



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 17, 2024 – 06:03 pm BST

PDB ID : 6S08  
Title : Crystal Structure of Properdin (TSR domains N1 & 456)  
Authors : van den Bos, R.M.; Pearce, N.M.; Gros, P.  
Deposited on : 2019-06-14  
Resolution : 2.03 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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 : 2.37.1  
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) : 2.37.1

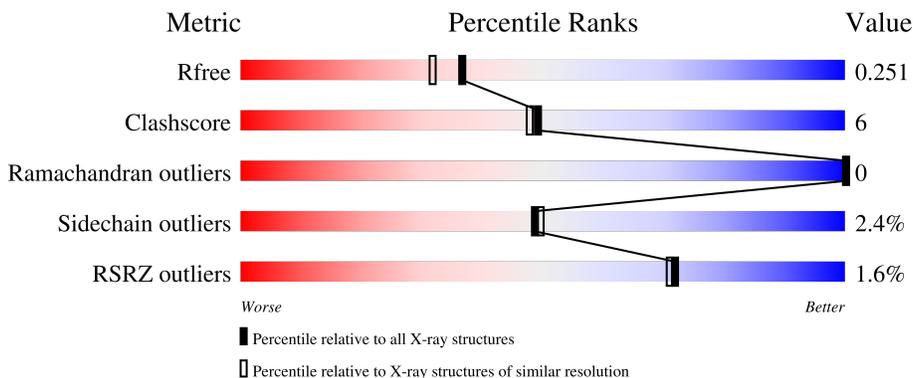
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	225	 80% 12% 8%
2	B	110	 76% 18% 5%
3	C	2	 100%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 2589 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 Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	206	1567	971	293	282	21	0	1	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	-	expression tag	UNP P27918
A	255	SER	-	expression tag	UNP P27918
A	470	ALA	-	expression tag	UNP P27918
A	471	ALA	-	expression tag	UNP P27918
A	472	ALA	-	expression tag	UNP P27918
A	473	HIS	-	expression tag	UNP P27918
A	474	HIS	-	expression tag	UNP P27918
A	475	HIS	-	expression tag	UNP P27918
A	476	HIS	-	expression tag	UNP P27918
A	477	HIS	-	expression tag	UNP P27918
A	478	HIS	-	expression tag	UNP P27918

- Molecule 2 is a protein called Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	105	776	476	137	151	12	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

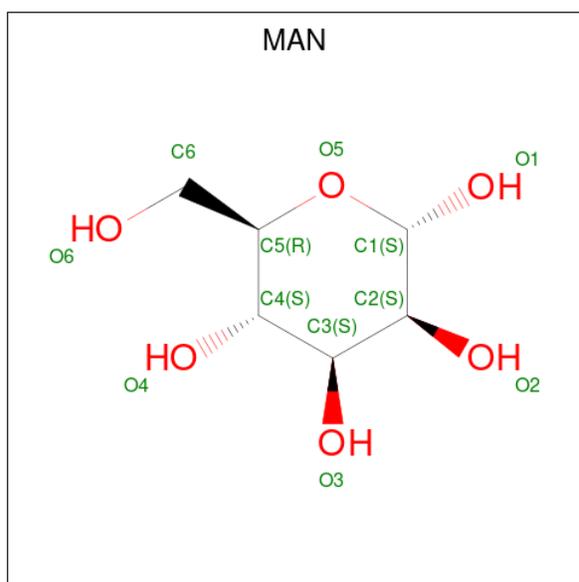
Chain	Residue	Modelled	Actual	Comment	Reference
B	133	ALA	-	expression tag	UNP P27918
B	134	ALA	-	expression tag	UNP P27918
B	135	ALA	-	expression tag	UNP P27918

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose.



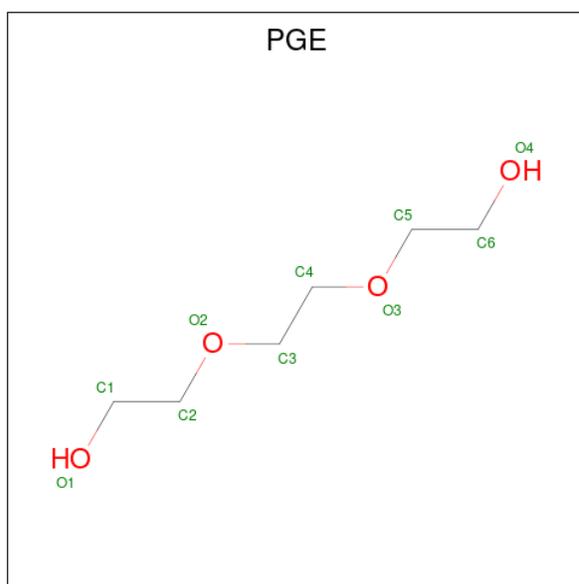
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).

