



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1M6B  
Title : Structure of the HER3 (ERBB3) Extracellular Domain  
Authors : Leahy, D.J.; Cho, H.-S.  
Deposited on : 2002-07-15  
Resolution : 2.60 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

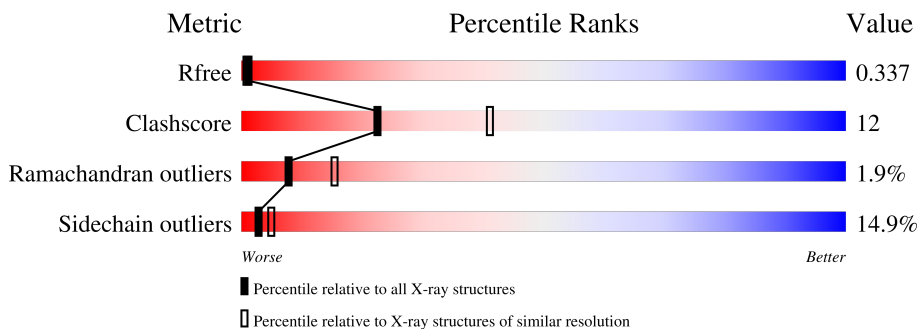
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	621	58% (green), 25% (yellow), 5% (orange), 12% (grey)
1	B	621	64% (green), 24% (yellow), 5% (orange), 6% (grey)
2	C	2	50% (yellow), 50% (orange)
2	D	2	50% (yellow), 50% (orange)

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	626	X	-	-	-
3	NAG	A	628	X	-	-	-
3	NAG	B	626	X	-	-	-
3	NAG	B	627	X	-	-	-
3	NAG	B	628	X	-	-	-
4	SO4	B	5001	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9012 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 Receptor protein-tyrosine kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	549	Total	C	N	O	S	0	0	0
			4206	2603	765	784	54			
1	B	584	Total	C	N	O	S	0	0	0
			4478	2766	813	840	59			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	VAL	ILE	engineered mutation	UNP P21860
B	61	VAL	ILE	engineered mutation	UNP P21860

- Molecule 2 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
			Total	C	N	O			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O S	0	0
			5	4 1		

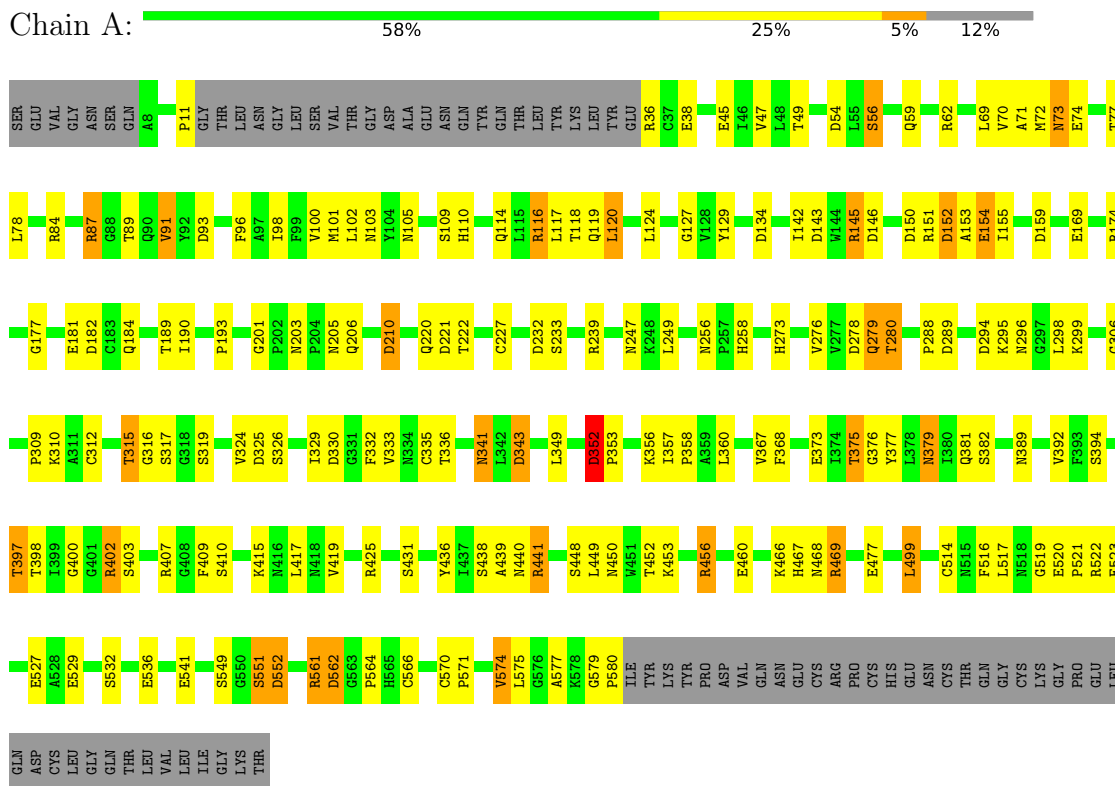
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	65	Total	O	0	0
			65	65		

