



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 01:49 AM EDT

PDB ID : 6GCC  
Title : Crystal structure of glutathione transferase Xi 3 mutant C56S from *Trametes versicolor* in complex with dextran-sulfate  
Authors : Schwartz, M.; Favier, F.; Didierjean, C.  
Deposited on : 2018-04-17  
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
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

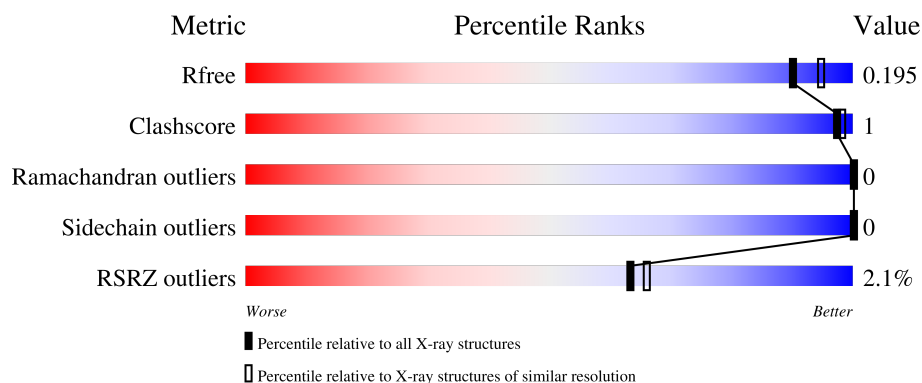
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

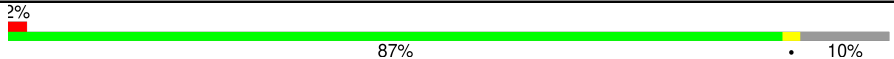

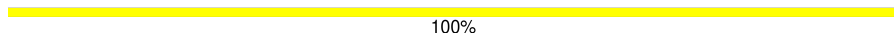
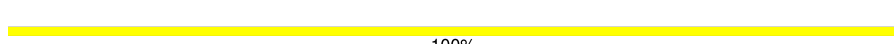
The reported resolution of this entry is 1.90 Å.

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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	325	
1	B	325	
2	C	3	
2	D	3	

## 2 Entry composition [i](#)

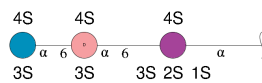
There are 3 unique types of molecules in this entry. The entry contains 10290 atoms, of which 4699 are hydrogens and 0 are deuteriums.

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 Glutathione transferase Xi 3 mutant C56S.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	H	N	O	S	0	0	0
			4690	1544	2325	390	429	2			
1	B	290	Total	C	H	N	O	S	0	1	0
			4688	1543	2326	389	428	2			

- Molecule 2 is an oligosaccharide called 3,4-di-O-sulfo-alpha-D-glucopyranose-(1-6)-3,4-di-O-sulfo-alpha-D-altropyranose-(1-6)-1,2,3,4-tetra-O-sulfo-alpha-D-allopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	3	Total	C	H	O	S	0	0	0
			90	18	24	40	8			
2	D	3	Total	C	H	O	S	0	0	0
			90	18	24	40	8			

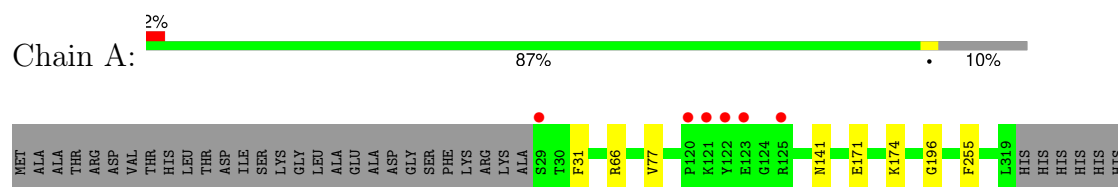
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	373	Total	O	0	0
			373	373		
3	B	359	Total	O	0	0
			359	359		

