



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 09:08 AM BST

PDB ID : 3B2U  
Title : Crystal structure of isolated domain III of the extracellular region of the epidermal growth factor receptor in complex with the Fab fragment of IMC-11F8  
Authors : Ferguson, K.M.; Li, S.; Kussie, P.  
Deposited on : 2007-10-19  
Resolution : 2.58 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.

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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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

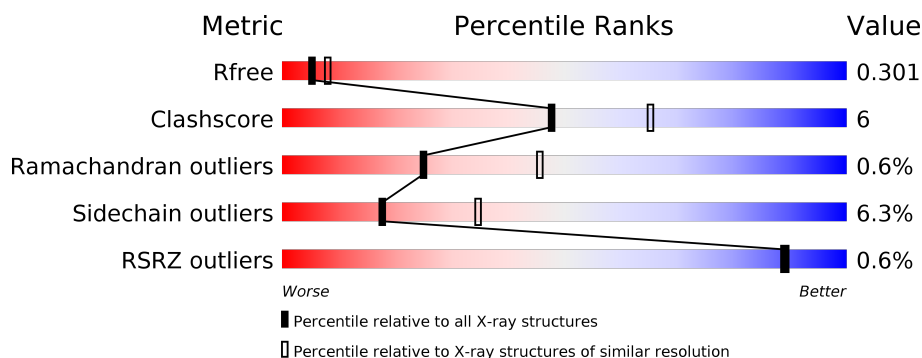
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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.





















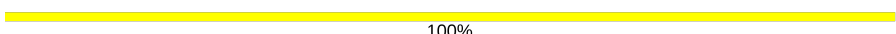



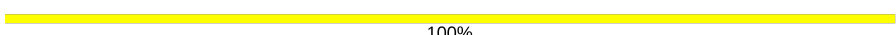
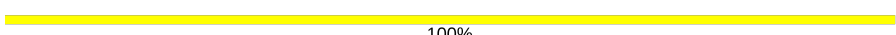
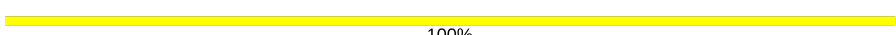
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 on 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	D	213	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	G	213	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	K	213	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	L	213	<div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	O	213	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	R	213	<div> <div>84%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	U	213	
1	X	213	
2	C	223	
2	F	223	
2	H	223	
2	J	223	
2	N	223	
2	Q	223	
2	T	223	
2	W	223	
3	A	214	
3	B	214	
3	E	214	
3	I	214	
3	M	214	
3	P	214	
3	S	214	
3	V	214	
4	Y	4	
4	c	4	
4	e	4	
5	Z	2	
5	b	2	
5	d	2	
5	g	2	

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Mol	Chain	Length	Quality of chain
5	l	2	 100%
5	n	2	 100%
5	p	2	 100%
6	a	3	 100%
6	f	3	 100%
6	i	3	 100%
6	j	3	 100%
6	k	3	 100%
6	m	3	 100%
6	o	3	 100%
7	h	5	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	e	4	X	-	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 39035 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 IMC-11F8 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1614	1008	272	329	5			
1	D	213	Total	C	N	O	S	0	0	0
			1605	1003	270	327	5			
1	G	213	Total	C	N	O	S	0	0	0
			1601	1002	269	325	5			
1	K	213	Total	C	N	O	S	0	0	0
			1598	999	265	329	5			
1	O	213	Total	C	N	O	S	0	0	0
			1606	1003	271	327	5			
1	R	213	Total	C	N	O	S	0	0	0
			1610	1005	271	329	5			
1	U	213	Total	C	N	O	S	0	0	0
			1618	1012	274	327	5			
1	X	213	Total	C	N	O	S	0	0	0
			1612	1008	270	329	5			

- Molecule 2 is a protein called IMC-11F8 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1603	1020	258	320	5			
2	C	213	Total	C	N	O	S	0	0	0
			1563	997	250	311	5			
2	F	215	Total	C	N	O	S	0	0	0
			1579	1004	254	316	5			
2	J	217	Total	C	N	O	S	0	0	0
			1591	1013	257	316	5			
2	N	218	Total	C	N	O	S	0	0	0
			1603	1018	258	322	5			
2	Q	217	Total	C	N	O	S	0	0	0
			1594	1015	256	318	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	216	Total	C	N	O	S	0	0	0
			1586	1011	253	317	5			
2	W	216	Total	C	N	O	S	0	0	0
			1595	1015	256	319	5			

- Molecule 3 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	195	Total	C	N	O	S	0	0	0
			1452	909	255	279	9			
3	B	194	Total	C	N	O	S	0	0	0
			1424	893	249	273	9			
3	E	194	Total	C	N	O	S	0	0	0
			1441	903	252	277	9			
3	I	193	Total	C	N	O	S	0	0	0
			1454	912	254	279	9			
3	M	195	Total	C	N	O	S	0	0	0
			1444	905	253	277	9			
3	P	193	Total	C	N	O	S	0	0	0
			1441	903	253	276	9			
3	S	194	Total	C	N	O	S	0	0	0
			1427	889	254	275	9			
3	V	193	Total	C	N	O	S	0	0	0
			1422	894	243	276	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	LEU	-	expression tag	UNP P00533
A	308	GLU	-	expression tag	UNP P00533
A	309	GLU	-	expression tag	UNP P00533
A	310	LYS	-	expression tag	UNP P00533
A	515	HIS	-	expression tag	UNP P00533
A	516	HIS	-	expression tag	UNP P00533
A	517	HIS	-	expression tag	UNP P00533
A	518	HIS	-	expression tag	UNP P00533
A	519	HIS	-	expression tag	UNP P00533
A	520	HIS	-	expression tag	UNP P00533
B	307	LEU	-	expression tag	UNP P00533
B	308	GLU	-	expression tag	UNP P00533
B	309	GLU	-	expression tag	UNP P00533
B	310	LYS	-	expression tag	UNP P00533

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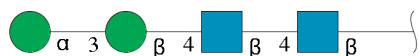
Chain	Residue	Modelled	Actual	Comment	Reference
B	515	HIS	-	expression tag	UNP P00533
B	516	HIS	-	expression tag	UNP P00533
B	517	HIS	-	expression tag	UNP P00533
B	518	HIS	-	expression tag	UNP P00533
B	519	HIS	-	expression tag	UNP P00533
B	520	HIS	-	expression tag	UNP P00533
E	307	LEU	-	expression tag	UNP P00533
E	308	GLU	-	expression tag	UNP P00533
E	309	GLU	-	expression tag	UNP P00533
E	310	LYS	-	expression tag	UNP P00533
E	515	HIS	-	expression tag	UNP P00533
E	516	HIS	-	expression tag	UNP P00533
E	517	HIS	-	expression tag	UNP P00533
E	518	HIS	-	expression tag	UNP P00533
E	519	HIS	-	expression tag	UNP P00533
E	520	HIS	-	expression tag	UNP P00533
I	307	LEU	-	expression tag	UNP P00533
I	308	GLU	-	expression tag	UNP P00533
I	309	GLU	-	expression tag	UNP P00533
I	310	LYS	-	expression tag	UNP P00533
I	515	HIS	-	expression tag	UNP P00533
I	516	HIS	-	expression tag	UNP P00533
I	517	HIS	-	expression tag	UNP P00533
I	518	HIS	-	expression tag	UNP P00533
I	519	HIS	-	expression tag	UNP P00533
I	520	HIS	-	expression tag	UNP P00533
M	307	LEU	-	expression tag	UNP P00533
M	308	GLU	-	expression tag	UNP P00533
M	309	GLU	-	expression tag	UNP P00533
M	310	LYS	-	expression tag	UNP P00533
M	515	HIS	-	expression tag	UNP P00533
M	516	HIS	-	expression tag	UNP P00533
M	517	HIS	-	expression tag	UNP P00533
M	518	HIS	-	expression tag	UNP P00533
M	519	HIS	-	expression tag	UNP P00533
M	520	HIS	-	expression tag	UNP P00533
P	307	LEU	-	expression tag	UNP P00533
P	308	GLU	-	expression tag	UNP P00533
P	309	GLU	-	expression tag	UNP P00533
P	310	LYS	-	expression tag	UNP P00533
P	515	HIS	-	expression tag	UNP P00533
P	516	HIS	-	expression tag	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
P	517	HIS	-	expression tag	UNP P00533
P	518	HIS	-	expression tag	UNP P00533
P	519	HIS	-	expression tag	UNP P00533
P	520	HIS	-	expression tag	UNP P00533
S	307	LEU	-	expression tag	UNP P00533
S	308	GLU	-	expression tag	UNP P00533
S	309	GLU	-	expression tag	UNP P00533
S	310	LYS	-	expression tag	UNP P00533
S	515	HIS	-	expression tag	UNP P00533
S	516	HIS	-	expression tag	UNP P00533
S	517	HIS	-	expression tag	UNP P00533
S	518	HIS	-	expression tag	UNP P00533
S	519	HIS	-	expression tag	UNP P00533
S	520	HIS	-	expression tag	UNP P00533
V	307	LEU	-	expression tag	UNP P00533
V	308	GLU	-	expression tag	UNP P00533
V	309	GLU	-	expression tag	UNP P00533
V	310	LYS	-	expression tag	UNP P00533
V	515	HIS	-	expression tag	UNP P00533
V	516	HIS	-	expression tag	UNP P00533
V	517	HIS	-	expression tag	UNP P00533
V	518	HIS	-	expression tag	UNP P00533
V	519	HIS	-	expression tag	UNP P00533
V	520	HIS	-	expression tag	UNP P00533

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
4	Y	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	c	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	e	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a



cetamido-2-deoxy-beta-D-glucopyranose.



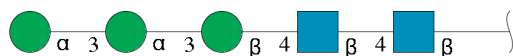
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	g	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	l	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	n	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	p	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 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.



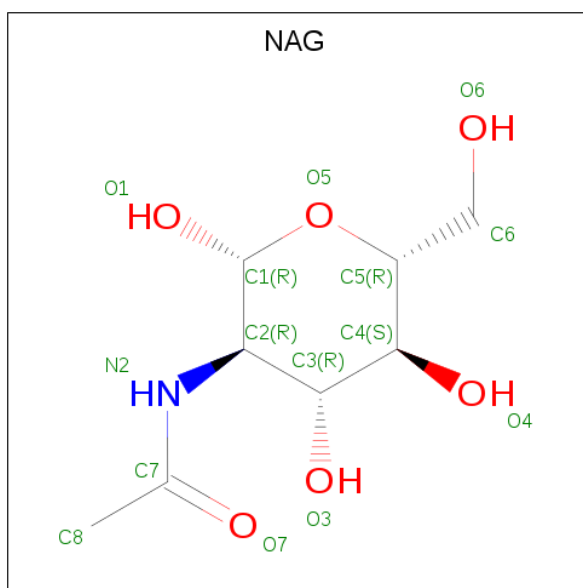
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	a	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	f	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	i	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	j	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	k	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	m	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	o	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-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
7	h	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



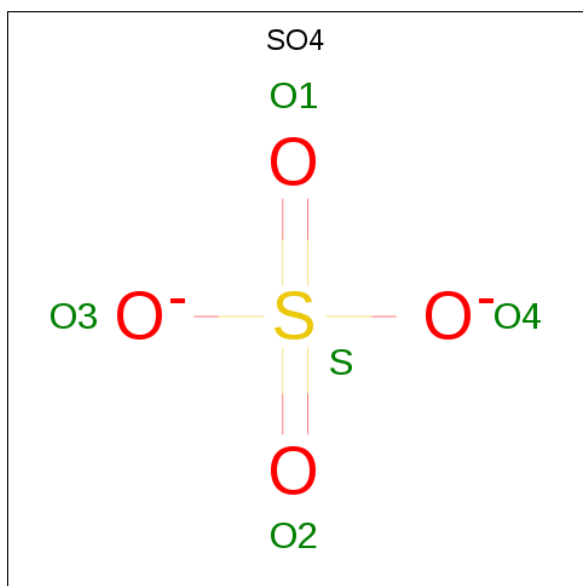
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	M	1	Total	C	N	O	0	0
			14	8	1	5		
8	P	1	Total	C	N	O	0	0
			14	8	1	5		
8	P	1	Total	C	N	O	0	0
			14	8	1	5		
8	S	1	Total	C	N	O	0	0
			14	8	1	5		
8	S	1	Total	C	N	O	0	0
			14	8	1	5		
8	V	1	Total	C	N	O	0	0
			14	8	1	5		
8	V	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	O S	0	0
			5	4 1		
9	G	1	Total	O S	0	0
			5	4 1		
9	E	1	Total	O S	0	0
			5	4 1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	K	1	Total	O	S	0	0
			5	4	1		
9	O	1	Total	O	S	0	0
			5	4	1		
9	U	1	Total	O	S	0	0
			5	4	1		
9	X	1	Total	O	S	0	0
			5	4	1		
9	V	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	56	Total	O	0	0
			56	56		
10	H	47	Total	O	0	0
			47	47		
10	A	30	Total	O	0	0
			30	30		
10	D	55	Total	O	0	0
			55	55		
10	C	45	Total	O	0	0
			45	45		
10	B	22	Total	O	0	0
			22	22		
10	G	50	Total	O	0	0
			50	50		
10	F	40	Total	O	0	0
			40	40		
10	E	30	Total	O	0	0
			30	30		
10	K	63	Total	O	0	0
			63	63		
10	J	44	Total	O	0	0
			44	44		
10	I	41	Total	O	0	0
			41	41		
10	O	57	Total	O	0	0
			57	57		
10	N	40	Total	O	0	0
			40	40		

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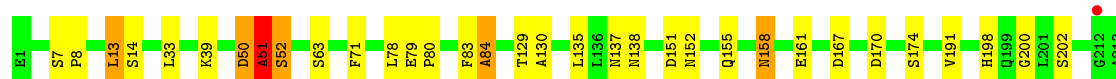
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	35	Total 35	O 35	0	0
10	R	62	Total 62	O 62	0	0
10	Q	51	Total 51	O 51	0	0
10	P	41	Total 41	O 41	0	0
10	U	42	Total 42	O 42	0	0
10	T	41	Total 41	O 41	0	0
10	S	23	Total 23	O 23	0	0
10	X	47	Total 47	O 47	0	0
10	W	50	Total 50	O 50	0	0
10	V	24	Total 24	O 24	0	0

### 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.

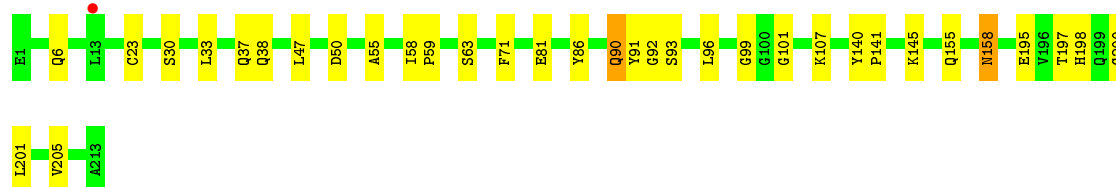
- Molecule 1: IMC-11F8 Fab Light chain

Chain L: 




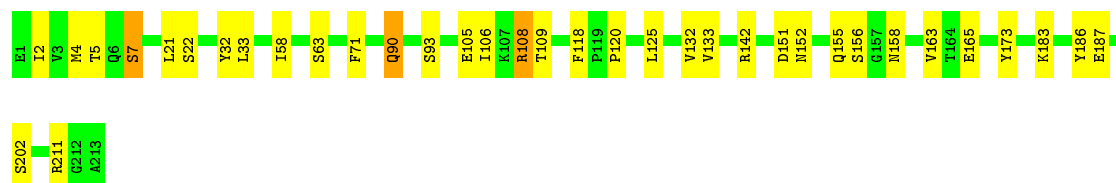
- Molecule 1: IMC-11F8 Fab Light chain

Chain D: 




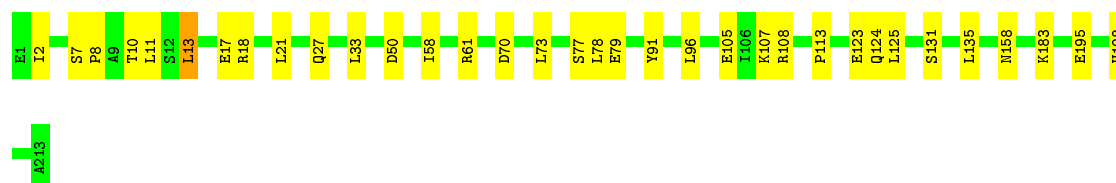
- Molecule 1: IMC-11F8 Fab Light chain

Chain G: 




- Molecule 1: IMC-11F8 Fab Light chain

Chain K: 