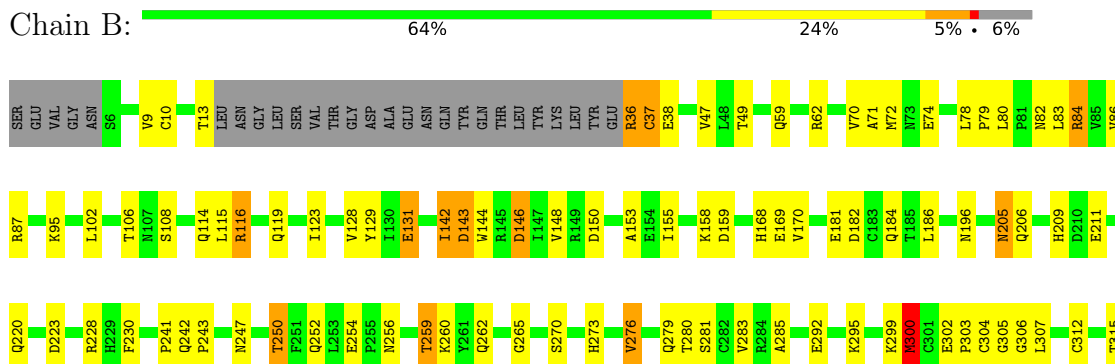
### 3 Residue-property plots i

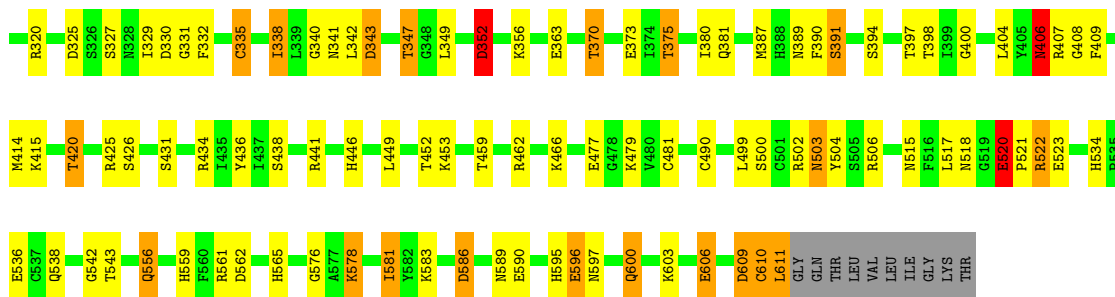
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Receptor protein-tyrosine kinase erbB-3



- Molecule 1: Receptor protein-tyrosine kinase erbB-3





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



MAG1  
MAG2

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



MAG1  
MAG2



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	236.26Å 49.62Å 190.86Å 90.00° 125.56° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 28.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-2.60) 90.7 (28.74-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.235 , 0.294 0.299 , 0.337	Depositor DCC
$R_{free}$ test set	2754 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.1	Xtrriage
Anisotropy	0.756	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 30.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	9012	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: NAG, SO4

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	0.56	0/4308	0.84	15/5845 (0.3%)
1	B	0.62	1/4586 (0.0%)	0.86	8/6222 (0.1%)
All	All	0.59	1/8894 (0.0%)	0.85	23/12067 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	MET	SD-CE	5.39	2.08	1.77

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ASP	CB-CG-OD2	8.78	126.20	118.30
1	A	221	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	146	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	143	ASP	CB-CG-OD2	6.24	123.91	118.30
1	B	325	ASP	CB-CG-OD2	6.20	123.88	118.30

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	4206	0	3996	79	0
1	B	4478	0	4242	123	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
3	A	98	0	91	0	0
3	B	84	0	78	2	0
4	B	5	0	0	4	0
5	A	20	0	0	3	0
5	B	65	0	0	7	0
All	All	9012	0	8457	202	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 12.

