



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 2, 2022 – 10:06 am BST

PDB ID : 2J6E  
Title : Crystal Structure of an Autoimmune Complex between a Human IgM Rheumatoid Factor and IgG1 Fc reveals a Novel Fc Epitope and Evidence for Affinity Maturation  
Authors : Duquerroy, S.; Stura, E.A.; Bressanelli, S.; Browne, H.; Beale, D.; Hamon, M.; Casali, P.; Vaney, M.C.; Rey, F.A.; Sutton, B.J.; Taussig, M.J.  
Deposited on : 2006-09-28  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.28.1  
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) : 2.28.1

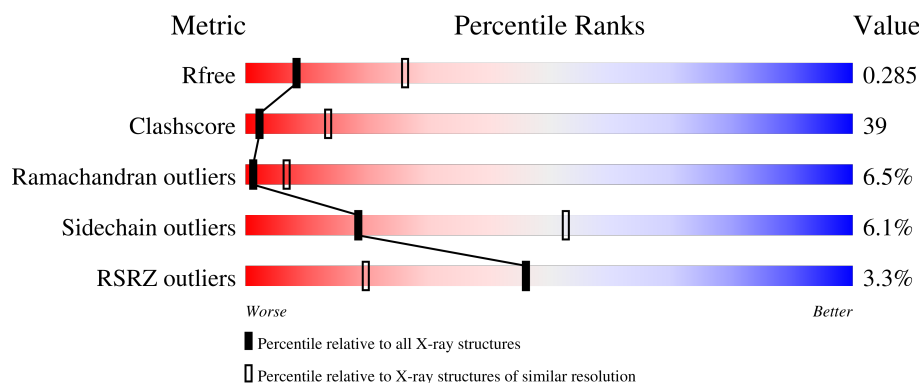
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



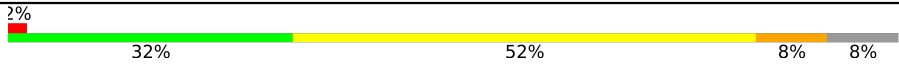

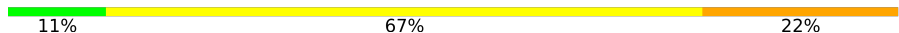
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	
1	B	232	
2	H	231	
2	I	231	
3	L	234	

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Mol	Chain	Length	Quality of chain
3	M	234	
4	C	9	
4	D	9	

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	NAG	C	5	X	-	-	-
8	MPD	A	504	-	-	X	X
8	MPD	A	505	-	-	-	X
8	MPD	A	506	-	-	-	X
8	MPD	B	503	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10195 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 IG GAMMA-1 CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	1
			1670	1062	282	320	6			
1	B	209	Total	C	N	O	S	0	0	1
			1667	1061	281	319	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	GLU	ASP	conflict	UNP P01857
B	270	GLU	ASP	conflict	UNP P01857

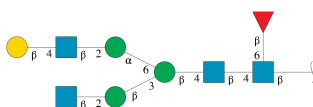
- Molecule 2 is a protein called IGM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1633	1029	275	323	6			
2	I	220	Total	C	N	O	S	0	0	0
			1660	1043	279	331	7			

- Molecule 3 is a protein called IGM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	1
			1587	993	270	320	4			
3	M	215	Total	C	N	O	S	0	0	0
			1602	1001	271	325	5			

- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	9	Total	C	N	O	0	0	0
			110	62	4	44			
4	D	9	Total	C	N	O	0	0	0
			110	62	4	44			

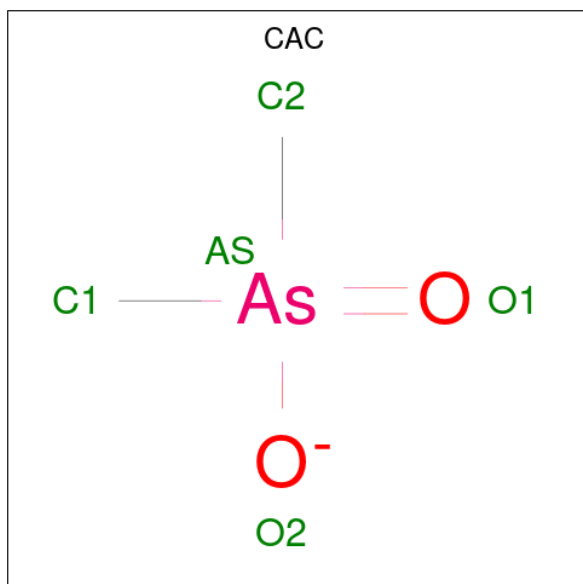
- Molecule 5 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cd	0	0
			1	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

