



wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2024 – 09:50 PM EDT

PDB ID : 6MGQ
Title : ERAP1 in the open conformation bound to 10mer phosphinic inhibitor DG014
Authors : Stern, L.J.; Maben, Z.
Deposited on : 2018-09-14
Resolution : 2.92 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

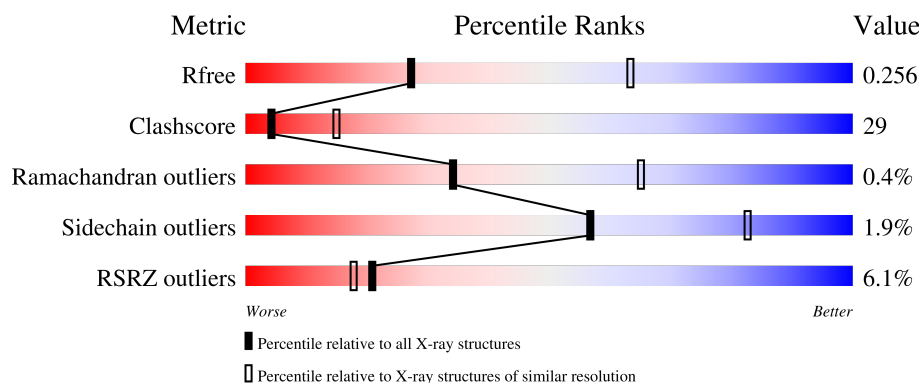
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	948	<div> <div>5%</div> <div> <div>52%</div> <div>38%</div> <div>9%</div> </div> </div>
1	B	948	<div> <div>6%</div> <div> <div>52%</div> <div>37%</div> <div>9%</div> </div> </div>
1	C	948	<div> <div>4%</div> <div> <div>51%</div> <div>38%</div> <div>11%</div> </div> </div>
2	D	10	<div> <div>30%</div> <div> <div>20%</div> <div>20%</div> <div>10%</div> <div>50%</div> </div> </div>
2	E	10	<div> <div>30%</div> <div> <div>20%</div> <div>20%</div> <div>10%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	10	
3	G	4	
4	H	2	
4	K	2	
4	L	2	
5	I	3	
5	J	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	I	1	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20671 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 Endoplasmic reticulum aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	861	Total	C	N	O	S	0	2	0
			6895	4438	1139	1284	34			
1	B	858	Total	C	N	O	S	0	2	0
			6705	4315	1104	1252	34			
1	C	843	Total	C	N	O	S	0	2	0
			6679	4299	1105	1243	32			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	ASP	GLY	conflict	UNP Q9NZ08
A	514	ARG	GLY	conflict	UNP Q9NZ08
A	528	ARG	LYS	conflict	UNP Q9NZ08
A	730	GLU	GLN	conflict	UNP Q9NZ08
A	949	LEU	-	expression tag	UNP Q9NZ08
A	950	GLU	-	expression tag	UNP Q9NZ08
A	951	ARG	-	expression tag	UNP Q9NZ08
A	952	MET	-	expression tag	UNP Q9NZ08
A	953	LEU	-	expression tag	UNP Q9NZ08
A	954	GLU	-	expression tag	UNP Q9NZ08
A	955	SER	-	expression tag	UNP Q9NZ08
A	956	ARG	-	expression tag	UNP Q9NZ08
A	957	GLY	-	expression tag	UNP Q9NZ08
A	958	PRO	-	expression tag	UNP Q9NZ08
A	959	PHE	-	expression tag	UNP Q9NZ08
A	960	GLU	-	expression tag	UNP Q9NZ08
A	961	GLN	-	expression tag	UNP Q9NZ08
A	962	LYS	-	expression tag	UNP Q9NZ08
A	963	LEU	-	expression tag	UNP Q9NZ08
A	964	ILE	-	expression tag	UNP Q9NZ08
A	965	SER	-	expression tag	UNP Q9NZ08
A	966	GLU	-	expression tag	UNP Q9NZ08
A	967	GLU	-	expression tag	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
A	968	ASP	-	expression tag	UNP Q9NZ08
A	969	LEU	-	expression tag	UNP Q9NZ08
A	970	ASN	-	expression tag	UNP Q9NZ08
A	971	MET	-	expression tag	UNP Q9NZ08
A	972	HIS	-	expression tag	UNP Q9NZ08
A	973	THR	-	expression tag	UNP Q9NZ08
A	974	GLU	-	expression tag	UNP Q9NZ08
A	975	HIS	-	expression tag	UNP Q9NZ08
A	976	HIS	-	expression tag	UNP Q9NZ08
A	977	HIS	-	expression tag	UNP Q9NZ08
A	978	HIS	-	expression tag	UNP Q9NZ08
A	979	HIS	-	expression tag	UNP Q9NZ08
A	980	HIS	-	expression tag	UNP Q9NZ08
B	346	ASP	GLY	conflict	UNP Q9NZ08
B	514	ARG	GLY	conflict	UNP Q9NZ08
B	528	ARG	LYS	conflict	UNP Q9NZ08
B	730	GLU	GLN	conflict	UNP Q9NZ08
B	949	LEU	-	expression tag	UNP Q9NZ08
B	950	GLU	-	expression tag	UNP Q9NZ08
B	951	ARG	-	expression tag	UNP Q9NZ08
B	952	MET	-	expression tag	UNP Q9NZ08
B	953	LEU	-	expression tag	UNP Q9NZ08
B	954	GLU	-	expression tag	UNP Q9NZ08
B	955	SER	-	expression tag	UNP Q9NZ08
B	956	ARG	-	expression tag	UNP Q9NZ08
B	957	GLY	-	expression tag	UNP Q9NZ08
B	958	PRO	-	expression tag	UNP Q9NZ08
B	959	PHE	-	expression tag	UNP Q9NZ08
B	960	GLU	-	expression tag	UNP Q9NZ08
B	961	GLN	-	expression tag	UNP Q9NZ08
B	962	LYS	-	expression tag	UNP Q9NZ08
B	963	LEU	-	expression tag	UNP Q9NZ08
B	964	ILE	-	expression tag	UNP Q9NZ08
B	965	SER	-	expression tag	UNP Q9NZ08
B	966	GLU	-	expression tag	UNP Q9NZ08
B	967	GLU	-	expression tag	UNP Q9NZ08
B	968	ASP	-	expression tag	UNP Q9NZ08
B	969	LEU	-	expression tag	UNP Q9NZ08
B	970	ASN	-	expression tag	UNP Q9NZ08
B	971	MET	-	expression tag	UNP Q9NZ08
B	972	HIS	-	expression tag	UNP Q9NZ08
B	973	THR	-	expression tag	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
B	974	GLU	-	expression tag	UNP Q9NZ08
B	975	HIS	-	expression tag	UNP Q9NZ08
B	976	HIS	-	expression tag	UNP Q9NZ08
B	977	HIS	-	expression tag	UNP Q9NZ08
B	978	HIS	-	expression tag	UNP Q9NZ08
B	979	HIS	-	expression tag	UNP Q9NZ08
B	980	HIS	-	expression tag	UNP Q9NZ08
C	346	ASP	GLY	conflict	UNP Q9NZ08
C	514	ARG	GLY	conflict	UNP Q9NZ08
C	528	ARG	LYS	conflict	UNP Q9NZ08
C	730	GLU	GLN	conflict	UNP Q9NZ08
C	949	LEU	-	expression tag	UNP Q9NZ08
C	950	GLU	-	expression tag	UNP Q9NZ08
C	951	ARG	-	expression tag	UNP Q9NZ08
C	952	MET	-	expression tag	UNP Q9NZ08
C	953	LEU	-	expression tag	UNP Q9NZ08
C	954	GLU	-	expression tag	UNP Q9NZ08
C	955	SER	-	expression tag	UNP Q9NZ08
C	956	ARG	-	expression tag	UNP Q9NZ08
C	957	GLY	-	expression tag	UNP Q9NZ08
C	958	PRO	-	expression tag	UNP Q9NZ08
C	959	PHE	-	expression tag	UNP Q9NZ08
C	960	GLU	-	expression tag	UNP Q9NZ08
C	961	GLN	-	expression tag	UNP Q9NZ08
C	962	LYS	-	expression tag	UNP Q9NZ08
C	963	LEU	-	expression tag	UNP Q9NZ08
C	964	ILE	-	expression tag	UNP Q9NZ08
C	965	SER	-	expression tag	UNP Q9NZ08
C	966	GLU	-	expression tag	UNP Q9NZ08
C	967	GLU	-	expression tag	UNP Q9NZ08
C	968	ASP	-	expression tag	UNP Q9NZ08
C	969	LEU	-	expression tag	UNP Q9NZ08
C	970	ASN	-	expression tag	UNP Q9NZ08
C	971	MET	-	expression tag	UNP Q9NZ08
C	972	HIS	-	expression tag	UNP Q9NZ08
C	973	THR	-	expression tag	UNP Q9NZ08
C	974	GLU	-	expression tag	UNP Q9NZ08
C	975	HIS	-	expression tag	UNP Q9NZ08
C	976	HIS	-	expression tag	UNP Q9NZ08
C	977	HIS	-	expression tag	UNP Q9NZ08
C	978	HIS	-	expression tag	UNP Q9NZ08
C	979	HIS	-	expression tag	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
C	980	HIS	-	expression tag	UNP Q9NZ08