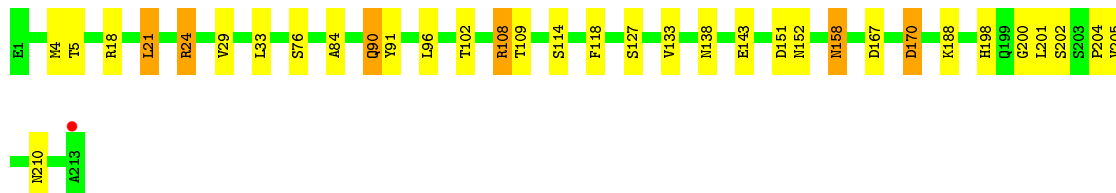
- Molecule 1: IMC-11F8 Fab Light chain

Chain O:  91% 8%




- Molecule 1: IMC-11F8 Fab Light chain

Chain R:  84% 13%




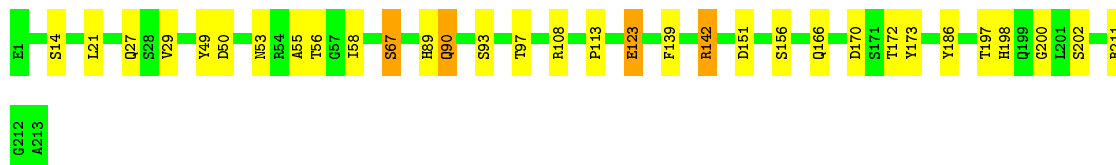
- Molecule 1: IMC-11F8 Fab Light chain

Chain U:  88% 10%




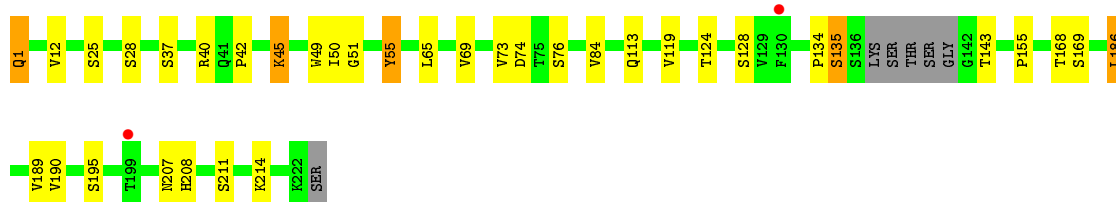
- Molecule 1: IMC-11F8 Fab Light chain

Chain X:  85% 13%



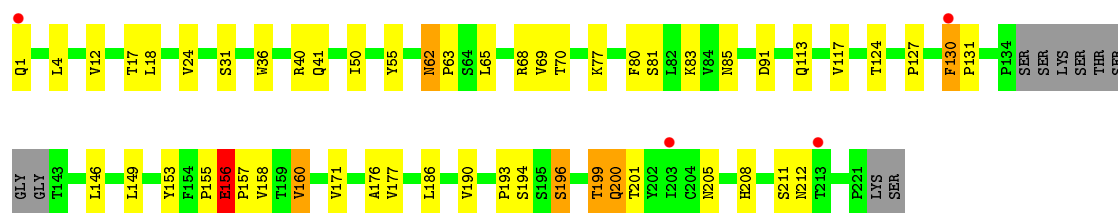
- Molecule 2: IMC-11F8 Fab Heavy chain

Chain H:  81% 14%

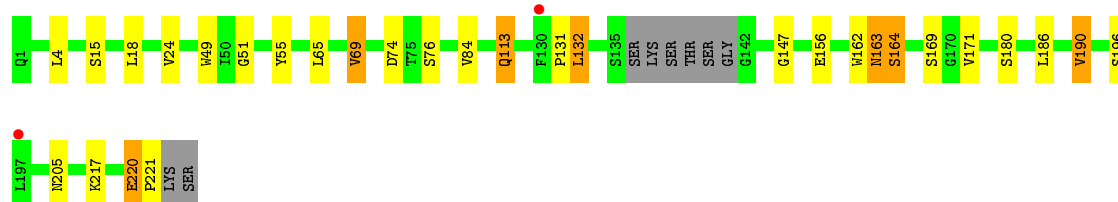
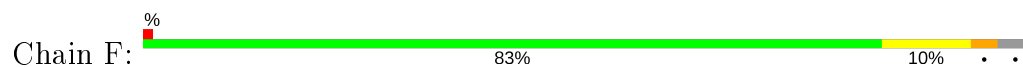


- Molecule 2: IMC-11F8 Fab Heavy chain

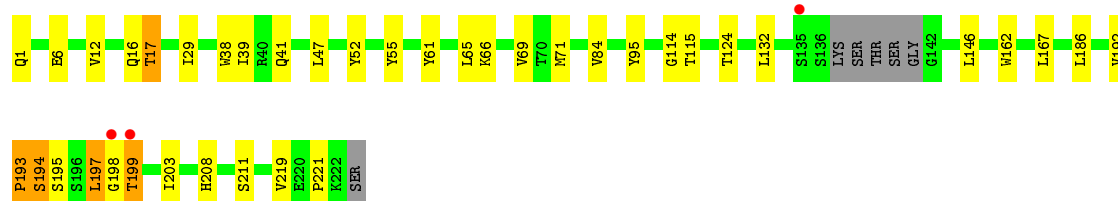
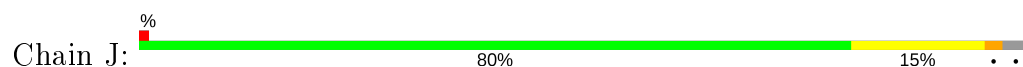
Chain C:  72% 21%



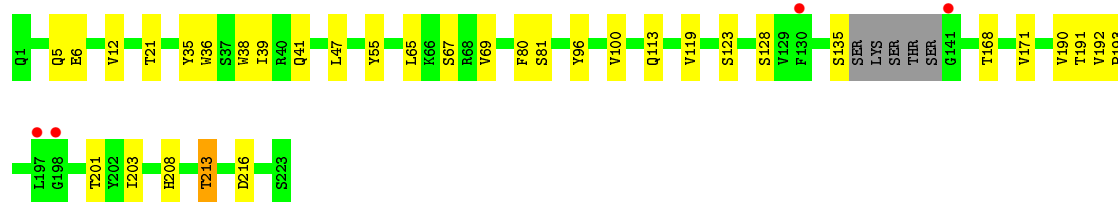
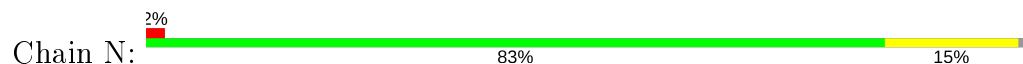
• Molecule 2: IMC-11F8 Fab Heavy chain



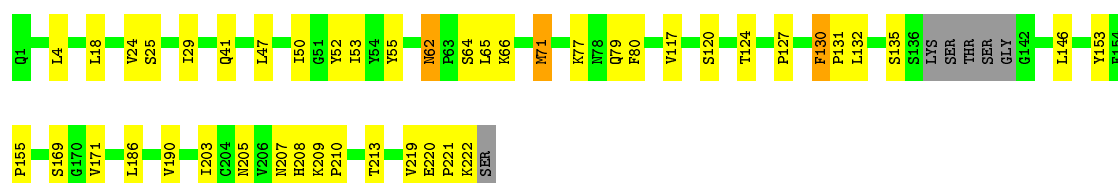
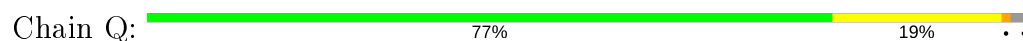
• Molecule 2: IMC-11F8 Fab Heavy chain



• Molecule 2: IMC-11F8 Fab Heavy chain

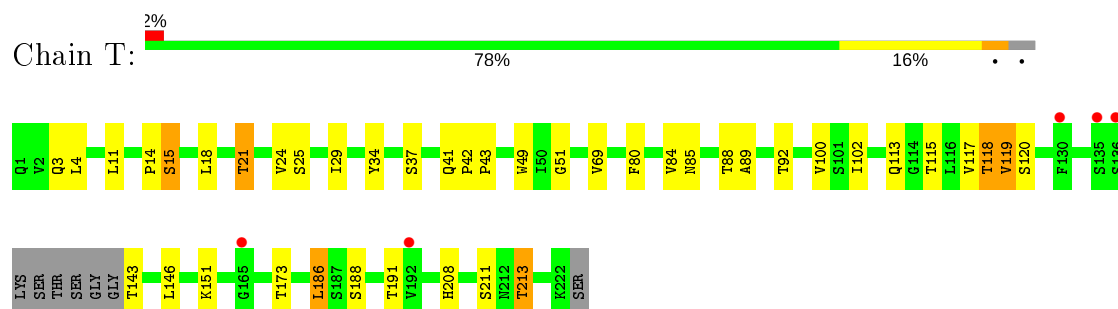


• Molecule 2: IMC-11F8 Fab Heavy chain

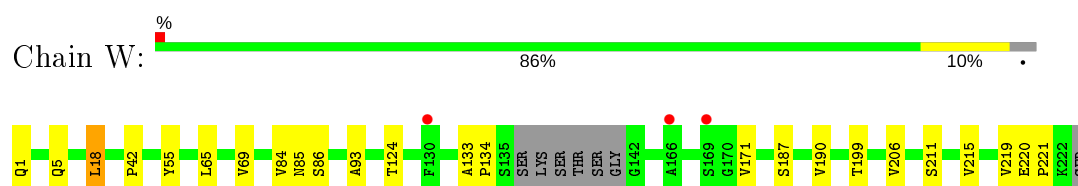




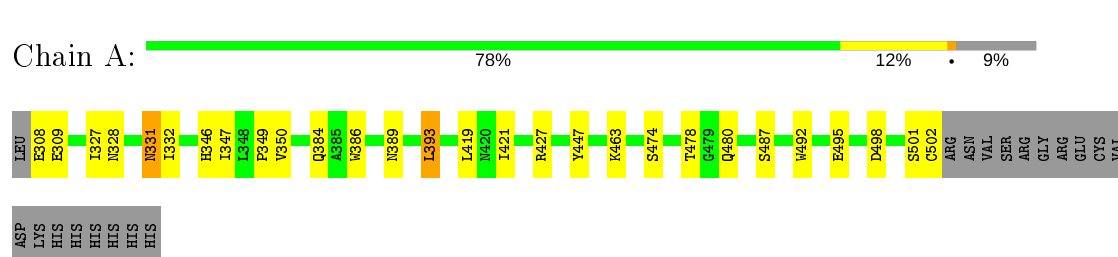
- Molecule 2: IMC-11F8 Fab Heavy chain



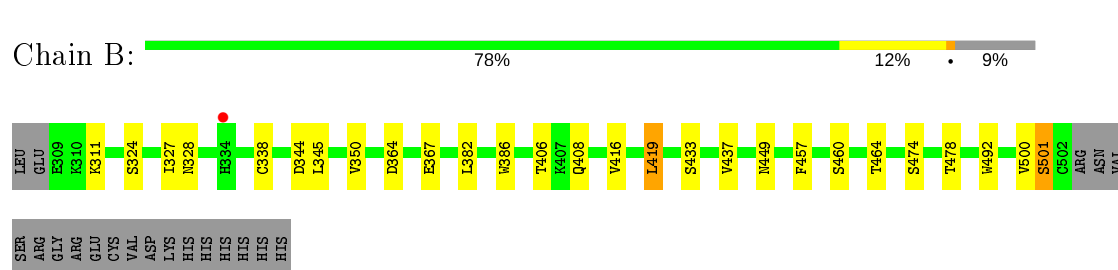
- Molecule 2: IMC-11F8 Fab Heavy chain



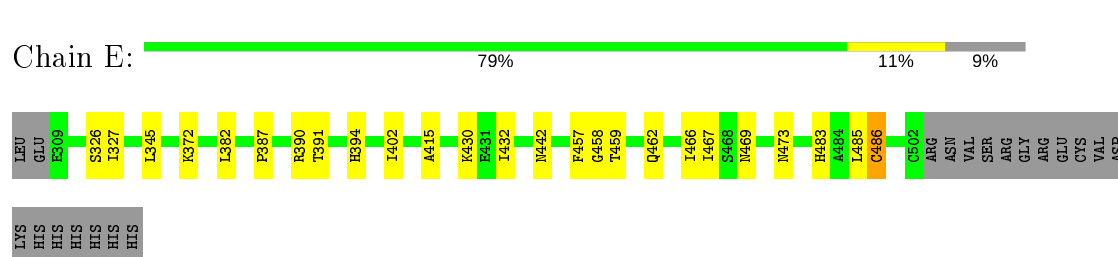
- Molecule 3: Epidermal growth factor receptor



- Molecule 3: Epidermal growth factor receptor

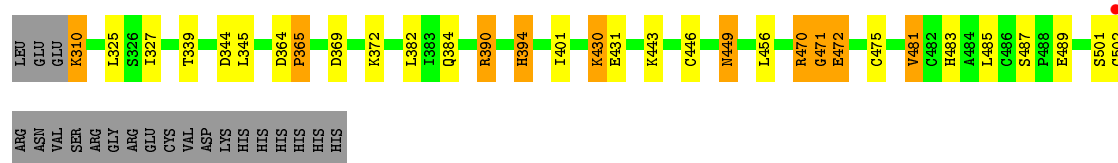


- Molecule 3: Epidermal growth factor receptor



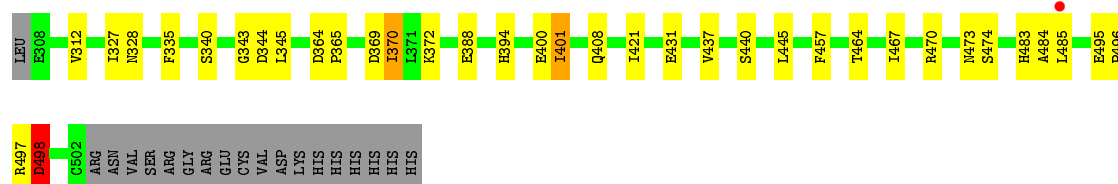
- Molecule 3: Epidermal growth factor receptor





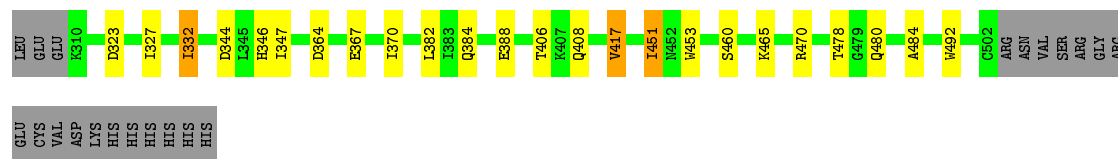
- Molecule 3: Epidermal growth factor receptor

Chain M: 74% 15% 9%



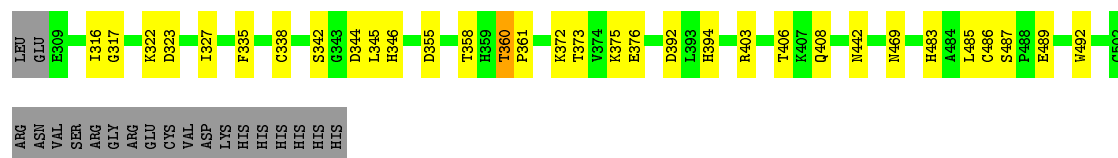
- Molecule 3: Epidermal growth factor receptor

Chain P: 79% 10% 10%



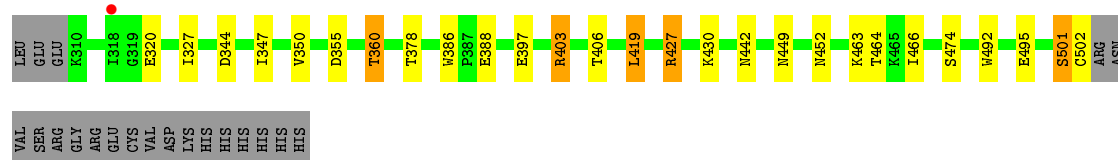
- Molecule 3: Epidermal growth factor receptor

Chain S: 76% 14% 9%



- Molecule 3: Epidermal growth factor receptor

Chain V: 78% 10% 10%



- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 100%



- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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

Chain l:  100%

MAG1  
MAG2

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

Chain n:  100%

MAG1  
MAG2

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

Chain p:  100%

MAG1  
MAG2

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

MAG1  
MAG2  
EMAG

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%

MAG1  
MAG2  
EMAG

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%

MAG1  
MAG2  
EMAG

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  100%

MAG1  
MAG2  
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  100%


MAG1  
MAG2  
BMA3

- Molecule 6: 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

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  100%

MAG1  
MAG2  
BMA3

- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.37Å 139.12Å 175.32Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	43.07 – 2.58 43.05 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.07-2.58) 98.9 (43.05-2.58)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.227 , 0.291 0.241 , 0.301	Depositor DCC
$R_{free}$ test set	11664 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 8.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.345 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	39035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% 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: SO4, BMA, NAG, MAN

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	D	0.56	0/1641	0.62	0/2235
1	G	0.58	0/1637	0.66	0/2228
1	K	0.56	0/1634	0.65	1/2226 (0.0%)
1	L	0.58	0/1650	0.69	0/2244
1	O	0.56	0/1642	0.67	0/2235
1	R	0.60	0/1646	0.66	0/2240
1	U	0.55	0/1654	0.64	0/2247
1	X	0.58	0/1648	0.69	1/2241 (0.0%)
2	C	0.57	0/1605	0.69	0/2205
2	F	0.59	0/1621	0.69	3/2225 (0.1%)
2	H	0.57	0/1645	0.68	1/2255 (0.0%)
2	J	0.57	0/1633	0.68	1/2239 (0.0%)
2	N	0.56	0/1645	0.66	0/2257
2	Q	0.57	0/1636	0.67	0/2244
2	T	0.55	0/1628	0.69	2/2234 (0.1%)
2	W	0.60	0/1637	0.67	1/2245 (0.0%)
3	A	0.53	0/1480	0.65	0/2011
3	B	0.55	0/1452	0.68	0/1979
3	E	0.56	0/1469	0.66	0/1997
3	I	0.57	0/1482	0.70	0/2011
3	M	0.52	0/1472	0.67	0/2003
3	P	0.58	0/1469	0.67	0/1997
3	S	0.52	0/1454	0.64	0/1978
3	V	0.53	0/1449	0.64	0/1972
All	All	0.56	0/37929	0.67	10/51748 (0.0%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	18	LEU	CA-CB-CG	6.22	129.60	115.30
1	X	21	LEU	CA-CB-CG	6.14	129.42	115.30
2	F	186	LEU	CA-CB-CG	5.96	129.00	115.30
2	H	186	LEU	CA-CB-CG	5.81	128.67	115.30
2	T	186	LEU	CA-CB-CG	5.73	128.48	115.30
2	J	186	LEU	CA-CB-CG	5.68	128.36	115.30
2	T	146	LEU	CA-CB-CG	5.57	128.11	115.30
1	K	135	LEU	CA-CB-CG	5.26	127.39	115.30
2	F	132	LEU	CA-CB-CG	5.20	127.26	115.30
2	F	156	GLU	N-CA-C	5.06	124.67	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	51	ALA	Peptide

