



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 09:54 AM EDT

PDB ID : 4GXU  
Title : Crystal structure of antibody 1F1 bound to the 1918 influenza hemagglutinin  
Authors : Ekiert, D.C.; Wilson, I.A.  
Deposited on : 2012-09-04  
Resolution : 3.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.35  
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) : 2.35

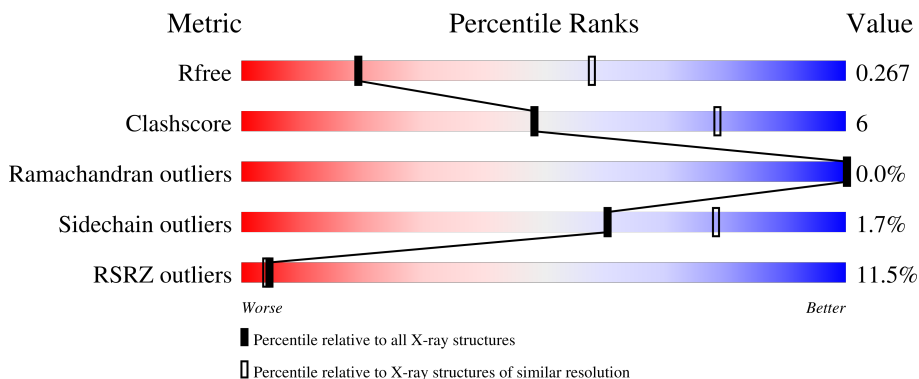
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.29 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	331	
1	C	331	
1	E	331	
1	G	331	
1	I	331	

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Mol	Chain	Length	Quality of chain
1	K	331	7% 87% 11%
2	B	176	7% 82% 14%
2	D	176	7% 83% 14%
2	F	176	7% 83% 14%
2	H	176	15% 81% 15%
2	J	176	10% 80% 16%
2	L	176	10% 85% 12%
3	M	231	7% 85% 14%
3	O	231	7% 45% 9% 46%
3	Q	231	23% 80% 18%
3	S	231	9% 47% 7% 46%
3	U	231	10% 43% 11% 46%
3	W	231	7% 45% 9% 46%
4	N	217	8% 88% 10%
4	P	217	9% 42% 9% 49%
4	R	217	24% 86% 12%
4	T	217	13% 39% 11% 49%
4	V	217	17% 39% 12% 49%
4	X	217	13% 42% 8% 49%
5	Y	3	33% 33% 33%
5	Z	3	100%
5	a	3	33% 67%
5	b	3	67% 33%
5	c	3	100%
5	d	3	67% 33%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	PCA	Q	1	-	-	-	X
4	PCA	P	1	-	-	-	X
4	PCA	R	1	-	-	-	X
4	PCA	X	1	-	-	-	X
5	BMA	a	3	-	-	-	X
6	NAG	B	201	-	-	-	X
6	NAG	I	401	-	-	-	X
6	NAG	J	201	-	-	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 38412 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	325	2568	1619	440	498	11	0	7	0
1	C	325	2576	1623	442	500	11	0	8	0
1	E	325	2576	1623	442	500	11	0	8	0
1	G	325	2576	1623	442	500	11	0	8	0
1	I	325	2576	1623	442	500	11	0	8	0
1	K	325	2576	1623	442	500	11	0	8	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q9WFX3
A	8	ASP	-	expression tag	UNP Q9WFX3
A	9	PRO	-	expression tag	UNP Q9WFX3
A	10	GLY	-	expression tag	UNP Q9WFX3
C	7	ALA	-	expression tag	UNP Q9WFX3
C	8	ASP	-	expression tag	UNP Q9WFX3
C	9	PRO	-	expression tag	UNP Q9WFX3
C	10	GLY	-	expression tag	UNP Q9WFX3
E	7	ALA	-	expression tag	UNP Q9WFX3
E	8	ASP	-	expression tag	UNP Q9WFX3
E	9	PRO	-	expression tag	UNP Q9WFX3
E	10	GLY	-	expression tag	UNP Q9WFX3
G	7	ALA	-	expression tag	UNP Q9WFX3
G	8	ASP	-	expression tag	UNP Q9WFX3
G	9	PRO	-	expression tag	UNP Q9WFX3
G	10	GLY	-	expression tag	UNP Q9WFX3
I	7	ALA	-	expression tag	UNP Q9WFX3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	8	ASP	-	expression tag	UNP Q9WFX3
I	9	PRO	-	expression tag	UNP Q9WFX3
I	10	GLY	-	expression tag	UNP Q9WFX3
K	7	ALA	-	expression tag	UNP Q9WFX3
K	8	ASP	-	expression tag	UNP Q9WFX3
K	9	PRO	-	expression tag	UNP Q9WFX3
K	10	GLY	-	expression tag	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	171	1399	873	241	279	6	0	3	0
2	D	171	1399	873	241	279	6	0	3	0
2	F	171	1399	873	241	279	6	0	3	0
2	H	171	1399	873	241	279	6	0	3	0
2	J	171	1399	873	241	279	6	0	3	0
2	L	171	1399	873	241	279	6	0	3	0

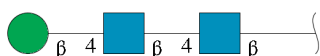
- Molecule 3 is a protein called Antibody 1F1, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	228	1758	1106	304	339	9	0	4	0
3	O	125	1003	632	178	187	6	0	2	0
3	Q	228	1766	1111	305	340	10	0	5	0
3	S	125	1003	632	178	187	6	0	2	0
3	U	125	1003	632	178	187	6	0	2	0
3	W	125	1003	632	178	187	6	0	2	0

- Molecule 4 is a protein called Antibody 1F1, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	214	Total	C	N	O	S	0	7	0
			1620	1019	268	329	4			
4	P	111	Total	C	N	O	S	0	7	0
			848	534	140	172	2			
4	R	214	Total	C	N	O	S	0	7	0
			1620	1019	268	329	4			
4	T	111	Total	C	N	O	S	0	7	0
			848	534	140	172	2			
4	V	111	Total	C	N	O	S	0	7	0
			848	534	140	172	2			
4	X	111	Total	C	N	O	S	0	7	0
			848	534	140	172	2			

- Molecule 5 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
5	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	Z	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	a	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	b	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	c	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	d	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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>).



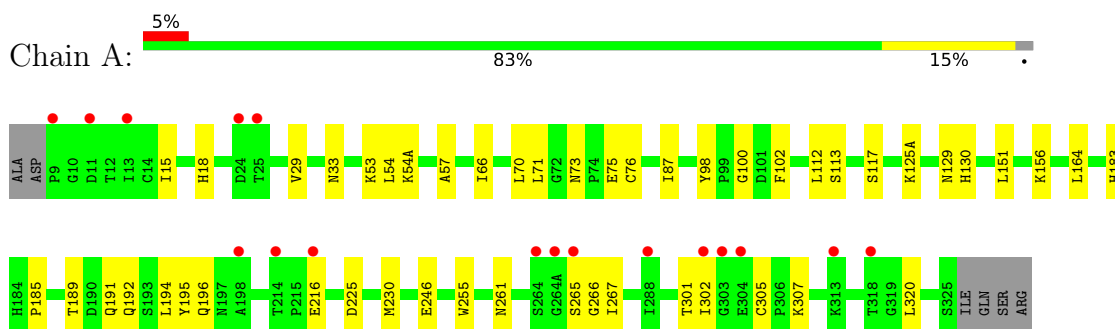
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	Total 14	8	1	5	0	0
6	B	1	Total 14	8	1	5	0	0
6	C	1	Total 14	8	1	5	0	0
6	D	1	Total 14	8	1	5	0	0
6	E	1	Total 14	8	1	5	0	0
6	F	1	Total 14	8	1	5	0	0
6	G	1	Total 14	8	1	5	0	0
6	H	1	Total 14	8	1	5	0	0
6	I	1	Total 14	8	1	5	0	0
6	J	1	Total 14	8	1	5	0	0
6	K	1	Total 14	8	1	5	0	0
6	L	1	Total 14	8	1	5	0	0



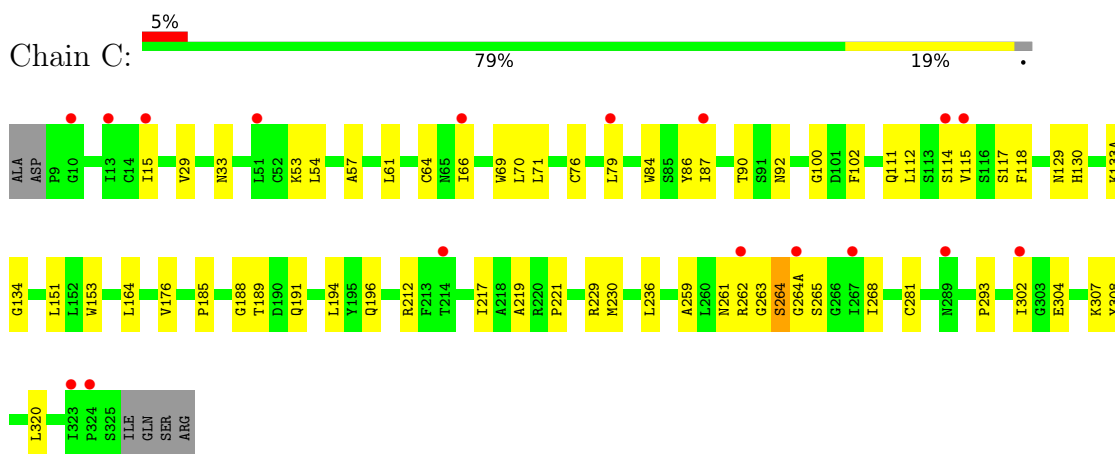
### 3 Residue-property plots [i](#)

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.

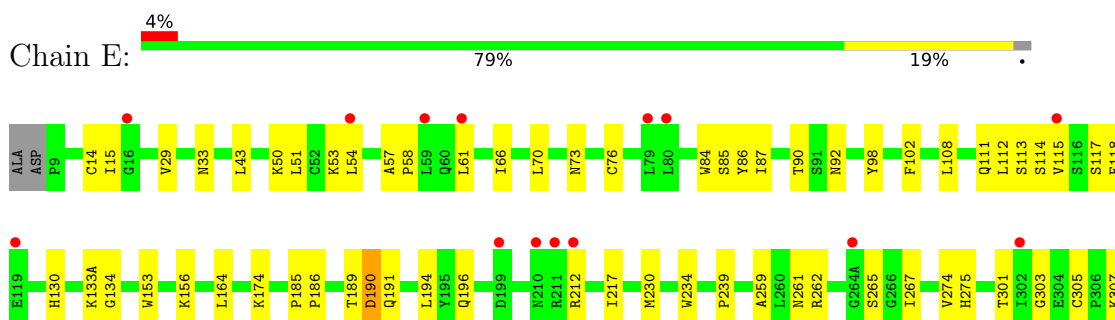
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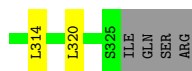


- Molecule 1: Hemagglutinin HA1 chain

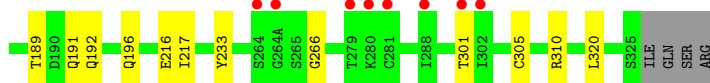
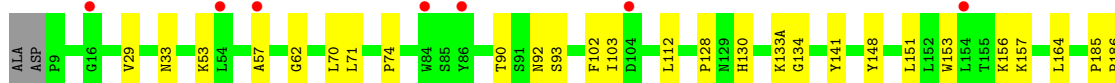
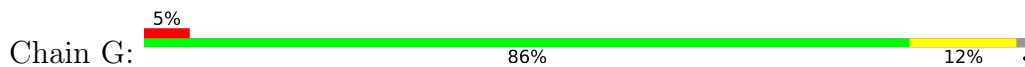


- Molecule 1: Hemagglutinin HA1 chain

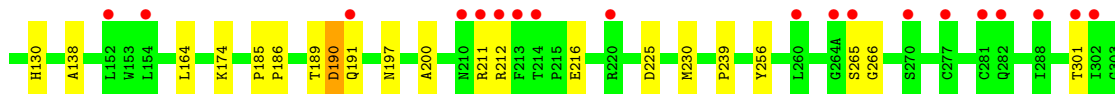
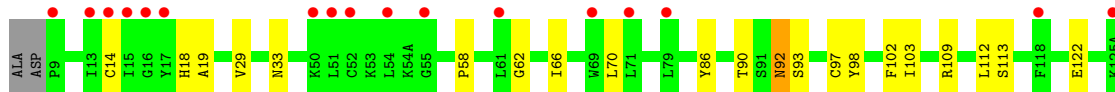
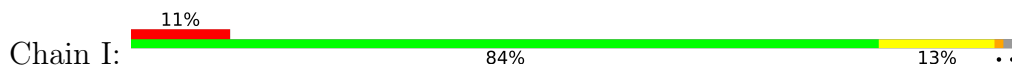




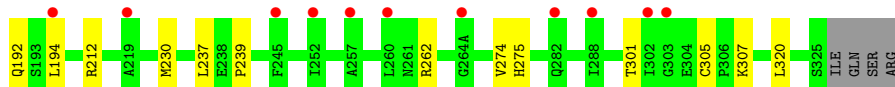
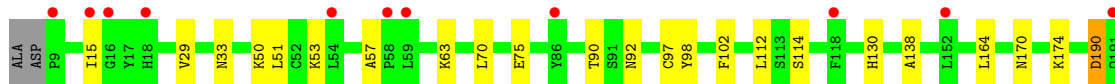
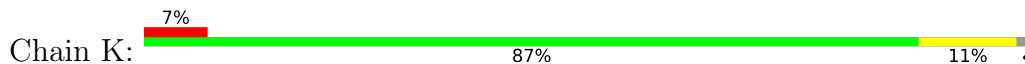
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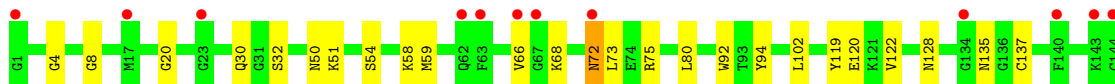
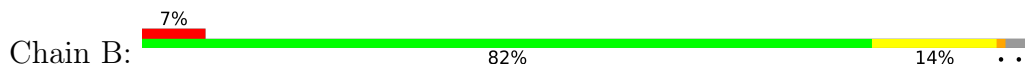
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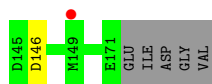


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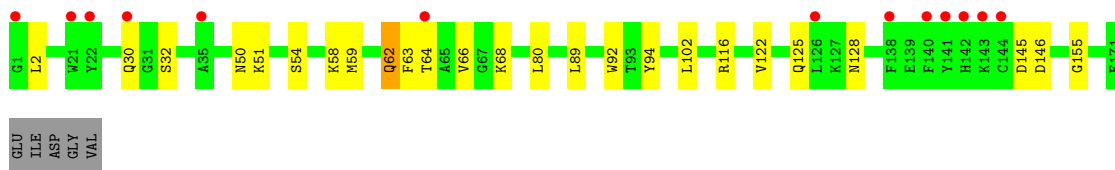
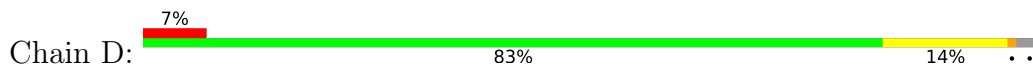


- Molecule 2: Hemagglutinin HA2 chain

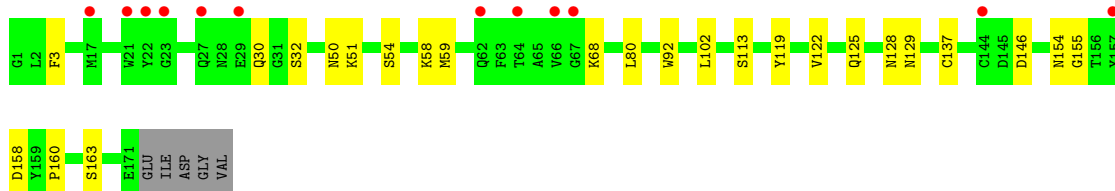
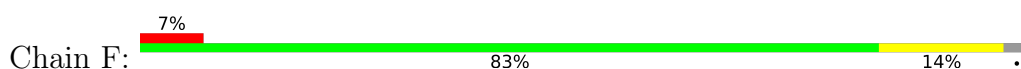




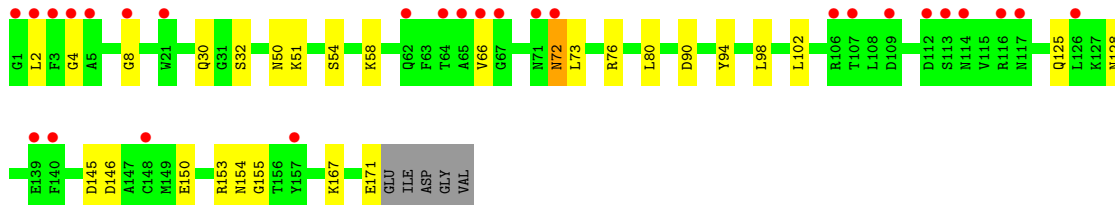
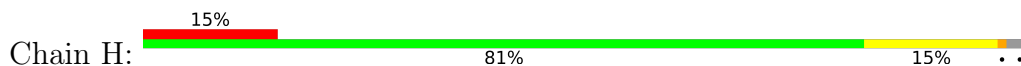
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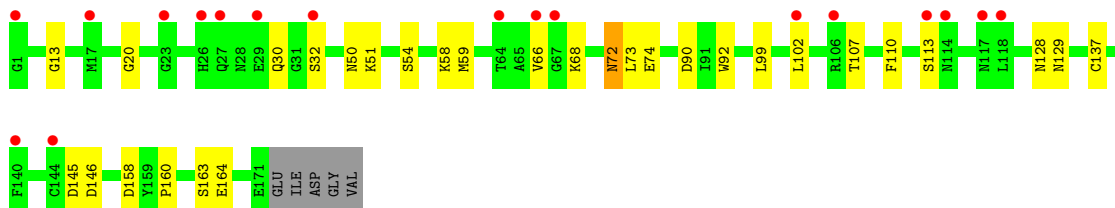
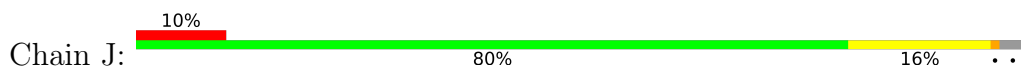
- Molecule 2: Hemagglutinin HA2 chain



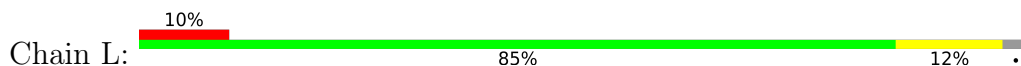
- Molecule 2: Hemagglutinin HA2 chain

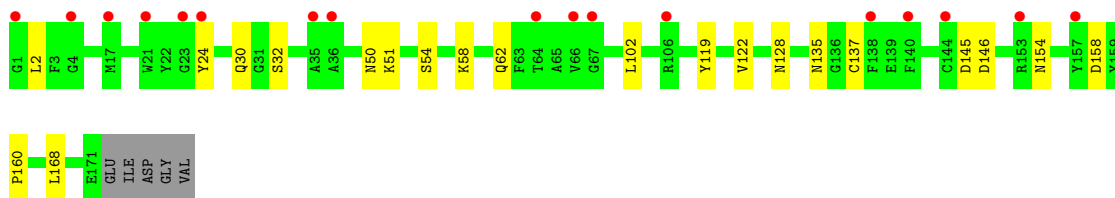


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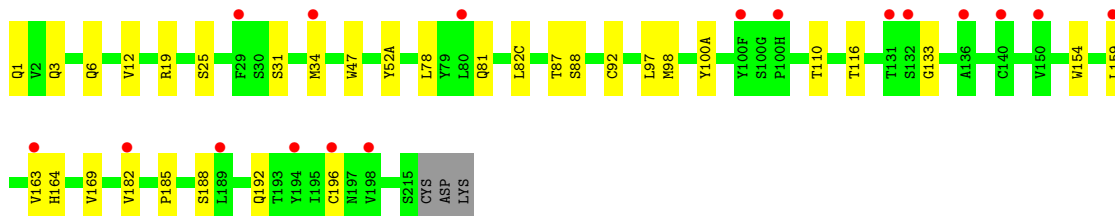
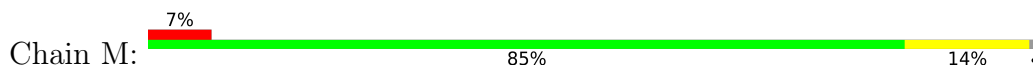