- Molecule 2 is a protein called Phosphinic inhibitor DG014.

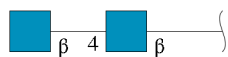
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	5	Total	C	N	O	P	0	0	0
			46	34	4	7	1			
2	E	5	Total	C	N	O	P	0	0	0
			46	34	4	7	1			
2	F	5	Total	C	N	O	P	0	0	0
			46	34	4	7	1			

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



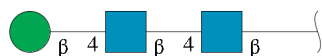
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	4	Total	C	N	O		0	0	0
			50	28	2	20				

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O		0	0	0
			28	16	2	10				
4	K	2	Total	C	N	O		0	0	0
			28	16	2	10				
4	L	2	Total	C	N	O		0	0	0
			28	16	2	10				

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



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		
6	C	1	Total	Zn	0	0
			1	1		

- Molecule 7 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	X	0	0
			1	1		
7	B	1	Total	X	0	0
			1	1		
7	C	1	Total	X	0	0
			1	1		

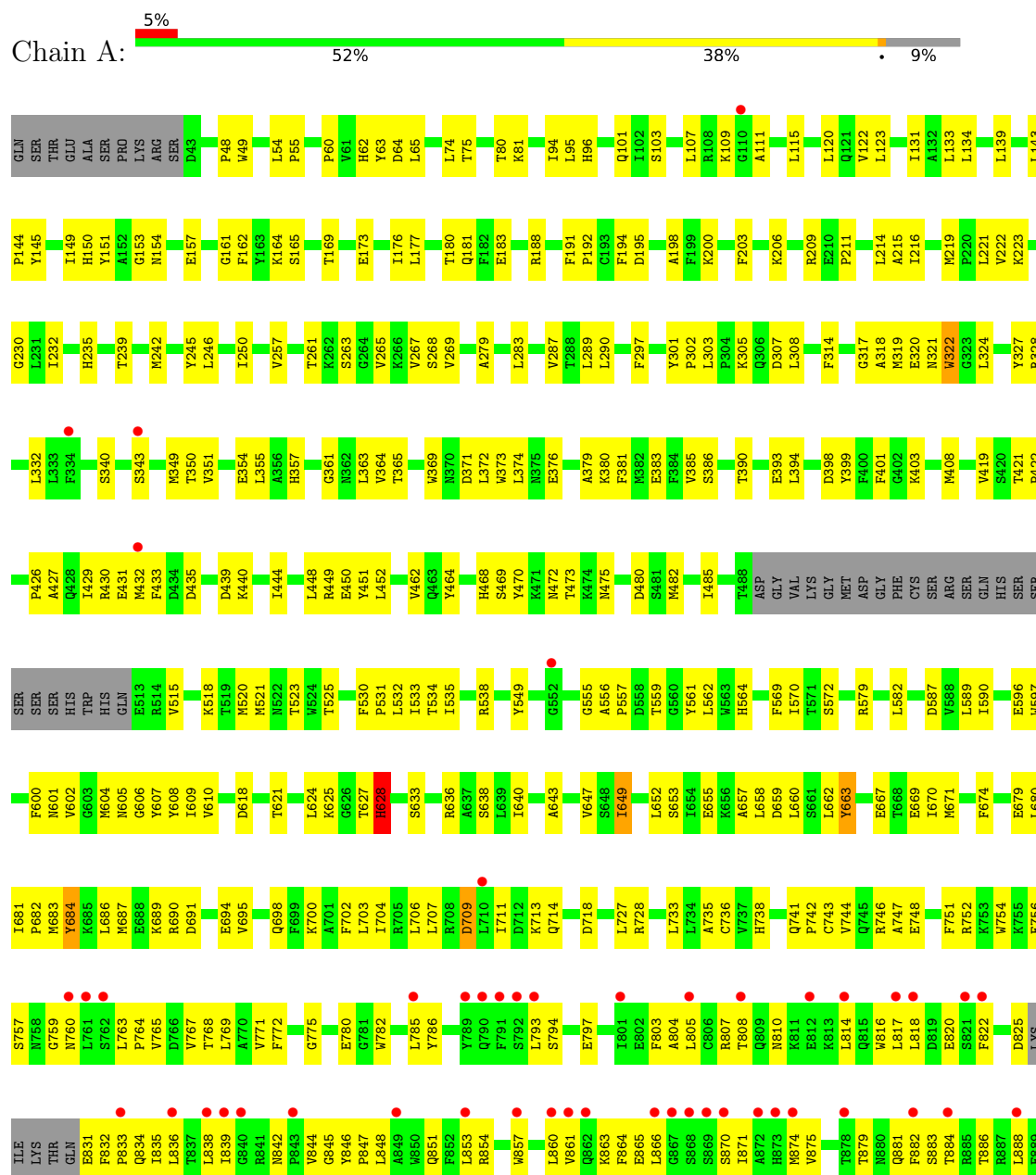
- Molecule 8 is water.

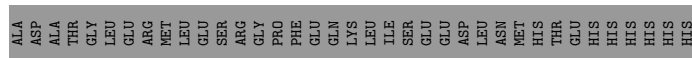
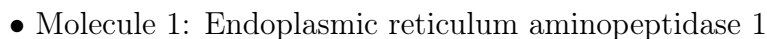
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	14	Total	O	0	0
			14	14		
8	B	14	Total	O	0	0
			14	14		
8	C	8	Total	O	0	0
			8	8		

