



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 19, 2024 – 12:05 PM EDT

PDB ID : 4Z7Q  
Title : Integrin alphaIIb beta3 in complex with AGDV-NH2 peptide  
Authors : Lin, F.-Y.; Zhu, J.; Springer, T.A.  
Deposited on : 2015-04-07  
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

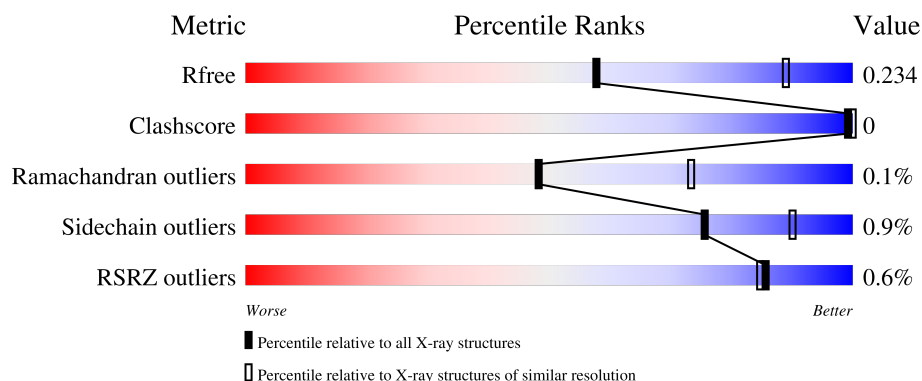
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

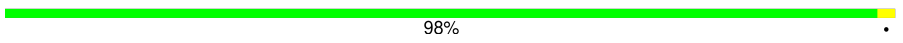
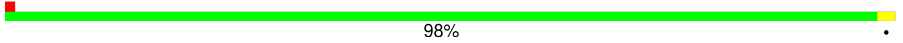
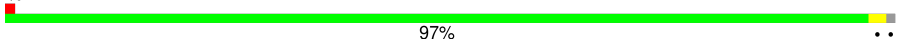
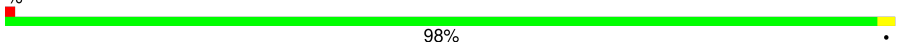
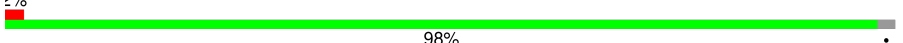
The reported resolution of this entry is 2.70 Å.

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.



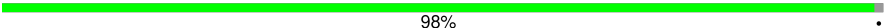
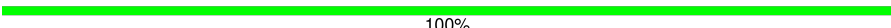
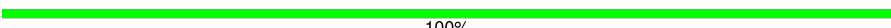
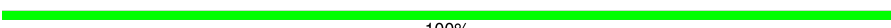


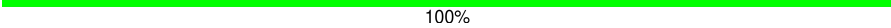
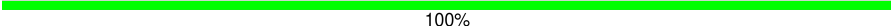
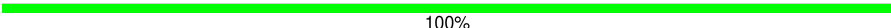
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	A	454	 98%
1	C	454	 98%
2	B	471	 97%
2	D	471	 98%
3	E	219	 98%

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Mol	Chain	Length	Quality of chain
3	H	219	 98%
4	F	214	 100%
4	L	214	 100%
5	G	5	 100%
5	I	5	 20% 100%
6	J	5	 40% 60%
7	K	2	 100%
7	N	2	 100%
8	M	3	 100%

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 42446 atoms, of which 20326 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	454	Total	C	H	N	O	S	0	7	0
			6882	2236	3366	606	666	8			
1	C	453	Total	C	H	N	O	S	0	6	0
			6839	2224	3337	604	666	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	466	Total	C	H	N	O	S	6	8	0
			7178	2262	3546	620	717	33			
2	D	471	Total	C	H	N	O	S	10	2	0
			7182	2260	3551	620	716	35			

- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	214	Total	C	H	N	O	S	0	0	0
			3221	1035	1590	264	326	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3242	1041	1600	266	329	6			

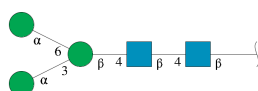
- Molecule 4 is a protein called Monoclonal antibody 10E5 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	0	0	0
			3190	1019	1553	268	341	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3190	1019	1553	268	341	9			

- Molecule 5 is a protein called Tetrapeptide AGDV-NH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	5	Total	C	H	N	O	0	0	1
			45	14	20	5	6			
5	I	5	Total	C	H	N	O	0	0	1
			45	14	20	5	6			

- Molecule 6 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.