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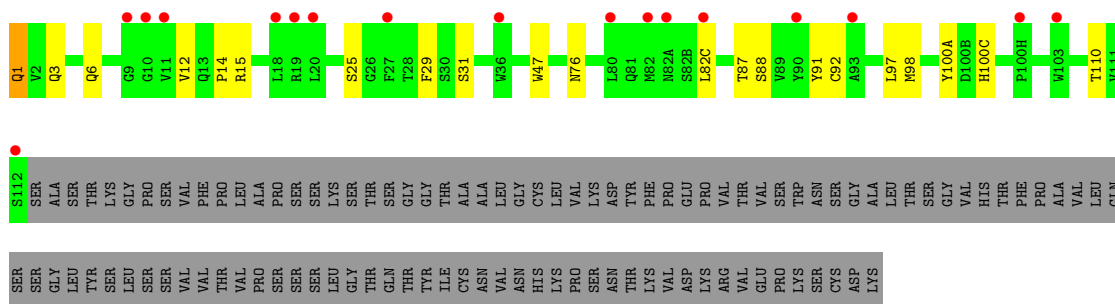
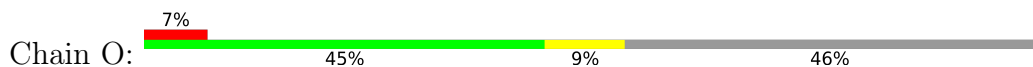




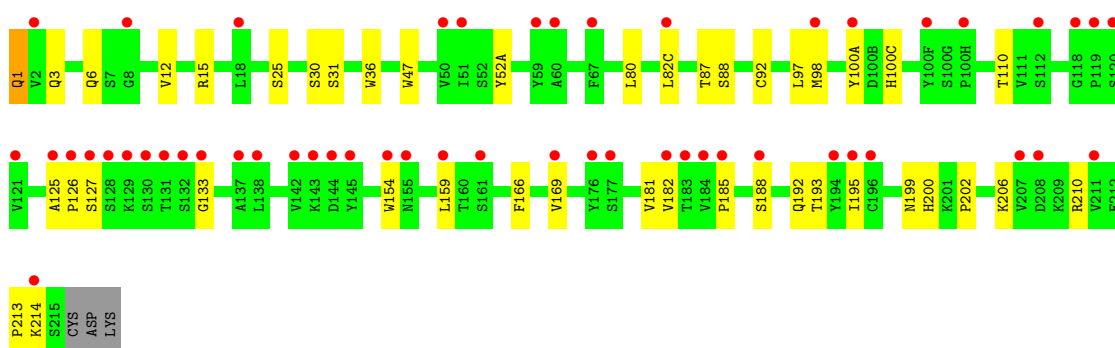
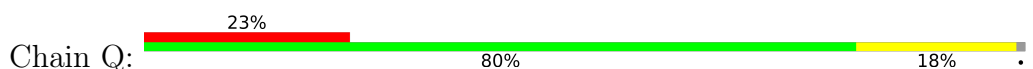
• Molecule 3: Antibody 1F1, heavy chain



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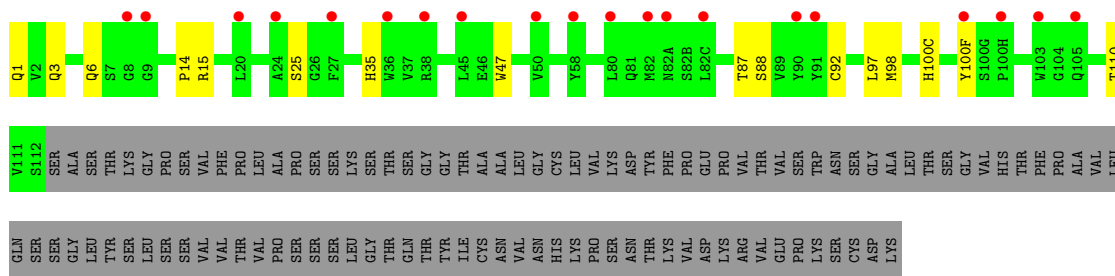


• Molecule 3: Antibody 1F1, heavy chain

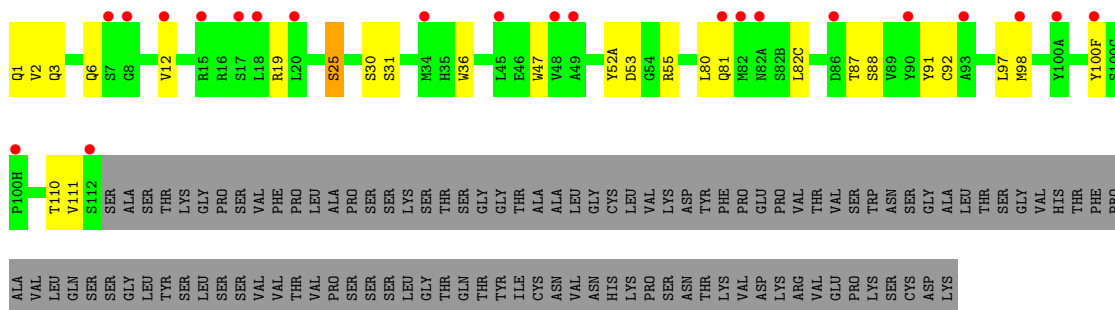


• Molecule 3: Antibody 1F1, heavy chain

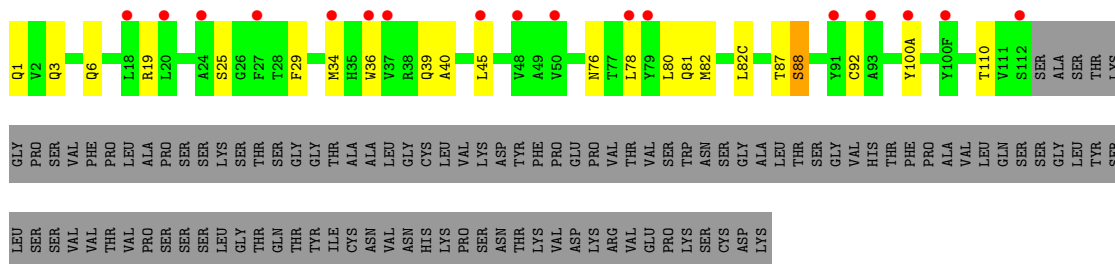




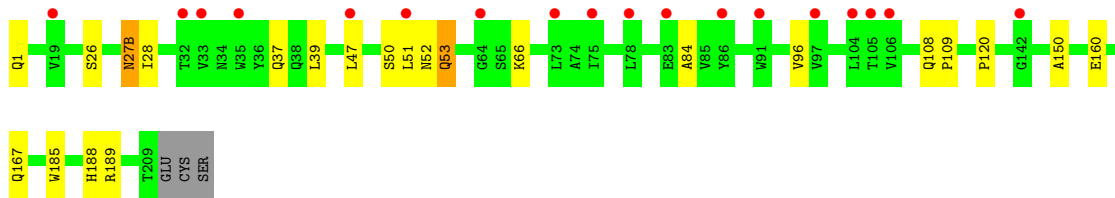
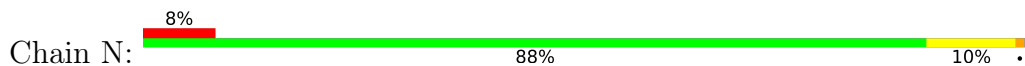
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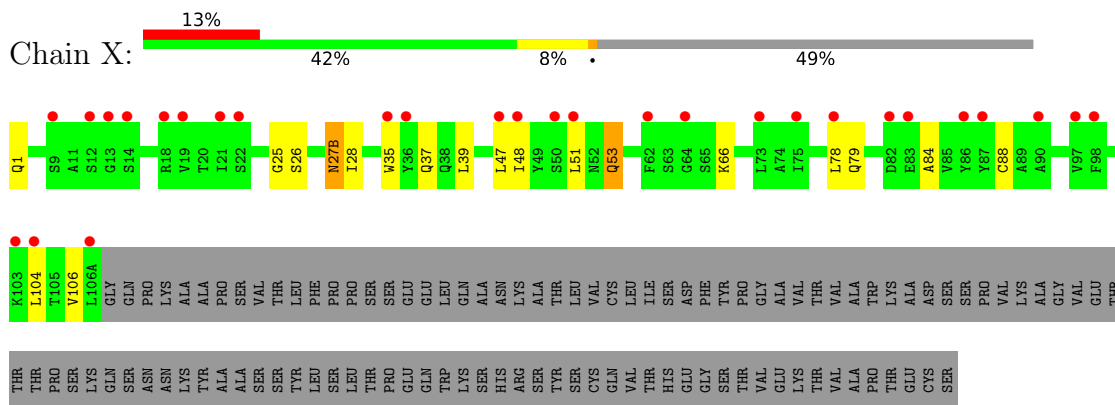
• Molecule 4: Antibody 1F1, light chain



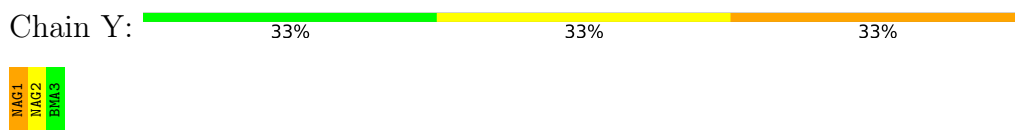
• Molecule 4: Antibody 1F1, light chain



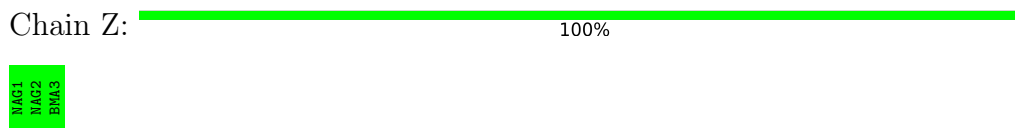




- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



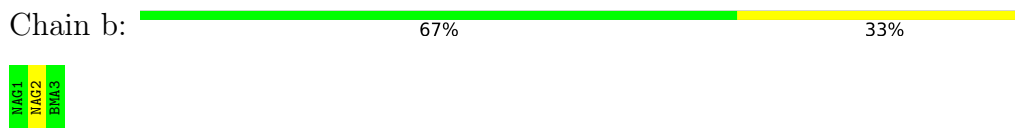
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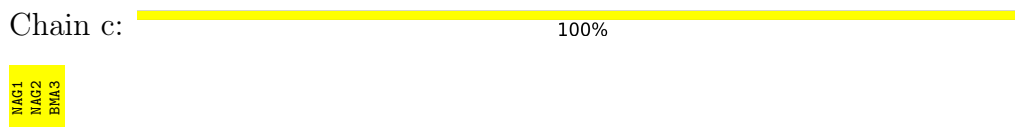
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- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  67% 33%

MAG1  
MAG2  
BMOA3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.71Å 176.27Å 168.12Å 90.00° 92.14° 90.00°	Depositor
Resolution (Å)	35.04 – 3.29 45.23 – 3.29	Depositor EDS
% Data completeness (in resolution range)	80.1 (35.04-3.29) 80.3 (45.23-3.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 3.32Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.219 , 0.255 0.227 , 0.267	Depositor DCC
$R_{free}$ test set	5439 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	104.3	Xtrriage
Anisotropy	0.548	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	38412	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, PCA, 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	0.29	0/2633	0.62	0/3588
1	C	0.33	0/2641	0.71	1/3599 (0.0%)
1	E	0.31	0/2641	0.65	0/3599
1	G	0.28	0/2641	0.60	0/3599
1	I	0.26	0/2641	0.57	0/3599
1	K	0.28	0/2641	0.60	0/3599
2	B	0.32	0/1426	0.59	0/1920
2	D	0.34	0/1426	0.64	1/1920 (0.1%)
2	F	0.34	0/1426	0.62	0/1920
2	H	0.31	0/1426	0.52	0/1920
2	J	0.32	0/1426	0.56	0/1920
2	L	0.35	0/1426	0.60	2/1920 (0.1%)
3	M	0.28	0/1794	0.59	0/2444
3	O	0.24	0/1020	0.55	0/1383
3	Q	0.26	0/1802	0.58	0/2454
3	S	0.24	0/1020	0.58	0/1383
3	U	0.27	0/1020	0.59	0/1383
3	W	0.26	0/1020	0.55	0/1383
4	N	0.27	0/1662	0.58	0/2276
4	P	0.24	0/869	0.57	0/1189
4	R	0.25	0/1662	0.60	1/2276 (0.0%)
4	T	0.24	0/869	0.57	0/1189
4	V	0.24	0/869	0.59	0/1189
4	X	0.23	0/869	0.53	0/1189
All	All	0.29	0/38870	0.60	5/52841 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	207	ALA	C-N-CD	6.38	141.80	128.40
1	C	264	SER	N-CA-C	5.96	127.09	111.00
2	D	62	GLN	N-CA-C	-5.55	96.03	111.00
2	L	168	LEU	CB-CG-CD1	-5.25	102.07	111.00
2	L	168	LEU	CA-CB-CG	5.04	126.90	115.30

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	2568	0	2488	39	0
1	C	2576	0	2493	54	1
1	E	2576	0	2493	51	0
1	G	2576	0	2493	30	0
1	I	2576	0	2493	32	0
1	K	2576	0	2493	23	0
2	B	1399	0	1312	22	0
2	D	1399	0	1312	24	0
2	F	1399	0	1312	19	0
2	H	1399	0	1312	22	0
2	J	1399	0	1312	25	0
2	L	1399	0	1312	13	0
3	M	1758	0	1718	20	0
3	O	1003	0	968	13	0
3	Q	1766	0	1726	26	0
3	S	1003	0	968	12	0
3	U	1003	0	968	18	0
3	W	1003	0	968	11	0
4	N	1620	0	1589	20	1
4	P	848	0	834	15	0
4	R	1620	0	1589	21	0
4	T	848	0	834	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	848	0	834	21	0
4	X	848	0	834	15	0
5	Y	39	0	34	1	0
5	Z	39	0	34	0	0
5	a	39	0	34	0	0
5	b	39	0	34	0	0
5	c	39	0	34	0	0
5	d	39	0	34	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
6	D	14	0	13	0	0
6	E	14	0	13	0	0
6	F	14	0	13	1	0
6	G	14	0	13	0	0
6	H	14	0	13	1	0
6	I	14	0	13	0	0
6	J	14	0	13	0	0
6	K	14	0	13	0	0
6	L	14	0	13	1	0
All	All	38412	0	37015	452	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 6.

