



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 03:51 PM BST

PDB ID : 1TU5  
Title : Crystal structure of bovine plasma copper-containing amine oxidase  
Authors : Lunelli, M.; Di Paolo, M.L.; Biadene, M.; Calderone, V.; Scarpa, M.; Battistutta, R.; Rigo, A.; Zanotti, G.  
Deposited on : 2004-06-24  
Resolution : 2.37 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

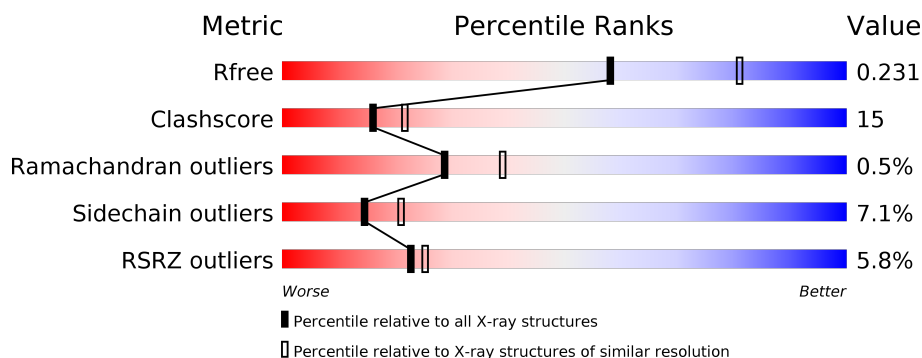
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	746	<div> <div>5%</div> <div> <div></div> <div>59%</div> <div>22%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	746	<div> <div>5%</div> <div> <div></div> <div>61%</div> <div>21%</div> <div>•</div> <div>15%</div> </div> </div>
2	C	3	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>
2	D	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	3	-	-	-	X
2	NAG	D	1	X	-	-	-
2	NAG	D	3	-	-	-	X
3	NAG	A	803	-	-	-	X
3	NAG	A	804	X	-	-	X
3	NAG	B	804	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10581 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.

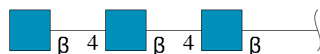
- Molecule 1 is a protein called Copper amine oxidase, liver isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	0	0
			5018	3217	862	920	19			
1	B	633	Total	C	N	O	S	0	0	0
			5018	3217	862	920	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	TPQ	TYR	modified residue	UNP Q29437
B	470	TPQ	TYR	modified residue	UNP Q29437

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			42	24	3	15			
2	D	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cu	0	0
			1	1		
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	A	2	Total	Ca	0	0
			2	2		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Cl	0	0
			2	2		
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	209	Total	O	0	0
			209	209		
7	B	201	Total	O	0	0
			201	201		

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.

- [illegible]

- Chain B:
- 
- 61% 21% 5% 15%
- | Amino Acid | Frequency (%) |
|------------|---------------|
| ARG        | 5             |
| GLU        | 61            |
| GLU        | 61            |
| GLY        | 61            |
| GLY        | 61            |
| VAL        | 61            |
| GLY        | 61            |
| SER        | 61            |
| GLU        | 61            |
| GLU        | 61            |
| GLY        | 61            |
| VAL        | 61            |
| GLY        | 61            |
| LVS        | 61            |
| GLN        | 61            |
| CYS        | 61            |
| HIS        | 61            |
| PRO        | 61            |
| SER        | 61            |
| SER        | 61            |
| LEU        | 61            |
| PRO        | 61            |
| PRO        | 61            |
| ARG        | 61            |
| ARG        | 61            |
| SER        | 61            |
| PRO        | 61            |
| SER        | 61            |
| CYS        | 61            |
| PRO        | 61            |
| ASP        | 61            |
| GLN        | 61            |
| TRP        | 61            |
| TRP        | 61            |
| THR        | 61            |
| HIS        | 61            |
| PRO        | 61            |
| ASP        | 61            |
| GLN        | 61            |
| SER        | 61            |
| SER        | 61            |
| Q57        | 21            |
| L58        | 21            |
| L62        | 21            |
| S63        | 21            |
| R64        | 21            |
| L67        | 21            |
| Y71        | 21            |
| L74        | 21            |
| L78        | 21            |
| L79        | 21            |





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.68Å 131.19Å 134.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.37 27.85 – 2.37	Depositor EDS
% Data completeness (in resolution range)	93.7 (25.00-2.37) 93.8 (27.85-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.36Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.237 0.203 , 0.231	Depositor DCC
$R_{free}$ test set	3719 reflections (7.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10581	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: CA, CU, NAG, TPQ, CL

