0.48	0.15	127,133,136,142	0
3	NAG	J	1	14/15	0.50	0.15	122,130,133,141	0
3	NAG	J	2	14/15	0.51	0.12	172,174,177,178	0
3	NAG	I	1	14/15	0.52	0.12	146,152,154,157	0
3	NAG	K	2	14/15	0.57	0.12	154,158,159,159	0
3	NAG	I	2	14/15	0.69	0.11	146,150,151,152	0

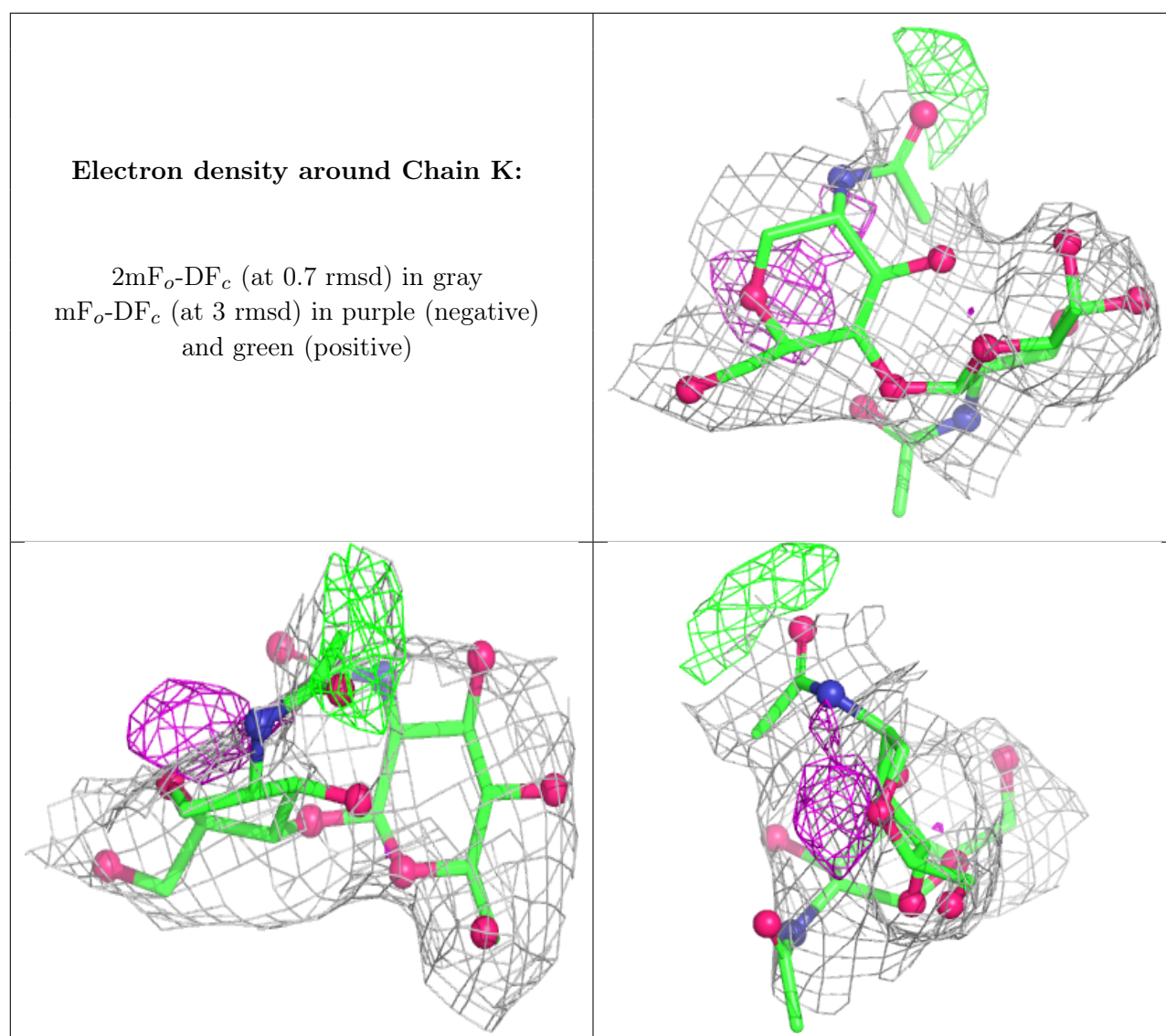
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain 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(Å ²)	Q<0.9
4	NAG	B	703	14/15	-0.32	0.17	236,240,241,242	0
4	NAG	D	701	14/15	-0.03	0.13	219,219,219,219	0
4	NAG	C	703	14/15	0.03	0.15	218,222,222,222	0
4	NAG	D	703	14/15	0.06	0.11	251,251,251,251	0
4	NAG	A	703	14/15	0.11	0.11	218,222,225,225	0
4	NAG	A	701	14/15	0.18	0.12	152,155,156,157	0
4	NAG	C	701	14/15	0.32	0.12	216,218,219,219	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	702	14/15	0.42	0.12	136,138,139,140	0
4	NAG	D	702	14/15	0.51	0.12	205,205,205,205	0
4	NAG	C	702	14/15	0.52	0.10	186,187,189,189	0
4	NAG	B	701	14/15	0.57	0.16	184,187,191,192	0
4	NAG	A	702	14/15	0.70	0.10	145,147,148,148	0
5	CA	F	402	1/1	0.87	0.08	96,96,96,96	0
5	CA	G	402	1/1	0.89	0.08	111,111,111,111	0
5	CA	G	401	1/1	0.93	0.05	79,79,79,79	0
5	CA	E	402	1/1	0.94	0.12	96,96,96,96	0
5	CA	F	401	1/1	0.97	0.07	76,76,76,76	0
5	CA	E	401	1/1	0.97	0.04	89,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.