3 Residue-property plots

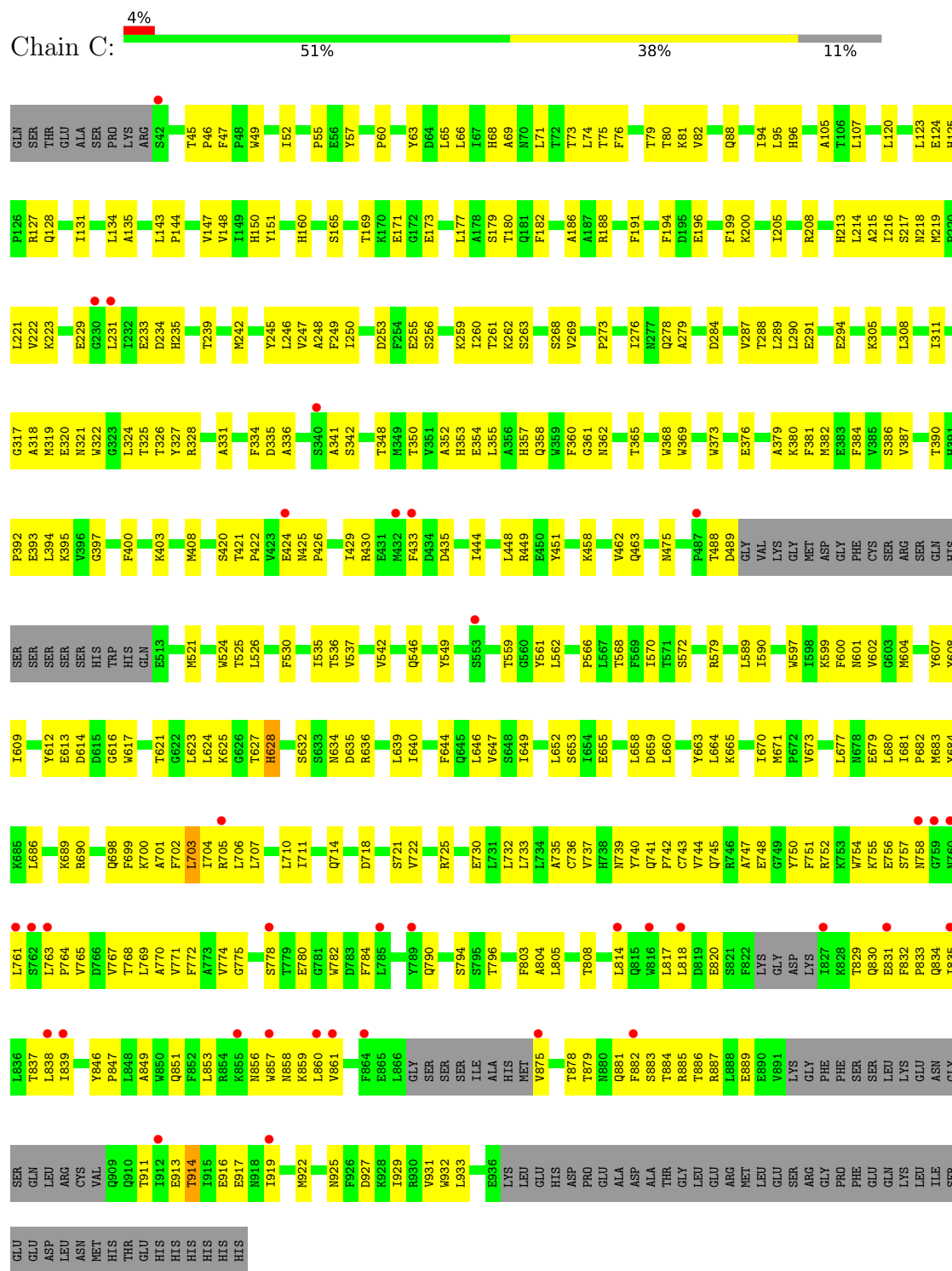
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

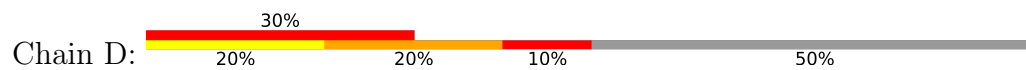


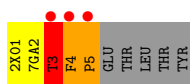


• Molecule 1: Endoplasmic reticulum aminopeptidase 1

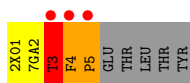
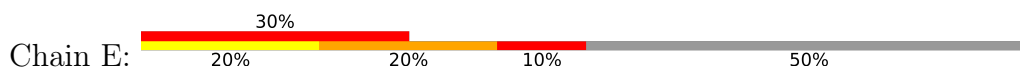


• Molecule 2: Phosphinic inhibitor DG014

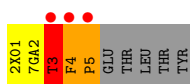
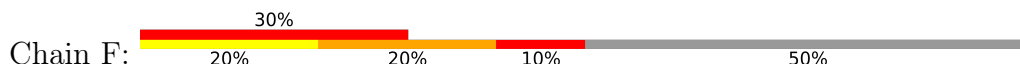




- Molecule 2: Phosphinic inhibitor DG014



- Molecule 2: Phosphinic inhibitor DG014



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



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



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



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



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

Chain I:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain J:  33% 67%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.14Å 234.70Å 132.28Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	56.06 – 2.92 67.31 – 2.92	Depositor EDS
% Data completeness (in resolution range)	81.7 (56.06-2.92) 74.5 (67.31-2.92)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.198 , 0.256 0.198 , 0.256	Depositor DCC
R_{free} test set	2987 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20671	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: ZN, 7GA, UNX, 2X0, MAN, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/7072	0.50	0/9601
1	B	0.32	0/6877	0.48	0/9357
1	C	0.32	0/6851	0.50	0/9318
2	D	3.53	4/26 (15.4%)	1.15	0/35
2	E	3.54	4/26 (15.4%)	1.11	0/35
2	F	3.53	4/26 (15.4%)	1.05	0/35
All	All	0.39	12/20878 (0.1%)	0.50	0/28381

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5	PRO	N-CD	10.84	1.63	1.47
2	E	5	PRO	N-CD	10.81	1.62	1.47
2	F	5	PRO	N-CD	10.80	1.62	1.47
2	F	5	PRO	N-CA	-8.31	1.33	1.47
2	D	5	PRO	N-CA	-8.26	1.33	1.47

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	6895	0	6764	346	0
1	B	6705	0	6432	391	0
1	C	6679	0	6464	347	0
2	D	46	0	47	49	0
2	E	46	0	48	66	0
2	F	46	0	48	63	0
3	G	50	0	43	0	0
4	H	28	0	25	2	0
4	K	28	0	25	1	0
4	L	28	0	25	3	0
5	I	39	0	34	9	0
5	J	39	0	34	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	14	0	0	2	0
8	B	14	0	0	1	0
8	C	8	0	0	0	0
All	All	20671	0	19989	1189	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 29.

The worst 5 of 1189 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:B:423:VAL:CG1	1:B:429:ILE:HG12	1.52	1.38
1:B:430:ARG:CB	2:E:1:2X0:H12	1.60	1.28
1:C:403:LYS:NZ	2:F:5:PRO:HD3	1.50	1.26
1:B:430:ARG:HB2	2:E:1:2X0:C18	1.68	1.23
1:C:426:PRO:O	1:C:430:ARG:HB2	1.32	1.22

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	855/948 (90%)	806 (94%)	47 (6%)	2 (0%)	47	77
1	B	854/948 (90%)	794 (93%)	55 (6%)	5 (1%)	25	57
1	C	835/948 (88%)	795 (95%)	38 (5%)	2 (0%)	47	77
2	D	2/10 (20%)	0	1 (50%)	1 (50%)	0	0
2	E	2/10 (20%)	0	1 (50%)	1 (50%)	0	0
2	F	2/10 (20%)	0	2 (100%)	0	100	100
All	All	2550/2874 (89%)	2395 (94%)	144 (6%)	11 (0%)	34	65

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	903	SER
1	C	820	GLU
1	B	795	SER
2	D	3	THR
1	B	46	PRO

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	756/846 (89%)	744 (98%)	12 (2%)	62	85
1	B	709/846 (84%)	694 (98%)	15 (2%)	53	80
1	C	717/846 (85%)	706 (98%)	11 (2%)	65	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	3/8 (38%)	2 (67%)	1 (33%)	0	0
2	E	3/8 (38%)	2 (67%)	1 (33%)	0	0
2	F	3/8 (38%)	2 (67%)	1 (33%)	0	0
All	All	2191/2562 (86%)	2150 (98%)	41 (2%)	57	83

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	268	SER
1	C	703	LEU
1	C	305	LYS
1	C	628	HIS
1	C	914	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	856	ASN
1	C	634	ASN
1	C	834	GLN
1	C	698	GLN
1	C	527	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 ⓘ