The worst 5 of 202 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:300:MET:CE	1:B:300:MET:SD	2.08	1.42
1:B:116:ARG:HG3	1:B:116:ARG:HH11	1.11	1.11
1:B:335:CYS:O	1:B:370:THR:HG22	1.56	1.03
1:B:452:THR:HG22	1:B:459:THR:HG21	1.42	1.00
1:B:578:LYS:HE2	1:B:578:LYS:H	1.31	0.96

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	545/621 (88%)	482 (88%)	52 (10%)	11 (2%)	<b>7</b> <b>14</b>
1	B	580/621 (93%)	525 (90%)	45 (8%)	10 (2%)	<b>9</b> <b>18</b>
All	All	1125/1242 (91%)	1007 (90%)	97 (9%)	21 (2%)	<b>8</b> <b>15</b>

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	SER
1	A	460	GLU
1	B	520	GLU
1	B	586	ASP
1	A	296	ASN

### 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	474/537 (88%)	398 (84%)	76 (16%)	2	4
1	B	506/537 (94%)	436 (86%)	70 (14%)	3	6
All	All	980/1074 (91%)	834 (85%)	146 (15%)	3	5

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	341	ASN
1	B	603	LYS
1	B	356	LYS
1	B	477	GLU
1	A	367	VAL

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	184	GLN
1	B	229	HIS
1	B	589	ASN
1	B	467	HIS
1	B	209	HIS

### 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](#)

4 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
2	NAG	C	1	2,1	14,14,15	0.82	0	17,19,21	1.63	4 (23%)
2	NAG	C	2	2	14,14,15	0.42	0	17,19,21	1.62	4 (23%)
2	NAG	D	1	2,1	14,14,15	0.45	0	17,19,21	1.28	2 (11%)
2	NAG	D	2	2	14,14,15	0.57	0	17,19,21	0.89	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
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	4.03	117.66	112.19
2	D	1	NAG	C1-O5-C5	3.38	116.77	112.19
2	C	1	NAG	C2-N2-C7	-2.93	118.73	122.90
2	C	2	NAG	C2-N2-C7	2.45	126.39	122.90
2	C	1	NAG	C4-C3-C2	2.39	114.51	111.02