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	0.57	2/5156 (0.0%)	0.83	7/7025 (0.1%)
1	B	0.55	0/5156	0.79	6/7025 (0.1%)
All	All	0.56	2/10312 (0.0%)	0.81	13/14050 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	VAL	CB-CG1	-6.81	1.38	1.52
1	A	142	VAL	CB-CG2	5.38	1.64	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	SER	N-CA-C	-9.93	84.20	111.00
1	A	446	PHE	N-CA-C	8.70	134.49	111.00
1	A	447	LEU	CA-CB-CG	-8.53	95.69	115.30
1	B	448	SER	N-CA-C	-8.41	88.30	111.00
1	B	446	PHE	N-CA-C	6.98	129.84	111.00

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	5018	0	4801	163	0
1	B	5018	0	4802	138	0
2	C	42	0	37	2	0
2	D	42	0	37	5	0
3	A	28	0	26	4	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	209	0	0	5	0
7	B	201	0	0	3	0
All	All	10581	0	9716	289	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 15.

The worst 5 of 289 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:591:LYS:N	1:A:591:LYS:HD3	1.63	1.09
1:B:232:ILE:HG12	1:B:240:HIS:CD2	1.87	1.08
1:B:591:LYS:H	1:B:591:LYS:CD	1.62	1.07
1:B:591:LYS:HD2	1:B:591:LYS:N	1.65	1.07
1:A:591:LYS:CD	1:A:591:LYS:H	1.63	1.02

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	628/746 (84%)	592 (94%)	33 (5%)	3 (0%)	29	39
1	B	628/746 (84%)	594 (95%)	31 (5%)	3 (0%)	29	39
All	All	1256/1492 (84%)	1186 (94%)	64 (5%)	6 (0%)	29	39

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	THR
1	A	81	ASP
1	A	235	GLY
1	A	233	THR
1	B	235	GLY

### 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	530/623 (85%)	491 (93%)	39 (7%)	13	19
1	B	530/623 (85%)	494 (93%)	36 (7%)	16	23
All	All	1060/1246 (85%)	985 (93%)	75 (7%)	14	21

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	639	THR
1	B	171	LEU
1	B	621	GLU
1	A	642	SER
1	A	700	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	184	ASN

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Mol	Chain	Res	Type
1	B	231	ASN
1	B	489	HIS
1	A	712	GLN
1	B	559	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
1	TPQ	B	470	1	13,14,15	2.77	7 (53%)	15,19,21	1.33	2 (13%)
1	TPQ	A	470	1	13,14,15	2.81	7 (53%)	15,19,21	1.22	1 (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
1	TPQ	B	470	1	-	2/5/22/24	0/1/1/1
1	TPQ	A	470	1	-	2/5/22/24	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	470	TPQ	C1-C2	-7.27	1.38	1.49
1	A	470	TPQ	C1-C2	-7.13	1.38	1.49
1	A	470	TPQ	O5-C5	3.33	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	470	TPQ	O5-C5	3.22	1.33	1.24
1	A	470	TPQ	O2-C2	3.20	1.33	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	TPQ	CB-CA-C	-3.02	105.81	111.47
1	B	470	TPQ	CB-CA-C	-2.86	106.10	111.47
1	B	470	TPQ	C6-C1-C2	2.16	120.30	118.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	470	TPQ	N-CA-CB-C1
1	B	470	TPQ	C-CA-CB-C1
1	A	470	TPQ	N-CA-CB-C1
1	A	470	TPQ	C-CA-CB-C1

There are no ring outliers.

No monomer is involved in short contacts.

## 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	NAG	C	1	1,2	14,14,15	0.57	0	17,19,21	0.98	1 (5%)
2	NAG	C	2	2	14,14,15	0.69	0	17,19,21	0.61	0
2	NAG	C	3	2	14,14,15	1.05	1 (7%)	17,19,21	1.07	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.82	1 (7%)	17,19,21	1.17	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	D	2	2	14,14,15	0.54	0	17,19,21	0.91	1 (5%)
2	NAG	D	3	2	14,14,15	0.73	0	17,19,21	0.85	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	C	3	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	3	2	-	5/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	NAG	C1-C2	3.35	1.57	1.52
2	D	1	NAG	O5-C5	2.02	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	3.00	116.26	112.19
2	C	3	NAG	C3-C4-C5	-2.52	105.75	110.24
2	C	1	NAG	C1-C2-N2	-2.46	106.28	110.49
2	D	2	NAG	C2-N2-C7	-2.36	119.55	122.90
2	D	1	NAG	C2-N2-C7	-2.15	119.84	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	1	NAG	C1

