



# wwPDB X-ray Structure Validation Summary Report

Nov 9, 2024 – 10:01 PM EST

PDB ID : 1HZH  
Title : CRYSTAL STRUCTURE OF THE INTACT HUMAN IGG B12 WITH BROAD AND POTENT ACTIVITY AGAINST PRIMARY HIV-1 ISOLATES: A TEMPLATE FOR HIV VACCINE DESIGN  
Authors : Sapphire, E.O.; Burton, D.R.; Wilson, I.A.  
Deposited on : 2001-01-24  
Resolution : 2.70 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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

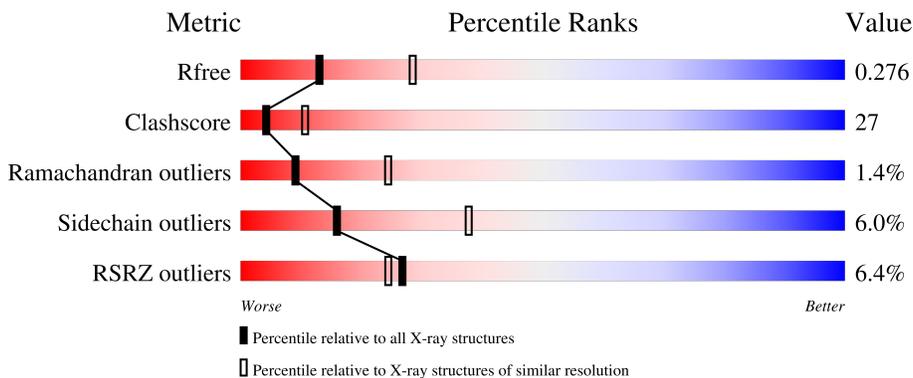
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	H	457	
1	K	457	
2	L	215	
2	M	215	
3	A	9	

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Mol	Chain	Length	Quality of chain
4	B	9	 44% 33% 22%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10647 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 IMMUNOGLOBULIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	457	3553	2252	600	685	16	0	0	0
1	K	444	3466	2202	583	665	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	225	ALA	VAL	conflict	UNP P0DOX5
K	225	ALA	VAL	conflict	UNP P0DOX5

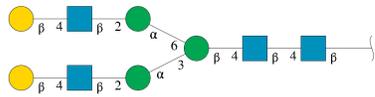
- Molecule 2 is a protein called IMMUNOGLOBULIN LIGHT CHAIN, Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	215	1668	1036	297	330	5	0	0	0
2	M	215	1668	1036	297	330	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

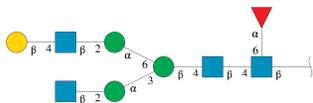
Chain	Residue	Modelled	Actual	Comment	Reference
L	202	ARG	SER	conflict	UNP Q8TCD0
M	202	ARG	SER	conflict	UNP Q8TCD0

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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
3	A	9	111	62	4	45	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-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	
			Total	C	N				O
4	B	9	110	62	4	44	0	0	0