All (452) 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)
4:X:27(B):ASN:HD22	4:X:28:ILE:H	1.15	0.95
4:R:27(B):ASN:HD22	4:R:28:ILE:H	1.14	0.95
4:T:27(B):ASN:HD22	4:T:28:ILE:H	1.15	0.94
4:V:27(B):ASN:HD22	4:V:28:ILE:H	1.15	0.94
4:P:27(B):ASN:HD22	4:P:28:ILE:H	1.13	0.91
4:N:27(B):ASN:HD22	4:N:28:ILE:H	1.13	0.90
1:C:129:ASN:ND2	3:Q:1:PCA:OE	2.05	0.89
1:C:111:GLN:O	1:C:114:SER:OG	1.94	0.85
1:G:156:LYS:NZ	4:T:50[A]:SER:OG	2.16	0.79
3:U:6:GLN:HE21	3:U:92:CYS:H	1.31	0.78
1:G:90:THR:OG1	1:G:92[A]:ASN:OD1	2.03	0.77
1:C:117:SER:OG	1:C:261:ASN:ND2	2.17	0.77
1:E:90:THR:OG1	1:E:92[A]:ASN:OD1	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:LEU:HD11	1:K:112:LEU:HD11	1.66	0.76
1:C:90:THR:OG1	1:C:92[A]:ASN:OD1	2.02	0.76
1:K:90:THR:OG1	1:K:92[A]:ASN:OD1	2.02	0.76
3:Q:6:GLN:HE21	3:Q:92:CYS:H	1.31	0.75
1:C:307:LYS:HE3	2:D:92:TRP:NE1	2.03	0.73
4:P:37:GLN:HB2	4:P:47[B]:LEU:HD11	1.71	0.73
1:E:196:GLN:NE2	4:R:52:ASN:OD1	2.22	0.71
2:J:30:GLN:HE22	2:J:146:ASP:H	1.38	0.71
1:I:70:LEU:HD11	1:I:112:LEU:HD11	1.73	0.71
3:M:169[A]:VAL:HG21	4:N:160:GLU:HB3	1.71	0.71
2:H:50:ASN:ND2	1:K:29:VAL:O	2.21	0.71
4:N:37:GLN:HB2	4:N:47[B]:LEU:HD11	1.72	0.70
4:T:37:GLN:HB2	4:T:47[B]:LEU:HD11	1.73	0.70
1:C:264(A):GLY:O	2:D:64:THR:HG22	1.92	0.69
4:X:37:GLN:HB2	4:X:47[B]:LEU:HD11	1.73	0.69
1:I:197:ASN:HB2	1:I:200:ALA:HB2	1.74	0.68
4:V:37:GLN:HB2	4:V:47[B]:LEU:HD11	1.73	0.68
4:R:37:GLN:HB2	4:R:47[B]:LEU:HD11	1.75	0.68
3:W:6:GLN:HE21	3:W:92:CYS:H	1.40	0.68
2:B:50:ASN:ND2	1:C:29:VAL:O	2.25	0.68
2:B:30:GLN:HE22	2:B:146:ASP:H	1.39	0.68
1:K:50:LYS:HD2	1:K:275:HIS:HB2	1.77	0.68
3:S:87:THR:HG23	3:S:110:THR:HA	1.76	0.67
2:D:30:GLN:HE22	2:D:146:ASP:H	1.42	0.67
4:N:27(B):ASN:ND2	4:N:28:ILE:H	1.92	0.67
2:D:50:ASN:ND2	1:E:29:VAL:O	2.27	0.67
4:X:27(B):ASN:ND2	4:X:28:ILE:H	1.92	0.66
1:E:117:SER:OG	1:E:261:ASN:ND2	2.29	0.66
3:M:6:GLN:HE21	3:M:92:CYS:H	1.42	0.66
1:A:216:GLU:OE1	1:E:212:ARG:HB3	1.96	0.66
4:X:26:SER:H	4:X:27(B):ASN:HD21	1.43	0.66
1:I:266:GLY:HA3	2:J:66:VAL:HG11	1.78	0.66
1:K:51:LEU:HB2	1:K:274:VAL:HG22	1.77	0.66
2:H:30:GLN:HE22	2:H:146:ASP:H	1.44	0.65
4:T:51:LEU:HD21	4:T:66:LYS:HG2	1.78	0.65
1:G:216:GLU:OE1	1:I:212:ARG:HB3	1.96	0.65
1:E:111:GLN:O	1:E:114:SER:OG	2.13	0.65
1:G:192:GLN:HE21	4:T:53:GLN:HB3	1.60	0.65
4:X:39:LEU:HD23	4:X:84:ALA:HB2	1.78	0.64
3:S:6:GLN:HE21	3:S:92:CYS:H	1.45	0.64
4:N:51:LEU:HD21	4:N:66:LYS:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:6:GLN:HE21	3:O:92:CYS:H	1.46	0.63
3:Q:126:PRO:HG2	3:Q:213:PRO:HA	1.80	0.63
3:Q:159:LEU:HD21	3:Q:182:VAL:HG11	1.80	0.63
4:P:26:SER:H	4:P:27(B):ASN:HD21	1.46	0.63
4:X:51:LEU:HD21	4:X:66:LYS:HG2	1.79	0.63
4:T:27(B):ASN:ND2	4:T:28:ILE:H	1.93	0.63
3:O:87:THR:HG23	3:O:110:THR:HA	1.81	0.63
1:G:29:VAL:O	2:J:50:ASN:ND2	2.29	0.62
4:R:27(B):ASN:ND2	4:R:28:ILE:H	1.91	0.62
1:C:114:SER:OG	1:C:262:ARG:NH1	2.30	0.62
1:A:70:LEU:HD11	1:A:112:LEU:HD11	1.82	0.62
4:P:27(B):ASN:ND2	4:P:28:ILE:H	1.92	0.62
2:L:30:GLN:HE22	2:L:146:ASP:H	1.48	0.62
1:A:156:LYS:NZ	4:N:50[A]:SER:OG	2.25	0.61
1:A:66[A]:ILE:HD11	1:A:87:ILE:HG21	1.82	0.61
4:R:26:SER:H	4:R:27(B):ASN:HD21	1.47	0.61
4:V:27(B):ASN:ND2	4:V:28:ILE:H	1.93	0.61
4:V:26:SER:H	4:V:27(B):ASN:HD21	1.46	0.61
3:S:35:HIS:HE1	3:S:100(F):TYR:HB3	1.66	0.61
4:X:78[B]:LEU:HD11	4:X:104:LEU:HD21	1.83	0.61
1:E:84:TRP:HH2	1:E:118:PHE:CE2	2.18	0.60
3:M:163:VAL:HG22	3:M:182:VAL:HG22	1.82	0.60
4:R:51:LEU:HD21	4:R:66:LYS:HG2	1.82	0.60
1:A:113:SER:O	1:A:265:SER:HB3	2.01	0.60
1:G:217:ILE:O	1:I:212:ARG:NH2	2.35	0.59
4:T:26:SER:H	4:T:27(B):ASN:HD21	1.50	0.59
1:A:29:VAL:O	2:F:50:ASN:ND2	2.35	0.58
2:J:30:GLN:NE2	2:J:146:ASP:H	2.00	0.58
3:M:87:THR:HG23	3:M:110:THR:HA	1.85	0.58
1:E:114:SER:OG	1:E:262:ARG:NH1	2.35	0.58
2:F:125:GLN:HE22	2:F:155:GLY:HA2	1.68	0.58
4:N:26:SER:H	4:N:27(B):ASN:HD21	1.49	0.58
2:F:30:GLN:HE22	2:F:146:ASP:H	1.52	0.58
4:X:26:SER:H	4:X:27(B):ASN:ND2	2.01	0.57
2:D:30:GLN:NE2	2:D:146:ASP:H	2.02	0.57
4:P:39:LEU:HD23	4:P:84:ALA:HB2	1.85	0.57
2:F:54:SER:O	2:F:58:LYS:HG2	2.05	0.57
4:R:26:SER:H	4:R:27(B):ASN:ND2	2.02	0.57
1:E:84:TRP:HH2	1:E:118:PHE:HE2	1.53	0.57
1:C:66[A]:ILE:HD11	1:C:87:ILE:HG21	1.85	0.57
1:C:302:ILE:HG12	2:D:66:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:SER:O	2:B:58:LYS:HG2	2.05	0.56
2:H:72[A]:ASN:HD22	2:H:73:LEU:N	2.03	0.56
1:I:216:GLU:OE1	1:K:212:ARG:HB3	2.04	0.56
2:B:72[A]:ASN:HD22	2:B:73:LEU:N	2.04	0.56
3:U:87:THR:HG23	3:U:110:THR:HA	1.87	0.56
1:A:15:ILE:HG12	2:B:119:TYR:HA	1.87	0.56
1:I:186:PRO:HB2	3:U:98[A]:MET:SD	2.46	0.56
3:U:19[A]:ARG:NH1	3:U:81:GLN:OE1	2.39	0.56
2:D:54:SER:O	2:D:58:LYS:HG2	2.06	0.56
1:G:185:PRO:HG2	1:G:191:GLN:HE21	1.71	0.56
1:A:192:GLN:HE21	4:N:53:GLN:HB3	1.71	0.55
1:C:53:LYS:HG2	1:C:57:ALA:HA	1.87	0.55
2:D:68:LYS:HE3	2:F:80:LEU:N	2.20	0.55
4:V:51:LEU:HD11	4:V:66:LYS:HB3	1.88	0.55
1:A:185:PRO:HG2	1:A:191:GLN:HE21	1.72	0.55
1:C:111:GLN:HB3	1:C:262:ARG:HH12	1.72	0.55
3:M:12:VAL:HG21	3:M:82(C):LEU:HD13	1.87	0.55
1:E:53:LYS:HG2	1:E:57:ALA:HA	1.88	0.55
1:E:54[A]:LEU:HD11	1:E:303:GLY:HA3	1.88	0.55
1:G:266:GLY:HA3	2:H:66:VAL:HG11	1.88	0.55
1:G:128:PRO:O	1:G:157:LYS:NZ	2.33	0.55
1:A:130:HIS:CE1	1:A:164:LEU:HB3	2.42	0.55
1:C:188:GLY:HA2	1:C:217:ILE:HD13	1.88	0.55
1:G:70:LEU:HD11	1:G:112:LEU:HD11	1.90	0.55
1:A:129:ASN:ND2	3:O:1:PCA:OE	2.40	0.54
1:G:196:GLN:NE2	4:T:52:ASN:OD1	2.40	0.54
2:H:125:GLN:NE2	2:H:155:GLY:HA2	2.22	0.54
3:M:164:HIS:CE1	4:N:167:GLN:HG2	2.42	0.54
4:T:26:SER:H	4:T:27(B):ASN:ND2	2.05	0.54
3:M:47:TRP:CG	4:N:96:VAL:HB	2.42	0.54
1:A:194:LEU:HD11	3:M:100(A):TYR:CZ	2.42	0.54
1:C:84:TRP:CZ3	1:C:118:PHE:HE2	2.25	0.54
1:C:114:SER:O	1:C:262:ARG:HA	2.07	0.54
4:V:25:GLY:HA3	4:V:27(B):ASN:HD21	1.73	0.54
2:J:72[A]:ASN:HD22	2:J:73:LEU:N	2.05	0.54
2:J:54:SER:O	2:J:58:LYS:HG2	2.08	0.54
4:P:26:SER:H	4:P:27(B):ASN:ND2	2.06	0.54
3:U:6:GLN:HE21	3:U:92:CYS:N	2.05	0.54
3:Q:169[A]:VAL:HG21	4:R:160:GLU:HB3	1.90	0.54
3:S:35:HIS:CE1	3:S:100(F):TYR:HB3	2.43	0.54
4:V:39:LEU:HD23	4:V:84:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:129:ASN:HD21	2:J:163:SER:HA	1.73	0.54
1:C:70:LEU:HD11	1:C:112:LEU:HD11	1.89	0.53
1:C:133(A):LYS:HD3	3:O:100(C):HIS:CD2	2.43	0.53
1:C:221:PRO:O	1:C:229:ARG:NH2	2.31	0.53
4:X:25:GLY:HA3	4:X:27(B):ASN:HD21	1.74	0.53
2:B:80:LEU:N	2:F:68:LYS:HE3	2.23	0.53
2:L:54:SER:O	2:L:58:LYS:HG2	2.08	0.53
4:X:79:GLN:O	4:X:106:VAL:HG21	2.08	0.53
1:I:310:ARG:NH1	2:J:90:ASP:OD1	2.39	0.53
4:V:26:SER:H	4:V:27(B):ASN:ND2	2.06	0.53
1:A:189:THR:HG22	3:M:97:LEU:HD23	1.89	0.52
4:N:150:ALA:HB1	4:N:188:HIS:CD2	2.44	0.52
1:I:97:CYS:HB2	1:I:138:ALA:O	2.09	0.52
1:C:196:GLN:NE2	4:P:52:ASN:OD1	2.40	0.52
1:E:185:PRO:HG2	1:E:191:GLN:HE21	1.74	0.52
4:X:35:TRP:HB2	4:X:48:ILE:HB	1.92	0.52
1:C:114:SER:HB2	1:C:263:GLY:H	1.74	0.52
2:H:2:LEU:O	2:J:113:SER:OG	2.28	0.52
4:R:35:TRP:HB2	4:R:48:ILE:HB	1.92	0.52
1:E:130:HIS:CE1	1:E:164:LEU:HB3	2.44	0.52
4:X:27(B):ASN:HD22	4:X:28:ILE:N	1.96	0.52
1:G:74:PRO:HB2	1:G:141:TYR:HB2	1.91	0.52
4:P:35:TRP:HB2	4:P:48:ILE:HB	1.91	0.52
3:Q:12:VAL:HG21	3:Q:82(C):LEU:HD13	1.92	0.52
1:C:29:VAL:CG2	2:D:102:LEU:HD23	2.40	0.52
1:C:54[A]:LEU:HD13	1:C:86:TYR:CE2	2.44	0.52
3:Q:154:TRP:HB3	3:Q:159:LEU:HD23	1.92	0.52
1:E:54[A]:LEU:HB3	1:E:85:SER:HB2	1.93	0.51
2:B:68:LYS:HE3	2:D:80:LEU:N	2.25	0.51
1:E:51:LEU:HB2	1:E:274:VAL:HG22	1.92	0.51
1:I:29:VAL:O	2:L:50:ASN:ND2	2.39	0.51
3:Q:47:TRP:CG	4:R:96:VAL:HB	2.46	0.51
1:E:66[A]:ILE:HD11	1:E:87:ILE:HG21	1.92	0.51
1:G:310:ARG:NH1	2:H:90:ASP:OD1	2.34	0.51
1:I:98:TYR:CD2	1:I:230:MET:HB2	2.46	0.51
1:G:29:VAL:HG11	2:J:51:LYS:HE2	1.93	0.51
1:I:90:THR:OG1	1:I:92[A]:ASN:OD1	2.21	0.51
2:H:51:LYS:HE2	1:K:29:VAL:HG11	1.93	0.51
1:C:281:CYS:HB2	1:C:304:GLU:O	2.10	0.50
3:O:12:VAL:HG21	3:O:82(C):LEU:HD13	1.93	0.50
1:I:130:HIS:CE1	1:I:164:LEU:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:130:HIS:CE1	1:K:164:LEU:HB3	2.47	0.50
3:Q:166:PHE:HE2	3:Q:181:VAL:HG12	1.76	0.50
4:R:14:SER:H	4:R:17:GLN:NE2	2.09	0.50
4:R:106(A):LEU:HA	4:R:140:TYR:OH	2.12	0.50
1:C:304:GLU:HG3	2:D:62:GLN:O	2.12	0.50
1:I:185:PRO:HG2	1:I:191:GLN:HE21	1.75	0.50
2:L:154:ASN:HB2	6:L:201:NAG:H82	1.94	0.50
3:W:87:THR:HG23	3:W:110:THR:HA	1.94	0.50
1:E:50:LYS:HD2	1:E:275:HIS:HB2	1.94	0.50
1:E:307:LYS:HE3	2:F:92:TRP:NE1	2.26	0.50
1:G:186:PRO:HB2	3:S:98[A]:MET:SD	2.51	0.50
3:S:14:PRO:O	3:S:15:ARG:HB2	2.12	0.50
1:C:15:ILE:HD11	2:D:122:VAL:HG21	1.94	0.49
3:U:6:GLN:NE2	3:U:92:CYS:H	2.05	0.49
1:I:225:ASP:OD1	3:U:52(A):TYR:OH	2.30	0.49
1:E:133(A):LYS:HD3	3:Q:100(C):HIS:CD2	2.48	0.49
3:S:47:TRP:CG	4:T:96:VAL:HB	2.47	0.49
1:E:113:SER:O	1:E:265:SER:HB3	2.12	0.49
1:E:114:SER:O	1:E:262:ARG:HA	2.12	0.49
4:R:51:LEU:HD11	4:R:66:LYS:HB3	1.94	0.49
1:C:61:LEU:HA	1:C:79:LEU:HD21	1.94	0.49
1:K:15:ILE:HG12	2:L:119:TYR:HA	1.95	0.49
2:B:51:LYS:HE2	1:C:29:VAL:HG11	1.94	0.49
1:I:62:GLY:O	1:I:93:SER:OG	2.20	0.49
1:A:29:VAL:HG11	2:F:51:LYS:HE2	1.94	0.49
1:C:76:CYS:HB3	1:C:79:LEU:HD12	1.94	0.49
4:P:80:SER:HA	4:P:106:VAL:HG11	1.95	0.49
4:V:35:TRP:CZ3	4:V:88:CYS:HB3	2.47	0.49
2:H:54:SER:O	2:H:58:LYS:HG2	2.13	0.49
3:M:159:LEU:HD21	3:M:182:VAL:HG11	1.94	0.49
1:C:29:VAL:HG21	2:D:102:LEU:HD23	1.95	0.49
4:P:83:GLU:HG3	4:P:104:LEU:O	2.13	0.49
1:C:293:PRO:HB3	2:D:59:MET:HG3	1.94	0.48
2:H:125:GLN:HE22	2:H:155:GLY:HA2	1.78	0.48
1:E:98:TYR:CD2	1:E:230:MET:HB2	2.48	0.48
1:K:97:CYS:HB2	1:K:138:ALA:O	2.13	0.48
4:N:39:LEU:HD23	4:N:84:ALA:HB2	1.94	0.48
4:V:51:LEU:HD21	4:V:66:LYS:HG2	1.94	0.48
1:A:307:LYS:HE3	2:B:92:TRP:CE2	2.48	0.48
4:N:27(B):ASN:HD22	4:N:28:ILE:N	1.96	0.48
1:E:70:LEU:HD11	1:E:112:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:189:THR:HG22	3:U:97:LEU:HD23	1.95	0.48
3:O:31:SER:O	3:O:98[B]:MET:HG3	2.14	0.48
4:R:39:LEU:HD23	4:R:84:ALA:HB2	1.96	0.48
4:V:14:SER:H	4:V:17:GLN:NE2	2.11	0.48
1:I:113:SER:O	1:I:265:SER:HB3	2.14	0.48
1:I:301:THR:HB	1:I:305:CYS:SG	2.53	0.48
4:N:51:LEU:HD11	4:N:66:LYS:HB3	1.96	0.48
1:K:192:GLN:HE21	4:X:53:GLN:NE2	2.12	0.47
1:E:307:LYS:HE3	2:F:92:TRP:CE2	2.49	0.47
4:R:27(B):ASN:HD22	4:R:28:ILE:N	1.97	0.47
1:A:307:LYS:HE3	2:B:92:TRP:NE1	2.29	0.47
3:Q:193:THR:HB	3:Q:210:ARG:HD3	1.95	0.47
1:C:236:LEU:HD11	1:C:262:ARG:NH2	2.30	0.47
1:E:115:VAL:HA	1:E:261:ASN:O	2.15	0.47
3:W:39:GLN:HB2	3:W:45:LEU:HD23	1.95	0.47
3:Q:36:TRP:CE2	3:Q:80:LEU:HB2	2.50	0.47
4:T:26:SER:N	4:T:27(B):ASN:HD21	2.13	0.47
1:A:29:VAL:HG21	2:B:102:LEU:HD23	1.97	0.47
1:E:73:ASN:HB3	1:E:76:CYS:SG	2.55	0.47
4:T:51:LEU:HD11	4:T:66:LYS:HD3	1.97	0.47
3:U:47:TRP:CG	4:V:96:VAL:HB	2.50	0.47
1:A:125(A):LYS:HD2	1:A:255:TRP:CH2	2.49	0.47
1:A:196:GLN:NE2	4:N:52:ASN:OD1	2.42	0.47
3:O:29:PHE:HB3	3:O:76:ASN:HD22	1.79	0.47
4:T:31:TYR:CZ	4:T:91:TRP:HD1	2.32	0.47
1:C:71:LEU:HD22	1:C:151:LEU:HD11	1.97	0.47
1:G:29:VAL:HG21	2:H:102:LEU:HD23	1.95	0.47
1:A:302:ILE:HG12	2:B:66:VAL:HG12	1.97	0.46
1:K:174:LYS:N	1:K:239:PRO:HG3	2.29	0.46
1:K:194:LEU:HD11	3:W:100(A):TYR:CZ	2.50	0.46
4:P:25:GLY:HA3	4:P:27(B):ASN:HD21	1.79	0.46
4:N:26:SER:H	4:N:27(B):ASN:ND2	2.13	0.46
3:U:100(F):TYR:HB2	4:V:91:TRP:CZ3	2.49	0.46
4:X:26:SER:N	4:X:27(B):ASN:HD21	2.11	0.46
1:A:18:HIS:HB2	2:B:20:GLY:O	2.15	0.46
1:C:130:HIS:CE1	1:C:164:LEU:HB3	2.49	0.46
2:H:154:ASN:HB2	6:H:201:NAG:H82	1.96	0.46
2:F:3:PHE:CE1	2:F:113:SER:HB2	2.51	0.46
4:T:27(B):ASN:HD22	4:T:28:ILE:N	1.98	0.46
4:V:35:TRP:HB2	4:V:48:ILE:HB	1.97	0.46
3:M:185:PRO:HG2	3:M:188:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:127:SER:HB3	3:Q:214:LYS:HD2	1.96	0.46
1:C:115:VAL:HA	1:C:261:ASN:O	2.16	0.46
4:T:14:SER:H	4:T:17:GLN:NE2	2.14	0.46
1:C:70:LEU:HD11	1:C:112:LEU:CD1	2.45	0.46
2:D:51:LYS:HE2	1:E:29:VAL:HG11	1.98	0.46
1:C:265:SER:O	2:D:66:VAL:HG21	2.16	0.46
2:H:80:LEU:N	2:J:68:LYS:HE3	2.30	0.46
4:V:27(B):ASN:HD22	4:V:28:ILE:N	1.98	0.46
1:A:183:HIS:ND1	1:A:195:TYR:OH	2.49	0.45
3:Q:30:SER:O	3:Q:52(A):TYR:HB2	2.16	0.45
3:Q:87:THR:HG23	3:Q:110:THR:HA	1.97	0.45
1:E:84:TRP:CH2	1:E:118:PHE:CE2	3.03	0.45
3:O:47:TRP:CG	4:P:96:VAL:HB	2.51	0.45
4:T:4:LEU:HB2	4:T:99:GLY:HA2	1.98	0.45
1:C:212:ARG:NH2	1:E:217:ILE:O	2.44	0.45
1:I:18:HIS:HB2	2:J:20:GLY:O	2.15	0.45
1:K:114:SER:OG	1:K:262:ARG:NH1	2.49	0.45
4:T:83:GLU:OE2	4:T:106:VAL:N	2.42	0.45
1:C:64:CYS:HB2	1:C:79:LEU:HD11	1.98	0.45
1:C:194:LEU:HD11	3:O:100(A):TYR:CZ	2.52	0.45
1:I:29:VAL:HG21	2:J:102:LEU:HD23	1.98	0.45
3:M:19[A]:ARG:NH1	3:M:81:GLN:OE1	2.44	0.45
3:M:164:HIS:HE1	4:N:167:GLN:HG2	1.82	0.45
3:Q:199:ASN:ND2	3:Q:206:LYS:HE2	2.31	0.45
3:U:31:SER:O	3:U:98[B]:MET:HG3	2.16	0.45
1:A:29:VAL:CG2	2:B:102:LEU:HD23	2.47	0.45
1:G:130:HIS:CE1	1:G:164:LEU:HB3	2.52	0.45
4:R:26:SER:N	4:R:27(B):ASN:HD21	2.12	0.45
3:W:34:MET:HB3	3:W:78:LEU:HD22	1.98	0.45
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.99	0.45
1:E:29:VAL:CG2	2:F:102:LEU:HD23	2.46	0.45
2:J:158:ASP:OD1	2:J:160:PRO:HD2	2.17	0.45
4:T:59:PRO:HB2	4:T:61:ARG:HG2	1.98	0.45
3:U:6:GLN:NE2	3:U:91:TYR:HA	2.32	0.45
4:V:35:TRP:CH2	4:V:88:CYS:HB3	2.52	0.45
1:C:189:THR:HG22	3:O:97:LEU:HD23	1.99	0.45
1:E:174:LYS:CA	1:E:239:PRO:HG3	2.46	0.45
3:Q:195:ILE:HG12	3:Q:210:ARG:HB2	1.98	0.45
1:E:54[B]:LEU:HD12	1:E:86:TYR:CD2	2.52	0.45
1:G:71:LEU:HD22	1:G:151:LEU:HD11	1.98	0.45
1:I:29:VAL:HG11	2:L:51:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASN:HB3	1:A:76:CYS:SG	2.57	0.44
1:A:185:PRO:HG2	1:A:191:GLN:NE2	2.32	0.44
1:K:53:LYS:HG2	1:K:57:ALA:HA	1.99	0.44
1:C:100:GLY:HA3	1:C:230:MET:O	2.16	0.44
3:O:6:GLN:HE21	3:O:91:TYR:HA	1.83	0.44
1:C:84:TRP:CH2	1:C:118:PHE:HE2	2.35	0.44
2:D:125:GLN:NE2	2:D:155:GLY:HA2	2.31	0.44
1:G:53:LYS:HG2	1:G:57:ALA:HA	1.99	0.44
1:E:15:ILE:HD11	2:F:122:VAL:HG21	1.99	0.44
1:A:71:LEU:HD22	1:A:151:LEU:HD11	1.99	0.44
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.99	0.44
1:G:29:VAL:CG2	2:H:102:LEU:HD23	2.48	0.44
3:M:154:TRP:CH2	3:M:196[B]:CYS:HB2	2.53	0.44
1:A:98:TYR:CD2	1:A:230:MET:HB2	2.53	0.44
1:A:266:GLY:HA3	2:B:66:VAL:HG11	1.98	0.44
2:H:150:GLU:OE2	2:H:153:ARG:NH1	2.51	0.44
1:I:19:ALA:HB2	2:J:13:GLY:HA3	1.99	0.44
1:I:29:VAL:CG2	2:J:102:LEU:HD23	2.48	0.44
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.99	0.44
2:B:4:GLY:O	2:B:8:GLY:HA3	2.18	0.44
1:E:15:ILE:HG12	2:F:119:TYR:HA	1.99	0.44
3:U:12:VAL:O	3:U:111:VAL:HA	2.18	0.44
1:A:54[A]:LEU:HG	1:A:54(A):LYS:HG2	2.00	0.44
1:C:111:GLN:O	1:C:262:ARG:NH1	2.51	0.44
2:F:30:GLN:HE22	2:F:146:ASP:N	2.14	0.44
2:F:129:ASN:HD21	2:F:163:SER:HA	1.83	0.44
1:G:134:GLY:HA3	1:G:153:TRP:HB3	2.00	0.44
4:N:108:GLN:HB2	4:N:109:PRO:HD2	2.00	0.44
3:Q:31:SER:O	3:Q:98[B]:MET:HG3	2.17	0.44
2:H:30:GLN:NE2	2:H:146:ASP:H	2.13	0.43
2:L:2:LEU:HD12	2:L:2:LEU:HA	1.77	0.43
4:N:120:PRO:HD2	4:N:185:TRP:CE2	2.53	0.43
1:A:225:ASP:OD1	3:M:52(A):TYR:OH	2.31	0.43
2:H:167:LYS:O	2:H:171:GLU:HG3	2.18	0.43
4:T:83:GLU:HG3	4:T:104:LEU:O	2.17	0.43
4:V:83:GLU:HG3	4:V:104:LEU:O	2.18	0.43
1:E:14:CYS:HA	2:F:137:CYS:HA	2.01	0.43
1:E:194:LEU:HD11	3:Q:100(A):TYR:OH	2.17	0.43
2:H:94:TYR:CE1	2:J:59:MET:SD	3.11	0.43
2:L:30:GLN:NE2	2:L:145:ASP:HB2	2.33	0.43
3:M:34:MET:HB3	3:M:78:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:TRP:CD1	1:C:79:LEU:HD13	2.53	0.43
2:L:158:ASP:OD1	2:L:160:PRO:HD2	2.19	0.43
3:W:19[A]:ARG:NH1	3:W:81:GLN:HB2	2.33	0.43
2:D:63:PHE:O	2:D:64:THR:C	2.56	0.43
2:J:30:GLN:NE2	2:J:145:ASP:HB2	2.34	0.43
4:R:4:LEU:HG	4:R:97[A]:VAL:HG12	2.00	0.43
4:T:4:LEU:HG	4:T:97[A]:VAL:HG12	2.00	0.43
2:D:2:LEU:HD12	2:D:2:LEU:HA	1.88	0.43
1:E:43:LEU:HB2	1:E:314:LEU:HB2	2.00	0.43
1:G:103[B]:ILE:HG13	1:G:233:TYR:CE2	2.54	0.43
2:H:30:GLN:NE2	2:H:145:ASP:HB2	2.34	0.43
4:V:47[A]:LEU:HD12	4:V:47[A]:LEU:HA	1.91	0.43
1:E:189:THR:HG22	3:Q:97:LEU:HD23	2.01	0.43
2:J:164:GLU:OE2	3:M:116:THR:HG21	2.19	0.43
1:E:58:PRO:HB3	1:E:86:TYR:CZ	2.54	0.43
1:K:29:VAL:CG2	2:L:102:LEU:HD23	2.49	0.43
4:P:51:LEU:HD21	4:P:66:LYS:HG2	2.01	0.43
1:C:308:TYR:CD2	2:D:89:LEU:HD13	2.53	0.43
2:D:30:GLN:NE2	2:D:145:ASP:HB2	2.34	0.43
4:V:38:GLN:HE21	4:V:87:TYR:HE2	1.65	0.43
1:C:268:ILE:HG23	1:C:302:ILE:HD11	2.00	0.42
1:G:189:THR:HG22	3:S:97:LEU:HD23	2.00	0.42
1:K:190:ASP:N	1:K:190:ASP:OD1	2.52	0.42
1:A:113:SER:HB3	1:A:266:GLY:HA2	2.00	0.42
2:H:76:ARG:NH2	2:J:74:GLU:OE2	2.52	0.42
1:G:185:PRO:HG2	1:G:191:GLN:NE2	2.33	0.42
1:I:58:PRO:HB3	1:I:86:TYR:CZ	2.54	0.42
2:J:129:ASN:ND2	2:J:163:SER:HA	2.33	0.42
1:A:117:SER:OG	1:A:261:ASN:ND2	2.47	0.42
2:H:98:LEU:HD21	2:J:99:LEU:HD13	2.01	0.42
4:P:27(B):ASN:HD22	4:P:28:ILE:N	1.96	0.42
3:W:29:PHE:CD2	3:W:76:ASN:HA	2.55	0.42
1:A:75:GLU:HG3	5:Y:1:NAG:HN2	1.83	0.42
2:J:107:THR:O	2:J:110:PHE:HB3	2.19	0.42
4:R:48:ILE:HA	4:R:53:GLN:O	2.20	0.42
2:B:135:ASN:OD1	2:B:137:CYS:HB2	2.20	0.42
1:E:185:PRO:HG2	1:E:191:GLN:NE2	2.34	0.42
1:K:63:LYS:HE3	1:K:75:GLU:HB3	2.01	0.42
3:Q:15:ARG:N	3:Q:82(C):LEU:O	2.36	0.42
3:W:36:TRP:CE2	3:W:80:LEU:HB2	2.55	0.42
1:C:115:VAL:HG11	1:C:118:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133(A):LYS:HD3	3:S:100(C):HIS:CD2	2.55	0.42
3:Q:195:ILE:HA	3:Q:210:ARG:HA	2.02	0.42
4:V:27(B):ASN:O	4:V:31:TYR:N	2.42	0.42
1:K:98:TYR:CD2	1:K:230:MET:HB2	2.54	0.42
1:A:246:GLU:OE2	1:C:219:ALA:HB3	2.20	0.41
2:B:59:MET:SD	2:D:94:TYR:CD1	3.13	0.41
1:I:174:LYS:HA	1:I:239:PRO:HG3	2.01	0.41
3:U:12:VAL:HG21	3:U:82(C):LEU:HD13	2.02	0.41
1:A:100:GLY:HA3	1:A:230:MET:O	2.20	0.41
1:E:186:PRO:HB2	3:Q:98[A]:MET:SD	2.60	0.41
3:Q:185:PRO:HG2	3:Q:188:SER:OG	2.19	0.41
3:U:30:SER:O	3:U:52(A):TYR:HB2	2.20	0.41
1:A:53:LYS:HG2	1:A:57:ALA:HA	2.01	0.41
1:G:71:LEU:O	1:G:148:TYR:HB3	2.20	0.41
3:Q:200:HIS:CD2	3:Q:202:PRO:HD2	2.55	0.41
3:U:36:TRP:CE2	3:U:80:LEU:HB2	2.54	0.41
1:A:301:THR:HB	1:A:305:CYS:SG	2.61	0.41
1:C:84:TRP:CH2	1:C:118:PHE:CE2	3.09	0.41
1:E:190:ASP:OD1	1:E:190:ASP:N	2.53	0.41
1:G:133(A):LYS:HB3	3:S:100(C):HIS:CG	2.56	0.41
1:I:66[B]:ILE:HD12	1:I:109:ARG:HG2	2.02	0.41
1:E:61:LEU:HD11	1:E:66[A]:ILE:HD13	2.03	0.41
1:E:174:LYS:HD2	1:E:259:ALA:HB1	2.02	0.41
1:G:301:THR:HB	1:G:305:CYS:SG	2.61	0.41
4:R:47[A]:LEU:HD21	4:R:62:PHE:CD1	2.55	0.41
1:C:176:VAL:HA	1:C:259:ALA:HA	2.03	0.41
1:E:87:ILE:HB	1:E:267:ILE:HG12	2.03	0.41
3:M:31:SER:O	3:M:98:MET:HG3	2.20	0.41
3:O:14:PRO:O	3:O:15:ARG:HB2	2.21	0.41
3:O:29:PHE:CD2	3:O:76:ASN:HA	2.56	0.41
4:P:26:SER:N	4:P:27(B):ASN:HD21	2.16	0.41
3:U:2:VAL:HA	3:U:25:SER:O	2.19	0.41
3:W:82:MET:HE2	3:W:82(C):LEU:HD21	2.03	0.41
2:B:94:TYR:CD1	2:F:59:MET:SD	3.13	0.41
1:E:108:LEU:HD22	1:E:234:TRP:CD1	2.56	0.41
1:G:62:GLY:O	1:G:93:SER:OG	2.27	0.41
1:E:156:LYS:HZ1	4:R:50[B]:SER:HB3	1.85	0.41
2:F:158:ASP:OD1	2:F:160:PRO:HD2	2.21	0.41
1:I:190:ASP:N	1:I:190:ASP:OD1	2.54	0.41
1:K:301:THR:HB	1:K:305:CYS:SG	2.61	0.41
2:L:24:TYR:HE2	2:L:122:VAL:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:108:GLN:HB2	4:R:109:PRO:HD2	2.02	0.41
4:T:7:PRO:HA	4:T:8:PRO:HD3	1.94	0.41
3:W:40:ALA:HA	3:W:88:SER:HA	2.03	0.41
1:A:87:ILE:HB	1:A:267:ILE:HG12	2.01	0.41
1:K:170:ASN:ND2	1:K:237:LEU:O	2.54	0.41
4:X:35:TRP:CZ3	4:X:88:CYS:HB3	2.56	0.41
2:B:120:GLU:CD	2:D:116:ARG:HH22	2.24	0.40
1:C:185:PRO:HG2	1:C:191:GLN:HE21	1.85	0.40
2:B:75:ARG:CZ	1:E:111:GLN:HE22	2.34	0.40
1:C:54[A]:LEU:HD13	1:C:86:TYR:HE2	1.87	0.40
1:C:307:LYS:HE3	2:D:92:TRP:CD1	2.56	0.40
1:I:122:GLU:HG3	1:I:256:TYR:CZ	2.55	0.40
2:L:135:ASN:OD1	2:L:137:CYS:HB2	2.21	0.40
1:E:108:LEU:HB2	1:E:234:TRP:CE2	2.57	0.40
1:I:103[B]:ILE:HG21	1:I:211:ARG:HH22	1.85	0.40
1:I:307:LYS:HE3	2:J:92:TRP:NE1	2.36	0.40
1:K:307:LYS:HD3	2:L:62:GLN:OE1	2.22	0.40
3:U:53:ASP:CG	3:U:55:ARG:HG3	2.41	0.40
4:V:85:VAL:HA	4:V:102:THR:O	2.22	0.40
2:F:154:ASN:HB2	6:F:201:NAG:H82	2.04	0.40
3:M:6:GLN:HE21	3:M:92:CYS:N	2.16	0.40
3:M:47:TRP:CD1	4:N:96:VAL:HB	2.56	0.40
3:Q:125:ALA:HB3	3:Q:214:LYS:HE3	2.03	0.40
1:E:301:THR:HB	1:E:305:CYS:SG	2.61	0.40
1:G:133(A):LYS:HB3	3:S:100(C):HIS:CD2	2.57	0.40
2:H:4:GLY:O	2:H:8:GLY:HA3	2.21	0.40
1:I:14:CYS:HA	2:J:137:CYS:HA	2.04	0.40
1:K:194:LEU:HD11	3:W:100(A):TYR:OH	2.22	0.40
3:S:100(F):TYR:HB2	4:T:91:TRP:CZ3	2.56	0.40

