



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2021 – 12:10 pm GMT

PDB ID : 7NP1  
Title : Crystal Structure of the SARS-CoV-2 Receptor Binding Domain in Complex with Antibody ION-360  
Authors : Hall, G.; Cowan, R.; Carr, M.  
Deposited on : 2021-02-26  
Resolution : 2.80 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 : 1.8.4 (270009), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

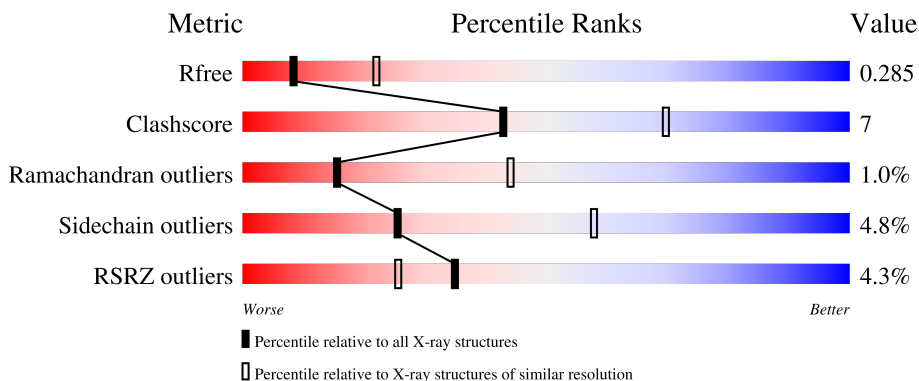
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	232	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 40px;">4%      59%      14%      •      26%</p>
1	B	232	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 40px;">7%      62%      10%      •      28%</p>
1	C	232	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 40px;">4%      64%      18%      18%</p>
1	D	232	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 40px;">8%      62%      16%      22%</p>
2	H	224	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 40px;">3%      83%      15%      •</p>

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Mol	Chain	Length	Quality of chain
2	I	224	
2	J	224	
2	K	224	
3	L	217	
3	M	217	
3	N	217	
3	O	217	
4	E	2	
4	F	2	

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	FUC	E	2	-	-	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 18843 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	171	1368	879	228	255	6	0	0	0
1	B	168	1346	865	225	251	5	0	0	0
1	C	190	1508	967	250	283	8	0	0	0
1	D	181	1445	927	239	272	7	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	540	ALA	-	expression tag	UNP P0DTC2
A	541	ALA	-	expression tag	UNP P0DTC2
A	542	ALA	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	SER	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2
A	550	HIS	-	expression tag	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	540	ALA	-	expression tag	UNP P0DTC2
B	541	ALA	-	expression tag	UNP P0DTC2
B	542	ALA	-	expression tag	UNP P0DTC2
B	543	GLY	-	expression tag	UNP P0DTC2
B	544	SER	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2

*Continued on next page...*

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Chain	Residue	Modelled	Actual	Comment	Reference
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
B	548	HIS	-	expression tag	UNP P0DTC2
B	549	HIS	-	expression tag	UNP P0DTC2
B	550	HIS	-	expression tag	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	542	ALA	-	expression tag	UNP P0DTC2
C	543	ALA	-	expression tag	UNP P0DTC2
C	544	ALA	-	expression tag	UNP P0DTC2
C	545	GLY	-	expression tag	UNP P0DTC2
C	546	SER	-	expression tag	UNP P0DTC2
C	547	HIS	-	expression tag	UNP P0DTC2
C	548	HIS	-	expression tag	UNP P0DTC2
C	549	HIS	-	expression tag	UNP P0DTC2
C	550	HIS	-	expression tag	UNP P0DTC2
C	551	HIS	-	expression tag	UNP P0DTC2
C	552	HIS	-	expression tag	UNP P0DTC2
D	?	-	HIS	deletion	UNP P0DTC2
D	?	-	ALA	deletion	UNP P0DTC2
D	542	ALA	-	expression tag	UNP P0DTC2
D	543	ALA	-	expression tag	UNP P0DTC2
D	544	ALA	-	expression tag	UNP P0DTC2
D	545	GLY	-	expression tag	UNP P0DTC2
D	546	SER	-	expression tag	UNP P0DTC2
D	547	HIS	-	expression tag	UNP P0DTC2
D	548	HIS	-	expression tag	UNP P0DTC2
D	549	HIS	-	expression tag	UNP P0DTC2
D	550	HIS	-	expression tag	UNP P0DTC2
D	551	HIS	-	expression tag	UNP P0DTC2
D	552	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1615	1014	272	323	6			
2	I	216	Total	C	N	O	S	0	1	0
			1597	1004	270	317	6			
2	J	218	Total	C	N	O	S	0	0	0
			1602	1007	270	319	6			
2	K	217	Total	C	N	O	S	0	0	0
			1598	1005	269	318	6			

- Molecule 3 is a protein called Immunoglobulin light chain.

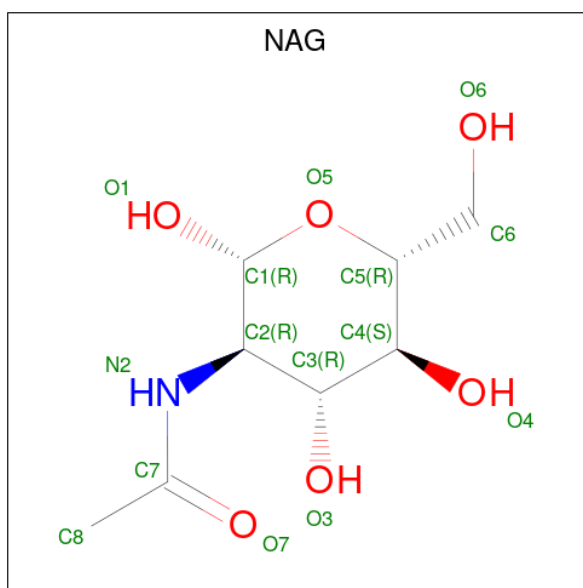
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	214	Total 1657	C 1036	N 278	O 338	S 5	0	1	0
3	M	214	Total 1652	C 1033	N 277	O 337	S 5	0	0	0
3	N	214	Total 1656	C 1035	N 279	O 337	S 5	0	1	0
3	O	214	Total 1652	C 1033	N 277	O 337	S 5	0	0	0

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	2	Total 24	C 14	N 1	O 9	0	0	0
4	F	2	Total 24	C 14	N 1	O 9	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

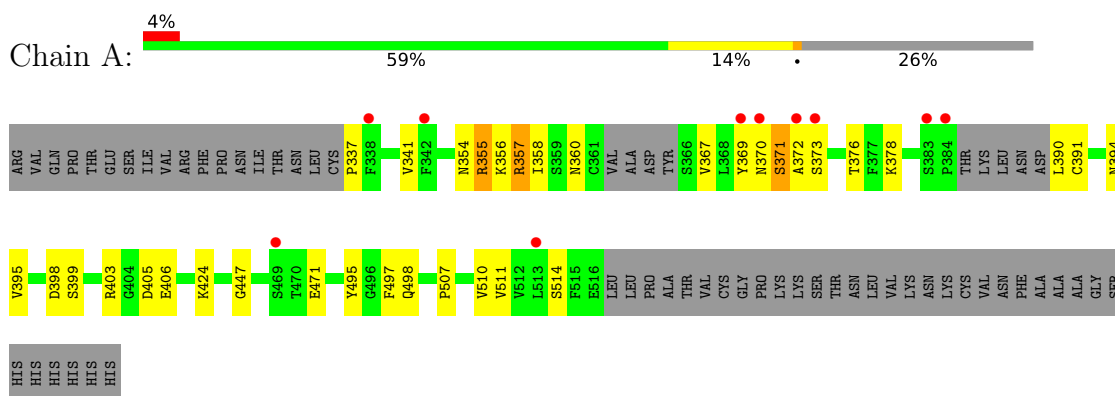
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	10	Total	O	0	0
			10	10		
6	C	7	Total	O	0	0
			7	7		
6	D	4	Total	O	0	0
			4	4		
6	H	3	Total	O	0	0
			3	3		
6	I	4	Total	O	0	0
			4	4		
6	J	3	Total	O	0	0
			3	3		
6	K	6	Total	O	0	0
			6	6		
6	L	5	Total	O	0	0
			5	5		
6	M	6	Total	O	0	0
			6	6		
6	N	6	Total	O	0	0
			6	6		
6	O	11	Total	O	0	0
			11	11		