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

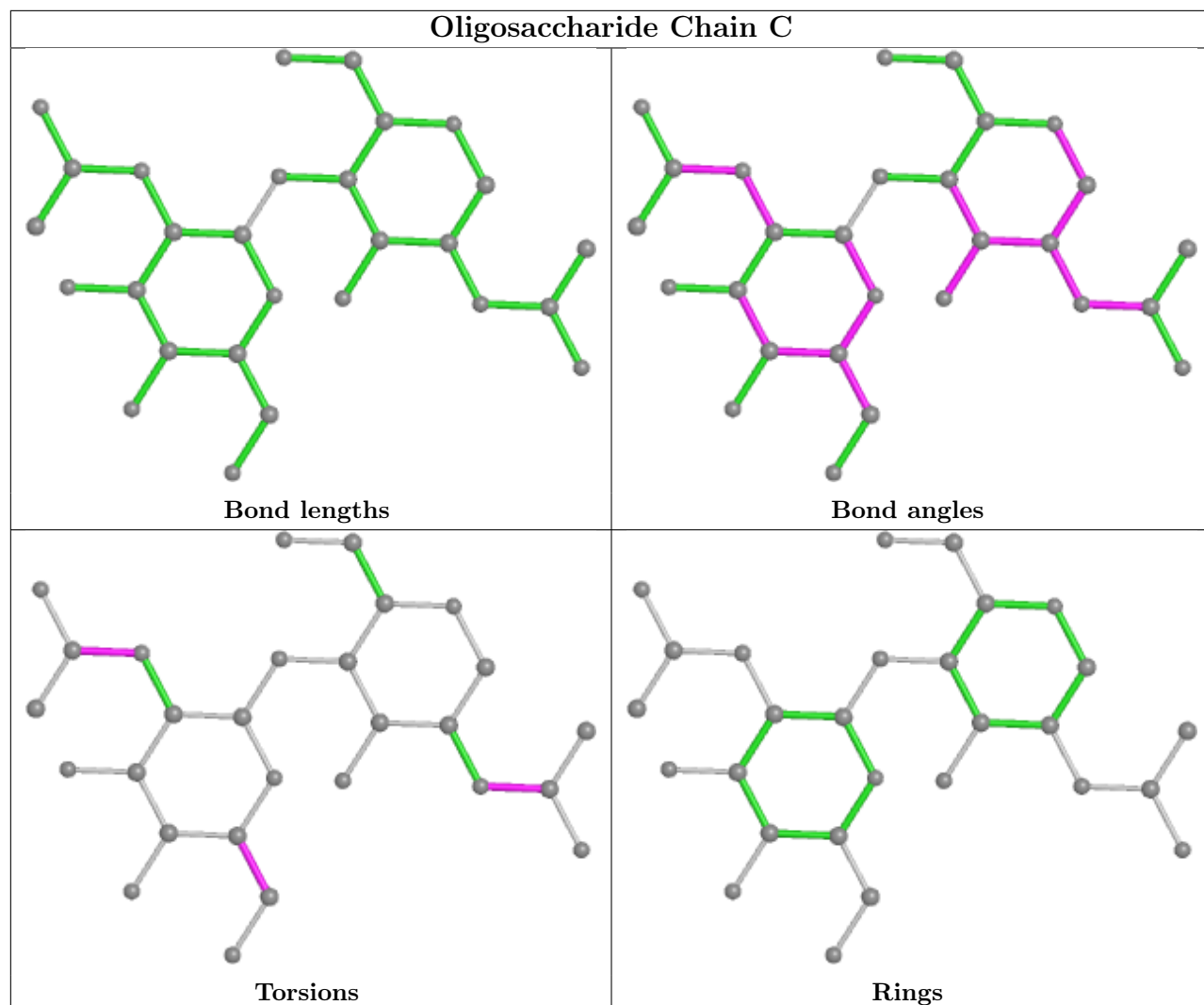
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2

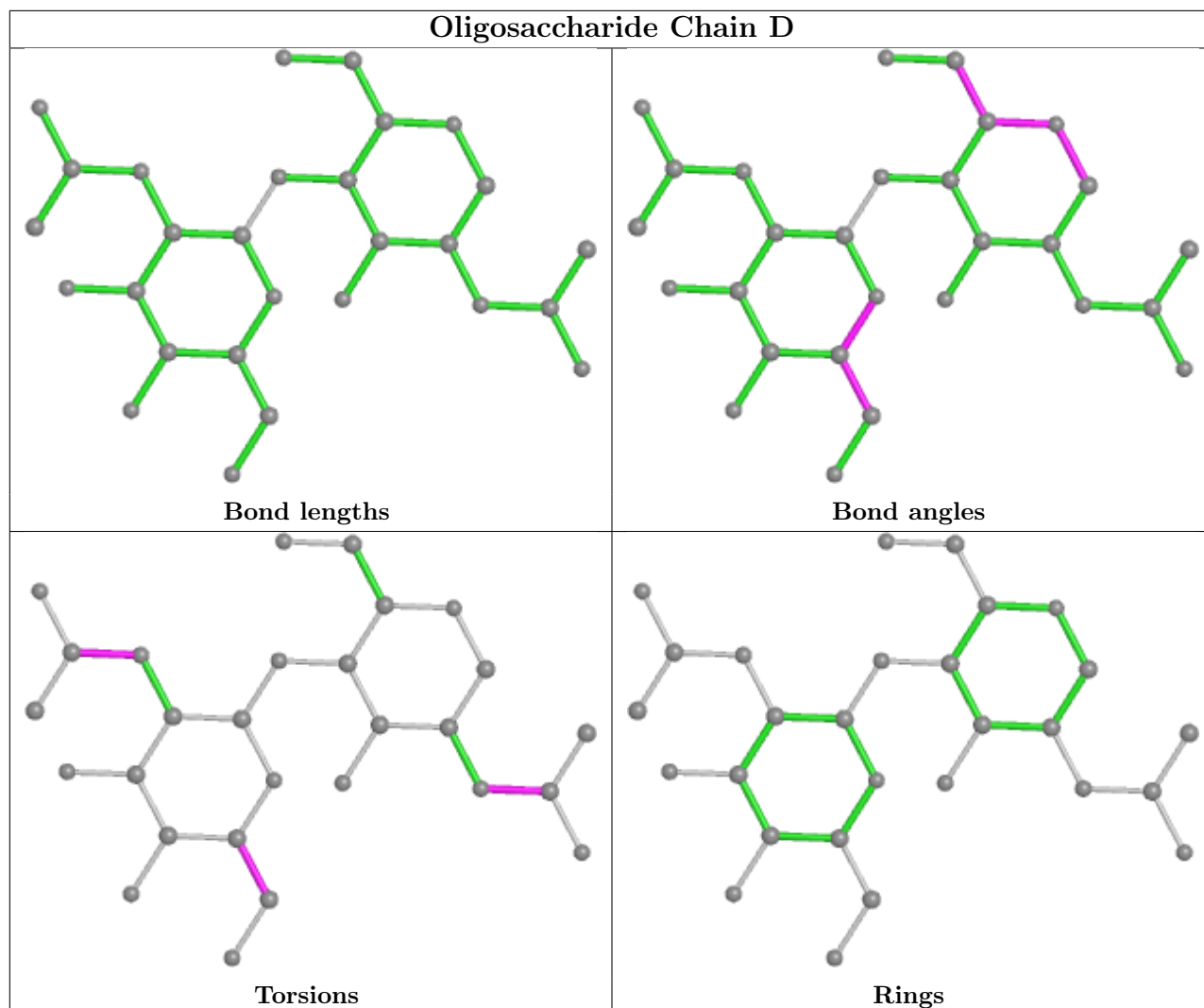
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	C	1	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](#)