## 5.2 Too-close contacts ⓘ

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	D	1605	0	1535	20	0
1	G	1601	0	1535	20	0
1	K	1598	0	1519	12	0
1	L	1614	0	1552	22	0
1	O	1606	0	1537	11	0
1	R	1610	0	1541	28	0
1	U	1618	0	1570	15	0
1	X	1612	0	1552	18	0
2	C	1563	0	1485	34	0
2	F	1579	0	1504	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1603	0	1541	20	0
2	J	1591	0	1525	19	0
2	N	1603	0	1528	11	0
2	Q	1594	0	1521	27	0
2	T	1586	0	1516	20	0
2	W	1595	0	1530	8	0
3	A	1452	0	1387	20	0
3	B	1424	0	1344	17	0
3	E	1441	0	1376	26	0
3	I	1454	0	1409	21	0
3	M	1444	0	1372	22	0
3	P	1441	0	1383	19	0
3	S	1427	0	1347	21	0
3	V	1422	0	1356	13	0
4	Y	50	0	43	0	0
4	c	50	0	43	0	0
4	e	50	0	43	0	0
5	Z	28	0	25	0	0
5	b	28	0	25	0	0
5	d	28	0	25	0	0
5	g	28	0	25	0	0
5	l	28	0	25	0	0
5	n	28	0	25	0	0
5	p	28	0	25	0	0
6	a	39	0	34	0	0
6	f	39	0	34	0	0
6	i	39	0	34	0	0
6	j	39	0	34	0	0
6	k	39	0	34	0	0
6	m	39	0	34	0	0
6	o	39	0	34	0	0
7	h	61	0	52	0	0
8	A	28	0	26	1	0
8	B	28	0	26	0	0
8	E	28	0	26	0	0
8	I	14	0	13	0	0
8	M	14	0	13	0	0
8	P	28	0	26	0	0
8	S	28	0	26	0	0
8	V	28	0	26	0	0
9	A	5	0	0	1	0
9	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	5	0	0	0	0
9	K	5	0	0	0	0
9	O	5	0	0	0	0
9	U	5	0	0	0	0
9	V	5	0	0	1	0
9	X	5	0	0	0	0
10	A	30	0	0	3	0
10	B	22	0	0	2	0
10	C	45	0	0	3	0
10	D	55	0	0	1	0
10	E	30	0	0	1	0
10	F	40	0	0	3	0
10	G	50	0	0	0	0
10	H	47	0	0	0	0
10	I	41	0	0	3	0
10	J	44	0	0	2	0
10	K	63	0	0	0	0
10	L	56	0	0	1	0
10	M	35	0	0	2	0
10	N	40	0	0	0	0
10	O	57	0	0	0	0
10	P	41	0	0	3	0
10	Q	51	0	0	3	0
10	R	62	0	0	2	0
10	S	23	0	0	2	0
10	T	41	0	0	1	0
10	U	42	0	0	1	0
10	V	24	0	0	1	0
10	W	50	0	0	1	0
10	X	47	0	0	2	0
All	All	39035	0	36241	448	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 6.

