



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 11, 2024 – 06:05 PM EDT

PDB ID : 8UDZ  
Title : The Structure of LTBP-49247 Fab Bound to TGFbeta1 Small Latent Complex  
Authors : Streich Jr., F.C.; Nicholls, S.B.; Boston, C.J.; Ramachandran, S.  
Deposited on : 2023-09-29  
Resolution : 2.21 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.

The types of validation reports are described at

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

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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 : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

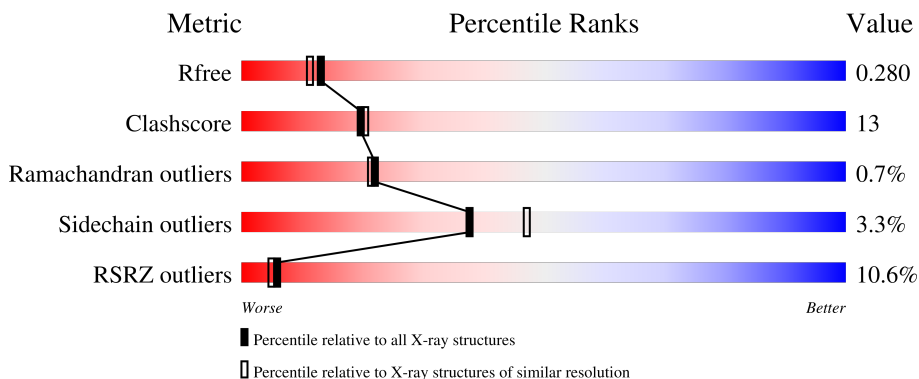
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	361	
1	B	361	
2	C	233	
2	E	233	
3	D	218	

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Mol	Chain	Length	Quality of chain
3	F	218	 88% 9% ..
4	G	5	 20% 80%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11329 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 Transforming growth factor beta-1 proprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	257	Total	C	N	O	S	0	0	0
			2062	1315	360	371	16			
1	B	294	Total	C	N	O	S	0	1	0
			2374	1520	413	424	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	SER	CYS	engineered mutation	UNP P01137
A	278	ALA	ARG	engineered mutation	UNP P01137
B	33	SER	CYS	engineered mutation	UNP P01137
B	278	ALA	ARG	engineered mutation	UNP P01137

- Molecule 2 is a protein called LTBP-49247 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	220	Total	C	N	O	S	0	0	0
			1654	1044	291	313	6			
2	E	223	Total	C	N	O	S	0	0	0
			1676	1057	295	318	6			

- Molecule 3 is a protein called LTBP-49247 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	214	Total	C	N	O	S	0	0	0
			1621	1006	270	340	5			
3	F	214	Total	C	N	O	S	0	0	0
			1621	1006	270	340	5			

- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	5	61	34	2	25	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	26	Total	O	0	0
			26	26		
6	B	30	Total	O	0	0
			30	30		
6	C	21	Total	O	0	0
			21	21		
6	D	30	Total	O	0	0
			30	30		

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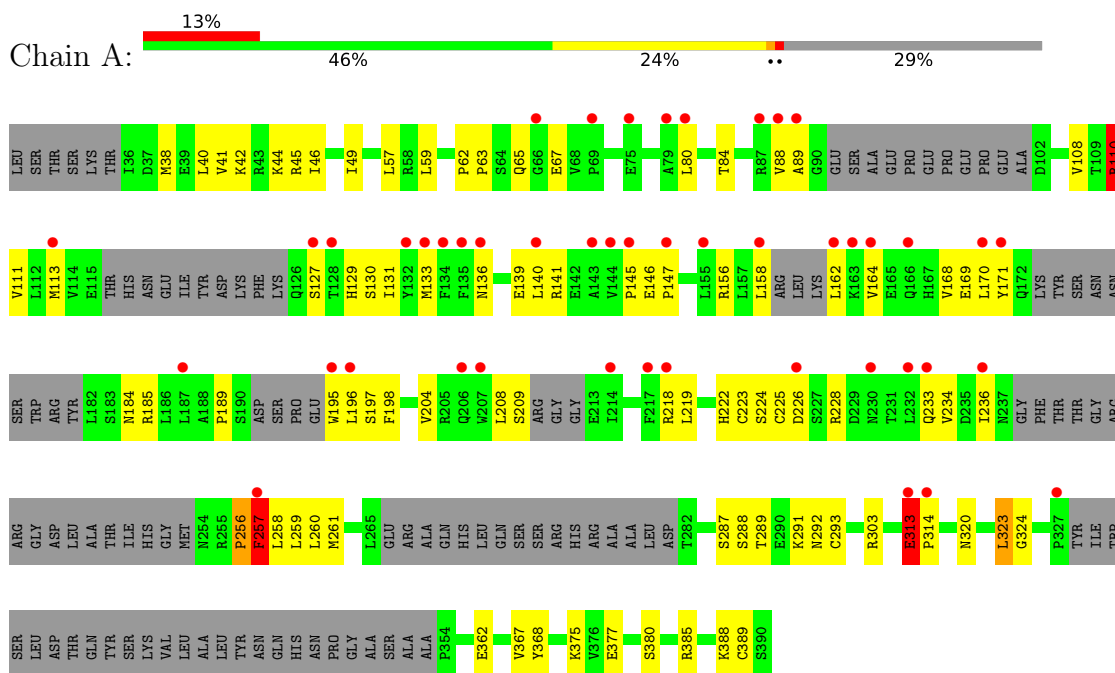
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	E	28	Total	O	0	0
			28	28		
6	F	97	Total	O	0	0
			97	97		

