



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 14, 2021 – 02:05 PM EDT

PDB ID : 7MXI  
Title : IgE-Fc in complex with DARPin<sub>s</sub> E2\_79 and E3\_53  
Authors : Pennington, L.F.; Jardetzky, T.J.  
Deposited on : 2021-05-19  
Resolution : 2.80 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](mailto: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.

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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	:	2.23.2
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)	:	2.23.2

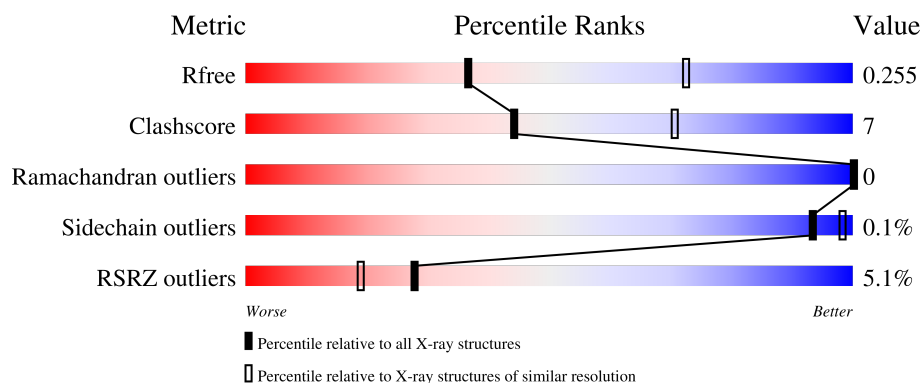
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	247	<div> <div>3%</div> <div>74%</div> <div>11%</div> <div>15%</div> </div>
1	B	247	<div> <div>70%</div> <div>15%</div> <div>15%</div> </div>
2	C	173	<div> <div>82%</div> <div>8%</div> <div>11%</div> </div>
2	D	173	<div> <div>82%</div> <div>8%</div> <div>11%</div> </div>
3	E	143	<div> <div>9%</div> <div>61%</div> <div>23%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	143	
4	G	3	
4	I	3	
5	H	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
4	NAG	G	2	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7485 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 IgE Fc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1604	1006	286	306	6			
1	B	211	Total	C	N	O	S	0	0	0
			1634	1024	296	308	6			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	299	ALA	-	expression tag	UNP P01854
A	300	PRO	-	expression tag	UNP P01854
A	301	MET	-	expression tag	UNP P01854
A	302	ALA	-	expression tag	UNP P01854
A	303	GLU	-	expression tag	UNP P01854
A	304	GLY	-	expression tag	UNP P01854
A	305	GLY	-	expression tag	UNP P01854
A	306	GLY	-	expression tag	UNP P01854
A	307	GLN	-	expression tag	UNP P01854
A	308	ASN	-	expression tag	UNP P01854
A	309	HIS	-	expression tag	UNP P01854
A	310	HIS	-	expression tag	UNP P01854
A	311	HIS	-	expression tag	UNP P01854
A	312	HIS	-	expression tag	UNP P01854
A	313	HIS	-	expression tag	UNP P01854
A	314	HIS	-	expression tag	UNP P01854
A	315	HIS	-	expression tag	UNP P01854
A	316	HIS	-	expression tag	UNP P01854
A	317	GLY	-	expression tag	UNP P01854
A	318	GLY	-	expression tag	UNP P01854
A	319	GLU	-	expression tag	UNP P01854
A	320	ASN	-	expression tag	UNP P01854
A	321	LEU	-	expression tag	UNP P01854
A	322	TYR	-	expression tag	UNP P01854
A	323	PHE	-	expression tag	UNP P01854

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Chain	Residue	Modelled	Actual	Comment	Reference
A	324	GLN	-	expression tag	UNP P01854
A	325	GLY	-	expression tag	UNP P01854
A	326	GLY	-	expression tag	UNP P01854
A	327	SER	-	expression tag	UNP P01854
B	299	ALA	-	expression tag	UNP P01854
B	300	PRO	-	expression tag	UNP P01854
B	301	MET	-	expression tag	UNP P01854
B	302	ALA	-	expression tag	UNP P01854
B	303	GLU	-	expression tag	UNP P01854
B	304	GLY	-	expression tag	UNP P01854
B	305	GLY	-	expression tag	UNP P01854
B	306	GLY	-	expression tag	UNP P01854
B	307	GLN	-	expression tag	UNP P01854
B	308	ASN	-	expression tag	UNP P01854
B	309	HIS	-	expression tag	UNP P01854
B	310	HIS	-	expression tag	UNP P01854
B	311	HIS	-	expression tag	UNP P01854
B	312	HIS	-	expression tag	UNP P01854
B	313	HIS	-	expression tag	UNP P01854
B	314	HIS	-	expression tag	UNP P01854
B	315	HIS	-	expression tag	UNP P01854
B	316	HIS	-	expression tag	UNP P01854
B	317	GLY	-	expression tag	UNP P01854
B	318	GLY	-	expression tag	UNP P01854
B	319	GLU	-	expression tag	UNP P01854
B	320	ASN	-	expression tag	UNP P01854
B	321	LEU	-	expression tag	UNP P01854
B	322	TYR	-	expression tag	UNP P01854
B	323	PHE	-	expression tag	UNP P01854
B	324	GLN	-	expression tag	UNP P01854
B	325	GLY	-	expression tag	UNP P01854
B	326	GLY	-	expression tag	UNP P01854
B	327	SER	-	expression tag	UNP P01854

- Molecule 2 is a protein called DARPin E3\_53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	154	Total	C	N	O	S	0	0	0
			1165	731	200	232	2			
2	D	154	Total	C	N	O	S	0	0	0
			1169	734	201	232	2			