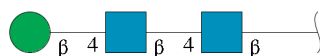
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	5	Total	C	H	N	O	0	0	0
			116	34	55	2	25			

- Molecule 7 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
7	K	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
7	N	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 8 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.

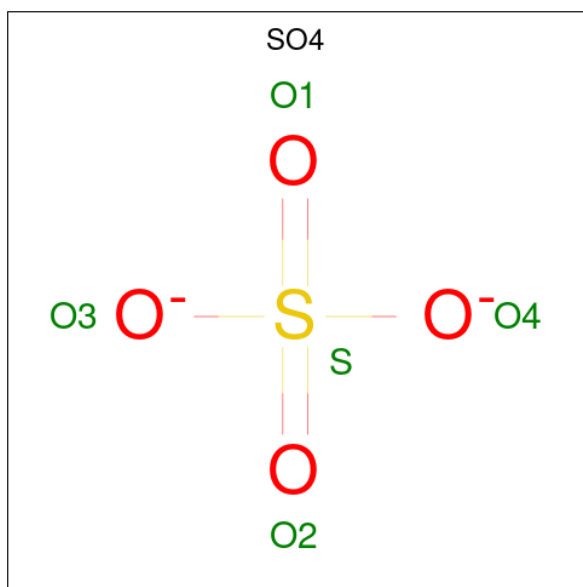


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	3	Total	C	H	N	O	0	0	0
			74	22	35	2	15			

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Ca	0	0
			4	4		
9	C	4	Total	Ca	0	0
			4	4		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

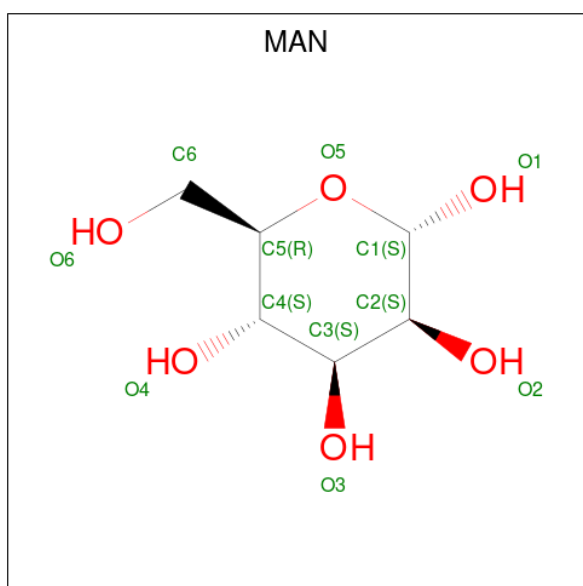
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	3	Total	Mn	0	0
			3	3		
12	D	3	Total	Mn	0	0
			3	3		

- Molecule 13 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
13	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
13	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 14 is alpha-D-mannopyranose (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total Cl 1 1	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	369	Total O 369 369	0	0
16	B	183	Total O 183 183	0	0
16	C	165	Total O 165 165	0	0
16	D	141	Total O 141 141	0	0
16	E	18	Total O 18 18	0	0
16	F	19	Total O 19 19	0	0
16	H	36	Total O 36 36	0	0
16	L	54	Total O 54 54	0	0
16	G	3	Total O 3 3	0	0
16	I	3	Total O 3 3	0	0

### 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: Integrin alpha-IIb

Chain A:  98%



- Molecule 1: Integrin alpha-IIb

Chain C:  98%



- Molecule 2: Integrin beta-3

Chain B:  97%



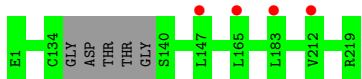
- Molecule 2: Integrin beta-3

Chain D:  98%



- Molecule 3: Monoclonal antibody 10E5 heavy chain

Chain E:  98%



- Molecule 3: Monoclonal antibody 10E5 heavy chain

Chain H:  98%



- Molecule 4: Monoclonal antibody 10E5 light chain

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Monoclonal antibody 10E5 light chain

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Tetrapeptide AGDV-NH<sub>2</sub>

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Tetrapeptide AGDV-NH<sub>2</sub>