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:C:264:SER:OG	4:N:189:ARG:N[2_444]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	330/331 (100%)	322 (98%)	8 (2%)	0	100	100
1	C	331/331 (100%)	324 (98%)	7 (2%)	0	100	100
1	E	331/331 (100%)	322 (97%)	9 (3%)	0	100	100
1	G	331/331 (100%)	324 (98%)	7 (2%)	0	100	100
1	I	331/331 (100%)	324 (98%)	7 (2%)	0	100	100
1	K	331/331 (100%)	322 (97%)	9 (3%)	0	100	100
2	B	172/176 (98%)	169 (98%)	3 (2%)	0	100	100
2	D	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	F	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	H	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	J	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	L	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
3	M	230/231 (100%)	224 (97%)	5 (2%)	1 (0%)	34	66
3	O	125/231 (54%)	123 (98%)	2 (2%)	0	100	100
3	Q	231/231 (100%)	225 (97%)	5 (2%)	1 (0%)	34	66
3	S	125/231 (54%)	123 (98%)	2 (2%)	0	100	100
3	U	125/231 (54%)	123 (98%)	2 (2%)	0	100	100
3	W	125/231 (54%)	123 (98%)	2 (2%)	0	100	100
4	N	219/217 (101%)	214 (98%)	5 (2%)	0	100	100
4	P	116/217 (54%)	113 (97%)	3 (3%)	0	100	100
4	R	219/217 (101%)	215 (98%)	4 (2%)	0	100	100
4	T	116/217 (54%)	113 (97%)	3 (3%)	0	100	100
4	V	116/217 (54%)	113 (97%)	3 (3%)	0	100	100
4	X	116/217 (54%)	113 (97%)	3 (3%)	0	100	100
All	All	4880/5730 (85%)	4779 (98%)	99 (2%)	2 (0%)	100	100



All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	133	GLY
3	Q	133	GLY

### 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	287/285 (101%)	284 (99%)	3 (1%)	76	86
1	C	288/285 (101%)	285 (99%)	3 (1%)	76	86
1	E	288/285 (101%)	284 (99%)	4 (1%)	67	82
1	G	288/285 (101%)	285 (99%)	3 (1%)	76	86
1	I	288/285 (101%)	282 (98%)	6 (2%)	53	75
1	K	288/285 (101%)	284 (99%)	4 (1%)	67	82
2	B	149/150 (99%)	145 (97%)	4 (3%)	44	71
2	D	149/150 (99%)	147 (99%)	2 (1%)	69	82
2	F	149/150 (99%)	147 (99%)	2 (1%)	69	82
2	H	149/150 (99%)	145 (97%)	4 (3%)	44	71
2	J	149/150 (99%)	145 (97%)	4 (3%)	44	71
2	L	149/150 (99%)	147 (99%)	2 (1%)	69	82
3	M	197/196 (100%)	193 (98%)	4 (2%)	55	76
3	O	106/196 (54%)	103 (97%)	3 (3%)	43	70
3	Q	198/196 (101%)	194 (98%)	4 (2%)	55	76
3	S	106/196 (54%)	103 (97%)	3 (3%)	43	70
3	U	106/196 (54%)	103 (97%)	3 (3%)	43	70
3	W	106/196 (54%)	103 (97%)	3 (3%)	43	70
4	N	185/181 (102%)	183 (99%)	2 (1%)	73	85
4	P	97/181 (54%)	95 (98%)	2 (2%)	53	75
4	R	185/181 (102%)	183 (99%)	2 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	T	97/181 (54%)	95 (98%)	2 (2%)	53	75
4	V	97/181 (54%)	95 (98%)	2 (2%)	53	75
4	X	97/181 (54%)	95 (98%)	2 (2%)	53	75
All	All	4198/4872 (86%)	4125 (98%)	73 (2%)	60	78

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	102	PHE
1	A	320	LEU
2	B	32	SER
2	B	72[A]	ASN
2	B	72[B]	ASN
2	B	128	ASN
1	C	33	ASN
1	C	102	PHE
1	C	320	LEU
2	D	32	SER
2	D	128	ASN
1	E	33	ASN
1	E	102	PHE
1	E	190	ASP
1	E	320	LEU
2	F	32	SER
2	F	128	ASN
1	G	33	ASN
1	G	102	PHE
1	G	320	LEU
2	H	32	SER
2	H	72[A]	ASN
2	H	72[B]	ASN
2	H	128	ASN
1	I	33	ASN
1	I	92[A]	ASN
1	I	92[B]	ASN
1	I	102	PHE
1	I	190	ASP
1	I	320	LEU
2	J	32	SER
2	J	72[A]	ASN