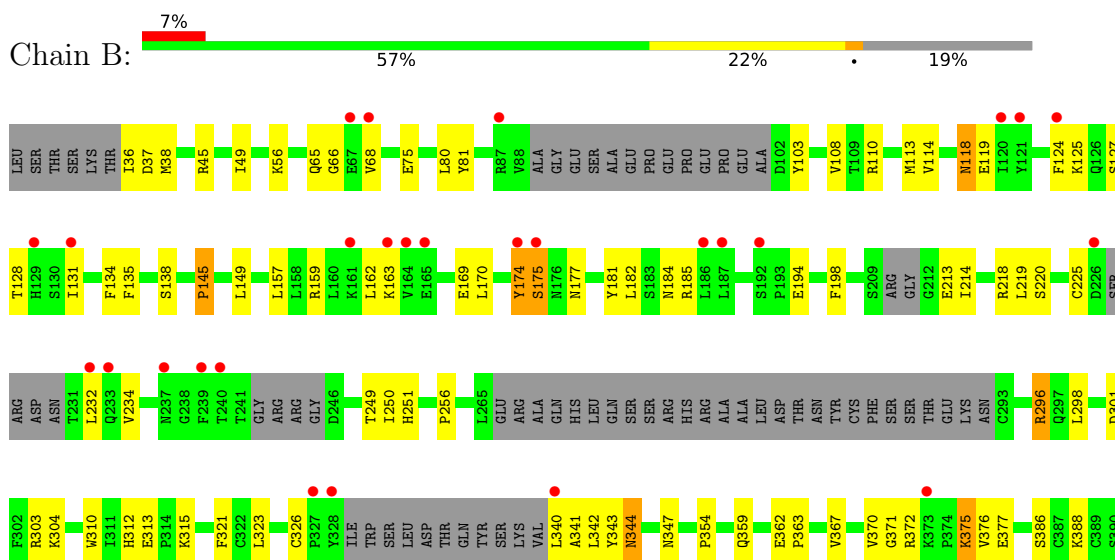
### 3 Residue-property plots i

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.

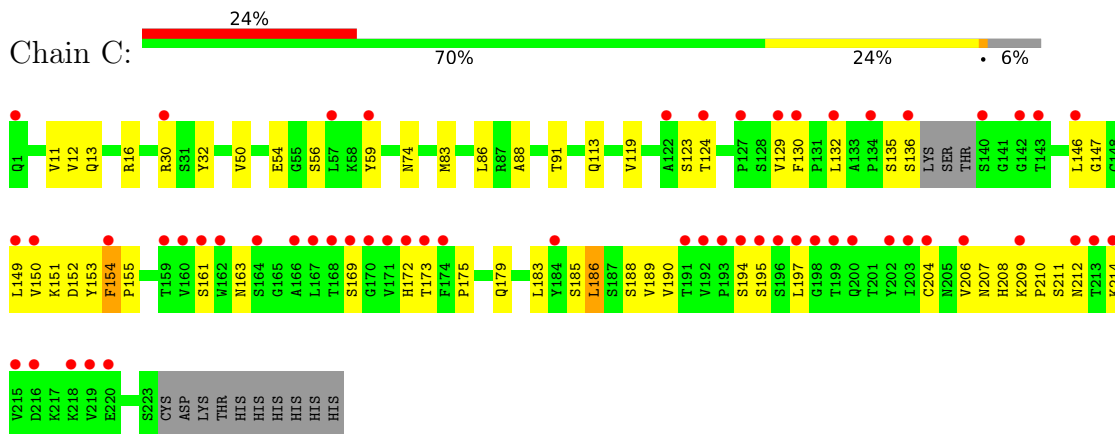
- Molecule 1: Transforming growth factor beta-1 proprotein