Chain I:  20%  100%



- Molecule 6: 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

Chain J:  40%  60%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1  
MAG2

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

100%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.44Å 144.24Å 104.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 2.70 48.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.94-2.70) 99.5 (48.94-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.188 , 0.236 0.192 , 0.234	Depositor DCC
$R_{free}$ test set	1078 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.7	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 80.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	42446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: GOL, NH2, MAN, SO4, NAG, MN, CA, BMA, CL

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	0.22	0/3633	0.40	0/4951
1	C	0.22	0/3618	0.38	0/4930
2	B	0.22	0/3728	0.39	0/5057
2	D	0.22	0/3710	0.38	0/5029
3	E	0.21	0/1673	0.37	0/2290
3	H	0.21	0/1684	0.38	0/2305
4	F	0.21	0/1673	0.36	0/2269
4	L	0.22	0/1673	0.37	0/2269
5	G	0.16	0/23	0.32	0/30
5	I	0.31	0/23	0.53	0/30
All	All	0.22	0/21438	0.38	0/29160

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3516	3366	3361	1	0
1	C	3502	3337	3320	1	0
2	B	3632	3546	3516	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3631	3551	3539	4	0
3	E	1631	1590	1590	0	0
3	H	1642	1600	1600	0	0
4	F	1637	1553	1553	0	0
4	L	1637	1553	1553	0	0
5	G	25	20	20	0	0
5	I	25	20	20	0	0
6	J	61	55	52	0	0
7	K	28	27	25	0	0
7	N	28	27	24	0	0
8	M	39	35	33	0	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
10	A	15	0	0	0	0
10	C	15	0	0	0	0
10	L	5	0	0	0	0
11	A	6	8	8	0	0
12	B	3	0	0	0	0
12	D	3	0	0	0	0
13	B	14	14	13	0	0
13	D	14	14	13	0	0
14	C	11	10	10	0	0
15	C	1	0	0	0	0
16	A	369	0	0	0	0
16	B	183	0	0	0	0
16	C	165	0	0	0	0
16	D	141	0	0	0	0
16	E	18	0	0	0	0
16	F	19	0	0	0	0
16	G	3	0	0	0	0
16	H	36	0	0	0	0
16	I	3	0	0	0	0
16	L	54	0	0	0	0
All	All	22120	20326	20250	7	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 0.

The worst 5 of 7 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)
2:B:288:ASP:OD1	2:B:289:TYR:N	2.43	0.52
2:D:371:ASN:HB2	2:D:398:SER:HB3	2.00	0.43
2:D:126:ASP:OD1	2:D:126:ASP:N	2.53	0.42
2:D:217:ASP:OD2	2:D:255:HIS:NE2	2.53	0.41
1:A:365:ASP:OD2	1:A:370:GLY:N	2.47	0.41

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	459/454 (101%)	439 (96%)	19 (4%)	1 (0%)	44	68
1	C	457/454 (101%)	437 (96%)	20 (4%)	0	100	100
2	B	472/471 (100%)	449 (95%)	21 (4%)	2 (0%)	30	55
2	D	471/471 (100%)	454 (96%)	17 (4%)	0	100	100
3	E	210/219 (96%)	197 (94%)	13 (6%)	0	100	100
3	H	212/219 (97%)	196 (92%)	16 (8%)	0	100	100
4	F	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
4	L	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
5	G	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
5	I	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	2711/2726 (99%)	2575 (95%)	133 (5%)	3 (0%)	48	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	375	LEU
2	B	157	VAL



### 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	368/362 (102%)	363 (99%)	5 (1%)	62	84
1	C	366/362 (101%)	360 (98%)	6 (2%)	58	82
2	B	420/416 (101%)	413 (98%)	7 (2%)	56	81
2	D	418/416 (100%)	415 (99%)	3 (1%)	81	93
3	E	186/189 (98%)	186 (100%)	0	100	100
3	H	187/189 (99%)	186 (100%)	1 (0%)	86	95
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
5	G	2/2 (100%)	2 (100%)	0	100	100
5	I	2/2 (100%)	2 (100%)	0	100	100
All	All	2325/2314 (100%)	2303 (99%)	22 (1%)	75	90

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	166	TYR
1	C	307	LEU
1	C	288	TYR
2	D	123	SER
2	B	76	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