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Mol	Chain	Res	Type
2	J	72 B	ASN
2	J	128	ASN
1	K	33	ASN
1	K	102	PHE
1	K	190	ASP
1	K	320	LEU
2	L	32	SER
2	L	128	ASN
3	M	3	GLN
3	M	25	SER
3	M	88	SER
3	M	192	GLN
4	N	27(B)	ASN
4	N	53	GLN
3	O	3	GLN
3	O	25	SER
3	O	88	SER
4	P	27(B)	ASN
4	P	53	GLN
3	Q	3	GLN
3	Q	25	SER
3	Q	88	SER
3	Q	192	GLN
4	R	27(B)	ASN
4	R	53	GLN
3	S	3	GLN
3	S	25	SER
3	S	88	SER
4	T	27(B)	ASN
4	T	53	GLN
3	U	3	GLN
3	U	25	SER
3	U	88	SER
4	V	27(B)	ASN
4	V	53	GLN
3	W	3	GLN
3	W	25	SER
3	W	88	SER
4	X	27(B)	ASN
4	X	53	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	192	GLN
1	A	196	GLN
1	A	197	ASN
1	A	250	ASN
2	B	30	GLN
2	B	43	ASN
2	B	125	GLN
2	B	128	ASN
2	B	129	ASN
1	C	129	ASN
1	C	191	GLN
1	C	197	ASN
1	C	250	ASN
1	C	261	ASN
2	D	30	GLN
2	D	43	ASN
2	D	125	GLN
2	D	128	ASN
2	D	129	ASN
1	E	129	ASN
1	E	191	GLN
1	E	197	ASN
1	E	250	ASN
1	E	261	ASN
2	F	30	GLN
2	F	43	ASN
2	F	125	GLN
2	F	128	ASN
2	F	129	ASN
1	G	191	GLN
1	G	192	GLN
1	G	197	ASN
1	G	250	ASN
2	H	30	GLN
2	H	43	ASN
2	H	125	GLN
2	H	128	ASN
2	H	129	ASN
1	I	191	GLN
1	I	197	ASN
1	I	250	ASN
2	J	30	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	43	ASN
2	J	125	GLN
2	J	128	ASN
2	J	129	ASN
1	K	191	GLN
1	K	197	ASN
1	K	250	ASN
2	L	30	GLN
2	L	43	ASN
2	L	125	GLN
2	L	128	ASN
2	L	129	ASN
3	M	3	GLN
3	M	39	GLN
3	M	164	HIS
3	M	192	GLN
4	N	17	GLN
4	N	27(B)	ASN
4	N	38	GLN
4	N	52	ASN
3	O	3	GLN
3	O	39	GLN
3	O	76	ASN
3	O	100(C)	HIS
4	P	17	GLN
4	P	27(B)	ASN
4	P	34	ASN
4	P	38	GLN
4	P	53	GLN
3	Q	3	GLN
3	Q	39	GLN
3	Q	164	HIS
3	Q	171	GLN
3	Q	192	GLN
4	R	17	GLN
4	R	27(B)	ASN
4	R	38	GLN
4	R	53	GLN
3	S	3	GLN
3	S	39	GLN
3	S	100(C)	HIS
4	T	17	GLN

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Mol	Chain	Res	Type
4	T	27(B)	ASN
4	T	38	GLN
3	U	3	GLN
3	U	39	GLN
4	V	17	GLN
4	V	27(B)	ASN
4	V	38	GLN
4	V	53	GLN
3	W	3	GLN
3	W	76	ASN
4	X	17	GLN
4	X	27(B)	ASN
4	X	53	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](#)

12 non-standard protein/DNA/RNA residues 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	PCA	X	1	4	7,8,9	1.77	1 (14%)	9,10,12	2.21	5 (55%)
4	PCA	R	1	4	7,8,9	1.84	1 (14%)	9,10,12	2.36	5 (55%)
3	PCA	W	1	3	7,8,9	1.83	1 (14%)	9,10,12	2.09	4 (44%)
3	PCA	U	1	3	7,8,9	1.81	1 (14%)	9,10,12	1.96	4 (44%)
4	PCA	P	1	4	7,8,9	1.91	1 (14%)	9,10,12	2.59	5 (55%)
3	PCA	Q	1	3	7,8,9	1.71	1 (14%)	9,10,12	2.07	4 (44%)
4	PCA	T	1	4	7,8,9	1.83	1 (14%)	9,10,12	2.26	6 (66%)
4	PCA	V	1	4	7,8,9	1.86	1 (14%)	9,10,12	2.52	5 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PCA	M	1	3	7,8,9	1.84	1 (14%)	9,10,12	2.15	4 (44%)
3	PCA	S	1	3	7,8,9	1.82	1 (14%)	9,10,12	2.06	4 (44%)
3	PCA	O	1	3	7,8,9	1.74	1 (14%)	9,10,12	2.06	4 (44%)
4	PCA	N	1	4	7,8,9	1.87	1 (14%)	9,10,12	2.52	6 (66%)

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	PCA	X	1	4	-	0/0/11/13	0/1/1/1
4	PCA	R	1	4	-	0/0/11/13	0/1/1/1
3	PCA	W	1	3	-	0/0/11/13	0/1/1/1
3	PCA	U	1	3	-	0/0/11/13	0/1/1/1
4	PCA	P	1	4	-	0/0/11/13	0/1/1/1
3	PCA	Q	1	3	-	0/0/11/13	0/1/1/1
4	PCA	T	1	4	-	0/0/11/13	0/1/1/1
4	PCA	V	1	4	-	0/0/11/13	0/1/1/1
3	PCA	M	1	3	-	0/0/11/13	0/1/1/1
3	PCA	S	1	3	-	0/0/11/13	0/1/1/1
3	PCA	O	1	3	-	0/0/11/13	0/1/1/1
4	PCA	N	1	4	-	0/0/11/13	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	1	PCA	CD-N	4.90	1.47	1.34
4	V	1	PCA	CD-N	4.76	1.47	1.34
3	M	1	PCA	CD-N	4.74	1.47	1.34
4	N	1	PCA	CD-N	4.72	1.47	1.34
3	S	1	PCA	CD-N	4.71	1.47	1.34
3	W	1	PCA	CD-N	4.71	1.47	1.34
4	R	1	PCA	CD-N	4.71	1.47	1.34
4	T	1	PCA	CD-N	4.70	1.47	1.34
3	U	1	PCA	CD-N	4.67	1.46	1.34
4	X	1	PCA	CD-N	4.55	1.46	1.34
3	O	1	PCA	CD-N	4.46	1.46	1.34
3	Q	1	PCA	CD-N	4.29	1.45	1.34

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	1	PCA	CB-CA-C	-4.28	106.81	112.70
4	V	1	PCA	OE-CD-CG	-3.93	119.90	126.76
4	P	1	PCA	OE-CD-CG	-3.84	120.07	126.76
4	N	1	PCA	OE-CD-CG	-3.83	120.08	126.76
4	N	1	PCA	CA-N-CD	-3.52	101.53	113.58
4	R	1	PCA	OE-CD-CG	-3.40	120.83	126.76
3	M	1	PCA	OE-CD-CG	-3.34	120.93	126.76
4	R	1	PCA	CB-CA-C	-3.30	108.16	112.70
3	W	1	PCA	OE-CD-CG	-3.26	121.07	126.76
4	V	1	PCA	CA-N-CD	-3.25	102.47	113.58
4	T	1	PCA	OE-CD-CG	-3.18	121.21	126.76
3	S	1	PCA	OE-CD-CG	-3.11	121.34	126.76
4	N	1	PCA	CB-CA-N	3.09	112.17	103.30
3	O	1	PCA	CA-N-CD	-3.09	103.02	113.58
3	Q	1	PCA	CA-N-CD	-3.08	103.04	113.58
4	P	1	PCA	CA-N-CD	-3.04	103.16	113.58
4	V	1	PCA	CB-CA-C	-2.99	108.59	112.70
4	R	1	PCA	CA-N-CD	-2.98	103.39	113.58
3	U	1	PCA	OE-CD-CG	-2.97	121.58	126.76
3	M	1	PCA	CA-N-CD	-2.97	103.42	113.58
4	T	1	PCA	CA-N-CD	-2.96	103.44	113.58
4	N	1	PCA	CG-CD-N	2.95	116.03	108.39
3	S	1	PCA	CA-N-CD	-2.94	103.51	113.58
4	X	1	PCA	CA-N-CD	-2.93	103.53	113.58
3	W	1	PCA	CA-N-CD	-2.91	103.62	113.58
4	X	1	PCA	OE-CD-CG	-2.89	121.72	126.76
3	O	1	PCA	OE-CD-CG	-2.88	121.73	126.76
3	Q	1	PCA	CG-CD-N	2.88	115.85	108.39
3	O	1	PCA	CB-CA-N	2.88	111.57	103.30
3	U	1	PCA	CA-N-CD	-2.85	103.81	113.58
4	T	1	PCA	CB-CA-C	-2.84	108.80	112.70
4	V	1	PCA	CG-CD-N	2.83	115.71	108.39
3	Q	1	PCA	CB-CA-N	2.76	111.23	103.30
4	X	1	PCA	CB-CA-C	-2.74	108.93	112.70
3	S	1	PCA	CB-CA-N	2.66	110.93	103.30
3	O	1	PCA	CG-CD-N	2.66	115.27	108.39
4	V	1	PCA	CB-CA-N	2.65	110.89	103.30
3	M	1	PCA	CB-CA-N	2.60	110.75	103.30
4	R	1	PCA	CG-CD-N	2.59	115.10	108.39
3	M	1	PCA	CG-CD-N	2.56	115.01	108.39
3	U	1	PCA	CB-CA-N	2.56	110.64	103.30
3	W	1	PCA	CB-CA-N	2.54	110.60	103.30
3	W	1	PCA	CG-CD-N	2.53	114.94	108.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	1	PCA	CG-CD-N	2.51	114.88	108.39
4	X	1	PCA	CG-CD-N	2.50	114.88	108.39
4	T	1	PCA	CG-CD-N	2.49	114.84	108.39
4	X	1	PCA	CB-CA-N	2.49	110.44	103.30
3	Q	1	PCA	OE-CD-CG	-2.48	122.43	126.76
3	S	1	PCA	CG-CD-N	2.48	114.80	108.39
4	T	1	PCA	CB-CA-N	2.46	110.35	103.30
4	P	1	PCA	CB-CA-N	2.45	110.34	103.30
3	U	1	PCA	CG-CD-N	2.43	114.67	108.39
4	R	1	PCA	CB-CA-N	2.39	110.16	103.30
4	N	1	PCA	CB-CA-C	-2.13	109.78	112.70
4	N	1	PCA	O-C-CA	-2.11	119.24	124.78
4	T	1	PCA	O-C-CA	-2.04	119.42	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	1	PCA	1	0
3	O	1	PCA	1	0

## 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
5	NAG	Y	1	5,1	14,14,15	0.51	0	17,19,21	1.17	4 (23%)
5	NAG	Y	2	5	14,14,15	0.60	0	17,19,21	1.11	1 (5%)
5	BMA	Y	3	5	11,11,12	0.69	0	15,15,17	0.75	0
5	NAG	Z	1	5,1	14,14,15	0.56	0	17,19,21	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	Z	2	5	14,14,15	0.50	0	17,19,21	0.84	0
5	BMA	Z	3	5	11,11,12	0.78	0	15,15,17	0.71	0
5	NAG	a	1	5,1	14,14,15	0.55	0	17,19,21	0.98	1 (5%)
5	NAG	a	2	5	14,14,15	0.57	0	17,19,21	1.14	1 (5%)
5	BMA	a	3	5	11,11,12	0.74	0	15,15,17	0.77	0
5	NAG	b	1	5,1	14,14,15	0.56	0	17,19,21	0.80	0
5	NAG	b	2	5	14,14,15	0.63	0	17,19,21	1.14	3 (17%)
5	BMA	b	3	5	11,11,12	0.73	0	15,15,17	0.74	0
5	NAG	c	1	5,1	14,14,15	0.54	0	17,19,21	1.03	2 (11%)
5	NAG	c	2	5	14,14,15	0.60	0	17,19,21	1.18	1 (5%)
5	BMA	c	3	5	11,11,12	1.04	2 (18%)	15,15,17	1.56	2 (13%)
5	NAG	d	1	5,1	14,14,15	0.55	0	17,19,21	0.66	0
5	NAG	d	2	5	14,14,15	0.63	0	17,19,21	1.29	1 (5%)
5	BMA	d	3	5	11,11,12	0.81	0	15,15,17	0.76	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
5	NAG	Y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	2/2/19/22	0/1/1/1
5	NAG	Z	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	3/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	2/2/19/22	0/1/1/1
5	NAG	a	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	a	2	5	-	4/6/23/26	0/1/1/1
5	BMA	a	3	5	-	2/2/19/22	0/1/1/1
5	NAG	b	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	3/6/23/26	0/1/1/1
5	BMA	b	3	5	-	0/2/19/22	0/1/1/1
5	NAG	c	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	3/6/23/26	0/1/1/1
5	BMA	c	3	5	-	0/2/19/22	0/1/1/1
5	NAG	d	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	d	3	5	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	3	BMA	C1-C2	2.43	1.57	1.52
5	c	3	BMA	C2-C3	2.27	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	3	BMA	C1-C2-C3	3.76	114.28	109.67
5	d	2	NAG	C4-C3-C2	3.66	116.39	111.02
5	c	2	NAG	C4-C3-C2	3.63	116.33	111.02
5	a	2	NAG	C4-C3-C2	3.15	115.64	111.02
5	Y	2	NAG	C4-C3-C2	3.13	115.61	111.02
5	c	3	BMA	O5-C1-C2	2.79	115.08	110.77
5	b	2	NAG	C3-C4-C5	2.48	114.67	110.24
5	Y	1	NAG	O4-C4-C3	-2.35	104.91	110.35
5	b	2	NAG	C4-C3-C2	2.34	114.45	111.02
5	c	1	NAG	O5-C1-C2	-2.24	107.75	111.29
5	Y	1	NAG	O5-C1-C2	-2.24	107.75	111.29
5	a	1	NAG	C4-C3-C2	2.23	114.28	111.02
5	Y	1	NAG	C1-O5-C5	2.16	115.12	112.19
5	Y	1	NAG	C2-N2-C7	-2.09	119.93	122.90
5	c	1	NAG	C1-O5-C5	2.07	115.00	112.19
5	b	2	NAG	O5-C1-C2	-2.00	108.12	111.29

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Z	2	NAG	C1-C2-N2-C7
5	Z	2	NAG	C8-C7-N2-C2
5	Z	2	NAG	O7-C7-N2-C2
5	a	1	NAG	C8-C7-N2-C2
5	a	1	NAG	O7-C7-N2-C2
5	b	2	NAG	C8-C7-N2-C2
5	b	2	NAG	O7-C7-N2-C2
5	c	2	NAG	C1-C2-N2-C7
5	c	2	NAG	C8-C7-N2-C2

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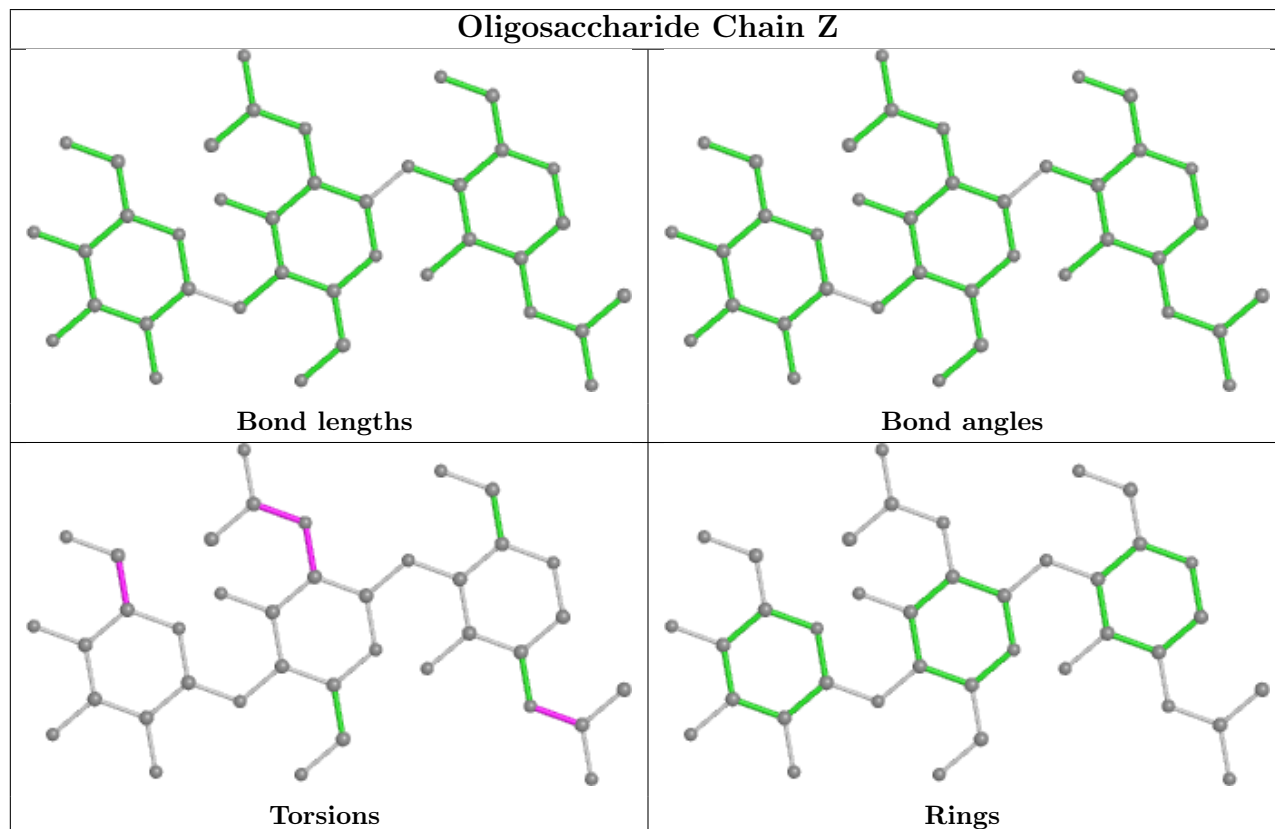
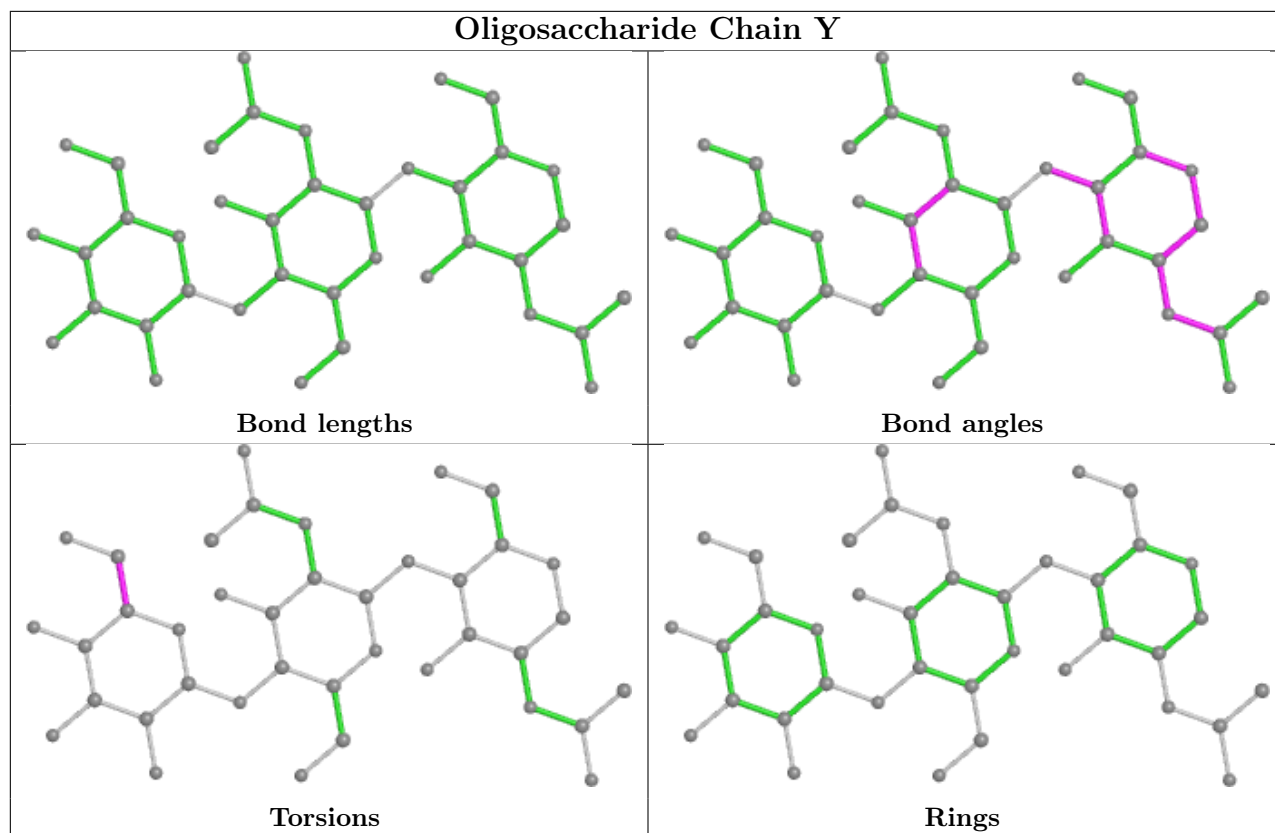
Mol	Chain	Res	Type	Atoms
5	c	2	NAG	O7-C7-N2-C2
5	a	2	NAG	C8-C7-N2-C2
5	a	2	NAG	O7-C7-N2-C2
5	d	2	NAG	C8-C7-N2-C2
5	d	2	NAG	O7-C7-N2-C2
5	a	3	BMA	O5-C5-C6-O6
5	d	3	BMA	O5-C5-C6-O6
5	a	3	BMA	C4-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	d	3	BMA	C4-C5-C6-O6
5	Y	3	BMA	C4-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
5	Z	3	BMA	C4-C5-C6-O6
5	c	1	NAG	C8-C7-N2-C2
5	Z	1	NAG	C8-C7-N2-C2
5	b	1	NAG	C8-C7-N2-C2
5	a	2	NAG	C4-C5-C6-O6
5	Z	3	BMA	O5-C5-C6-O6
5	c	1	NAG	O7-C7-N2-C2
5	b	2	NAG	O5-C5-C6-O6
5	Z	1	NAG	O7-C7-N2-C2
5	b	1	NAG	O7-C7-N2-C2