14 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	$\# Z  > 2$
3	NAG	A	623	1	14,14,15	0.69	0	17,19,21	1.31	3 (17%)
4	SO4	B	5001	-	4,4,4	0.22	0	6,6,6	0.32	0
3	NAG	B	622	1	14,14,15	0.68	0	17,19,21	3.03	6 (35%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	622	1	14,14,15	0.43	0	17,19,21	2.24	2 (11%)
3	NAG	A	630	1	14,14,15	0.67	0	17,19,21	1.68	3 (17%)
3	NAG	B	626	1	14,14,15	0.68	0	17,19,21	1.93	6 (35%)
3	NAG	B	628	1	14,14,15	0.69	0	17,19,21	1.65	2 (11%)
3	NAG	A	626	1	14,14,15	0.62	0	17,19,21	1.15	2 (11%)
3	NAG	B	627	1	14,14,15	0.57	0	17,19,21	1.52	2 (11%)
3	NAG	A	627	1	14,14,15	0.62	0	17,19,21	1.53	4 (23%)
3	NAG	A	628	1	14,14,15	0.73	0	17,19,21	1.76	4 (23%)
3	NAG	B	623	1	14,14,15	0.70	0	17,19,21	1.63	4 (23%)
3	NAG	A	629	1	14,14,15	0.79	1 (7%)	17,19,21	1.62	4 (23%)
3	NAG	B	629	1	14,14,15	1.02	1 (7%)	17,19,21	1.55	3 (17%)

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	A	623	1	-	0/6/23/26	0/1/1/1
3	NAG	B	622	1	-	4/6/23/26	0/1/1/1
3	NAG	B	626	1	1/1/5/7	6/6/23/26	0/1/1/1
3	NAG	A	622	1	-	3/6/23/26	0/1/1/1
3	NAG	B	628	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	A	630	1	-	4/6/23/26	0/1/1/1
3	NAG	A	626	1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	B	627	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	A	627	1	-	4/6/23/26	0/1/1/1
3	NAG	A	628	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	B	623	1	-	4/6/23/26	0/1/1/1
3	NAG	A	629	1	-	0/6/23/26	0/1/1/1
3	NAG	B	629	1	-	5/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	629	NAG	C1-C2	2.99	1.56	1.52
3	A	629	NAG	C1-C2	2.43	1.56	1.52