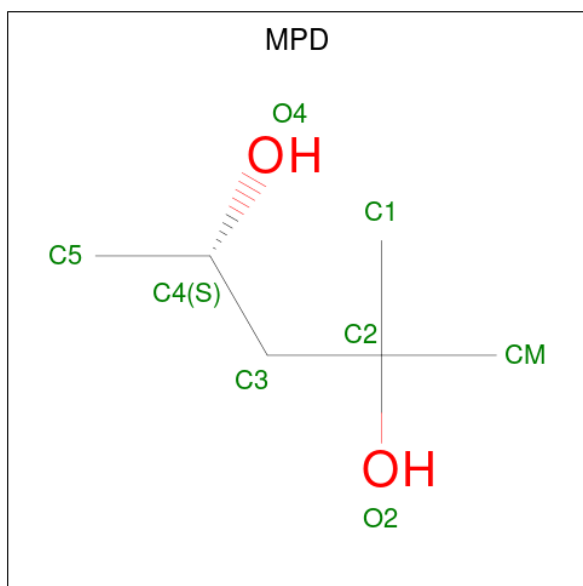
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



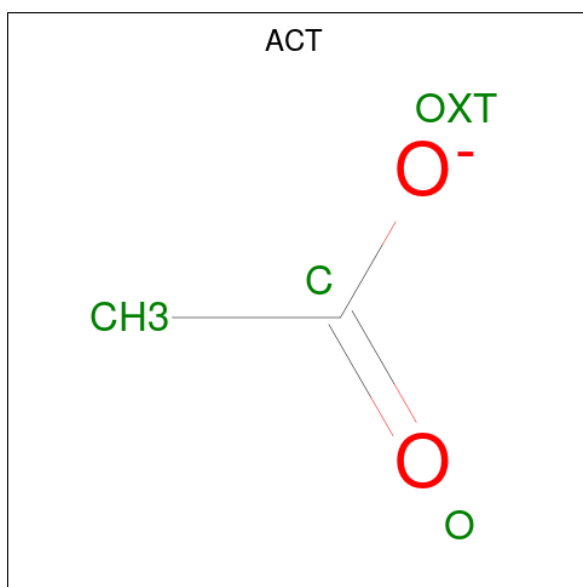
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			8	6	2		
8	A	1	Total	C	O	0	0
			8	6	2		
8	A	1	Total	C	O	0	0
			8	6	2		
8	B	1	Total	C	O	0	0
			8	6	2		
8	B	1	Total	C	O	0	0
			8	6	2		
8	M	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is water.

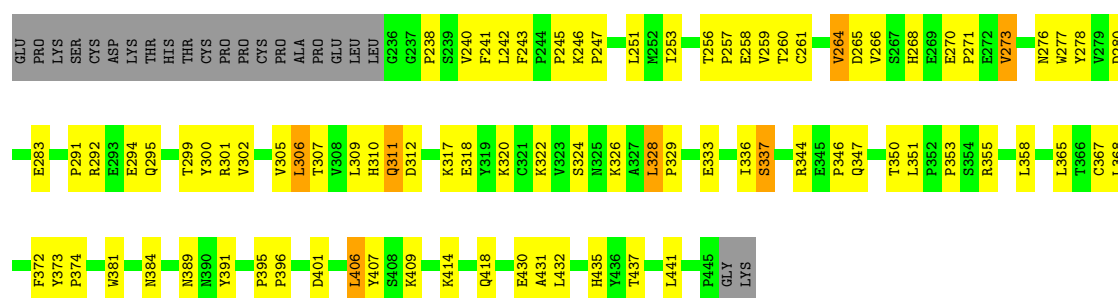
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	32	Total	O	0	0
			32	32		
10	B	16	Total	O	0	0
			16	16		
10	H	9	Total	O	0	0
			9	9		
10	I	20	Total	O	0	0
			20	20		
10	L	4	Total	O	0	0
			4	4		
10	M	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

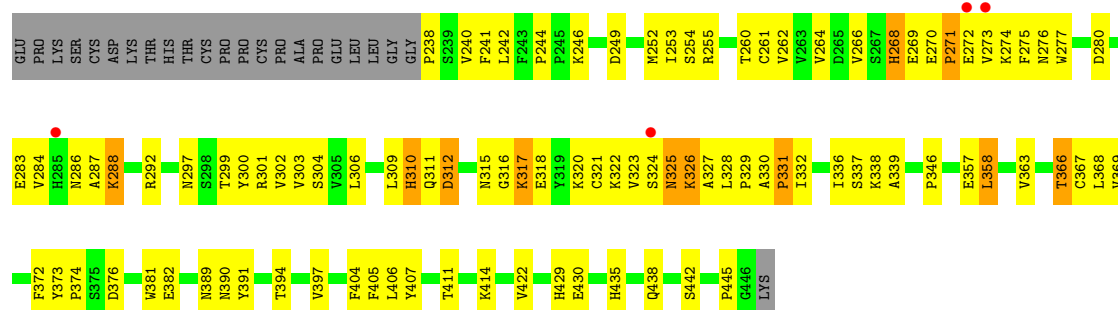
#### • Molecule 1: IG GAMMA-1 CHAIN C REGION

Chain A: 



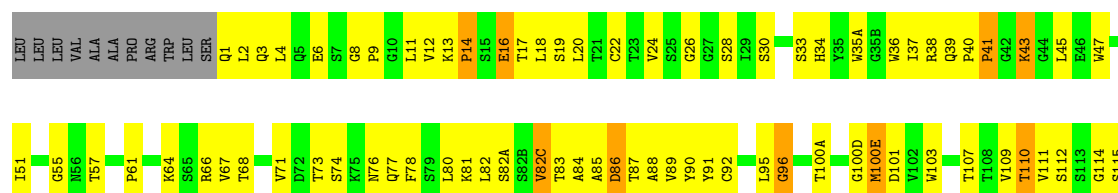
#### • Molecule 1: IG GAMMA-1 CHAIN C REGION