- Molecule 3 is a protein called Anti-IgE Inhibitor E2\_79.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total 896	C 559	N 160	O 176	S 1	0	0	0
3	F	120	Total 901	C 564	N 162	O 174	S 1	0	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	MET	-	initiating methionine	UNP L7MTK7
E	-5	ARG	-	expression tag	UNP L7MTK7
E	-4	GLY	-	expression tag	UNP L7MTK7
E	-3	SER	-	expression tag	UNP L7MTK7
E	-2	HIS	-	expression tag	UNP L7MTK7
E	-1	HIS	-	expression tag	UNP L7MTK7
E	0	HIS	-	expression tag	UNP L7MTK7
E	1	HIS	-	expression tag	UNP L7MTK7
E	2	HIS	-	expression tag	UNP L7MTK7
E	3	HIS	-	expression tag	UNP L7MTK7
E	4	GLY	-	expression tag	UNP L7MTK7
E	5	SER	-	expression tag	UNP L7MTK7
E	6	ASP	-	expression tag	UNP L7MTK7
E	7	ASP	-	expression tag	UNP L7MTK7
E	8	ASP	-	expression tag	UNP L7MTK7
E	9	ASP	-	expression tag	UNP L7MTK7
E	10	LYS	-	expression tag	UNP L7MTK7
E	11	SER	-	expression tag	UNP L7MTK7
E	12	SER	-	expression tag	UNP L7MTK7
E	13	ASP	-	expression tag	UNP L7MTK7
E	14	LEU	-	expression tag	UNP L7MTK7
E	15	GLY	-	expression tag	UNP L7MTK7
E	16	LYS	-	expression tag	UNP L7MTK7
E	17	LYS	-	expression tag	UNP L7MTK7
E	18	LEU	-	expression tag	UNP L7MTK7
E	19	LEU	-	expression tag	UNP L7MTK7
E	20	GLU	-	expression tag	UNP L7MTK7
E	21	ALA	-	expression tag	UNP L7MTK7
E	22	ALA	-	expression tag	UNP L7MTK7
E	23	ARG	-	expression tag	UNP L7MTK7
E	24	ALA	-	expression tag	UNP L7MTK7
E	25	GLY	-	expression tag	UNP L7MTK7
E	26	GLN	-	expression tag	UNP L7MTK7
E	27	ASP	-	expression tag	UNP L7MTK7
E	28	ASP	-	expression tag	UNP L7MTK7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	29	GLU	-	expression tag	UNP L7MTK7
E	30	VAL	-	expression tag	UNP L7MTK7
E	31	ARG	-	expression tag	UNP L7MTK7
E	32	ILE	-	expression tag	UNP L7MTK7
E	33	LEU	-	expression tag	UNP L7MTK7
E	34	THR	-	expression tag	UNP L7MTK7
E	35	ALA	-	expression tag	UNP L7MTK7
E	36	ASN	-	expression tag	UNP L7MTK7
E	37	GLY	-	expression tag	UNP L7MTK7
E	38	ALA	-	expression tag	UNP L7MTK7
E	39	ASP	-	expression tag	UNP L7MTK7
E	40	VAL	-	expression tag	UNP L7MTK7
E	41	ASN	-	expression tag	UNP L7MTK7
E	42	ALA	-	expression tag	UNP L7MTK7
E	43	ASN	-	expression tag	UNP L7MTK7
E	44	ASP	-	expression tag	UNP L7MTK7
E	45	TYR	-	expression tag	UNP L7MTK7
E	46	TRP	-	expression tag	UNP L7MTK7
E	47	GLY	-	expression tag	UNP L7MTK7
E	48	HIS	-	expression tag	UNP L7MTK7
E	49	THR	-	expression tag	UNP L7MTK7
E	50	PRO	-	expression tag	UNP L7MTK7
E	51	LEU	-	expression tag	UNP L7MTK7
E	52	HIS	-	expression tag	UNP L7MTK7
E	53	LEU	-	expression tag	UNP L7MTK7
E	54	ALA	-	expression tag	UNP L7MTK7
E	55	ALA	-	expression tag	UNP L7MTK7
E	136	ASN	-	expression tag	UNP L7MTK7
F	-6	MET	-	initiating methionine	UNP L7MTK7
F	-5	ARG	-	expression tag	UNP L7MTK7
F	-4	GLY	-	expression tag	UNP L7MTK7
F	-3	SER	-	expression tag	UNP L7MTK7
F	-2	HIS	-	expression tag	UNP L7MTK7
F	-1	HIS	-	expression tag	UNP L7MTK7
F	0	HIS	-	expression tag	UNP L7MTK7
F	1	HIS	-	expression tag	UNP L7MTK7
F	2	HIS	-	expression tag	UNP L7MTK7
F	3	HIS	-	expression tag	UNP L7MTK7
F	4	GLY	-	expression tag	UNP L7MTK7
F	5	SER	-	expression tag	UNP L7MTK7
F	6	ASP	-	expression tag	UNP L7MTK7
F	7	ASP	-	expression tag	UNP L7MTK7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	8	ASP	-	expression tag	UNP L7MTK7
F	9	ASP	-	expression tag	UNP L7MTK7
F	10	LYS	-	expression tag	UNP L7MTK7
F	11	SER	-	expression tag	UNP L7MTK7
F	12	SER	-	expression tag	UNP L7MTK7
F	13	ASP	-	expression tag	UNP L7MTK7
F	14	LEU	-	expression tag	UNP L7MTK7
F	15	GLY	-	expression tag	UNP L7MTK7
F	16	LYS	-	expression tag	UNP L7MTK7
F	17	LYS	-	expression tag	UNP L7MTK7
F	18	LEU	-	expression tag	UNP L7MTK7
F	19	LEU	-	expression tag	UNP L7MTK7
F	20	GLU	-	expression tag	UNP L7MTK7
F	21	ALA	-	expression tag	UNP L7MTK7
F	22	ALA	-	expression tag	UNP L7MTK7
F	23	ARG	-	expression tag	UNP L7MTK7
F	24	ALA	-	expression tag	UNP L7MTK7
F	25	GLY	-	expression tag	UNP L7MTK7
F	26	GLN	-	expression tag	UNP L7MTK7
F	27	ASP	-	expression tag	UNP L7MTK7
F	28	ASP	-	expression tag	UNP L7MTK7
F	29	GLU	-	expression tag	UNP L7MTK7
F	30	VAL	-	expression tag	UNP L7MTK7
F	31	ARG	-	expression tag	UNP L7MTK7
F	32	ILE	-	expression tag	UNP L7MTK7
F	33	LEU	-	expression tag	UNP L7MTK7
F	34	THR	-	expression tag	UNP L7MTK7
F	35	ALA	-	expression tag	UNP L7MTK7
F	36	ASN	-	expression tag	UNP L7MTK7
F	37	GLY	-	expression tag	UNP L7MTK7
F	38	ALA	-	expression tag	UNP L7MTK7
F	39	ASP	-	expression tag	UNP L7MTK7
F	40	VAL	-	expression tag	UNP L7MTK7
F	41	ASN	-	expression tag	UNP L7MTK7
F	42	ALA	-	expression tag	UNP L7MTK7
F	43	ASN	-	expression tag	UNP L7MTK7
F	44	ASP	-	expression tag	UNP L7MTK7
F	45	TYR	-	expression tag	UNP L7MTK7
F	46	TRP	-	expression tag	UNP L7MTK7
F	47	GLY	-	expression tag	UNP L7MTK7
F	48	HIS	-	expression tag	UNP L7MTK7
F	49	THR	-	expression tag	UNP L7MTK7