16 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	G	1	3,1	14,14,15	0.29	0	17,19,21	0.60	0
3	NAG	G	2	3	14,14,15	0.17	0	17,19,21	0.52	0
3	BMA	G	3	3	11,11,12	0.66	0	15,15,17	0.83	0
3	MAN	G	4	3	11,11,12	1.43	2 (18%)	15,15,17	1.24	1 (6%)
4	NAG	H	1	1,4	14,14,15	0.26	0	17,19,21	0.50	0
4	NAG	H	2	4	14,14,15	0.37	0	17,19,21	0.46	0
5	NAG	I	1	1,5	14,14,15	0.37	0	17,19,21	1.14	1 (5%)
5	NAG	I	2	5	14,14,15	0.31	0	17,19,21	0.87	1 (5%)
5	BMA	I	3	5	11,11,12	0.29	0	15,15,17	0.81	0
5	NAG	J	1	1,5	14,14,15	0.38	0	17,19,21	0.59	0
5	NAG	J	2	5	14,14,15	0.30	0	17,19,21	0.77	1 (5%)
5	BMA	J	3	5	11,11,12	1.14	2 (18%)	15,15,17	1.73	4 (26%)
4	NAG	K	1	1,4	14,14,15	0.18	0	17,19,21	0.51	0
4	NAG	K	2	4	14,14,15	0.57	0	17,19,21	0.64	0
4	NAG	L	1	1,4	14,14,15	0.32	0	17,19,21	0.50	0
4	NAG	L	2	4	14,14,15	0.27	0	17,19,21	0.77	1 (5%)

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	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	1/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	NAG	J	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	4	MAN	C4-C3	2.82	1.59	1.52
3	G	4	MAN	C1-C2	2.42	1.57	1.52
5	J	3	BMA	C4-C3	2.39	1.58	1.52
5	J	3	BMA	C4-C5	2.02	1.57	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	3	BMA	C1-C2-C3	-4.29	104.39	109.67
5	J	3	BMA	O5-C1-C2	-3.16	105.90	110.77
5	I	1	NAG	C2-N2-C7	-3.10	118.49	122.90
3	G	4	MAN	C1-O5-C5	2.55	115.65	112.19
5	J	2	NAG	O4-C4-C5	-2.51	103.06	109.30

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	2	NAG	C3-C2-N2-C7
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 18 short contacts:

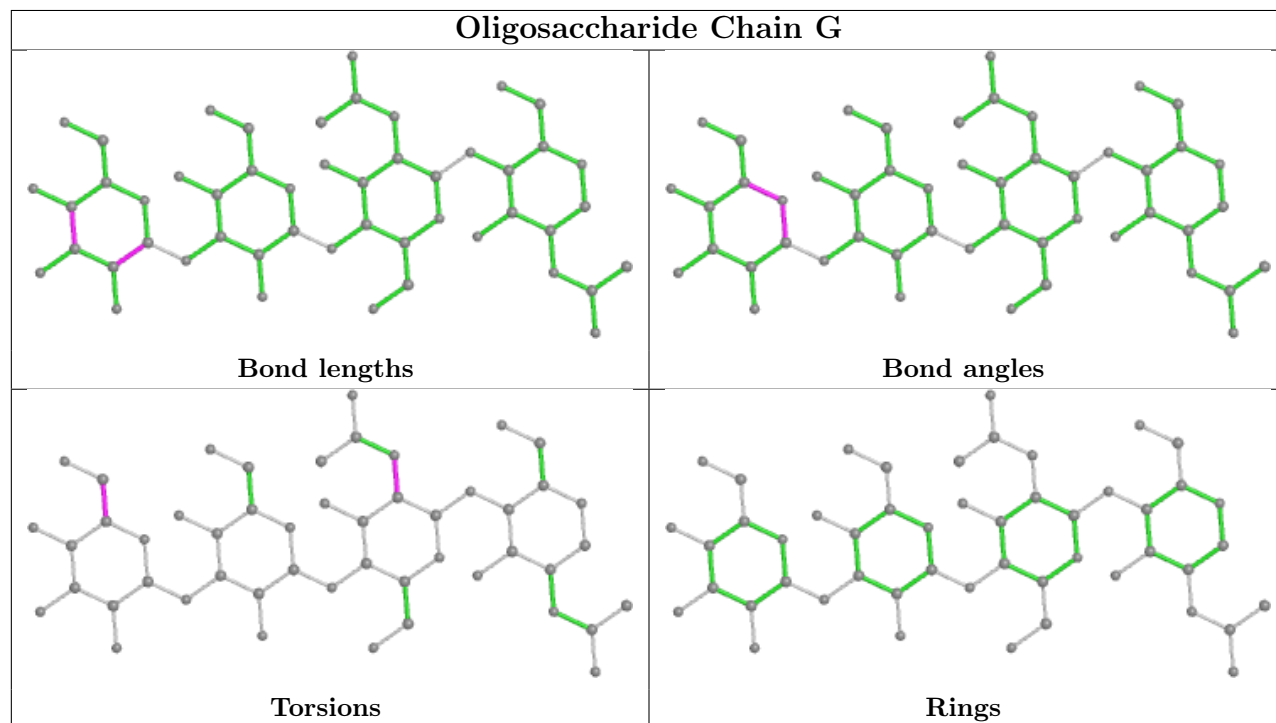
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	2	0
4	L	1	NAG	1	0
4	K	1	NAG	1	0
5	J	3	BMA	1	0
5	J	2	NAG	1	0
4	L	2	NAG	3	0
5	J	1	NAG	2	0

