



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 09:56 AM BST

PDB ID : 6N4Y
Title : Metabotropic Glutamate Receptor 5 Extracellular Domain with Nb43
Authors : Koehl, A.; Hu, H.; Feng, D.; Sun, B.; Chu, M.; Weis, W.I.; Mathiesen, J.M.;
Skiniotis, G.; Kobilka, B.K.
Deposited on : 2018-11-20
Resolution : 3.26 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 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 : 2.13.1
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) : 2.13.1

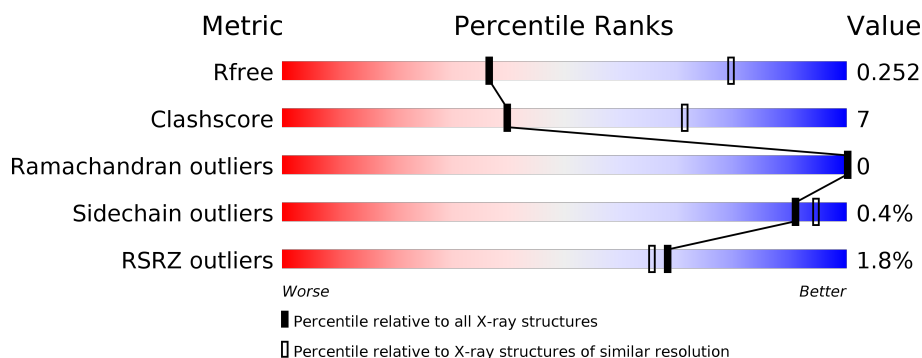
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 on 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	596	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 69%, yellow 69%, yellow 84%, grey 84%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 69% 15% 15% </div> </div>
1	B	596	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 69%, yellow 69%, yellow 87%, grey 87%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 69% 18% 13% </div> </div>
1	C	596	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 68%, yellow 68%, yellow 80%, grey 80%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 68% 12% 19% </div> </div>
1	D	596	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 0%, green 71%, yellow 71%, yellow 85%, grey 85%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 71% 14% 14% </div> </div>
2	E	123	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 87%, yellow 87%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 87% 13% </div> </div>
2	F	123	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 86%, yellow 86%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 86% 14% </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	123	
2	H	123	
3	I	3	
4	J	7	
5	K	5	
6	L	6	

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	FUC	I	3	-	-	-	X
4	MAN	J	4	-	-	-	X
4	MAN	J	5	-	-	-	X
7	NAG	A	601	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19626 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 Metabotropic glutamate receptor 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			3937	2485	671	745	36			
1	B	517	Total	C	N	O	S	0	0	0
			4018	2537	689	754	38			
1	C	480	Total	C	N	O	S	0	0	0
			3737	2363	638	702	34			
1	D	511	Total	C	N	O	S	0	0	0
			3947	2490	671	748	38			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP P41594
A	-15	LEU	-	expression tag	UNP P41594
A	-14	LEU	-	expression tag	UNP P41594
A	-13	VAL	-	expression tag	UNP P41594
A	-12	ASN	-	expression tag	UNP P41594
A	-11	GLN	-	expression tag	UNP P41594
A	-10	SER	-	expression tag	UNP P41594
A	-9	HIS	-	expression tag	UNP P41594
A	-8	GLN	-	expression tag	UNP P41594
A	-7	GLY	-	expression tag	UNP P41594
A	-6	PHE	-	expression tag	UNP P41594
A	-5	ASN	-	expression tag	UNP P41594
A	-4	LYS	-	expression tag	UNP P41594
A	-3	GLU	-	expression tag	UNP P41594
A	-2	HIS	-	expression tag	UNP P41594
A	-1	THR	-	expression tag	UNP P41594
A	0	SER	-	expression tag	UNP P41594
A	1	LYS	-	expression tag	UNP P41594
A	2	MET	-	expression tag	UNP P41594
A	3	VAL	-	expression tag	UNP P41594
A	4	SER	-	expression tag	UNP P41594

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	-	expression tag	UNP P41594
A	6	ILE	-	expression tag	UNP P41594
A	7	VAL	-	expression tag	UNP P41594
A	8	LEU	-	expression tag	UNP P41594
A	9	TYR	-	expression tag	UNP P41594
A	10	VAL	-	expression tag	UNP P41594
A	11	LEU	-	expression tag	UNP P41594
A	12	LEU	-	expression tag	UNP P41594
A	13	ALA	-	expression tag	UNP P41594
A	14	ALA	-	expression tag	UNP P41594
A	15	ALA	-	expression tag	UNP P41594
A	16	ALA	-	expression tag	UNP P41594
A	17	HIS	-	expression tag	UNP P41594
A	18	SER	-	expression tag	UNP P41594
A	19	ALA	-	expression tag	UNP P41594
A	20	PHE	-	expression tag	UNP P41594
A	572	HIS	-	expression tag	UNP P41594
A	573	HIS	-	expression tag	UNP P41594
A	574	HIS	-	expression tag	UNP P41594
A	575	HIS	-	expression tag	UNP P41594
A	576	HIS	-	expression tag	UNP P41594
A	577	HIS	-	expression tag	UNP P41594
A	578	HIS	-	expression tag	UNP P41594
A	579	HIS	-	expression tag	UNP P41594
B	-16	MET	-	initiating methionine	UNP P41594
B	-15	LEU	-	expression tag	UNP P41594
B	-14	LEU	-	expression tag	UNP P41594
B	-13	VAL	-	expression tag	UNP P41594
B	-12	ASN	-	expression tag	UNP P41594
B	-11	GLN	-	expression tag	UNP P41594
B	-10	SER	-	expression tag	UNP P41594
B	-9	HIS	-	expression tag	UNP P41594
B	-8	GLN	-	expression tag	UNP P41594
B	-7	GLY	-	expression tag	UNP P41594
B	-6	PHE	-	expression tag	UNP P41594
B	-5	ASN	-	expression tag	UNP P41594
B	-4	LYS	-	expression tag	UNP P41594
B	-3	GLU	-	expression tag	UNP P41594
B	-2	HIS	-	expression tag	UNP P41594
B	-1	THR	-	expression tag	UNP P41594
B	0	SER	-	expression tag	UNP P41594
B	1	LYS	-	expression tag	UNP P41594

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	expression tag	UNP P41594
B	3	VAL	-	expression tag	UNP P41594
B	4	SER	-	expression tag	UNP P41594
B	5	ALA	-	expression tag	UNP P41594
B	6	ILE	-	expression tag	UNP P41594
B	7	VAL	-	expression tag	UNP P41594
B	8	LEU	-	expression tag	UNP P41594
B	9	TYR	-	expression tag	UNP P41594
B	10	VAL	-	expression tag	UNP P41594
B	11	LEU	-	expression tag	UNP P41594
B	12	LEU	-	expression tag	UNP P41594
B	13	ALA	-	expression tag	UNP P41594
B	14	ALA	-	expression tag	UNP P41594
B	15	ALA	-	expression tag	UNP P41594
B	16	ALA	-	expression tag	UNP P41594
B	17	HIS	-	expression tag	UNP P41594
B	18	SER	-	expression tag	UNP P41594
B	19	ALA	-	expression tag	UNP P41594
B	20	PHE	-	expression tag	UNP P41594
B	572	HIS	-	expression tag	UNP P41594
B	573	HIS	-	expression tag	UNP P41594
B	574	HIS	-	expression tag	UNP P41594
B	575	HIS	-	expression tag	UNP P41594
B	576	HIS	-	expression tag	UNP P41594
B	577	HIS	-	expression tag	UNP P41594
B	578	HIS	-	expression tag	UNP P41594
B	579	HIS	-	expression tag	UNP P41594
C	-16	MET	-	initiating methionine	UNP P41594
C	-15	LEU	-	expression tag	UNP P41594
C	-14	LEU	-	expression tag	UNP P41594
C	-13	VAL	-	expression tag	UNP P41594
C	-12	ASN	-	expression tag	UNP P41594
C	-11	GLN	-	expression tag	UNP P41594
C	-10	SER	-	expression tag	UNP P41594
C	-9	HIS	-	expression tag	UNP P41594
C	-8	GLN	-	expression tag	UNP P41594
C	-7	GLY	-	expression tag	UNP P41594
C	-6	PHE	-	expression tag	UNP P41594
C	-5	ASN	-	expression tag	UNP P41594
C	-4	LYS	-	expression tag	UNP P41594
C	-3	GLU	-	expression tag	UNP P41594
C	-2	HIS	-	expression tag	UNP P41594