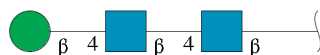
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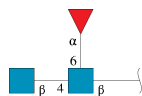
Chain	Residue	Modelled	Actual	Comment	Reference
F	50	PRO	-	expression tag	UNP L7MTK7
F	51	LEU	-	expression tag	UNP L7MTK7
F	52	HIS	-	expression tag	UNP L7MTK7
F	53	LEU	-	expression tag	UNP L7MTK7
F	54	ALA	-	expression tag	UNP L7MTK7
F	55	ALA	-	expression tag	UNP L7MTK7
F	136	ASN	-	expression tag	UNP L7MTK7

- Molecule 4 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
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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.

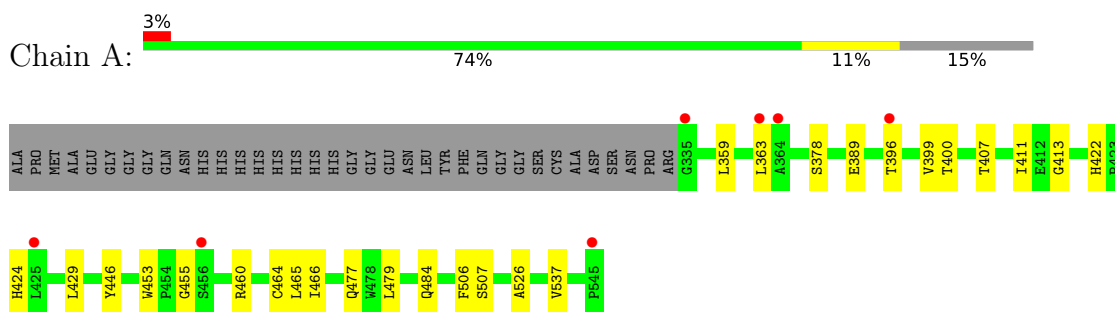


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

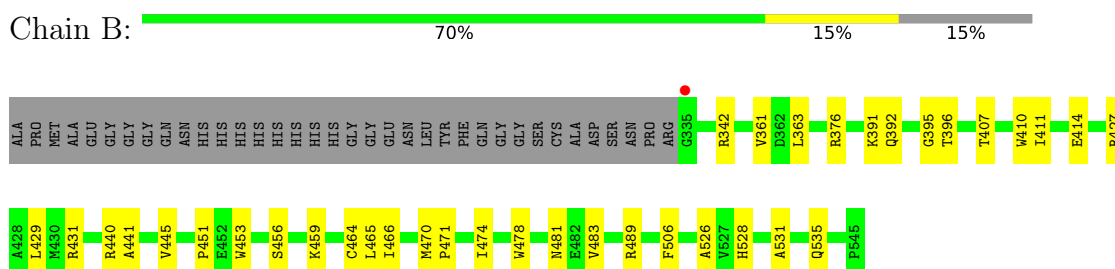
### 3 Residue-property plots [i](#)