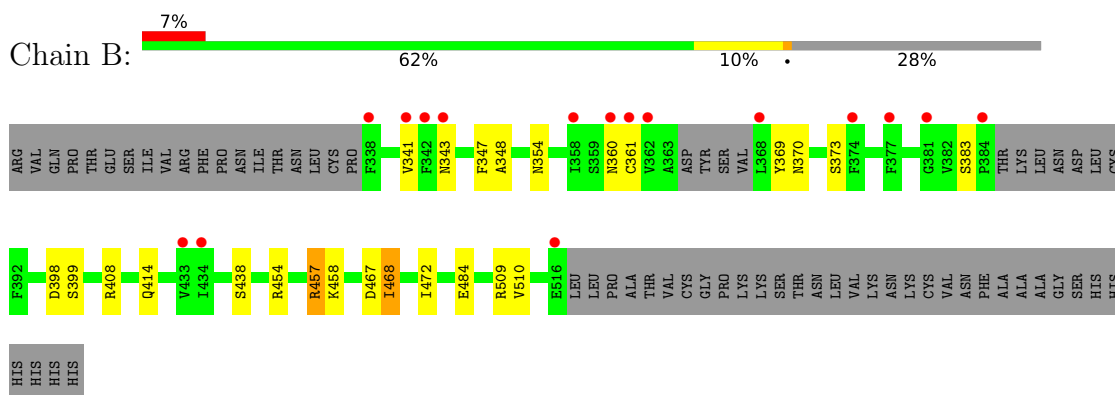
### 3 Residue-property plots [i](#)

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.

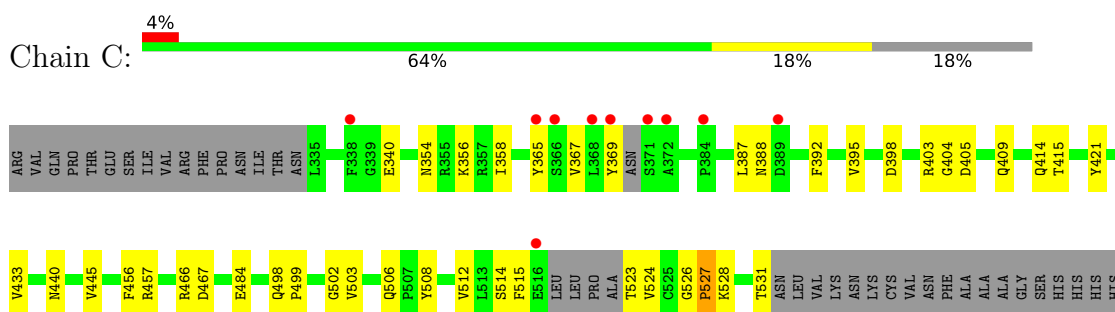
- Molecule 1: Spike protein S1



- Molecule 1: Spike protein S1



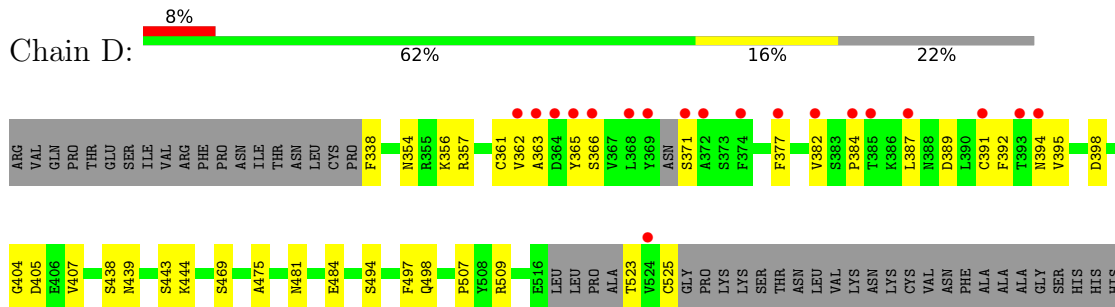
- Molecule 1: Spike protein S1





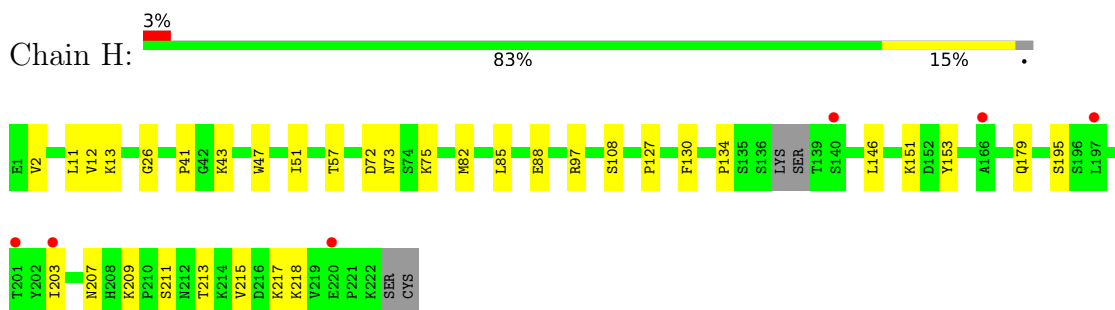
HIS  
HIS

• Molecule 1: Spike protein S1

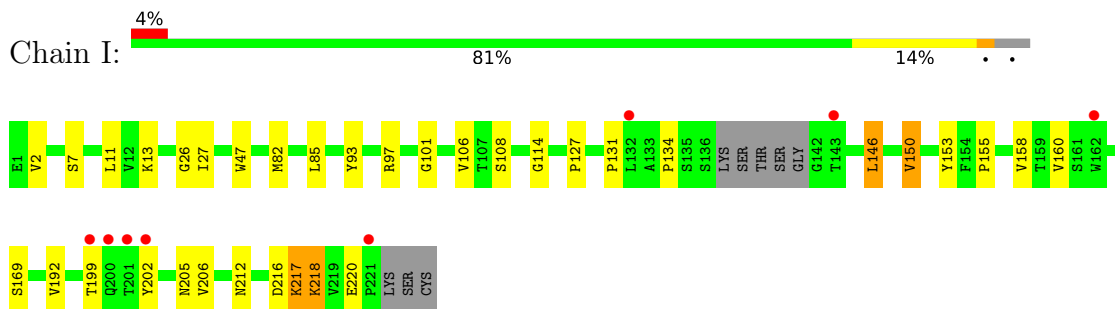


HIS  
HIS  
HIS

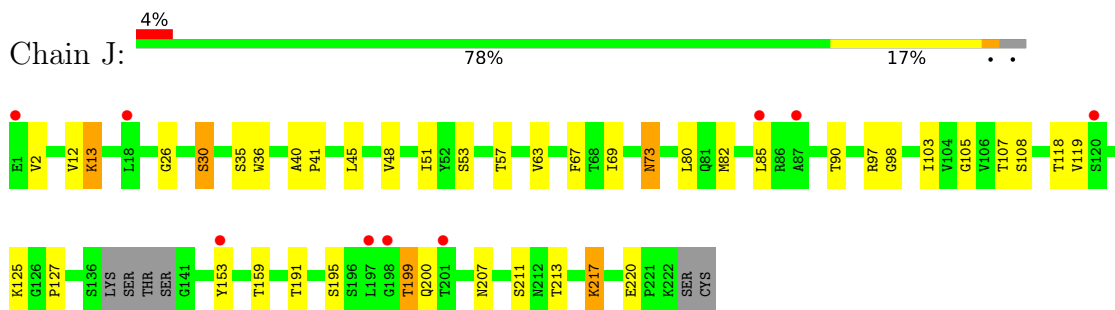
• Molecule 2: Immunoglobulin gamma-1 heavy chain