12 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	$\# Z  > 2$
6	NAG	J	1	2,6	14,14,15	0.35	0	17,19,21	0.51	0
6	NAG	J	2	6	14,14,15	0.33	0	17,19,21	0.49	0
6	BMA	J	3	6	11,11,12	0.90	1 (9%)	15,15,17	0.89	0
6	MAN	J	4	6	11,11,12	0.72	0	15,15,17	1.08	2 (13%)
6	MAN	J	5	6	11,11,12	0.90	0	15,15,17	1.04	1 (6%)
7	NAG	K	1	2,7	14,14,15	0.27	0	17,19,21	0.42	0
7	NAG	K	2	7	14,14,15	0.21	0	17,19,21	0.50	0
8	NAG	M	1	2,8	14,14,15	0.16	0	17,19,21	0.48	0
8	NAG	M	2	8	14,14,15	0.33	0	17,19,21	0.38	0
8	BMA	M	3	8	11,11,12	0.63	0	15,15,17	0.72	0
7	NAG	N	1	2,7	14,14,15	0.21	0	17,19,21	0.47	0
7	NAG	N	2	7	14,14,15	0.50	0	17,19,21	0.58	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
6	NAG	J	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	1/2/19/22	0/1/1/1
7	NAG	K	1	2,7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	K	2	7	-	4/6/23/26	0/1/1/1
8	NAG	M	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	M	2	8	-	0/6/23/26	0/1/1/1
8	BMA	M	3	8	-	0/2/19/22	0/1/1/1
7	NAG	N	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	3	BMA	O5-C1	-2.04	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	4	MAN	C1-O5-C5	3.01	116.22	112.19
6	J	5	MAN	O2-C2-C3	-2.28	105.42	110.15
6	J	4	MAN	O2-C2-C3	-2.24	105.52	110.15

There are no chirality outliers.

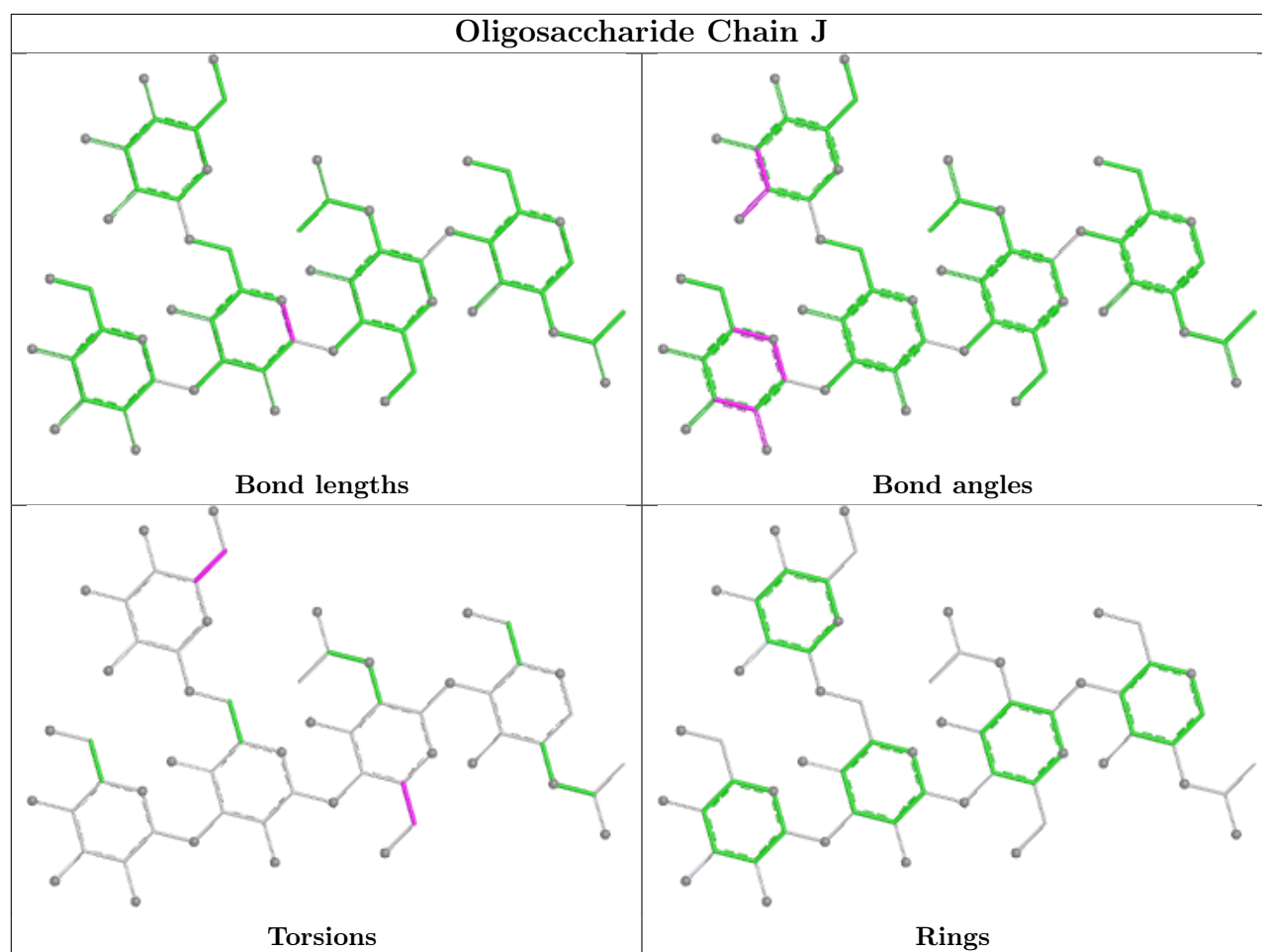
5 of 11 torsion outliers are listed below:

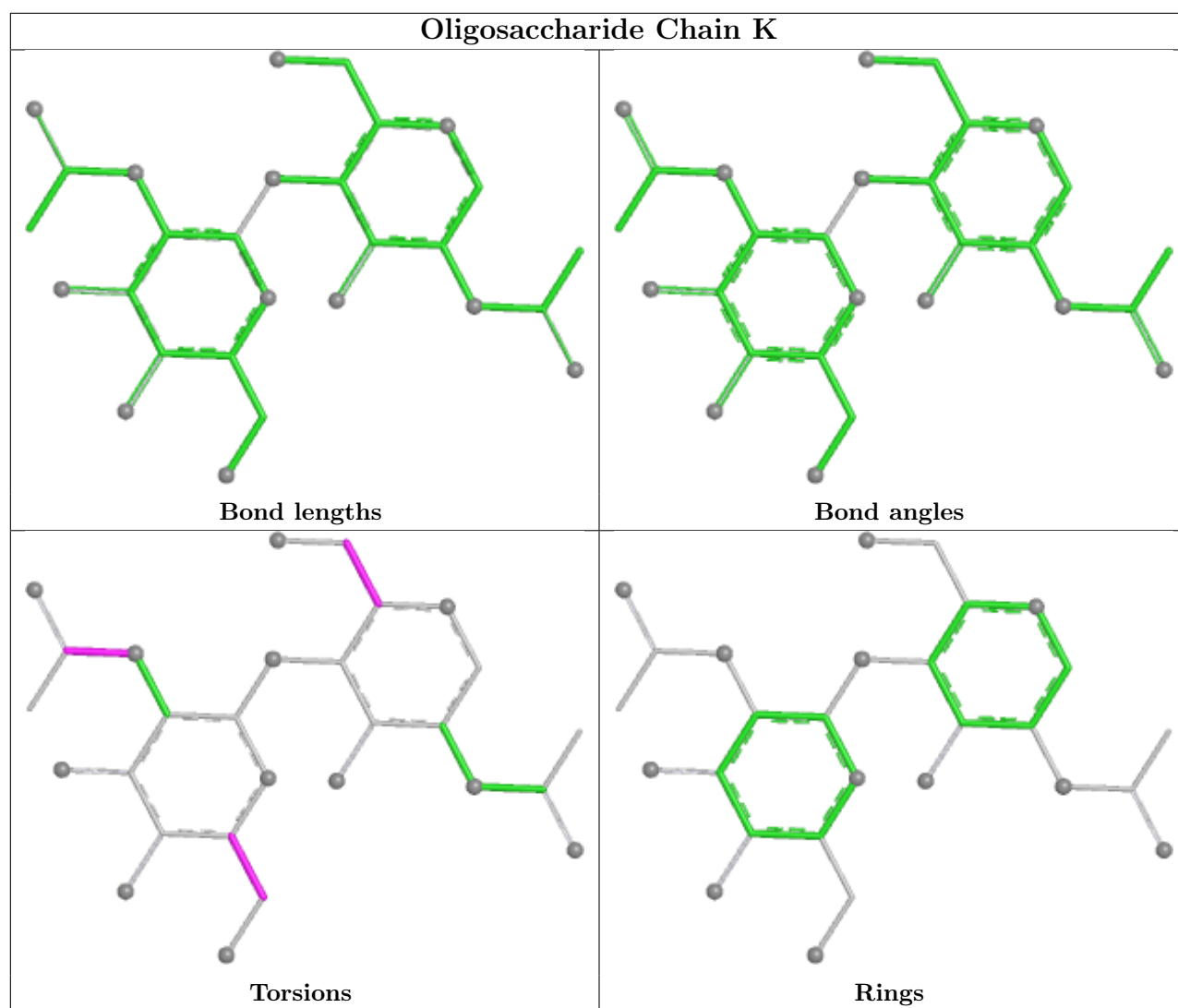
Mol	Chain	Res	Type	Atoms
7	K	1	NAG	C4-C5-C6-O6
7	K	2	NAG	C4-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
7	K	1	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6