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	THR	-	expression tag	UNP P41594
C	0	SER	-	expression tag	UNP P41594
C	1	LYS	-	expression tag	UNP P41594
C	2	MET	-	expression tag	UNP P41594
C	3	VAL	-	expression tag	UNP P41594
C	4	SER	-	expression tag	UNP P41594
C	5	ALA	-	expression tag	UNP P41594
C	6	ILE	-	expression tag	UNP P41594
C	7	VAL	-	expression tag	UNP P41594
C	8	LEU	-	expression tag	UNP P41594
C	9	TYR	-	expression tag	UNP P41594
C	10	VAL	-	expression tag	UNP P41594
C	11	LEU	-	expression tag	UNP P41594
C	12	LEU	-	expression tag	UNP P41594
C	13	ALA	-	expression tag	UNP P41594
C	14	ALA	-	expression tag	UNP P41594
C	15	ALA	-	expression tag	UNP P41594
C	16	ALA	-	expression tag	UNP P41594
C	17	HIS	-	expression tag	UNP P41594
C	18	SER	-	expression tag	UNP P41594
C	19	ALA	-	expression tag	UNP P41594
C	20	PHE	-	expression tag	UNP P41594
C	572	HIS	-	expression tag	UNP P41594
C	573	HIS	-	expression tag	UNP P41594
C	574	HIS	-	expression tag	UNP P41594
C	575	HIS	-	expression tag	UNP P41594
C	576	HIS	-	expression tag	UNP P41594
C	577	HIS	-	expression tag	UNP P41594
C	578	HIS	-	expression tag	UNP P41594
C	579	HIS	-	expression tag	UNP P41594
D	-16	MET	-	initiating methionine	UNP P41594
D	-15	LEU	-	expression tag	UNP P41594
D	-14	LEU	-	expression tag	UNP P41594
D	-13	VAL	-	expression tag	UNP P41594
D	-12	ASN	-	expression tag	UNP P41594
D	-11	GLN	-	expression tag	UNP P41594
D	-10	SER	-	expression tag	UNP P41594
D	-9	HIS	-	expression tag	UNP P41594
D	-8	GLN	-	expression tag	UNP P41594
D	-7	GLY	-	expression tag	UNP P41594
D	-6	PHE	-	expression tag	UNP P41594
D	-5	ASN	-	expression tag	UNP P41594

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	LYS	-	expression tag	UNP P41594
D	-3	GLU	-	expression tag	UNP P41594
D	-2	HIS	-	expression tag	UNP P41594
D	-1	THR	-	expression tag	UNP P41594
D	0	SER	-	expression tag	UNP P41594
D	1	LYS	-	expression tag	UNP P41594
D	2	MET	-	expression tag	UNP P41594
D	3	VAL	-	expression tag	UNP P41594
D	4	SER	-	expression tag	UNP P41594
D	5	ALA	-	expression tag	UNP P41594
D	6	ILE	-	expression tag	UNP P41594
D	7	VAL	-	expression tag	UNP P41594
D	8	LEU	-	expression tag	UNP P41594
D	9	TYR	-	expression tag	UNP P41594
D	10	VAL	-	expression tag	UNP P41594
D	11	LEU	-	expression tag	UNP P41594
D	12	LEU	-	expression tag	UNP P41594
D	13	ALA	-	expression tag	UNP P41594
D	14	ALA	-	expression tag	UNP P41594
D	15	ALA	-	expression tag	UNP P41594
D	16	ALA	-	expression tag	UNP P41594
D	17	HIS	-	expression tag	UNP P41594
D	18	SER	-	expression tag	UNP P41594
D	19	ALA	-	expression tag	UNP P41594
D	20	PHE	-	expression tag	UNP P41594
D	572	HIS	-	expression tag	UNP P41594
D	573	HIS	-	expression tag	UNP P41594
D	574	HIS	-	expression tag	UNP P41594
D	575	HIS	-	expression tag	UNP P41594
D	576	HIS	-	expression tag	UNP P41594
D	577	HIS	-	expression tag	UNP P41594
D	578	HIS	-	expression tag	UNP P41594
D	579	HIS	-	expression tag	UNP P41594

- Molecule 2 is a protein called Nanobody 43.

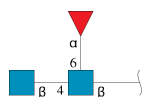
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	123	Total	C	N	O	S	0	0	0
			933	580	161	187	5			
2	F	123	Total	C	N	O	S	0	0	0
			927	577	158	187	5			
2	G	123	Total	C	N	O	S	0	0	0
			929	577	160	187	5			

Continued on next page...

Continued from previous page...

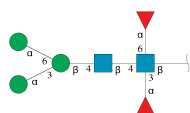
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	119	Total	C	N	O	S	0	0	0
			893	558	152	178	5			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



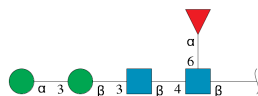
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	3	Total	C	N	O		0	0	0
			38	22	2	14				

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	7	Total	C	N	O		0	0	0
			81	46	2	33				

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

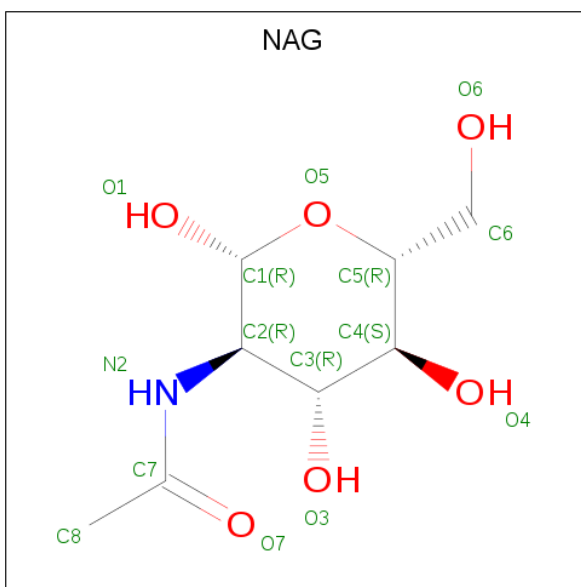


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	5	Total	C	N	O		0	0	0
			60	34	2	24				

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

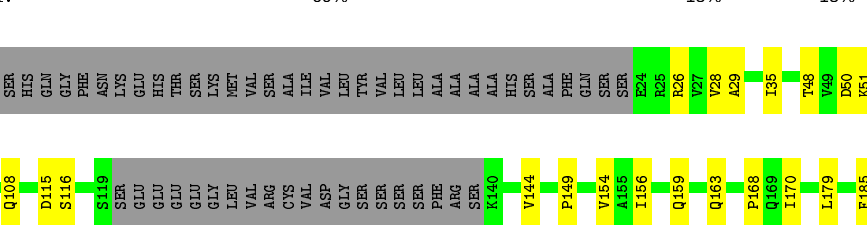
A 4x4 grid with a 180-degree rotation. The grid contains green circles, blue squares, and red triangles. The rotation is indicated by a curved arrow labeled '180°'.