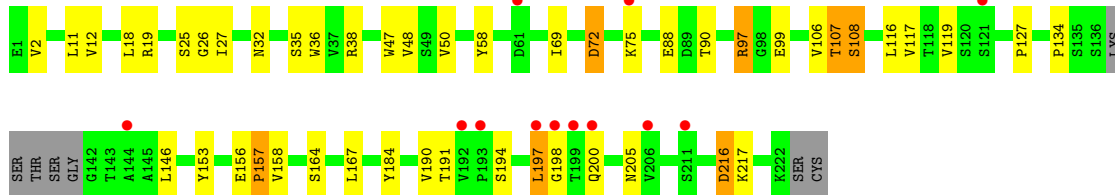
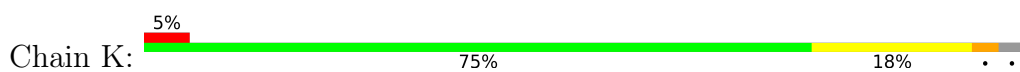
• Molecule 2: Immunoglobulin gamma-1 heavy chain



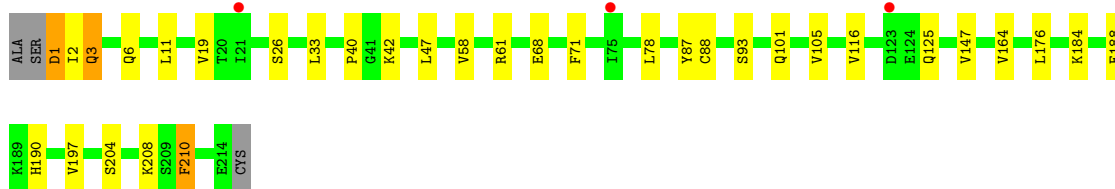
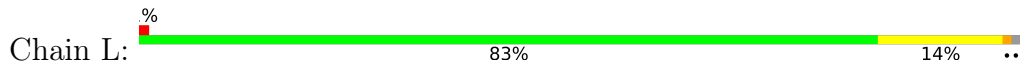
• Molecule 2: Immunoglobulin gamma-1 heavy chain



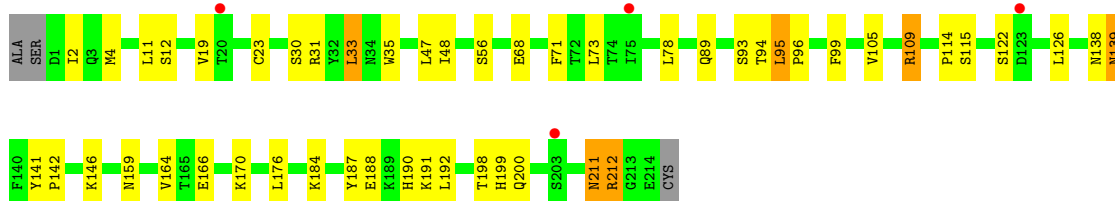
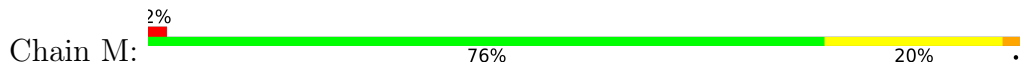
• Molecule 2: Immunoglobulin gamma-1 heavy chain



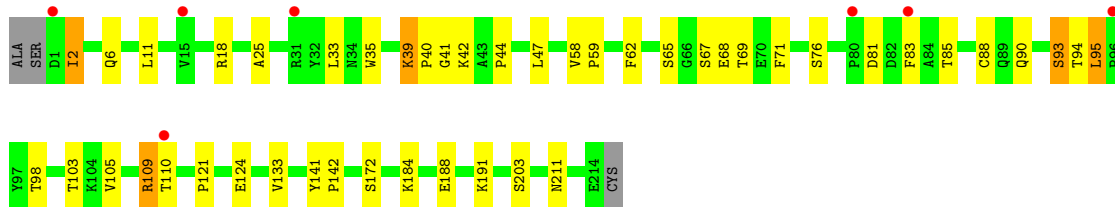
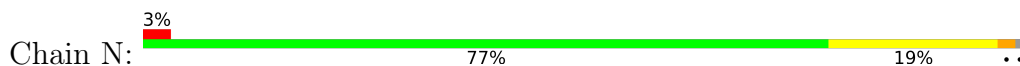
- Molecule 3: Immunoglobulin light chain



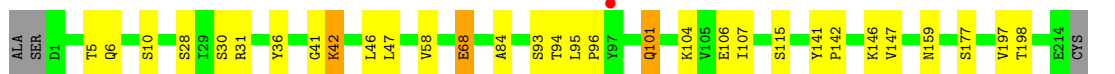
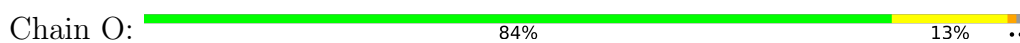
- Molecule 3: Immunoglobulin light chain



- Molecule 3: Immunoglobulin light chain



- Molecule 3: Immunoglobulin light chain



- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

IMAGE  
FUC2

- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

IMAGE  
FUC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.05Å 107.90Å 181.63Å 90.00° 99.45° 90.00°	Depositor
Resolution (Å)	48.28 – 2.80 48.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.28-2.80) 99.8 (48.28-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.81Å)	Xtrriage
Refinement program	PDB-REDO v1.0, PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.232 , 0.281 0.237 , 0.285	Depositor DCC
$R_{free}$ test set	8477 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.7	Xtrriage
Anisotropy	0.419	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	18843	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8134e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC

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	0.30	0/1406	0.54	0/1906
1	B	0.31	0/1383	0.52	0/1875
1	C	0.30	0/1548	0.53	0/2100
1	D	0.30	0/1483	0.54	0/2012
2	H	0.28	0/1649	0.55	0/2245
2	I	0.28	0/1634	0.56	0/2225
2	J	0.29	0/1636	0.57	0/2227
2	K	0.31	0/1632	0.58	1/2222 (0.0%)
3	L	0.28	0/1696	0.57	0/2302
3	M	0.29	0/1688	0.56	0/2291
3	N	0.30	0/1695	0.60	0/2301
3	O	0.28	0/1688	0.58	0/2291
All	All	0.29	0/19138	0.56	1/25997 (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
3	L	0	1
3	M	0	1
3	N	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	216	ASP	CB-CG-OD1	-5.05	113.75	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	1	ASP	Peptide
3	M	95	LEU	Peptide
3	N	83	PHE	Peptide

## 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	1368	0	1288	22	0
1	B	1346	0	1264	15	0
1	C	1508	0	1432	22	0
1	D	1445	0	1361	20	1
2	H	1615	0	1594	17	1
2	I	1597	0	1579	19	0
2	J	1602	0	1582	26	0
2	K	1598	0	1579	29	0
3	L	1657	0	1610	20	0
3	M	1652	0	1604	24	0
3	N	1656	0	1606	28	0
3	O	1652	0	1604	18	0
4	E	24	0	22	0	0
4	F	24	0	22	0	0
5	B	14	0	13	1	0
5	D	14	0	13	0	0
6	A	6	0	0	0	0
6	B	10	0	0	0	0
6	C	7	0	0	1	0
6	D	4	0	0	0	0
6	H	3	0	0	0	0
6	I	4	0	0	0	0
6	J	3	0	0	0	0
6	K	6	0	0	0	0
6	L	5	0	0	0	0
6	M	6	0	0	0	0
6	N	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	O	11	0	0	1	0
All	All	18843	0	18173	251	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 7.