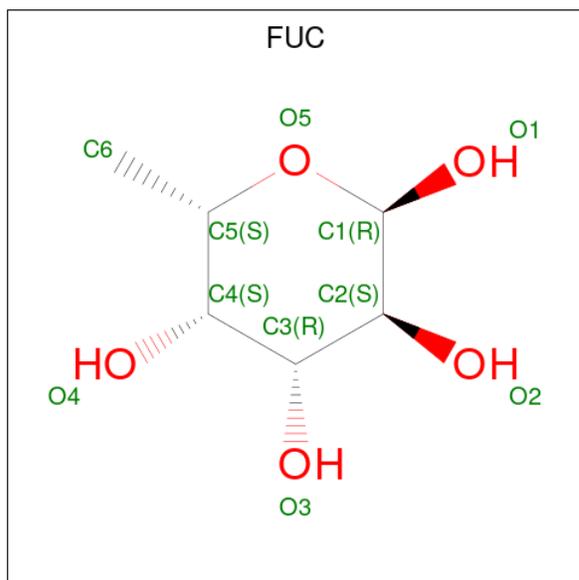


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O	0	0
			10 6 4		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na	0	0
			1 1		

- Molecule 7 is alpha-L-fucopyranose (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		

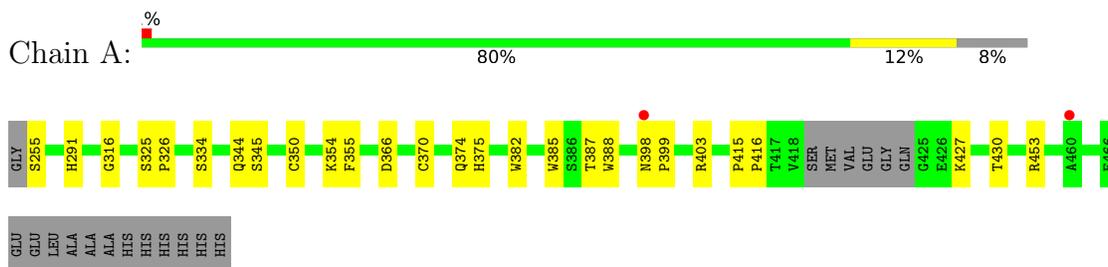
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	82	Total	O	0	0
			82	82		
8	B	34	Total	O	0	0
			34	34		

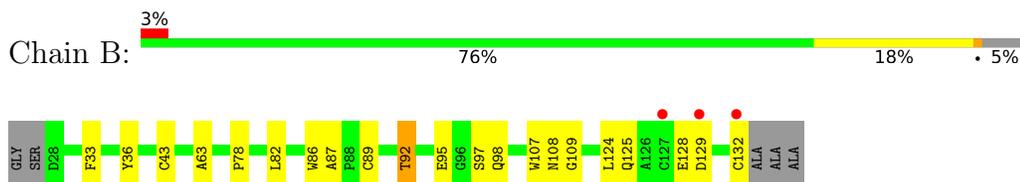
### 3 Residue-property plots [i](#)

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.

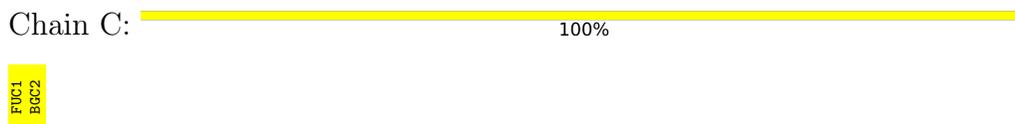
- Molecule 1: Properdin



- Molecule 2: Properdin



- Molecule 3: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.00Å 114.86Å 39.82Å 90.00° 99.56° 90.00°	Depositor
Resolution (Å)	79.61 – 2.03 79.61 – 2.03	Depositor EDS
% Data completeness (in resolution range)	54.5 (79.61-2.03) 54.5 (79.61-2.03)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.77 (at 2.03Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.212 , 0.248 0.217 , 0.251	Depositor DCC
$R_{free}$ test set	879 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtrriage
Anisotropy	0.036	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, PGE, MAN, NA, 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	0.63	0/1623	0.82	0/2220
2	B	0.68	0/795	0.84	0/1083
All	All	0.65	0/2418	0.83	0/3303

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1567	0	1445	15	0
2	B	776	0	686	12	0
3	C	21	0	19	0	0
4	A	77	0	70	3	0
4	B	11	0	10	1	0
5	A	10	0	14	3	0
6	A	1	0	0	0	0
7	B	10	0	10	1	0
8	A	82	0	0	0	0
8	B	34	0	0	0	0
All	All	2589	0	2254	28	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.

