



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:43 AM UTC

PDB ID : 6N4Y / pdb_00006n4y
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.;
Skinotitis, 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 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

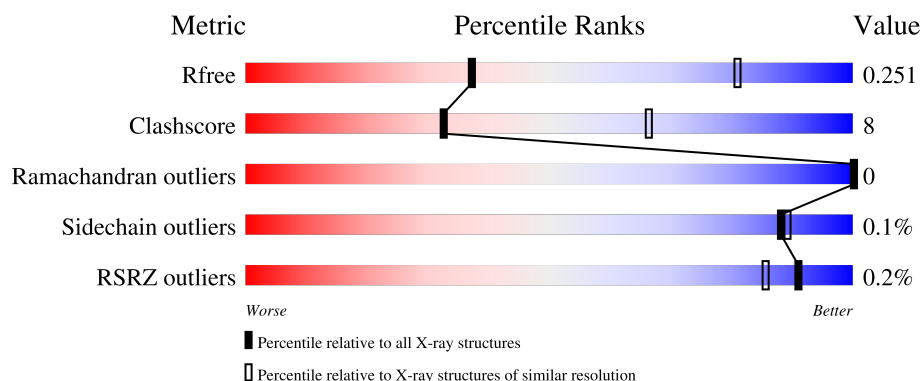
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (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 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	596	 69% 16% 15%
1	B	596	 68% 18% 13%
1	C	596	 66% 14% 19%
1	D	596	 69% 16% 14%
2	E	123	 86% 14%

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Mol	Chain	Length	Quality of chain
2	F	123	85% 15%
2	G	123	82% 18%
2	H	123	% 76% 20% .
3	I	3	100%
4	J	7	14% 71% 14%
5	K	5	20% 60% 20%
6	L	6	50% 50%

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

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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

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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

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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

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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.

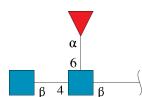
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	123	Total	C	N	O	S	0	0	0
			933	580	161	187	5			
2	F	123	Total	C	N	O	S	0	0	0
			927	577	158	187	5			
2	G	123	Total	C	N	O	S	0	0	0
			929	577	160	187	5			

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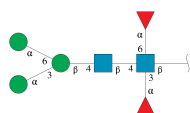
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	119	Total	C	N	O	S	0	0	0
			893	558	152	178	5			

- 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.



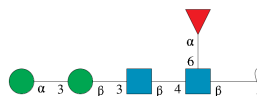
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	3	Total	C	N	O		0	0	0
			38	22	2	14				

- 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				

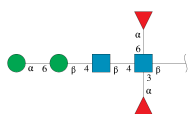
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

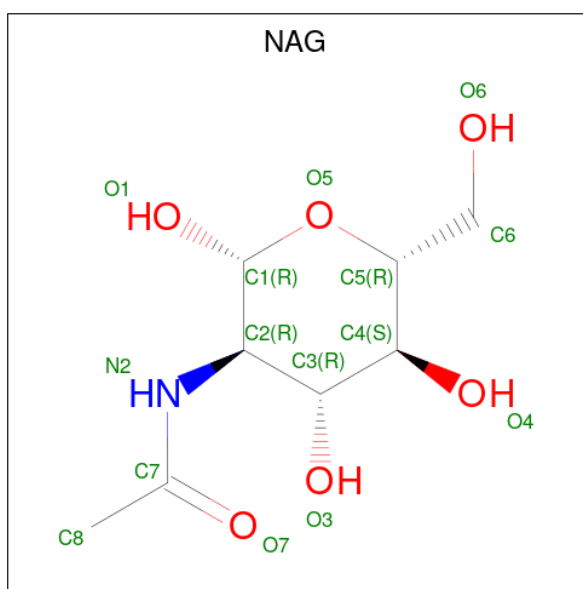
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	6	Total	C	N	O	0	0	0
			70	40	2	28			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