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

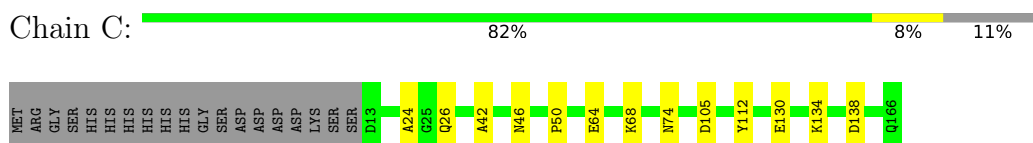
- Molecule 1: IgE Fc



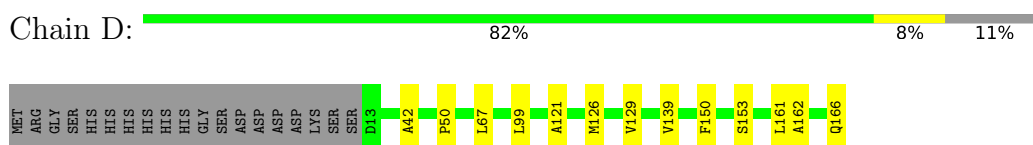
- Molecule 1: IgE Fc



- Molecule 2: DARPin E3\_53

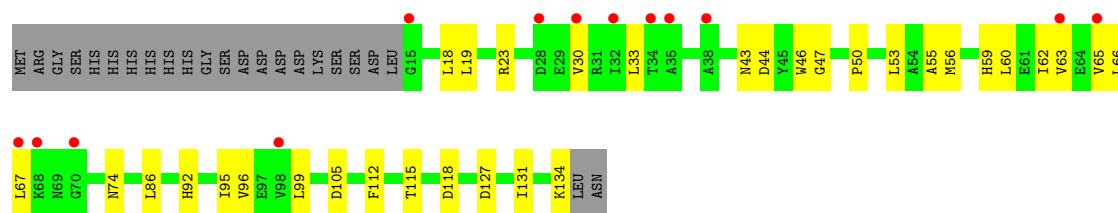


- Molecule 2: DARPin E3\_53

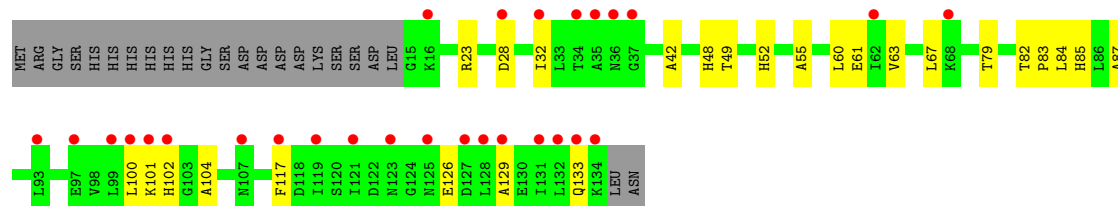


- Molecule 3: Anti-IgE Inhibitor E2\_79





● Molecule 3: Anti-IgE Inhibitor E2\_79



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



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.91Å 137.79Å 88.25Å 90.00° 105.68° 90.00°	Depositor
Resolution (Å)	38.74 – 2.80 38.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.74-2.80) 98.7 (38.74-2.80)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.213 , 0.256 0.213 , 0.255	Depositor DCC
$R_{free}$ test set	1278 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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	0.32	0/1646	0.53	0/2255
1	B	0.34	0/1677	0.64	2/2291 (0.1%)
2	C	0.28	0/1183	0.48	0/1608
2	D	0.28	0/1187	0.49	0/1612
3	E	0.31	0/910	0.59	0/1239
3	F	0.31	0/915	0.53	0/1243
All	All	0.31	0/7518	0.55	2/10248 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	427	ARG	CA-CB-CG	5.97	126.53	113.40
1	B	427	ARG	CB-CG-CD	5.72	126.48	111.60

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	1604	0	1518	23	0
1	B	1634	0	1581	22	1
2	C	1165	0	1129	9	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1169	0	1140	7	0
3	E	896	0	864	24	0
3	F	901	0	884	19	0
4	G	39	0	34	0	0
4	I	39	0	34	1	0
5	H	38	0	34	0	0
All	All	7485	0	7218	97	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 97 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)
3:E:50:PRO:HB2	3:E:66:LEU:HD21	1.69	0.74
2:C:74:ASN:HD21	2:C:105:ASP:H	1.35	0.73
1:A:453:TRP:HD1	1:A:455:GLY:H	1.37	0.71
3:F:82:THR:HG22	3:F:85:HIS:ND1	2.06	0.70
1:B:391:LYS:HE2	1:B:395:GLY:HA2	1.76	0.68

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:LYS:NZ	2:C:138:ASP:OD2[1_655]	2.18	0.02

## 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	209/247 (85%)	208 (100%)	1 (0%)	0	<b>100</b> <b>100</b>

*Continued on next page...*

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	209/247 (85%)	204 (98%)	5 (2%)	0	100	100
2	C	152/173 (88%)	150 (99%)	2 (1%)	0	100	100
2	D	152/173 (88%)	147 (97%)	5 (3%)	0	100	100
3	E	118/143 (82%)	115 (98%)	3 (2%)	0	100	100
3	F	118/143 (82%)	114 (97%)	4 (3%)	0	100	100
All	All	958/1126 (85%)	938 (98%)	20 (2%)	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	172/212 (81%)	172 (100%)	0	100	100
1	B	179/212 (84%)	179 (100%)	0	100	100
2	C	118/136 (87%)	118 (100%)	0	100	100
2	D	119/136 (88%)	119 (100%)	0	100	100
3	E	89/113 (79%)	88 (99%)	1 (1%)	73	92
3	F	90/113 (80%)	90 (100%)	0	100	100
All	All	767/922 (83%)	766 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	112	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	46	ASN

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Mol	Chain	Res	Type
2	C	74	ASN
3	F	78	ASN
3	E	74	ASN
1	B	417	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 ⓘ

9 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	$\# Z  > 2$
4	NAG	G	1	4,1	14,14,15	0.52	0	17,19,21	0.40	0
4	NAG	G	2	4	14,14,15	0.50	0	17,19,21	0.72	0
4	BMA	G	3	4	11,11,12	1.00	1 (9%)	15,15,17	1.30	2 (13%)
5	NAG	H	1	1,5	14,14,15	0.29	0	17,19,21	0.41	0
5	NAG	H	2	5	14,14,15	0.22	0	17,19,21	0.71	0
5	FUC	H	3	5	10,10,11	1.23	2 (20%)	14,14,16	1.18	2 (14%)
4	NAG	I	1	4,1	14,14,15	0.46	0	17,19,21	1.09	1 (5%)
4	NAG	I	2	4	14,14,15	0.26	0	17,19,21	1.57	2 (11%)
4	BMA	I	3	4	11,11,12	0.42	0	15,15,17	1.26	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.