The worst 5 of 28 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)
1:A:387:THR:HA	4:A:508:MAN:O2	2.04	0.57
1:A:374:GLN:OE1	1:A:375:HIS:CE1	2.59	0.55
1:A:325:SER:OG	5:A:507:PGE:H52	2.07	0.54
2:B:33:PHE:CG	2:B:43:CYS:HB3	2.44	0.52
1:A:255:SER:HB2	1:A:291:HIS:HB2	1.93	0.49

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	203/225 (90%)	196 (97%)	7 (3%)	0	100	100
2	B	103/110 (94%)	99 (96%)	4 (4%)	0	100	100
All	All	306/335 (91%)	295 (96%)	11 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	170/191 (89%)	168 (99%)	2 (1%)	71	75
2	B	82/89 (92%)	78 (95%)	4 (5%)	25	20
All	All	252/280 (90%)	246 (98%)	6 (2%)	49	49

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	92	THR
2	B	129	ASP
2	B	132	CYS
1	A	427	LYS
1	A	334	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	375	HIS
1	A	443	GLN
1	A	445	GLN
2	B	98	GLN
2	B	125	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](#)

2 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	$\# Z  > 2$
3	FUC	C	1	3,1	10,10,11	0.63	0	14,14,16	1.48	3 (21%)
3	BGC	C	2	3	11,11,12	0.60	0	15,15,17	1.66	3 (20%)

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
3	FUC	C	1	3,1	-	-	0/1/1/1
3	BGC	C	2	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	BGC	O4-C4-C3	-3.12	103.14	110.35
3	C	2	BGC	C1-C2-C3	-3.07	105.89	109.67
3	C	1	FUC	C1-O5-C5	2.64	118.77	112.78
3	C	1	FUC	O5-C5-C6	2.20	112.06	107.33
3	C	2	BGC	O4-C4-C5	2.11	114.54	109.30

There are no chirality outliers.