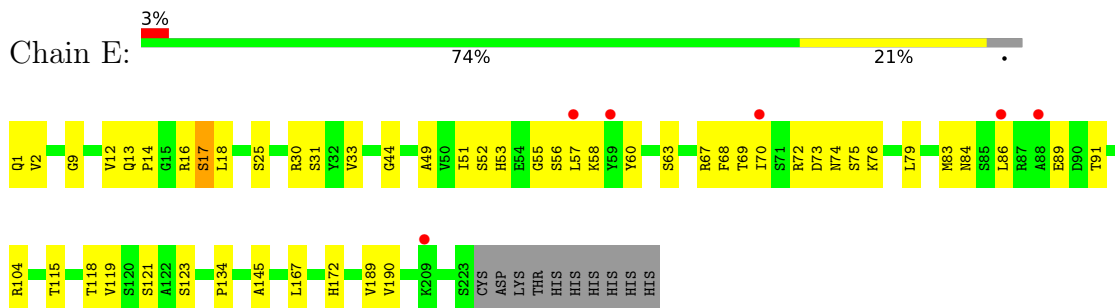
- Molecule 1: Transforming growth factor beta-1 proprotein



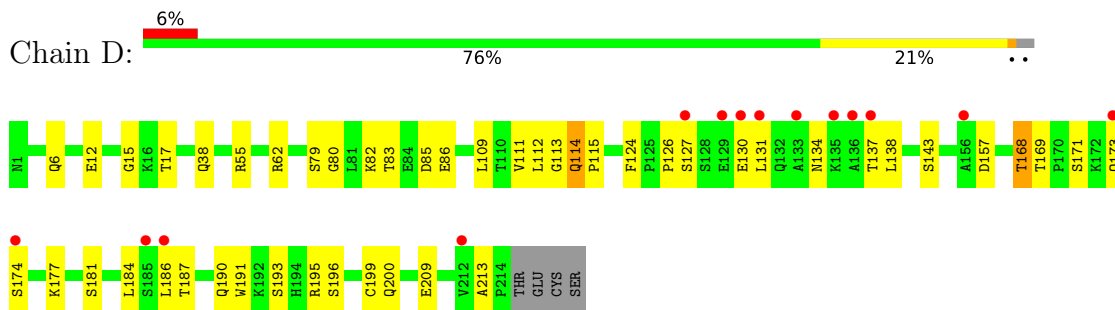
- Molecule 2: LTBP-49247 Fab Heavy Chain



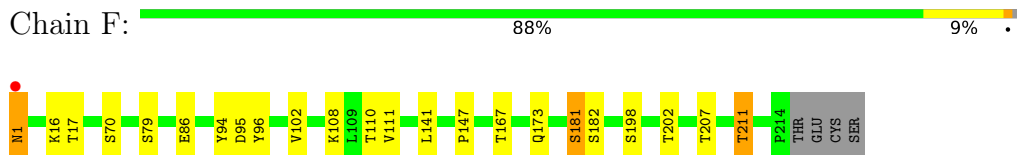
- Molecule 2: LTBP-49247 Fab Heavy Chain



- Molecule 3: LTBP-49247 Fab Light Chain



- Molecule 3: LTBP-49247 Fab Light Chain



- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose





MAC1  
MAC2  
BMA3  
MAN4  
MAN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.50Å 141.91Å 186.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.50 – 2.21 73.50 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.5 (73.50-2.21) 99.5 (73.50-2.21)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.232 , 0.264 0.245 , 0.280	Depositor DCC
$R_{free}$ test set	4891 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.3	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11329	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, MAN, 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	0.48	1/2102 (0.0%)	0.68	0/2838
1	B	0.48	0/2432	0.65	0/3292
2	C	0.47	0/1693	0.68	1/2300 (0.0%)
2	E	0.43	0/1716	0.65	0/2332
3	D	0.47	0/1660	0.64	0/2267
3	F	0.53	0/1660	0.68	0/2267
All	All	0.48	1/11263 (0.0%)	0.66	1/15296 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	PHE	CE2-CZ	5.37	1.47	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	186	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain

## 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	2062	0	2067	85	0
1	B	2374	0	2373	69	0
2	C	1654	0	1641	47	0
2	E	1676	0	1667	40	0
3	D	1621	0	1544	37	0
3	F	1621	0	1544	23	0
4	G	61	0	52	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	26	0	0	1	0
6	B	30	0	0	1	0
6	C	21	0	0	0	0
6	D	30	0	0	1	0
6	E	28	0	0	0	0
6	F	97	0	0	2	0
All	All	11329	0	10914	280	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 13.