'-' means no outliers of that kind were identified.

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	FUC	C2-C3	2.74	1.56	1.52
5	H	3	FUC	C1-C2	2.41	1.57	1.52
4	G	3	BMA	C4-C5	2.15	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	C4-C3-C2	-4.77	104.03	111.02
4	I	1	NAG	O4-C4-C3	-3.40	102.48	110.35
4	I	3	BMA	C1-C2-C3	2.93	113.27	109.67
5	H	3	FUC	C1-C2-C3	2.48	112.71	109.67
4	G	3	BMA	C1-C2-C3	-2.33	106.80	109.67

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

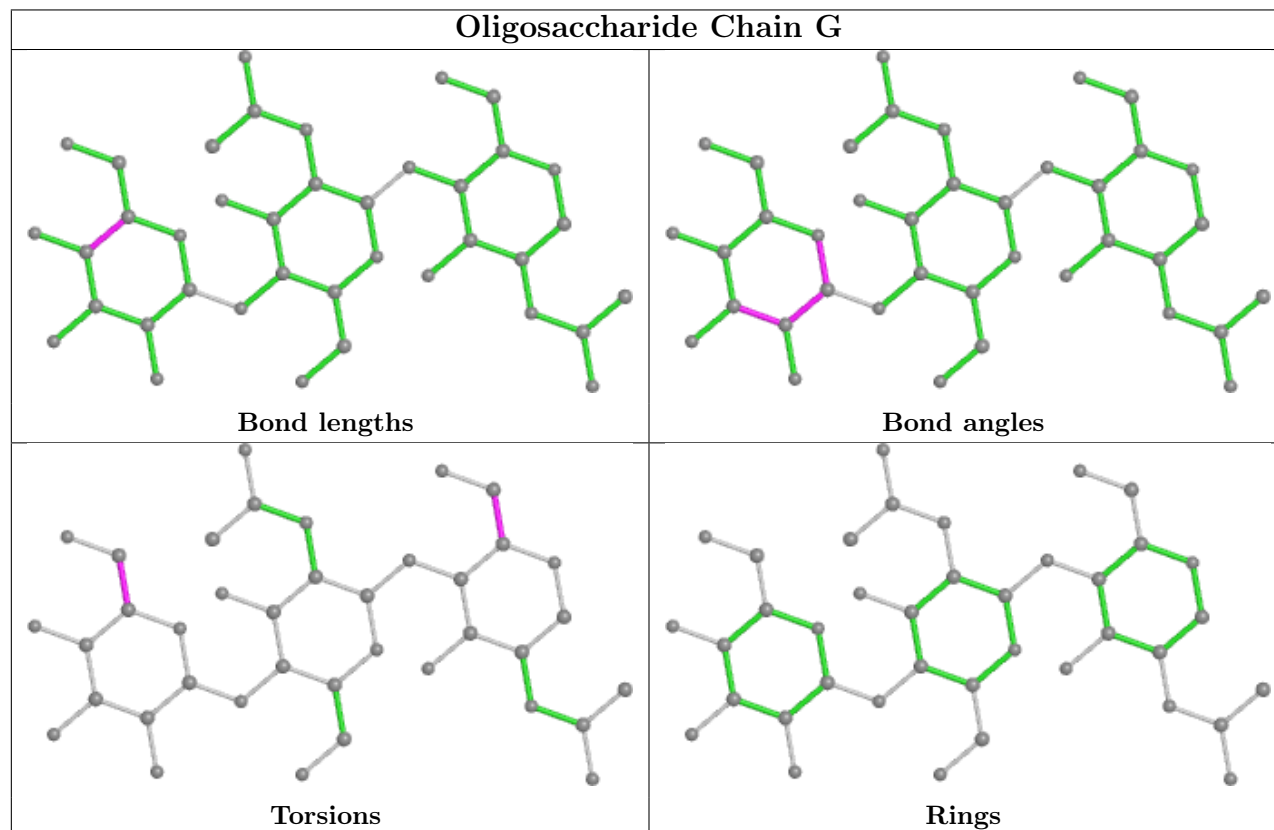
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	G	1	NAG	O5-C5-C6-O6