All (251) 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)
3:N:109:ARG:HG3	3:N:109:ARG:HH11	1.39	0.87
2:K:90:THR:HG22	2:K:119:VAL:H	1.40	0.85
3:O:6:GLN:H	3:O:101:GLN:HE22	1.26	0.83
2:K:164:SER:H	2:K:205:ASN:HD21	1.22	0.82
1:D:365:TYR:HD1	1:D:387:LEU:HB3	1.45	0.80
2:J:40:ALA:HB1	2:J:41:PRO:HD2	1.63	0.80
3:O:104:LYS:NZ	6:O:301:HOH:O	2.18	0.76
3:L:2:ILE:O	3:L:26:SER:OG	2.02	0.76
1:C:484:GLU:OE2	2:I:13:LYS:NZ	2.18	0.75
2:I:134:PRO:HG3	2:I:146:LEU:HB3	1.68	0.75
2:J:45:LEU:HD21	3:N:44:PRO:HG2	1.69	0.74
2:I:205:ASN:ND2	2:I:216:ASP:OD1	2.15	0.73
3:N:6:GLN:OE1	3:N:103:THR:OG1	2.07	0.73
1:D:438:SER:HB3	1:D:509:ARG:HD2	1.71	0.72
2:J:90:THR:HG23	2:J:118:THR:HA	1.71	0.72
2:I:82:MET:HB3	2:I:85:LEU:HD21	1.73	0.70
3:M:19:VAL:HG21	3:M:78:LEU:HD13	1.73	0.70
2:H:203:ILE:HD11	2:H:218:LYS:HE2	1.74	0.69
3:N:109:ARG:HD2	3:N:172:SER:HB2	1.74	0.69
2:K:11:LEU:HD12	2:K:12:VAL:H	1.59	0.68
3:N:2:ILE:HD12	3:N:2:ILE:H	1.60	0.67
3:L:47:LEU:HA	3:L:58:VAL:HG21	1.76	0.67
1:D:365:TYR:CD1	1:D:387:LEU:HB3	2.30	0.66
3:N:90:GLN:HE21	3:N:98:THR:HG22	1.60	0.66
1:C:457:ARG:NH1	1:C:467:ASP:OD2	2.29	0.65
1:C:433:VAL:HG12	1:C:512:VAL:HG22	1.79	0.65
2:K:164:SER:H	2:K:205:ASN:ND2	1.93	0.65
2:H:134:PRO:HG3	2:H:146:LEU:HB3	1.77	0.64
2:H:211:SER:HG	2:H:213:THR:HG1	1.43	0.63
1:C:358:ILE:HB	1:C:395:VAL:HG13	1.79	0.63
2:K:194:SER:O	2:K:197:LEU:HG	2.00	0.62
3:L:6:GLN:HB2	3:L:101:GLN:NE2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2:VAL:HG22	2:I:26:GLY:HA3	1.82	0.61
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.82	0.61
2:J:35:SER:OG	2:J:98:GLY:O	2.18	0.61
1:A:355:ARG:HD3	1:A:398:ASP:OD1	2.01	0.60
2:I:218:LYS:HD2	2:I:220:GLU:OE1	2.02	0.60
3:M:11:LEU:HD22	3:M:105:VAL:HG22	1.83	0.60
2:H:72:ASP:OD2	2:H:75:LYS:HE2	2.02	0.60
1:C:456:PHE:CZ	2:J:105:GLY:HA3	2.36	0.59
2:H:151:LYS:NZ	2:H:179:GLN:HE22	1.99	0.59
3:M:146:LYS:HB3	3:M:198:THR:HB	1.85	0.59
2:I:192:VAL:HG21	2:I:202:TYR:OH	2.03	0.59
2:J:159:THR:HG22	2:J:207:ASN:HB3	1.84	0.59
1:A:372:ALA:O	1:A:373:SER:OG	2.20	0.59
2:I:27:ILE:HD12	2:I:97:ARG:HG3	1.84	0.59
1:B:454:ARG:HD3	1:B:457:ARG:HG3	1.85	0.58
3:L:147:VAL:HG22	3:L:197:VAL:HG22	1.84	0.58
3:O:147:VAL:HG12	3:O:197:VAL:HG22	1.84	0.58
2:K:97:ARG:O	2:K:108:SER:HA	2.04	0.58
3:L:11:LEU:HD22	3:L:105:VAL:HG22	1.85	0.58
2:K:164:SER:N	2:K:205:ASN:HD21	1.99	0.57
3:M:170:LYS:HA	3:M:170:LYS:HE2	1.85	0.57
3:O:6:GLN:N	3:O:101:GLN:HE22	1.99	0.57
1:C:409:GLN:HA	1:C:414:GLN:HG2	1.85	0.57
1:C:526:GLY:O	1:C:528:LYS:N	2.37	0.57
3:O:5:THR:HA	3:O:101:GLN:HE22	1.70	0.57
1:D:363:ALA:HB1	1:D:365:TYR:CZ	2.39	0.56
1:B:347:PHE:CD1	1:B:509:ARG:HD3	2.41	0.56
1:D:361:CYS:HA	1:D:362:VAL:HB	1.88	0.56
1:C:340:GLU:OE1	1:C:356:LYS:NZ	2.35	0.55
1:D:357:ARG:HE	1:D:394:ASN:HD21	1.53	0.55
2:J:13:LYS:N	2:J:13:LYS:HD2	2.21	0.55
3:L:6:GLN:HB2	3:L:101:GLN:HE22	1.70	0.55
3:N:39:LYS:NZ	3:N:81:ASP:O	2.37	0.55
2:I:27:ILE:CD1	2:I:97:ARG:HG3	2.37	0.55
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.88	0.55
3:N:109:ARG:HG3	3:N:109:ARG:NH1	2.15	0.55
3:O:5:THR:HA	3:O:101:GLN:NE2	2.21	0.55
1:A:403:ARG:HB2	1:A:406:GLU:HG3	1.89	0.54
2:H:51:ILE:HG13	2:H:57:THR:HG22	1.88	0.54
2:K:134:PRO:HG3	2:K:146:LEU:HB3	1.90	0.54
2:H:41:PRO:O	2:H:43:LYS:HE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:25:ALA:HB3	3:N:69:THR:HA	1.89	0.54
2:H:11:LEU:HD12	2:H:12:VAL:H	1.73	0.54
3:O:6:GLN:H	3:O:101:GLN:NE2	2.02	0.54
1:A:356:LYS:HD3	1:A:357:ARG:N	2.23	0.53
2:I:101:GLY:HA3	2:I:106:VAL:HG12	1.90	0.53
3:M:30:SER:OG	3:M:31:ARG:N	2.41	0.53
1:D:363:ALA:HB1	1:D:365:TYR:CE2	2.44	0.53
2:K:197:LEU:HD12	2:K:198:GLY:H	1.75	0.52
1:C:445:VAL:HG12	1:C:499:PRO:HG2	1.90	0.52
3:N:47:LEU:HA	3:N:58:VAL:HG21	1.91	0.52
1:A:367:VAL:HA	1:A:370:ASN:ND2	2.24	0.52
2:K:11:LEU:HD12	2:K:12:VAL:N	2.22	0.52
3:O:47:LEU:HA	3:O:58:VAL:HG21	1.90	0.52
1:B:408:ARG:NH1	1:B:414:GLN:OE1	2.43	0.52
3:L:19:VAL:HG21	3:L:78:LEU:HD13	1.91	0.52
1:C:354:ASN:O	1:C:398:ASP:HA	2.10	0.51
2:H:82:MET:HB3	2:H:85:LEU:HD21	1.91	0.51
2:J:127:PRO:HB3	2:J:153:TYR:HB3	1.92	0.51
1:A:403:ARG:HG3	1:A:495:TYR:CE1	2.45	0.51
1:C:388:ASN:HB3	1:C:527:PRO:HD2	1.91	0.51
3:L:2:ILE:HG13	3:L:93:SER:HB3	1.92	0.51
1:D:354:ASN:O	1:D:398:ASP:HA	2.10	0.51
2:K:47:TRP:HE1	2:K:50:VAL:HG13	1.74	0.51
2:K:88:GLU:OE2	2:K:88:GLU:N	2.30	0.51
3:L:6:GLN:HE22	3:L:87:TYR:HA	1.74	0.51
3:M:199:HIS:CD2	3:M:200:GLN:H	2.27	0.51
1:B:467:ASP:O	1:B:468:ILE:HG12	2.10	0.51
1:C:421:TYR:OH	2:J:53:SER:O	2.19	0.51
2:J:199:THR:HG23	2:J:200:GLN:OE1	2.09	0.51
3:M:114:PRO:HD3	3:M:199:HIS:ND1	2.25	0.51
3:L:164:VAL:HG22	3:L:176:LEU:HD12	1.92	0.51
3:N:109:ARG:NH1	3:N:110:THR:O	2.44	0.51
1:B:343:ASN:OD1	5:B:601:NAG:N2	2.44	0.50
1:A:403:ARG:HH21	1:A:405:ASP:HB2	1.76	0.50
3:N:94:THR:O	3:N:95:LEU:HB2	2.10	0.50
3:N:11:LEU:HD22	3:N:105:VAL:HG22	1.93	0.50
2:K:50:VAL:CG2	2:K:58:TYR:HB2	2.42	0.50
1:D:392:PHE:O	1:D:523:THR:N	2.45	0.49
3:N:59:PRO:HG2	3:N:62:PHE:HE2	1.78	0.49
3:O:30:SER:OG	3:O:31:ARG:N	2.46	0.49
3:M:35:TRP:CE2	3:M:73:LEU:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:156:GLU:HB3	2:K:157:PRO:HA	1.94	0.49
3:M:89:GLN:HB2	3:M:99:PHE:CD1	2.48	0.49
1:B:408:ARG:HH22	1:B:414:GLN:HE22	1.61	0.49
3:N:184:LYS:O	3:N:188:GLU:HG2	2.12	0.49
1:B:347:PHE:CE1	1:B:509:ARG:HB3	2.48	0.48
3:L:1:ASP:O	3:L:3:GLN:NE2	2.46	0.48
1:D:405:ASP:OD1	1:D:405:ASP:N	2.44	0.48
1:D:384:PRO:HA	1:D:387:LEU:HD23	1.96	0.48
2:H:97:ARG:O	2:H:108:SER:HA	2.14	0.48
2:J:51:ILE:HD12	2:J:57:THR:HG22	1.95	0.48
3:M:47:LEU:O	3:M:48:ILE:HD13	2.14	0.48
1:D:365:TYR:CE1	1:D:387:LEU:HD12	2.48	0.47