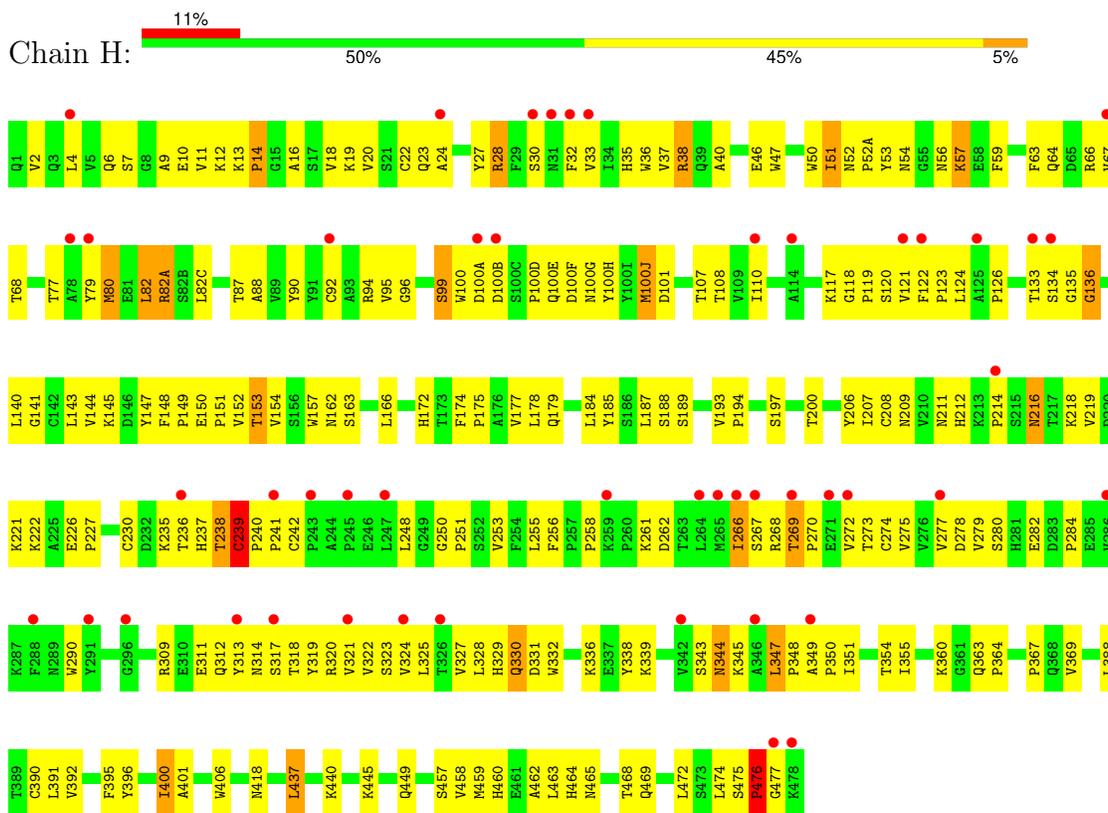
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	15	Total	O	0	0
			15	15		
5	K	38	Total	O	0	0
			38	38		
5	L	6	Total	O	0	0
			6	6		
5	M	12	Total	O	0	0
			12	12		

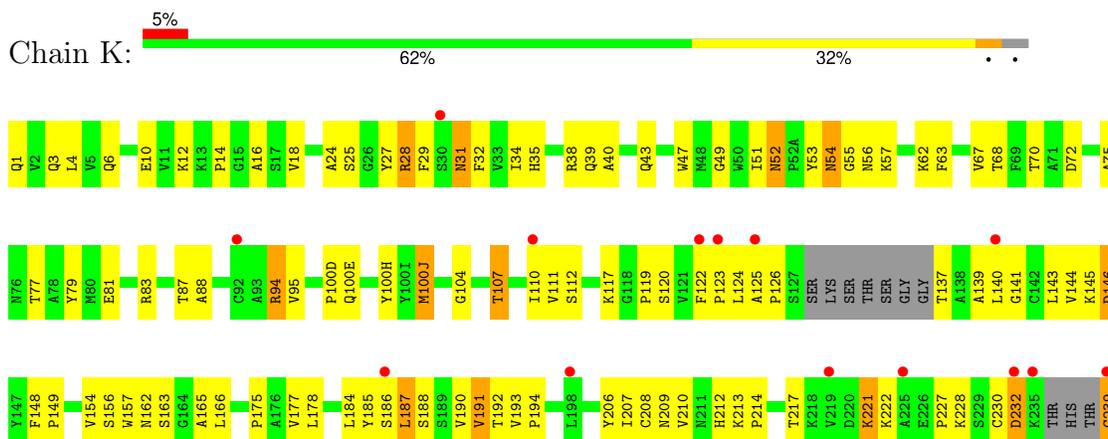
### 3 Residue-property plots

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: IMMUNOGLOBULIN HEAVY CHAIN