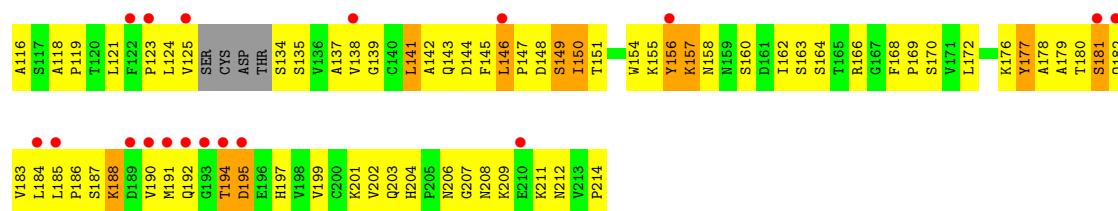
Chain B: 



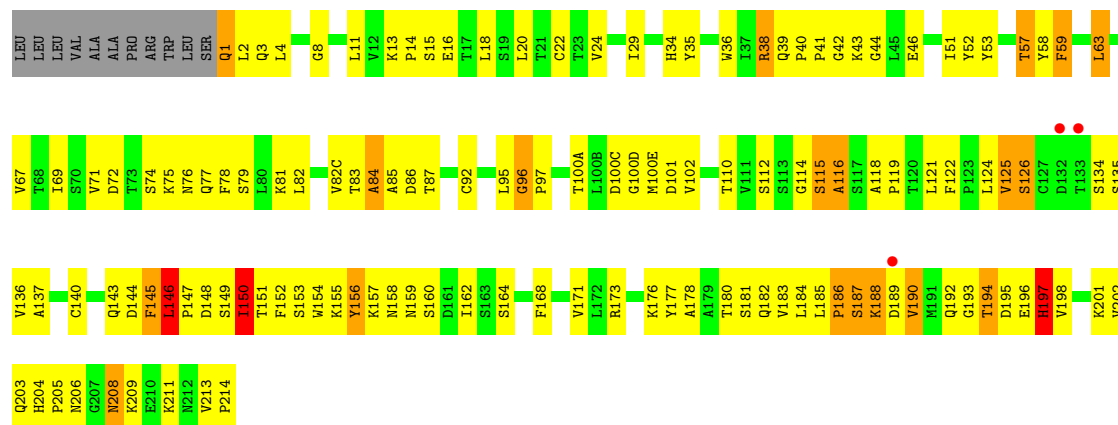
#### • Molecule 2: IGM

Chain H: 

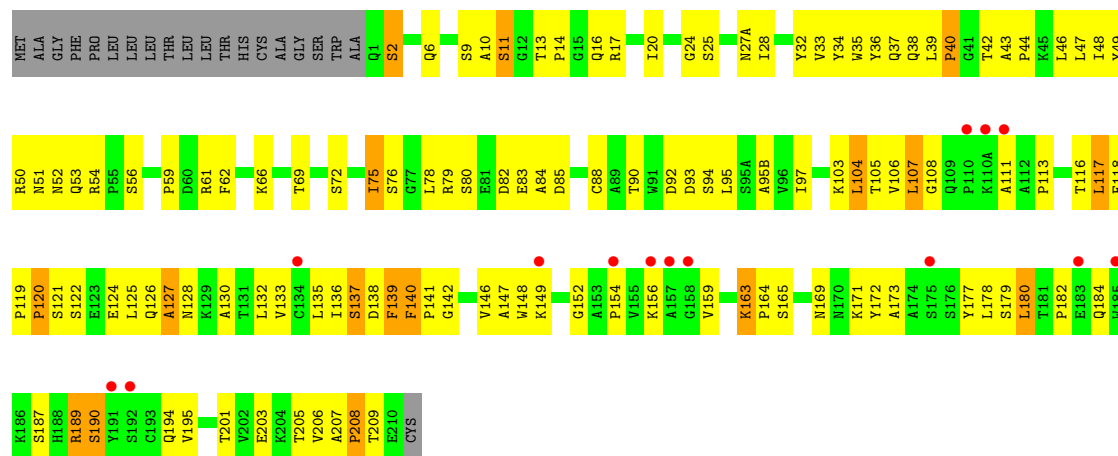




### • Molecule 2: IGM

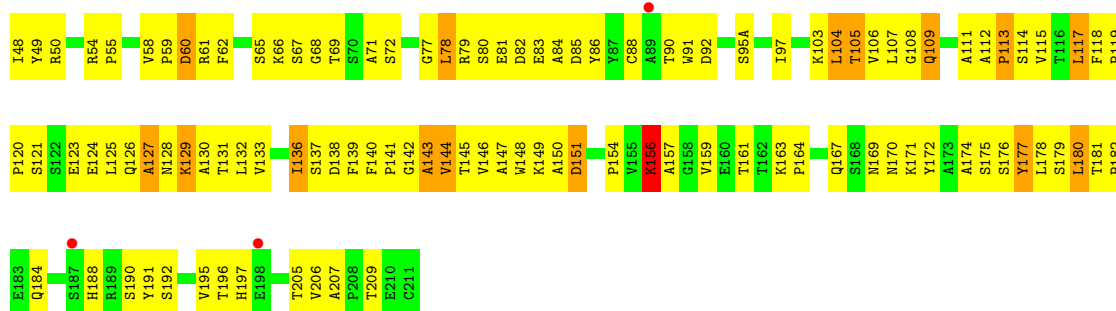


### • Molecule 3: IGM



### • Molecule 3: IGM





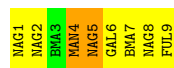
- Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 22% 22% 56%



- Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 11% 67% 22%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	241.98Å 75.61Å 102.40Å 90.00° 91.13° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00 24.72 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (25.00-3.00) 97.9 (24.72-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.223 , 0.288 0.221 , 0.285	Depositor DCC
$R_{free}$ test set	2601 reflections (7.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.3	Xtriage
Anisotropy	0.113	Xtriage
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>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10195	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: FUL, ZN, GAL, MPD, NAG, MAN, BMA, CD, ACT, CAC

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	0.51	0/1716	0.68	0/2338
1	B	0.43	0/1713	0.65	1/2335 (0.0%)
2	H	0.34	0/1672	0.62	0/2275
2	I	0.38	0/1699	0.69	1/2312 (0.0%)
3	L	0.35	0/1626	0.60	0/2220
3	M	0.34	0/1641	0.62	0/2238
All	All	0.40	0/10067	0.65	2/13718 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	PRO	N-CA-CB	5.66	110.09	103.30
2	I	92	CYS	CA-CB-SG	5.06	123.11	114.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1670	0	1635	84	0
1	B	1667	0	1631	93	0
2	H	1633	0	1596	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1660	0	1617	129	0
3	L	1587	0	1548	147	0
3	M	1602	0	1559	155	0
4	C	110	0	94	14	0
4	D	110	0	94	15	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	5	0	0	0	0
8	A	24	0	42	17	0
8	B	16	0	28	0	0
8	M	8	0	14	2	0
9	A	8	0	6	0	0
9	B	4	0	3	0	0
9	H	4	0	3	0	0
10	A	32	0	0	0	0
10	B	16	0	0	1	0
10	H	9	0	0	0	0
10	I	20	0	0	1	0
10	L	4	0	0	0	0
10	M	3	0	0	0	0
All	All	10195	0	9870	772	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 39.

The worst 5 of 772 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:L:16:GLN:HG2	3:L:17:ARG:H	1.18	1.09
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.35	1.06
3:M:79:ARG:HB3	3:M:79:ARG:NH1	1.82	0.95
3:L:80:SER:HA	3:L:106:VAL:HG11	1.48	0.94
2:I:96:GLY:HA3	2:I:100(A):THR:HG21	1.49	0.94

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	A	208/232 (90%)	194 (93%)	11 (5%)	3 (1%)	11	43
1	B	207/232 (89%)	173 (84%)	26 (13%)	8 (4%)	3	17
2	H	212/231 (92%)	152 (72%)	40 (19%)	20 (9%)	0	3
2	I	216/231 (94%)	171 (79%)	23 (11%)	22 (10%)	0	2
3	L	212/234 (91%)	152 (72%)	45 (21%)	15 (7%)	1	5
3	M	213/234 (91%)	153 (72%)	45 (21%)	15 (7%)	1	6
All	All	1268/1394 (91%)	995 (78%)	190 (15%)	83 (6%)	1	7

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	43	LYS
2	H	86	ASP
2	H	96	GLY
2	H	149	SER
2	H	156	TYR

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/215 (90%)	181 (93%)	13 (7%)	16	49
1	B	194/215 (90%)	185 (95%)	9 (5%)	27	64
2	H	185/198 (93%)	176 (95%)	9 (5%)	25	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	189/198 (96%)	177 (94%)	12 (6%)	18	51
3	L	177/193 (92%)	165 (93%)	12 (7%)	16	48
3	M	179/193 (93%)	166 (93%)	13 (7%)	14	44
All	All	1118/1212 (92%)	1050 (94%)	68 (6%)	18	53

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	60	ASP
3	M	104	LEU
3	M	156	LYS
2	H	82(C)	VAL
2	H	74	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	208	ASN
3	M	126	GLN
2	I	56	ASN
3	M	184	GLN
3	L	169	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 ⓘ

18 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	NAG	C	1	1,4	14,14,15	0.60	0	17,19,21	1.04	1 (5%)
4	NAG	C	2	4	14,14,15	0.55	0	17,19,21	0.94	0
4	BMA	C	3	4	11,11,12	0.67	0	15,15,17	0.73	0
4	MAN	C	4	4	11,11,12	0.47	0	15,15,17	0.55	0
4	NAG	C	5	4	14,14,15	0.66	0	17,19,21	1.11	1 (5%)
4	GAL	C	6	4	11,11,12	0.43	0	15,15,17	0.53	0
4	BMA	C	7	4	11,11,12	0.72	0	15,15,17	0.94	1 (6%)
4	NAG	C	8	4	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
4	FUL	C	9	4	10,10,11	0.47	0	14,14,16	0.92	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.66	0	17,19,21	0.74	0
4	NAG	D	2	4	14,14,15	0.68	0	17,19,21	0.67	0
4	BMA	D	3	4	11,11,12	0.58	0	15,15,17	0.44	0
4	MAN	D	4	4	11,11,12	0.57	0	15,15,17	0.85	1 (6%)
4	NAG	D	5	4	14,14,15	0.55	0	17,19,21	1.00	2 (11%)
4	GAL	D	6	4	11,11,12	0.49	0	15,15,17	0.39	0
4	BMA	D	7	4	11,11,12	0.73	0	15,15,17	0.76	0
4	NAG	D	8	4	14,14,15	0.58	0	17,19,21	0.63	0
4	FUL	D	9	4	10,10,11	0.45	0	14,14,16	0.58	0