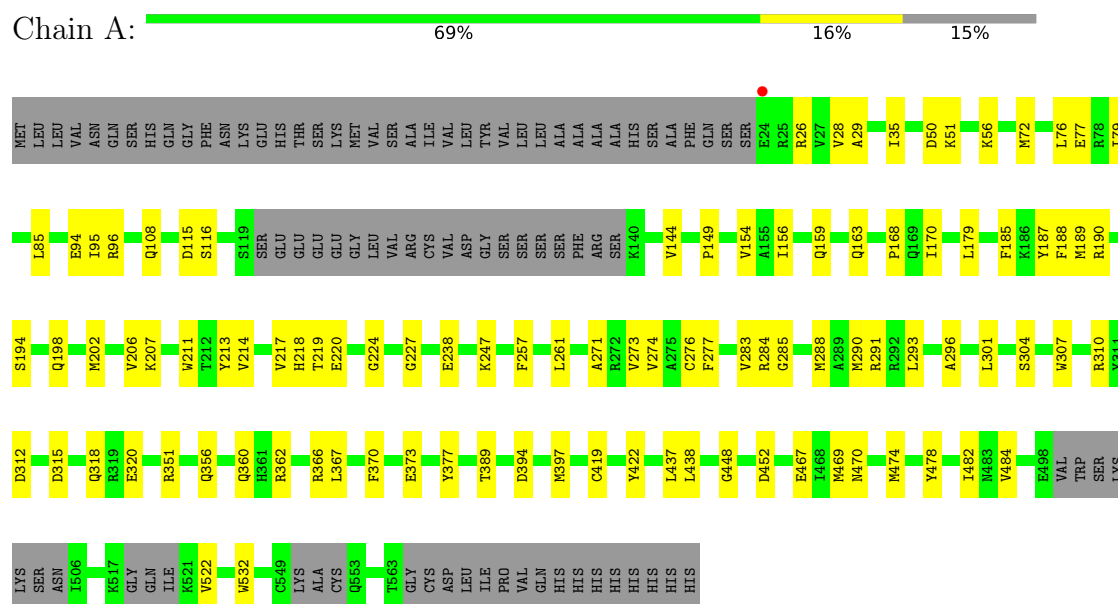


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

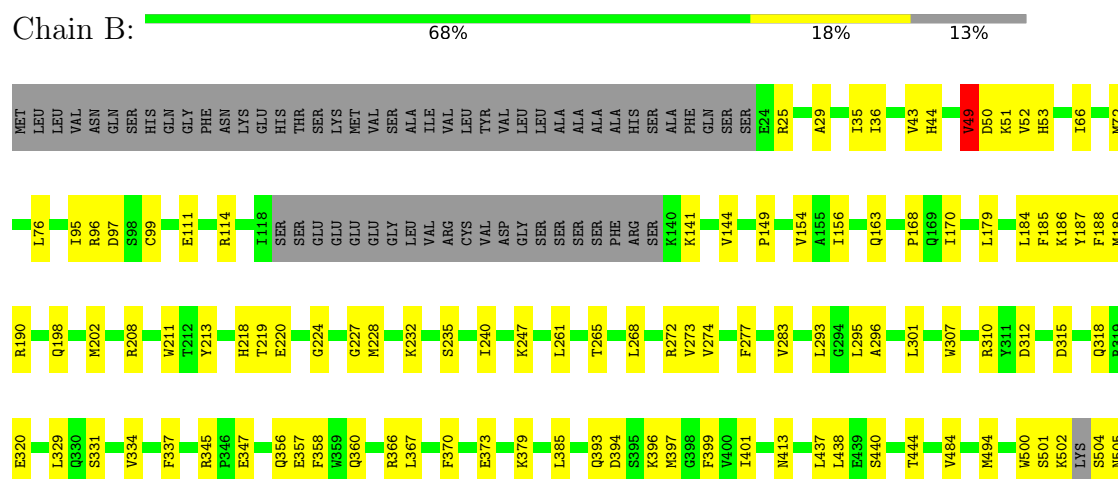
3 Residue-property plots

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

• Molecule 1: Metabotropic glutamate receptor 5



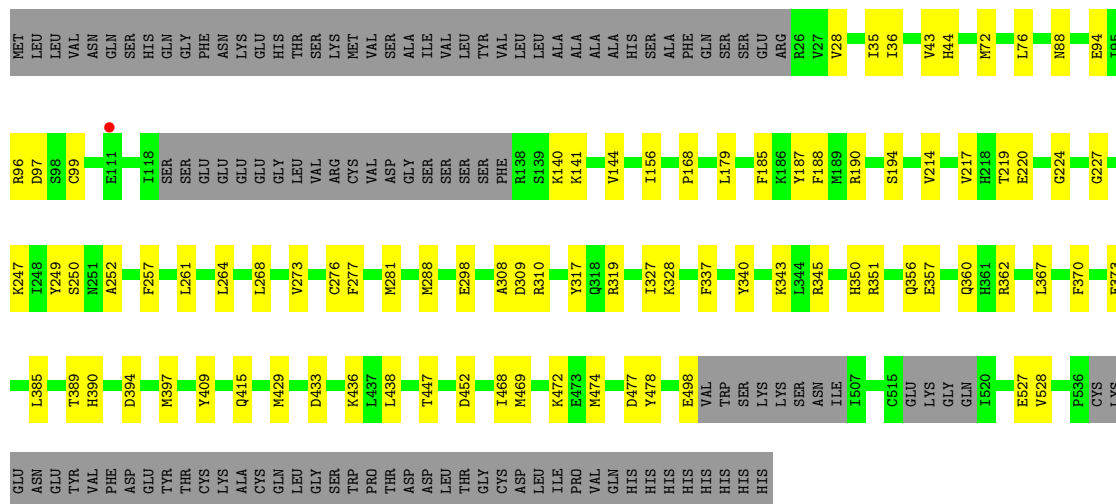
• Molecule 1: Metabotropic glutamate receptor 5





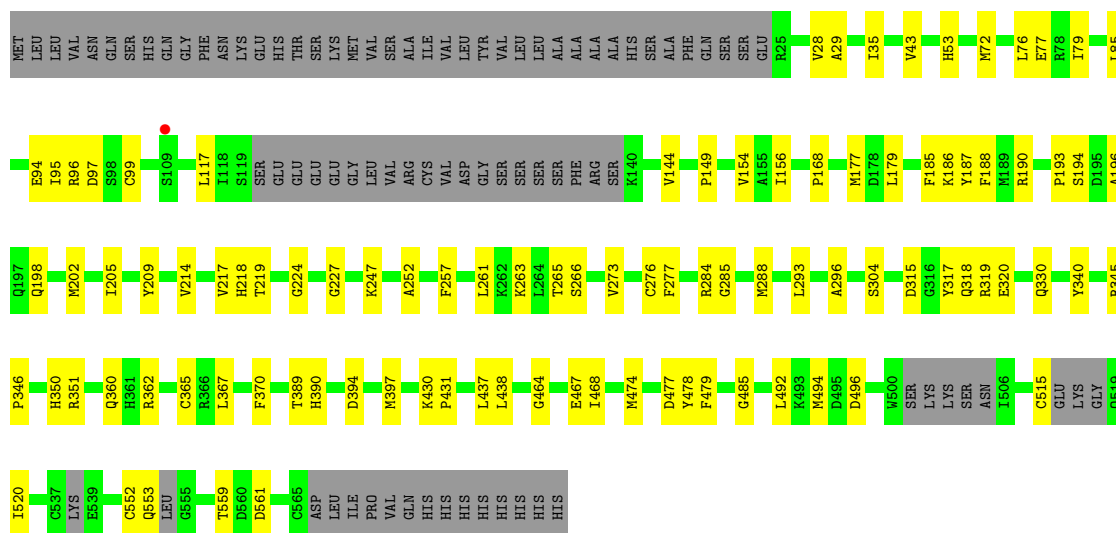
• Molecule 1: Metabotropic glutamate receptor 5