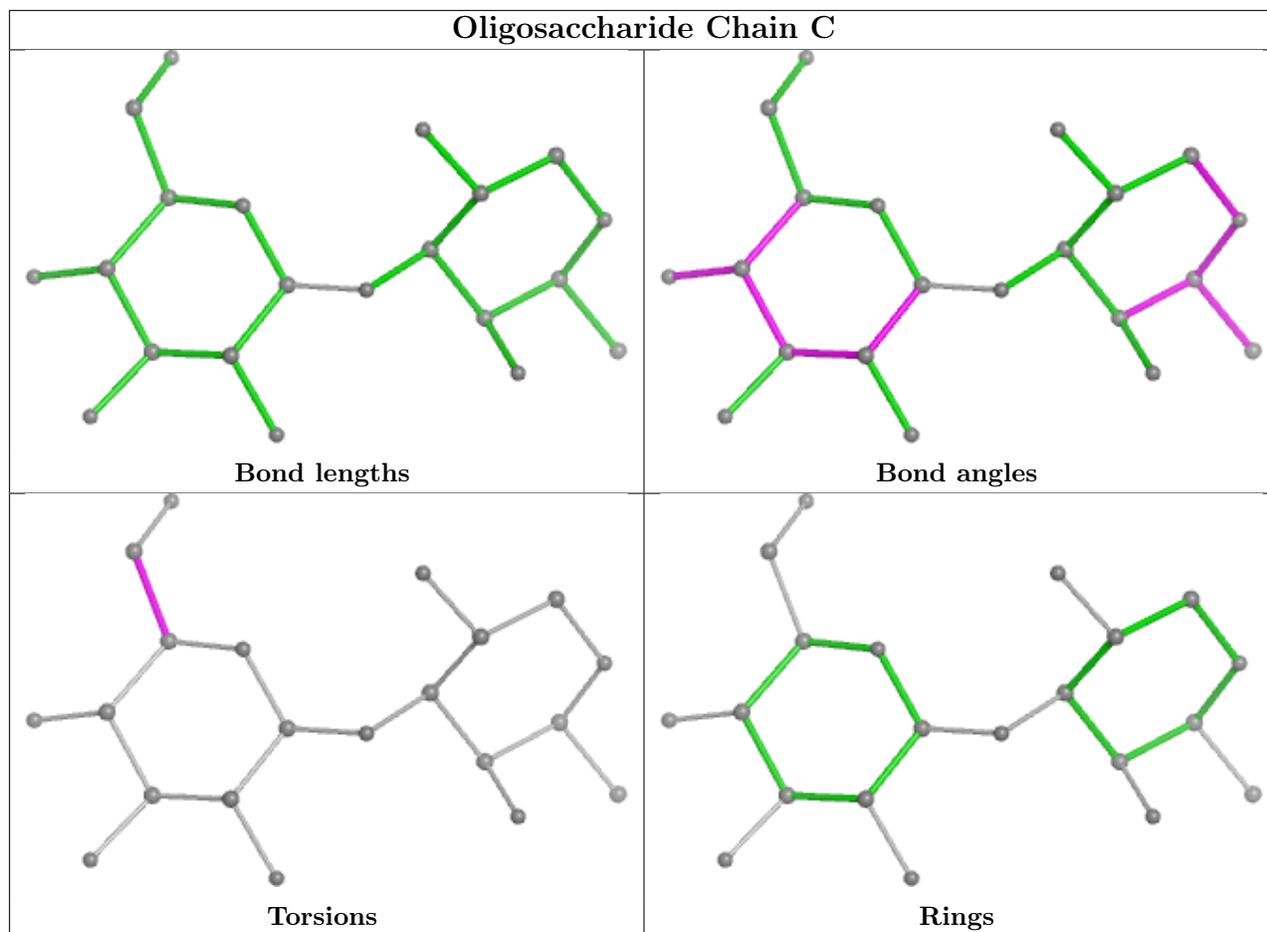
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	BGC	C4-C5-C6-O6
3	C	2	BGC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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
7	FUC	B	201	2	10,10,11	0.59	0	14,14,16	1.59	3 (21%)
4	MAN	A	502	1	11,11,12	0.41	0	15,15,17	1.42	3 (20%)
4	MAN	A	501	1	11,11,12	0.37	0	15,15,17	1.69	1 (6%)
4	MAN	A	508	1	11,11,12	0.57	0	15,15,17	0.81	1 (6%)
5	PGE	A	507	-	9,9,9	0.37	0	8,8,8	0.34	0
4	MAN	A	503	1	11,11,12	0.76	0	15,15,17	1.54	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	B	200	2	11,11,12	0.82	0	15,15,17	2.33	3 (20%)
4	MAN	A	504	1	11,11,12	0.55	0	15,15,17	1.29	2 (13%)
4	MAN	A	506	1	11,11,12	0.41	0	15,15,17	2.28	3 (20%)
4	MAN	A	505	1	11,11,12	0.60	0	15,15,17	1.58	2 (13%)

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
7	FUC	B	201	2	-	-	0/1/1/1
4	MAN	A	502	1	-	0/2/19/22	0/1/1/1
4	MAN	A	501	1	-	0/2/19/22	0/1/1/1
4	MAN	A	508	1	-	0/2/19/22	1/1/1/1
5	PGE	A	507	-	-	3/7/7/7	-
4	MAN	A	503	1	-	2/2/19/22	0/1/1/1
4	MAN	B	200	2	-	1/2/19/22	0/1/1/1
4	MAN	A	504	1	-	0/2/19/22	0/1/1/1
4	MAN	A	506	1	-	1/2/19/22	0/1/1/1
4	MAN	A	505	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	506	MAN	C1-O5-C5	7.01	121.69	112.19
4	B	200	MAN	O5-C5-C6	5.66	116.08	107.20
4	A	501	MAN	C1-O5-C5	5.63	119.82	112.19
4	B	200	MAN	C1-O5-C5	5.43	119.55	112.19
4	A	505	MAN	O5-C5-C6	3.86	113.25	107.20

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	MAN	O5-C5-C6-O6
4	A	506	MAN	O5-C5-C6-O6
4	A	503	MAN	C4-C5-C6-O6
5	A	507	PGE	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	507	PGE	C3-C4-O3-C5

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	508	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	201	FUC	1	0
4	A	508	MAN	1	0
5	A	507	PGE	3	0
4	A	503	MAN	1	0
4	B	200	MAN	1	0
4	A	504	MAN	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	206/225 (91%)	0.04	2 (0%) 82 82	14, 25, 53, 62	0
2	B	105/110 (95%)	0.21	3 (2%) 51 51	12, 27, 70, 105	0
All	All	311/335 (92%)	0.09	5 (1%) 72 71	12, 26, 58, 105	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	ALA	3.7
2	B	132	CYS	2.8
1	A	398	ASN	2.2
2	B	127	CYS	2.0
2	B	129	ASP	2.0