3:L:6:GLN:NE2	3:L:88:CYS:H	2.12	0.47
2:K:127:PRO:HB3	2:K:153:TYR:HB3	1.96	0.47
1:D:361:CYS:HB3	1:D:362:VAL:C	2.34	0.47
3:N:124:GLU:OE1	3:N:124:GLU:N	2.43	0.47
1:C:523:THR:HG23	1:C:524:VAL:HG13	1.97	0.47
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.95	0.47
2:K:2:VAL:HG22	2:K:26:GLY:HA3	1.97	0.47
3:L:6:GLN:HE21	3:L:88:CYS:H	1.63	0.47
1:C:503:VAL:HA	1:C:506:GLN:HE21	1.80	0.47
2:I:127:PRO:HB2	2:I:150:VAL:HG23	1.96	0.47
3:O:94:THR:C	3:O:96:PRO:HD2	2.35	0.47
1:C:456:PHE:HZ	2:J:105:GLY:HA3	1.77	0.46
1:C:523:THR:N	6:C:601:HOH:O	2.47	0.46
3:N:141:TYR:CD1	3:N:142:PRO:HA	2.50	0.46
1:B:438:SER:CB	1:B:509:ARG:HG3	2.45	0.46
2:K:35:SER:OG	2:K:50:VAL:HG12	2.15	0.46
1:B:472:ILE:HD12	1:B:484:GLU:HG2	1.97	0.46
2:J:211:SER:OG	2:J:213:THR:OG1	2.24	0.46
3:N:35:TRP:CZ3	3:N:88:CYS:HB3	2.50	0.46
2:J:63:VAL:HB	2:J:67:PHE:CD2	2.51	0.46
2:K:167:LEU:HD21	2:K:190:VAL:HG21	1.98	0.46
3:M:138:ASN:OD1	3:M:139:ASN:ND2	2.49	0.46
2:J:2:VAL:HG22	2:J:26:GLY:HA3	1.98	0.46
1:A:471:GLU:OE2	1:A:471:GLU:N	2.49	0.46
2:I:127:PRO:HB3	2:I:153:TYR:HB3	1.97	0.46
2:I:217:LYS:HD2	2:I:217:LYS:HA	1.86	0.46
2:K:38:ARG:HG2	2:K:48:VAL:CG2	2.45	0.46
1:D:497:PHE:CE2	1:D:507:PRO:HB3	2.51	0.45
2:K:72:ASP:OD2	2:K:75:LYS:N	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:116:LEU:HD12	2:K:117:VAL:N	2.31	0.45
1:C:502:GLY:O	1:C:506:GLN:HG3	2.17	0.45
3:M:93:SER:OG	3:M:94:THR:O	2.35	0.45
2:J:103:ILE:O	2:J:107:THR:HG23	2.16	0.45
3:M:141:TYR:CG	3:M:142:PRO:HA	2.52	0.45
3:O:141:TYR:CG	3:O:142:PRO:HA	2.52	0.45
1:B:354:ASN:O	1:B:398:ASP:HA	2.16	0.45
2:I:131:PRO:O	3:M:122:SER:OG	2.35	0.45
3:N:33:LEU:HD22	3:N:71:PHE:CG	2.52	0.45
1:A:399:SER:HA	1:A:510:VAL:O	2.16	0.45
1:B:348:ALA:HB2	1:B:354:ASN:OD1	2.16	0.45
2:J:82:MET:HB3	2:J:85:LEU:HD21	1.99	0.45
1:A:370:ASN:OD1	1:A:371:SER:N	2.50	0.44
2:H:82:MET:HE2	2:H:85:LEU:HD21	1.99	0.44
2:K:156:GLU:HG3	2:K:184:TYR:CE2	2.51	0.44
3:L:184:LYS:O	3:L:188:GLU:HG3	2.16	0.44
3:M:187:TYR:O	3:M:212:ARG:NH1	2.49	0.44
3:N:94:THR:O	3:N:94:THR:OG1	2.32	0.44
2:K:18:LEU:HD12	2:K:19:ARG:H	1.81	0.44
2:J:217:LYS:HD2	2:J:217:LYS:HA	1.66	0.44
3:M:33:LEU:HD22	3:M:71:PHE:CG	2.52	0.44
3:M:191:LYS:HG3	3:M:211:ASN:OD1	2.17	0.44
2:J:45:LEU:HD21	3:N:44:PRO:CG	2.45	0.44
3:N:2:ILE:HD12	3:N:2:ILE:N	2.29	0.44
3:N:2:ILE:HD13	3:N:90:GLN:NE2	2.33	0.44
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.53	0.44
1:A:367:VAL:HA	1:A:370:ASN:HD21	1.81	0.44
1:A:369:TYR:O	1:A:372:ALA:HB2	2.18	0.44
1:C:392:PHE:CD2	1:C:515:PHE:HB3	2.53	0.44
2:H:43:LYS:HA	2:H:43:LYS:HD3	1.88	0.44
3:M:109:ARG:HE	3:M:109:ARG:HB2	1.62	0.44
1:A:376:THR:HG23	1:A:378:LYS:HE3	1.99	0.44
2:J:12:VAL:O	2:J:119:VAL:HA	2.17	0.44
2:K:50:VAL:HG23	2:K:58:TYR:HB2	2.00	0.44
2:J:36:TRP:NE1	2:J:80:LEU:HB2	2.33	0.43
3:O:41:GLY:O	3:O:42:LYS:HD2	2.18	0.43
1:A:356:LYS:HG3	1:A:358:ILE:HD11	2.00	0.43
3:N:2:ILE:HD11	3:N:93:SER:HB2	2.00	0.43
3:M:164:VAL:HG22	3:M:176:LEU:HD12	2.01	0.43
1:A:398:ASP:O	1:A:511:VAL:HA	2.18	0.43
3:O:36:TYR:CE1	3:O:46:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:SER:HA	1:B:510:VAL:O	2.18	0.43
3:N:121:PRO:HD3	3:N:133:VAL:HG22	2.01	0.43
1:D:338:PHE:HE2	1:D:365:TYR:CD2	2.37	0.43
2:H:213:THR:HG22	2:H:215:VAL:HG23	2.01	0.43
2:H:130:PHE:CE2	3:L:125:GLN:HG3	2.54	0.43
3:O:106:GLU:HG2	3:O:107:ILE:N	2.34	0.43
3:L:116:VAL:O	3:L:208:LYS:HE2	2.18	0.43
1:A:354:ASN:O	1:A:398:ASP:HA	2.18	0.43
2:K:107:THR:O	2:K:108:SER:HB2	2.19	0.43
2:I:97:ARG:O	2:I:108:SER:HA	2.17	0.43
2:K:36:TRP:HD1	2:K:69:ILE:HD12	1.83	0.43
2:J:36:TRP:O	2:J:48:VAL:HG12	2.19	0.42
3:L:2:ILE:CG1	3:L:93:SER:HB3	2.49	0.42
1:B:408:ARG:NH2	1:B:414:GLN:HE22	2.17	0.42
1:C:440:ASN:OD1	1:C:440:ASN:N	2.50	0.42
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.54	0.42
3:O:159:ASN:OD1	3:O:159:ASN:N	2.52	0.42
3:M:212:ARG:HG3	3:M:212:ARG:HH11	1.84	0.42
2:J:13:LYS:HD2	2:J:13:LYS:H	1.84	0.42
1:A:403:ARG:NH2	1:A:405:ASP:HB2	2.35	0.42
2:J:36:TRP:HD1	2:J:69:ILE:HD12	1.85	0.42
3:N:2:ILE:HD11	3:N:93:SER:CB	2.49	0.42
3:N:41:GLY:O	3:N:42:LYS:HD3	2.20	0.42
1:A:337:PRO:HD2	1:A:360:ASN:HD21	1.85	0.42
2:H:207:ASN:HD21	2:H:209:LYS:HG3	1.84	0.42
2:I:11:LEU:HB2	2:I:155:PRO:HG3	2.01	0.42
3:O:101:GLN:CD	3:O:101:GLN:H	2.22	0.42
2:J:30:SER:HB3	2:J:73:ASN:ND2	2.35	0.41
1:D:443:SER:O	1:D:444:LYS:HD2	2.19	0.41
3:O:146:LYS:HB3	3:O:198:THR:HB	2.01	0.41
1:A:358:ILE:HB	1:A:395:VAL:CG1	2.50	0.41
2:K:99:GLU:O	2:K:99:GLU:HG2	2.21	0.41
3:N:191:LYS:HE2	3:N:211:ASN:HB3	2.02	0.41
1:C:404:GLY:HA2	1:C:508:TYR:CD1	2.55	0.41
2:H:2:VAL:HG22	2:H:26:GLY:HA3	2.03	0.41
2:I:160:VAL:HG12	2:I:206:VAL:HG22	2.02	0.41
1:D:475:ALA:HB1	2:K:32:ASN:HD21	1.84	0.41
2:I:192:VAL:HG21	2:I:202:TYR:CZ	2.55	0.41
3:M:188:GLU:HA	3:M:212:ARG:NH1	2.35	0.41
1:A:447:GLY:HA2	1:A:498:GLN:HG2	2.03	0.41
3:O:28:SER:OG	3:O:68:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ARG:NH2	1:C:405:ASP:OD1	2.54	0.41
1:D:438:SER:O	1:D:507:PRO:HG2	2.21	0.41
1:C:365:TYR:CD2	1:C:387:LEU:HB3	2.56	0.40
2:K:27:ILE:HD13	2:K:27:ILE:HA	1.98	0.40
3:M:2:ILE:HD12	3:M:2:ILE:N	2.36	0.40
3:M:199:HIS:CD2	3:M:200:GLN:N	2.89	0.40
1:B:472:ILE:CD1	1:B:484:GLU:HG2	2.52	0.40
3:L:210:PHE:CD1	3:L:210:PHE:C	2.94	0.40
3:M:4:MET:HE2	3:M:23:CYS:SG	2.62	0.40
1:D:404:GLY:O	1:D:407:VAL:HG23	2.22	0.40
2:I:93:TYR:O	2:I:114:GLY:HA2	2.21	0.40
2:J:97:ARG:O	2:J:108:SER:HA	2.21	0.40
1:D:382:VAL:HG22	1:D:387:LEU:HD22	2.03	0.40
3:L:42:LYS:HA	3:L:42:LYS:HD2	1.89	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:D:484:GLU:OE1	2:H:13:LYS:NZ[2_556]	2.09	0.11