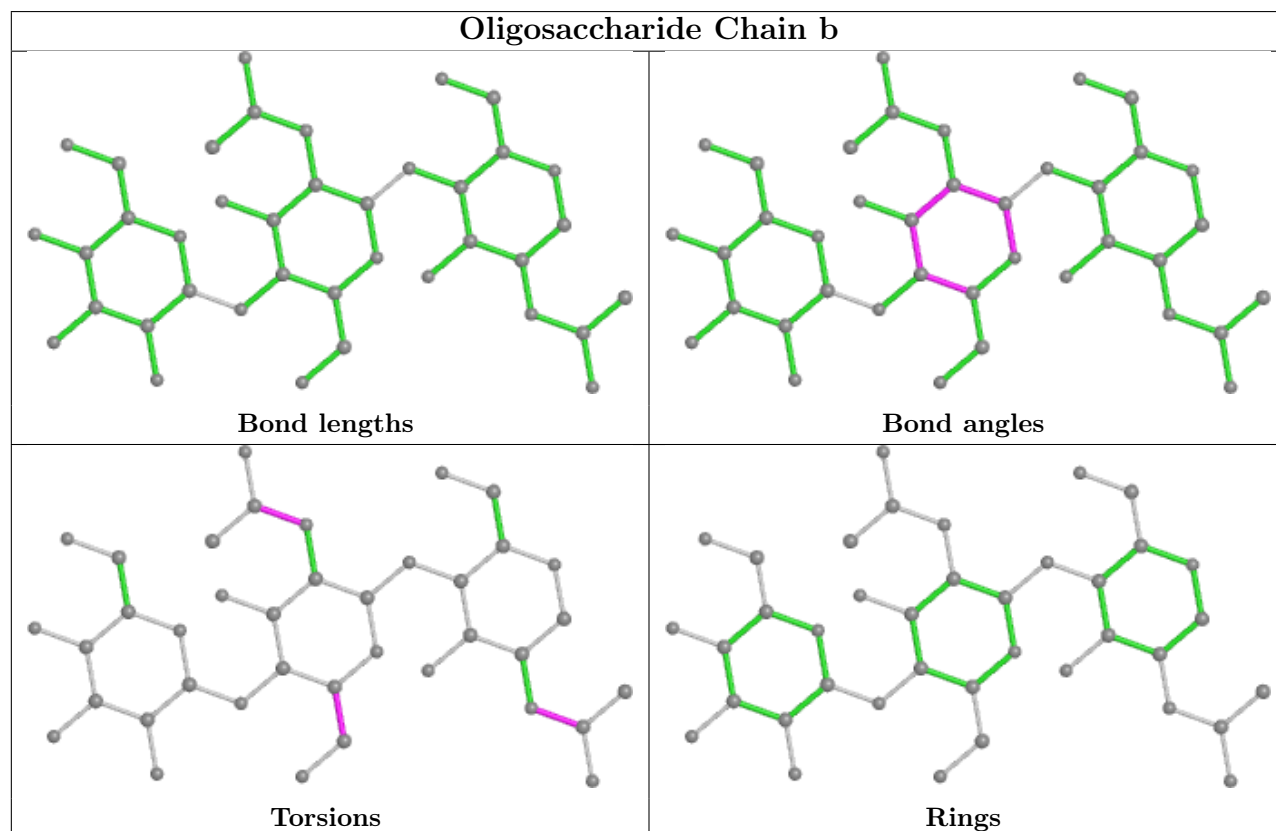
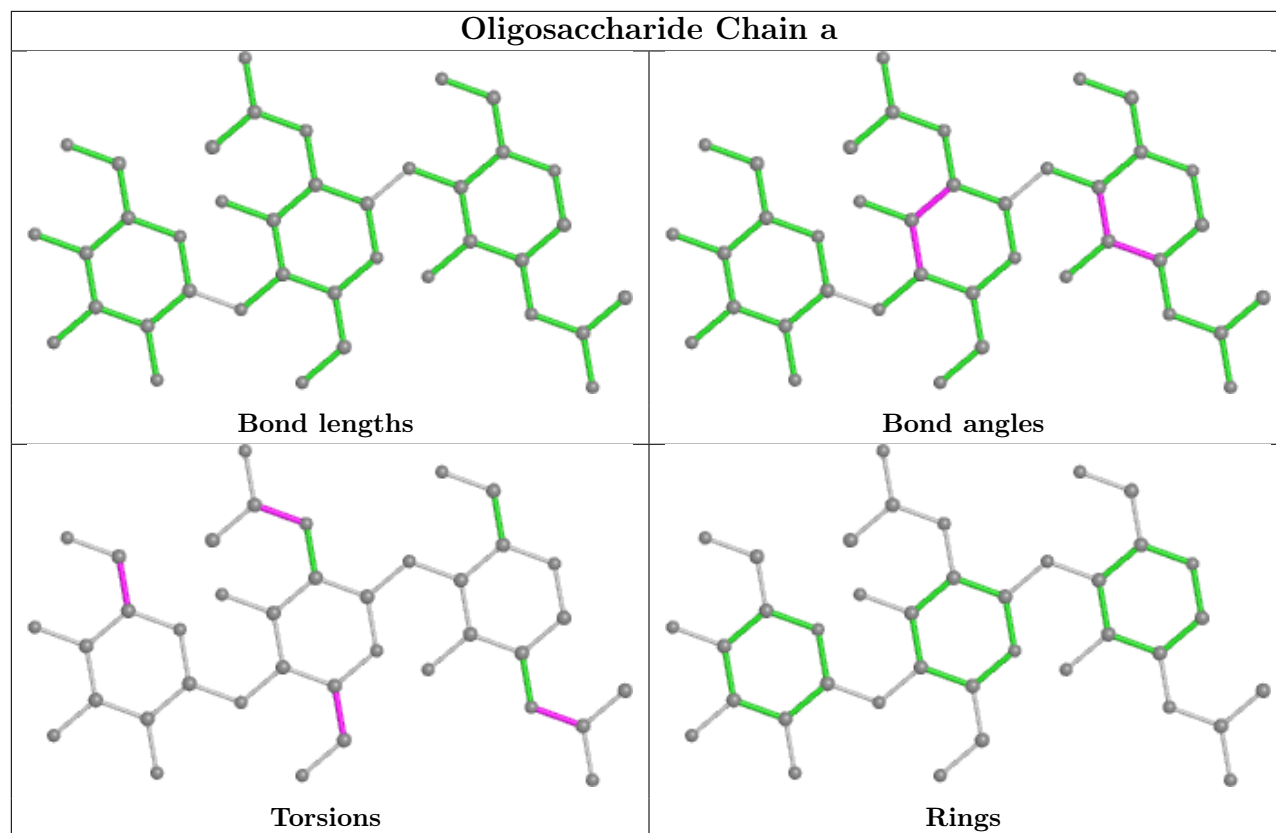
There are no ring outliers.

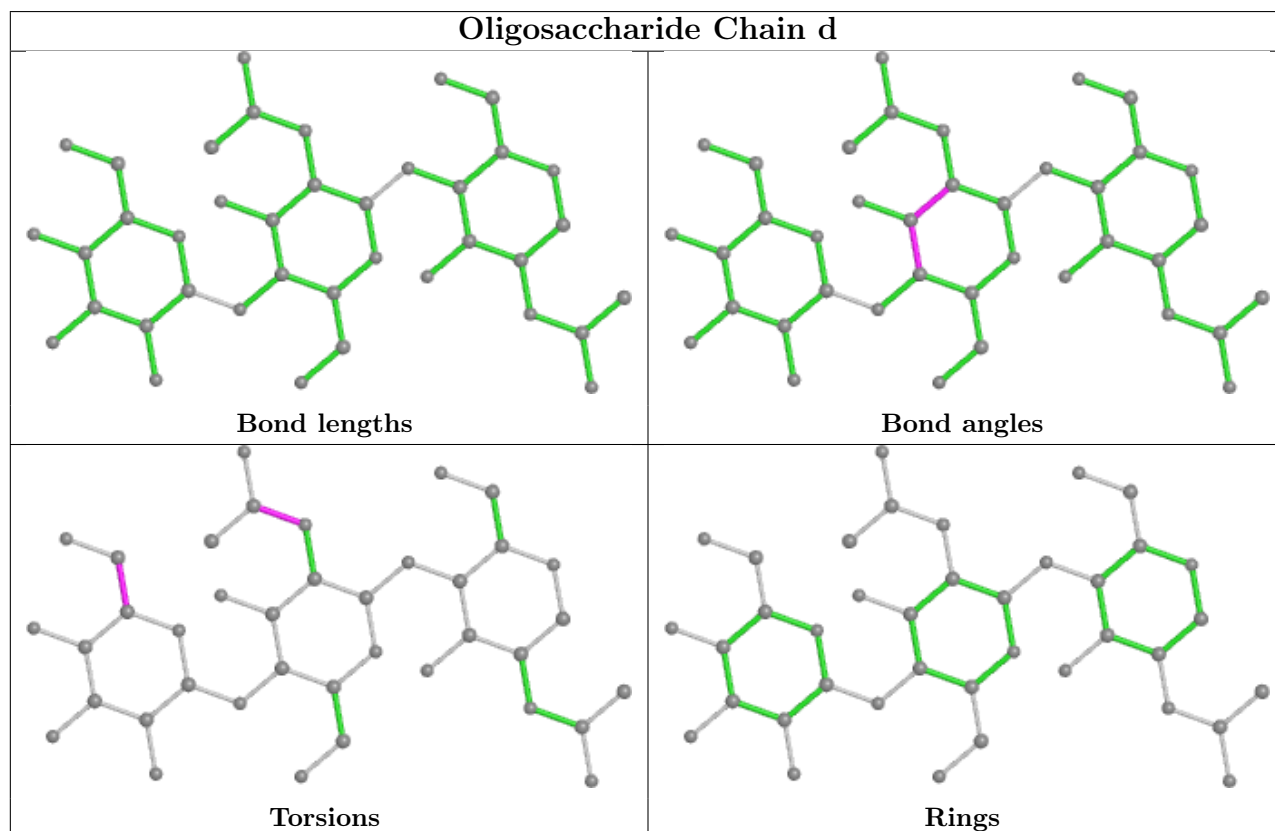
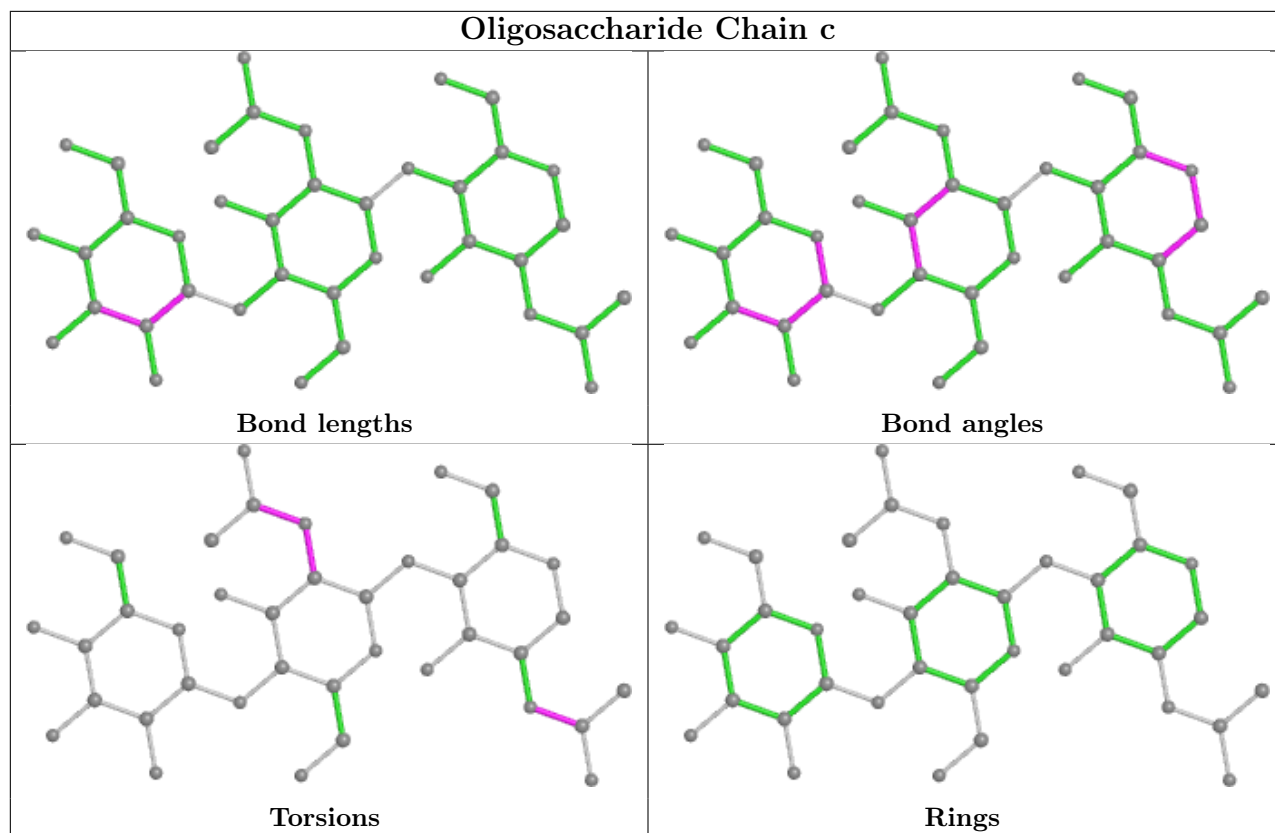
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	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

12 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
6	NAG	A	401	1	14,14,15	0.43	0	17,19,21	1.13	1 (5%)
6	NAG	I	401	1	14,14,15	0.56	0	17,19,21	1.16	2 (11%)
6	NAG	F	201	2	14,14,15	0.53	0	17,19,21	1.11	1 (5%)
6	NAG	L	201	2	14,14,15	0.48	0	17,19,21	2.18	2 (11%)
6	NAG	B	201	2	14,14,15	0.55	0	17,19,21	0.94	1 (5%)
6	NAG	C	401	1	14,14,15	0.51	0	17,19,21	1.60	2 (11%)
6	NAG	E	401	1	14,14,15	0.58	0	17,19,21	1.07	1 (5%)
6	NAG	D	201	2	14,14,15	0.52	0	17,19,21	0.65	0
6	NAG	J	201	2	14,14,15	0.46	0	17,19,21	0.84	1 (5%)
6	NAG	K	401	1	14,14,15	0.54	0	17,19,21	1.52	2 (11%)
6	NAG	H	201	2	14,14,15	0.50	0	17,19,21	0.71	0
6	NAG	G	401	1	14,14,15	0.66	0	17,19,21	0.77	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	A	401	1	-	2/6/23/26	0/1/1/1
6	NAG	I	401	1	-	3/6/23/26	0/1/1/1
6	NAG	F	201	2	-	4/6/23/26	0/1/1/1
6	NAG	L	201	2	-	2/6/23/26	0/1/1/1
6	NAG	B	201	2	-	0/6/23/26	0/1/1/1
6	NAG	C	401	1	-	3/6/23/26	0/1/1/1
6	NAG	E	401	1	-	6/6/23/26	0/1/1/1
6	NAG	D	201	2	-	2/6/23/26	0/1/1/1
6	NAG	J	201	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	K	401	1	-	4/6/23/26	0/1/1/1
6	NAG	H	201	2	-	2/6/23/26	0/1/1/1
6	NAG	G	401	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	201	NAG	C1-O5-C5	8.02	123.06	112.19
6	K	401	NAG	C1-O5-C5	4.72	118.58	112.19
6	C	401	NAG	C1-O5-C5	4.38	118.13	112.19
6	C	401	NAG	O5-C1-C2	4.30	118.07	111.29
6	A	401	NAG	C1-O5-C5	3.62	117.09	112.19
6	I	401	NAG	C1-O5-C5	3.58	117.04	112.19
6	F	201	NAG	C1-O5-C5	3.43	116.85	112.19
6	L	201	NAG	C2-N2-C7	2.65	126.68	122.90
6	E	401	NAG	C1-O5-C5	2.60	115.71	112.19
6	K	401	NAG	C1-C2-N2	2.52	114.80	110.49
6	J	201	NAG	O5-C5-C6	2.47	111.07	107.20
6	I	401	NAG	O5-C1-C2	2.39	115.06	111.29
6	B	201	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	NAG	C8-C7-N2-C2
6	A	401	NAG	O7-C7-N2-C2
6	C	401	NAG	C8-C7-N2-C2
6	C	401	NAG	O7-C7-N2-C2
6	E	401	NAG	C8-C7-N2-C2
6	E	401	NAG	O7-C7-N2-C2
6	F	201	NAG	C8-C7-N2-C2
6	F	201	NAG	O7-C7-N2-C2
6	G	401	NAG	C3-C2-N2-C7
6	G	401	NAG	C8-C7-N2-C2
6	G	401	NAG	O7-C7-N2-C2
6	K	401	NAG	C1-C2-N2-C7
6	K	401	NAG	C8-C7-N2-C2
6	K	401	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	L	201	NAG	C8-C7-N2-C2
6	L	201	NAG	O7-C7-N2-C2
6	H	201	NAG	C8-C7-N2-C2
6	H	201	NAG	O7-C7-N2-C2
6	E	401	NAG	C1-C2-N2-C7
6	F	201	NAG	C4-C5-C6-O6
6	F	201	NAG	O5-C5-C6-O6
6	D	201	NAG	C8-C7-N2-C2
6	D	201	NAG	O7-C7-N2-C2
6	G	401	NAG	O5-C5-C6-O6
6	K	401	NAG	O5-C5-C6-O6
6	I	401	NAG	O5-C5-C6-O6
6	G	401	NAG	C4-C5-C6-O6
6	C	401	NAG	O5-C5-C6-O6
6	I	401	NAG	C8-C7-N2-C2
6	E	401	NAG	C4-C5-C6-O6
6	E	401	NAG	C3-C2-N2-C7
6	I	401	NAG	O7-C7-N2-C2
6	E	401	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	201	NAG	1	0
6	L	201	NAG	1	0
6	H	201	NAG	1	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