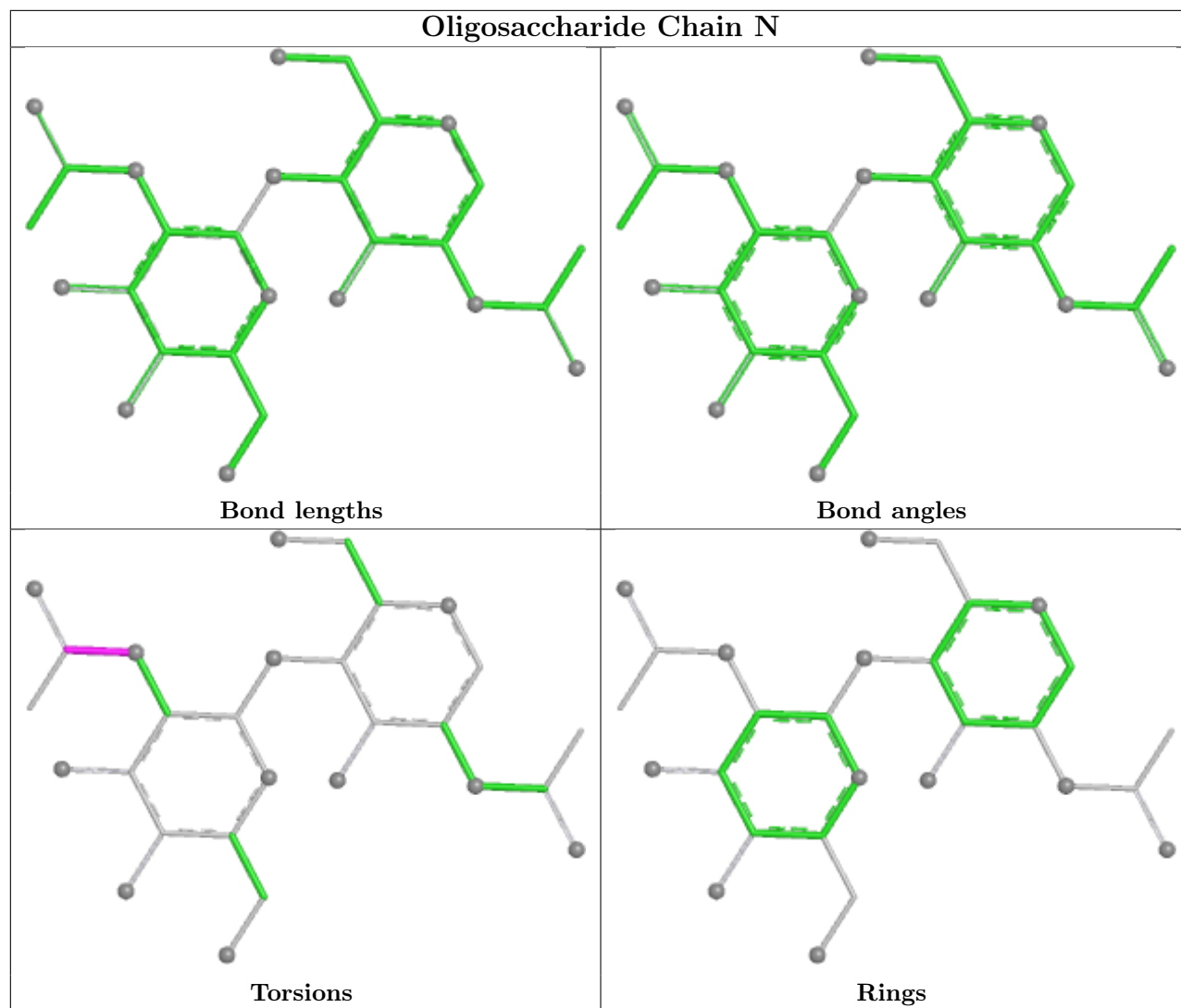
There are no ring outliers.