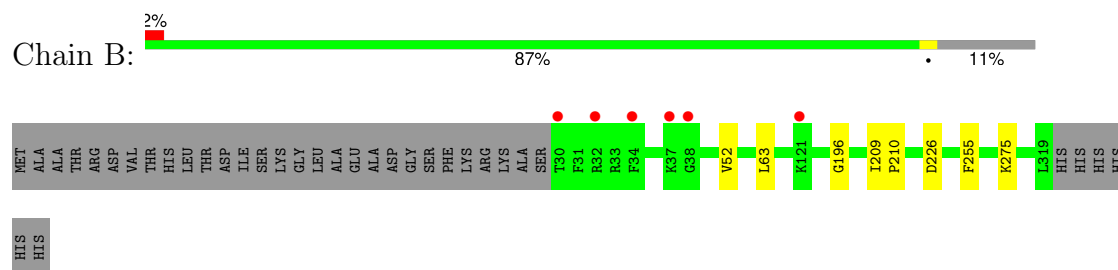
### 3 Residue-property plots [i](#)

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: Glutathione transferase Xi 3 mutant C56S



- Molecule 1: Glutathione transferase Xi 3 mutant C56S



- Molecule 2: 3,4-di-O-sulfo-alpha-D-glucopyranose-(1-6)-3,4-di-O-sulfo-alpha-D-altropyranose-(1-6)-1,2,3,4-tetra-O-sulfo-alpha-D-allopyranose



- Molecule 2: 3,4-di-O-sulfo-alpha-D-glucopyranose-(1-6)-3,4-di-O-sulfo-alpha-D-altropyranose-(1-6)-1,2,3,4-tetra-O-sulfo-alpha-D-allopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.26Å 72.26Å 317.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.01 – 1.90 46.01 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (46.01-1.90) 97.0 (46.01-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.55 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.160 , 0.193 0.164 , 0.195	Depositor DCC
$R_{free}$ test set	3357 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: TUG, TUJ, 5LT

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	0.56	0/2436	0.64	0/3321
1	B	0.54	0/2436	0.63	0/3322
All	All	0.55	0/4872	0.64	0/6643

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	2365	2325	2325	4	0
1	B	2362	2326	2325	4	0
2	C	66	24	0	0	0
2	D	66	24	0	0	0
3	A	373	0	0	0	0
3	B	359	0	0	0	0
All	All	5591	4699	4650	8	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 1.

All (8) 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:171:GLU:HA	1:A:174:LYS:HE2	1.82	0.61
1:B:52:VAL:HG21	1:B:63:LEU:HD21	1.98	0.45
1:B:209:ILE:HB	1:B:210:PRO:HD3	2.01	0.43
1:A:196:GLY:HA3	1:A:255:PHE:CD1	2.55	0.42
1:B:196:GLY:HA3	1:B:255:PHE:CD1	2.55	0.41
1:A:66:ARG:CZ	1:A:77:VAL:HG23	2.51	0.41
1:B:226:ASP:OD1	1:B:275:LYS:NZ	2.53	0.40
1:A:31:PHE:O	1:A:141:ASN:HA	2.21	0.40

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	289/325 (89%)	283 (98%)	6 (2%)	0	100	100
1	B	289/325 (89%)	286 (99%)	3 (1%)	0	100	100
All	All	578/650 (89%)	569 (98%)	9 (2%)	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	252/279 (90%)	252 (100%)	0	100	100
1	B	252/279 (90%)	252 (100%)	0	100	100
All	All	504/558 (90%)	504 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

6 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
2	TUJ	C	1	2	28,28,28	1.71	8 (28%)	36,45,45	2.45	15 (41%)
2	TUG	C	2	2	19,19,20	1.45	4 (21%)	23,29,31	2.60	12 (52%)
2	5LT	C	3	2	19,19,20	1.37	4 (21%)	23,29,31	3.00	8 (34%)
2	TUJ	D	1	2	28,28,28	1.84	8 (28%)	36,45,45	2.87	18 (50%)
2	TUG	D	2	2	19,19,20	1.49	4 (21%)	23,29,31	2.73	12 (52%)
2	5LT	D	3	2	19,19,20	1.47	4 (21%)	23,29,31	3.44	7 (30%)