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



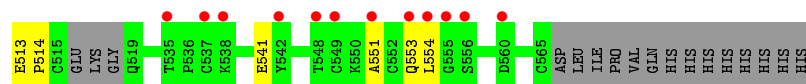
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 14	C 8	N 1	O 5	0	0
7	B	1	Total 14	C 8	N 1	O 5	0	0
7	C	1	Total 14	C 8	N 1	O 5	0	0
7	D	1	Total 14	C 8	N 1	O 5	0	0

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.

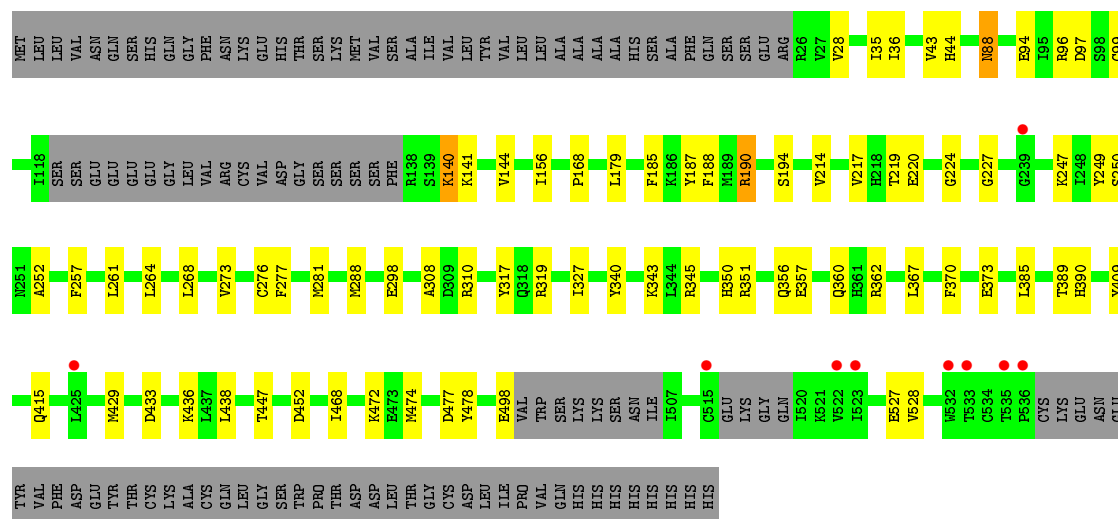
- Chain A: 

- Chain B:

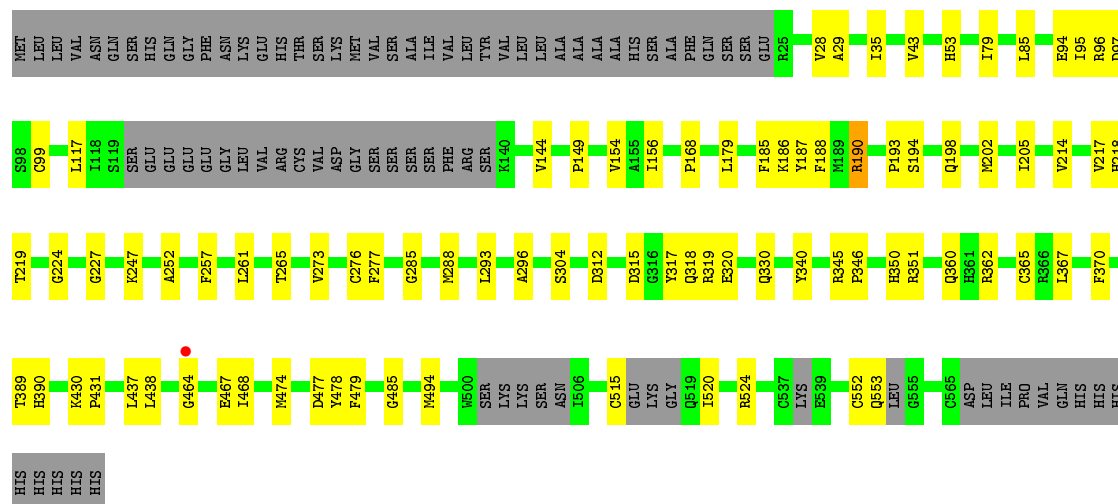
Item	Category
Q329	Green
Q330	Green
S331	Green
V334	Green
F337	Green
R345	Green
E337	Green
F358	Green
Q359	Green
Q360	Green
R366	Green
L367	Green
F370	Green
E373	Green
K379	Green
L385	Green
Q393	Green
K396	Green
F399	Green
V400	Green
I401	Green
N413	Green
L437	Green
L438	Green
E439	Green
S440	Green
T444	Green
V464	Green
M464	Green
W500	Green
S501	Green
K502	Green
L515	Green
S504	Green
N505	Green
I506	Green
S509	Green
R86	Green
D87	Green
S98	Green
C99	Green
E111	Green
Y213	Green
H218	Green
T219	Green
E220	Green
G224	Green
G227	Green
M228	Green
K232	Green
S235	Green
I240	Green
K247	Green
L261	Green
T265	Green
L268	Green
R272	Green
V273	Green
V274	Green
F277	Green
V283	Green
L293	Green
G294	Green
L295	Green
A296	Green
L301	Green
S304	Green
W307	Green
R310	Green
Y311	Green
D312	Green
D315	Green
Q318	Green
R319	Green
E320	Green
R114	Green
I118	Green
SER	Green
SER	Green
GLU	Green
GLU	Green
GLU	Green
GLU	Green
GLY	Green
LEU	Green
VAL	Green
ARG	Green
CYS	Green
VAL	Green
ASP	Green
GLY	Green
SER	Green
SER	Green
SER	Green
SER	Green
PHE	Green
ARG	Green
SER	Green
K141	Green
V144	Green
P149	Green
V154	Green
A155	Green
I156	Green
Q163	Green
P168	Green
Q169	Green
I170	Green
L179	Green
L184	Green
F185	Green
K186	Green
Y187	Green
F188	Green
M189	Green
R190	Green
Q198	Green
VAL	Yellow
LEU	Yellow
VAL	Yellow
ASN	Yellow
GLN	Yellow
SER	Yellow
GLN	Yellow
PHE	Yellow
ASN	Yellow
LYS	Yellow
GLU	Yellow
HIS	Yellow
THR	Yellow
SER	Yellow
LYS	Yellow
MET	Yellow
VAL	Yellow
SER	Yellow
SER	Yellow
ILE	Yellow
VAL	Yellow
LEU	Yellow
TVR	Yellow
VAL	Yellow
LEU	Yellow
ALA	Yellow
ALA	Yellow
ALA	Yellow
HIS	Yellow
SER	Yellow
ALA	Yellow
PHE	Yellow
GLN	Yellow
SER	Yellow
SER	Yellow
P24	Yellow
R25	Yellow
A29	Yellow
I35	Yellow
I36	Yellow
V43	Yellow
H44	Yellow
V49	Yellow
D50	Yellow
K51	Yellow
V52	Yellow
H53	Yellow
I66	Yellow
T65	Yellow



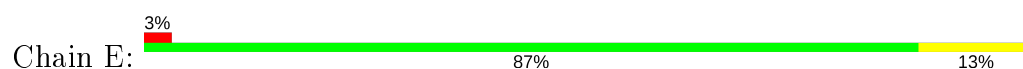
• Molecule 1: Metabotropic glutamate receptor 5



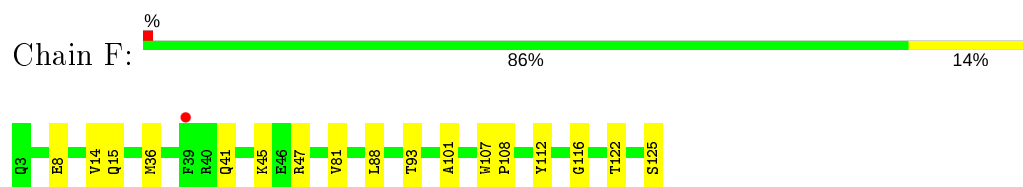
• Molecule 1: Metabotropic glutamate receptor 5