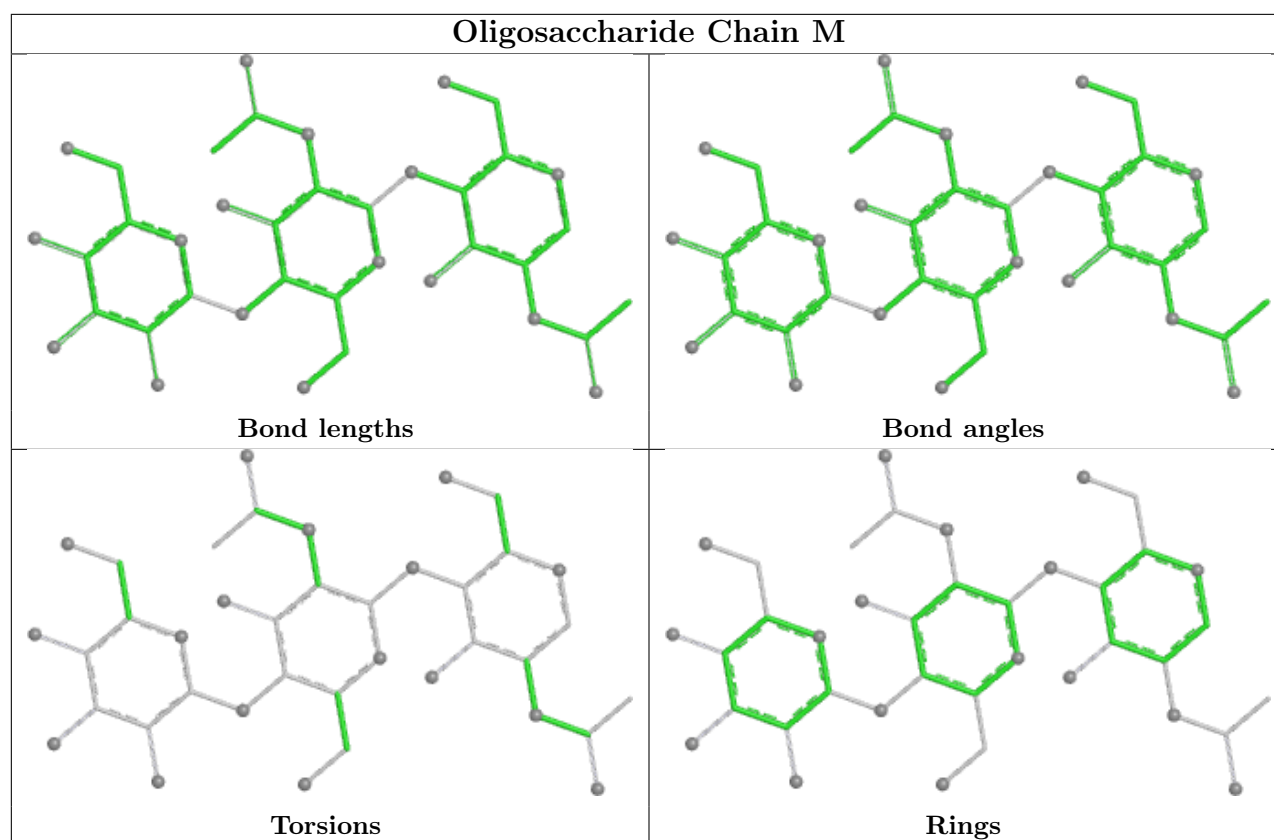
No monomer is involved in short contacts.

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](#)