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
2	TUJ	C	1	2	-	5/20/42/42	0/1/1/1
2	TUG	C	2	2	-	10/12/29/32	0/1/1/1
2	5LT	C	3	2	-	8/12/29/32	0/1/1/1
2	TUJ	D	1	2	-	5/20/42/42	0/1/1/1
2	TUG	D	2	2	-	10/12/29/32	0/1/1/1
2	5LT	D	3	2	-	8/12/29/32	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	TUJ	O1-S1	4.34	1.70	1.57
2	C	1	TUJ	O1-S1	4.02	1.69	1.57
2	D	1	TUJ	O4-S4	3.73	1.68	1.57
2	D	1	TUJ	O2-C2	-3.69	1.38	1.46
2	C	1	TUJ	O4-S4	3.56	1.68	1.57
2	D	1	TUJ	O3-S3	3.51	1.67	1.57
2	C	1	TUJ	O3-S3	3.33	1.67	1.57
2	C	2	TUG	O4-S4	3.28	1.67	1.57
2	D	3	5LT	O4-C4	-3.09	1.39	1.46
2	D	2	TUG	O4-C4	-3.07	1.39	1.46
2	C	1	TUJ	O2-S2	3.05	1.66	1.57
2	D	1	TUJ	O2-S2	3.03	1.66	1.57
2	C	1	TUJ	O2-C2	-3.03	1.39	1.46
2	D	3	5LT	O3-S1	2.98	1.66	1.57
2	D	2	TUG	O3-C3	-2.93	1.39	1.46
2	D	2	TUG	O4-S4	2.88	1.66	1.57
2	C	2	TUG	O3-C3	-2.80	1.40	1.46
2	C	1	TUJ	O4-C4	-2.74	1.40	1.46
2	C	3	5LT	O3-C3	-2.73	1.40	1.46
2	C	3	5LT	O3-S1	2.72	1.65	1.57
2	C	2	TUG	O3-S3	2.72	1.65	1.57
2	D	2	TUG	O3-S3	2.69	1.65	1.57
2	D	3	5LT	O4-S2	2.66	1.65	1.57
2	D	1	TUJ	O4-C4	-2.57	1.40	1.46
2	C	3	5LT	O4-S2	2.57	1.65	1.57
2	D	1	TUJ	C2-C3	2.52	1.57	1.52
2	D	3	5LT	O3-C3	-2.48	1.40	1.46
2	C	3	5LT	O4-C4	-2.45	1.40	1.46
2	C	2	TUG	O4-C4	-2.41	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	TUJ	C2-C3	2.23	1.56	1.52
2	C	1	TUJ	O3-C3	-2.05	1.41	1.46
2	D	1	TUJ	O3-C3	-2.04	1.41	1.46