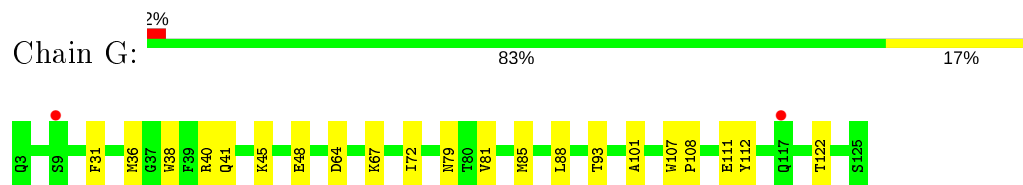
• Molecule 2: Nanobody 43



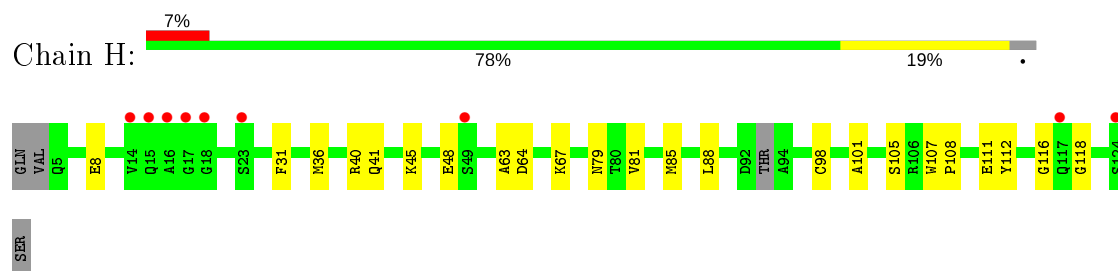
- Molecule 2: Nanobody 43



- Molecule 2: Nanobody 43



- Molecule 2: Nanobody 43



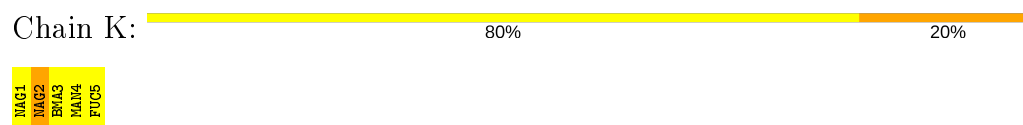
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



MAN1	MAN2	MAN3	MAN4	FUC5	FUC6
------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.53Å 158.39Å 111.96Å 90.00° 101.93° 90.00°	Depositor
Resolution (Å)	38.87 – 3.26 39.60 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.87-3.26) 91.7 (39.60-3.26)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.199 , 0.251 0.200 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19626	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.41% 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: FUC, BMA, NAG, MAN

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	0.26	0/4023	0.48	0/5446
1	B	0.30	0/4107	0.50	0/5560
1	C	0.25	0/3819	0.48	0/5164
1	D	0.26	0/4032	0.48	0/5457
2	E	0.27	0/955	0.50	0/1293
2	F	0.27	0/949	0.48	0/1286
2	G	0.26	0/951	0.50	0/1289
2	H	0.25	0/914	0.51	0/1238
All	All	0.27	0/19750	0.49	0/26733

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	3937	0	3736	56	0
1	B	4018	0	3834	73	0
1	C	3737	0	3585	53	0
1	D	3947	0	3733	54	0
2	E	933	0	869	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	927	0	858	10	0
2	G	929	0	858	14	0
2	H	893	0	822	15	0
3	I	38	0	34	0	0
4	J	81	0	70	2	0
5	K	60	0	52	1	0
6	L	70	0	61	0	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
All	All	19626	0	18564	277	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 7.

The worst 5 of 277 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)
1:D:345:ARG:HD3	1:D:346:PRO:HD2	1.58	0.84
1:C:472:LYS:HD2	1:C:498:GLU:HG3	1.69	0.74
1:C:268:LEU:HD11	1:C:298:GLU:HB3	1.71	0.72
1:D:515:CYS:HB3	1:D:520:ILE:HB	1.70	0.72
1:C:527:GLU:HG2	1:C:528:VAL:HG23	1.71	0.72

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	497/596 (83%)	469 (94%)	28 (6%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	509/596 (85%)	482 (95%)	27 (5%)	0	100	100
1	C	472/596 (79%)	449 (95%)	23 (5%)	0	100	100
1	D	499/596 (84%)	476 (95%)	23 (5%)	0	100	100
2	E	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
2	F	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
2	G	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
2	H	115/123 (94%)	113 (98%)	2 (2%)	0	100	100
All	All	2455/2876 (85%)	2340 (95%)	115 (5%)	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 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	422/520 (81%)	421 (100%)	1 (0%)	93	96
1	B	432/520 (83%)	430 (100%)	2 (0%)	88	93
1	C	402/520 (77%)	399 (99%)	3 (1%)	84	90
1	D	422/520 (81%)	420 (100%)	2 (0%)	88	93
2	E	96/97 (99%)	96 (100%)	0	100	100
2	F	95/97 (98%)	95 (100%)	0	100	100
2	G	95/97 (98%)	95 (100%)	0	100	100
2	H	90/97 (93%)	90 (100%)	0	100	100
All	All	2054/2468 (83%)	2046 (100%)	8 (0%)	91	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	88	ASN
1	D	524	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	190	ARG
1	B	506	ILE
1	C	140	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	413	ASN
1	C	108	GLN
1	D	74	HIS
1	B	350	HIS
1	C	166	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 ⓘ

21 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	1,3	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
3	NAG	I	2	3	14,14,15	0.40	0	17,19,21	0.60	0
3	FUC	I	3	3	10,10,11	1.10	0	14,14,16	1.20	1 (7%)
4	NAG	J	1	1,4	14,14,15	1.06	1 (7%)	17,19,21	0.75	0
4	NAG	J	2	4	14,14,15	0.64	1 (7%)	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	J	3	4	11,11,12	1.22	2 (18%)	15,15,17	1.31	2 (13%)
4	MAN	J	4	4	11,11,12	0.74	0	15,15,17	0.99	2 (13%)
4	MAN	J	5	4	11,11,12	0.61	0	15,15,17	1.06	2 (13%)
4	FUC	J	6	4	10,10,11	1.46	2 (20%)	14,14,16	1.34	3 (21%)
4	FUC	J	7	4	10,10,11	0.77	0	14,14,16	0.88	0
5	NAG	K	1	1,5	14,14,15	0.33	0	17,19,21	0.81	1 (5%)
5	NAG	K	2	5	14,14,15	0.65	1 (7%)	17,19,21	0.64	0
5	BMA	K	3	5	11,11,12	0.69	0	15,15,17	0.98	1 (6%)
5	MAN	K	4	5	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
5	FUC	K	5	5	10,10,11	0.69	0	14,14,16	0.80	0
6	NAG	L	1	1,6	14,14,15	0.30	0	17,19,21	0.59	0
6	NAG	L	2	6	14,14,15	0.27	0	17,19,21	0.50	0
6	BMA	L	3	6	11,11,12	0.70	0	15,15,17	0.81	0
6	MAN	L	4	6	11,11,12	0.75	0	15,15,17	1.17	2 (13%)
6	FUC	L	5	6	10,10,11	0.69	0	14,14,16	0.96	1 (7%)
6	FUC	L	6	6	10,10,11	0.90	1 (10%)	14,14,16	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
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	FUC	I	3	3	-	-	0/1/1/1
4	NAG	J	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
4	FUC	J	6	4	-	-	0/1/1/1
4	FUC	J	7	4	-	-	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
5	FUC	K	5	5	-	-	0/1/1/1
6	NAG	L	1	1,6	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1
6	MAN	L	4	6	-	0/2/19/22	0/1/1/1
6	FUC	L	5	6	-	-	0/1/1/1
6	FUC	L	6	6	-	-	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	NAG	O5-C1	-3.70	1.37	1.43
4	J	6	FUC	C1-C2	2.87	1.58	1.52
4	J	3	BMA	O3-C3	2.65	1.49	1.43
5	K	2	NAG	O5-C1	-2.24	1.40	1.43
4	J	2	NAG	O5-C1	-2.20	1.40	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	NAG	C1-O5-C5	3.43	116.84	112.19
4	J	3	BMA	O3-C3-C2	3.39	116.49	109.99
4	J	5	MAN	C1-O5-C5	3.02	116.28	112.19
6	L	4	MAN	C1-O5-C5	2.97	116.21	112.19
5	K	4	MAN	C1-O5-C5	2.74	115.91	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