Chain C: 66% 14% 19%



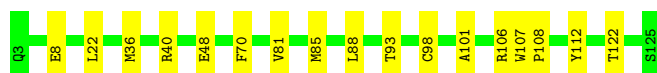
• Molecule 1: Metabotropic glutamate receptor 5

Chain D: 69% 16% 14%



• Molecule 2: Nanobody 43

Chain E: 86% 14%



- Molecule 2: Nanobody 43

Chain F:  85% 15%



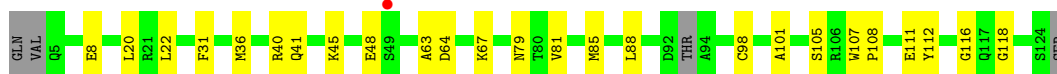
- Molecule 2: Nanobody 43

Chain G:  82% 18%

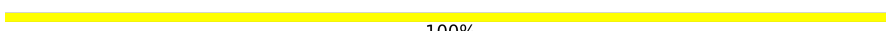


- Molecule 2: Nanobody 43

Chain H:  76% 20%

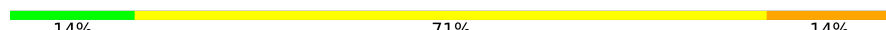


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

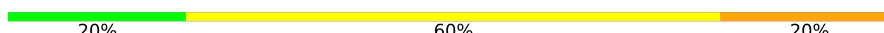


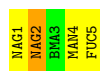
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  14% 71% 14%



- 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

Chain K:  20% 60% 20%



- 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



HA01
HA02
BOL3
HA04
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 38.87 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.87-3.26) 91.5 (38.87-3.26)	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 , 0.251	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)	0.31 , 45.3	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: BMA, NAG, MAN, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/4023	0.40	0/5446
1	B	0.28	1/4107 (0.0%)	0.47	2/5560 (0.0%)
1	C	0.14	0/3819	0.41	0/5164
1	D	0.14	0/4032	0.41	0/5457
2	E	0.13	0/955	0.42	0/1293
2	F	0.12	0/949	0.39	0/1286
2	G	0.13	0/951	0.40	0/1289
2	H	0.12	0/914	0.41	0/1238
All	All	0.18	1/19750 (0.0%)	0.42	2/26733 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	505	ASN	CA-C	-5.80	1.47	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	VAL	N-CA-C	8.85	119.64	110.62
1	B	507	ILE	CB-CA-C	-6.14	102.32	110.98

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	59	0
1	B	4018	0	3834	77	0
1	C	3737	0	3585	58	0
1	D	3947	0	3733	62	0
2	E	933	0	869	12	0
2	F	927	0	858	11	0
2	G	929	0	858	15	0
2	H	893	0	822	17	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	302	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 8.

The worst 5 of 302 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
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%)	422 (100%)	0	100	100
1	B	432/520 (83%)	429 (99%)	3 (1%)	76	79
1	C	402/520 (77%)	402 (100%)	0	100	100
1	D	422/520 (81%)	422 (100%)	0	100	100
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%)	2051 (100%)	3 (0%)	88	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	49	VAL
1	B	506	ILE
1	B	507	ILE

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

Mol	Chain	Res	Type
1	D	198	GLN
2	G	76	ASN
2	H	61	HIS
2	G	61	HIS
1	C	108	GLN

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	3,1	14,14,15	0.38	0	17,19,21	0.94	1 (5%)
3	NAG	I	2	3	14,14,15	0.43	0	17,19,21	0.61	1 (5%)
3	FUC	I	3	3	10,10,11	1.09	0	14,14,16	1.13	1 (7%)
4	NAG	J	1	4,1	14,14,15	1.02	1 (7%)	17,19,21	0.76	0
4	NAG	J	2	4	14,14,15	0.61	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	1.20	2 (18%)	15,15,17	1.22	2 (13%)
4	MAN	J	4	4	11,11,12	0.73	0	15,15,17	0.98	2 (13%)
4	MAN	J	5	4	11,11,12	0.60	0	15,15,17	1.04	2 (13%)
4	FUC	J	6	4	10,10,11	1.44	2 (20%)	14,14,16	1.22	2 (14%)
4	FUC	J	7	4	10,10,11	0.75	0	14,14,16	0.80	0
5	NAG	K	1	5,1	14,14,15	0.32	0	17,19,21	0.83	1 (5%)
5	NAG	K	2	5	14,14,15	0.63	1 (7%)	17,19,21	0.65	0
5	BMA	K	3	5	11,11,12	0.68	0	15,15,17	0.87	0
5	MAN	K	4	5	11,11,12	0.60	0	15,15,17	1.00	2 (13%)
5	FUC	K	5	5	10,10,11	0.66	0	14,14,16	0.73	0
6	NAG	L	1	6,1	14,14,15	0.29	0	17,19,21	0.61	0
6	NAG	L	2	6	14,14,15	0.28	0	17,19,21	0.51	0
6	BMA	L	3	6	11,11,12	0.69	0	15,15,17	0.75	0
6	MAN	L	4	6	11,11,12	0.72	0	15,15,17	1.11	2 (13%)
6	FUC	L	5	6	10,10,11	0.69	0	14,14,16	0.90	1 (7%)
6	FUC	L	6	6	10,10,11	0.88	1 (10%)	14,14,16	0.71	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	3,1	-	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	4,1	-	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	5,1	-	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	6,1	-	0/6/23/26	0/1/1/1

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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	-3.50	1.37	1.43
4	J	6	FUC	C1-C2	2.74	1.58	1.52
4	J	3	BMA	O3-C3	2.53	1.49	1.43
4	J	6	FUC	C4-C5	2.16	1.57	1.52
5	K	2	NAG	O5-C1	-2.11	1.40	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	NAG	C1-O5-C5	3.48	116.84	112.19
4	J	3	BMA	O3-C3-C2	3.15	116.49	110.05
4	J	5	MAN	C1-O5-C5	3.06	116.28	112.19
6	L	4	MAN	C1-O5-C5	3.00	116.21	112.19
5	K	4	MAN	C1-O5-C5	2.78	115.91	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