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	5LT	C2-C3-C4	-12.14	101.99	111.03
2	C	3	5LT	C2-C3-C4	-9.01	104.32	111.03
2	D	1	TUJ	O1-C1-C2	8.87	122.55	107.17
2	C	1	TUJ	O1-C1-C2	6.36	118.19	107.17
2	D	1	TUJ	C1-O1-S1	-6.08	109.80	117.80
2	C	2	TUG	C2-C3-C4	5.70	115.27	111.03
2	D	3	5LT	C4-O4-S2	5.47	132.16	119.04
2	D	2	TUG	C2-C3-C4	5.34	115.01	111.03
2	D	2	TUG	O43-S4-O4	5.18	118.27	106.37
2	C	3	5LT	C3-O3-S1	4.97	130.97	119.04
2	D	3	5LT	C3-O3-S1	4.76	130.47	119.04
2	C	1	TUJ	O5-C5-C6	4.73	118.17	106.44
2	D	1	TUJ	O5-C5-C6	4.72	118.13	106.44
2	C	1	TUJ	C1-O1-S1	-4.71	111.59	117.80
2	C	3	5LT	C1-C2-C3	-4.67	102.90	109.29
2	C	2	TUG	O43-S4-O4	4.64	117.03	106.37
2	D	3	5LT	C1-C2-C3	-4.43	103.23	109.29
2	C	3	5LT	C4-O4-S2	4.41	129.61	119.04
2	D	3	5LT	O2-C2-C1	4.37	119.22	109.22
2	D	1	TUJ	C6-C5-C4	-4.32	101.23	113.38
2	C	2	TUG	O5-C5-C6	4.28	115.99	107.66
2	D	1	TUJ	O12-S1-O11	-4.23	95.91	112.24
2	C	1	TUJ	C2-C3-C4	4.20	119.64	110.43
2	D	2	TUG	O5-C5-C6	4.11	115.66	107.66
2	C	3	5LT	O4-C4-C3	-3.99	99.85	108.56
2	D	1	TUJ	C2-C3-C4	3.92	119.03	110.43
2	C	1	TUJ	C6-C5-C4	-3.92	102.37	113.38
2	D	2	TUG	C4-O4-S4	3.88	128.35	119.04
2	C	2	TUG	O5-C5-C4	3.69	116.69	110.06
2	C	3	5LT	O2-C2-C1	3.64	117.55	109.22
2	D	2	TUG	C6-C5-C4	-3.61	103.23	113.38
2	C	2	TUG	O33-S3-O3	3.50	114.42	106.37
2	C	1	TUJ	O12-S1-O11	-3.47	98.86	112.24
2	D	2	TUG	O5-C5-C4	3.47	116.28	110.06
2	D	1	TUJ	C1-C2-C3	3.46	117.48	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	TUJ	O2-C2-C1	3.37	112.11	107.58
2	D	2	TUG	C3-C4-C5	3.28	117.30	110.58
2	C	1	TUJ	O13-S1-O1	3.19	113.71	106.37
2	D	1	TUJ	O33-S3-O3	3.18	113.69	106.37
2	D	2	TUG	O33-S3-O3	3.07	113.43	106.37
2	D	1	TUJ	O4-C4-C3	2.98	115.06	108.56
2	C	2	TUG	C6-C5-C4	-2.92	105.18	113.38
2	D	2	TUG	C3-O3-S3	-2.90	112.08	119.04
2	C	2	TUG	C3-C4-C5	2.87	116.46	110.58
2	D	1	TUJ	O5-C1-C2	-2.82	104.02	109.49
2	C	1	TUJ	O33-S3-O3	2.81	112.84	106.37
2	D	1	TUJ	O13-S1-O11	-2.65	99.29	108.56
2	C	1	TUJ	O31-S3-O32	-2.59	102.24	112.24
2	C	1	TUJ	O5-C1-O1	2.58	114.72	107.90
2	D	3	5LT	O2-C2-C3	2.56	115.98	109.99
2	C	1	TUJ	O42-S4-O41	-2.52	102.51	112.24
2	C	2	TUG	C4-O4-S4	2.52	125.08	119.04
2	D	2	TUG	O42-S4-O41	-2.51	102.56	112.24
2	C	2	TUG	C1-O5-C5	2.46	115.48	112.19
2	D	1	TUJ	O5-C1-O1	2.45	114.37	107.90
2	D	1	TUJ	O2-C2-C3	-2.42	103.28	108.56
2	C	1	TUJ	O2-C2-C1	2.35	110.73	107.58
2	C	2	TUG	O5-C1-C2	-2.34	105.20	110.79
2	D	1	TUJ	O42-S4-O41	-2.34	103.20	112.24
2	D	2	TUG	O43-S4-O41	-2.30	100.52	108.56
2	D	2	TUG	O6-C6-C5	2.30	119.15	111.33
2	D	1	TUJ	O31-S3-O32	-2.27	103.47	112.24
2	C	3	5LT	O5-C5-C4	-2.27	105.99	110.06
2	C	2	TUG	O42-S4-O41	-2.26	103.52	112.24
2	C	1	TUJ	O4-C4-C3	2.23	113.43	108.56
2	C	2	TUG	O43-S4-O41	-2.23	100.74	108.56
2	D	3	5LT	O4-C4-C3	-2.13	103.91	108.56
2	C	1	TUJ	O22-S2-O21	-2.11	104.09	112.24
2	C	3	5LT	C1-O5-C5	2.10	115.00	112.19
2	D	1	TUJ	O22-S2-O21	-2.05	104.31	112.24
2	D	1	TUJ	O43-S4-O4	2.04	111.05	106.37
2	C	1	TUJ	O23-S2-O2	2.01	111.00	106.37