- Molecule 1: IMMUNOGLOBULIN HEAVY CHAIN







## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	271.32Å 271.32Å 175.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.65 – 2.70 29.65 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.7 (29.65-2.70) 91.6 (29.65-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.61Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.229 , 0.273 0.233 , 0.276	Depositor DCC
$R_{free}$ test set	6305 reflections (10.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 67.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for $-1/3^*h+1/3^*k+4/3^*l,-k,2/3^*h+1/3^*k+1/3^*l$ 0.012 for $-2/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+4/3^*l,-1/3^*h+1/3^*k+1/3^*l$ 0.006 for $-h,1/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+1/3^*l$	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: FUC, NAG, BMA, MAN, GAL

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	H	0.37	0/3654	0.62	0/4983
1	K	0.40	0/3563	0.64	0/4859
2	L	0.34	0/1704	0.60	0/2306
2	M	0.38	0/1704	0.63	0/2306
All	All	0.38	0/10625	0.62	0/14454

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	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	136	GLY	Mainchain

### 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	H	3553	0	3460	231	1
1	K	3466	0	3373	152	0
2	L	1668	0	1621	69	0
2	M	1668	0	1621	110	0
3	A	111	0	94	11	0
4	B	110	0	94	7	0
5	H	15	0	0	2	0
5	K	38	0	0	0	0
5	L	6	0	0	0	0
5	M	12	0	0	1	0
All	All	10647	0	10263	556	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 27.

The worst 5 of 556 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:K:261:LYS:HE2	1:K:265:MET:HE1	1.09	1.06
1:H:400:ILE:HD11	1:H:458:VAL:HG13	1.38	1.05
1:K:221:LYS:HE3	1:K:221:LYS:HA	1.39	1.04
2:M:1:GLU:HG3	2:M:2:ILE:H	1.18	1.03
2:M:100:GLN:H	2:M:100:GLN:NE2	1.56	1.03

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:H:136:GLY:CA	1:H:136:GLY:CA[4_557]	1.86	0.34

## 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	H	455/457 (100%)	400 (88%)	48 (10%)	7 (2%)	8	22
1	K	438/457 (96%)	402 (92%)	30 (7%)	6 (1%)	9	24
2	L	213/215 (99%)	193 (91%)	17 (8%)	3 (1%)	9	24
2	M	213/215 (99%)	195 (92%)	15 (7%)	3 (1%)	9	24
All	All	1319/1344 (98%)	1190 (90%)	110 (8%)	19 (1%)	9	24

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	99	SER
1	H	239	CYS
1	H	476	PRO
1	H	477	GLY
1	K	16	ALA

### 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	H	405/405 (100%)	376 (93%)	29 (7%)	12	30
1	K	395/405 (98%)	378 (96%)	17 (4%)	25	52
2	L	187/187 (100%)	179 (96%)	8 (4%)	25	52
2	M	187/187 (100%)	171 (91%)	16 (9%)	8	21
All	All	1174/1184 (99%)	1104 (94%)	70 (6%)	16	38

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	63	SER
2	M	74	THR
2	M	143	GLU
1	H	418	ASN
1	H	400	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	452	ASN
2	L	147	GLN
1	K	460	HIS
2	L	42	GLN
2	L	198	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](#)