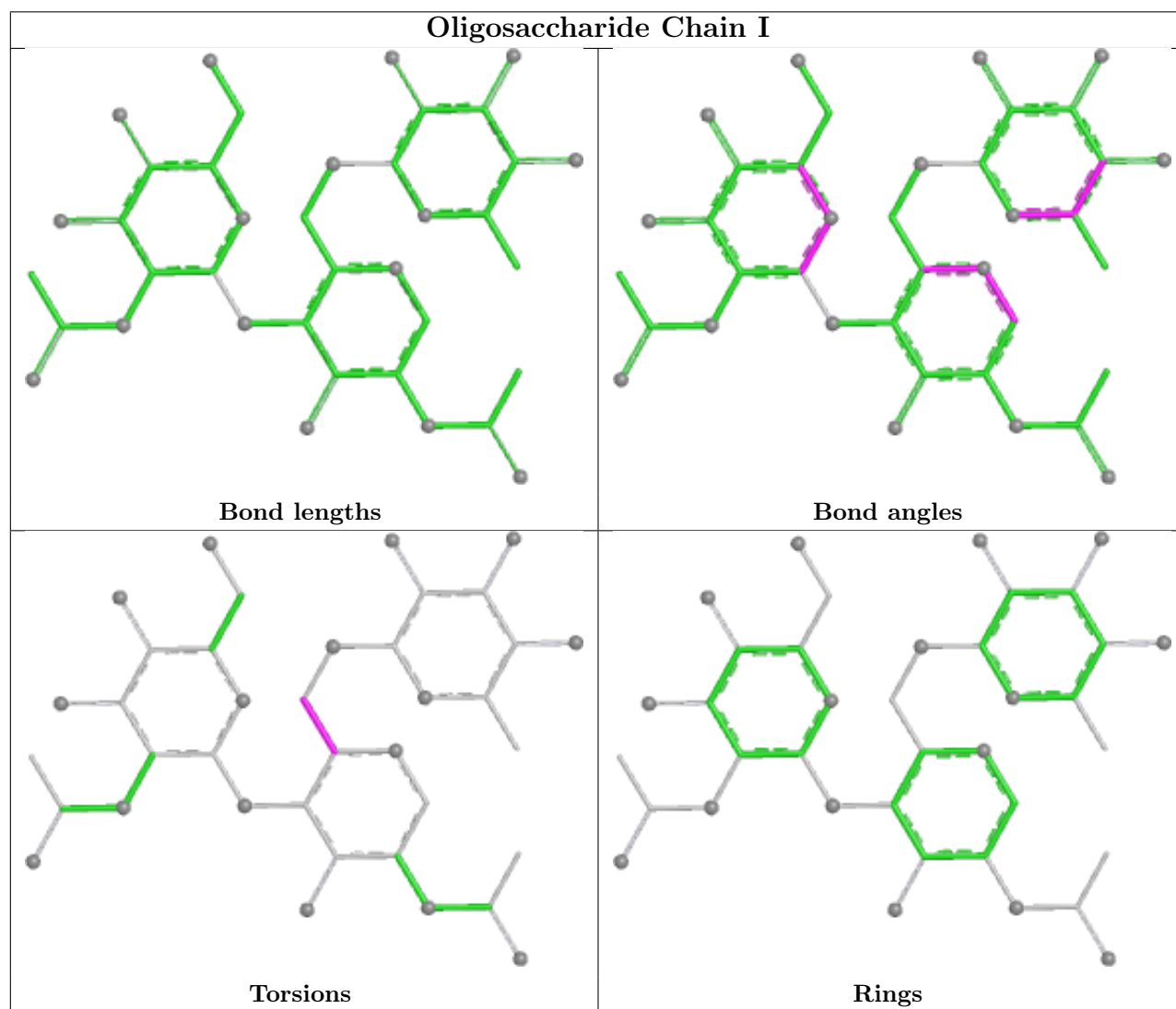
Mol	Chain	Res	Type	Atoms
4	J	3	BMA	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6