The worst 5 of 280 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:F:17:THR:HG22	3:F:79:SER:CA	1.75	1.16
3:F:17:THR:CG2	3:F:79:SER:HA	1.88	1.03
3:F:17:THR:HG22	3:F:79:SER:HA	0.97	0.97
2:C:30:ARG:HG3	2:C:74:ASN:ND2	1.83	0.94
2:E:49:ALA:HB1	2:E:70:ILE:HD11	1.55	0.88

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	237/361 (66%)	223 (94%)	11 (5%)	3 (1%)	12	9
1	B	281/361 (78%)	258 (92%)	20 (7%)	3 (1%)	14	11
2	C	216/233 (93%)	204 (94%)	11 (5%)	1 (0%)	29	30
2	E	221/233 (95%)	211 (96%)	9 (4%)	1 (0%)	29	30
3	D	212/218 (97%)	201 (95%)	10 (5%)	1 (0%)	29	30
3	F	212/218 (97%)	205 (97%)	7 (3%)	0	100	100
All	All	1379/1624 (85%)	1302 (94%)	68 (5%)	9 (1%)	22	21

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	SER
2	C	154	PHE
1	A	313	GLU
2	E	56	SER
1	B	251	HIS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/321 (73%)	225 (96%)	9 (4%)	33	41
1	B	265/321 (83%)	256 (97%)	9 (3%)	37	46
2	C	182/195 (93%)	175 (96%)	7 (4%)	33	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	185/195 (95%)	181 (98%)	4 (2%)	52 64
3	D	187/191 (98%)	179 (96%)	8 (4%)	29 35
3	F	187/191 (98%)	183 (98%)	4 (2%)	53 65
All	All	1240/1414 (88%)	1199 (97%)	41 (3%)	38 47

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

Mol	Chain	Res	Type
3	D	127	SER
2	E	75	SER
3	D	143	SER
3	D	199	CYS
3	F	1	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	134	ASN
3	D	190	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

5 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	1,4	14,14,15	0.35	0	17,19,21	0.65	0
4	NAG	G	2	4	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
4	BMA	G	3	4	11,11,12	1.04	0	15,15,17	1.39	3 (20%)
4	MAN	G	4	4	11,11,12	1.60	3 (27%)	15,15,17	1.14	2 (13%)
4	MAN	G	5	4	11,11,12	1.58	3 (27%)	15,15,17	1.50	4 (26%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5	MAN	C2-C3	3.50	1.57	1.52
4	G	4	MAN	C1-C2	3.24	1.59	1.52
4	G	5	MAN	C1-C2	2.59	1.58	1.52
4	G	4	MAN	O5-C5	2.45	1.48	1.43
4	G	5	MAN	O5-C5	2.16	1.47	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5	MAN	C1-O5-C5	3.60	117.07	112.19
4	G	4	MAN	C1-O5-C5	3.13	116.43	112.19
4	G	5	MAN	C1-C2-C3	2.69	112.98	109.67
4	G	2	NAG	C1-O5-C5	2.58	115.69	112.19
4	G	3	BMA	C1-O5-C5	2.56	115.67	112.19

There are no chirality outliers.