All (448) 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:F:113:GLN:HG3	10:F:248:HOH:O	1.36	1.21
1:R:24:ARG:HG2	1:R:24:ARG:HH11	1.09	1.11
3:E:327:ILE:HD11	3:E:345:LEU:HD22	1.35	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:GLN:HE21	2:H:1:GLN:HA	1.14	1.07
1:X:142:ARG:HH11	1:X:142:ARG:HG2	1.18	1.06
1:U:48:ILE:HG13	10:U:249:HOH:O	1.56	1.06
2:H:69:VAL:HG12	2:H:84:VAL:HG22	1.46	0.94
3:M:497:ARG:H	3:M:498:ASP:HB2	1.32	0.92
2:W:220:GLU:HG3	2:W:221:PRO:HD2	1.51	0.92
3:M:497:ARG:N	3:M:498:ASP:HB2	1.85	0.92
3:M:437:VAL:HB	3:M:464:THR:HG22	1.53	0.91
3:M:327:ILE:HD11	3:M:345:LEU:HD22	1.56	0.87
2:H:1:GLN:NE2	2:H:1:GLN:HA	1.86	0.87
1:G:32:TYR:CD2	3:E:467:ILE:HD11	2.10	0.87
3:I:327:ILE:HD11	3:I:345:LEU:HD22	1.58	0.86
2:C:130:PHE:HB2	2:C:131:PRO:HD2	1.56	0.85
3:E:442:ASN:HD22	3:E:469:ASN:HD21	1.26	0.83
1:R:133:VAL:HG11	2:Q:132:LEU:HD22	1.61	0.83
1:R:24:ARG:NH1	1:R:24:ARG:HG2	1.89	0.82
2:N:203:ILE:HD11	2:N:216:ASP:HB3	1.61	0.81
1:X:198:HIS:HD2	1:X:200:GLY:H	1.26	0.81
1:U:38:GLN:HE22	2:T:41:GLN:HE22	1.27	0.81
3:A:327:ILE:HD11	3:A:332:ILE:HD12	1.63	0.81
1:G:2:ILE:HG22	1:G:4:MET:CE	2.09	0.81
2:C:156:GLU:HG2	2:C:156:GLU:O	1.79	0.80
1:L:51:ALA:HB3	1:L:52:SER:HB2	1.63	0.80
2:J:61:TYR:HE2	2:J:71:MET:HE2	1.45	0.80
1:X:142:ARG:CG	1:X:142:ARG:HH11	1.93	0.79
2:J:69:VAL:HG12	2:J:84:VAL:HG22	1.67	0.77
2:C:1:GLN:HA	10:C:263:HOH:O	1.83	0.77
1:R:198:HIS:HD2	1:R:200:GLY:H	1.32	0.77
3:B:364:ASP:HB3	3:B:367:GLU:OE1	1.84	0.76
2:T:69:VAL:HG22	2:T:84:VAL:HG22	1.66	0.76
1:R:21:LEU:HD23	1:R:102:THR:HG21	1.69	0.74
2:C:4:LEU:HD23	2:C:24:VAL:HG22	1.68	0.73
1:R:29:VAL:HG11	1:R:90:GLN:HG3	1.71	0.72
1:X:198:HIS:CD2	1:X:200:GLY:H	2.07	0.72
1:D:37:GLN:HB2	1:D:47:LEU:HD11	1.71	0.71
1:R:158:ASN:H	1:R:158:ASN:HD22	1.40	0.70
3:E:473:ASN:HB3	10:E:4229:HOH:O	1.92	0.69
2:C:130:PHE:HE2	2:C:149:LEU:HD23	1.54	0.69
1:O:198:HIS:HD2	1:O:200:GLY:H	1.38	0.69
1:L:198:HIS:HD2	1:L:200:GLY:H	1.41	0.69
2:Q:127:PRO:HB3	2:Q:153:TYR:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:327:ILE:HD11	3:E:345:LEU:CD2	2.19	0.68
3:P:470:ARG:HH22	3:P:478:THR:HG21	1.58	0.68
3:P:384:GLN:HB3	3:P:417:VAL:HG13	1.75	0.68
3:I:470:ARG:HD3	3:I:475:CYS:SG	2.34	0.67
3:M:497:ARG:CA	3:M:498:ASP:HB2	2.24	0.67
3:A:474:SER:HB3	9:A:1:SO4:O1	1.94	0.67
3:A:328:ASN:H	3:A:331:ASN:HD21	1.40	0.67
1:R:198:HIS:CD2	1:R:200:GLY:H	2.12	0.67
1:G:155:GLN:HE21	1:G:158:ASN:HD21	1.43	0.66
3:A:327:ILE:HD11	3:A:332:ILE:CD1	2.25	0.66
2:C:193:PRO:HB2	2:C:196:SER:HB2	1.76	0.66
2:J:17:THR:HG22	10:J:253:HOH:O	1.96	0.66
1:G:32:TYR:CG	3:E:467:ILE:HD11	2.31	0.66
3:V:419:LEU:H	3:V:442:ASN:ND2	1.94	0.65
1:R:118:PHE:HB2	1:R:133:VAL:CG1	2.26	0.65
2:F:69:VAL:HG12	2:F:84:VAL:HG22	1.78	0.65
3:S:360:THR:HB	10:S:4216:HOH:O	1.97	0.65
2:J:192:VAL:HB	2:J:193:PRO:HD2	1.76	0.65
2:T:173:THR:HG22	2:T:188:SER:OG	1.96	0.65
3:E:442:ASN:HB2	3:E:469:ASN:HD22	1.62	0.65
1:K:21:LEU:HD12	1:K:73:LEU:HD23	1.79	0.64
1:K:124:GLN:HE22	1:K:131:SER:HB2	1.62	0.64
2:Q:124:THR:HG22	2:Q:155:PRO:HD3	1.80	0.64
1:U:198:HIS:HD2	1:U:200:GLY:H	1.44	0.64
1:R:108:ARG:HD3	1:R:109:THR:O	1.96	0.64
1:X:142:ARG:NH1	1:X:142:ARG:HG2	1.97	0.64
2:H:207:ASN:HD21	2:H:214:LYS:HE2	1.62	0.64
3:P:344:ASP:OD1	3:P:406:THR:HG23	1.98	0.64
2:N:192:VAL:HB	2:N:193:PRO:HD2	1.79	0.63
1:D:158:ASN:H	1:D:158:ASN:HD22	1.47	0.63
1:D:90:GLN:HE22	1:D:93:SER:H	1.47	0.63
1:O:90:GLN:HE22	1:O:93:SER:H	1.47	0.62
2:T:211:SER:OG	2:T:213:THR:HG22	1.98	0.62
2:F:74:ASP:OD1	2:F:76:SER:HB3	1.98	0.62
3:S:338:CYS:O	3:S:373:THR:HG23	1.98	0.62
2:W:69:VAL:HG22	2:W:84:VAL:HG22	1.81	0.62
3:B:437:VAL:HB	3:B:464:THR:HG22	1.82	0.62
3:E:459:THR:H	3:E:462:GLN:HE21	1.45	0.62
2:H:42:PRO:HB2	2:H:45:LYS:HD3	1.82	0.61
1:D:6:GLN:HE21	1:D:99:GLY:HA3	1.65	0.61
3:I:483:HIS:HD2	3:I:485:LEU:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:158:ASN:HD22	1:O:158:ASN:H	1.49	0.60
3:B:386:TRP:CB	3:B:419:LEU:HG	2.32	0.60
2:H:55:TYR:OH	3:A:384:GLN:NE2	2.35	0.60
2:T:88:THR:O	2:T:119:VAL:HG21	2.01	0.60
3:I:471:GLY:O	10:I:4213:HOH:O	2.16	0.60
2:C:156:GLU:CG	2:C:156:GLU:O	2.50	0.60
1:G:33:LEU:HD22	1:G:71:PHE:CG	2.36	0.60
3:S:317:GLY:O	3:S:322:LYS:HA	2.02	0.60
2:N:208:HIS:HB3	2:N:213:THR:HG23	1.84	0.59
2:Q:62:ASN:HD22	2:Q:64:SER:H	1.50	0.59
3:I:310:LYS:N	3:I:339:THR:HG1	1.99	0.59
3:I:401:ILE:HG23	3:I:431:GLU:HB3	1.84	0.59
2:H:134:PRO:O	2:H:135:SER:HB2	2.03	0.59
1:L:198:HIS:CD2	1:L:200:GLY:H	2.19	0.59
2:T:88:THR:C	2:T:119:VAL:HG21	2.22	0.59
3:V:360:THR:HB	10:V:4217:HOH:O	2.02	0.59
2:W:5:GLN:HG3	10:W:259:HOH:O	2.02	0.59
2:Q:203:ILE:HD11	10:Q:262:HOH:O	2.01	0.59
3:P:451:ILE:HD11	3:P:453:TRP:CD2	2.38	0.58
3:E:483:HIS:HD2	3:E:485:LEU:H	1.50	0.58
3:M:457:PHE:HZ	3:M:464:THR:HG23	1.68	0.58
2:C:199:THR:HG22	2:C:200:GLN:H	1.67	0.58
3:M:484:ALA:O	3:M:485:LEU:HB2	2.03	0.58
3:P:470:ARG:NH2	3:P:478:THR:HG21	2.19	0.58
2:C:130:PHE:HB2	2:C:131:PRO:CD	2.29	0.58
3:V:378:THR:HA	3:V:403:ARG:HB2	1.85	0.58
3:E:442:ASN:HD22	3:E:469:ASN:ND2	1.97	0.58
3:I:446:CYS:SG	3:I:470:ARG:HD3	2.44	0.58
1:U:198:HIS:CD2	1:U:200:GLY:H	2.21	0.58
3:B:386:TRP:HB2	3:B:419:LEU:HG	1.86	0.57
3:B:492:TRP:HA	10:B:4218:HOH:O	2.04	0.57
3:E:459:THR:H	3:E:462:GLN:NE2	2.02	0.57
2:H:189:VAL:HG12	2:H:190:VAL:N	2.19	0.57
1:D:155:GLN:HB3	1:D:158:ASN:HD21	1.70	0.57
3:S:376:GLU:OE1	3:S:403:ARG:NH1	2.38	0.57
3:V:474:SER:HB2	9:V:1:SO4:O4	2.04	0.57
3:A:386:TRP:CE2	3:A:393:LEU:HD12	2.40	0.57
3:E:387:PRO:HG2	3:E:390:ARG:HD2	1.87	0.57
1:G:2:ILE:HG22	1:G:4:MET:HE1	1.86	0.57
2:F:163:ASN:O	2:F:164:SER:HB2	2.04	0.56
3:M:401:ILE:HG23	3:M:431:GLU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:24:ARG:CG	1:R:24:ARG:HH11	1.98	0.56
2:T:89:ALA:HA	2:T:119:VAL:CG2	2.35	0.56
1:G:105:GLU:HG2	1:G:106:ILE:N	2.20	0.56
3:V:355:ASP:HB3	3:V:360:THR:HG23	1.88	0.56
1:R:138:ASN:ND2	1:R:170:ASP:OD1	2.39	0.56
2:F:171:VAL:HG22	2:F:190:VAL:CG1	2.36	0.56
2:J:52:TYR:C	2:J:71:MET:HE3	2.27	0.55
3:S:355:ASP:HB3	3:S:360:THR:HG23	1.87	0.55
2:T:18:LEU:HD11	2:T:117:VAL:HG11	1.89	0.55
2:C:65:LEU:HD13	2:C:69:VAL:HG21	1.89	0.55
2:Q:77:LYS:O	2:Q:79:GLN:HG3	2.06	0.55
2:Q:52:TYR:C	2:Q:71:MET:CE	2.76	0.55
3:I:471:GLY:O	3:I:472:GLU:CB	2.55	0.54
1:L:167:ASP:HB3	1:L:170:ASP:OD1	2.08	0.54
2:Q:41:GLN:HG2	10:Q:263:HOH:O	2.06	0.54
2:W:220:GLU:HG3	2:W:221:PRO:CD	2.32	0.54
1:D:55:ALA:HB3	1:D:58:ILE:HD13	1.90	0.54
1:G:2:ILE:HG22	1:G:4:MET:HE3	1.89	0.54
2:Q:52:TYR:C	2:Q:71:MET:HE1	2.28	0.54
3:I:369:ASP:OD2	3:I:390:ARG:NH2	2.41	0.54
1:L:161:GLU:HG3	10:L:225:HOH:O	2.07	0.54
3:B:327:ILE:HD11	3:B:345:LEU:HD22	1.90	0.53
3:P:327:ILE:HG12	3:P:347:ILE:HG12	1.91	0.53
3:M:369:ASP:O	3:M:372:LYS:HG3	2.08	0.53
2:C:62:ASN:HD22	2:C:63:PRO:CD	2.20	0.53
1:G:183:LYS:O	1:G:187:GLU:HG2	2.09	0.53
3:B:457:PHE:HZ	3:B:464:THR:HG23	1.73	0.53
3:A:328:ASN:H	3:A:331:ASN:ND2	2.06	0.52
3:B:500:VAL:O	3:B:501:SER:CB	2.57	0.52
1:R:143:GLU:HG2	1:X:197:THR:HG21	1.90	0.52
2:W:206:VAL:HB	2:W:215:VAL:HG13	1.91	0.52
2:C:199:THR:O	2:C:200:GLN:C	2.47	0.52
3:E:466:ILE:O	3:E:467:ILE:HD13	2.10	0.52
2:H:12:VAL:O	2:H:119:VAL:HA	2.09	0.52
2:C:18:LEU:HD12	2:C:117:VAL:HG11	1.91	0.52
2:J:208:HIS:ND1	2:J:211:SER:HB3	2.25	0.52
1:R:158:ASN:H	1:R:158:ASN:ND2	2.08	0.52
3:S:327:ILE:HD11	3:S:345:LEU:HD22	1.90	0.52
2:C:208:HIS:ND1	2:C:211:SER:HB3	2.24	0.52
2:C:62:ASN:HD22	2:C:63:PRO:HD2	1.72	0.52
3:M:328:ASN:HB2	10:M:4228:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:478:THR:HG23	3:P:480:GLN:HE21	1.74	0.52
3:P:451:ILE:HD11	3:P:453:TRP:CE3	2.45	0.52
2:C:62:ASN:HD22	2:C:63:PRO:N	2.08	0.51
3:A:327:ILE:HG22	3:A:346:HIS:O	2.10	0.51
1:X:49:TYR:O	1:X:53:ASN:HB2	2.10	0.51
1:G:32:TYR:CE2	3:E:467:ILE:HD11	2.46	0.51
2:H:207:ASN:ND2	2:H:214:LYS:HE2	2.26	0.51
3:B:344:ASP:OD1	3:B:406:THR:HG23	2.10	0.51
1:R:29:VAL:HG11	1:R:90:GLN:CG	2.40	0.51
2:J:61:TYR:CE2	2:J:71:MET:HE2	2.35	0.51
1:X:142:ARG:HB3	10:X:246:HOH:O	2.10	0.51
2:J:38:TRP:O	2:J:39:ILE:HG13	2.10	0.51
3:M:440:SER:HA	3:M:467:ILE:O	2.11	0.51
2:J:12:VAL:HG13	2:J:16:GLN:HE21	1.75	0.51
2:J:38:TRP:C	2:J:39:ILE:HG13	2.31	0.51
2:F:4:LEU:HD22	2:F:24:VAL:HG22	1.92	0.51
1:R:118:PHE:HB2	1:R:133:VAL:HG13	1.93	0.51
2:T:34:TYR:HA	2:T:100:VAL:O	2.11	0.51
2:T:89:ALA:HA	2:T:119:VAL:HG22	1.92	0.50
3:S:483:HIS:HD2	3:S:485:LEU:H	1.58	0.50
2:T:18:LEU:CD1	2:T:117:VAL:HG11	2.41	0.50
2:F:18:LEU:C	2:F:18:LEU:HD23	2.32	0.50
2:J:197:LEU:O	2:J:199:THR:N	2.41	0.50
1:X:166:GLN:HG3	1:X:173:TYR:CZ	2.46	0.50
2:F:131:PRO:HD3	2:F:217:LYS:HE2	1.94	0.50
2:H:1:GLN:NE2	2:H:1:GLN:CA	2.68	0.50
1:U:201:LEU:O	1:U:202:SER:HB2	2.10	0.50
1:G:108:ARG:NH1	1:G:109:THR:O	2.39	0.50
3:E:442:ASN:ND2	3:E:469:ASN:HD21	2.03	0.50
2:Q:208:HIS:HB3	2:Q:213:THR:HB	1.93	0.50
1:D:38:GLN:HE22	2:C:41:GLN:HE22	1.59	0.49
1:R:118:PHE:HB2	1:R:133:VAL:HG12	1.94	0.49
3:S:358:THR:OG1	3:S:360:THR:HG22	2.12	0.49
1:D:141:PRO:O	1:D:198:HIS:HE1	1.95	0.49
1:D:33:LEU:HD22	1:D:71:PHE:CG	2.47	0.49
2:F:147:GLY:HA2	2:F:162:TRP:CH2	2.47	0.49
2:T:92:THR:HG23	2:T:118:THR:HA	1.93	0.49
2:Q:130:PHE:HB2	2:Q:131:PRO:CD	2.42	0.49
3:A:327:ILE:CG2	3:A:347:ILE:HG12	2.43	0.49
1:K:13:LEU:HD13	1:K:78:LEU:HD11	1.94	0.49
1:U:47:LEU:HB2	1:U:48:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:89:HIS:HD2	1:X:97:THR:O	1.95	0.49
2:J:193:PRO:O	2:J:194:SER:CB	2.59	0.49
3:S:442:ASN:HD22	3:S:469:ASN:HD21	1.61	0.49
2:N:6:GLU:OE1	2:N:96:TYR:HA	2.13	0.49
3:B:386:TRP:HB3	3:B:419:LEU:HG	1.95	0.49
1:D:63:SER:HB3	10:D:251:HOH:O	2.12	0.49
3:E:483:HIS:O	3:E:486:CYS:HB2	2.13	0.48
2:N:38:TRP:C	2:N:39:ILE:HG13	2.33	0.48
2:Q:171:VAL:HG22	2:Q:190:VAL:HG22	1.95	0.48
2:Q:52:TYR:O	2:Q:71:MET:HE1	2.13	0.48
3:B:500:VAL:O	3:B:501:SER:HB2	2.13	0.48
3:E:458:GLY:H	3:E:462:GLN:HE22	1.60	0.48
2:N:12:VAL:O	2:N:119:VAL:HA	2.12	0.48
3:S:344:ASP:OD1	3:S:406:THR:HG23	2.12	0.48
2:T:208:HIS:HB3	2:T:213:THR:HG23	1.95	0.48
3:A:427:ARG:HA	3:A:492:TRP:CD1	2.48	0.48
1:L:191:VAL:HG11	1:G:5:THR:HG21	1.96	0.48
1:L:33:LEU:HD13	1:L:71:PHE:CD1	2.49	0.48
1:X:27:GLN:OE1	10:X:254:HOH:O	2.20	0.48
1:K:7:SER:HA	1:K:8:PRO:C	2.34	0.48
1:G:120:PRO:HD3	1:G:132:VAL:HG22	1.95	0.48
3:M:483:HIS:O	3:M:484:ALA:HB3	2.13	0.48
2:C:171:VAL:HG22	2:C:190:VAL:HG22	1.96	0.47
3:I:481:VAL:HG22	10:I:4230:HOH:O	2.13	0.47
1:U:201:LEU:O	1:U:202:SER:CB	2.60	0.47
3:E:442:ASN:HB2	3:E:469:ASN:ND2	2.27	0.47
2:H:124:THR:HG22	2:H:155:PRO:HD3	1.95	0.47
3:M:400:GLU:C	3:M:401:ILE:HG12	2.34	0.47
3:E:442:ASN:H	3:E:469:ASN:ND2	2.12	0.47
2:F:171:VAL:HG22	2:F:190:VAL:HG12	1.96	0.47
2:T:14:PRO:O	2:T:15:SER:HB3	2.13	0.47
3:A:350:VAL:HG13	10:A:4216:HOH:O	2.15	0.47
2:C:124:THR:HG22	2:C:155:PRO:HD3	1.96	0.47
2:C:68:ARG:NH2	2:C:91:ASP:OD2	2.47	0.47
1:L:155:GLN:HB3	1:L:158:ASN:HD21	1.80	0.47
1:R:21:LEU:HD23	1:R:102:THR:CG2	2.40	0.47
2:H:49:TRP:CZ2	2:H:51:GLY:HA2	2.49	0.47
1:L:138:ASN:H	1:L:174:SER:HB3	1.80	0.47
3:P:492:TRP:HA	10:P:4232:HOH:O	2.15	0.47
3:P:384:GLN:NE2	10:P:4223:HOH:O	2.48	0.47
3:B:328:ASN:HB2	10:B:4203:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:167:ASP:OD2	1:R:170:ASP:HB2	2.15	0.47
3:V:419:LEU:HB2	3:V:442:ASN:ND2	2.30	0.47
1:L:135:LEU:HD22	2:H:189:VAL:HG11	1.97	0.46
1:L:50:ASP:O	1:L:52:SER:HB3	2.15	0.46
3:P:364:ASP:HB3	3:P:367:GLU:HG3	1.97	0.46
1:D:140:TYR:CG	1:D:141:PRO:HA	2.51	0.46
2:F:49:TRP:CZ2	2:F:51:GLY:HA2	2.50	0.46
2:Q:62:ASN:ND2	2:Q:64:SER:H	2.14	0.46
2:T:21:THR:HG22	10:T:243:HOH:O	2.14	0.46
2:W:171:VAL:HG22	2:W:190:VAL:HG22	1.96	0.46
3:P:484:ALA:HA	10:P:4234:HOH:O	2.15	0.46
2:Q:71:MET:HB2	2:Q:71:MET:HE2	1.68	0.46
3:E:382:LEU:HD12	3:E:415:ALA:HB3	1.98	0.46
2:T:11:LEU:HD12	2:T:118:THR:O	2.16	0.46
2:W:133:ALA:HA	2:W:134:PRO:HD3	1.76	0.46
1:K:2:ILE:HG12	1:K:27:GLN:HB2	1.96	0.46
1:D:201:LEU:HD13	1:D:205:VAL:HG23	1.98	0.46
2:Q:130:PHE:HB2	2:Q:131:PRO:HD2	1.96	0.46
3:A:308:GLU:HA	3:A:309:GLU:HA	1.74	0.46
2:C:130:PHE:CE2	2:C:149:LEU:HD23	2.44	0.46
1:X:123:GLU:HG2	1:X:123:GLU:H	1.42	0.46
3:M:484:ALA:O	3:M:485:LEU:CB	2.64	0.45
1:G:118:PHE:HB2	1:G:133:VAL:HG13	1.99	0.45
2:Q:209:LYS:CB	2:Q:210:PRO:HD3	2.46	0.45
3:S:335:PHE:HA	3:S:338:CYS:SG	2.55	0.45
1:L:51:ALA:CB	1:L:52:SER:HB2	2.39	0.45
2:T:29:ILE:HD11	2:T:80:PHE:HB3	1.97	0.45
1:U:19:ALA:HB3	1:U:75:ILE:HB	1.98	0.45
3:I:382:LEU:HD11	3:I:384:GLN:HE21	1.80	0.45
1:O:175:LEU:HD23	1:O:176:SER:N	2.31	0.45
1:O:35:TRP:CE2	1:O:73:LEU:HB2	2.51	0.45
3:V:397:GLU:HB2	3:V:427:ARG:HD2	1.98	0.45
3:V:427:ARG:HG3	3:V:427:ARG:H	1.58	0.45
1:X:186:TYR:CE2	1:X:211:ARG:HD3	2.51	0.45
2:C:157:PRO:O	2:C:208:HIS:HD2	2.00	0.45
2:C:4:LEU:CD2	2:C:24:VAL:HG22	2.41	0.45
2:C:77:LYS:HA	10:C:257:HOH:O	2.15	0.45
1:G:186:TYR:CZ	1:G:211:ARG:HG3	2.51	0.45
2:Q:18:LEU:HD12	2:Q:117:VAL:HG11	1.99	0.45
3:I:471:GLY:O	3:I:472:GLU:HB3	2.17	0.45
3:P:382:LEU:HD11	3:P:384:GLN:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:327:ILE:HG21	3:A:347:ILE:HG12	1.99	0.45
3:E:459:THR:N	3:E:462:GLN:HE21	2.15	0.45
3:M:495:GLU:O	3:M:498:ASP:HB3	2.16	0.45
2:Q:41:GLN:HB2	2:Q:47:LEU:HD23	1.99	0.45
2:Q:29:ILE:HD11	2:Q:80:PHE:HD1	1.82	0.45
3:V:386:TRP:HB2	3:V:419:LEU:HG	1.98	0.45
3:V:501:SER:O	3:V:502:CYS:HB2	2.17	0.45
1:G:90:GLN:HE22	1:G:93:SER:H	1.63	0.45
1:O:24:ARG:HH12	1:U:210:ASN:HD21	1.63	0.45
2:Q:53:ILE:N	2:Q:71:MET:HE3	2.32	0.45
2:C:62:ASN:ND2	2:C:63:PRO:HD2	2.32	0.44
3:I:372:LYS:NZ	3:I:394:HIS:CE1	2.84	0.44
1:U:47:LEU:CB	1:U:48:ILE:HD12	2.48	0.44
2:F:147:GLY:HA2	2:F:162:TRP:HH2	1.82	0.44
3:P:478:THR:CG2	3:P:480:GLN:NE2	2.80	0.44
3:S:322:LYS:O	3:S:323:ASP:HB2	2.18	0.44
2:J:197:LEU:HD22	2:J:221:PRO:HG3	2.00	0.44
1:L:151:ASP:O	1:L:152:ASN:HB2	2.17	0.44
3:P:384:GLN:HB3	3:P:417:VAL:CG1	2.47	0.44
3:S:442:ASN:HB2	3:S:469:ASN:HD22	1.82	0.44
1:U:142:ARG:HD3	1:U:142:ARG:O	2.17	0.44
3:A:349:PRO:HD2	10:A:4216:HOH:O	2.18	0.44
2:C:85:ASN:HB2	10:F:250:HOH:O	2.17	0.44
1:D:58:ILE:HA	1:D:59:PRO:HD3	1.88	0.44
1:D:90:GLN:NE2	1:D:92:GLY:H	2.15	0.44
3:I:483:HIS:CD2	3:I:485:LEU:H	2.33	0.44
2:J:95:TYR:O	2:J:114:GLY:HA2	2.18	0.44
1:L:79:GLU:O	1:L:80:PRO:C	2.56	0.44
2:N:41:GLN:HB2	2:N:47:LEU:HD23	2.00	0.44
3:S:316:ILE:HD12	3:S:316:ILE:H	1.81	0.44
2:Q:169:SER:HB3	10:Q:257:HOH:O	2.18	0.44
1:K:113:PRO:HD3	1:K:198:HIS:CD2	2.53	0.44
1:X:55:ALA:HB3	1:X:58:ILE:HD13	1.99	0.44
2:F:169:SER:HA	10:F:240:HOH:O	2.18	0.44
2:N:171:VAL:HG22	2:N:190:VAL:HG13	2.00	0.44
2:H:208:HIS:ND1	2:H:211:SER:HB3	2.33	0.43
3:S:355:ASP:HB3	3:S:360:THR:CG2	2.47	0.43
2:Q:220:GLU:O	2:Q:222:LYS:N	2.50	0.43
3:V:427:ARG:HA	3:V:492:TRP:CD1	2.52	0.43
3:A:487:SER:OG	3:A:501:SER:HB2	2.18	0.43
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:197:LEU:C	2:J:199:THR:H	2.22	0.43
1:U:187:GLU:HA	1:U:211:ARG:HE	1.82	0.43
2:N:36:TRP:HB3	2:N:80:PHE:CZ	2.54	0.43
3:A:478:THR:OG1	3:A:480:GLN:NE2	2.51	0.43
2:C:36:TRP:HB3	2:C:80:PHE:CZ	2.54	0.43
3:S:360:THR:HA	3:S:361:PRO:HD3	1.75	0.43
1:X:113:PRO:HB3	1:X:139:PHE:HB3	2.00	0.43
3:E:372:LYS:NZ	3:E:394:HIS:CD2	2.87	0.43
2:F:162:TRP:O	2:F:164:SER:N	2.39	0.43
1:O:163:VAL:O	1:O:163:VAL:HG13	2.18	0.43
2:H:189:VAL:CG1	2:H:190:VAL:N	2.82	0.43
3:I:443:LYS:O	3:I:470:ARG:HB3	2.19	0.43
3:S:487:SER:C	3:S:489:GLU:H	2.22	0.43
2:Q:4:LEU:HD22	2:Q:24:VAL:HG22	2.00	0.43
1:U:112:ALA:HB1	1:U:201:LEU:HD13	2.01	0.43
3:B:457:PHE:HZ	3:B:464:THR:CG2	2.32	0.43
1:O:198:HIS:CD2	1:O:200:GLY:H	2.25	0.43
3:P:332:ILE:CD1	3:P:370:ILE:HG12	2.49	0.43
3:V:419:LEU:HB2	3:V:442:ASN:HD22	1.83	0.43
2:F:220:GLU:HB2	2:F:221:PRO:HD2	2.01	0.43
3:M:343:GLY:HA3	10:M:4236:HOH:O	2.19	0.43
2:C:160:VAL:HA	2:C:205:ASN:O	2.19	0.42
1:K:61:ARG:CZ	1:K:79:GLU:HG3	2.49	0.42
1:L:50:ASP:O	1:L:51:ALA:HB3	2.19	0.42
3:M:483:HIS:O	3:M:484:ALA:CB	2.66	0.42
2:Q:52:TYR:C	2:Q:71:MET:HE3	2.39	0.42
1:R:204:PRO:HD3	10:R:261:HOH:O	2.19	0.42
3:S:492:TRP:HA	10:S:4222:HOH:O	2.18	0.42
3:B:478:THR:HG22	3:B:478:THR:O	2.18	0.42
1:D:145:LYS:HB3	1:D:197:THR:HB	2.01	0.42
1:D:91:TYR:HA	1:D:96:LEU:HD22	2.00	0.42
1:G:7:SER:O	1:G:22:SER:HB3	2.19	0.42
2:H:73:VAL:HG12	2:H:74:ASP:N	2.34	0.42
1:L:13:LEU:HD13	1:L:78:LEU:HD11	2.01	0.42
3:M:312:VAL:HG12	3:M:340:SER:HB2	2.01	0.42
1:X:90:GLN:HE22	1:X:93:SER:H	1.67	0.42
1:D:158:ASN:N	1:D:158:ASN:HD22	2.08	0.42
2:J:52:TYR:HB3	10:J:251:HOH:O	2.18	0.42
1:L:83:PHE:O	1:L:84:ALA:HB2	2.19	0.42
3:M:457:PHE:CZ	3:M:464:THR:HG23	2.53	0.42
2:W:42:PRO:HA	2:W:93:ALA:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:327:ILE:CD1	3:E:345:LEU:HD22	2.26	0.42
3:I:364:ASP:HA	3:I:365:PRO:HD2	1.83	0.42
1:L:137:ASN:HA	1:L:174:SER:HB3	2.00	0.42
3:S:483:HIS:CD2	3:S:485:LEU:H	2.35	0.42
1:L:7:SER:HA	1:L:8:PRO:C	2.40	0.42
3:E:402:ILE:O	3:E:432:ILE:HA	2.20	0.42
3:P:478:THR:CG2	3:P:480:GLN:HE21	2.33	0.42
2:T:4:LEU:HD22	2:T:24:VAL:HG22	2.02	0.42
1:U:33:LEU:HD13	1:U:71:PHE:CD1	2.55	0.42
1:X:170:ASP:HB3	1:X:172:THR:HG23	2.02	0.42
1:R:24:ARG:NH1	1:R:24:ARG:CG	2.68	0.42
2:C:18:LEU:O	2:C:83:LYS:HA	2.20	0.42
1:L:129:THR:HG22	1:L:130:ALA:N	2.35	0.42
1:O:158:ASN:HD22	1:O:158:ASN:N	2.11	0.42
3:I:487:SER:OG	3:I:489:GLU:HB2	2.20	0.42
1:R:4:MET:HE1	1:R:33:LEU:HD12	2.02	0.42
3:V:464:THR:HG22	3:V:466:ILE:HG13	2.01	0.42
3:A:389:ASN:HD22	8:A:3891:NAG:H83	1.85	0.41
3:A:419:LEU:HB2	3:A:421:ILE:HG12	2.01	0.41
2:H:40:ARG:HB3	2:H:50:ILE:HD11	2.02	0.41
3:M:364:ASP:HA	3:M:365:PRO:HD2	1.75	0.41
3:B:382:LEU:HD13	3:B:408:GLN:NE2	2.34	0.41
2:C:40:ARG:HD3	2:C:50:ILE:HD11	2.02	0.41
1:K:91:TYR:HA	1:K:96:LEU:HD22	2.01	0.41
1:O:50:ASP:O	1:O:52:SER:N	2.53	0.41
1:R:210:ASN:ND2	10:R:272:HOH:O	2.52	0.41
1:D:140:TYR:CD1	1:D:141:PRO:HA	2.55	0.41
3:E:467:ILE:HA	3:E:467:ILE:HD13	1.71	0.41
2:H:73:VAL:CG1	2:H:74:ASP:N	2.84	0.41
2:H:74:ASP:OD2	2:H:76:SER:HB2	2.20	0.41
3:I:382:LEU:HD11	3:I:384:GLN:NE2	2.35	0.41
2:N:5:GLN:HG3	2:N:113:GLN:OE1	2.20	0.41
1:R:158:ASN:ND2	1:R:158:ASN:N	2.68	0.41
1:U:125:LEU:HA	1:U:125:LEU:HD23	1.88	0.41
1:D:198:HIS:HD2	1:D:200:GLY:H	1.68	0.41
3:P:465:LYS:HB3	3:P:465:LYS:HE3	1.76	0.41
3:A:427:ARG:HD2	10:A:4222:HOH:O	2.20	0.41
2:C:12:VAL:HG22	10:C:268:HOH:O	2.21	0.41
3:I:430:LYS:HB3	3:I:430:LYS:HE2	1.78	0.41
2:J:41:GLN:HB2	2:J:47:LEU:HD13	2.03	0.41
3:P:478:THR:HG23	3:P:480:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:50:ILE:HG23	2:Q:65:LEU:HD13	2.01	0.41
1:R:201:LEU:HD13	1:R:205:VAL:HG23	2.02	0.41
3:A:495:GLU:HB2	3:A:498:ASP:OD2	2.21	0.41
3:B:311:LYS:HB3	3:B:338:CYS:HA	2.02	0.41
1:K:11:LEU:HD23	1:K:11:LEU:HA	1.92	0.41
1:K:123:GLU:OE2	1:K:123:GLU:N	2.39	0.41
1:K:125:LEU:HD22	1:K:183:LYS:HG3	2.02	0.41
1:K:17:GLU:O	1:K:77:SER:HA	2.20	0.41
1:L:158:ASN:ND2	1:L:158:ASN:H	2.18	0.41
1:O:123:GLU:HG2	1:O:123:GLU:H	1.61	0.41
2:Q:29:ILE:HD11	2:Q:80:PHE:CD1	2.56	0.41
1:R:151:ASP:O	1:R:152:ASN:HB2	2.21	0.41
1:R:91:TYR:HA	1:R:96:LEU:HD22	2.02	0.41
1:R:158:ASN:HD22	1:R:158:ASN:N	2.05	0.41
2:C:208:HIS:ND1	2:C:211:SER:CB	2.84	0.41
2:J:162:TRP:HA	2:J:203:ILE:O	2.21	0.41
1:L:158:ASN:H	1:L:158:ASN:HD22	1.68	0.41
2:C:176:ALA:HB2	2:C:186:LEU:HD12	2.03	0.40
1:G:2:ILE:CG2	1:G:4:MET:HE1	2.49	0.40
2:T:42:PRO:HA	2:T:43:PRO:HD3	1.98	0.40
1:X:29:VAL:CG1	1:X:29:VAL:O	2.68	0.40
3:E:457:PHE:HB3	3:E:462:GLN:NE2	2.37	0.40
2:J:6:GLU:HB2	2:J:115:THR:HG23	2.03	0.40
1:G:151:ASP:O	1:G:152:ASN:HB2	2.22	0.40
1:G:142:ARG:HD3	1:G:173:TYR:CE2	2.56	0.40
3:I:449:ASN:ND2	10:I:4223:HOH:O	2.53	0.40
3:I:430:LYS:HA	3:I:456:LEU:CD1	2.51	0.40
3:M:335:PHE:HB2	3:M:370:ILE:HD11	2.04	0.40
2:N:35:TYR:HB2	2:N:100:VAL:HB	2.02	0.40
1:D:86:TYR:O	1:D:101:GLY:HA2	2.21	0.40
3:M:421:ILE:HD12	3:M:445:LEU:HD13	2.03	0.40
3:S:442:ASN:H	3:S:469:ASN:ND2	2.18	0.40
3:B:416:VAL:HG12	3:B:419:LEU:HD22	2.04	0.40
3:S:316:ILE:HD13	3:S:346:HIS:H	1.86	0.40
2:T:49:TRP:CZ2	2:T:51:GLY:HA2	2.57	0.40