Of 26 ligands modelled in this entry, 15 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z  > 2$
10	SO4	C	507	-	4,4,4	0.24	0	6,6,6	0.06	0
10	SO4	C	508	-	4,4,4	0.23	0	6,6,6	0.07	0
11	GOL	A	508	-	5,5,5	0.38	0	5,5,5	0.17	0
13	NAG	B	2004	2	14,14,15	0.19	0	17,19,21	0.45	0
10	SO4	A	506	-	4,4,4	0.24	0	6,6,6	0.08	0
10	SO4	A	505	-	4,4,4	0.24	0	6,6,6	0.07	0
10	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.08	0
13	NAG	D	503	2	14,14,15	0.54	0	17,19,21	0.50	0
10	SO4	A	507	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	MAN	C	505	-	11,11,12	0.65	0	15,15,17	1.04	2 (13%)
10	SO4	C	506	-	4,4,4	0.23	0	6,6,6	0.08	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
14	MAN	C	505	-	-	2/2/19/22	0/1/1/1
11	GOL	A	508	-	-	2/4/4/4	-
13	NAG	D	503	2	-	2/6/23/26	0/1/1/1
13	NAG	B	2004	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	505	MAN	C1-O5-C5	2.68	115.78	112.19
14	C	505	MAN	O2-C2-C3	-2.36	105.26	110.15

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	2004	NAG	O5-C5-C6-O6
13	D	503	NAG	O5-C5-C6-O6
13	D	503	NAG	C4-C5-C6-O6
14	C	505	MAN	O5-C5-C6-O6
13	B	2004	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	454/454 (100%)	-0.67	1 (0%) 92 91	30, 57, 99, 178	6 (1%)
1	C	453/454 (99%)	-0.37	3 (0%) 84 83	39, 81, 126, 186	4 (0%)
2	B	466/471 (98%)	-0.19	3 (0%) 85 85	35, 99, 196, 236	6 (1%)
2	D	471/471 (100%)	-0.16	3 (0%) 85 85	40, 103, 177, 274	2 (0%)
3	E	214/219 (97%)	0.24	4 (1%) 66 65	84, 169, 249, 306	0
3	H	216/219 (98%)	-0.00	0 100 100	54, 128, 199, 226	0
4	F	214/214 (100%)	0.13	0 100 100	86, 157, 230, 269	0
4	L	214/214 (100%)	-0.30	0 100 100	61, 112, 157, 222	0
5	G	4/5 (80%)	0.29	0 100 100	67, 72, 77, 89	0
5	I	4/5 (80%)	1.28	1 (25%) 2 2	88, 96, 97, 113	0
All	All	2710/2726 (99%)	-0.23	15 (0%) 85 85	30, 98, 200, 306	18 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	129[A]	TRP	8.5
1	A	454	VAL	5.1
1	C	1	LEU	4.0
5	I	408	ALA	3.2
3	E	147	LEU	3.1

### 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 ⓘ

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands ⓘ

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(Å <sup>2</sup> )	Q<0.9
14	MAN	C	505	11/12	0.69	0.10	105,127,152,153	0
12	MN	D	501	1/1	0.77	0.16	373,373,373,373	0
13	NAG	B	2004	14/15	0.78	0.10	112,139,164,168	0
10	SO4	C	508	5/5	0.78	0.12	128,134,137,137	0
10	SO4	L	301	5/5	0.82	0.10	119,121,128,136	0
10	SO4	C	507	5/5	0.83	0.10	142,142,158,159	0
13	NAG	D	503	14/15	0.84	0.10	90,120,136,151	0
12	MN	B	2002	1/1	0.84	0.22	341,341,341,341	0
11	GOL	A	508	6/6	0.87	0.14	69,95,115,117	0
10	SO4	A	506	5/5	0.90	0.17	115,126,130,141	0
10	SO4	C	506	5/5	0.91	0.17	145,159,162,164	0
10	SO4	A	507	5/5	0.91	0.10	88,93,107,118	0
10	SO4	A	505	5/5	0.92	0.19	135,139,148,160	0
12	MN	D	509	1/1	0.94	0.10	126,126,126,126	0
15	CL	C	509	1/1	0.95	0.10	100,100,100,100	0
9	CA	C	504	1/1	0.98	0.08	76,76,76,76	0
9	CA	A	501	1/1	0.98	0.04	65,65,65,65	0
9	CA	A	502	1/1	0.99	0.04	58,58,58,58	0
12	MN	D	502	1/1	0.99	0.05	81,81,81,81	0
9	CA	A	503	1/1	0.99	0.04	47,47,47,47	0
9	CA	A	504	1/1	0.99	0.07	65,65,65,65	0
9	CA	C	501	1/1	0.99	0.03	116,116,116,116	0
9	CA	C	502	1/1	0.99	0.03	77,77,77,77	0
12	MN	B	2003	1/1	0.99	0.04	74,74,74,74	0
12	MN	B	2001	1/1	1.00	0.04	49,49,49,49	0
9	CA	C	503	1/1	1.00	0.04	75,75,75,75	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.