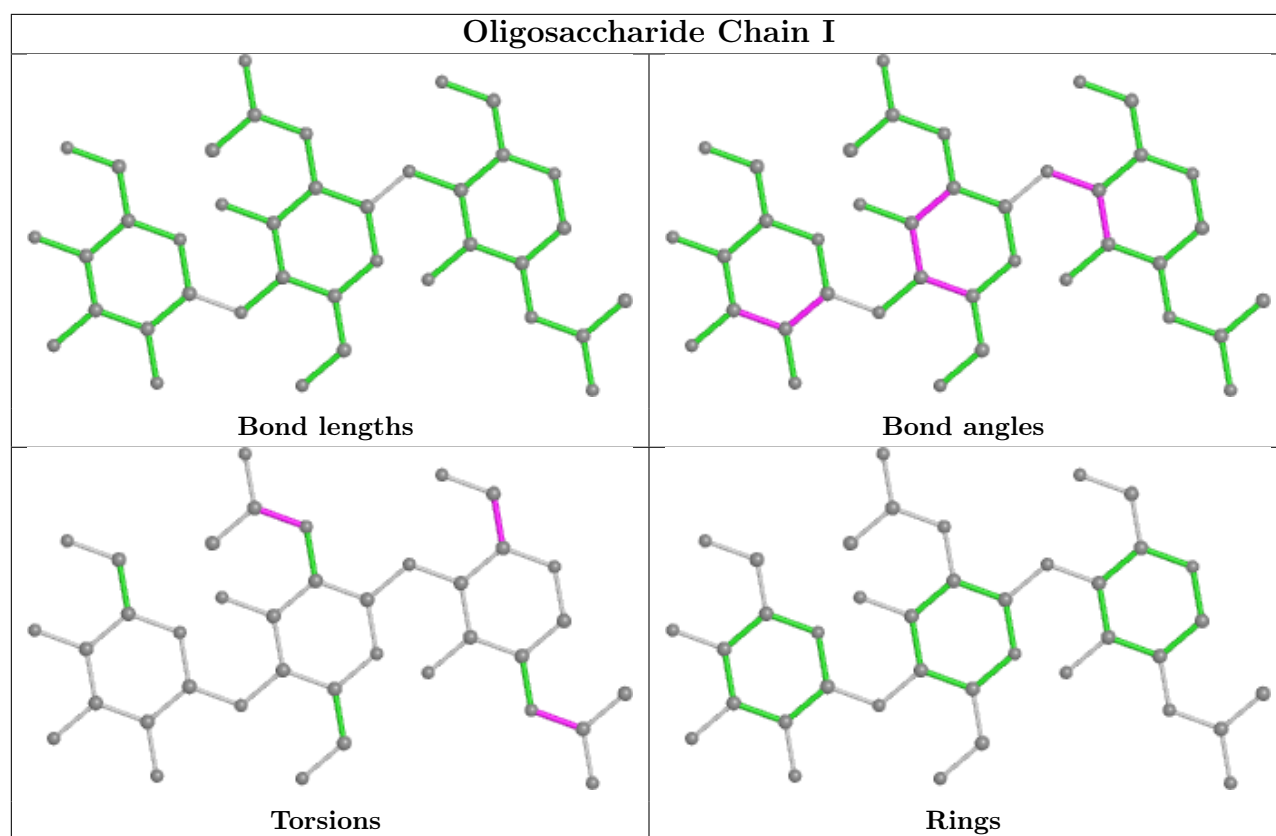
There are no ring outliers.

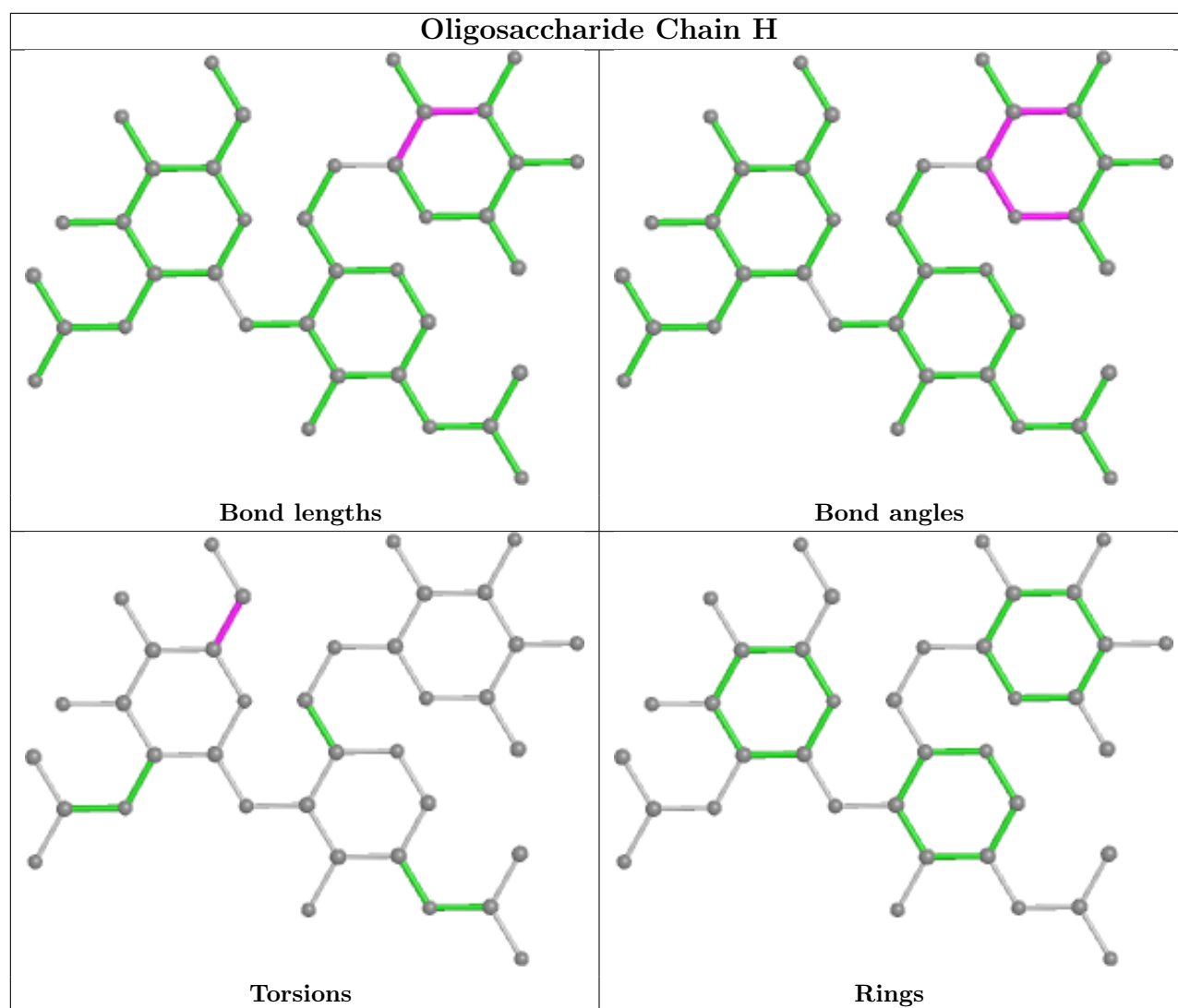
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	NAG	1	0