There are no symmetry-related clashes.

## 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	D	211/213 (99%)	204 (97%)	6 (3%)	1 (0%)	29	50
1	G	211/213 (99%)	201 (95%)	10 (5%)	0	100	100
1	K	211/213 (99%)	201 (95%)	10 (5%)	0	100	100
1	L	211/213 (99%)	203 (96%)	5 (2%)	3 (1%)	11	21
1	O	211/213 (99%)	199 (94%)	11 (5%)	1 (0%)	29	50
1	R	211/213 (99%)	205 (97%)	5 (2%)	1 (0%)	29	50
1	U	211/213 (99%)	200 (95%)	10 (5%)	1 (0%)	29	50
1	X	211/213 (99%)	200 (95%)	9 (4%)	2 (1%)	17	34
2	C	209/223 (94%)	199 (95%)	8 (4%)	2 (1%)	15	31
2	F	211/223 (95%)	197 (93%)	11 (5%)	3 (1%)	11	21
2	H	213/223 (96%)	199 (93%)	12 (6%)	2 (1%)	17	34
2	J	213/223 (96%)	198 (93%)	11 (5%)	4 (2%)	8	14
2	N	214/223 (96%)	203 (95%)	11 (5%)	0	100	100
2	Q	213/223 (96%)	198 (93%)	14 (7%)	1 (0%)	29	50
2	T	212/223 (95%)	201 (95%)	10 (5%)	1 (0%)	29	50
2	W	212/223 (95%)	205 (97%)	7 (3%)	0	100	100
3	A	193/214 (90%)	188 (97%)	4 (2%)	1 (0%)	29	50
3	B	192/214 (90%)	184 (96%)	7 (4%)	1 (0%)	29	50
3	E	192/214 (90%)	185 (96%)	7 (4%)	0	100	100
3	I	191/214 (89%)	181 (95%)	8 (4%)	2 (1%)	15	31
3	M	193/214 (90%)	177 (92%)	14 (7%)	2 (1%)	15	31
3	P	191/214 (89%)	178 (93%)	12 (6%)	1 (0%)	29	50
3	S	192/214 (90%)	176 (92%)	16 (8%)	0	100	100
3	V	191/214 (89%)	179 (94%)	12 (6%)	0	100	100
All	All	4920/5200 (95%)	4661 (95%)	230 (5%)	29 (1%)	25	45

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	51	ALA
1	L	52	SER
2	C	200	GLN
3	B	501	SER
2	F	164	SER
2	J	194	SER
3	I	472	GLU
3	M	498	ASP
1	U	202	SER
2	H	195	SER
2	J	197	LEU
3	I	471	GLY
2	Q	221	PRO
1	X	67	SER
2	J	193	PRO
1	X	151	ASP
1	L	84	ALA
2	F	15	SER
1	O	51	ALA
3	P	460	SER
2	H	135	SER
3	A	447	TYR
1	D	30	SER
2	F	163	ASN
2	J	198	GLY
1	R	84	ALA
2	C	156	GLU
3	M	496	PRO
2	T	102	ILE

### 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	D	177/181 (98%)	170 (96%)	7 (4%)	31 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	176/181 (97%)	165 (94%)	11 (6%)	18	35
1	K	176/181 (97%)	164 (93%)	12 (7%)	16	30
1	L	179/181 (99%)	172 (96%)	7 (4%)	32	56
1	O	177/181 (98%)	168 (95%)	9 (5%)	24	44
1	R	178/181 (98%)	165 (93%)	13 (7%)	14	27
1	U	180/181 (99%)	168 (93%)	12 (7%)	16	31
1	X	179/181 (99%)	169 (94%)	10 (6%)	21	40
2	C	174/192 (91%)	156 (90%)	18 (10%)	7	12
2	F	177/192 (92%)	167 (94%)	10 (6%)	21	40
2	H	181/192 (94%)	168 (93%)	13 (7%)	14	27
2	J	178/192 (93%)	165 (93%)	13 (7%)	14	27
2	N	180/192 (94%)	167 (93%)	13 (7%)	14	27
2	Q	178/192 (93%)	165 (93%)	13 (7%)	14	27
2	T	178/192 (93%)	162 (91%)	16 (9%)	9	17
2	W	180/192 (94%)	169 (94%)	11 (6%)	18	36
3	A	158/188 (84%)	154 (98%)	4 (2%)	47	70
3	B	153/188 (81%)	146 (95%)	7 (5%)	27	49
3	E	157/188 (84%)	153 (98%)	4 (2%)	47	70
3	I	161/188 (86%)	149 (92%)	12 (8%)	13	26
3	M	156/188 (83%)	146 (94%)	10 (6%)	17	34
3	P	158/188 (84%)	151 (96%)	7 (4%)	28	51
3	S	153/188 (81%)	145 (95%)	8 (5%)	23	44
3	V	155/188 (82%)	138 (89%)	17 (11%)	6	10
All	All	4099/4488 (91%)	3842 (94%)	257 (6%)	18	35

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	13	LEU
1	L	14	SER
1	L	39	LYS
1	L	50	ASP
1	L	63	SER
1	L	158	ASN

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Mol	Chain	Res	Type
1	L	202	SER
2	H	1	GLN
2	H	25	SER
2	H	28	SER
2	H	37	SER
2	H	45	LYS
2	H	55	TYR
2	H	65	LEU
2	H	113	GLN
2	H	128	SER
2	H	143	THR
2	H	168	THR
2	H	169	SER
2	H	186	LEU
3	A	331	ASN
3	A	393	LEU
3	A	463	LYS
3	A	502	CYS
1	D	23	CYS
1	D	50	ASP
1	D	81	GLU
1	D	90	GLN
1	D	107	LYS
1	D	158	ASN
1	D	195	GLU
2	C	17	THR
2	C	31	SER
2	C	55	TYR
2	C	62	ASN
2	C	70	THR
2	C	81	SER
2	C	113	GLN
2	C	130	PHE
2	C	146	LEU
2	C	156	GLU
2	C	158	VAL
2	C	160	VAL
2	C	177	VAL
2	C	194	SER
2	C	196	SER
2	C	199	THR
2	C	201	THR

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Mol	Chain	Res	Type
2	C	212	ASN
3	B	324	SER
3	B	350	VAL
3	B	419	LEU
3	B	433	SER
3	B	449	ASN
3	B	460	SER
3	B	474	SER
1	G	7	SER
1	G	21	LEU
1	G	58	ILE
1	G	63	SER
1	G	90	GLN
1	G	108	ARG
1	G	125	LEU
1	G	156	SER
1	G	163	VAL
1	G	165	GLU
1	G	202	SER
2	F	55	TYR
2	F	65	LEU
2	F	69	VAL
2	F	113	GLN
2	F	132	LEU
2	F	180	SER
2	F	190	VAL
2	F	196	SER
2	F	205	ASN
2	F	220	GLU
3	E	326	SER
3	E	391	THR
3	E	430	LYS
3	E	486	CYS
1	K	10	THR
1	K	13	LEU
1	K	18	ARG
1	K	33	LEU
1	K	50	ASP
1	K	58	ILE
1	K	70	ASP
1	K	105	GLU
1	K	107	LYS

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Mol	Chain	Res	Type
1	K	108	ARG
1	K	158	ASN
1	K	195	GLU
2	J	1	GLN
2	J	17	THR
2	J	29	ILE
2	J	55	TYR
2	J	65	LEU
2	J	66	LYS
2	J	124	THR
2	J	132	LEU
2	J	146	LEU
2	J	167	LEU
2	J	195	SER
2	J	199	THR
2	J	219	VAL
3	I	310	LYS
3	I	325	LEU
3	I	344	ASP
3	I	365	PRO
3	I	390	ARG
3	I	394	HIS
3	I	430	LYS
3	I	449	ASN
3	I	470	ARG
3	I	481	VAL
3	I	501	SER
3	I	502	CYS
1	O	33	LEU
1	O	73	LEU
1	O	74	THR
1	O	90	GLN
1	O	108	ARG
1	O	123	GLU
1	O	156	SER
1	O	158	ASN
1	O	201	LEU
2	N	21	THR
2	N	55	TYR
2	N	65	LEU
2	N	67	SER
2	N	69	VAL

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Mol	Chain	Res	Type
2	N	81	SER
2	N	123	SER
2	N	128	SER
2	N	135	SER
2	N	168	THR
2	N	191	THR
2	N	201	THR
2	N	213	THR
3	M	344	ASP
3	M	370	ILE
3	M	388	GLU
3	M	394	HIS
3	M	401	ILE
3	M	408	GLN
3	M	470	ARG
3	M	473	ASN
3	M	474	SER
3	M	498	ASP
1	R	5	THR
1	R	18	ARG
1	R	21	LEU
1	R	24	ARG
1	R	76	SER
1	R	90	GLN
1	R	108	ARG
1	R	114	SER
1	R	127	SER
1	R	158	ASN
1	R	170	ASP
1	R	188	LYS
1	R	202	SER
2	Q	25	SER
2	Q	55	TYR
2	Q	62	ASN
2	Q	66	LYS
2	Q	71	MET
2	Q	120	SER
2	Q	130	PHE
2	Q	135	SER
2	Q	146	LEU
2	Q	186	LEU
2	Q	205	ASN

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Mol	Chain	Res	Type
2	Q	207	ASN
2	Q	219	VAL
3	P	323	ASP
3	P	332	ILE
3	P	346	HIS
3	P	388	GLU
3	P	408	GLN
3	P	417	VAL
3	P	451	ILE
1	U	50	ASP
1	U	126	LYS
1	U	129	THR
1	U	136	LEU
1	U	142	ARG
1	U	156	SER
1	U	169	LYS
1	U	197	THR
1	U	199	GLN
1	U	201	LEU
1	U	203	SER
1	U	211	ARG
2	T	3	GLN
2	T	15	SER
2	T	21	THR
2	T	25	SER
2	T	37	SER
2	T	85	ASN
2	T	113	GLN
2	T	115	THR
2	T	118	THR
2	T	119	VAL
2	T	120	SER
2	T	143	THR
2	T	151	LYS
2	T	186	LEU
2	T	191	THR
2	T	213	THR
3	S	342	SER
3	S	360	THR
3	S	372	LYS
3	S	375	LYS
3	S	392	ASP

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Mol	Chain	Res	Type
3	S	394	HIS
3	S	408	GLN
3	S	486	CYS
1	X	14	SER
1	X	50	ASP
1	X	56	THR
1	X	67	SER
1	X	90	GLN
1	X	108	ARG
1	X	123	GLU
1	X	142	ARG
1	X	156	SER
1	X	202	SER
2	W	1	GLN
2	W	18	LEU
2	W	55	TYR
2	W	65	LEU
2	W	85	ASN
2	W	86	SER
2	W	124	THR
2	W	187	SER
2	W	199	THR
2	W	211	SER
2	W	219	VAL
3	V	320	GLU
3	V	327	ILE
3	V	344	ASP
3	V	347	ILE
3	V	350	VAL
3	V	360	THR
3	V	388	GLU
3	V	403	ARG
3	V	406	THR
3	V	419	LEU
3	V	427	ARG
3	V	430	LYS
3	V	449	ASN
3	V	452	ASN
3	V	463	LYS
3	V	495	GLU
3	V	501	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such

sidechains are listed below:

Mol	Chain	Res	Type
1	L	124	GLN
1	L	137	ASN
1	L	155	GLN
1	L	158	ASN
1	L	198	HIS
2	H	1	GLN
2	H	172	HIS
2	H	179	GLN
2	H	207	ASN
3	A	331	ASN
3	A	384	GLN
3	A	452	ASN
3	A	480	GLN
3	A	483	HIS
1	D	6	GLN
1	D	38	GLN
1	D	42	GLN
1	D	90	GLN
1	D	124	GLN
1	D	158	ASN
1	D	198	HIS
2	C	62	ASN
2	C	113	GLN
3	B	314	ASN
3	B	394	HIS
3	B	408	GLN
3	B	480	GLN
1	G	90	GLN
1	G	155	GLN
2	F	5	GLN
2	F	79	GLN
3	E	411	GLN
3	E	452	ASN
3	E	462	GLN
3	E	469	ASN
3	E	483	HIS
1	K	42	GLN
1	K	124	GLN
1	K	158	ASN
1	K	160	GLN
2	J	5	GLN
2	J	16	GLN