18 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	A	1	3	14,14,15	0.45	0	17,19,21	0.87	0
3	NAG	A	2	3	14,14,15	0.37	0	17,19,21	0.89	1 (5%)
3	BMA	A	3	3	11,11,12	0.49	0	15,15,17	0.79	1 (6%)
3	MAN	A	4	3	11,11,12	0.57	0	15,15,17	0.69	0
3	NAG	A	5	3	14,14,15	0.64	0	17,19,21	0.86	1 (5%)
3	GAL	A	6	3	11,11,12	0.46	0	15,15,17	0.37	0
3	MAN	A	7	3	11,11,12	0.70	0	15,15,17	0.57	0
3	NAG	A	8	3	14,14,15	0.65	0	17,19,21	1.02	1 (5%)
3	GAL	A	9	3	11,11,12	0.56	0	15,15,17	0.29	0
4	NAG	B	1	4	14,14,15	0.43	0	17,19,21	1.02	1 (5%)
4	NAG	B	2	4	14,14,15	0.49	0	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	B	3	4	11,11,12	0.67	0	15,15,17	0.59	0
4	MAN	B	4	4	11,11,12	0.79	0	15,15,17	0.57	0
4	NAG	B	5	4	14,14,15	0.53	0	17,19,21	1.04	1 (5%)
4	GAL	B	6	4	11,11,12	0.55	0	15,15,17	0.33	0
4	MAN	B	7	4	11,11,12	0.57	0	15,15,17	1.10	1 (6%)
4	NAG	B	8	4	14,14,15	0.59	0	17,19,21	0.67	0
4	FUC	B	9	4	10,10,11	0.58	0	14,14,16	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1	3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	2/6/23/26	0/1/1/1
3	BMA	A	3	3	-	0/2/19/22	0/1/1/1
3	MAN	A	4	3	-	0/2/19/22	0/1/1/1
3	NAG	A	5	3	-	0/6/23/26	0/1/1/1
3	GAL	A	6	3	-	2/2/19/22	0/1/1/1
3	MAN	A	7	3	-	2/2/19/22	0/1/1/1
3	NAG	A	8	3	-	2/6/23/26	0/1/1/1
3	GAL	A	9	3	-	2/2/19/22	0/1/1/1
4	NAG	B	1	4	-	4/6/23/26	0/1/1/1
4	NAG	B	2	4	-	1/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
4	NAG	B	5	4	-	2/6/23/26	0/1/1/1
4	GAL	B	6	4	-	0/2/19/22	0/1/1/1
4	MAN	B	7	4	-	2/2/19/22	0/1/1/1
4	NAG	B	8	4	-	3/6/23/26	0/1/1/1
4	FUC	B	9	4	-	-	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	8	NAG	C2-N2-C7	-3.04	118.82	122.90
4	B	5	NAG	C2-N2-C7	-2.91	119.00	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	NAG	C2-N2-C7	-2.89	119.03	122.90
4	B	2	NAG	C2-N2-C7	-2.69	119.30	122.90
3	A	2	NAG	C2-N2-C7	-2.64	119.36	122.90