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







## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	211/247 (85%)	-0.02	7 (3%) 46 36	27, 50, 95, 109	0
1	B	211/247 (85%)	-0.12	1 (0%) 91 88	28, 46, 83, 107	0
2	C	154/173 (89%)	-0.23	0 100 100	32, 45, 62, 78	0
2	D	154/173 (89%)	-0.18	0 100 100	33, 48, 71, 85	0
3	E	120/143 (83%)	0.56	13 (10%) 5 3	47, 71, 101, 110	0
3	F	120/143 (83%)	1.07	28 (23%) 0 0	71, 107, 127, 136	0
All	All	970/1126 (86%)	0.11	49 (5%) 28 19	27, 53, 111, 136	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	65	VAL	4.6
3	E	67	LEU	4.3
3	F	100	LEU	4.2
3	F	132	LEU	4.2
1	A	545	PRO	3.9

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

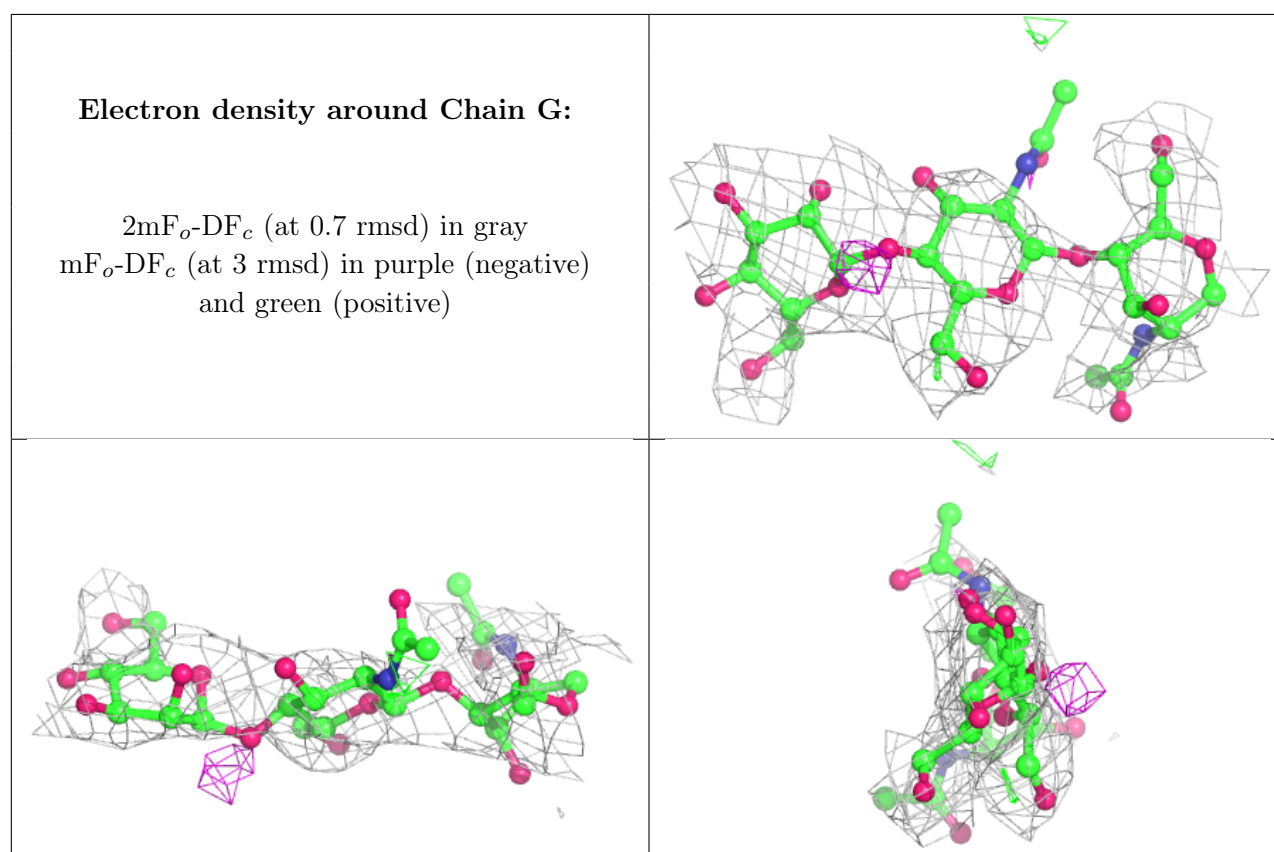
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 95<sup>th</sup> 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.