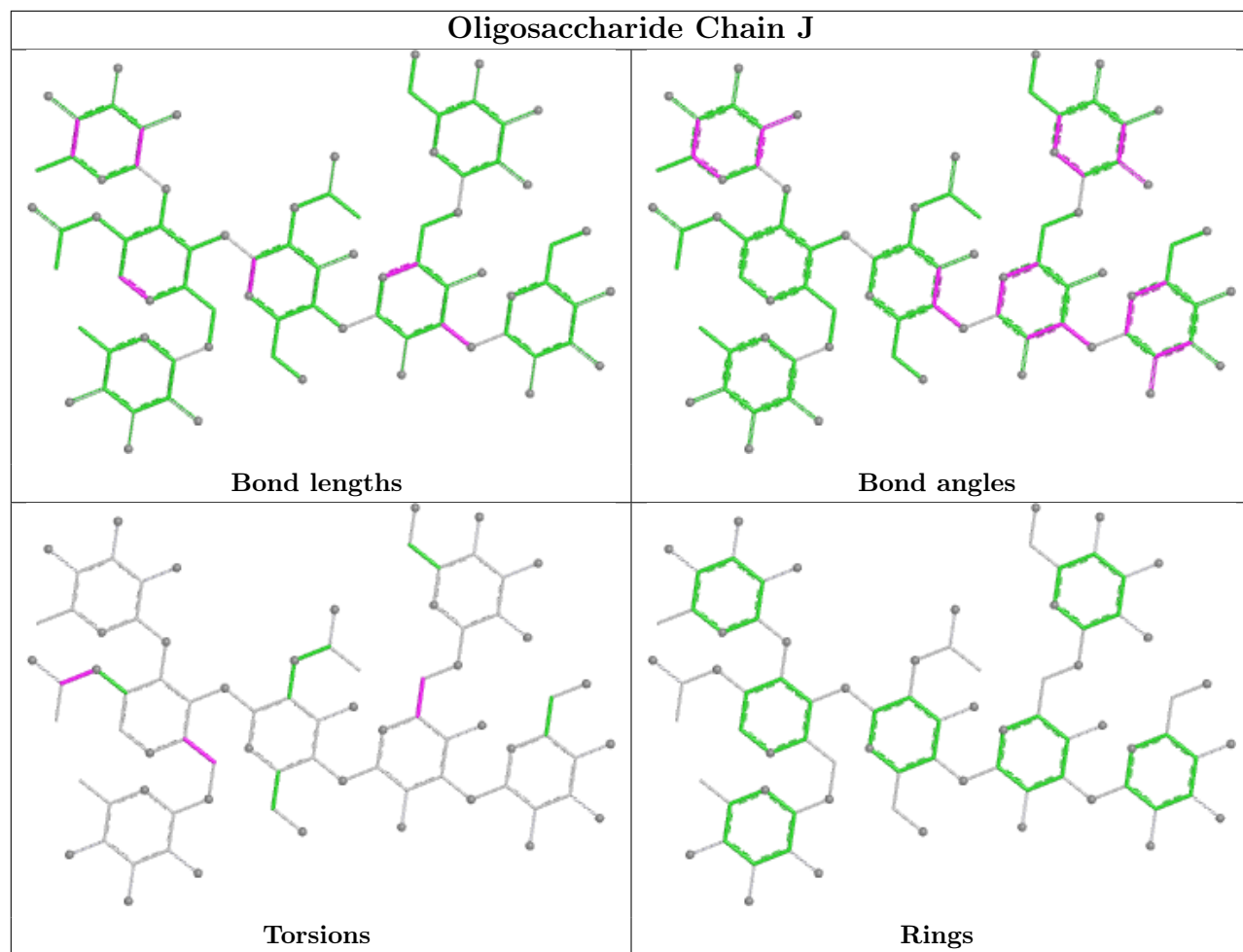
There are no ring outliers.

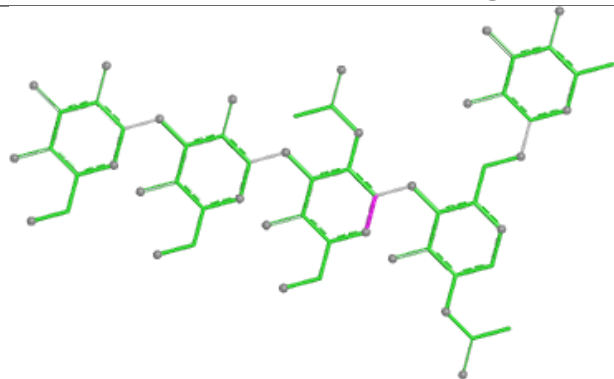
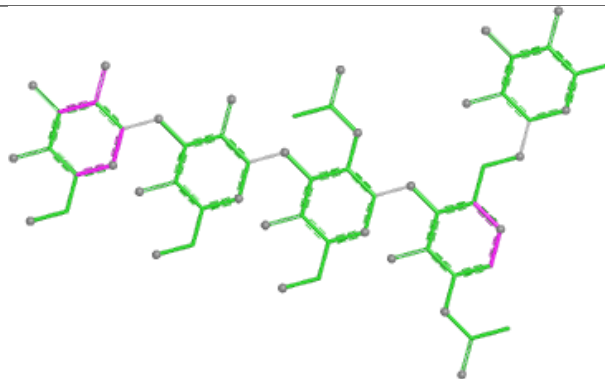
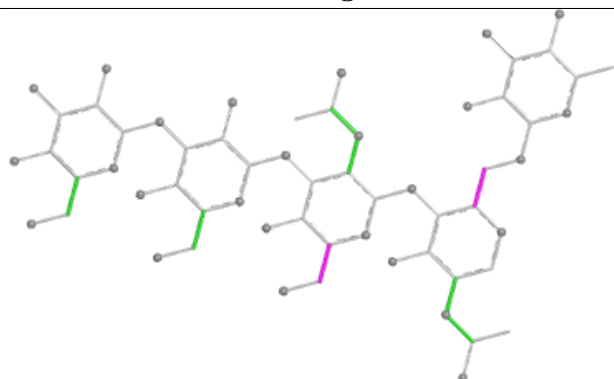
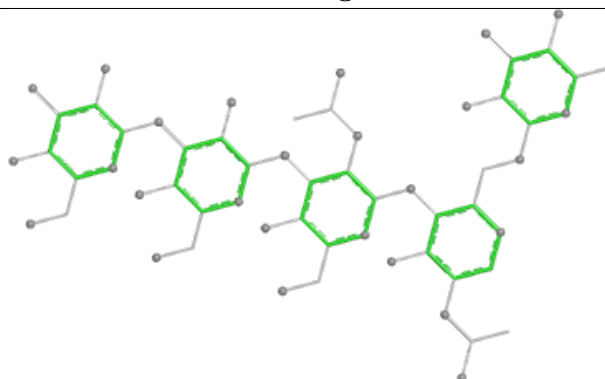
3 monomers are involved in 3 short contacts:

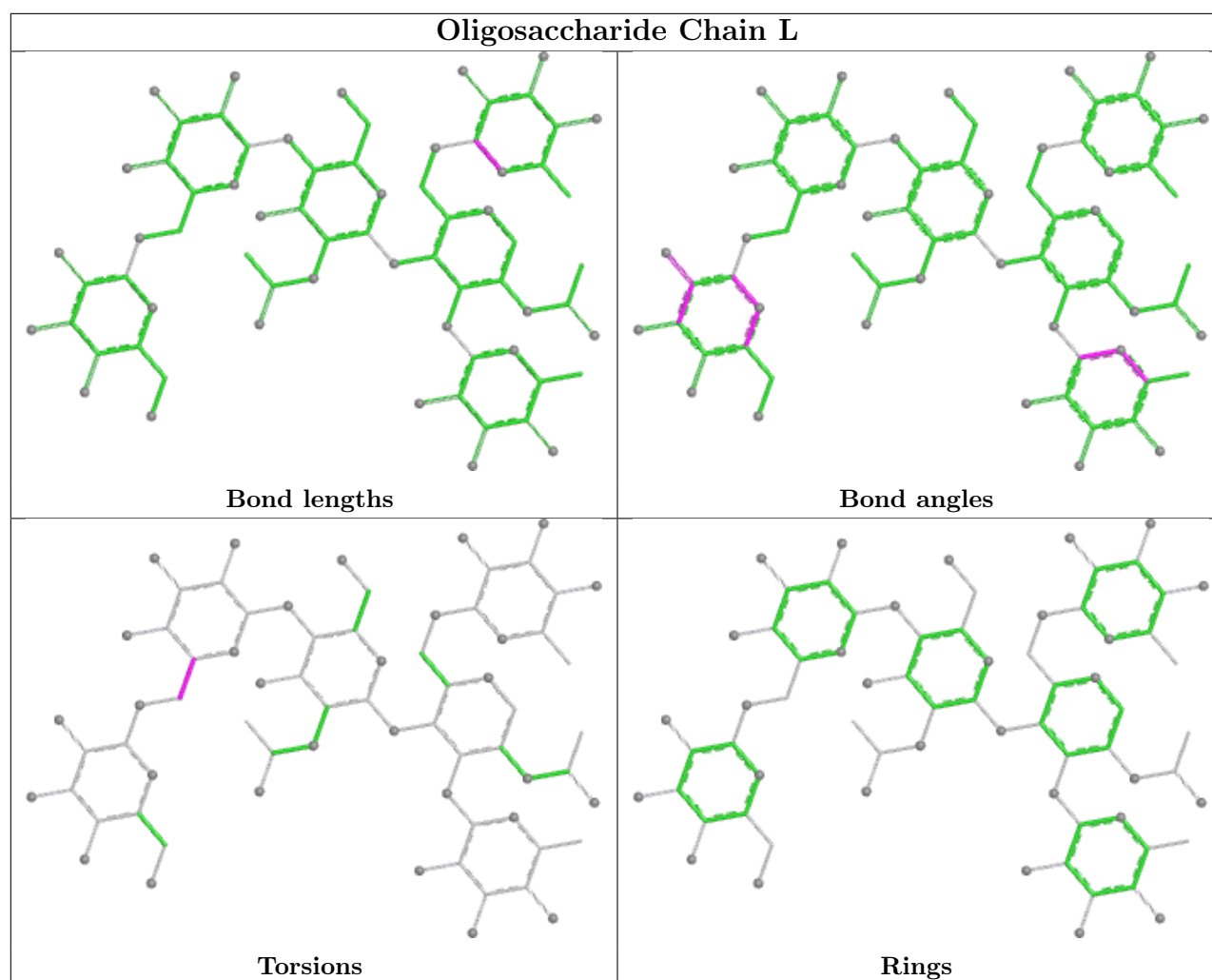
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	2	NAG	1	0
5	K	5	FUC	1	0
4	J	3	BMA	2	0

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





Oligosaccharide Chain K**Bond lengths****Bond angles****Torsions****Rings**



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	A	601	1	14,14,15	0.26	0	17,19,21	0.38	0
7	NAG	C	606	1	14,14,15	0.65	1 (7%)	17,19,21	0.64	1 (5%)
7	NAG	B	608	1	14,14,15	0.54	0	17,19,21	0.61	1 (5%)
7	NAG	D	607	1	14,14,15	0.54	0	17,19,21	0.53	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	A	601	1	-	0/6/23/26	0/1/1/1
7	NAG	C	606	1	-	0/6/23/26	0/1/1/1
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	606	NAG	C1-C2	2.07	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	606	NAG	C1-O5-C5	2.12	115.03	112.19
7	B	608	NAG	C1-O5-C5	2.03	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 [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	507/596 (85%)	-0.30	1 (0%) 91 85	43, 71, 114, 131	0
1	B	517/596 (86%)	-0.23	1 (0%) 91 85	48, 73, 118, 148	0
1	C	480/596 (80%)	-0.32	1 (0%) 91 85	46, 69, 109, 135	0
1	D	511/596 (85%)	-0.19	1 (0%) 91 85	46, 80, 123, 141	0
2	E	123/123 (100%)	-0.28	0 100 100	63, 77, 102, 121	0
2	F	123/123 (100%)	-0.39	0 100 100	62, 78, 100, 125	0
2	G	123/123 (100%)	-0.27	0 100 100	55, 78, 109, 126	0
2	H	119/123 (96%)	-0.03	1 (0%) 82 68	67, 95, 122, 128	0
All	All	2503/2876 (87%)	-0.26	5 (0%) 91 85	43, 75, 116, 148	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	49	SER	2.7
1	A	24	GLU	2.4
1	B	519	GLN	2.3
1	D	109	SER	2.3
1	C	111	GLU	2.2