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

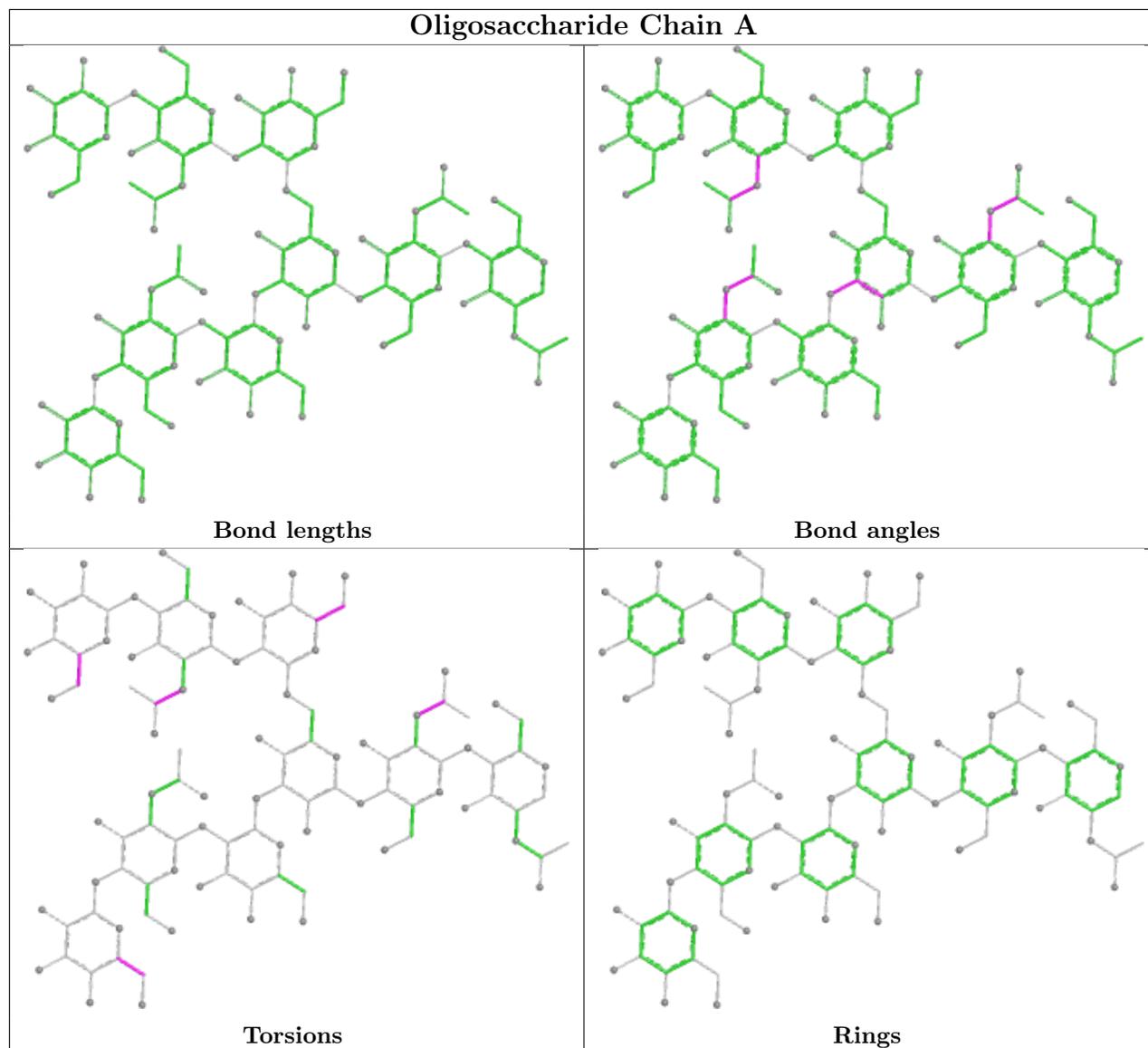
Mol	Chain	Res	Type	Atoms
4	B	8	NAG	C3-C2-N2-C7
4	B	8	NAG	C8-C7-N2-C2
4	B	8	NAG	O7-C7-N2-C2
4	B	7	MAN	O5-C5-C6-O6
3	A	6	GAL	C4-C5-C6-O6