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

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

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5	NAG	C2-N2-C7	-2.86	118.83	122.90
4	D	4	MAN	C1-O5-C5	2.68	115.82	112.19
4	D	5	NAG	C4-C3-C2	-2.51	107.34	111.02
4	C	8	NAG	C2-N2-C7	-2.37	119.52	122.90
4	D	5	NAG	C2-N2-C7	-2.28	119.65	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	5	NAG	C1

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C8-C7-N2-C2
4	C	2	NAG	O7-C7-N2-C2
4	C	5	NAG	C8-C7-N2-C2
4	C	5	NAG	O7-C7-N2-C2
4	C	8	NAG	C8-C7-N2-C2

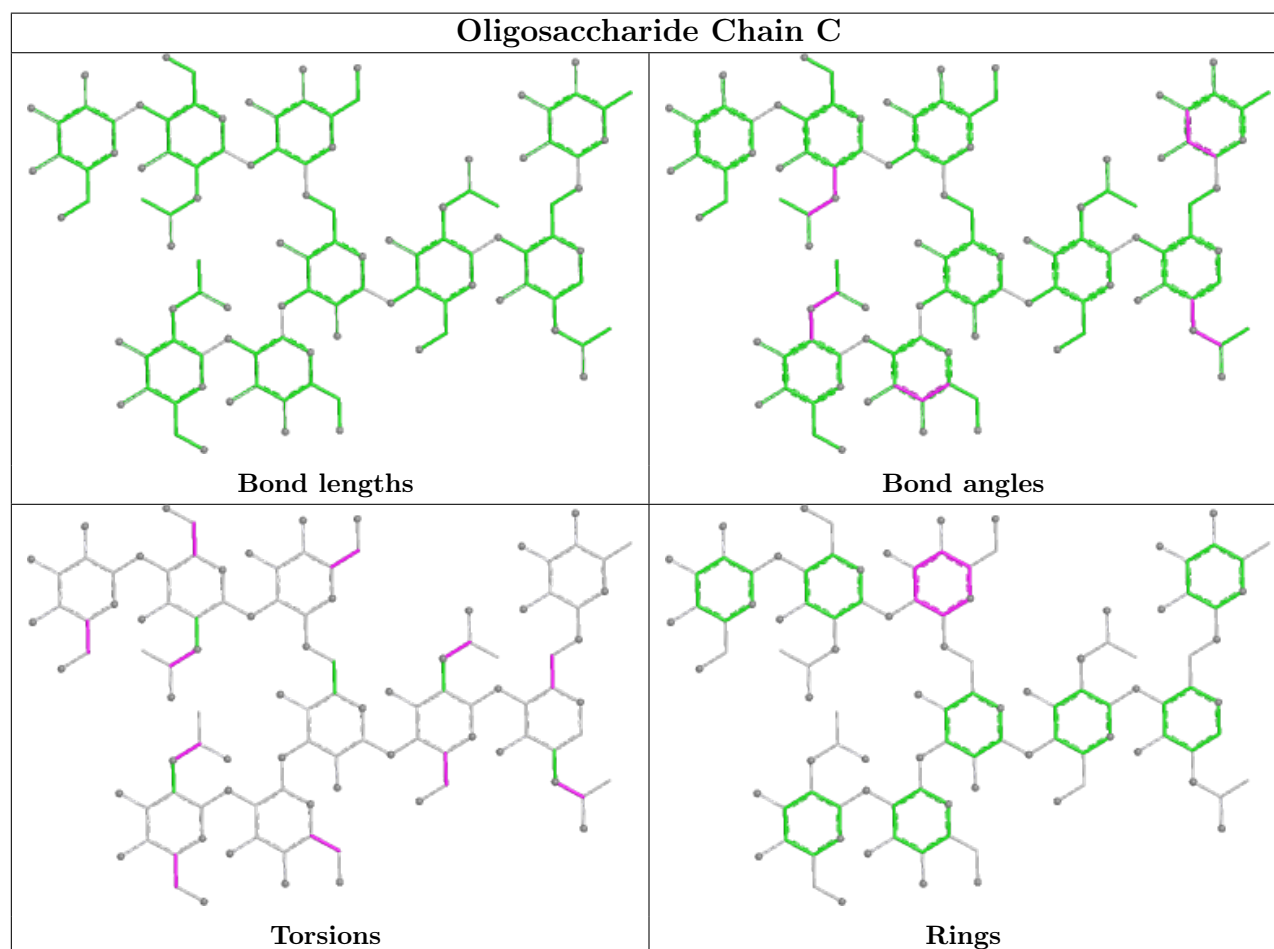
All (2) ring outliers are listed below:

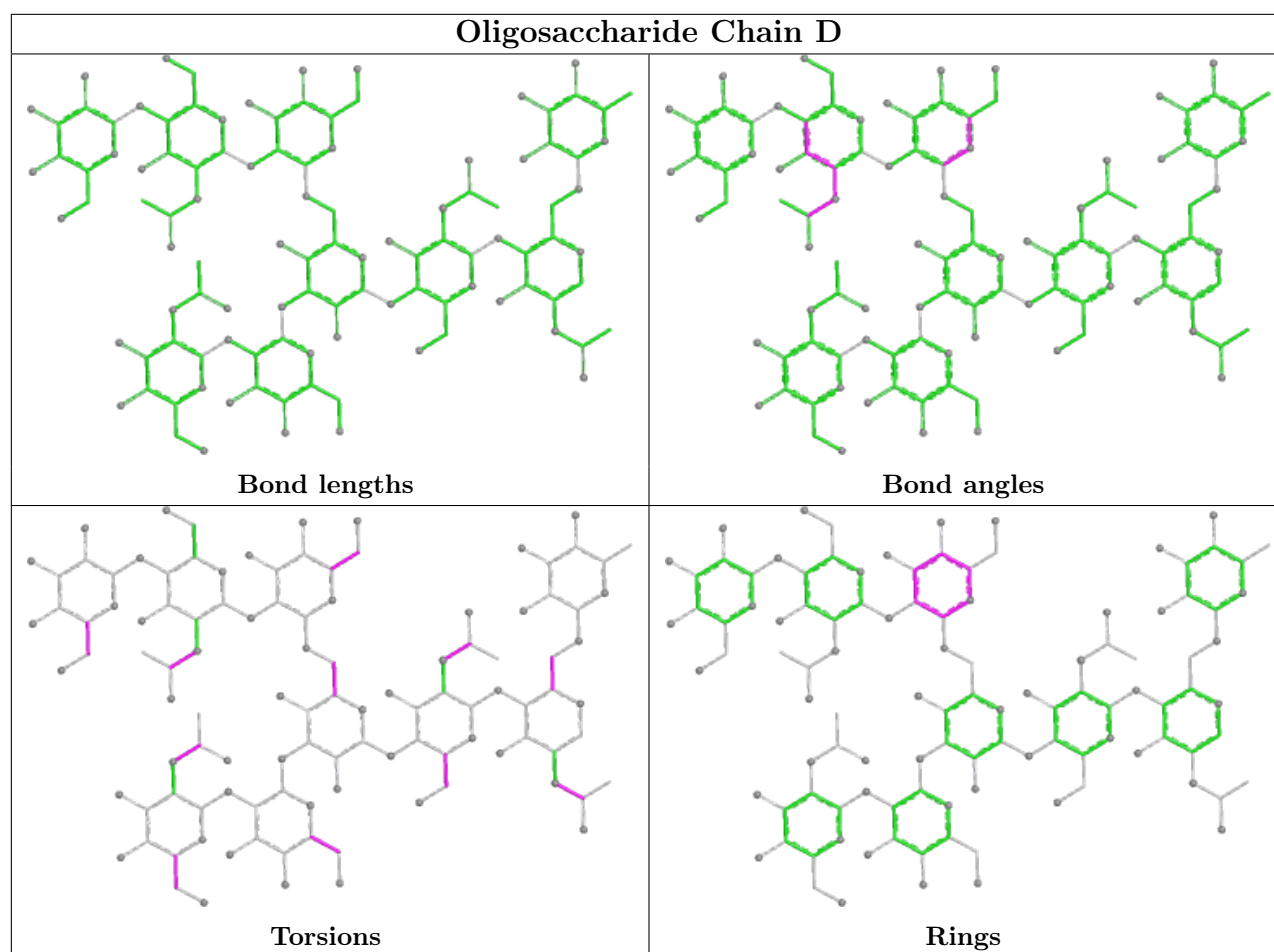
Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C1-C2-C3-C4-C5-O5
4	C	4	MAN	C1-C2-C3-C4-C5-O5

15 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5	NAG	4	0
4	C	6	GAL	5	0
4	C	9	FUL	2	0
4	D	2	NAG	5	0
4	C	8	NAG	2	0
4	C	1	NAG	2	0
4	C	5	NAG	3	0
4	D	8	NAG	2	0
4	D	9	FUL	1	0
4	D	1	NAG	2	0
4	D	4	MAN	3	0
4	D	6	GAL	3	0
4	C	2	NAG	4	0
4	D	7	BMA	2	0
4	C	7	BMA	2	0