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Mol	Chain	Res	Type
2	J	200	GLN
3	I	394	HIS
3	I	398	ASN
3	I	449	ASN
3	I	483	HIS
1	O	90	GLN
1	O	124	GLN
1	O	158	ASN
1	O	189	HIS
1	O	198	HIS
2	N	5	GLN
2	N	200	GLN
3	M	408	GLN
3	M	483	HIS
1	R	42	GLN
1	R	124	GLN
1	R	137	ASN
1	R	158	ASN
1	R	160	GLN
1	R	198	HIS
1	R	210	ASN
2	Q	16	GLN
2	Q	62	ASN
2	Q	207	ASN
3	P	480	GLN
3	P	483	HIS
1	U	38	GLN
1	U	53	ASN
1	U	198	HIS
3	S	469	ASN
3	S	480	GLN
3	S	483	HIS
1	X	27	GLN
1	X	42	GLN
1	X	89	HIS
1	X	90	GLN
1	X	137	ASN
1	X	198	HIS
2	W	1	GLN
3	V	384	GLN
3	V	442	ASN
3	V	452	ASN



### 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 ⓘ

52 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	Y	1	3,4	14,14,15	0.57	0	17,19,21	1.21	2 (11%)
4	NAG	Y	2	4	14,14,15	0.55	0	17,19,21	0.99	1 (5%)
4	BMA	Y	3	4	11,11,12	0.97	0	15,15,17	1.34	2 (13%)
4	MAN	Y	4	4	11,11,12	1.49	2 (18%)	15,15,17	2.40	6 (40%)
5	NAG	Z	1	3,5	14,14,15	0.64	0	17,19,21	1.06	2 (11%)
5	NAG	Z	2	5	14,14,15	0.57	0	17,19,21	0.74	0
6	NAG	a	1	3,6	14,14,15	0.50	0	17,19,21	1.09	2 (11%)
6	NAG	a	2	6	14,14,15	0.51	0	17,19,21	1.24	1 (5%)
6	BMA	a	3	6	11,11,12	0.66	0	15,15,17	1.07	1 (6%)
5	NAG	b	1	3,5	14,14,15	0.58	0	17,19,21	1.11	2 (11%)
5	NAG	b	2	5	14,14,15	0.73	1 (7%)	17,19,21	1.69	4 (23%)
4	NAG	c	1	3,4	14,14,15	0.67	0	17,19,21	1.29	2 (11%)
4	NAG	c	2	4	14,14,15	0.63	0	17,19,21	0.97	1 (5%)
4	BMA	c	3	4	11,11,12	0.69	0	15,15,17	0.80	0
4	MAN	c	4	4	11,11,12	1.31	1 (9%)	15,15,17	3.13	8 (53%)
5	NAG	d	1	3,5	14,14,15	0.52	0	17,19,21	1.03	1 (5%)
5	NAG	d	2	5	14,14,15	0.41	0	17,19,21	1.42	2 (11%)
4	NAG	e	1	3,4	14,14,15	0.59	0	17,19,21	1.41	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	e	2	4	14,14,15	0.65	0	17,19,21	1.16	1 (5%)
4	BMA	e	3	4	11,11,12	0.82	0	15,15,17	2.28	4 (26%)
4	MAN	e	4	4	11,11,12	0.67	0	15,15,17	0.62	0
6	NAG	f	1	3,6	14,14,15	0.53	0	17,19,21	1.66	4 (23%)
6	NAG	f	2	6	14,14,15	0.64	0	17,19,21	1.36	2 (11%)
6	BMA	f	3	6	11,11,12	0.63	0	15,15,17	1.17	2 (13%)
5	NAG	g	1	3,5	14,14,15	0.59	0	17,19,21	1.89	4 (23%)
5	NAG	g	2	5	14,14,15	0.48	0	17,19,21	1.22	2 (11%)
7	NAG	h	1	3,7	14,14,15	0.58	0	17,19,21	1.09	2 (11%)
7	NAG	h	2	7	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
7	BMA	h	3	7	11,11,12	0.69	0	15,15,17	1.18	2 (13%)
7	MAN	h	4	7	11,11,12	1.50	2 (18%)	15,15,17	2.40	6 (40%)
7	MAN	h	5	7	11,11,12	1.51	2 (18%)	15,15,17	1.34	1 (6%)
6	NAG	i	1	3,6	14,14,15	0.57	0	17,19,21	1.35	2 (11%)
6	NAG	i	2	6	14,14,15	0.57	0	17,19,21	1.08	1 (5%)
6	BMA	i	3	6	11,11,12	0.72	0	15,15,17	1.04	1 (6%)
6	NAG	j	1	3,6	14,14,15	0.66	0	17,19,21	1.37	2 (11%)
6	NAG	j	2	6	14,14,15	0.55	0	17,19,21	1.03	1 (5%)
6	BMA	j	3	6	11,11,12	0.77	0	15,15,17	0.98	1 (6%)
6	NAG	k	1	3,6	14,14,15	0.63	0	17,19,21	1.21	2 (11%)
6	NAG	k	2	6	14,14,15	0.70	0	17,19,21	1.55	3 (17%)
6	BMA	k	3	6	11,11,12	0.80	0	15,15,17	1.36	1 (6%)
5	NAG	l	1	3,5	14,14,15	0.55	0	17,19,21	1.35	2 (11%)
5	NAG	l	2	5	14,14,15	0.53	0	17,19,21	1.80	4 (23%)
6	NAG	m	1	3,6	14,14,15	0.59	0	17,19,21	1.03	1 (5%)
6	NAG	m	2	6	14,14,15	0.64	0	17,19,21	1.44	3 (17%)
6	BMA	m	3	6	11,11,12	0.62	0	15,15,17	1.33	3 (20%)
5	NAG	n	1	3,5	14,14,15	0.65	0	17,19,21	2.05	4 (23%)
5	NAG	n	2	5	14,14,15	0.59	0	17,19,21	1.73	4 (23%)
6	NAG	o	1	3,6	14,14,15	0.44	0	17,19,21	1.14	3 (17%)
6	NAG	o	2	6	14,14,15	0.68	0	17,19,21	1.18	2 (11%)
6	BMA	o	3	6	11,11,12	0.65	0	15,15,17	0.91	1 (6%)
5	NAG	p	1	3,5	14,14,15	0.62	0	17,19,21	1.60	3 (17%)
5	NAG	p	2	5	14,14,15	0.42	0	17,19,21	1.67	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Y	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Y	3	4	-	0/2/19/22	0/1/1/1
4	MAN	Y	4	4	-	0/2/19/22	0/1/1/1
5	NAG	Z	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	4/6/23/26	0/1/1/1
6	NAG	a	1	3,6	-	3/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	BMA	a	3	6	-	2/2/19/22	0/1/1/1
5	NAG	b	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	3/6/23/26	0/1/1/1
4	NAG	c	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	0/6/23/26	0/1/1/1
4	BMA	c	3	4	-	2/2/19/22	0/1/1/1
4	MAN	c	4	4	-	2/2/19/22	1/1/1/1
5	NAG	d	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	2/6/23/26	0/1/1/1
4	NAG	e	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
4	BMA	e	3	4	-	2/2/19/22	0/1/1/1
4	MAN	e	4	4	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	f	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	BMA	f	3	6	-	2/2/19/22	0/1/1/1
5	NAG	g	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	g	2	5	-	2/6/23/26	0/1/1/1
7	NAG	h	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	h	2	7	-	2/6/23/26	0/1/1/1
7	BMA	h	3	7	-	1/2/19/22	0/1/1/1
7	MAN	h	4	7	-	0/2/19/22	0/1/1/1
7	MAN	h	5	7	-	0/2/19/22	1/1/1/1
6	NAG	i	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	i	2	6	-	1/6/23/26	0/1/1/1
6	BMA	i	3	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	j	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	j	2	6	-	2/6/23/26	0/1/1/1
6	BMA	j	3	6	-	2/2/19/22	0/1/1/1
6	NAG	k	1	3,6	-	1/6/23/26	0/1/1/1
6	NAG	k	2	6	-	2/6/23/26	0/1/1/1
6	BMA	k	3	6	-	2/2/19/22	0/1/1/1
5	NAG	l	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	l	2	5	-	5/6/23/26	0/1/1/1
6	NAG	m	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	m	2	6	-	0/6/23/26	0/1/1/1
6	BMA	m	3	6	-	2/2/19/22	0/1/1/1
5	NAG	n	1	3,5	-	6/6/23/26	0/1/1/1
5	NAG	n	2	5	-	5/6/23/26	0/1/1/1
6	NAG	o	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	o	2	6	-	2/6/23/26	0/1/1/1
6	BMA	o	3	6	-	0/2/19/22	0/1/1/1
5	NAG	p	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	p	2	5	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	h	4	MAN	O5-C1	3.22	1.48	1.43
4	Y	4	MAN	O5-C1	3.13	1.48	1.43
7	h	5	MAN	O5-C5	2.65	1.48	1.43
7	h	5	MAN	C2-C3	2.53	1.56	1.52
4	c	4	MAN	O5-C1	-2.37	1.39	1.43
7	h	4	MAN	C6-C5	2.10	1.58	1.51
4	Y	4	MAN	C6-C5	2.09	1.58	1.51
5	b	2	NAG	C1-C2	2.08	1.55	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	c	4	MAN	C2-C3-C4	-7.90	97.22	110.89
4	e	3	BMA	C1-C2-C3	6.58	117.75	109.67
7	h	4	MAN	O3-C3-C4	5.53	123.13	110.35
4	Y	4	MAN	O3-C3-C4	5.50	123.08	110.35
4	c	4	MAN	O2-C2-C1	-4.23	100.49	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	4	MAN	O5-C1-C2	-4.22	104.25	110.77
7	h	4	MAN	O5-C1-C2	-4.20	104.29	110.77
6	k	3	BMA	O5-C5-C6	4.16	113.73	107.20
5	g	1	NAG	C1-O5-C5	4.14	117.80	112.19
5	n	2	NAG	O5-C5-C6	4.00	113.48	107.20
6	k	2	NAG	C4-C3-C2	3.95	116.80	111.02
5	n	1	NAG	C1-O5-C5	3.94	117.53	112.19
6	f	1	NAG	C1-O5-C5	3.93	117.52	112.19
6	m	2	NAG	C4-C3-C2	3.89	116.72	111.02
5	p	2	NAG	C4-C3-C2	-3.89	105.32	111.02
6	k	2	NAG	O5-C1-C2	-3.87	105.18	111.29
6	a	2	NAG	C1-O5-C5	3.83	117.38	112.19
4	c	4	MAN	O3-C3-C4	-3.79	101.58	110.35
6	f	1	NAG	O5-C5-C6	3.77	113.11	107.20
4	e	1	NAG	C1-O5-C5	3.71	117.21	112.19
5	p	2	NAG	C1-O5-C5	3.67	117.16	112.19
5	n	1	NAG	O5-C1-C2	-3.65	105.52	111.29
4	Y	1	NAG	C1-O5-C5	3.64	117.13	112.19
6	m	3	BMA	O5-C5-C6	3.62	112.87	107.20
5	g	1	NAG	O5-C1-C2	-3.60	105.60	111.29
5	n	2	NAG	C3-C4-C5	3.60	116.66	110.24
4	c	4	MAN	O5-C5-C6	3.57	112.80	107.20
6	j	1	NAG	C1-O5-C5	3.55	117.01	112.19
5	p	1	NAG	C1-O5-C5	3.44	116.86	112.19
5	l	2	NAG	C2-N2-C7	3.43	127.78	122.90
4	Y	4	MAN	O3-C3-C2	-3.42	103.44	109.99
5	d	2	NAG	C4-C3-C2	-3.42	106.01	111.02
5	b	2	NAG	O5-C5-C6	3.38	112.50	107.20
7	h	4	MAN	O3-C3-C2	-3.37	103.54	109.99
5	n	1	NAG	C2-N2-C7	3.36	127.68	122.90
5	g	1	NAG	C3-C4-C5	3.32	116.16	110.24
4	e	3	BMA	C2-C3-C4	3.26	116.53	110.89
5	l	1	NAG	C1-O5-C5	3.25	116.60	112.19
6	f	2	NAG	C1-O5-C5	3.22	116.55	112.19
7	h	3	BMA	O3-C3-C4	3.17	117.67	110.35
5	p	1	NAG	O5-C1-C2	-3.14	106.33	111.29
5	d	2	NAG	C1-O5-C5	3.13	116.43	112.19
4	c	4	MAN	O2-C2-C3	-3.11	103.91	110.14
4	c	4	MAN	C1-O5-C5	3.09	116.38	112.19
5	d	1	NAG	C1-O5-C5	3.08	116.37	112.19
5	l	2	NAG	C3-C4-C5	3.08	115.74	110.24
5	l	1	NAG	O5-C1-C2	-3.08	106.43	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	2	NAG	O5-C5-C6	3.05	111.98	107.20
6	i	1	NAG	C1-O5-C5	3.04	116.31	112.19
5	n	2	NAG	C2-N2-C7	3.02	127.21	122.90
4	e	3	BMA	C3-C4-C5	3.02	115.62	110.24
6	f	2	NAG	C4-C3-C2	3.00	115.42	111.02
4	c	1	NAG	O5-C1-C2	-2.98	106.58	111.29
5	l	2	NAG	C4-C3-C2	2.96	115.35	111.02
6	i	2	NAG	C1-O5-C5	2.95	116.19	112.19
5	b	2	NAG	C4-C3-C2	2.93	115.31	111.02
4	Y	3	BMA	C1-O5-C5	-2.91	108.25	112.19
6	a	1	NAG	O5-C1-C2	-2.87	106.76	111.29
5	n	1	NAG	C3-C4-C5	2.81	115.24	110.24
6	k	1	NAG	O5-C5-C6	2.77	111.55	107.20
5	b	2	NAG	C2-N2-C7	2.76	126.83	122.90
4	c	1	NAG	O5-C5-C6	2.75	111.52	107.20
6	k	2	NAG	O4-C4-C3	-2.67	104.18	110.35
7	h	1	NAG	C1-O5-C5	2.64	115.77	112.19
4	Y	3	BMA	C1-C2-C3	2.64	112.91	109.67
6	m	2	NAG	O5-C1-C2	-2.63	107.14	111.29
5	b	1	NAG	C2-N2-C7	-2.59	119.21	122.90
6	o	1	NAG	O5-C1-C2	-2.59	107.19	111.29
6	o	3	BMA	C1-C2-C3	2.59	112.85	109.67
4	e	2	NAG	C1-O5-C5	2.56	115.66	112.19
7	h	5	MAN	O5-C1-C2	2.55	114.71	110.77
7	h	4	MAN	C3-C4-C5	2.53	114.75	110.24
5	b	1	NAG	O5-C1-C2	-2.51	107.32	111.29
5	l	2	NAG	O5-C1-C2	-2.51	107.33	111.29
7	h	2	NAG	C1-O5-C5	2.49	115.57	112.19
5	b	2	NAG	O5-C1-C2	2.48	115.21	111.29
7	h	4	MAN	O6-C6-C5	2.48	119.81	111.29
6	f	3	BMA	C1-O5-C5	2.47	115.54	112.19
4	Y	4	MAN	C3-C4-C5	2.47	114.65	110.24
4	c	4	MAN	C3-C4-C5	-2.46	105.84	110.24
4	Y	4	MAN	O6-C6-C5	2.46	119.74	111.29
4	e	3	BMA	C1-O5-C5	2.46	115.52	112.19
6	j	2	NAG	C4-C3-C2	2.44	114.59	111.02
6	f	3	BMA	C3-C4-C5	2.43	114.58	110.24
5	n	2	NAG	O5-C1-C2	-2.43	107.44	111.29
6	o	2	NAG	C4-C3-C2	2.43	114.58	111.02
6	i	1	NAG	C4-C3-C2	2.40	114.54	111.02
5	g	1	NAG	C1-C2-N2	2.32	114.46	110.49
5	Z	1	NAG	C1-O5-C5	2.27	115.27	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	2	NAG	C1-C2-N2	-2.26	106.63	110.49
7	h	4	MAN	C2-C3-C4	-2.26	106.99	110.89
7	h	1	NAG	O5-C5-C6	2.22	110.68	107.20
4	Y	4	MAN	C2-C3-C4	-2.21	107.07	110.89
6	o	1	NAG	C1-O5-C5	2.21	115.19	112.19
6	m	2	NAG	O4-C4-C3	-2.20	105.26	110.35
5	p	1	NAG	C1-C2-N2	2.19	114.23	110.49
7	h	3	BMA	O5-C5-C6	2.19	110.64	107.20
6	i	3	BMA	O5-C5-C6	2.18	110.63	107.20
4	Y	1	NAG	O5-C1-C2	-2.18	107.85	111.29
6	f	1	NAG	O7-C7-C8	-2.17	118.02	122.06
4	c	2	NAG	O5-C1-C2	-2.17	107.87	111.29
5	p	2	NAG	O5-C5-C6	2.16	110.59	107.20
6	k	1	NAG	C2-N2-C7	-2.16	119.83	122.90
6	m	3	BMA	C1-O5-C5	-2.13	109.31	112.19
5	Z	1	NAG	O5-C1-C2	-2.11	107.96	111.29
6	m	3	BMA	C2-C3-C4	2.10	114.53	110.89
6	o	1	NAG	O7-C7-C8	-2.09	118.17	122.06
4	e	1	NAG	O5-C5-C6	2.08	110.47	107.20
6	m	1	NAG	C1-O5-C5	2.07	115.00	112.19
4	Y	2	NAG	O5-C1-C2	-2.07	108.01	111.29
4	c	4	MAN	O4-C4-C5	2.07	114.43	109.30
6	a	1	NAG	O7-C7-C8	-2.07	118.22	122.06
6	a	3	BMA	C1-O5-C5	-2.04	109.42	112.19
6	j	1	NAG	C3-C4-C5	2.03	113.86	110.24
6	f	1	NAG	O5-C1-C2	-2.03	108.08	111.29
4	e	1	NAG	O5-C1-C2	-2.03	108.09	111.29
6	o	2	NAG	O4-C4-C3	-2.03	105.67	110.35
6	j	3	BMA	C3-C4-C5	2.02	113.84	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	e	4	MAN	C1