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	622	NAG	C2-N2-C7	-8.24	111.17	122.90
3	A	622	NAG	C1-O5-C5	7.93	122.93	112.19
3	A	630	NAG	C1-O5-C5	5.60	119.78	112.19
3	B	622	NAG	C1-O5-C5	5.59	119.76	112.19
3	A	628	NAG	O5-C1-C2	-4.98	103.42	111.29

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	626	NAG	C1
3	A	628	NAG	C1
3	B	626	NAG	C1
3	B	627	NAG	C1
3	B	628	NAG	C1

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	622	NAG	C8-C7-N2-C2
3	A	622	NAG	O7-C7-N2-C2
3	A	628	NAG	C8-C7-N2-C2
3	A	628	NAG	O7-C7-N2-C2
3	A	630	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5001	SO4	4	0
3	B	627	NAG	2	0

## 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

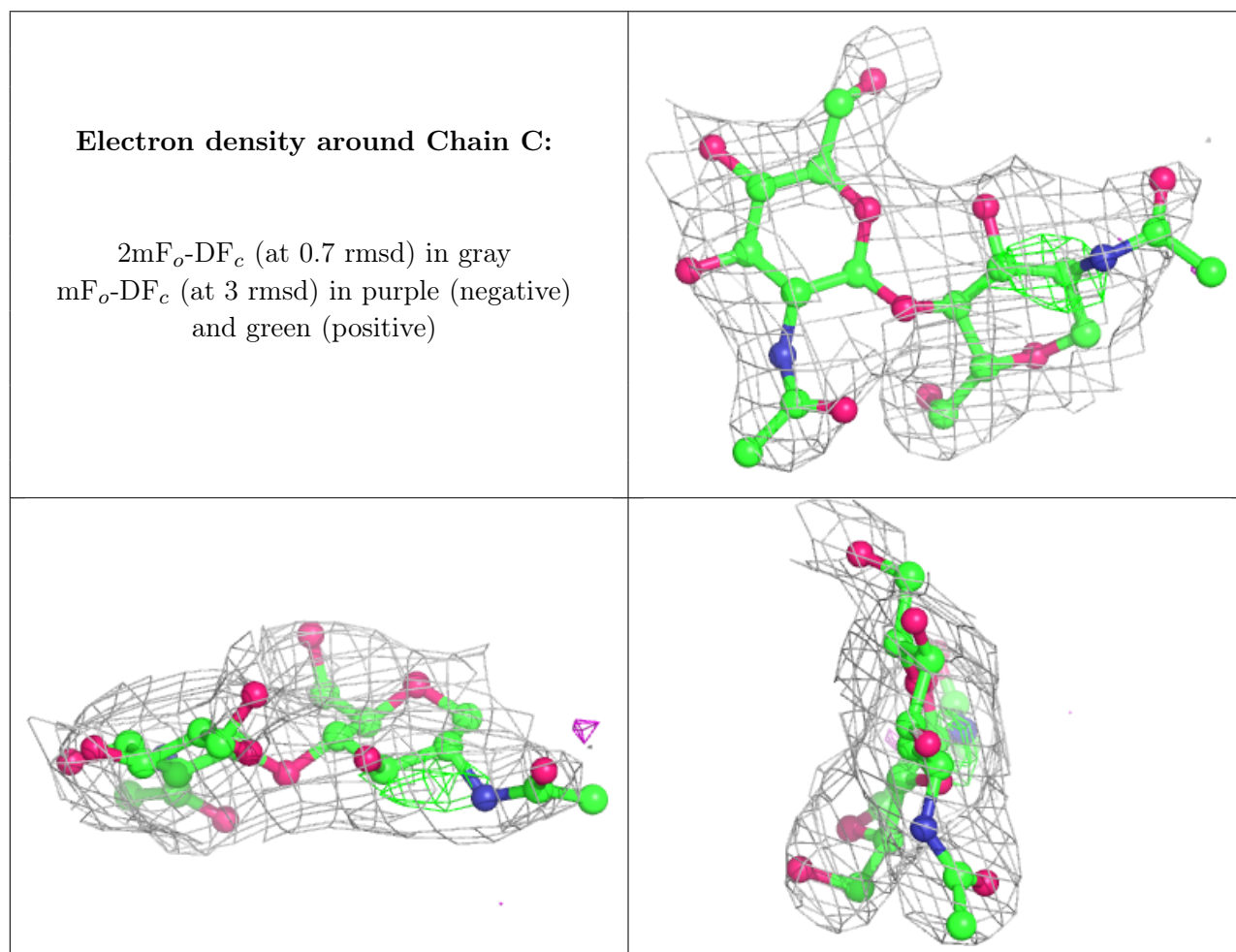
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