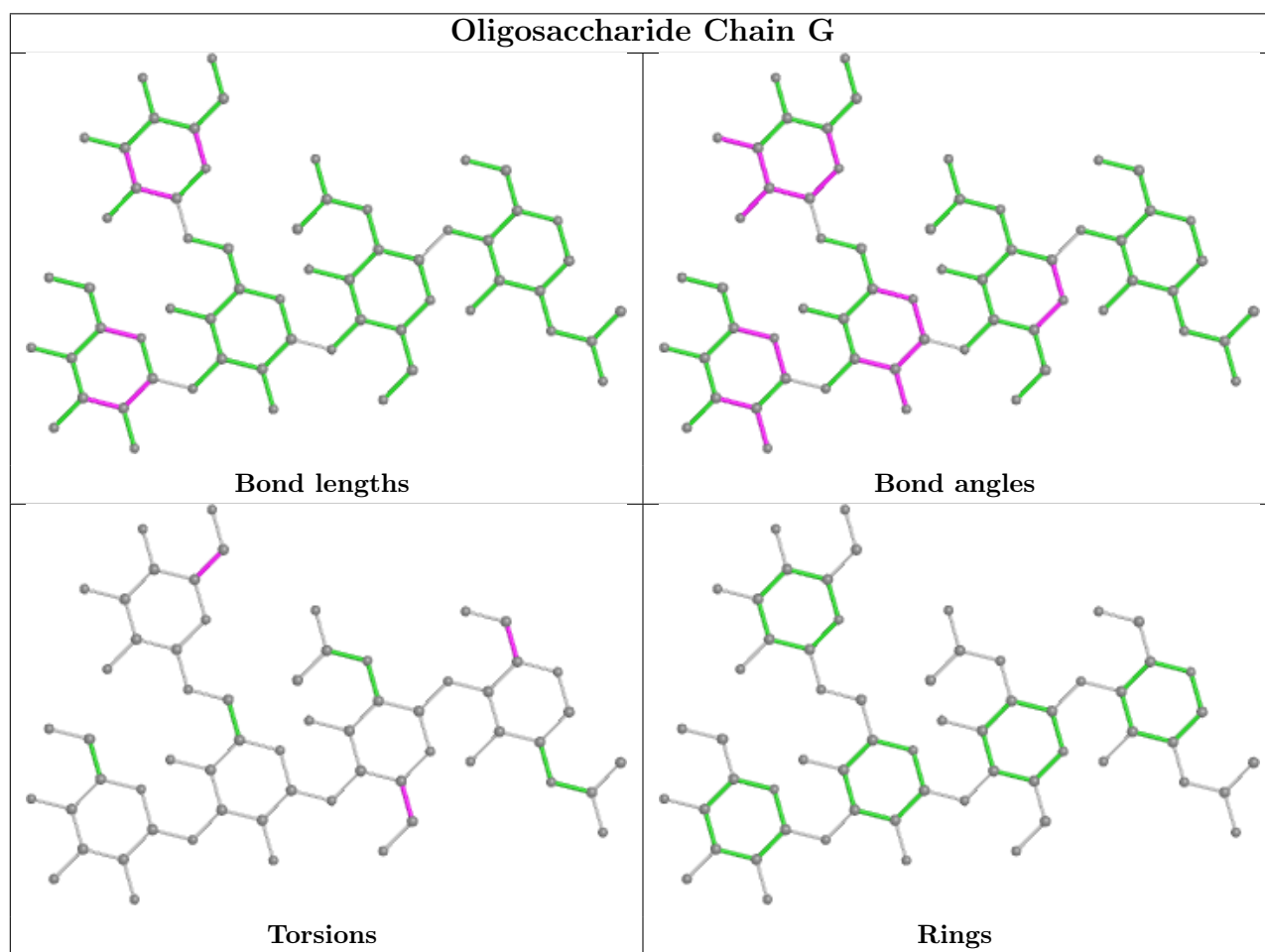
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	NAG	O5-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

2 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
5	NAG	A	401	1	14,14,15	0.38	0	17,19,21	0.49	0
5	NAG	B	401	1	14,14,15	0.72	0	17,19,21	0.68	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
5	NAG	A	401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	NAG	C1-O5-C5	2.32	115.33	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	NAG	C4-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	B	401	NAG	O5-C5-C6-O6
5	B	401	NAG	C4-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

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	257/361 (71%)	0.93	46 (17%) <b>1</b> <b>1</b>	30, 95, 128, 136	0
1	B	294/361 (81%)	0.68	27 (9%) <b>9</b> <b>7</b>	49, 76, 119, 140	0
2	C	220/233 (94%)	1.32	57 (25%) <b>0</b> <b>0</b>	44, 88, 159, 186	0
2	E	223/233 (95%)	0.36	6 (2%) 54 52	54, 79, 114, 132	0
3	D	214/218 (98%)	0.64	14 (6%) <b>18</b> <b>17</b>	45, 78, 131, 158	0
3	F	214/218 (98%)	0.50	1 (0%) <b>91</b> <b>90</b>	43, 55, 81, 112	0
All	All	1422/1624 (87%)	0.74	151 (10%) <b>6</b> <b>5</b>	30, 76, 132, 186	0

The worst 5 of 151 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	191	THR	12.0
1	B	121	TYR	11.4
2	C	162	TRP	10.0
2	C	198	GLY	9.4
1	B	124	PHE	8.1