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	b	2	NAG	C8-C7-N2-C2
5	b	2	NAG	O7-C7-N2-C2
5	n	1	NAG	C3-C2-N2-C7
5	n	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	n	1	NAG	O7-C7-N2-C2
5	l	2	NAG	C8-C7-N2-C2
5	l	2	NAG	O7-C7-N2-C2
5	Z	2	NAG	C8-C7-N2-C2
5	Z	2	NAG	O7-C7-N2-C2
6	f	2	NAG	C8-C7-N2-C2
6	f	2	NAG	O7-C7-N2-C2
5	n	2	NAG	C3-C2-N2-C7
5	n	2	NAG	C8-C7-N2-C2
5	n	2	NAG	O7-C7-N2-C2
5	n	2	NAG	O5-C5-C6-O6
5	l	2	NAG	O5-C5-C6-O6
4	c	4	MAN	O5-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
6	a	3	BMA	O5-C5-C6-O6
5	p	2	NAG	O5-C5-C6-O6
6	f	1	NAG	C8-C7-N2-C2
7	h	2	NAG	C8-C7-N2-C2
4	e	3	BMA	O5-C5-C6-O6
6	j	1	NAG	O5-C5-C6-O6
4	e	3	BMA	C4-C5-C6-O6
5	p	2	NAG	C4-C5-C6-O6
6	a	3	BMA	C4-C5-C6-O6
5	n	2	NAG	C4-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	n	1	NAG	C4-C5-C6-O6
6	f	3	BMA	O5-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
5	n	1	NAG	O5-C5-C6-O6
4	c	3	BMA	O5-C5-C6-O6
5	l	2	NAG	C4-C5-C6-O6
5	g	1	NAG	C8-C7-N2-C2
6	f	1	NAG	O7-C7-N2-C2
7	h	2	NAG	O7-C7-N2-C2
5	d	2	NAG	O5-C5-C6-O6
6	j	3	BMA	O5-C5-C6-O6
6	m	3	BMA	O5-C5-C6-O6
5	b	2	NAG	C1-C2-N2-C7
5	l	2	NAG	C1-C2-N2-C7
6	a	2	NAG	C4-C5-C6-O6
4	c	4	MAN	C4-C5-C6-O6
6	o	2	NAG	C4-C5-C6-O6

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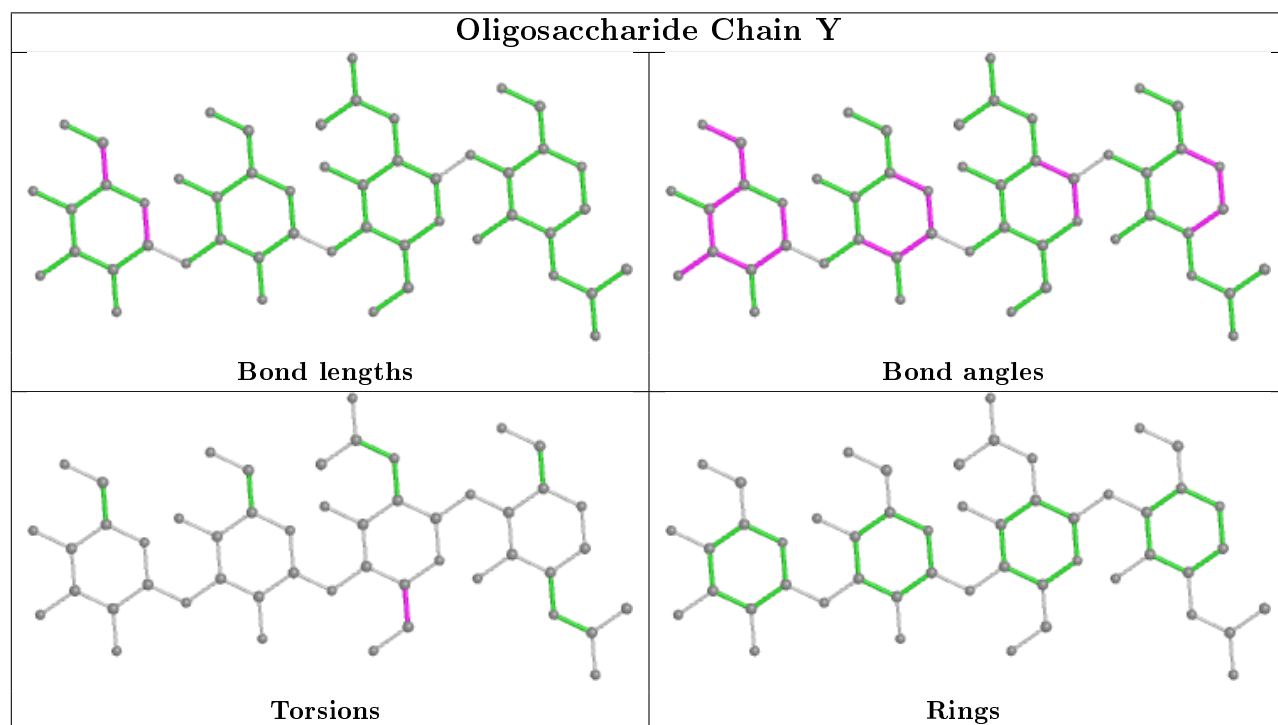
Mol	Chain	Res	Type	Atoms
5	g	2	NAG	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
6	j	3	BMA	C4-C5-C6-O6
5	g	1	NAG	O7-C7-N2-C2
6	i	1	NAG	C8-C7-N2-C2
6	o	2	NAG	O5-C5-C6-O6
6	j	2	NAG	O5-C5-C6-O6
6	f	1	NAG	C4-C5-C6-O6
4	c	3	BMA	C4-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
6	f	3	BMA	C4-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
6	j	1	NAG	C4-C5-C6-O6
6	i	1	NAG	O7-C7-N2-C2
6	k	3	BMA	C4-C5-C6-O6
6	k	2	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
6	k	3	BMA	O5-C5-C6-O6
6	o	1	NAG	C4-C5-C6-O6
4	e	4	MAN	C4-C5-C6-O6
6	k	2	NAG	O5-C5-C6-O6
4	e	4	MAN	O5-C5-C6-O6
6	j	2	NAG	C4-C5-C6-O6
6	o	1	NAG	O5-C5-C6-O6
6	m	3	BMA	C4-C5-C6-O6
5	n	1	NAG	C1-C2-N2-C7
6	k	1	NAG	C4-C5-C6-O6
6	a	1	NAG	C8-C7-N2-C2
7	h	3	BMA	C4-C5-C6-O6
6	a	1	NAG	O7-C7-N2-C2
6	a	1	NAG	C4-C5-C6-O6
6	i	2	NAG	C4-C5-C6-O6

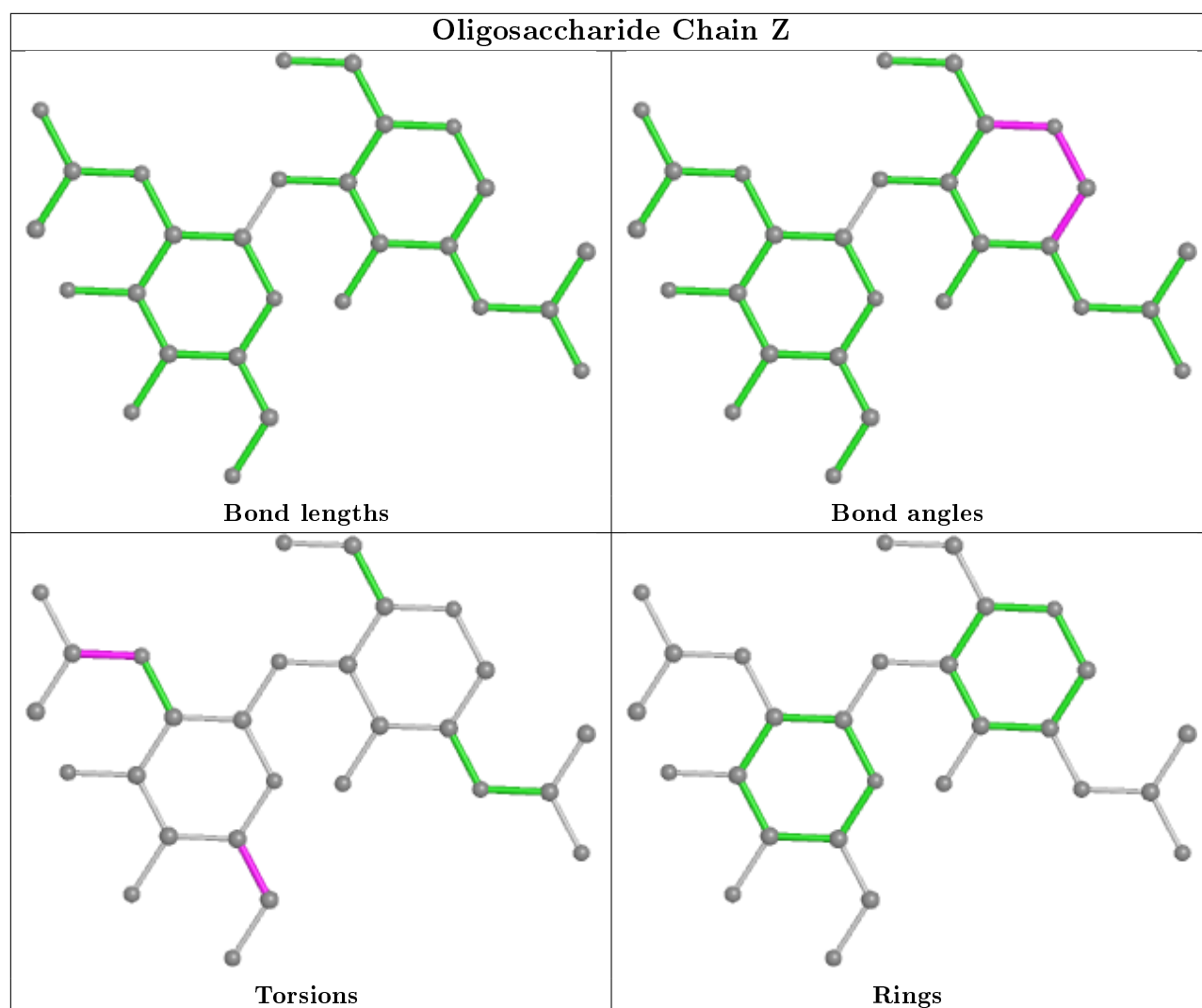
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	h	5	MAN	C1-C2-C3-C4-C5-O5
4	c	4	MAN	C1-C2-C3-C4-C5-O5

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](#)

22 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	$\# Z  > 2$
8	NAG	P	3371	3	14,14,15	0.57	0	17,19,21	1.10	1 (5%)
9	SO4	U	214	-	4,4,4	0.17	0	6,6,6	0.13	0
8	NAG	E	3891	3	14,14,15	0.60	0	17,19,21	1.23	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	SO4	E	1	-	4,4,4	0.14	0	6,6,6	0.48	0
8	NAG	A	3371	3	14,14,15	0.59	0	17,19,21	1.24	2 (11%)
8	NAG	S	3371	3	14,14,15	0.68	1 (7%)	17,19,21	1.63	5 (29%)
8	NAG	S	3891	3	14,14,15	0.66	0	17,19,21	1.42	2 (11%)
8	NAG	V	3371	3	14,14,15	0.51	0	17,19,21	1.32	2 (11%)
8	NAG	A	3891	3	14,14,15	0.50	0	17,19,21	1.73	4 (23%)
8	NAG	B	3891	3	14,14,15	0.59	0	17,19,21	1.87	5 (29%)
9	SO4	V	1	-	4,4,4	0.18	0	6,6,6	0.17	0
9	SO4	G	214	-	4,4,4	0.13	0	6,6,6	0.26	0
8	NAG	B	3371	3	14,14,15	0.56	0	17,19,21	1.16	1 (5%)
9	SO4	O	214	-	4,4,4	0.12	0	6,6,6	0.15	0
9	SO4	K	214	-	4,4,4	0.15	0	6,6,6	0.26	0
8	NAG	M	3371	3	14,14,15	0.68	1 (7%)	17,19,21	2.06	3 (17%)
8	NAG	I	3371	3	14,14,15	0.74	1 (7%)	17,19,21	1.10	1 (5%)
9	SO4	X	214	-	4,4,4	0.13	0	6,6,6	0.19	0
9	SO4	A	1	-	4,4,4	0.13	0	6,6,6	0.12	0
8	NAG	P	3891	3	14,14,15	0.63	0	17,19,21	2.17	2 (11%)
8	NAG	V	3891	3	14,14,15	0.47	0	17,19,21	1.88	4 (23%)
8	NAG	E	3371	3	14,14,15	0.55	0	17,19,21	1.30	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	P	3371	3	-	2/6/23/26	0/1/1/1
8	NAG	V	3371	3	-	2/6/23/26	0/1/1/1
8	NAG	I	3371	3	-	2/6/23/26	0/1/1/1
8	NAG	E	3891	3	-	5/6/23/26	0/1/1/1
8	NAG	A	3371	3	-	3/6/23/26	0/1/1/1
8	NAG	A	3891	3	-	4/6/23/26	0/1/1/1
8	NAG	B	3891	3	-	2/6/23/26	0/1/1/1
8	NAG	B	3371	3	-	3/6/23/26	0/1/1/1
8	NAG	S	3371	3	-	5/6/23/26	0/1/1/1
8	NAG	M	3371	3	-	5/6/23/26	0/1/1/1
8	NAG	V	3891	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	S	3891	3	-	3/6/23/26	0/1/1/1
8	NAG	P	3891	3	-	2/6/23/26	0/1/1/1
8	NAG	E	3371	3	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	3371	NAG	C1-C2	2.39	1.55	1.52
8	M	3371	NAG	C1-C2	2.20	1.55	1.52
8	S	3371	NAG	C1-C2	2.06	1.55	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	3891	NAG	C1-O5-C5	7.55	122.42	112.19
8	M	3371	NAG	C1-O5-C5	6.21	120.61	112.19
8	V	3891	NAG	C1-O5-C5	5.52	119.67	112.19
8	A	3891	NAG	C1-O5-C5	4.60	118.42	112.19
8	M	3371	NAG	O5-C1-C2	4.22	117.95	111.29
8	S	3891	NAG	C4-C3-C2	4.15	117.10	111.02
8	B	3371	NAG	C1-O5-C5	3.72	117.23	112.19
8	B	3891	NAG	C3-C4-C5	-3.58	103.85	110.24
8	P	3891	NAG	O5-C5-C6	3.36	112.47	107.20
8	B	3891	NAG	O5-C5-C6	3.25	112.29	107.20
8	B	3891	NAG	C1-O5-C5	3.18	116.50	112.19
8	A	3371	NAG	C1-O5-C5	3.16	116.48	112.19
8	S	3371	NAG	C1-O5-C5	3.14	116.44	112.19
8	V	3891	NAG	C4-C3-C2	-2.96	106.68	111.02
8	E	3891	NAG	C1-O5-C5	2.90	116.12	112.19
8	I	3371	NAG	C1-O5-C5	2.87	116.08	112.19
8	A	3891	NAG	C4-C3-C2	-2.82	106.89	111.02
8	M	3371	NAG	C2-N2-C7	2.79	126.88	122.90
8	S	3371	NAG	C1-C2-N2	2.76	115.20	110.49
8	V	3371	NAG	C1-O5-C5	2.73	115.89	112.19
8	V	3891	NAG	O5-C1-C2	-2.68	107.06	111.29
8	S	3371	NAG	C2-N2-C7	2.67	126.71	122.90
8	V	3371	NAG	C3-C4-C5	2.60	114.87	110.24
8	A	3371	NAG	C2-N2-C7	2.59	126.59	122.90
8	P	3371	NAG	C1-O5-C5	2.59	115.69	112.19
8	B	3891	NAG	C1-C2-N2	-2.50	106.21	110.49
8	A	3891	NAG	O5-C1-C2	-2.45	107.42	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	3891	NAG	O5-C5-C6	2.38	110.94	107.20
8	S	3371	NAG	O5-C5-C6	2.38	110.93	107.20
8	S	3371	NAG	C3-C4-C5	-2.32	106.11	110.24
8	E	3371	NAG	O5-C1-C2	2.22	114.79	111.29
8	B	3891	NAG	O3-C3-C2	2.20	114.02	109.47
8	E	3371	NAG	O5-C5-C6	2.13	110.54	107.20
8	V	3891	NAG	C1-C2-N2	2.11	114.10	110.49
8	A	3891	NAG	O7-C7-C8	-2.03	118.28	122.06
8	E	3371	NAG	O7-C7-C8	-2.01	118.31	122.06