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	165/232 (71%)	156 (94%)	9 (6%)	0	100 100
1	B	162/232 (70%)	148 (91%)	12 (7%)	2 (1%)	13 39
1	C	184/232 (79%)	174 (95%)	9 (5%)	1 (0%)	29 61
1	D	175/232 (75%)	163 (93%)	11 (6%)	1 (1%)	25 56
2	H	216/224 (96%)	209 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	213/224 (95%)	206 (97%)	7 (3%)	0	100	100
2	J	214/224 (96%)	204 (95%)	9 (4%)	1 (0%)	29	61
2	K	213/224 (95%)	204 (96%)	6 (3%)	3 (1%)	11	34
3	L	213/217 (98%)	201 (94%)	9 (4%)	3 (1%)	11	34
3	M	212/217 (98%)	200 (94%)	7 (3%)	5 (2%)	6	20
3	N	213/217 (98%)	197 (92%)	12 (6%)	4 (2%)	8	26
3	O	212/217 (98%)	199 (94%)	10 (5%)	3 (1%)	11	34
All	All	2392/2692 (89%)	2261 (94%)	108 (4%)	23 (1%)	15	44

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	370	ASN
2	J	199	THR
3	M	96	PRO
3	N	40	PRO
3	N	95	LEU
3	O	95	LEU
1	B	468	ILE
1	C	527	PRO
2	K	158	VAL
3	M	68	GLU
3	M	192	LEU
3	N	68	GLU
1	D	439	ASN
3	L	3	GLN
3	M	139	ASN
3	O	68	GLU
3	O	84	ALA
2	K	108	SER
3	L	68	GLU
3	M	95	LEU
3	L	40	PRO
3	N	39	LYS
2	K	157	PRO

### 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	148/202 (73%)	139 (94%)	9 (6%)	18	48
1	B	144/202 (71%)	136 (94%)	8 (6%)	21	51
1	C	165/202 (82%)	158 (96%)	7 (4%)	30	63
1	D	157/202 (78%)	145 (92%)	12 (8%)	13	36
2	H	182/186 (98%)	177 (97%)	5 (3%)	44	78
2	I	180/186 (97%)	170 (94%)	10 (6%)	21	51
2	J	180/186 (97%)	172 (96%)	8 (4%)	28	61
2	K	180/186 (97%)	170 (94%)	10 (6%)	21	51
3	L	190/191 (100%)	186 (98%)	4 (2%)	53	84
3	M	189/191 (99%)	177 (94%)	12 (6%)	18	46
3	N	189/191 (99%)	180 (95%)	9 (5%)	25	58
3	O	189/191 (99%)	183 (97%)	6 (3%)	39	73
All	All	2093/2316 (90%)	1993 (95%)	100 (5%)	25	58