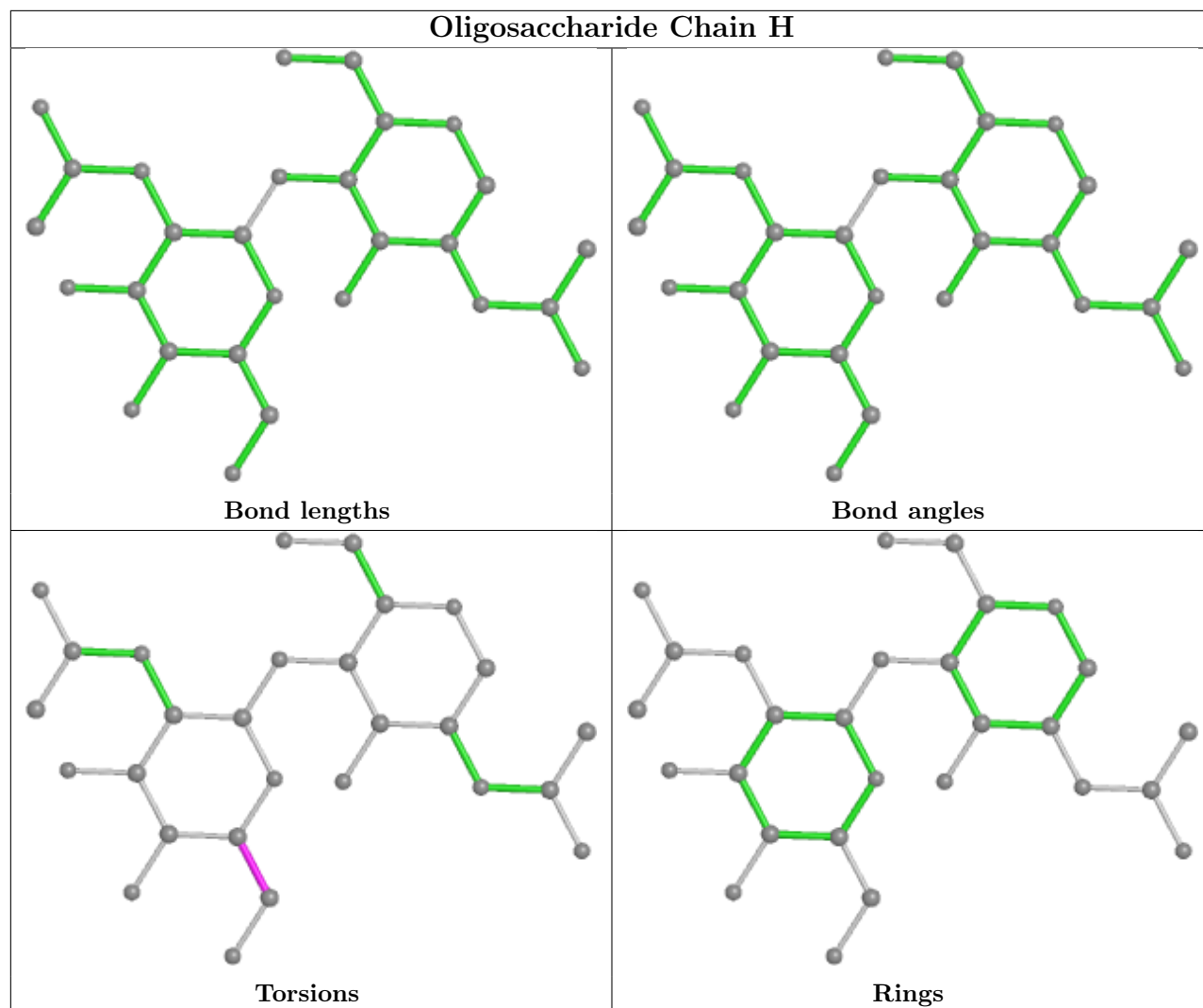
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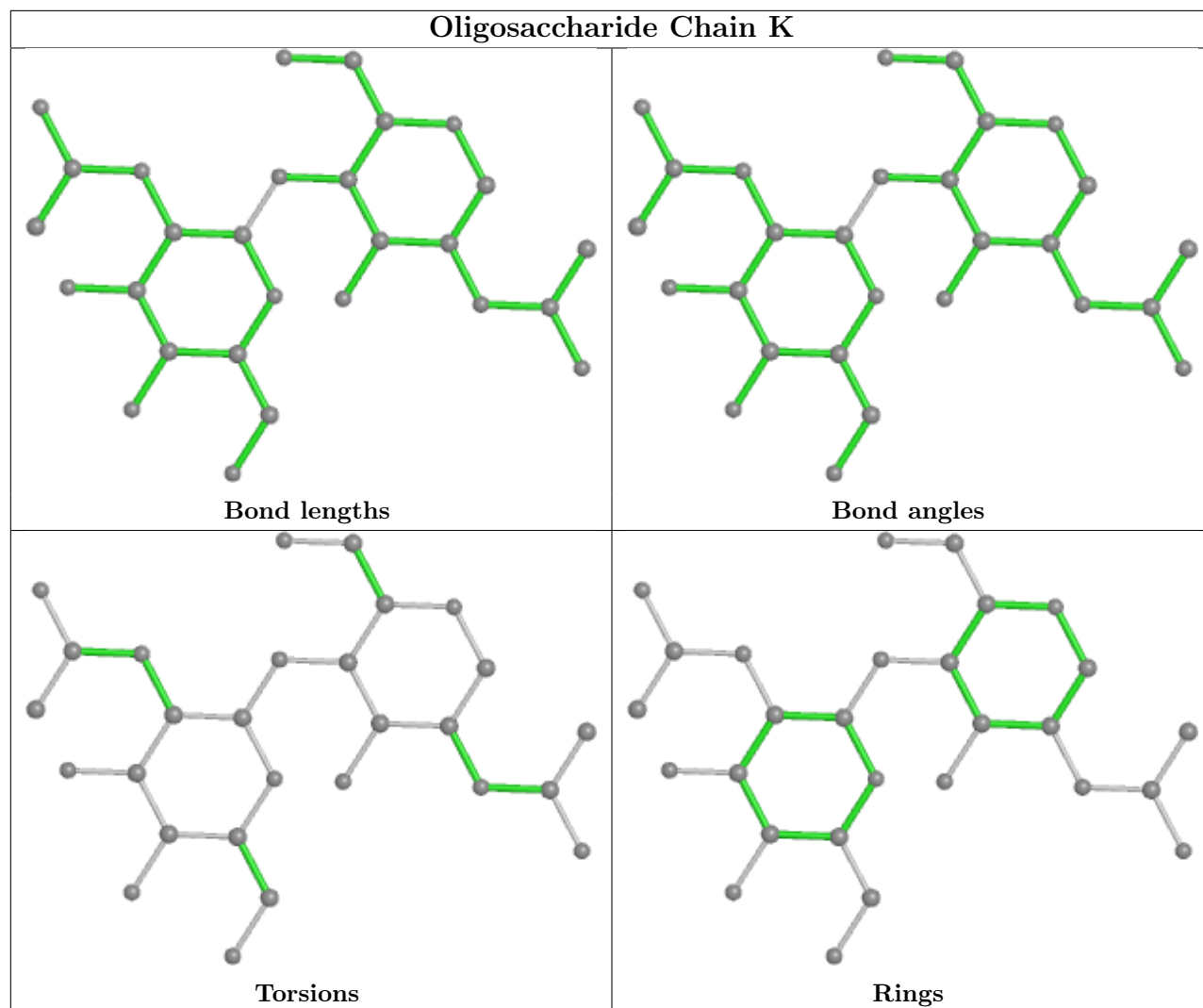
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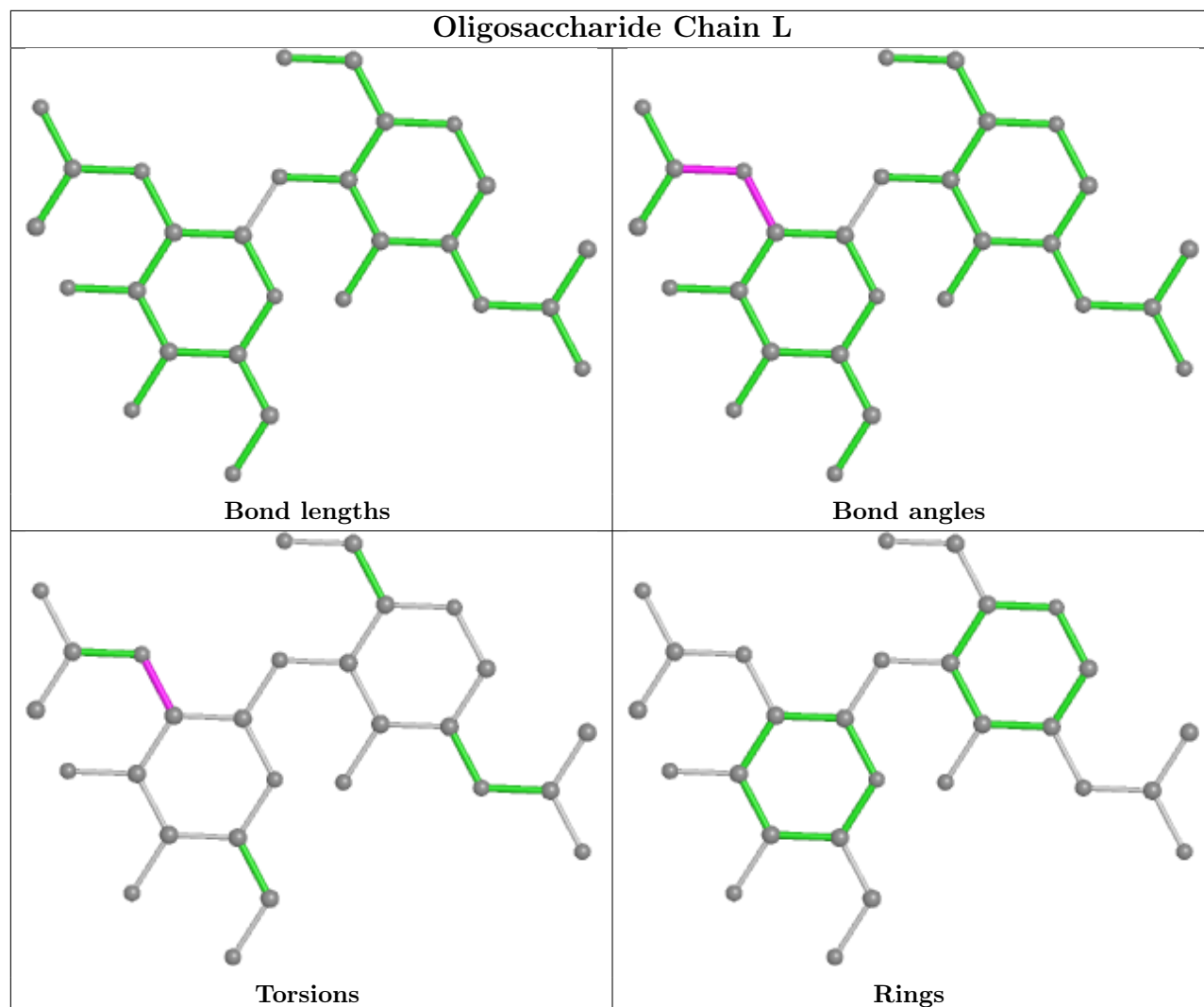
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1	NAG	9	0