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	325/331 (98%)	0.56	17 (5%) 27 25	43, 86, 149, 213	0
1	C	325/331 (98%)	0.39	17 (5%) 27 25	31, 71, 134, 219	0
1	E	325/331 (98%)	0.44	14 (4%) 35 34	37, 74, 129, 199	0
1	G	325/331 (98%)	0.44	15 (4%) 32 30	60, 104, 146, 175	0
1	I	325/331 (98%)	0.51	38 (11%) 4 4	65, 109, 151, 202	0
1	K	325/331 (98%)	0.40	22 (6%) 17 17	62, 100, 134, 148	0
2	B	171/176 (97%)	0.55	13 (7%) 13 13	43, 107, 161, 207	0
2	D	171/176 (97%)	0.67	13 (7%) 13 13	33, 109, 150, 171	0
2	F	171/176 (97%)	0.51	12 (7%) 16 16	37, 102, 155, 189	0
2	H	171/176 (97%)	0.86	27 (15%) 2 2	58, 102, 152, 206	0
2	J	171/176 (97%)	0.78	18 (10%) 6 6	53, 109, 154, 177	0
2	L	171/176 (97%)	0.68	17 (9%) 7 7	46, 99, 139, 172	0
3	M	227/231 (98%)	0.40	17 (7%) 14 13	49, 90, 151, 210	0
3	O	124/231 (53%)	0.67	17 (13%) 3 2	62, 113, 148, 161	0
3	Q	227/231 (98%)	1.20	52 (22%) 0 1	67, 135, 212, 241	0
3	S	124/231 (53%)	0.80	20 (16%) 1 2	100, 143, 179, 191	0
3	U	124/231 (53%)	1.08	22 (17%) 1 1	98, 141, 183, 212	0
3	W	124/231 (53%)	0.63	17 (13%) 3 2	101, 132, 164, 180	0
4	N	213/217 (98%)	0.36	18 (8%) 10 10	46, 77, 116, 156	0
4	P	110/217 (50%)	0.77	19 (17%) 1 1	73, 119, 158, 165	0
4	R	213/217 (98%)	0.98	52 (24%) 0 0	80, 156, 205, 251	0
4	T	110/217 (50%)	1.08	29 (26%) 0 0	113, 160, 179, 215	0
4	V	110/217 (50%)	1.73	37 (33%) 0 0	137, 171, 215, 247	0
4	X	110/217 (50%)	0.98	29 (26%) 0 0	112, 148, 185, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4792/5730 (83%)	0.65	552 (11%) 4 4	31, 106, 176, 251	0

All (552) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	V	89	ALA	16.0
3	Q	130	SER	13.5
3	Q	129	LYS	12.0
1	A	264(A)	GLY	11.8
3	Q	126	PRO	10.1
4	V	90	ALA	9.9
4	V	21	ILE	9.9
3	U	93	ALA	9.3
4	V	22	SER	8.7
4	V	86	TYR	8.3
4	R	2	PRO	8.0
4	T	86	TYR	7.6
1	G	264(A)	GLY	7.5
3	Q	132	SER	7.0
3	U	18	LEU	7.0
4	V	82	ASP	6.9
3	Q	119	PRO	6.7
2	H	1	GLY	6.6
1	E	79	LEU	6.6
4	V	36	TYR	6.4
3	Q	184	VAL	6.3
4	V	19[A]	VAL	6.2
3	Q	127	SER	5.8
3	S	100(F)	TYR	5.8
3	U	112	SER	5.8
3	Q	138	LEU	5.8
4	V	34	ASN	5.7
3	U	17	SER	5.6
4	X	19[A]	VAL	5.5
4	V	13	GLY	5.4
3	Q	100(F)	TYR	5.3
4	X	106(A)	LEU	5.3
1	K	302	ILE	5.2
4	V	20	THR	5.2
1	I	210	ASN	5.2
1	C	114	SER	5.2
2	L	64	THR	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	Q	131	THR	5.0
4	X	62	PHE	5.0
3	Q	194	TYR	5.0
4	V	75	ILE	5.0
4	X	75	ILE	5.0
3	O	10	GLY	4.9
4	V	80	SER	4.9
4	N	104	LEU	4.9
4	V	37	GLN	4.9
1	G	280	LYS	4.9
4	V	97[A]	VAL	4.8
4	T	106(A)	LEU	4.8
2	J	117	ASN	4.8
4	R	106(A)	LEU	4.7
4	T	97[A]	VAL	4.7
4	R	191	TYR	4.7
3	O	82	MET	4.7
3	U	81	GLN	4.7
4	T	82	ASP	4.7
2	L	21	TRP	4.7
2	D	138	PHE	4.6
3	M	131	THR	4.6
3	Q	183	THR	4.6
3	Q	142	VAL	4.5
4	V	33	VAL	4.5
1	G	301	THR	4.5
4	R	28	ILE	4.5
2	L	24	TYR	4.5
2	H	4	GLY	4.5
3	M	132	SER	4.5
3	O	9	GLY	4.5
4	R	185	TRP	4.5
4	V	88	CYS	4.5
4	X	14	SER	4.4
4	T	2	PRO	4.4
4	V	98	PHE	4.4
2	H	64	THR	4.4
3	W	112	SER	4.4
2	F	157	TYR	4.4
3	Q	128	SER	4.4
2	L	1	GLY	4.3
2	D	143	LYS	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	R	133	VAL	4.3
4	T	47[A]	LEU	4.3
4	R	125	LEU	4.3
1	A	9	PRO	4.3
4	R	90	ALA	4.3
3	Q	144	ASP	4.3
2	H	72[A]	ASN	4.3
2	D	141	TYR	4.2
2	J	23	GLY	4.2
3	S	36	TRP	4.2
3	S	9	GLY	4.2
4	R	118	PHE	4.2
3	S	100(H)	PRO	4.2
4	R	193	CYS	4.2
4	T	104	LEU	4.2
4	P	106(A)	LEU	4.1
1	A	302	ILE	4.1
3	W	78	LEU	4.1
4	X	47[A]	LEU	4.1
3	Q	182	VAL	4.1
2	H	62	GLN	4.1
1	I	302	ILE	4.1
4	V	44	PRO	4.1
3	O	11	VAL	4.1
4	X	78[A]	LEU	4.0
2	B	144	CYS	4.0
2	F	17	MET	4.0
4	R	107	GLY	4.0
3	S	90	TYR	4.0
3	U	45	LEU	4.0
4	R	19[A]	VAL	4.0
2	H	65	ALA	4.0
4	V	73	LEU	4.0
4	T	40	PRO	4.0
4	X	73	LEU	4.0
4	X	86	TYR	3.9
1	I	304	GLU	3.9
1	E	302	ILE	3.9
2	D	140	PHE	3.9
2	J	140	PHE	3.9
3	O	82(A)	ASN	3.9
2	B	140	PHE	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	X	18	ARG	3.9
4	V	83	GLU	3.9
1	G	54[A]	LEU	3.9
4	N	91	TRP	3.9
4	V	35	TRP	3.9
3	Q	143	LYS	3.8
4	X	21	ILE	3.8
1	G	302	ILE	3.8
1	I	16	GLY	3.8
2	B	72[A]	ASN	3.8
4	R	106	VAL	3.8
4	R	146	VAL	3.8
2	D	1	GLY	3.7
3	Q	207	VAL	3.7
1	A	264	SER	3.7
4	R	174	ALA	3.7
2	B	67	GLY	3.7
4	X	13	GLY	3.7
3	Q	120	SER	3.7
3	Q	214	LYS	3.7
4	V	2	PRO	3.6
4	V	106	VAL	3.6
1	A	13	ILE	3.6
1	G	279	THR	3.6
4	R	132	LEU	3.6
4	R	129	LYS	3.6
3	W	18	LEU	3.6
2	J	66	VAL	3.6
1	E	80	LEU	3.6
3	Q	185	PRO	3.6
3	Q	159	LEU	3.6
3	O	18	LEU	3.6
3	U	48	VAL	3.6
4	V	106(A)	LEU	3.6
4	P	2	PRO	3.6
2	J	27	GLN	3.6
3	U	34	MET	3.6
1	K	264(A)	GLY	3.6
4	R	98	PHE	3.5
1	K	257	ALA	3.5
4	V	104	LEU	3.5
3	Q	67	PHE	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	J	67	GLY	3.5
3	Q	51	ILE	3.5
2	B	134	GLY	3.5
2	D	144	CYS	3.5
2	F	64	THR	3.5
1	G	288	ILE	3.5
4	N	51	LEU	3.5
4	T	91	TRP	3.4
4	V	28	ILE	3.4
1	I	79	LEU	3.4
4	N	47[A]	LEU	3.4
4	P	47[A]	LEU	3.4
3	Q	188	SER	3.4
4	N	142	GLY	3.4
3	Q	125	ALA	3.4
3	S	105	GLN	3.4
3	M	100(F)	TYR	3.4
3	W	45	LEU	3.4
4	P	73	LEU	3.4
4	V	47[A]	LEU	3.4
1	C	13	ILE	3.4
2	H	112	ASP	3.4
2	H	140	PHE	3.4
3	Q	137	ALA	3.4
3	S	103	TRP	3.4
2	J	144	CYS	3.4
1	A	288	ILE	3.4
3	Q	121	VAL	3.3
3	W	36	TRP	3.3
1	I	301	THR	3.3
1	K	260	LEU	3.3
4	N	19[A]	VAL	3.3
4	V	11	ALA	3.3
3	M	189	LEU	3.3
3	Q	161	SER	3.3
4	T	78[A]	LEU	3.3
3	M	140[A]	CYS	3.3
4	V	87	TYR	3.3
4	R	12	SER	3.3
4	V	12	SER	3.3
4	T	99	GLY	3.3
1	A	303	GLY	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	117	ASN	3.2
1	A	25	THR	3.2
3	S	38	ARG	3.2
2	H	114	ASN	3.2
1	I	61	LEU	3.2
2	L	153	ARG	3.2
3	W	34	MET	3.2
2	L	66	VAL	3.2
3	Q	177	SER	3.2
4	R	149	LYS	3.2
2	B	1	GLY	3.2
3	Q	50	VAL	3.2
1	I	15	ILE	3.2
2	L	23	GLY	3.2
4	N	105	THR	3.2
3	W	93	ALA	3.2
3	Q	2	VAL	3.2
3	Q	154	TRP	3.2
1	C	302	ILE	3.2
3	O	82(C)	LEU	3.2
4	P	13	GLY	3.2
4	T	35	TRP	3.2
2	J	114	ASN	3.2
2	B	23	GLY	3.1
1	A	11	ASP	3.1
2	F	67	GLY	3.1
4	X	35	TRP	3.1
4	P	105	THR	3.1
3	Q	133	GLY	3.1
4	T	21	ILE	3.1
2	D	35	ALA	3.1
1	I	51	LEU	3.1
2	J	106	ARG	3.1
3	Q	112	SER	3.1
1	C	79	LEU	3.1
1	K	58	PRO	3.1
3	O	103	TRP	3.1
4	R	192	SER	3.1
4	R	104	LEU	3.1
2	J	17	MET	3.0
2	H	148	CYS	3.0
1	K	219	ALA	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	8	GLY	3.0
4	R	21	ILE	3.0
4	P	80	SER	3.0
4	X	22	SER	3.0
2	H	113	SER	3.0
4	X	48	ILE	3.0
1	A	24	ASP	3.0
4	N	35	TRP	3.0
4	P	82	ASP	3.0
2	H	109	ASP	3.0
2	J	32	SER	3.0
3	Q	145	TYR	3.0
3	Q	82(C)	LEU	3.0
1	C	264(A)	GLY	3.0
3	Q	155	ASN	3.0
4	P	86	TYR	3.0
4	N	106	VAL	3.0
3	Q	8	GLY	3.0
4	R	175	SER	3.0
4	R	195	VAL	3.0
3	U	20	LEU	3.0
1	I	214[A]	THR	3.0
3	U	82	MET	3.0
3	Q	59	TYR	3.0
4	P	3	VAL	3.0
4	R	148	TRP	2.9
4	T	33	VAL	2.9
4	R	105	THR	2.9
1	I	69	TRP	2.9
4	P	21	ILE	2.9
1	C	115	VAL	2.9
3	S	82(C)	LEU	2.9
1	C	289	ASN	2.9
2	B	17	MET	2.9
4	P	35	TRP	2.9
4	R	117	LEU	2.9
4	T	19[A]	VAL	2.9
3	S	82	MET	2.8
2	B	62	GLN	2.8
2	H	66	VAL	2.8
1	I	264(A)	GLY	2.8
4	R	178	LEU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	W	37	VAL	2.8
4	R	155	VAL	2.8
4	N	86	TYR	2.8
4	T	46	LEU	2.8
4	R	207	ALA	2.8
4	R	13	GLY	2.8
4	R	83	GLU	2.8
2	L	144	CYS	2.8
2	H	67	GLY	2.8
2	J	26	HIS	2.8
4	T	88	CYS	2.8
4	R	116	THR	2.8
3	O	80	LEU	2.7
2	F	66	VAL	2.7
3	W	48	VAL	2.7
2	H	21	TRP	2.7
4	T	23	CYS	2.7
1	I	260	LEU	2.7
4	X	12	SER	2.7
4	X	90	ALA	2.7
1	K	152	LEU	2.7
4	R	78[A]	LEU	2.7
2	F	27	GLN	2.7
4	R	22	SER	2.7
3	S	27	PHE	2.7
4	P	98	PHE	2.7
4	X	64	GLY	2.7
1	I	13	ILE	2.7
1	I	71	LEU	2.7
2	B	66	VAL	2.7
4	V	3	VAL	2.7
3	M	198	VAL	2.7
3	Q	211	VAL	2.7
2	L	157	TYR	2.7
3	U	90	TYR	2.7
1	C	10	GLY	2.7
3	S	20	LEU	2.7
3	W	27	PHE	2.7
1	K	194	LEU	2.7
3	O	20	LEU	2.7
3	U	82(A)	ASN	2.7
2	H	139	GLU	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	S	80	LEU	2.6
1	K	282	GLN	2.6
3	U	12	VAL	2.6
2	H	3	PHE	2.6
4	R	23	CYS	2.6
4	X	97[A]	VAL	2.6
4	X	50[A]	SER	2.6
4	P	88	CYS	2.6
2	J	113	SER	2.6
3	W	79	TYR	2.6
3	M	196[A]	CYS	2.6
1	E	115	VAL	2.6
2	F	23	GLY	2.6
3	Q	169[A]	VAL	2.6
4	V	91	TRP	2.6
4	R	14	SER	2.6
3	U	49	ALA	2.6
4	T	90	ALA	2.6
3	U	98[A]	MET	2.6
1	K	54[A]	LEU	2.6
4	T	89	ALA	2.6
4	T	73	LEU	2.6
2	H	106	ARG	2.6
1	G	264	SER	2.6
4	P	104	LEU	2.6
2	F	21	TRP	2.6
4	T	36	TYR	2.6
3	Q	18	LEU	2.6
3	Q	100(A)	TYR	2.5
3	U	86	ASP	2.5
1	K	15	ILE	2.5
1	I	9	PRO	2.5
3	S	82(A)	ASN	2.5
3	U	100(F)	TYR	2.5
2	L	36	ALA	2.5
1	I	118	PHE	2.5
2	D	64	THR	2.5
4	T	4	LEU	2.5
4	V	4	LEU	2.5
1	C	214[A]	THR	2.5
2	L	106	ARG	2.5
1	K	86	TYR	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	W	50	VAL	2.5
4	N	33	VAL	2.5
4	N	73	LEU	2.5
1	I	211	ARG	2.5
2	D	142	HIS	2.5
4	R	75	ILE	2.5
1	E	211	ARG	2.4
1	I	125(A)	LYS	2.4
2	D	21	TRP	2.4
3	Q	118	GLY	2.4
4	X	104	LEU	2.4
1	I	152	LEU	2.4
3	U	8	GLY	2.4
4	R	86	TYR	2.4
2	H	116	ARG	2.4
3	U	15	ARG	2.4
1	C	323	ILE	2.4
3	U	100(H)	PRO	2.4
4	R	73	LEU	2.4
1	A	265	SER	2.4
3	W	100(F)	TYR	2.4
4	T	50[A]	SER	2.4
1	C	262	ARG	2.4
1	E	212	ARG	2.4
1	K	16	GLY	2.4
2	L	4	GLY	2.4
2	B	63	PHE	2.4
2	B	143	LYS	2.4
1	K	191	GLN	2.4
1	G	16	GLY	2.4
3	S	50	VAL	2.4
3	W	100(A)	TYR	2.4
4	R	89	ALA	2.4
3	O	36	TRP	2.4
2	F	144	CYS	2.4
2	L	140	PHE	2.4
3	S	58	TYR	2.4
2	D	126	LEU	2.4
4	N	78[A]	LEU	2.4
4	P	14	SER	2.4
4	T	3	VAL	2.4
3	Q	196[A]	CYS	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	O	100(H)	PRO	2.4
4	T	20	THR	2.4
4	R	47[A]	LEU	2.4
3	Q	60	ALA	2.4
1	E	199	ASP	2.3
2	L	35	ALA	2.3
1	I	52	CYS	2.3
1	I	288	ILE	2.3
3	Q	195	ILE	2.3
4	R	111	ALA	2.3
3	S	8	GLY	2.3
1	A	318	THR	2.3
1	G	281	CYS	2.3
1	I	17	TYR	2.3
2	J	102	LEU	2.3
1	K	9	PRO	2.3
1	I	154	LEU	2.3
3	M	159	LEU	2.3
4	T	11	ALA	2.3
1	I	191	GLN	2.3
3	M	80	LEU	2.3
3	S	91	TYR	2.3
1	K	303	GLY	2.3
1	K	18	HIS	2.3
4	R	91	TRP	2.3
1	K	245	PHE	2.3
3	M	163	VAL	2.3
3	Q	208	ASP	2.3
1	E	61	LEU	2.3
1	K	118	PHE	2.3
3	O	90	TYR	2.3
3	U	100(A)	TYR	2.3
4	N	75	ILE	2.3
1	E	16	GLY	2.3
2	H	71	ASN	2.3
4	P	78[A]	LEU	2.3
1	C	267	ILE	2.3
4	T	44	PRO	2.2
1	I	282	GLN	2.2
1	E	264(A)	GLY	2.2
3	M	194	TYR	2.2
4	P	106	VAL	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	W	24	ALA	2.2
1	A	313	LYS	2.2
1	I	305	CYS	2.2
3	O	19[A]	ARG	2.2
1	E	54[A]	LEU	2.2
1	G	86	TYR	2.2
1	G	84	TRP	2.2
1	E	210	ASN	2.2
1	I	277	CYS	2.2
1	G	154	LEU	2.2
1	I	212	ARG	2.2
3	M	34	MET	2.2
3	Q	98[A]	MET	2.2
4	N	97[A]	VAL	2.2
2	D	30	GLN	2.2
2	L	17	MET	2.2
2	L	138	PHE	2.2
2	D	22	TYR	2.2
2	B	149	MET	2.2
1	I	265	SER	2.2
3	M	29	PHE	2.2
1	K	288	ILE	2.2
1	I	55	GLY	2.2
4	R	150	ALA	2.2
1	G	104	ASP	2.2
1	E	59	LEU	2.2
1	C	324	PRO	2.2
4	N	83	GLU	2.2
1	C	51	LEU	2.1
2	F	22	TYR	2.1
4	N	64	GLY	2.1
4	X	103	LYS	2.1
1	A	214[A]	THR	2.1
3	O	93	ALA	2.1
1	C	66[A]	ILE	2.1
1	I	50	LYS	2.1
4	X	9	SER	2.1
3	Q	176	TYR	2.1
1	C	15	ILE	2.1
1	I	213	PHE	2.1
4	X	98	PHE	2.1
3	Q	100(H)	PRO	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	M	182	VAL	2.1
2	J	118	LEU	2.1
3	S	45	LEU	2.1
3	S	24	ALA	2.1
4	X	51	LEU	2.1
3	U	7	SER	2.1
2	H	2	LEU	2.1
1	A	304	GLU	2.1
1	G	57	ALA	2.1
4	R	140	TYR	2.1
4	V	14	SER	2.1
4	V	45	LYS	2.1
4	N	32	THR	2.1
4	R	131	THR	2.1
2	H	157	TYR	2.1
2	F	62	GLN	2.1
4	V	62	PHE	2.1
4	P	89	ALA	2.1
4	X	87	TYR	2.1
1	C	87	ILE	2.1
1	K	252	ILE	2.1
1	I	54[A]	LEU	2.1
3	O	27	PHE	2.1
1	I	220	ARG	2.1
2	H	107	THR	2.1
2	J	64	THR	2.1
3	M	150	VAL	2.1
1	K	59	LEU	2.1
2	H	126	LEU	2.1
2	J	1	GLY	2.1
3	W	20	LEU	2.1
1	I	270	SER	2.0
4	X	82	ASP	2.0
4	X	83	GLU	2.0
1	I	281	CYS	2.0
2	H	5	ALA	2.0
4	R	182	PRO	2.0
3	M	136	ALA	2.0
4	R	25	GLY	2.0
4	R	141	PRO	2.0
4	R	186	LYS	2.0
2	J	29	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
3	O	112	SER	2.0
2	L	67	GLY	2.0
3	W	91	TYR	2.0
4	T	12	SER	2.0
1	A	198	ALA	2.0
3	M	100(H)	PRO	2.0
1	A	216	GLU	2.0
1	E	119	GLU	2.0
2	F	29	GLU	2.0
1	I	14	CYS	2.0
4	X	36	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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.