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	VAL
1	A	355	ARG
1	A	357	ARG
1	A	371	SER
1	A	390	LEU
1	A	391	CYS
1	A	394	ASN
1	A	424	LYS
1	A	514	SER
1	B	341	VAL
1	B	360	ASN
1	B	361	CYS
1	B	369	TYR
1	B	373	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	383	SER
1	B	457	ARG
1	B	458	LYS
1	C	367	VAL
1	C	369	TYR
1	C	415	THR
1	C	466	ARG
1	C	498	GLN
1	C	514	SER
1	C	531	THR
1	D	356	LYS
1	D	366	SER
1	D	371	SER
1	D	377	PHE
1	D	389	ASP
1	D	391	CYS
1	D	395	VAL
1	D	469	SER
1	D	481	ASN
1	D	494	SER
1	D	498	GLN
1	D	525	CYS
2	H	47	TRP
2	H	73	ASN
2	H	88	GLU
2	H	195	SER
2	H	217	LYS
2	I	7	SER
2	I	47	TRP
2	I	146	LEU
2	I	150	VAL
2	I	158	VAL
2	I	169	SER
2	I	199	THR
2	I	212	ASN
2	I	217	LYS
2	I	218	LYS
2	J	13	LYS
2	J	30	SER
2	J	73	ASN
2	J	125	LYS
2	J	191	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	195	SER
2	J	217	LYS
2	J	220	GLU
2	K	25	SER
2	K	72	ASP
2	K	97	ARG
2	K	106	VAL
2	K	107	THR
2	K	191	THR
2	K	197	LEU
2	K	200	GLN
2	K	216	ASP
2	K	217	LYS
3	L	61	ARG
3	L	190	HIS
3	L	204	SER
3	L	210	PHE
3	M	12	SER
3	M	33	LEU
3	M	56	SER
3	M	109	ARG
3	M	115	SER
3	M	126	LEU
3	M	159	ASN
3	M	166	GLU
3	M	184	LYS
3	M	190	HIS
3	M	211	ASN
3	M	212	ARG
3	N	2	ILE
3	N	18	ARG
3	N	65	SER
3	N	67	SER
3	N	76	SER
3	N	85	THR
3	N	93	SER
3	N	109	ARG
3	N	203	SER
3	O	10	SER
3	O	42	LYS
3	O	93	SER
3	O	101	GLN

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Mol	Chain	Res	Type
3	O	115	SER
3	O	177	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	450	ASN
2	H	179	GLN
2	H	207	ASN
2	K	179	GLN
2	K	200	GLN
2	K	205	ASN
3	O	101	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](#)

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

## 5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

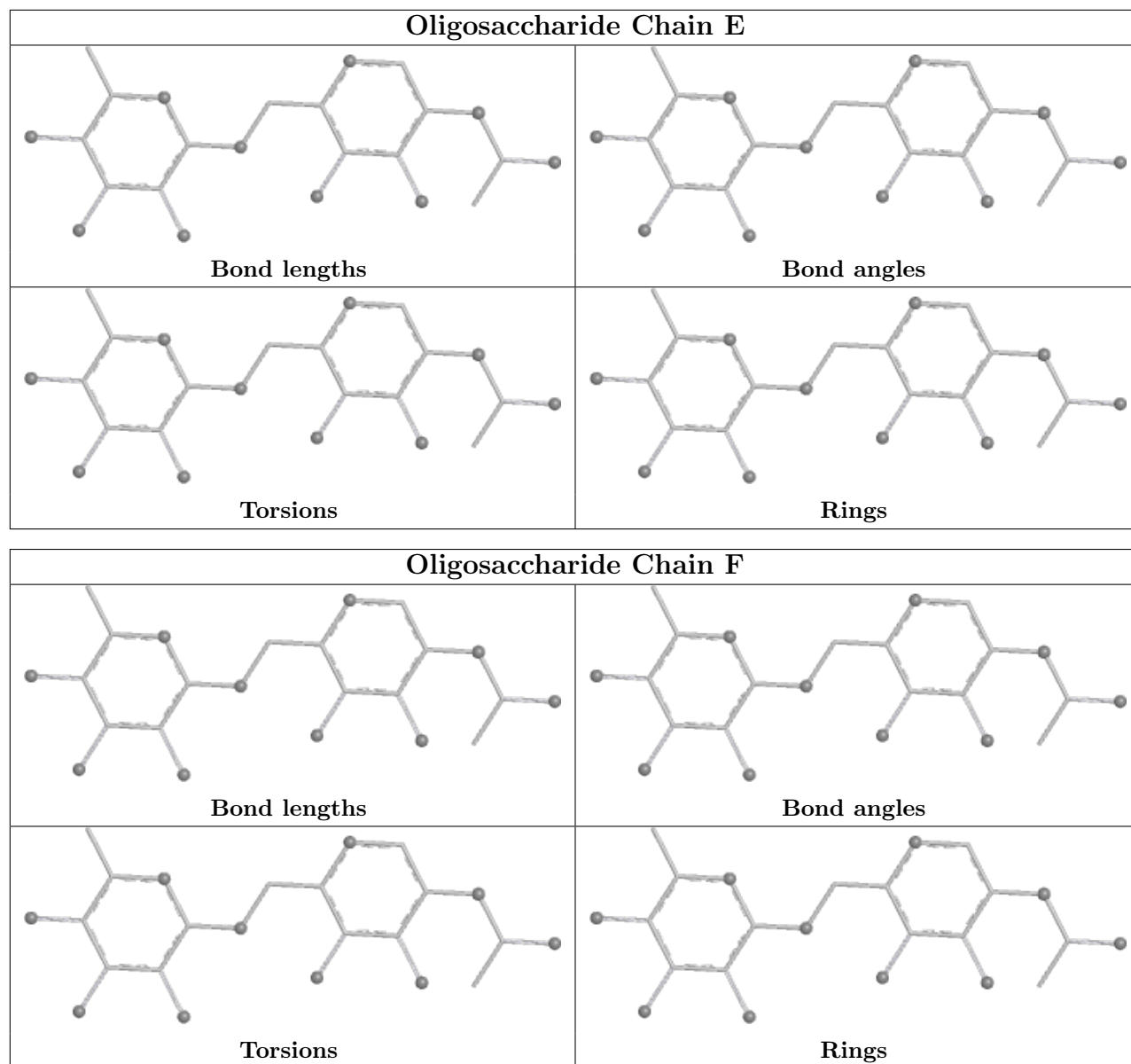
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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	171/232 (73%)	0.49	10 (5%) 23 15	42, 59, 88, 106	0
1	B	168/232 (72%)	0.57	16 (9%) 8 4	39, 63, 92, 107	0
1	C	190/232 (81%)	0.24	10 (5%) 26 17	35, 59, 86, 100	0
1	D	181/232 (78%)	0.49	19 (10%) 6 3	40, 67, 108, 143	0
2	H	220/224 (98%)	0.30	6 (2%) 54 44	34, 55, 87, 119	0
2	I	216/224 (96%)	0.30	8 (3%) 41 31	34, 56, 91, 103	0
2	J	218/224 (97%)	0.28	9 (4%) 37 27	41, 72, 94, 110	0
2	K	217/224 (96%)	0.36	12 (5%) 25 16	52, 69, 92, 114	0
3	L	214/217 (98%)	0.03	3 (1%) 75 70	41, 58, 73, 85	0
3	M	214/217 (98%)	0.14	4 (1%) 66 59	46, 67, 85, 99	0
3	N	214/217 (98%)	0.29	7 (3%) 46 36	39, 64, 93, 117	0
3	O	214/217 (98%)	0.12	1 (0%) 91 88	40, 59, 79, 93	0
All	All	2437/2692 (90%)	0.29	105 (4%) 35 25	34, 63, 92, 143	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	192	VAL	6.6
1	D	364	ASP	6.4
1	D	387	LEU	6.4
2	H	201	THR	5.0
1	D	362	VAL	5.0
1	D	369	TYR	4.8
1	B	338	PHE	4.8
3	M	203	SER	4.5
2	I	199	THR	4.5
2	K	144	ALA	4.4
2	J	201	THR	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	I	202	TYR	4.0
2	K	199	THR	3.8
2	K	193	PRO	3.8
1	A	384	PRO	3.7
1	B	381	GLY	3.7
1	D	371	SER	3.6
3	N	80	PRO	3.6
2	H	220	GLU	3.6
2	K	206	VAL	3.6
1	D	524	VAL	3.6
1	A	338	PHE	3.6
2	K	197	LEU	3.5
1	A	372	ALA	3.5
2	J	197	LEU	3.5
2	I	201	THR	3.5
2	K	211	SER	3.4
1	A	370	ASN	3.4
1	B	342	PHE	3.4
2	J	120	SER	3.3
2	J	198	GLY	3.3
1	B	377	PHE	3.3
1	D	393	THR	3.3
1	D	372	ALA	3.2
2	I	221	PRO	3.2
1	B	384	PRO	3.2
1	A	369	TYR	3.2
1	D	365	TYR	3.1
1	D	394	ASN	3.1
2	J	87	ALA	3.0
3	N	1	ASP	3.0
2	H	140	SER	2.9
2	I	200	GLN	2.9
2	H	197	LEU	2.9
1	B	358	ILE	2.8
3	N	83	PHE	2.8
1	D	385	THR	2.7
3	L	75	ILE	2.7
1	B	374	PHE	2.7
1	C	366	SER	2.7
2	K	198	GLY	2.7
1	B	343	ASN	2.6
1	B	361	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	L	123	ASP	2.6
1	C	516	GLU	2.6
3	M	20	THR	2.5
1	D	377	PHE	2.5
1	C	369	TYR	2.5
2	J	1	GLU	2.5
1	D	391	CYS	2.4
2	J	85	LEU	2.4
1	A	383	SER	2.4
1	D	368	LEU	2.4
1	B	368	LEU	2.4
2	I	132	LEU	2.4
3	N	96	PRO	2.4
3	O	97	TYR	2.4
1	C	389	ASP	2.4
2	K	121	SER	2.4
1	B	516	GLU	2.4
1	B	434	ILE	2.3
2	H	203	ILE	2.3
3	N	31[A]	ARG	2.3
1	C	371	SER	2.3
2	J	18	LEU	2.3
1	A	373	SER	2.3
1	B	433	VAL	2.3
1	B	341	VAL	2.2
1	B	362	VAL	2.2
1	A	342	PHE	2.2
1	C	365	TYR	2.2
1	D	374	PHE	2.2
3	M	75	ILE	2.2
1	B	360	ASN	2.2
1	C	338	PHE	2.2
1	C	368	LEU	2.2
1	D	384	PRO	2.2
3	N	15	VAL	2.2
1	D	363	ALA	2.2
2	H	166	ALA	2.1
2	K	200	GLN	2.1
2	I	143	THR	2.1
3	M	123	ASP	2.1
2	K	61	ASP	2.1
1	C	384	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	382	VAL	2.1
2	I	162	TRP	2.1
1	A	469	SER	2.1
1	A	513	LEU	2.1
1	C	372	ALA	2.0
3	N	110	THR	2.0
1	D	366	SER	2.0
2	K	75	LYS	2.0
3	L	21	ILE	2.0
2	J	153	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