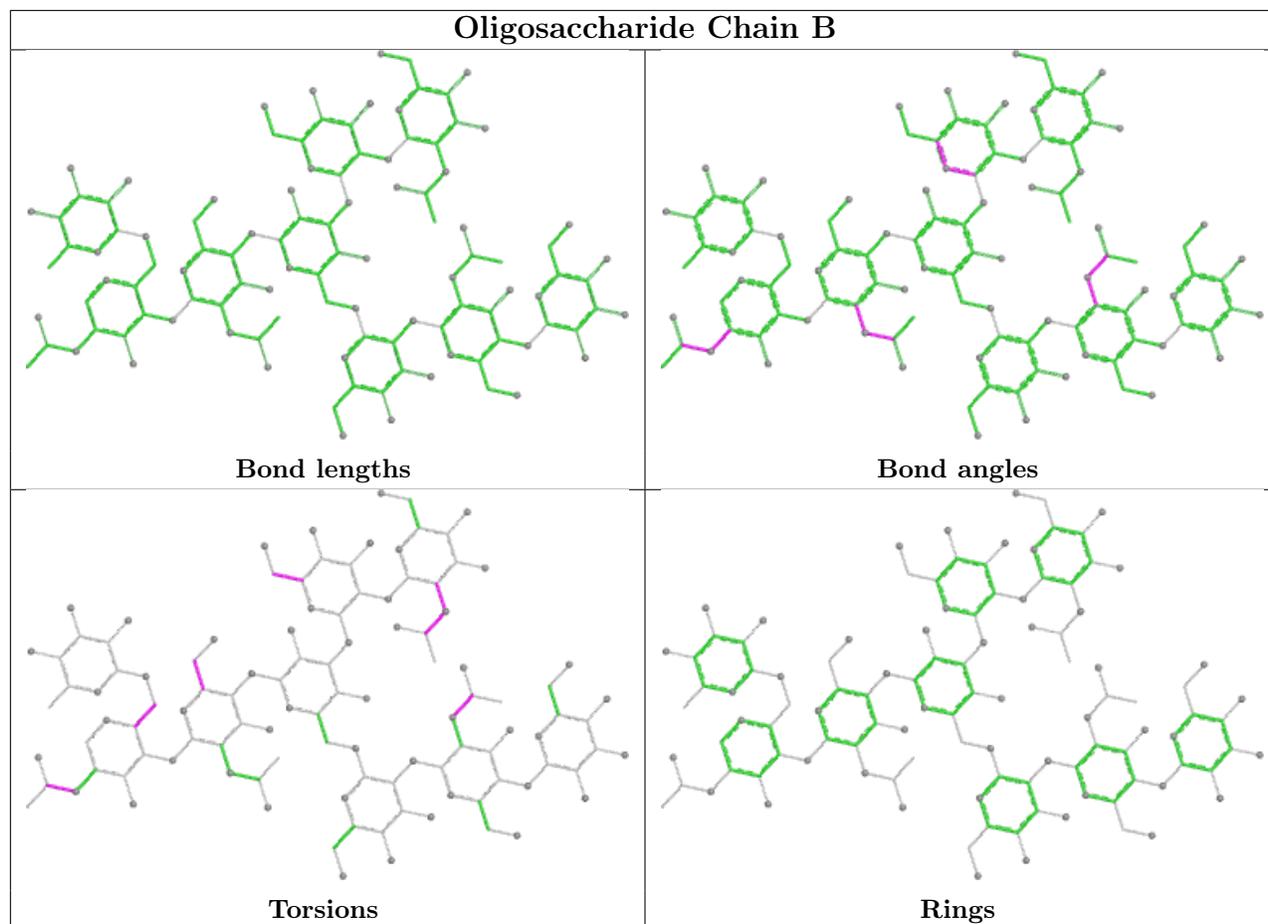
There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5	NAG	3	0
3	A	1	NAG	5	0
3	A	8	NAG	2	0
4	B	1	NAG	4	0
4	B	2	NAG	2	0
4	B	8	NAG	1	0
3	A	2	NAG	1	0
3	A	6	GAL	3	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	H	457/457 (100%)	0.63	48 (10%) 13 12	29, 97, 181, 199	0
1	K	444/457 (97%)	0.08	21 (4%) 37 35	28, 67, 159, 197	0
2	L	215/215 (100%)	0.35	6 (2%) 55 53	43, 89, 146, 164	0
2	M	215/215 (100%)	0.30	10 (4%) 37 35	36, 77, 167, 193	0
All	All	1331/1344 (99%)	0.35	85 (6%) 27 24	28, 83, 167, 199	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	134	SER	7.0
1	H	288	PHE	4.4
1	H	265	MET	4.3
1	H	267	SER	4.3
1	K	219	VAL	4.1

### 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](#)

SUGAR-RSR INFOmissingINFO

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.