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	TUG	C5-C4-O4-S4
2	C	2	TUG	C3-C4-O4-S4
2	C	3	5LT	C2-C3-O3-S1
2	C	3	5LT	C4-C3-O3-S1
2	C	3	5LT	C5-C4-O4-S2
2	C	3	5LT	C4-O4-S2-O23
2	C	3	5LT	C4-O4-S2-O21
2	C	3	5LT	C4-O4-S2-O22
2	D	2	TUG	C5-C4-O4-S4
2	D	2	TUG	C4-O4-S4-O41
2	D	3	5LT	C2-C3-O3-S1
2	D	3	5LT	C5-C4-O4-S2
2	D	2	TUG	O5-C5-C6-O6
2	C	3	5LT	O5-C5-C6-O6
2	D	3	5LT	O5-C5-C6-O6
2	D	3	5LT	C4-C5-C6-O6
2	C	3	5LT	C4-C5-C6-O6
2	C	2	TUG	O5-C5-C6-O6
2	D	2	TUG	C4-C5-C6-O6
2	C	2	TUG	C4-C5-C6-O6
2	C	1	TUJ	C1-O1-S1-O12
2	C	1	TUJ	C2-O2-S2-O21
2	C	1	TUJ	C2-O2-S2-O22
2	C	2	TUG	C4-O4-S4-O41
2	C	2	TUG	C4-O4-S4-O42
2	C	2	TUG	C3-O3-S3-O32
2	D	1	TUJ	C1-O1-S1-O12
2	D	1	TUJ	C2-O2-S2-O21
2	D	1	TUJ	C2-O2-S2-O22
2	D	2	TUG	C4-O4-S4-O42
2	D	3	5LT	C4-O4-S2-O21
2	D	3	5LT	C4-O4-S2-O22
2	C	1	TUJ	C2-O2-S2-O23
2	C	2	TUG	C4-O4-S4-O43
2	C	2	TUG	C3-O3-S3-O33
2	D	1	TUJ	C2-O2-S2-O23
2	D	2	TUG	C4-O4-S4-O43
2	D	3	5LT	C4-O4-S2-O23
2	C	1	TUJ	C1-O1-S1-O11
2	C	2	TUG	C3-O3-S3-O31
2	D	1	TUJ	C1-O1-S1-O11
2	D	2	TUG	C3-C4-O4-S4
2	D	3	5LT	C4-C3-O3-S1

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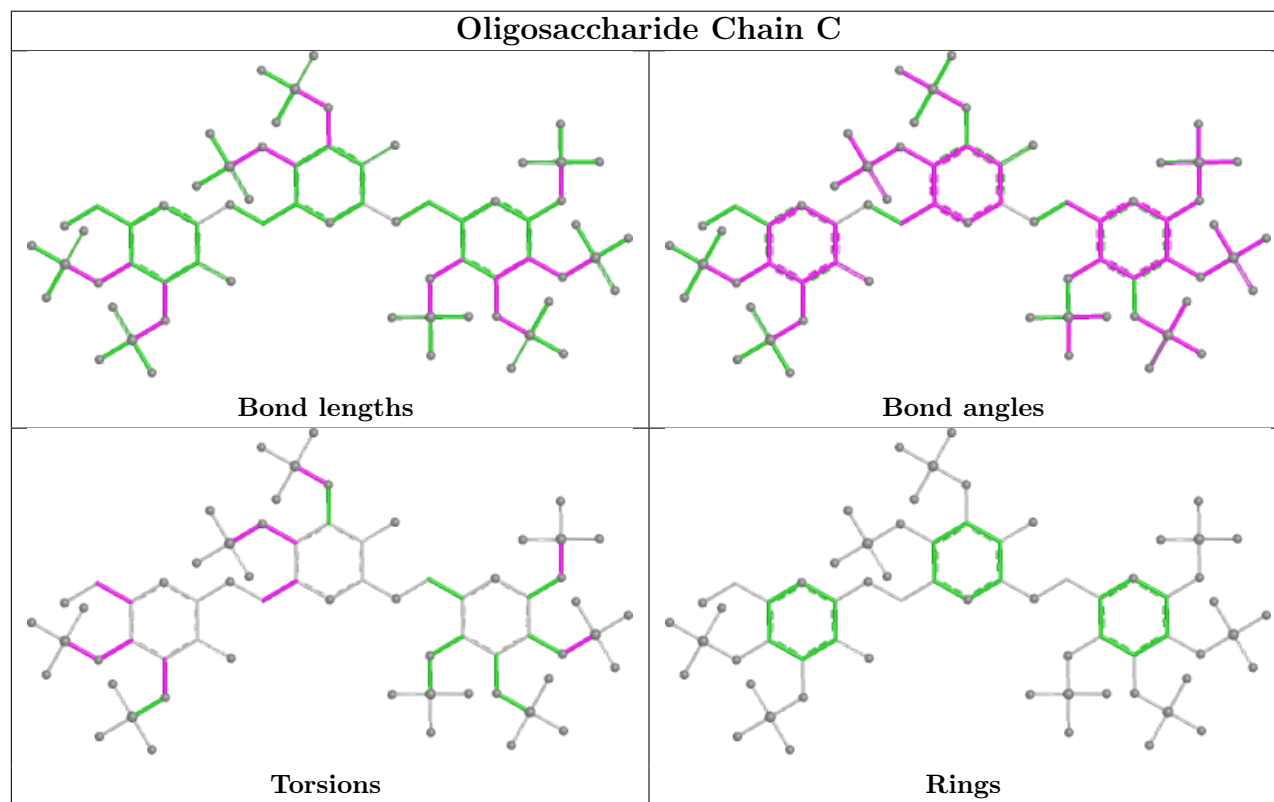
*Continued from previous page...*