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	3891	NAG	C3-C2-N2-C7
8	E	3891	NAG	C8-C7-N2-C2
8	E	3891	NAG	O7-C7-N2-C2
8	A	3371	NAG	C8-C7-N2-C2
8	A	3371	NAG	O7-C7-N2-C2
8	S	3371	NAG	C1-C2-N2-C7
8	S	3371	NAG	C8-C7-N2-C2
8	S	3371	NAG	O7-C7-N2-C2
8	S	3891	NAG	C8-C7-N2-C2
8	S	3891	NAG	O7-C7-N2-C2
8	V	3371	NAG	C8-C7-N2-C2
8	V	3371	NAG	O7-C7-N2-C2
8	A	3891	NAG	C8-C7-N2-C2
8	A	3891	NAG	O7-C7-N2-C2
8	B	3371	NAG	C8-C7-N2-C2
8	B	3371	NAG	O7-C7-N2-C2
8	M	3371	NAG	C3-C2-N2-C7
8	M	3371	NAG	O7-C7-N2-C2
8	I	3371	NAG	C8-C7-N2-C2
8	I	3371	NAG	O7-C7-N2-C2
8	V	3891	NAG	C8-C7-N2-C2
8	V	3891	NAG	O7-C7-N2-C2
8	E	3371	NAG	C8-C7-N2-C2
8	E	3371	NAG	O7-C7-N2-C2
8	M	3371	NAG	C8-C7-N2-C2
8	P	3371	NAG	C8-C7-N2-C2
8	A	3891	NAG	O5-C5-C6-O6
8	P	3371	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	P	3891	NAG	O5-C5-C6-O6
8	M	3371	NAG	C4-C5-C6-O6
8	P	3891	NAG	C4-C5-C6-O6
8	M	3371	NAG	O5-C5-C6-O6
8	A	3891	NAG	C4-C5-C6-O6
8	E	3371	NAG	C4-C5-C6-O6
8	S	3371	NAG	C4-C5-C6-O6
8	V	3891	NAG	O5-C5-C6-O6
8	S	3371	NAG	O5-C5-C6-O6
8	E	3371	NAG	O5-C5-C6-O6
8	B	3891	NAG	C4-C5-C6-O6
8	E	3891	NAG	O5-C5-C6-O6
8	E	3891	NAG	C4-C5-C6-O6
8	A	3371	NAG	C4-C5-C6-O6
8	S	3891	NAG	O5-C5-C6-O6
8	B	3891	NAG	O5-C5-C6-O6
8	B	3371	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	3891	NAG	1	0
9	V	1	SO4	1	0
9	A	1	SO4	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	D	213/213 (100%)	-0.14	1 (0%) 91 90	15, 26, 31, 33	0
1	G	213/213 (100%)	-0.08	0 100 100	17, 26, 32, 34	0
1	K	213/213 (100%)	-0.20	0 100 100	18, 27, 33, 35	0
1	L	213/213 (100%)	-0.10	1 (0%) 91 90	18, 26, 32, 35	0
1	O	213/213 (100%)	-0.16	0 100 100	18, 26, 33, 36	0
1	R	213/213 (100%)	-0.10	1 (0%) 91 90	16, 25, 31, 35	0
1	U	213/213 (100%)	-0.15	0 100 100	18, 26, 31, 34	0
1	X	213/213 (100%)	-0.11	0 100 100	15, 26, 32, 33	0
2	C	213/223 (95%)	0.16	4 (1%) 66 64	20, 27, 39, 41	0
2	F	215/223 (96%)	0.04	2 (0%) 84 83	20, 28, 39, 47	0
2	H	217/223 (97%)	0.07	2 (0%) 84 83	17, 27, 40, 44	0
2	J	217/223 (97%)	0.16	3 (1%) 75 73	19, 28, 38, 42	0
2	N	218/223 (97%)	-0.01	4 (1%) 68 66	18, 28, 39, 49	0
2	Q	217/223 (97%)	-0.07	0 100 100	19, 28, 39, 42	0
2	T	216/223 (96%)	0.10	5 (2%) 60 57	19, 28, 40, 43	0
2	W	216/223 (96%)	0.01	3 (1%) 75 73	19, 27, 39, 44	0
3	A	195/214 (91%)	-0.12	0 100 100	18, 28, 38, 45	0
3	B	194/214 (90%)	-0.09	1 (0%) 91 90	19, 29, 40, 45	0
3	E	194/214 (90%)	-0.03	0 100 100	15, 28, 40, 46	0
3	I	193/214 (90%)	-0.08	1 (0%) 91 90	17, 26, 40, 48	0
3	M	195/214 (91%)	-0.03	1 (0%) 91 90	16, 27, 42, 47	0
3	P	193/214 (90%)	-0.08	0 100 100	18, 27, 38, 47	0
3	S	194/214 (90%)	-0.13	0 100 100	17, 29, 40, 44	0
3	V	193/214 (90%)	-0.13	1 (0%) 91 90	19, 27, 39, 42	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4984/5200 (95%)	-0.05	30 (0%) 89 89	15, 27, 38, 49	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	135	SER	3.1
2	N	198	GLY	3.1
3	M	485	LEU	2.9
2	C	1	GLN	2.9
2	J	198	GLY	2.8
2	T	136	SER	2.8
2	J	199	THR	2.6
2	W	130	PHE	2.5
2	T	135	SER	2.5
2	H	130	PHE	2.4
2	T	130	PHE	2.4
3	I	502	CYS	2.4
2	N	141	GLY	2.4
2	W	166	ALA	2.4
1	R	213	ALA	2.3
2	N	197	LEU	2.3
2	T	165	GLY	2.2
2	T	192	VAL	2.2
2	C	203	ILE	2.2
2	C	213	THR	2.2
2	N	130	PHE	2.2
2	F	197	LEU	2.1
2	C	130	PHE	2.1
3	B	334	HIS	2.1
1	L	212	GLY	2.1
2	H	199	THR	2.1
3	V	318	ILE	2.1
2	W	169	SER	2.1
1	D	13	LEU	2.0
2	F	130	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

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.

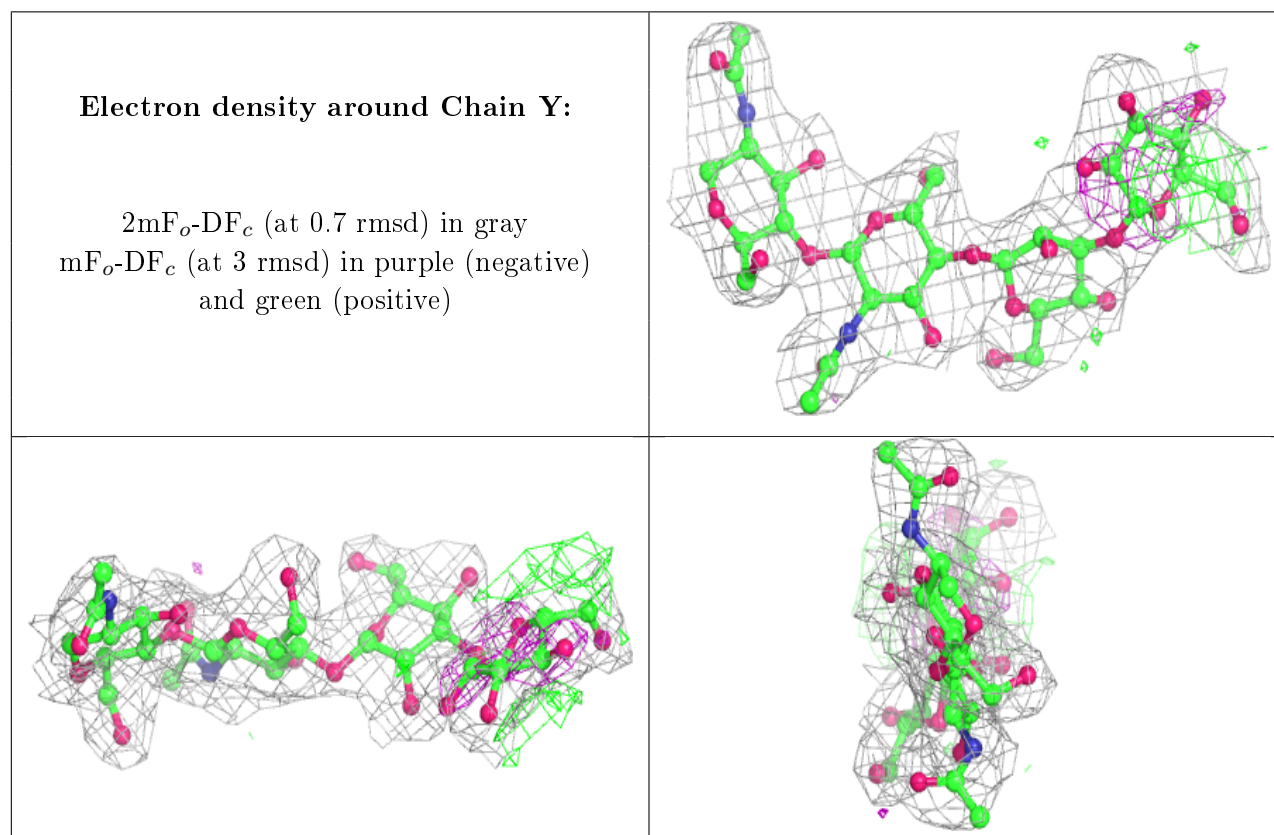
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MAN	e	4	11/12	0.63	0.33	23,31,33,35	0
7	MAN	h	4	11/12	0.66	0.27	23,31,33,35	0
6	BMA	k	3	11/12	0.67	0.20	50,52,53,54	0
4	MAN	Y	4	11/12	0.71	0.27	23,31,33,35	0
6	BMA	m	3	11/12	0.73	0.22	50,52,53,53	0
6	BMA	j	3	11/12	0.75	0.24	62,64,64,65	0
6	BMA	f	3	11/12	0.76	0.22	43,44,45,45	0
7	BMA	h	3	11/12	0.78	0.24	45,48,50,55	0
7	MAN	h	5	11/12	0.80	0.39	26,33,34,36	0
5	NAG	d	2	14/15	0.80	0.16	47,50,52,52	0
4	BMA	e	3	11/12	0.81	0.25	54,59,62,63	0
6	BMA	a	3	11/12	0.82	0.17	49,50,51,52	0
5	NAG	n	2	14/15	0.83	0.22	47,53,56,56	0
5	NAG	b	2	14/15	0.85	0.25	49,52,54,54	0
5	NAG	Z	2	14/15	0.85	0.24	49,52,52,52	0
6	BMA	i	3	11/12	0.85	0.18	43,45,46,46	0
5	NAG	l	2	14/15	0.86	0.14	47,50,50,50	0
4	BMA	c	3	11/12	0.87	0.23	45,46,48,51	0
4	BMA	Y	3	11/12	0.87	0.14	49,50,53,56	0
5	NAG	g	2	14/15	0.88	0.14	49,51,53,53	0
6	NAG	f	1	14/15	0.88	0.17	33,36,37,40	0
6	NAG	i	1	14/15	0.89	0.15	35,40,42,43	0
4	MAN	c	4	11/12	0.89	0.17	23,31,33,35	0
6	BMA	o	3	11/12	0.90	0.17	44,45,47,48	0
5	NAG	p	2	14/15	0.90	0.17	42,45,47,47	0
6	NAG	a	2	14/15	0.92	0.17	38,41,44,48	0
6	NAG	o	2	14/15	0.92	0.15	34,37,40,42	0
7	NAG	h	2	14/15	0.92	0.15	26,33,36,41	0
6	NAG	i	2	14/15	0.92	0.21	44,45,46,47	0
6	NAG	j	2	14/15	0.92	0.15	50,56,59,60	0
6	NAG	f	2	14/15	0.93	0.23	43,44,45,45	0
5	NAG	d	1	14/15	0.93	0.14	32,36,39,43	0
6	NAG	j	1	14/15	0.93	0.15	35,39,43,48	0
6	NAG	m	2	14/15	0.93	0.15	37,41,43,47	0
6	NAG	k	2	14/15	0.93	0.13	36,41,42,47	0
5	NAG	p	1	14/15	0.93	0.14	32,38,39,41	0
5	NAG	n	1	14/15	0.93	0.17	36,41,44,47	0

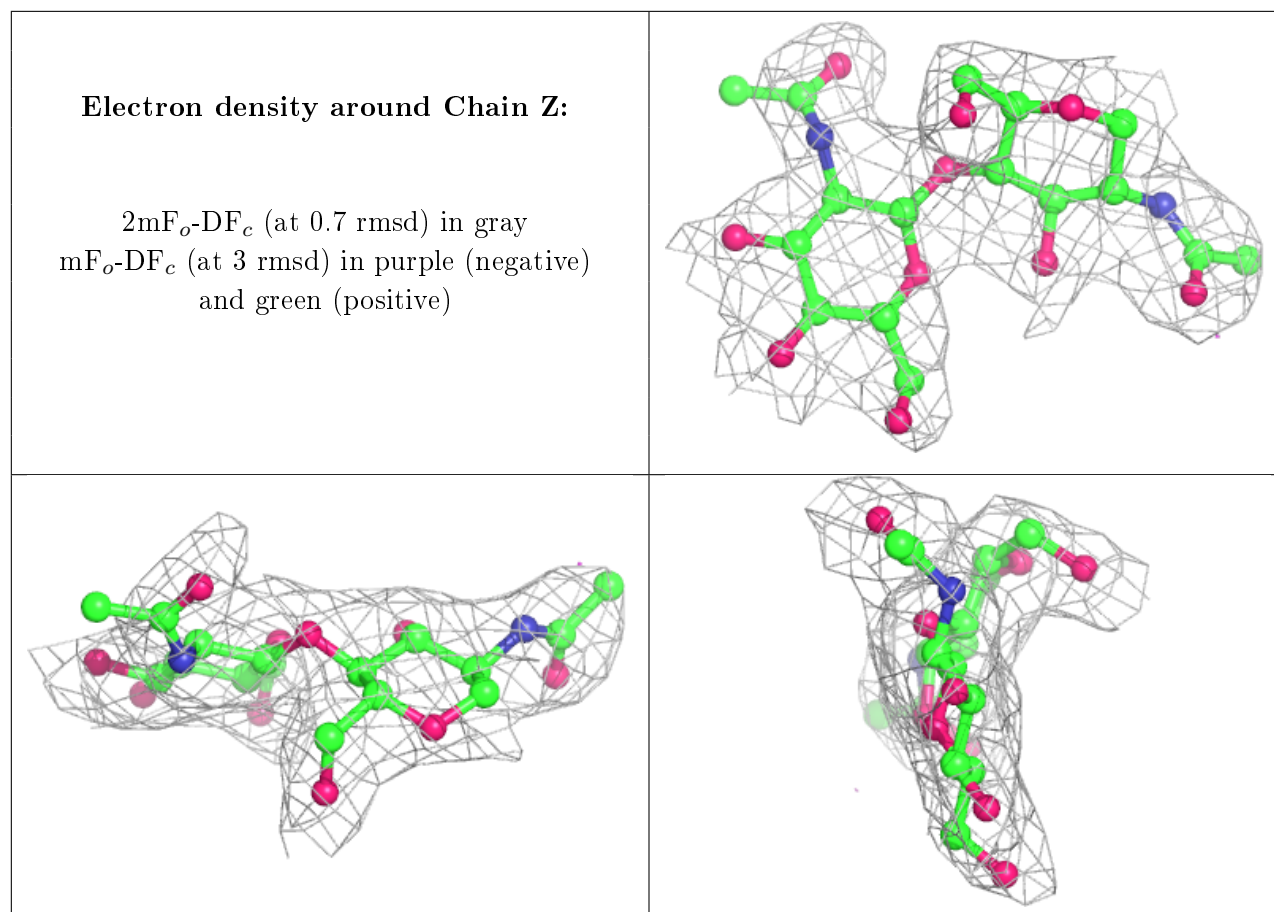
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	e	2	14/15	0.93	0.17	32,36,41,47	0
5	NAG	l	1	14/15	0.94	0.14	32,38,42,46	0
4	NAG	Y	2	14/15	0.94	0.14	37,40,43,47	0
5	NAG	g	1	14/15	0.94	0.15	33,38,43,46	0
5	NAG	b	1	14/15	0.94	0.14	34,37,40,45	0
5	NAG	Z	1	14/15	0.95	0.17	37,40,42,45	0
6	NAG	a	1	14/15	0.95	0.16	28,31,33,37	0
4	NAG	c	2	14/15	0.96	0.14	32,34,37,41	0
7	NAG	h	1	14/15	0.96	0.12	18,27,28,30	0
6	NAG	o	1	14/15	0.96	0.18	22,25,29,33	0
6	NAG	m	1	14/15	0.96	0.12	25,27,30,33	0
4	NAG	Y	1	14/15	0.97	0.13	27,31,34,38	0
4	NAG	c	1	14/15	0.97	0.10	17,22,27,29	0
4	NAG	e	1	14/15	0.97	0.13	22,25,27,30	0
6	NAG	k	1	14/15	0.98	0.13	18,22,26,31	0

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





## 6.4 Ligands ⓘ

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
8	NAG	V	3371	14/15	0.75	0.33	45,48,52,52	0
8	NAG	B	3371	14/15	0.77	0.27	47,50,52,52	0
8	NAG	I	3371	14/15	0.78	0.20	43,47,48,49	0
8	NAG	P	3891	14/15	0.78	0.20	41,44,47,49	0
8	NAG	E	3891	14/15	0.79	0.21	40,43,46,46	0
8	NAG	B	3891	14/15	0.80	0.20	44,46,51,52	0
8	NAG	S	3891	14/15	0.80	0.18	44,46,50,51	0
8	NAG	A	3371	14/15	0.82	0.19	45,46,47,47	0
8	NAG	A	3891	14/15	0.82	0.17	40,42,44,44	0
8	NAG	S	3371	14/15	0.83	0.27	40,41,43,43	0
8	NAG	V	3891	14/15	0.84	0.15	40,43,45,45	0
8	NAG	P	3371	14/15	0.86	0.16	39,42,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	E	3371	14/15	0.86	0.13	43,45,47,48	0
8	NAG	M	3371	14/15	0.87	0.21	42,45,47,47	0
9	SO4	X	214	5/5	0.88	0.16	69,70,70,70	0
9	SO4	E	1	5/5	0.90	0.15	56,57,58,58	0
9	SO4	K	214	5/5	0.91	0.18	67,68,68,69	0
9	SO4	U	214	5/5	0.94	0.14	76,77,77,78	0
9	SO4	G	214	5/5	0.94	0.11	63,63,63,64	0
9	SO4	A	1	5/5	0.95	0.13	50,50,51,51	0
9	SO4	O	214	5/5	0.96	0.11	70,70,70,71	0
9	SO4	V	1	5/5	0.97	0.11	59,60,60,60	0

## 6.5 Other polymers

There are no such residues in this entry.