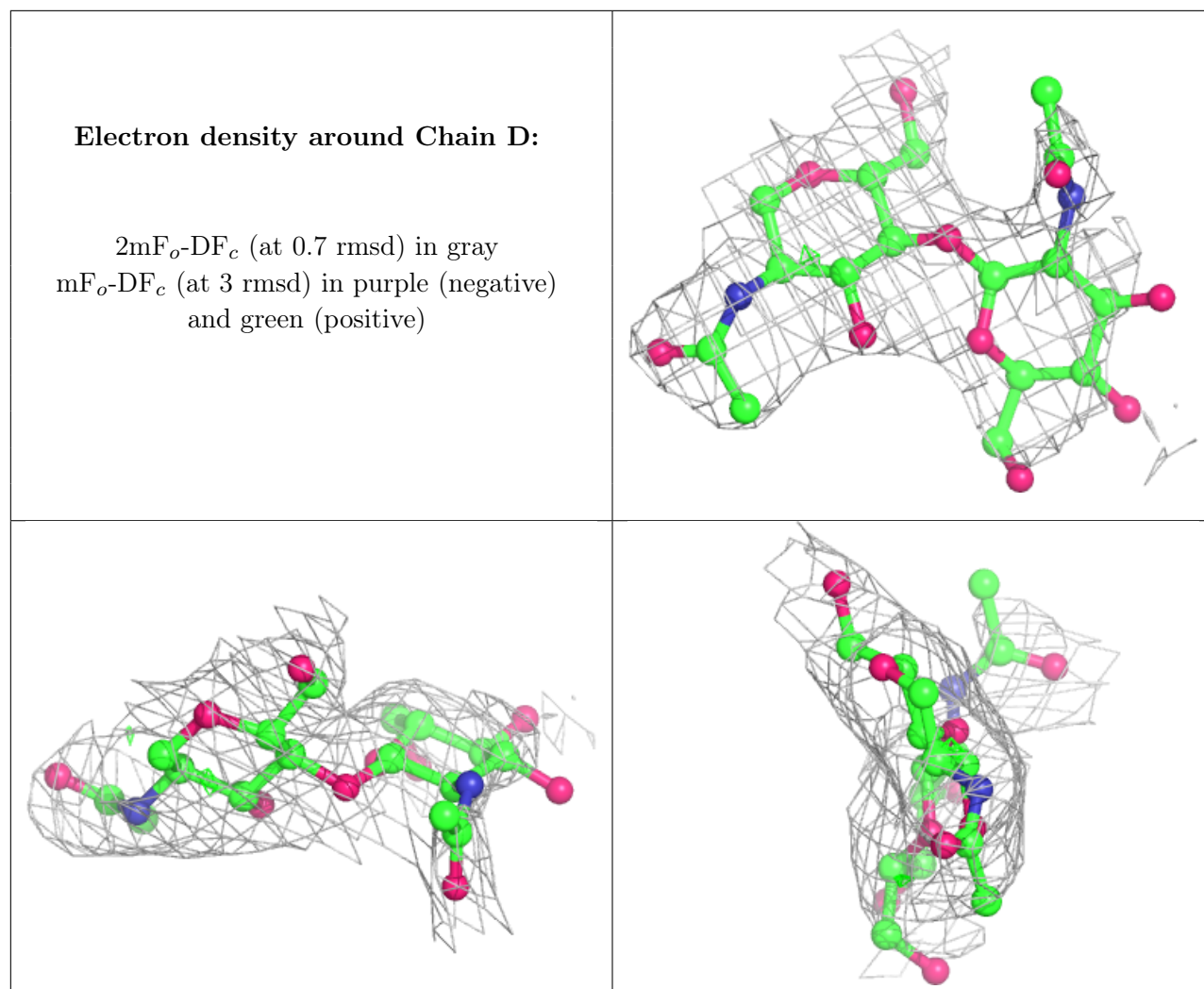
Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.

## 6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.