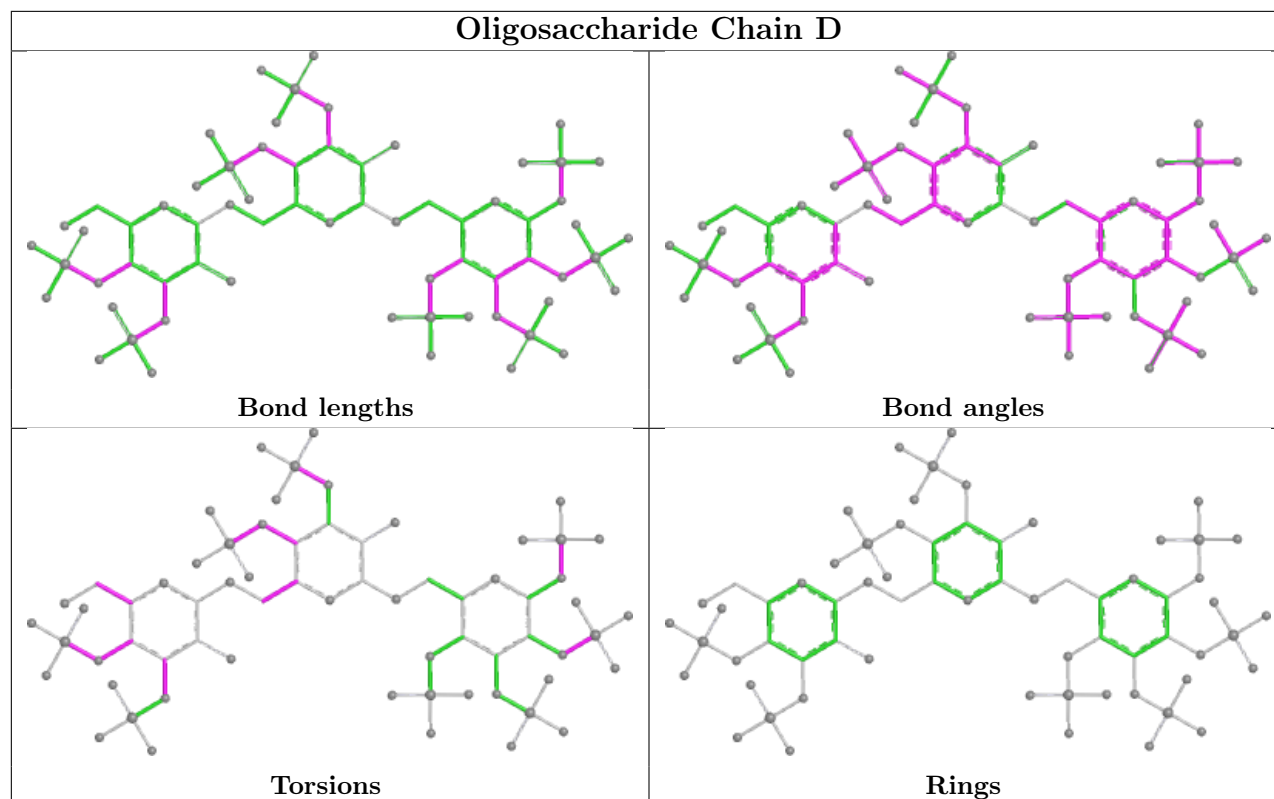
Mol	Chain	Res	Type	Atoms
2	D	2	TUG	C3-O3-S3-O33
2	D	2	TUG	C3-O3-S3-O32
2	D	2	TUG	C3-O3-S3-O31

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](#)

There are no ligands in this entry.