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,

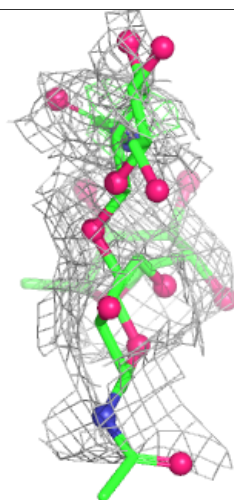
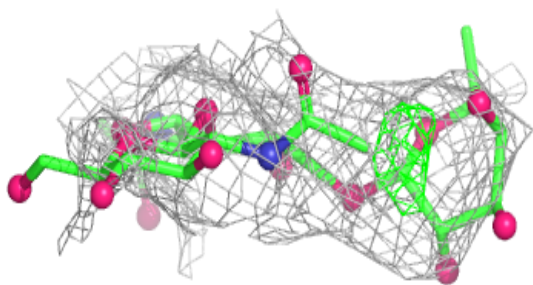
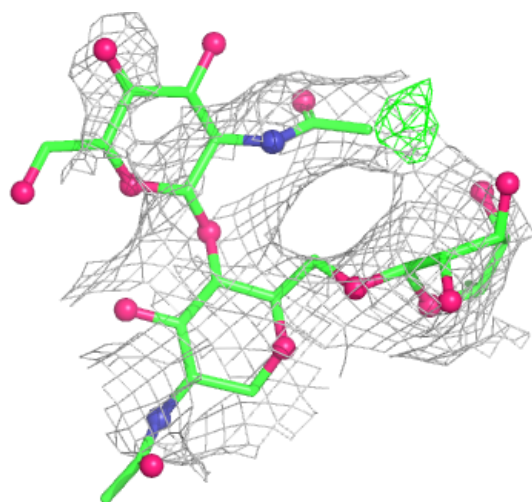
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FUC	J	7	10/11	0.23	0.15	103,127,136,138	0
4	MAN	J	4	11/12	0.37	0.14	116,140,148,149	0
3	NAG	I	2	14/15	0.37	0.15	120,159,165,170	0
4	NAG	J	1	14/15	0.65	0.10	89,120,129,133	0
5	FUC	K	5	10/11	0.65	0.14	133,140,143,143	0
3	FUC	I	3	10/11	0.67	0.15	124,138,147,147	0
5	MAN	K	4	11/12	0.68	0.14	125,132,140,140	0
5	NAG	K	2	14/15	0.68	0.10	135,147,159,167	0
4	NAG	J	2	14/15	0.69	0.11	110,127,132,136	0
5	BMA	K	3	11/12	0.73	0.09	112,129,137,138	0
4	FUC	J	6	10/11	0.75	0.10	106,114,126,131	0
5	NAG	K	1	14/15	0.75	0.12	121,141,160,162	0
6	MAN	L	4	11/12	0.76	0.12	81,96,103,106	0
4	MAN	J	5	11/12	0.79	0.12	91,118,141,142	0
4	BMA	J	3	11/12	0.81	0.09	109,123,130,139	0
6	FUC	L	6	10/11	0.81	0.11	83,95,108,109	0
3	NAG	I	1	14/15	0.82	0.09	122,140,155,157	0
6	NAG	L	2	14/15	0.85	0.09	93,102,112,115	0
6	BMA	L	3	11/12	0.85	0.08	90,101,111,113	0
6	FUC	L	5	10/11	0.90	0.11	90,109,123,127	0
6	NAG	L	1	14/15	0.90	0.10	93,102,115,120	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.

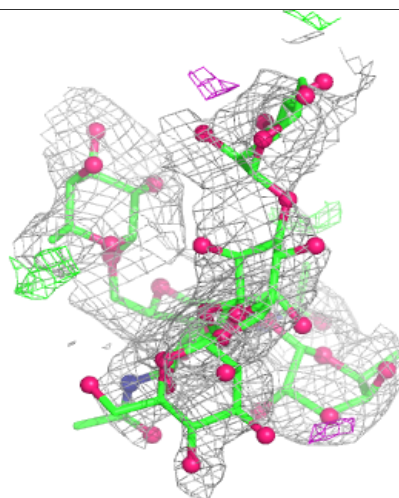
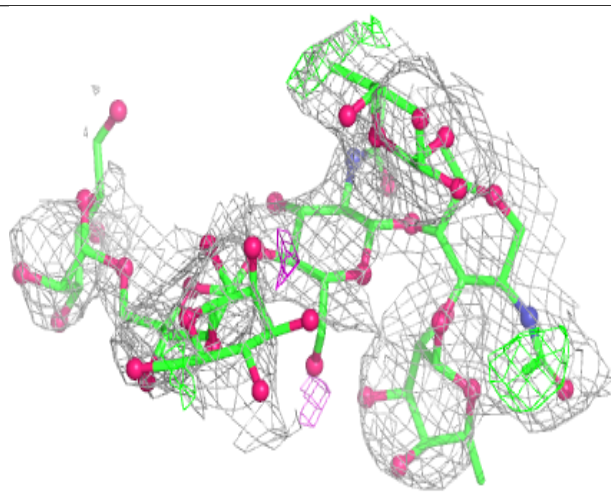
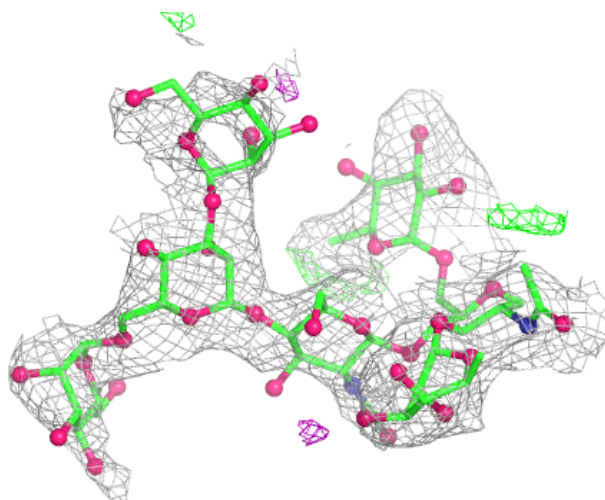
Electron density around Chain I:

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



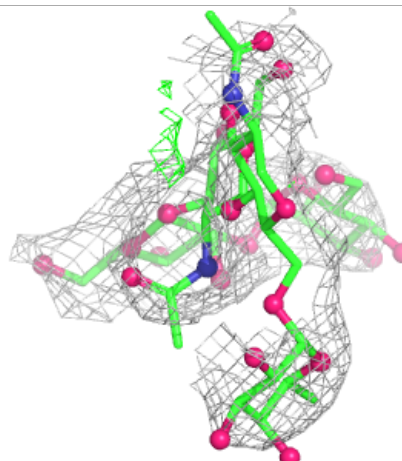
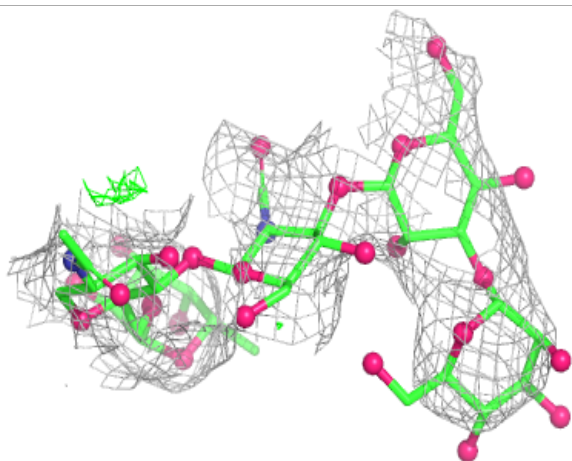
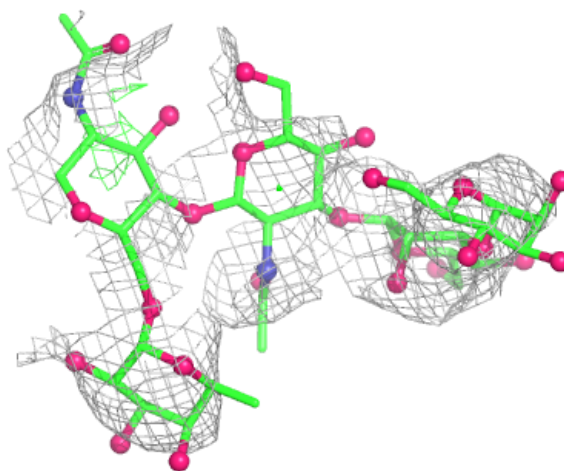
Electron density around Chain J:

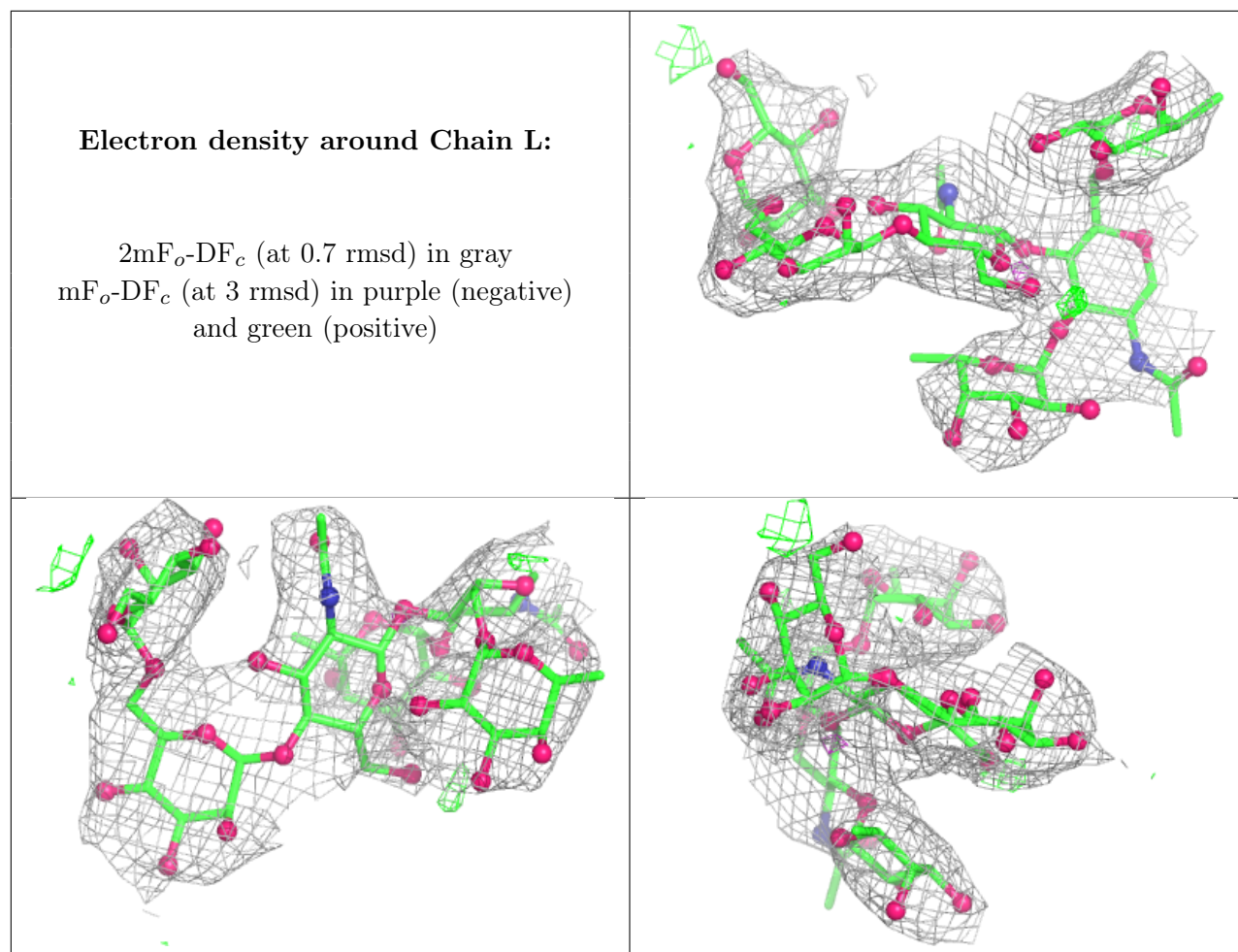
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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($\text{\AA}^2$)	Q<0.9
7	NAG	A	601	14/15	0.41	0.14	95,135,152,159	0
7	NAG	C	606	14/15	0.57	0.12	108,135,142,144	0
7	NAG	D	607	14/15	0.72	0.10	87,113,123,135	0
7	NAG	B	608	14/15	0.74	0.12	93,118,134,138	0

6.5 Other polymers [i](#)

There are no such residues in this entry.