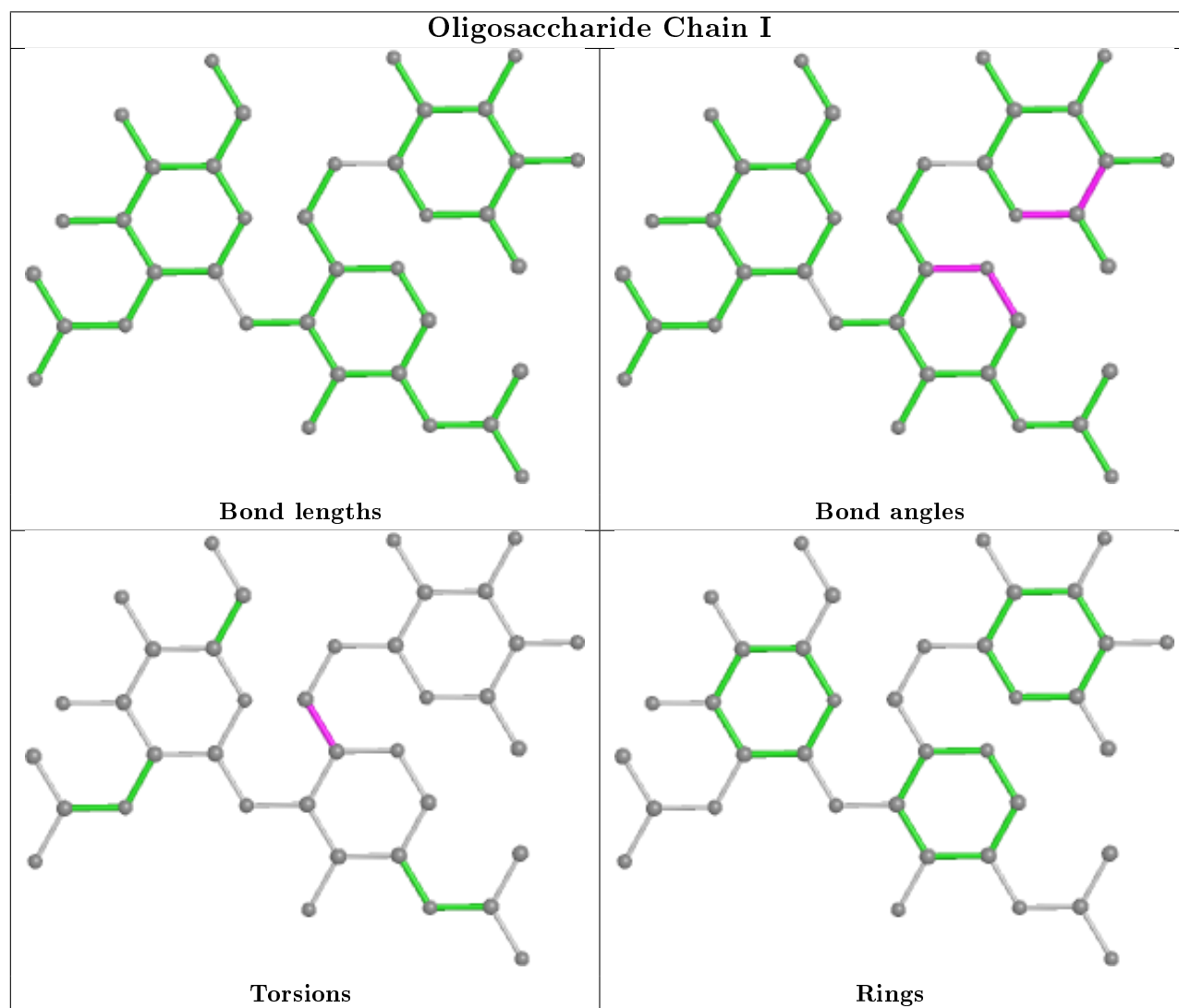
Mol	Chain	Res	Type	Atoms
4	J	3	BMA	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6

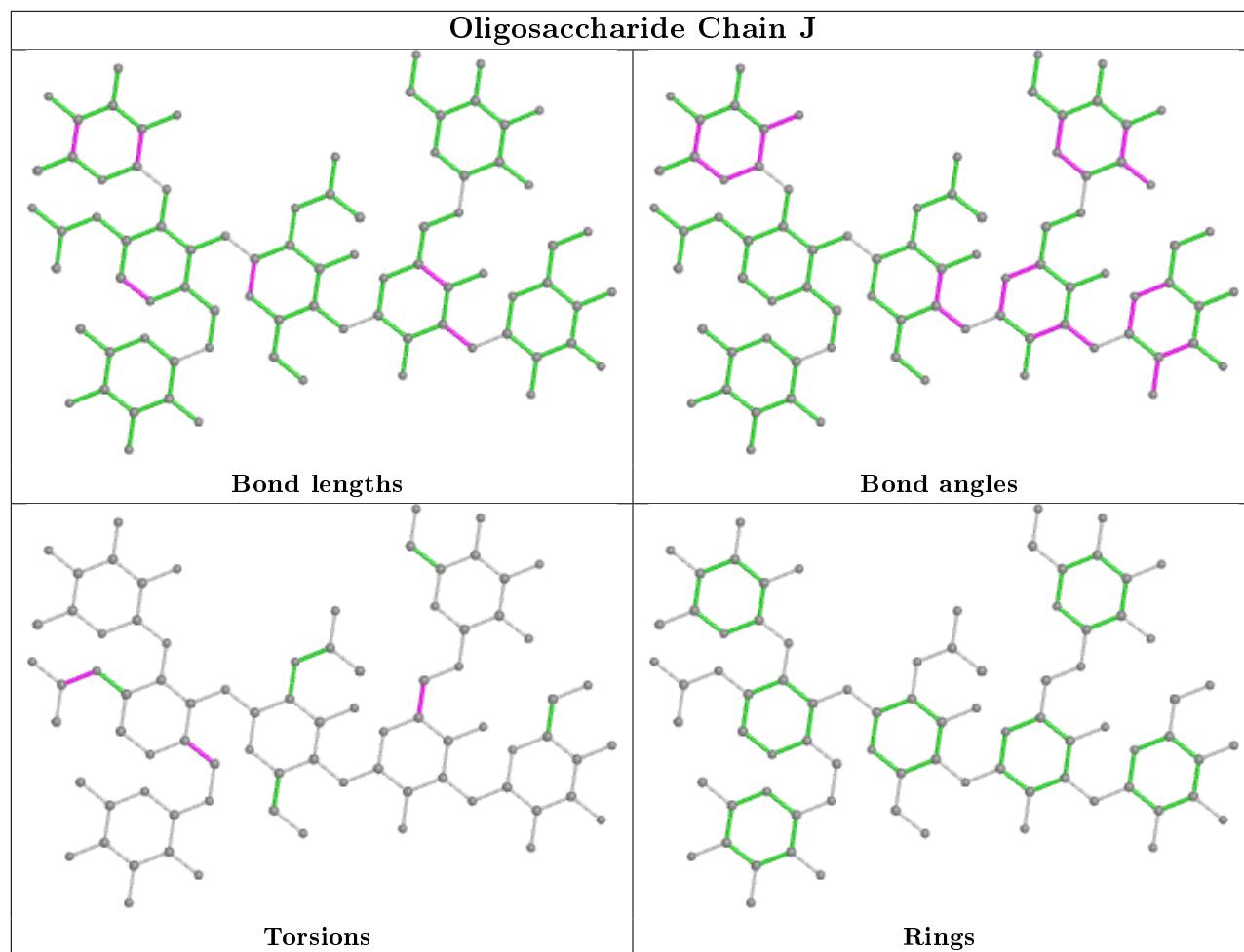
There are no ring outliers.