## 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	291/325 (89%)	-0.26	6 (2%) 63 66	13, 18, 32, 54	0
1	B	290/325 (89%)	-0.14	6 (2%) 63 66	13, 19, 34, 50	0
All	All	581/650 (89%)	-0.20	12 (2%) 63 66	13, 19, 33, 54	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	LYS	5.0
1	A	123	GLU	3.5
1	A	29	SER	3.5
1	B	30	THR	3.2
1	B	32	ARG	2.8
1	B	34	PHE	2.5
1	B	37	LYS	2.5
1	B	38	GLY	2.4
1	A	122	TYR	2.2
1	A	125	ARG	2.2
1	B	121	LYS	2.2
1	A	120	PRO	2.1

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

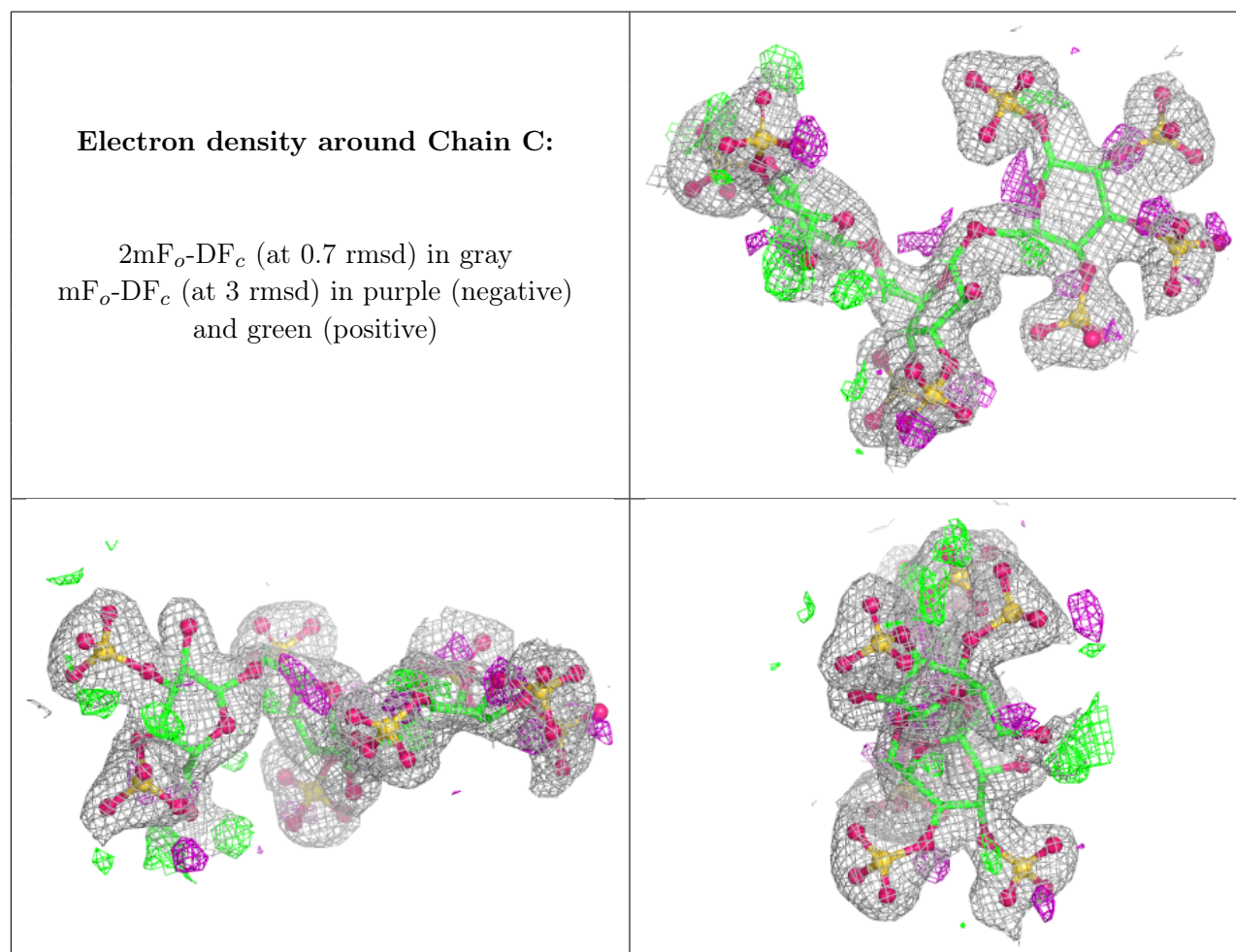
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