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.

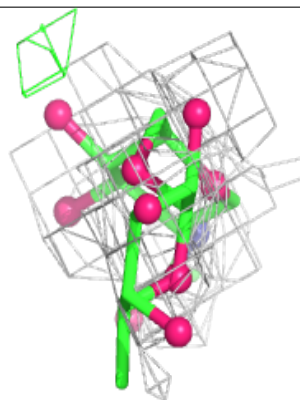
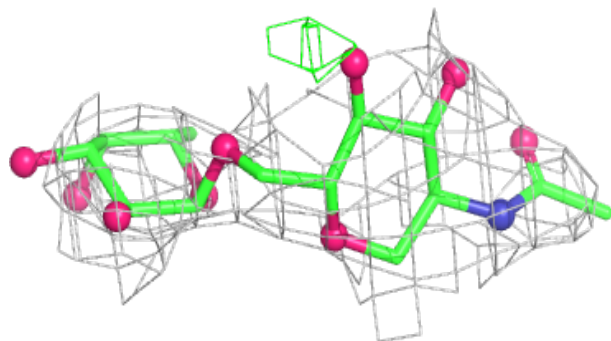
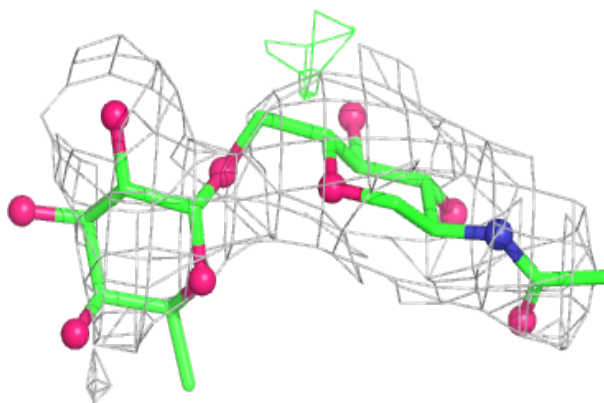
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
4	FUC	E	2	10/11	0.58	0.48	140,158,166,168	0
4	NAG	E	1	14/15	0.79	0.28	105,119,140,152	0
4	NAG	F	1	14/15	0.85	0.25	71,87,104,106	0
4	FUC	F	2	10/11	0.85	0.24	107,117,122,123	0

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.

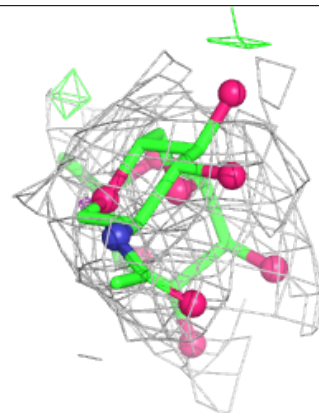
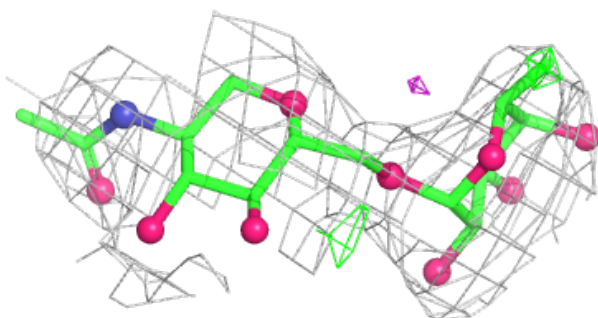
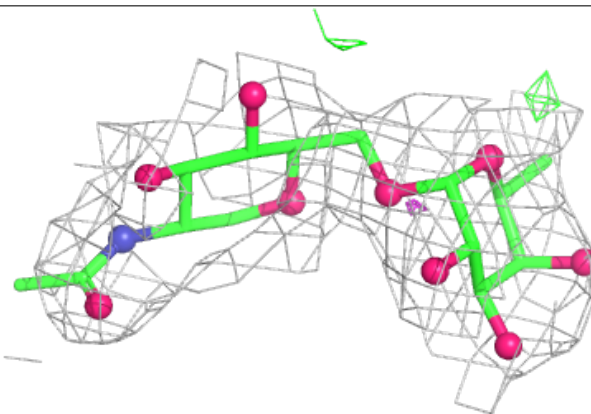


**Electron density around Chain E:**

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

**Electron density around Chain F:**

$2mF_o-DF_c$  (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
5	NAG	B	601	14/15	0.48	0.28	120,132,146,147	0
5	NAG	D	601	14/15	0.67	0.32	111,125,133,138	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.