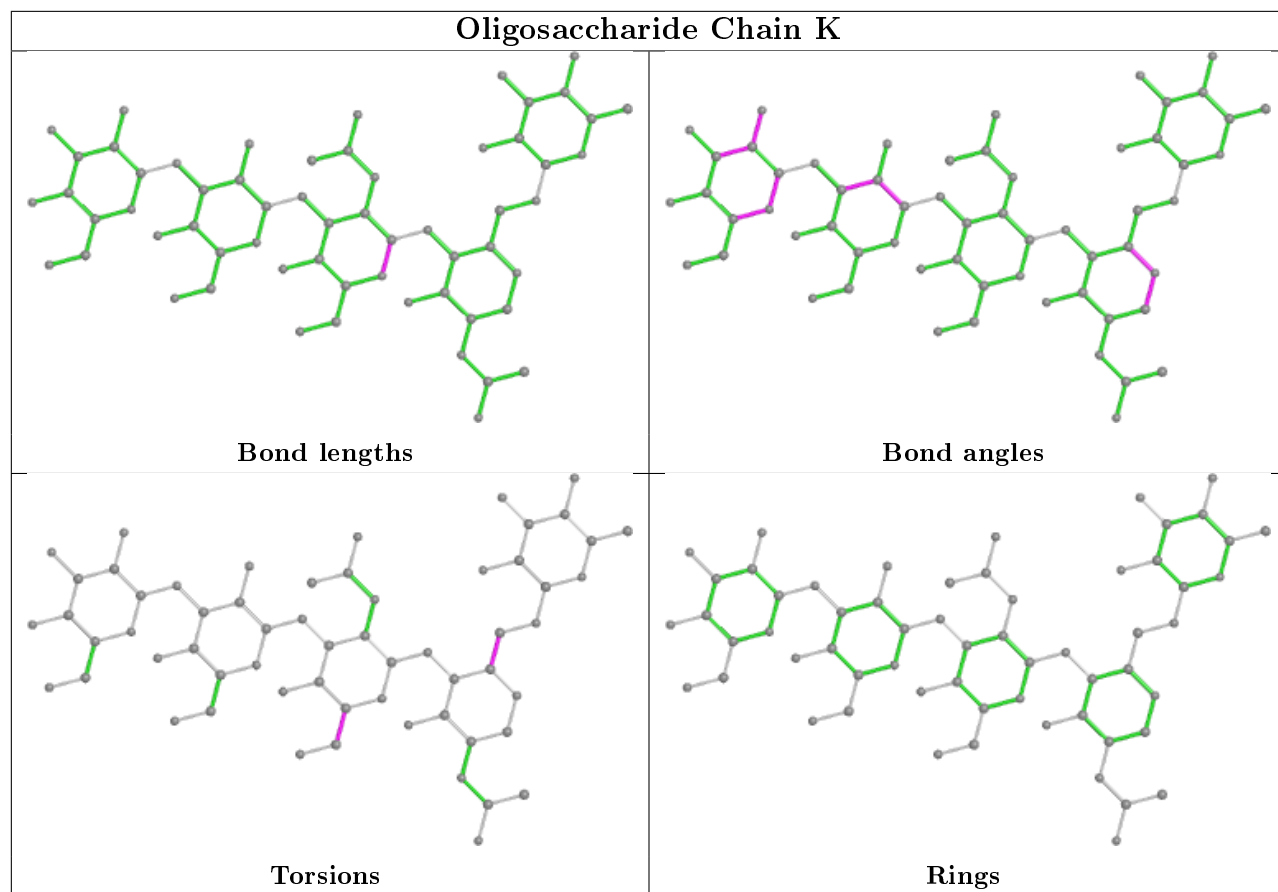
3 monomers are involved in 3 short contacts:

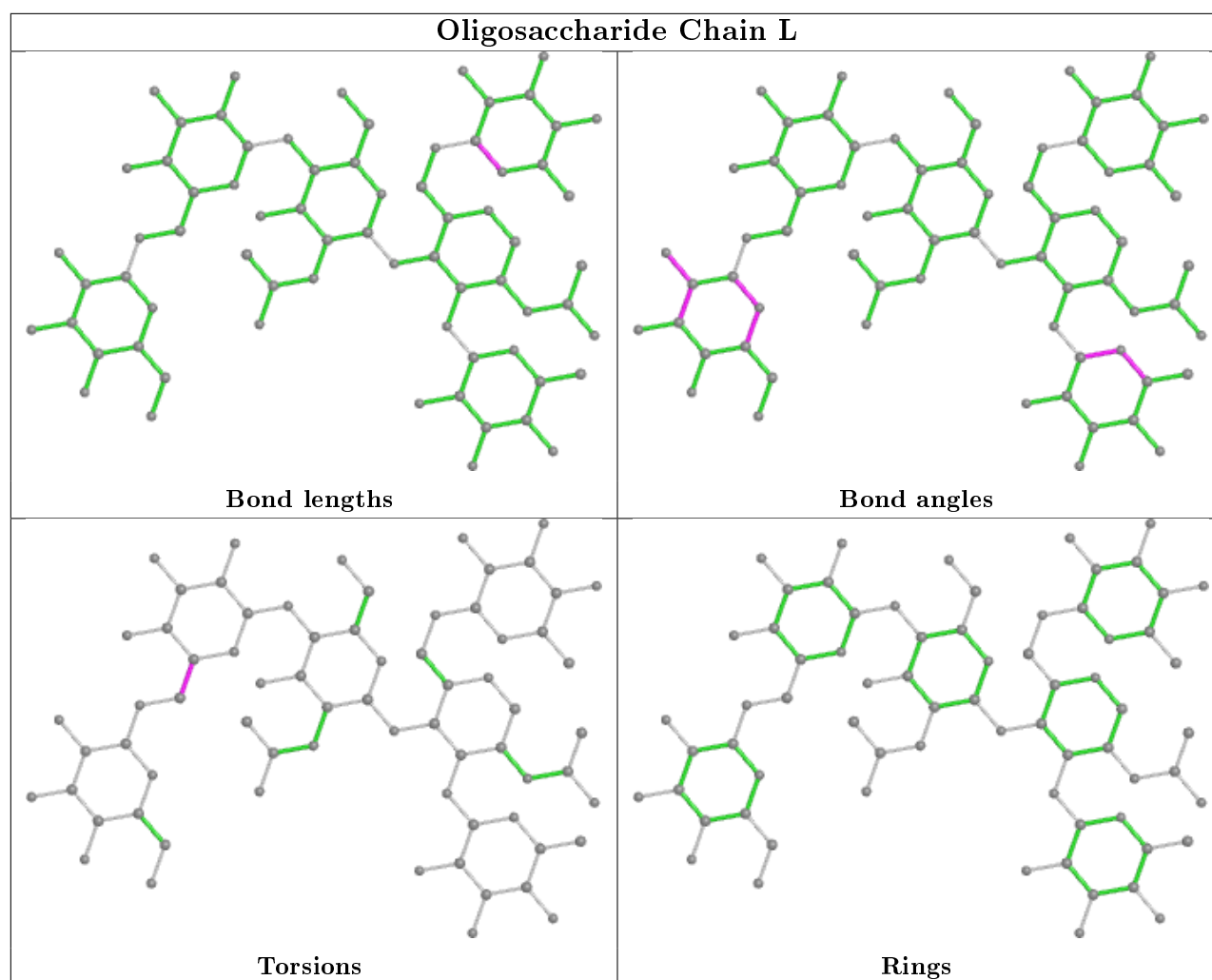
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	2	NAG	1	0
4	J	3	BMA	2	0
5	K	5	FUC	1	0