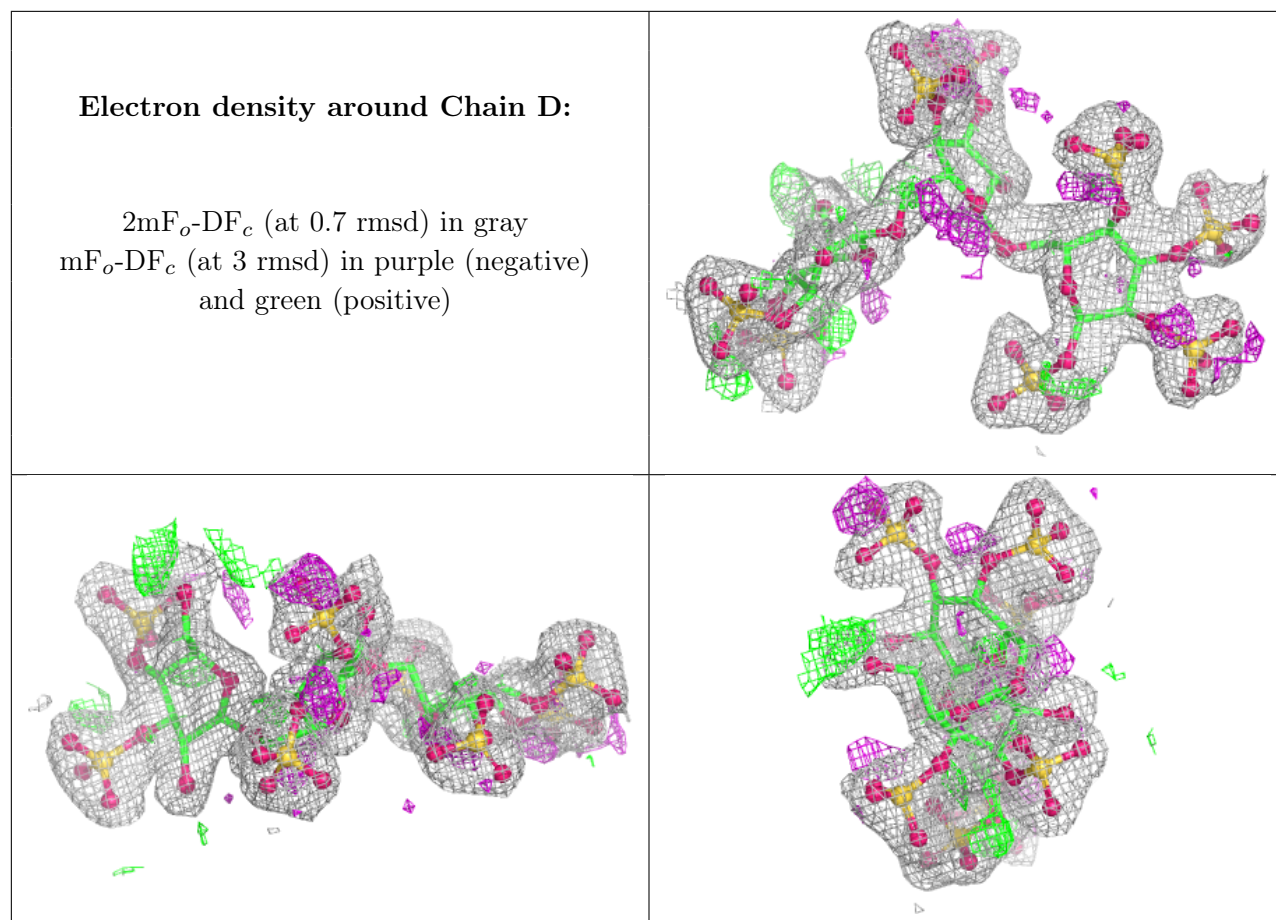
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 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
2	TUJ	C	1	28/28	0.90	0.22	25,52,72,83	0
2	TUG	D	2	19/20	0.92	0.17	31,42,51,59	0
2	TUJ	D	1	28/28	0.93	0.17	23,46,70,84	0
2	TUG	C	2	19/20	0.93	0.20	30,45,57,65	0
2	5LT	C	3	19/20	0.95	0.14	25,37,49,61	0
2	5LT	D	3	19/20	0.96	0.12	26,36,46,56	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.