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

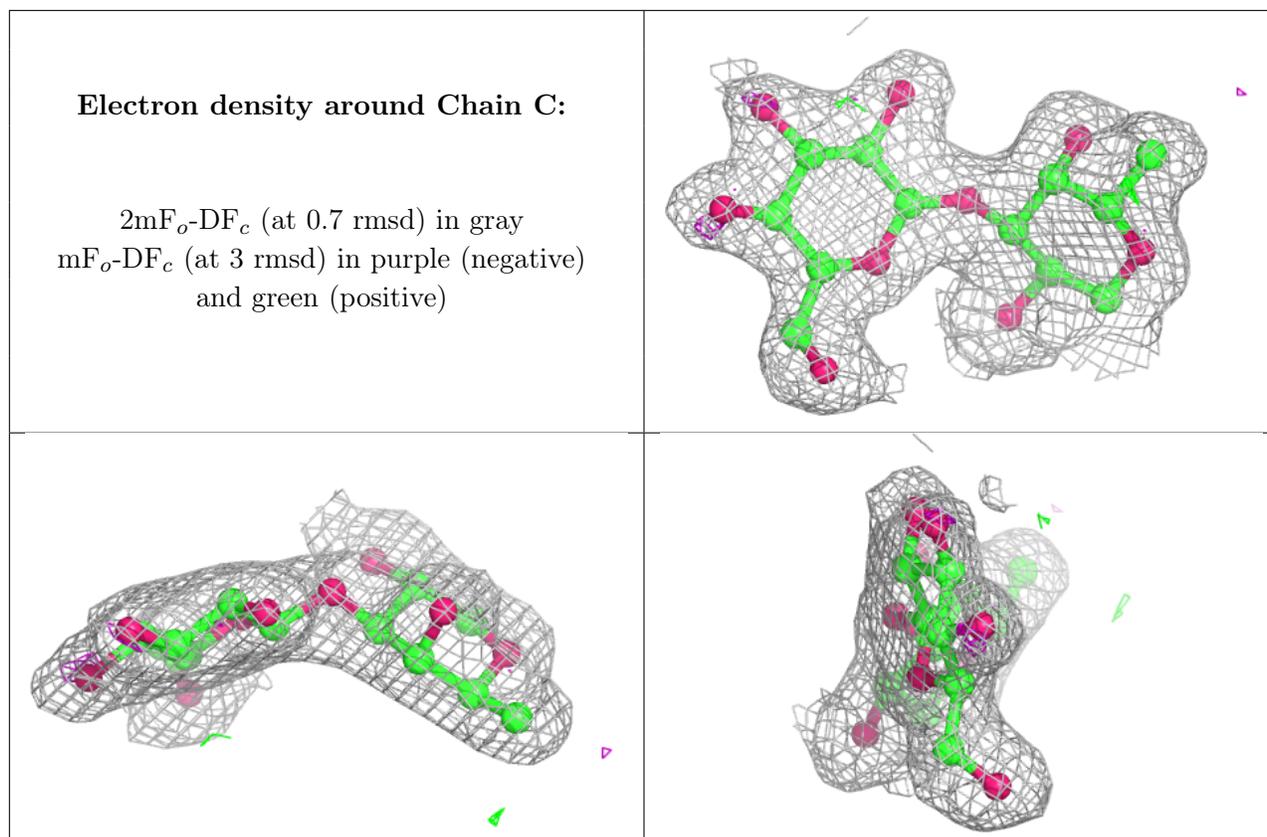
There are no non-standard protein/DNA/RNA residues in this entry.

### 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
3	FUC	C	1	10/11	0.95	0.11	21,22,24,24	0
3	BGC	C	2	11/12	0.96	0.13	19,23,25,26	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 [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
7	FUC	B	201	10/11	0.75	0.23	99,101,102,107	0
4	MAN	B	200	11/12	0.81	0.17	31,36,39,39	0
5	PGE	A	507	10/10	0.86	0.18	29,31,32,34	0
4	MAN	A	508	11/12	0.86	0.22	43,46,50,51	0
4	MAN	A	503	11/12	0.92	0.12	30,34,35,36	0
4	MAN	A	502	11/12	0.94	0.08	27,30,31,32	0
4	MAN	A	504	11/12	0.95	0.09	24,27,28,29	0
4	MAN	A	505	11/12	0.95	0.09	21,23,25,25	0
4	MAN	A	501	11/12	0.96	0.10	20,22,23,23	0
6	NA	A	509	1/1	0.96	0.14	27,27,27,27	0
4	MAN	A	506	11/12	0.96	0.09	20,24,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.