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





## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	ACT	H	301	-	1,3,3	1.36	0	0,3,3	-	-
8	MPD	B	502	-	7,7,7	0.49	0	9,10,10	0.45	0
8	MPD	B	503	-	7,7,7	0.55	0	9,10,10	0.46	0
8	MPD	M	301	-	7,7,7	0.50	0	9,10,10	0.50	0
9	ACT	B	504	-	1,3,3	0.43	0	0,3,3	-	-
9	ACT	A	508	-	1,3,3	1.28	0	0,3,3	-	-
8	MPD	A	505	-	7,7,7	0.63	0	9,10,10	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ACT	A	507	-	1,3,3	0.87	0	0,3,3	-	-
8	MPD	A	504	-	7,7,7	0.55	0	9,10,10	0.49	0
8	MPD	A	506	-	7,7,7	0.74	0	9,10,10	0.62	0
7	CAC	A	503	6	0,4,4	-	-	0,6,6	-	-

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	MPD	B	502	-	-	0/5/5/5	-
8	MPD	B	503	-	-	2/5/5/5	-
8	MPD	M	301	-	-	1/5/5/5	-
8	MPD	A	505	-	-	0/5/5/5	-
8	MPD	A	504	-	-	0/5/5/5	-
8	MPD	A	506	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	506	MPD	C1-C2-C3-C4
8	B	503	MPD	C1-C2-C3-C4
8	B	503	MPD	O2-C2-C3-C4
8	M	301	MPD	O2-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	301	MPD	2	0
8	A	505	MPD	2	0
8	A	504	MPD	13	0
8	A	506	MPD	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	127:CYS	C	132:ASP	N	15.42

## 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	210/232 (90%)	-0.67	0 <span>100</span> <span>100</span>	24, 39, 56, 68	0
1	B	209/232 (90%)	-0.27	4 (1%) <span>66</span> <span>37</span>	23, 56, 131, 140	0
2	H	216/231 (93%)	0.19	18 (8%) <span>11</span> <span>3</span>	32, 77, 151, 152	0
2	I	220/231 (95%)	-0.30	3 (1%) <span>75</span> <span>49</span>	24, 56, 133, 146	0
3	L	214/234 (91%)	0.21	14 (6%) <span>18</span> <span>5</span>	36, 89, 151, 152	0
3	M	215/234 (91%)	0.02	4 (1%) <span>66</span> <span>37</span>	45, 95, 138, 141	0
All	All	1284/1394 (92%)	-0.13	43 (3%) <span>46</span> <span>20</span>	23, 67, 148, 152	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	194	THR	4.9
1	B	324	SER	4.8
2	H	184	LEU	4.8
2	H	146	LEU	4.6
3	L	183	GLU	3.4

### 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](#)

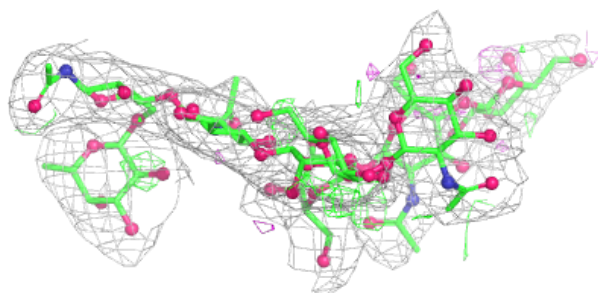
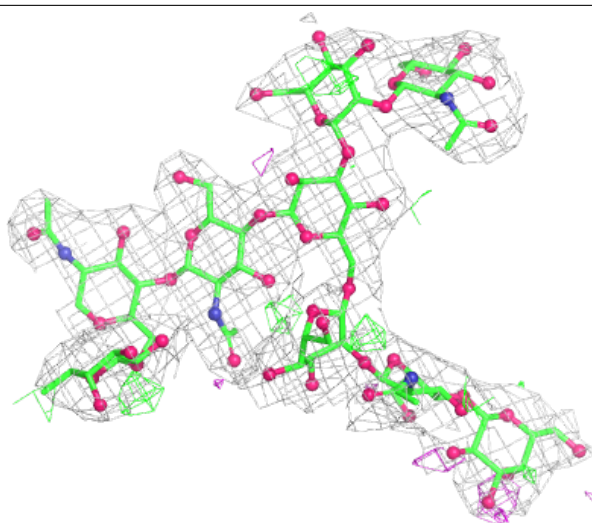
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