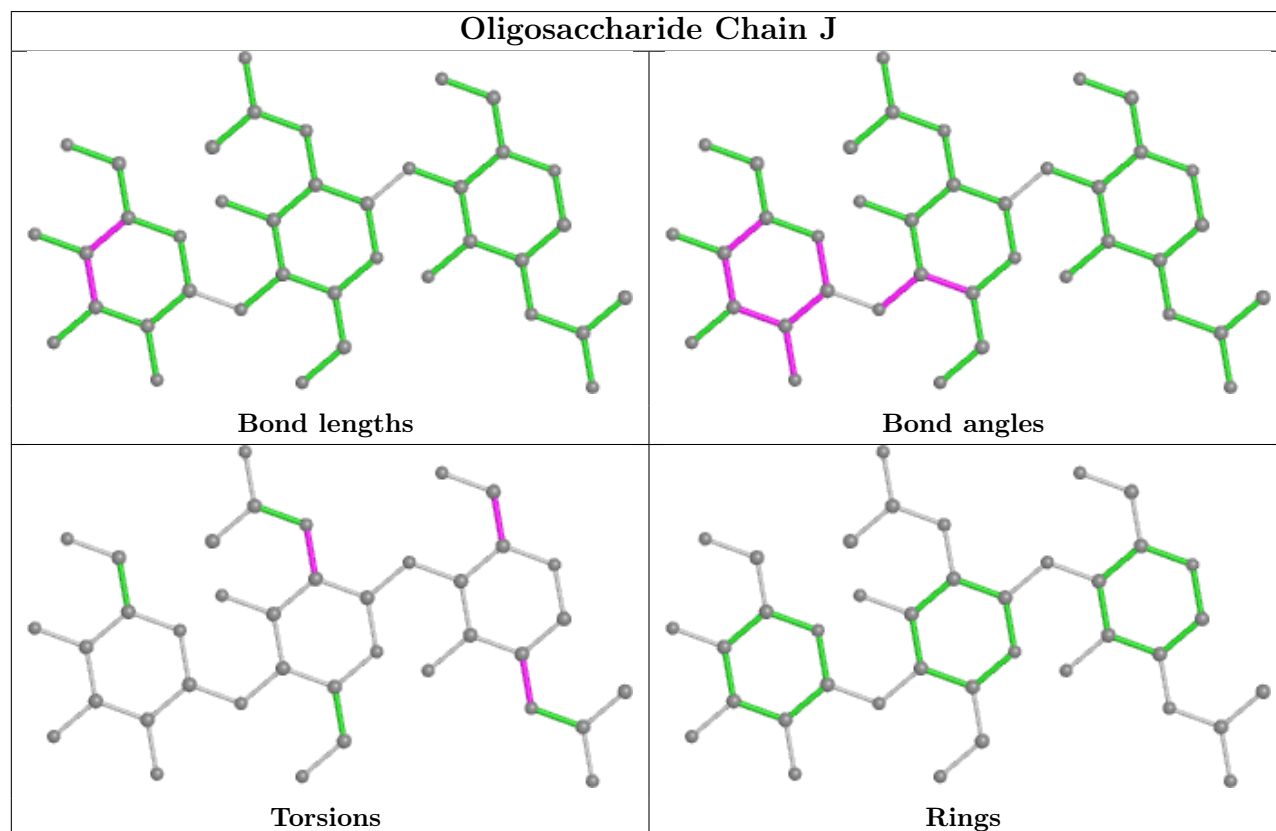
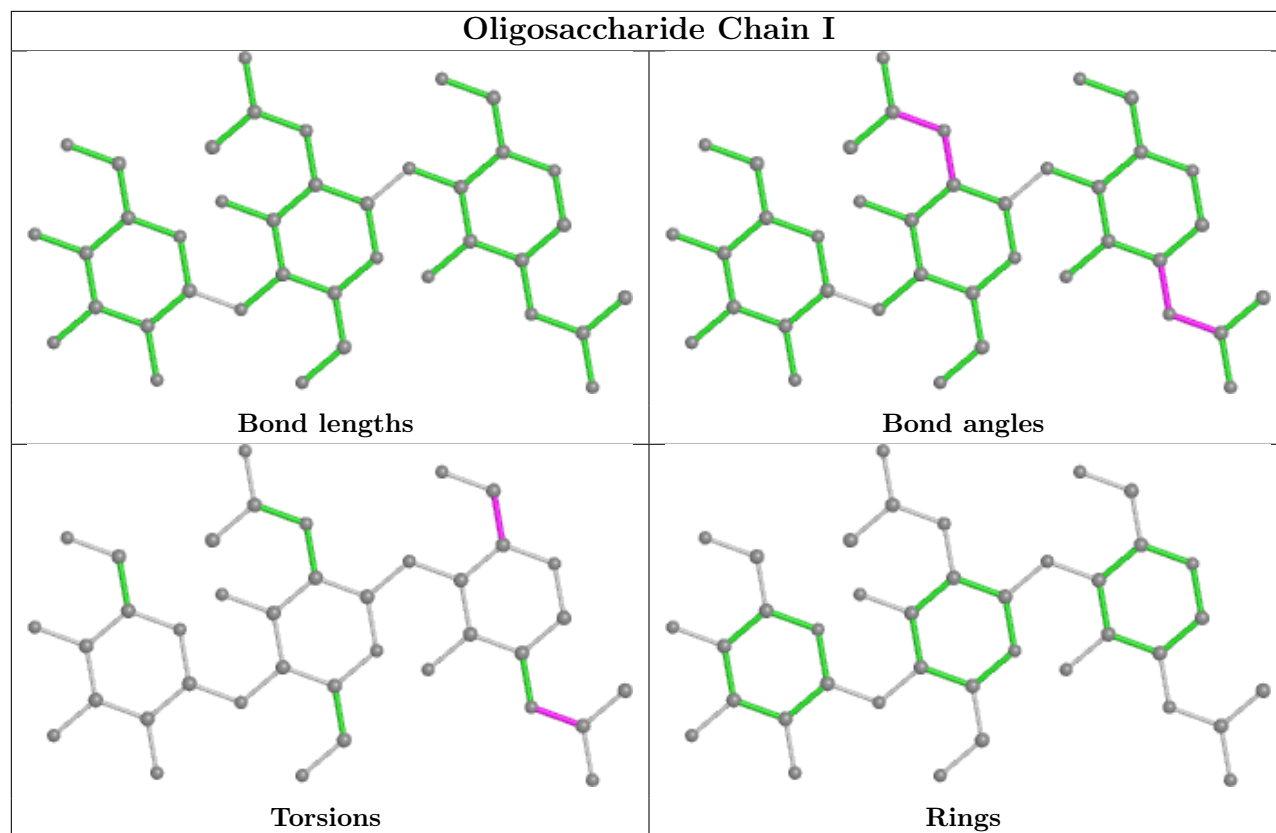
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic and 3 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	861/948 (90%)	0.32	52 (6%) 21 18	16, 50, 138, 178	0
1	B	858/948 (90%)	0.43	61 (7%) 16 13	27, 71, 167, 231	0
1	C	843/948 (88%)	0.20	36 (4%) 35 32	21, 51, 140, 197	0
2	D	3/10 (30%)	6.69	3 (100%) 0 0	56, 56, 58, 70	3 (100%)
2	E	3/10 (30%)	10.82	3 (100%) 0 0	54, 54, 61, 66	3 (100%)
2	F	3/10 (30%)	8.62	3 (100%) 0 0	60, 60, 63, 72	3 (100%)
All	All	2571/2874 (89%)	0.35	158 (6%) 21 18	16, 58, 151, 231	9 (0%)