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	NAG	C8-C7-N2-C2

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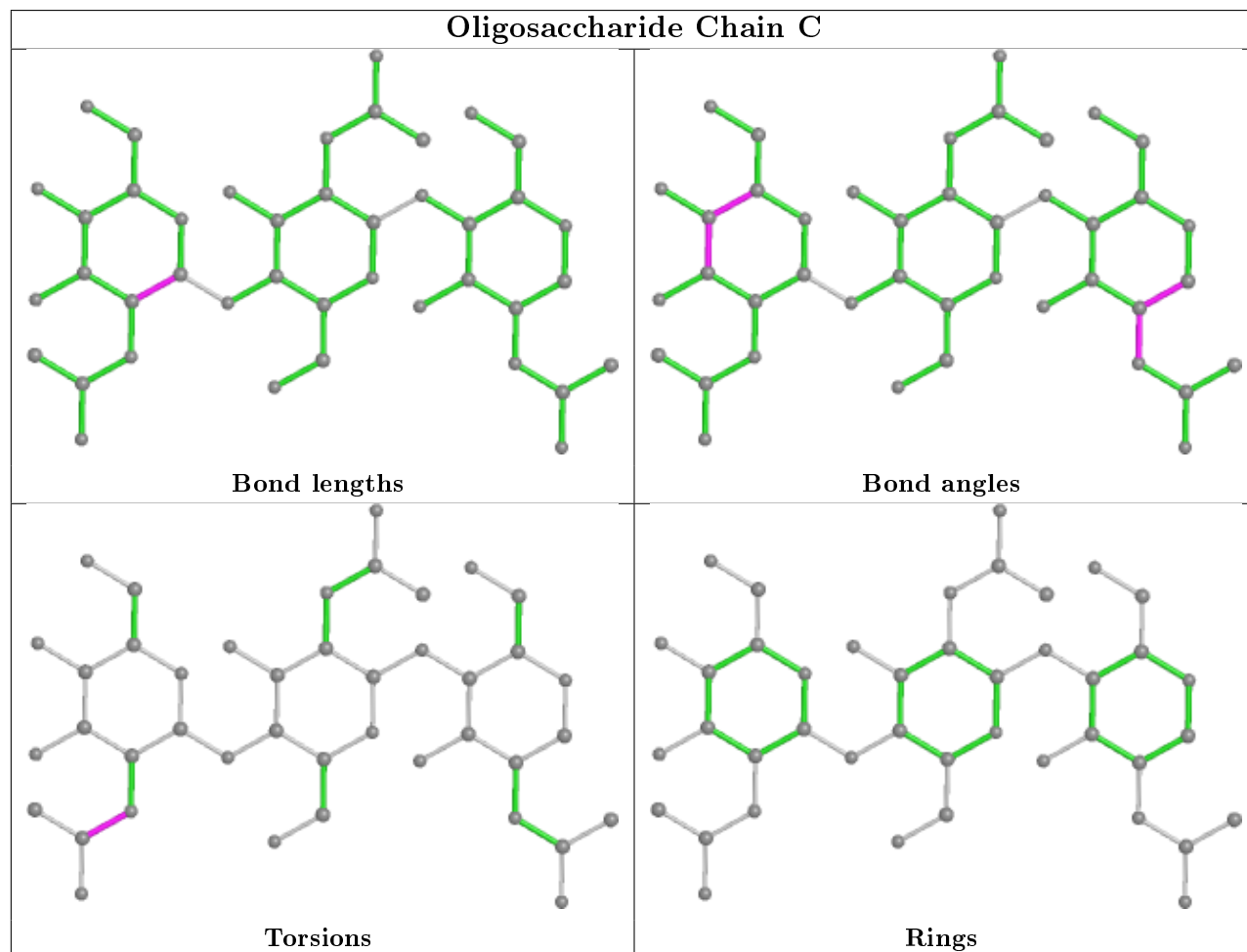
Mol	Chain	Res	Type	Atoms
2	C	3	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

There are no ring outliers.