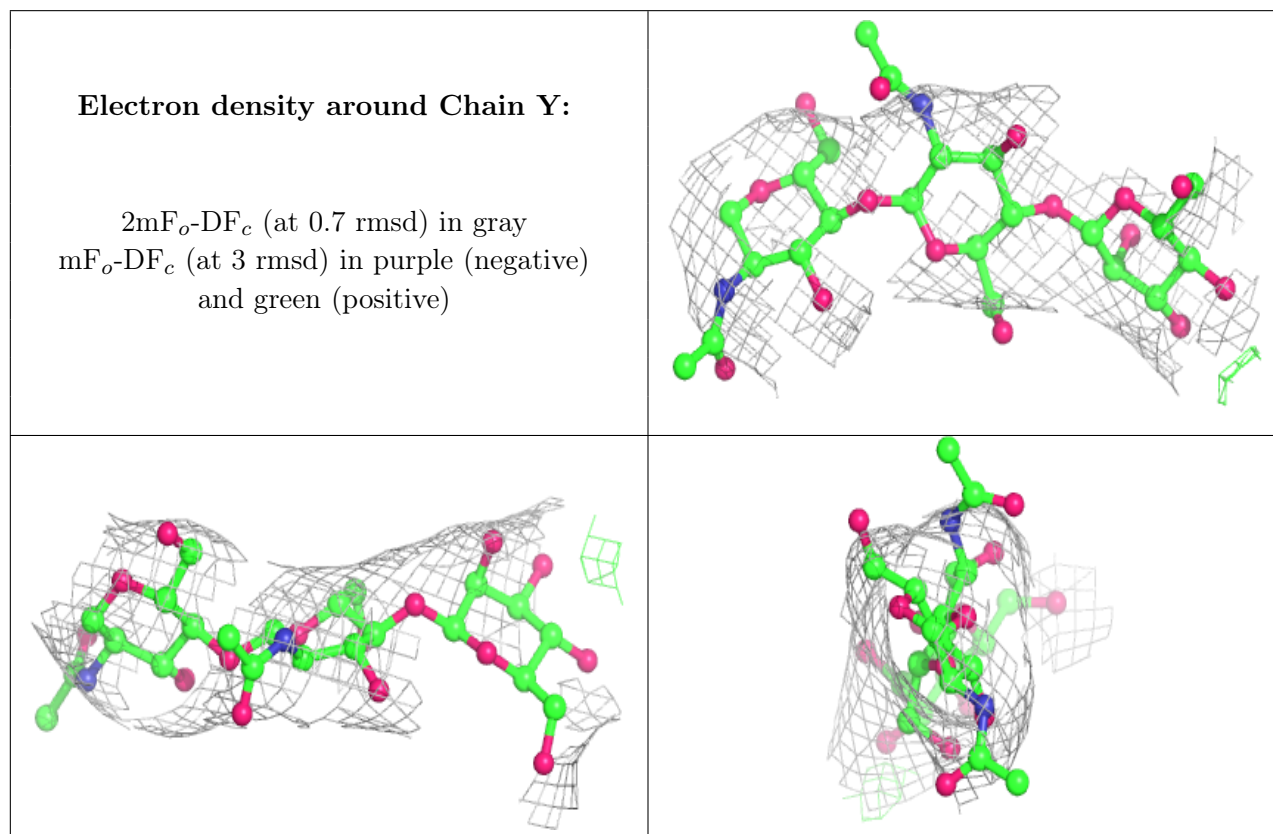
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PCA	R	1	8/9	0.41	0.53	203,208,217,222	0
3	PCA	S	1	8/9	0.55	0.37	199,209,211,212	0
4	PCA	V	1	8/9	0.58	0.34	206,209,213,215	0
4	PCA	X	1	8/9	0.67	0.41	207,212,215,218	0
4	PCA	N	1	8/9	0.68	0.26	172,194,204,208	0
3	PCA	M	1	8/9	0.69	0.29	120,132,139,146	0
4	PCA	P	1	8/9	0.70	0.60	124,132,163,169	0
4	PCA	T	1	8/9	0.71	0.33	193,201,222,228	0
3	PCA	Q	1	8/9	0.74	0.56	155,160,163,164	0
3	PCA	O	1	8/9	0.84	0.14	151,153,157,160	0
3	PCA	U	1	8/9	0.89	0.15	170,178,182,187	0
3	PCA	W	1	8/9	0.91	0.14	195,198,202,208	0

## 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.

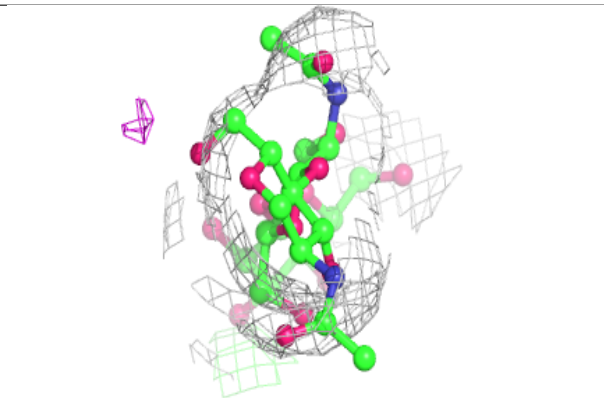
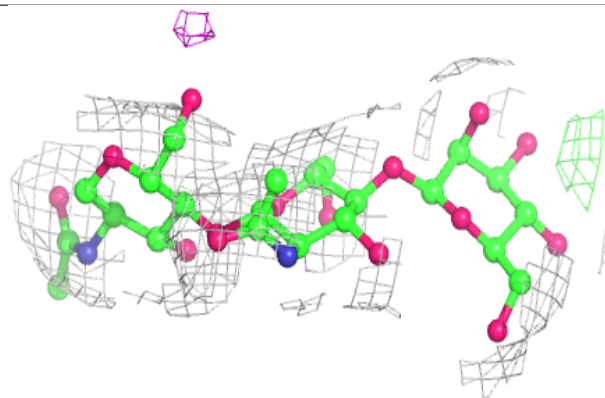
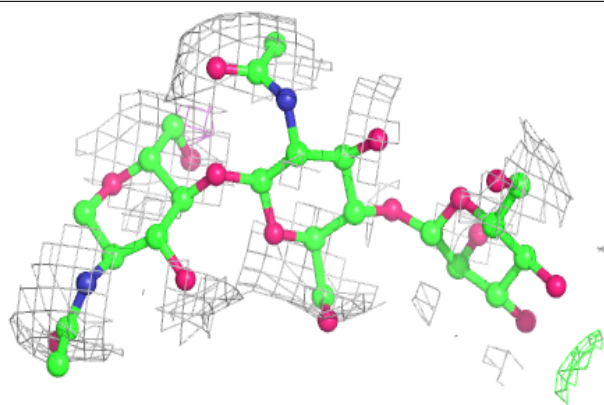
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BMA	a	3	11/12	0.68	0.46	122,134,154,160	0
5	BMA	Y	3	11/12	0.82	0.14	101,127,129,135	0
5	BMA	b	3	11/12	0.84	0.20	114,120,128,131	0
5	BMA	Z	3	11/12	0.86	0.23	83,104,113,124	0
5	BMA	d	3	11/12	0.87	0.21	122,132,138,140	0
5	NAG	Y	2	14/15	0.89	0.32	107,118,131,133	0
5	BMA	c	3	11/12	0.89	0.28	99,117,171,172	0
5	NAG	Z	2	14/15	0.89	0.20	96,100,107,110	0
5	NAG	Y	1	14/15	0.90	0.30	99,109,118,126	0
5	NAG	d	2	14/15	0.90	0.20	116,120,133,135	0
5	NAG	a	1	14/15	0.90	0.22	50,70,80,81	0
5	NAG	c	2	14/15	0.91	0.16	100,126,130,138	0
5	NAG	a	2	14/15	0.91	0.20	67,77,90,107	0
5	NAG	Z	1	14/15	0.92	0.23	62,79,94,98	0
5	NAG	b	2	14/15	0.93	0.14	108,124,132,133	0
5	NAG	c	1	14/15	0.93	0.13	78,102,106,113	0
5	NAG	b	1	14/15	0.94	0.15	78,90,99,99	0
5	NAG	d	1	14/15	0.94	0.23	65,106,114,116	0

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

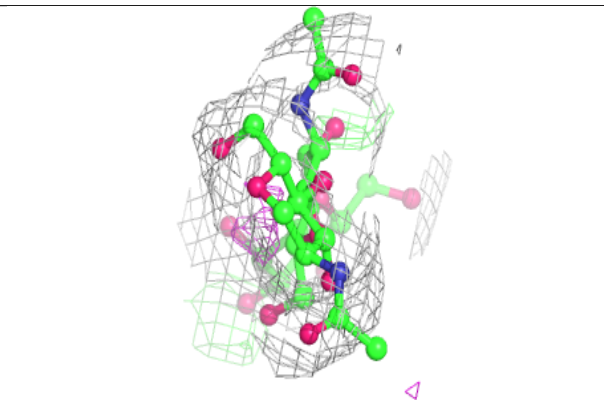
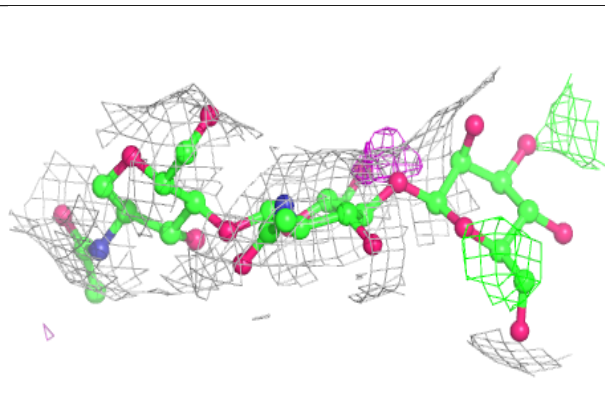
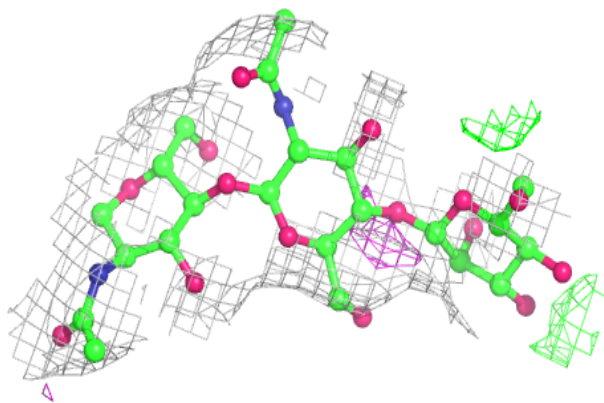


**Electron density around Chain Z:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

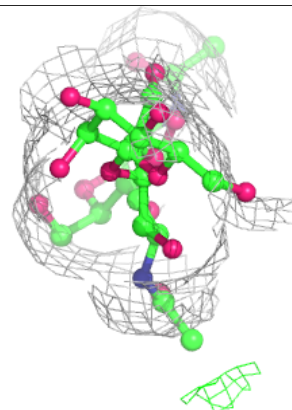
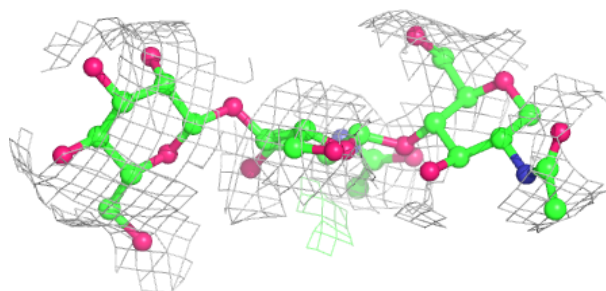
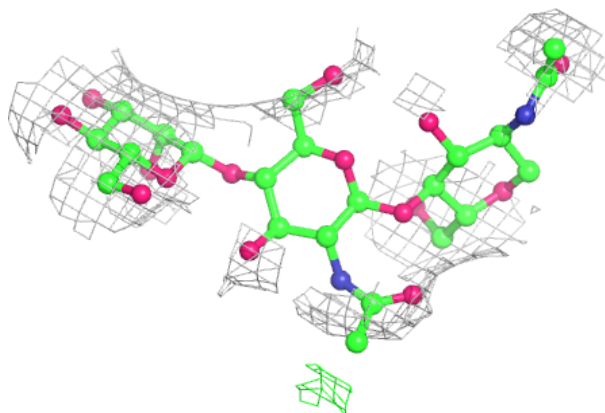
**Electron density around Chain a:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

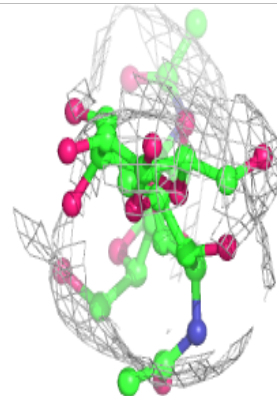
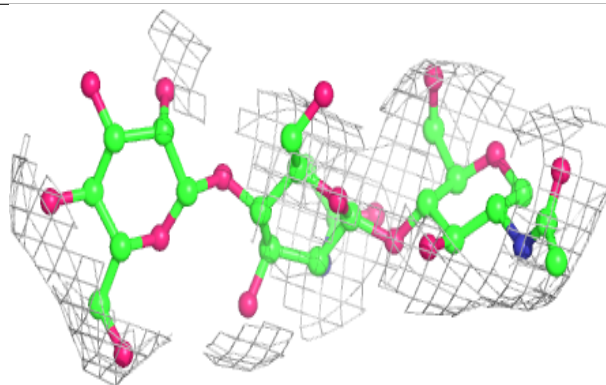
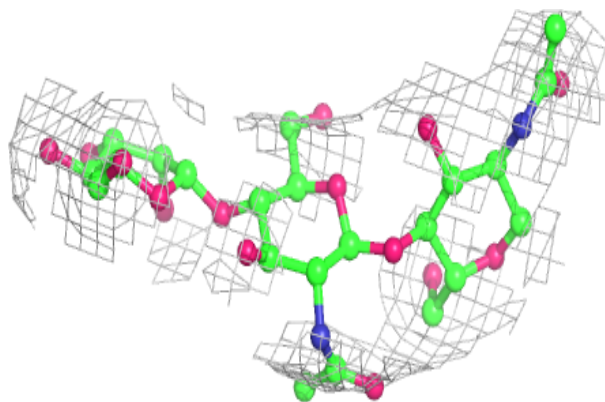


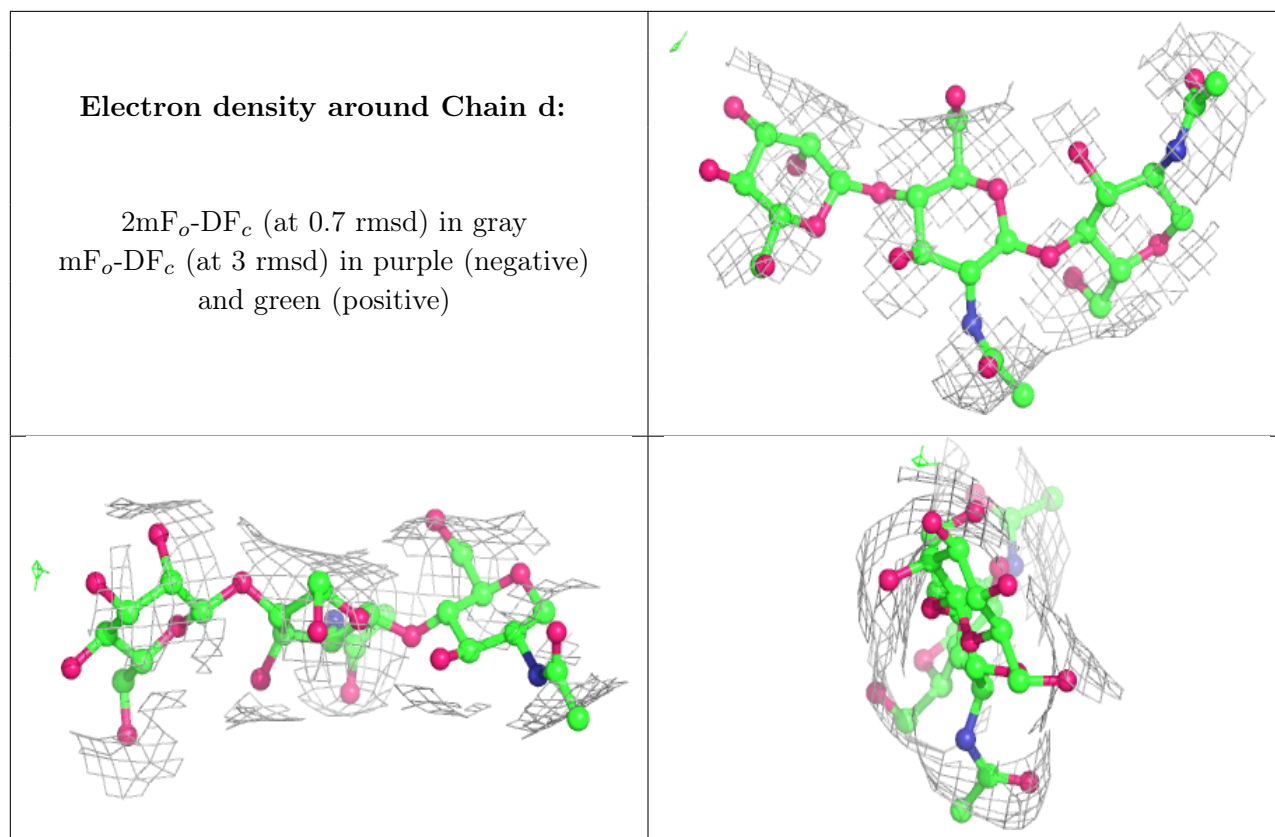
**Electron density around Chain b:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain c:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.4 Ligands [i](#)

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
6	NAG	I	401	14/15	0.58	0.58	179,188,220,226	0
6	NAG	F	201	14/15	0.59	0.33	163,181,186,191	0
6	NAG	J	201	14/15	0.64	0.44	122,141,152,153	0
6	NAG	B	201	14/15	0.71	0.40	153,170,177,180	0
6	NAG	A	401	14/15	0.74	0.39	152,185,198,200	0
6	NAG	H	201	14/15	0.74	0.38	135,152,165,168	0
6	NAG	E	401	14/15	0.75	0.26	186,209,213,218	0
6	NAG	C	401	14/15	0.76	0.28	151,163,173,176	0
6	NAG	D	201	14/15	0.78	0.27	139,164,173,176	0
6	NAG	L	201	14/15	0.78	0.38	140,174,180,183	0
6	NAG	G	401	14/15	0.81	0.19	175,184,195,196	0
6	NAG	K	401	14/15	0.87	0.25	116,156,174,182	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.