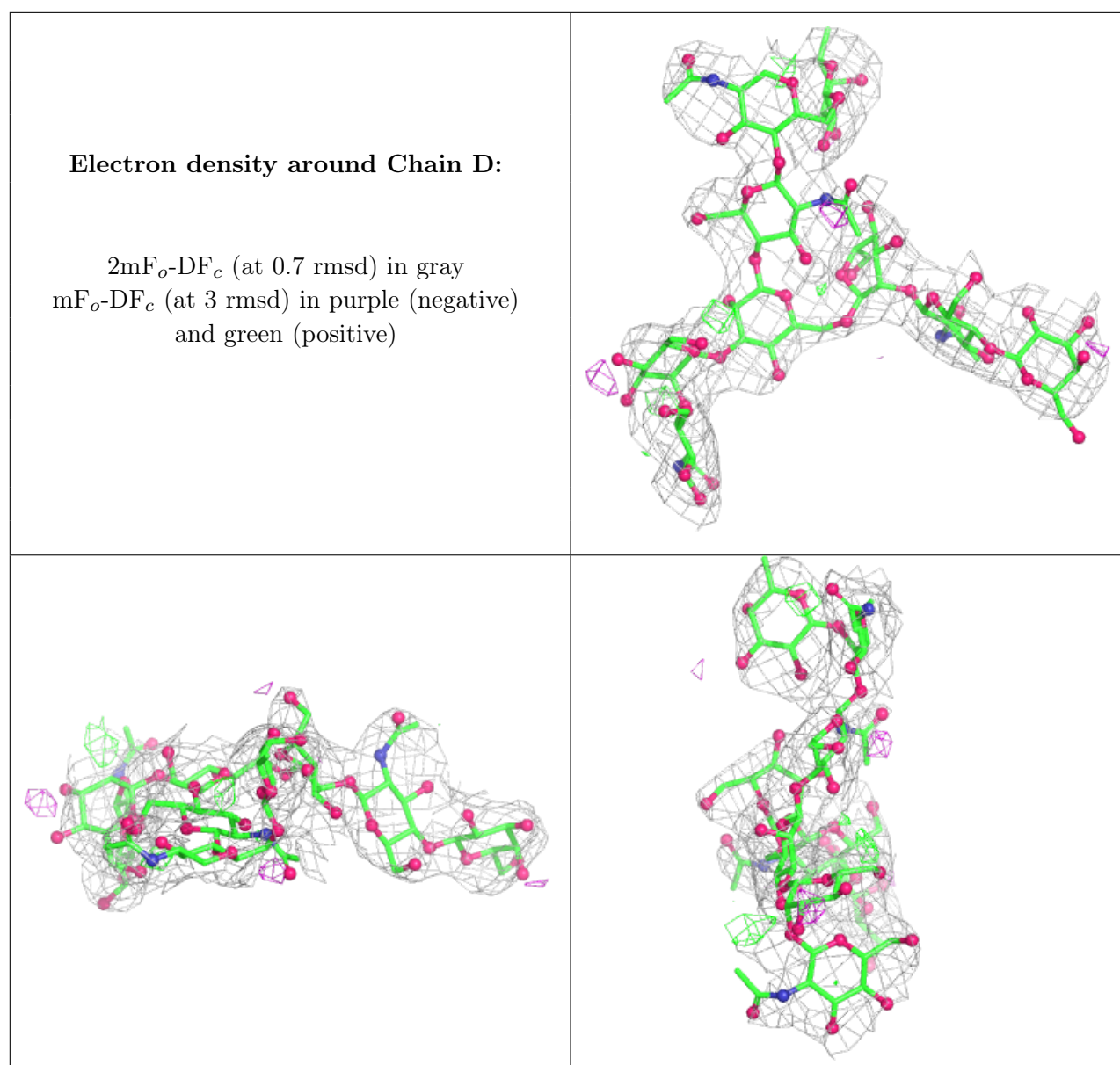
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FUL	D	9	10/11	0.80	0.25	119,119,120,120	0
4	NAG	D	8	14/15	0.81	0.26	119,121,122,122	0
4	BMA	D	7	11/12	0.83	0.27	112,117,118,119	0
4	MAN	D	4	11/12	0.84	0.32	108,109,110,110	0
4	NAG	C	8	14/15	0.84	0.23	88,91,92,92	0
4	NAG	D	1	14/15	0.84	0.22	118,122,123,123	0
4	NAG	D	2	14/15	0.84	0.19	120,122,126,126	0
4	NAG	D	5	14/15	0.85	0.17	106,107,108,109	0
4	GAL	D	6	11/12	0.86	0.23	108,108,109,110	0
4	GAL	C	6	11/12	0.88	0.24	53,56,61,61	0
4	BMA	D	3	11/12	0.88	0.23	112,117,119,120	0
4	BMA	C	7	11/12	0.89	0.19	71,78,82,83	0
4	MAN	C	4	11/12	0.93	0.11	49,50,52,54	0
4	NAG	C	5	14/15	0.93	0.15	50,51,57,59	0
4	FUL	C	9	10/11	0.95	0.14	45,48,51,51	0
4	BMA	C	3	11/12	0.95	0.11	45,47,51,62	0
4	NAG	C	1	14/15	0.97	0.15	32,34,40,45	0
4	NAG	C	2	14/15	0.97	0.13	34,36,39,40	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 C:**

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





## 6.4 Ligands ⓘ

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
8	MPD	A	506	8/8	0.72	0.50	81,81,81,81	0
8	MPD	A	504	8/8	0.73	0.48	92,95,96,98	0
9	ACT	H	301	4/4	0.75	0.30	81,81,81,81	0
8	MPD	B	503	8/8	0.76	0.52	82,83,84,84	0
8	MPD	A	505	8/8	0.76	0.59	81,83,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ZN	B	501	1/1	0.77	0.15	143,143,143,143	0
8	MPD	B	502	8/8	0.82	0.17	81,83,83,84	0
9	ACT	A	508	4/4	0.85	0.32	85,85,85,85	0
8	MPD	M	301	8/8	0.88	0.29	81,81,81,81	0
9	ACT	B	504	4/4	0.94	0.22	81,81,81,81	0
9	ACT	A	507	4/4	0.96	0.21	64,65,65,66	0
6	ZN	A	502	1/1	0.98	0.04	43,43,43,43	0
7	CAC	A	503	5/5	0.98	0.09	83,84,84,87	0
5	CD	A	501	1/1	0.99	0.06	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.