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](#)

4 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	B	608	1	14,14,15	0.51	0	17,19,21	0.59	1 (5%)
7	NAG	D	607	1	14,14,15	0.50	0	17,19,21	0.52	0
7	NAG	C	606	1	14,14,15	0.62	0	17,19,21	0.62	1 (5%)
7	NAG	A	601	1	14,14,15	0.25	0	17,19,21	0.36	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	B	608	1	-	1/6/23/26	0/1/1/1
7	NAG	D	607	1	-	2/6/23/26	0/1/1/1
7	NAG	C	606	1	-	0/6/23/26	0/1/1/1
7	NAG	A	601	1	-	0/6/23/26	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(°)
7	C	606	NAG	C1-O5-C5	2.09	115.03	112.19
7	B	608	NAG	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	607	NAG	O5-C5-C6-O6
7	D	607	NAG	C4-C5-C6-O6
7	B	608	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	507/596 (85%)	-0.10	6 (1%) 79 77	43, 71, 114, 131	0
1	B	517/596 (86%)	-0.06	13 (2%) 57 53	48, 73, 118, 148	0
1	C	480/596 (80%)	-0.16	9 (1%) 66 64	46, 69, 109, 135	0
1	D	511/596 (85%)	-0.09	1 (0%) 95 95	46, 80, 123, 141	0
2	E	123/123 (100%)	0.05	4 (3%) 46 43	63, 77, 102, 121	0
2	F	123/123 (100%)	0.04	1 (0%) 86 86	62, 78, 100, 125	0
2	G	123/123 (100%)	0.03	2 (1%) 72 69	55, 78, 109, 126	0
2	H	119/123 (96%)	0.35	9 (7%) 13 12	67, 95, 122, 128	0
All	All	2503/2876 (87%)	-0.06	45 (1%) 68 65	43, 75, 116, 148	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	VAL	4.1
1	C	536	PRO	4.0
1	B	560	ASP	3.9
1	B	556	SER	3.6
1	B	549	CYS	3.4

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

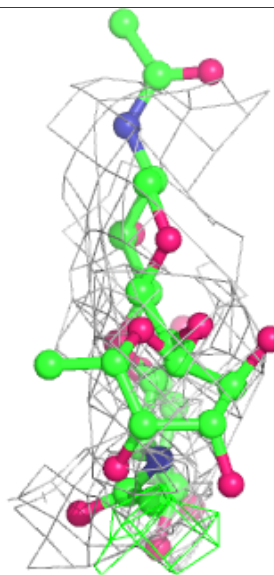
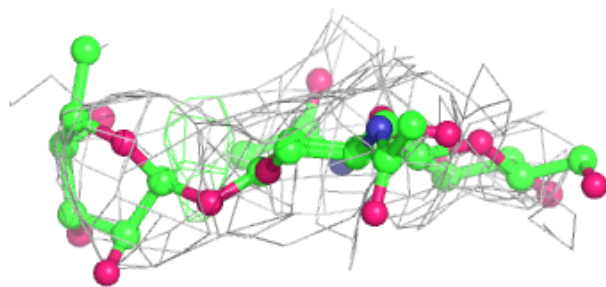
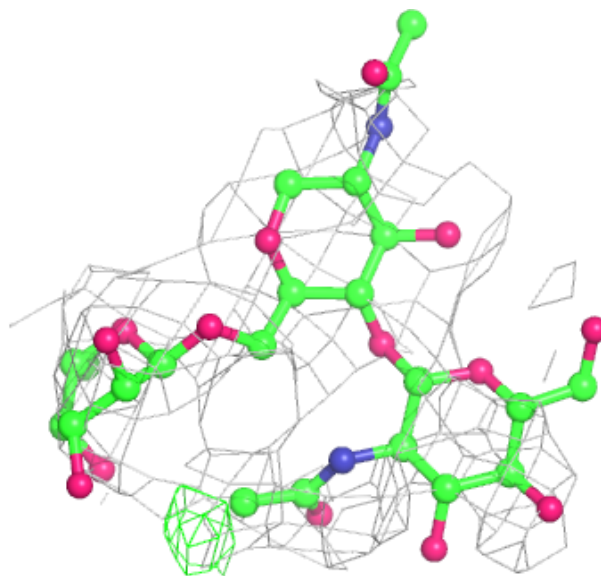
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	I	2	14/15	0.56	0.40	120,159,165,170	0
4	MAN	J	4	11/12	0.69	0.50	116,140,148,149	0
5	NAG	K	1	14/15	0.77	0.19	121,141,160,162	0
3	NAG	I	1	14/15	0.77	0.30	122,140,155,157	0
3	FUC	I	3	10/11	0.77	0.46	124,138,147,147	0
4	MAN	J	5	11/12	0.77	0.42	91,118,141,142	0
5	NAG	K	2	14/15	0.77	0.33	135,147,159,167	0
4	FUC	J	7	10/11	0.79	0.23	103,127,136,138	0
6	MAN	L	4	11/12	0.80	0.33	81,96,103,106	0
5	MAN	K	4	11/12	0.84	0.47	125,132,140,140	0
4	BMA	J	3	11/12	0.86	0.29	109,123,130,139	0
5	FUC	K	5	10/11	0.86	0.29	133,140,143,143	0
6	BMA	L	3	11/12	0.86	0.18	90,101,111,113	0
5	BMA	K	3	11/12	0.86	0.24	112,129,137,138	0
4	NAG	J	2	14/15	0.86	0.30	110,127,132,136	0
6	NAG	L	2	14/15	0.88	0.24	93,102,112,115	0
6	NAG	L	1	14/15	0.89	0.26	93,102,115,120	0
4	NAG	J	1	14/15	0.90	0.12	89,120,129,133	0
6	FUC	L	6	10/11	0.91	0.20	83,95,108,109	0
4	FUC	J	6	10/11	0.92	0.17	106,114,126,131	0
6	FUC	L	5	10/11	0.92	0.42	90,109,123,127	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.