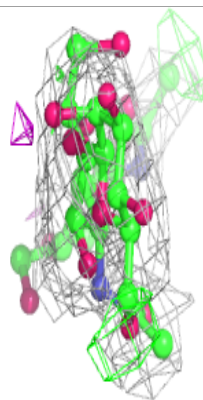
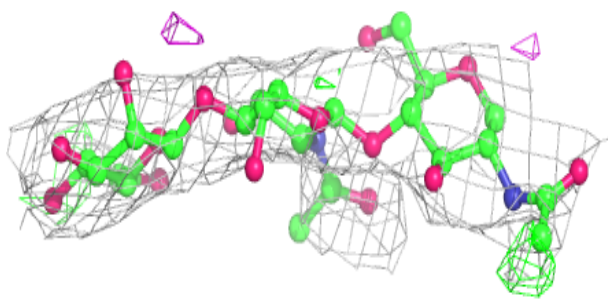
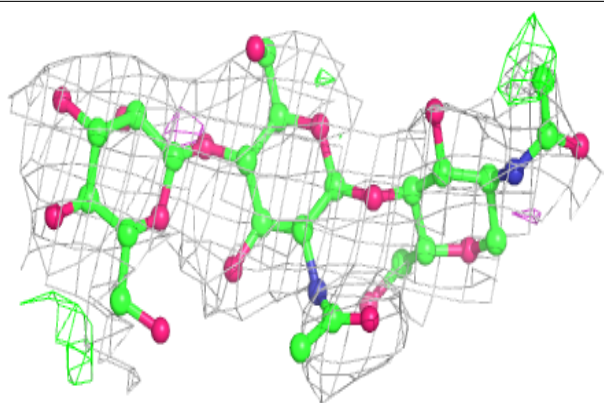
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	G	2	14/15	0.62	0.42	89,116,127,133	0
4	BMA	G	3	11/12	0.65	0.28	72,98,108,109	0
5	FUC	H	3	10/11	0.67	0.31	78,89,106,128	0
4	NAG	G	1	14/15	0.73	0.39	109,118,127,131	0
4	NAG	I	2	14/15	0.78	0.27	85,91,104,107	0
4	NAG	I	1	14/15	0.78	0.30	105,112,118,129	0
4	BMA	I	3	11/12	0.81	0.33	77,88,95,97	0
5	NAG	H	2	14/15	0.83	0.20	87,91,99,100	0
5	NAG	H	1	14/15	0.84	0.17	77,84,94,96	0

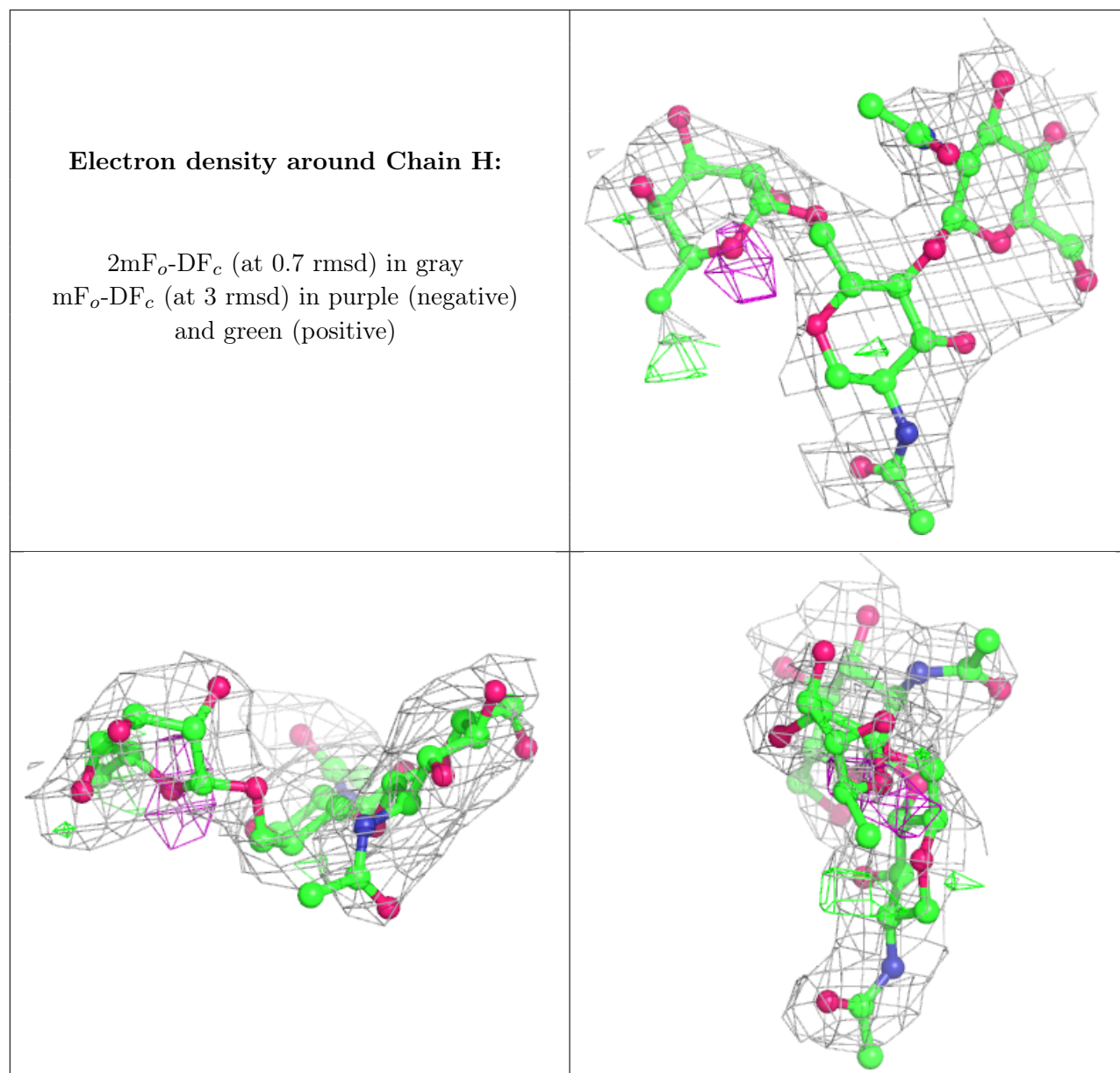
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**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)





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.