The worst 5 of 158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	3	THR	16.0
1	B	792	SER	12.9
2	E	5	PRO	11.8
2	F	5	PRO	11.4
2	D	3	THR	9.1

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

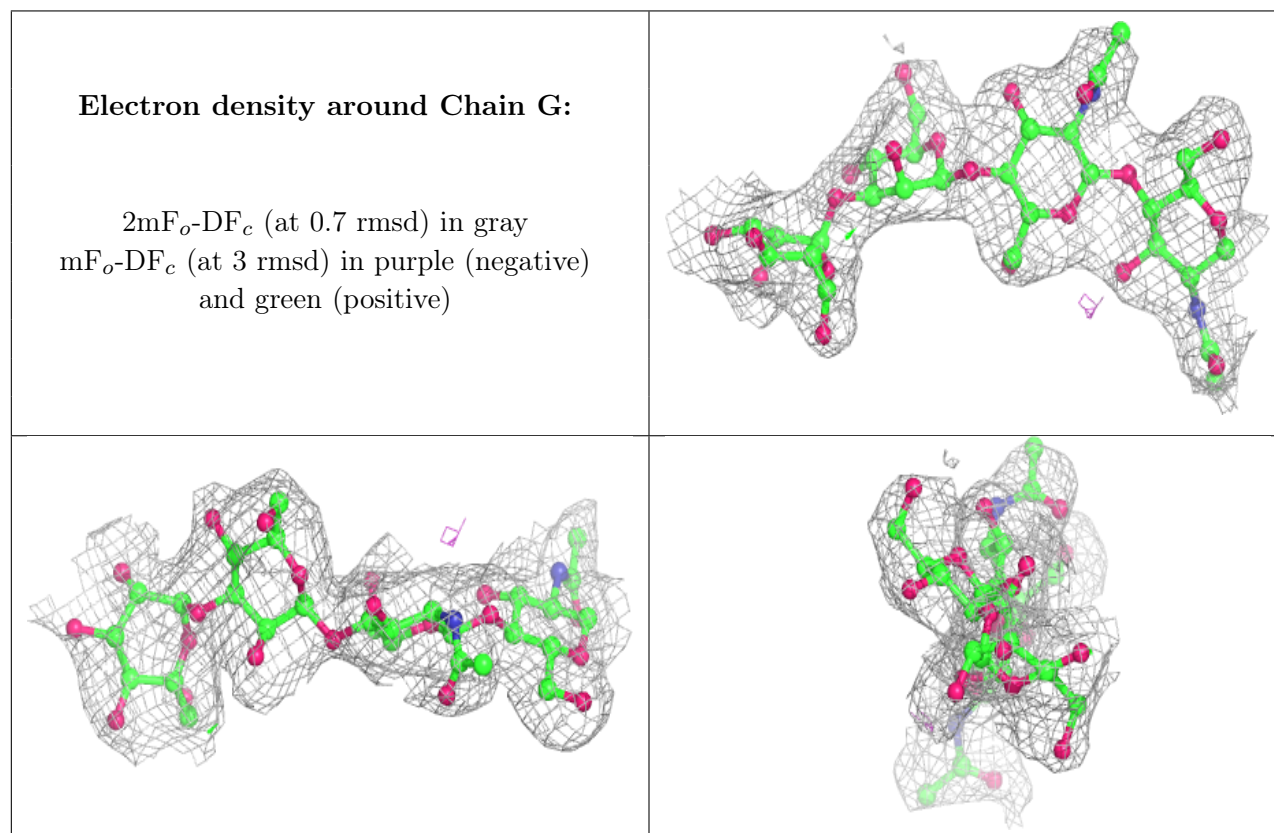
There are no non-standard protein/DNA/RNA residues in this entry.

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.

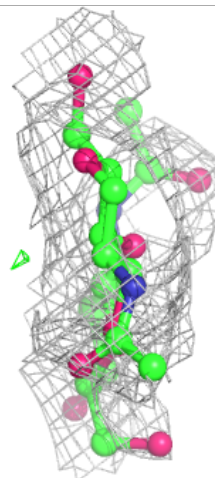
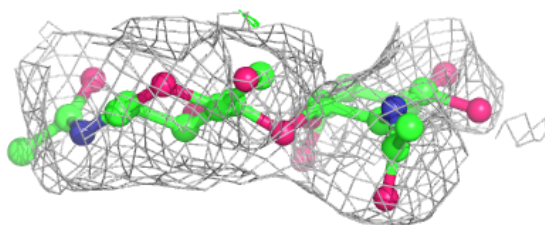
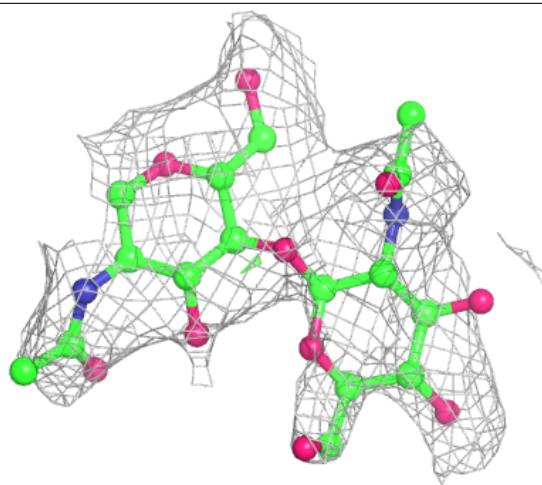
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	J	2	14/15	0.61	0.27	82,105,114,117	0
4	NAG	H	2	14/15	0.66	0.34	82,103,117,121	0
5	NAG	J	1	14/15	0.76	0.28	80,100,110,112	0
4	NAG	L	2	14/15	0.76	0.32	98,111,114,115	0
5	BMA	J	3	11/12	0.77	0.24	95,109,119,119	0
5	BMA	I	3	11/12	0.78	0.21	86,98,109,112	0
5	NAG	I	2	14/15	0.78	0.23	94,108,114,116	0
4	NAG	H	1	14/15	0.79	0.20	72,88,102,113	0
5	NAG	I	1	14/15	0.81	0.23	66,83,96,102	0
4	NAG	K	2	14/15	0.84	0.30	68,77,85,86	0
4	NAG	L	1	14/15	0.86	0.22	71,89,103,107	0
3	MAN	G	4	11/12	0.87	0.20	52,64,78,78	0
3	NAG	G	1	14/15	0.89	0.15	48,63,69,71	0
3	BMA	G	3	11/12	0.90	0.14	54,67,80,80	0
4	NAG	K	1	14/15	0.91	0.25	57,69,75,79	0
3	NAG	G	2	14/15	0.92	0.16	60,68,74,80	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.