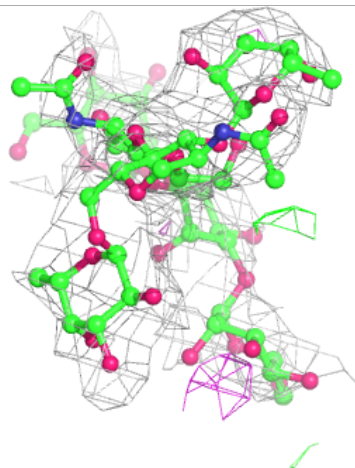
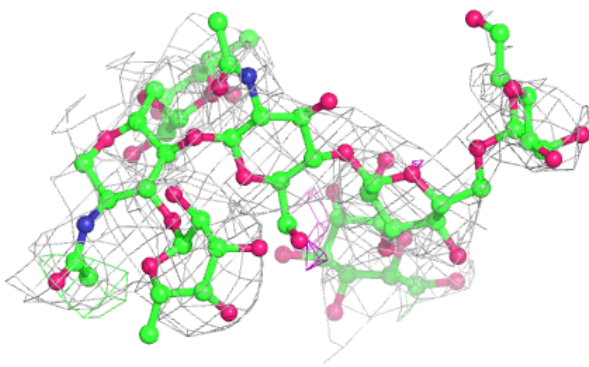
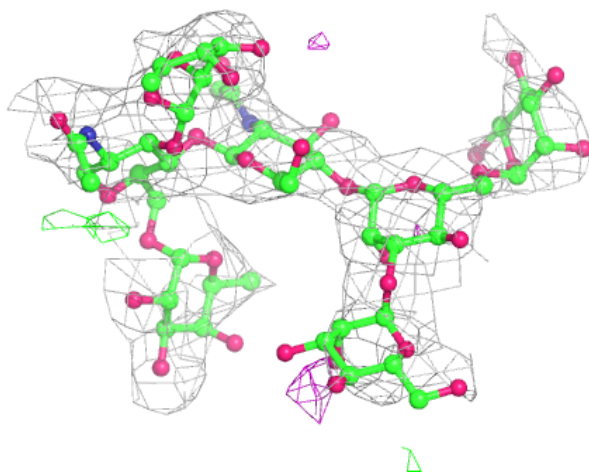
Electron density around Chain I:

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



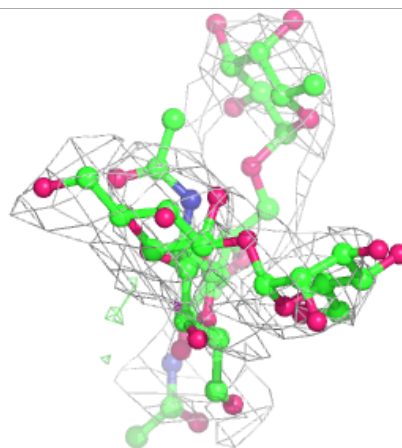
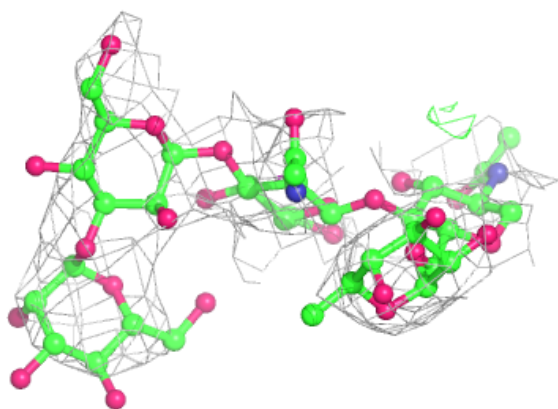
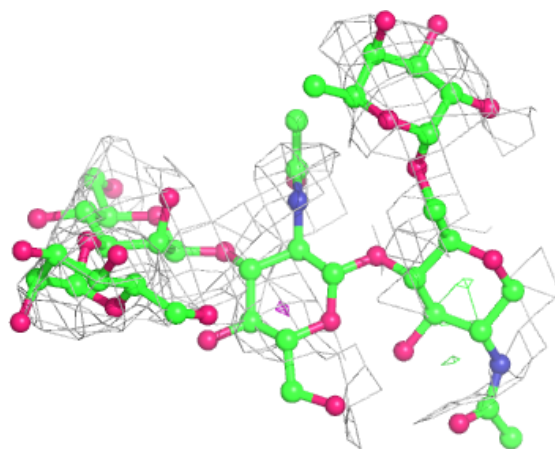
Electron density around Chain J:

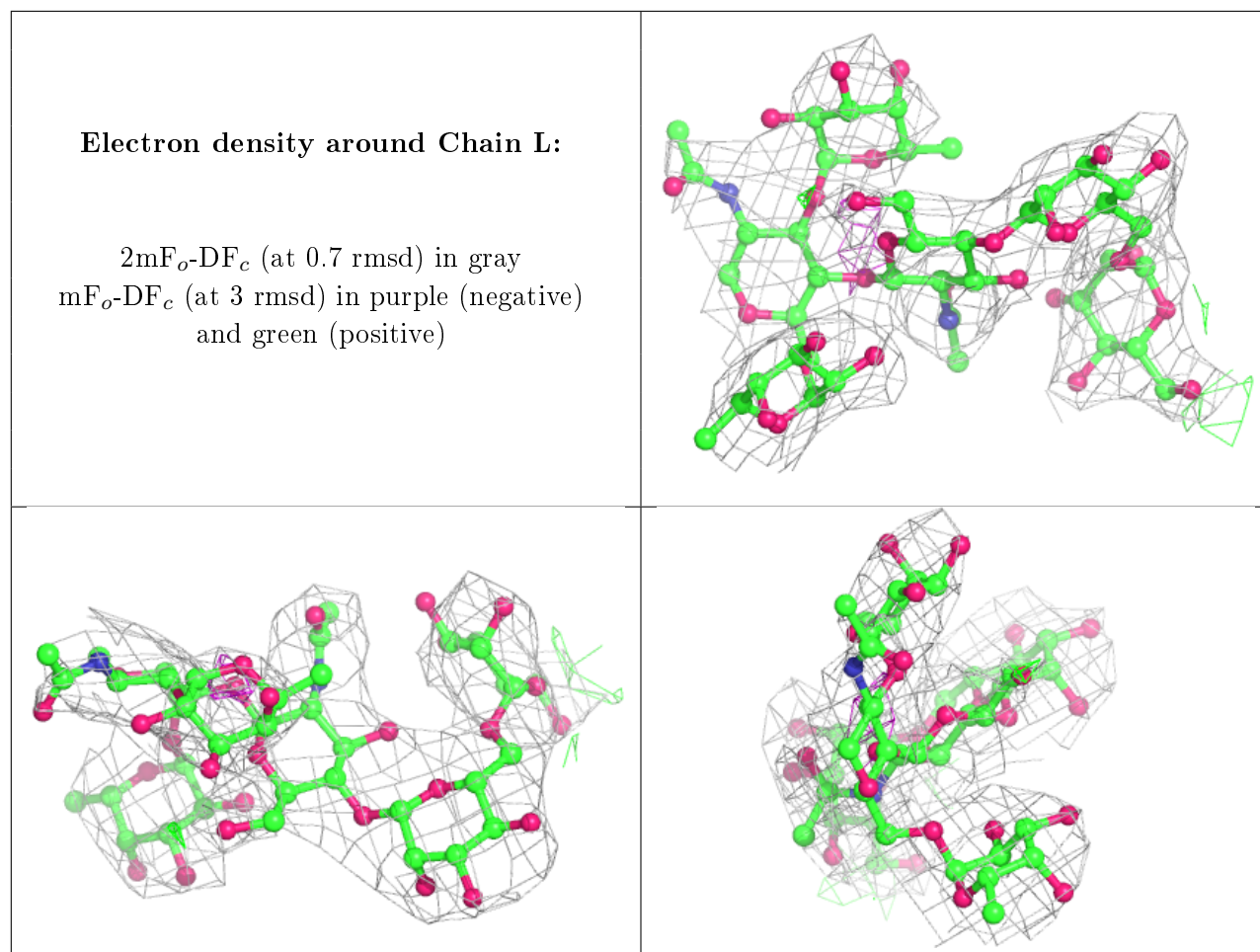
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
7	NAG	A	601	14/15	0.63	0.42	95,135,152,159	0
7	NAG	B	608	14/15	0.79	0.25	93,118,134,138	0
7	NAG	C	606	14/15	0.82	0.20	108,135,142,144	0
7	NAG	D	607	14/15	0.85	0.26	87,113,123,135	0

6.5 Other polymers [i](#)

There are no such residues in this entry.