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

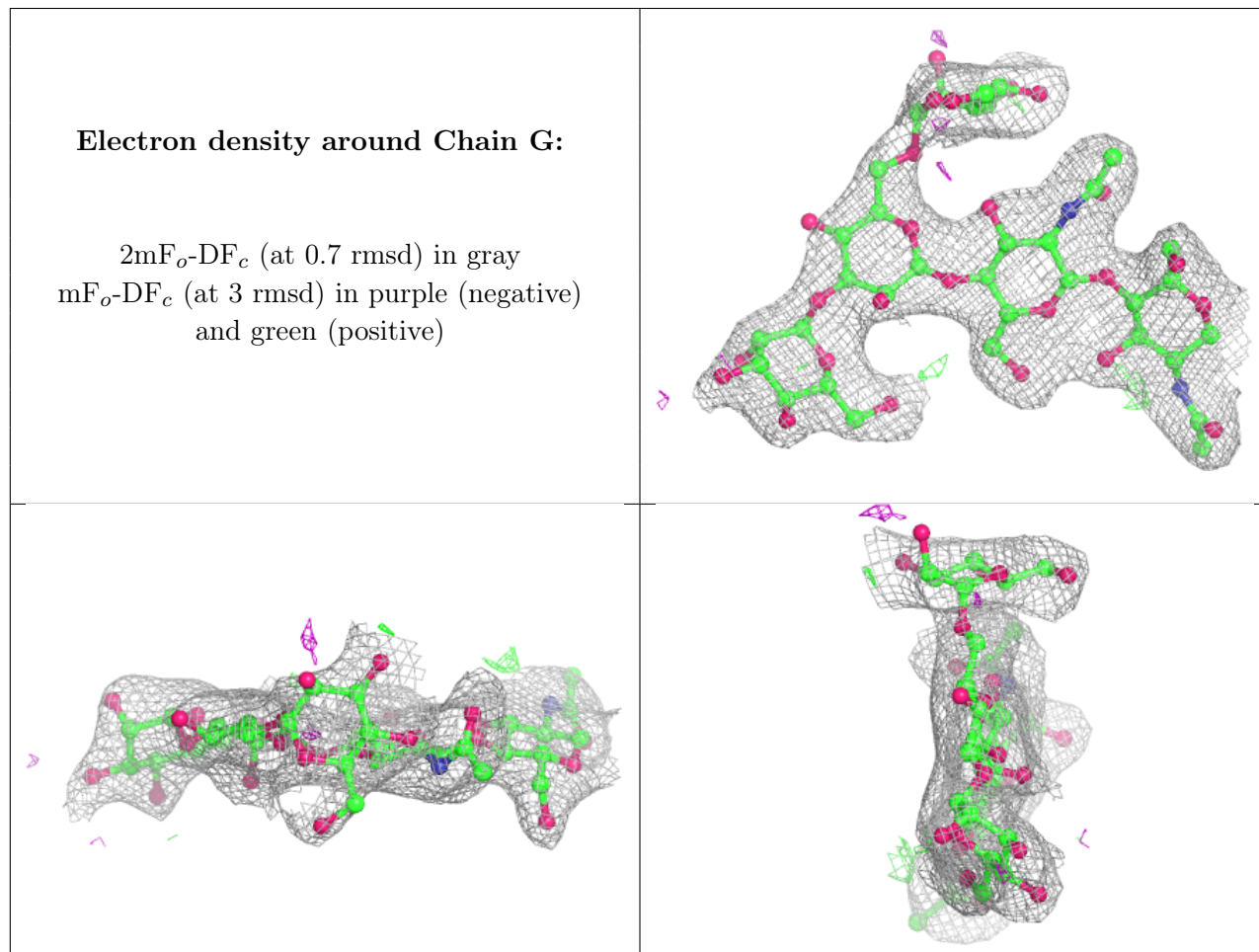
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 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	MAN	G	5	11/12	0.62	0.22	107,113,115,120	0
4	NAG	G	2	14/15	0.88	0.12	78,85,93,95	0
4	BMA	G	3	11/12	0.90	0.13	86,91,100,110	0
4	MAN	G	4	11/12	0.91	0.14	79,81,86,86	0
4	NAG	G	1	14/15	0.95	0.11	66,72,79,84	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.



## 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, 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
5	NAG	B	401	14/15	0.80	0.14	104,111,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	401	14/15	0.82	0.24	110,120,125,125	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.