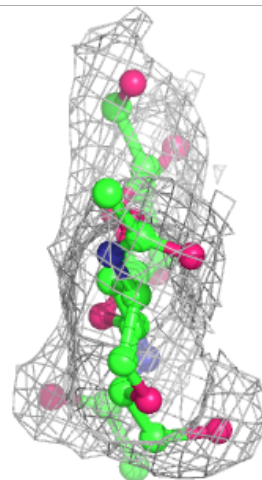
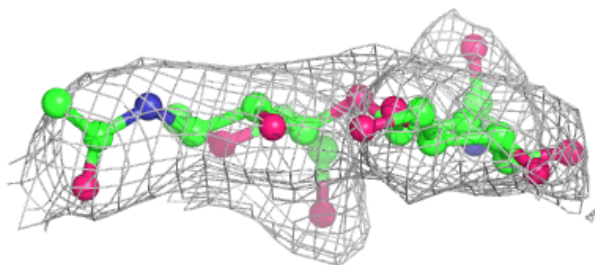
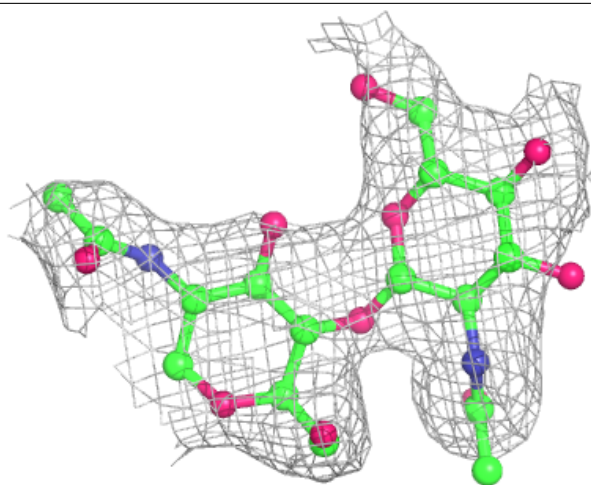
Electron density around Chain H:

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



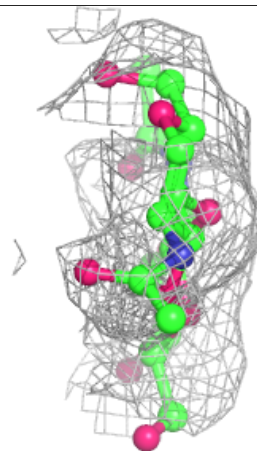
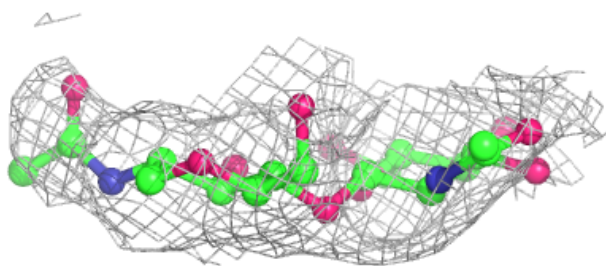
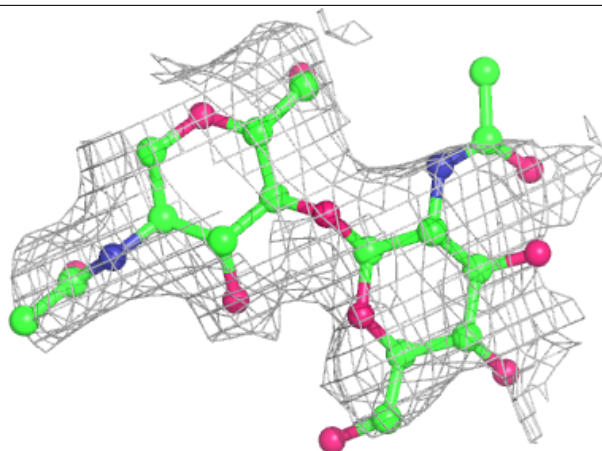
Electron density around Chain K:

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



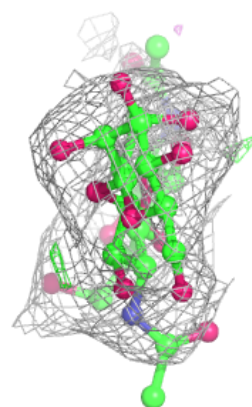
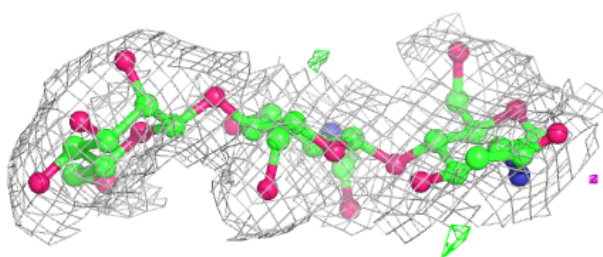
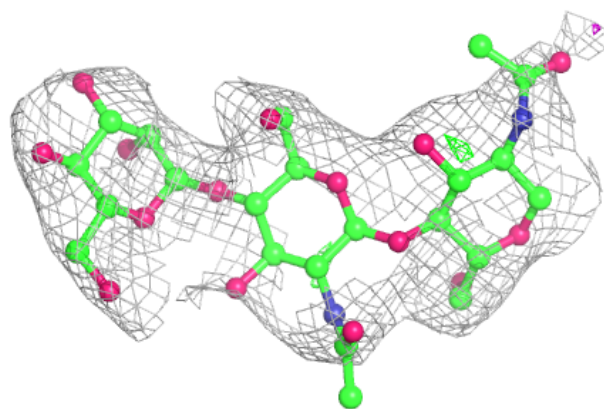
Electron density around Chain L:

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

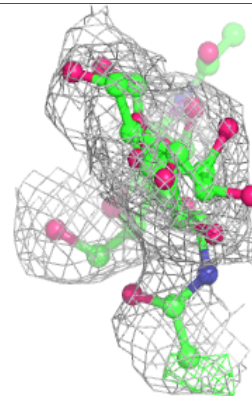
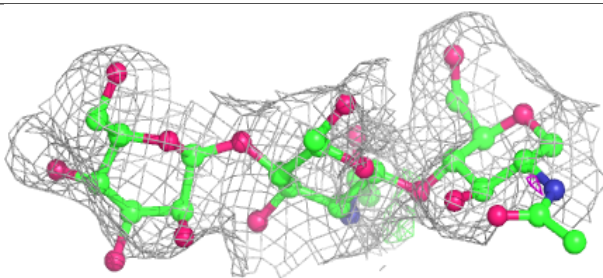
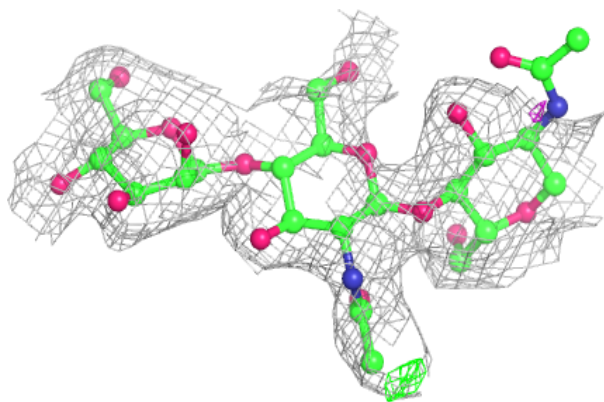


Electron density around Chain I:

$2mF_o-DF_c$ (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)



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	UNX	B	1002	1/1	0.70	0.37	27,27,27,27	0
7	UNX	C	1002	1/1	0.90	0.46	35,35,35,35	0
7	UNX	A	1002	1/1	0.94	0.24	35,35,35,35	0
6	ZN	C	1001	1/1	0.98	0.09	25,25,25,25	0
6	ZN	B	1001	1/1	0.98	0.11	36,36,36,36	0
6	ZN	A	1001	1/1	0.99	0.12	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.