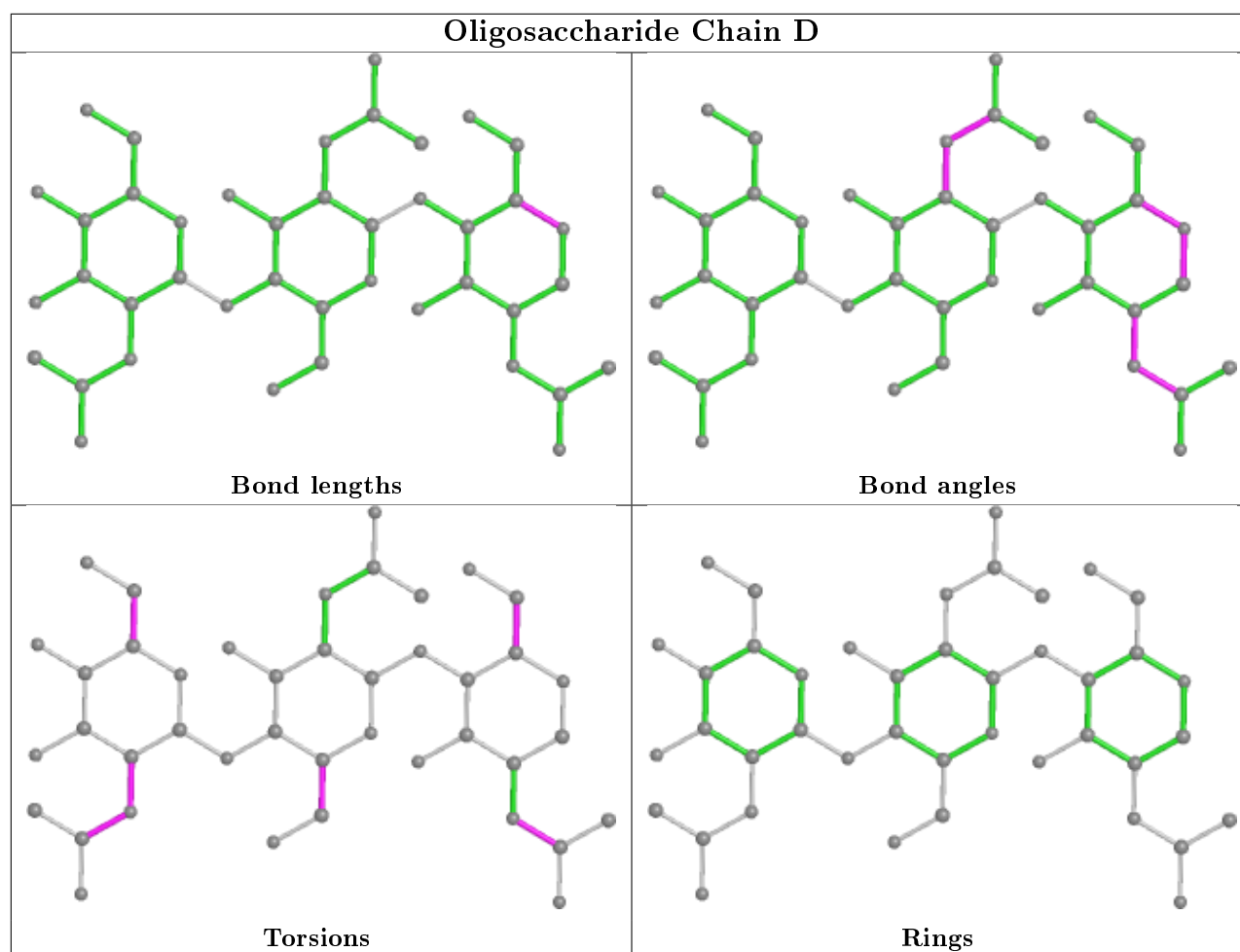
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	D	2	NAG	4	0
2	C	3	NAG	1	0
2	D	3	NAG	5	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 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z  > 2$
3	NAG	B	804	1	14,14,15	0.74	0	17,19,21	0.81	1 (5%)
3	NAG	A	803	1	14,14,15	0.72	0	17,19,21	1.04	1 (5%)
3	NAG	A	804	1	14,14,15	0.58	0	17,19,21	0.69	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
3	NAG	B	804	1	-	2/6/23/26	0/1/1/1
3	NAG	A	803	1	-	3/6/23/26	0/1/1/1
3	NAG	A	804	1	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	NAG	O5-C1-C2	-2.12	107.94	111.29
3	B	804	NAG	C2-N2-C7	-2.05	119.99	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	804	NAG	C1

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	804	NAG	C8-C7-N2-C2
3	A	804	NAG	O7-C7-N2-C2
3	A	803	NAG	C3-C2-N2-C7
3	B	804	NAG	C8-C7-N2-C2
3	B	804	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	NAG	2	0
3	A	804	NAG	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	632/746 (84%)	0.30	37 (5%) 22 24	11, 25, 50, 114	0
1	B	632/746 (84%)	0.37	36 (5%) 23 26	9, 25, 48, 115	0
All	All	1264/1492 (84%)	0.33	73 (5%) 23 25	9, 25, 49, 115	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	446	PHE	16.7
1	A	447	LEU	15.1
1	B	451	PHE	14.7
1	A	444	SER	14.6
1	A	450	TYR	14.6

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

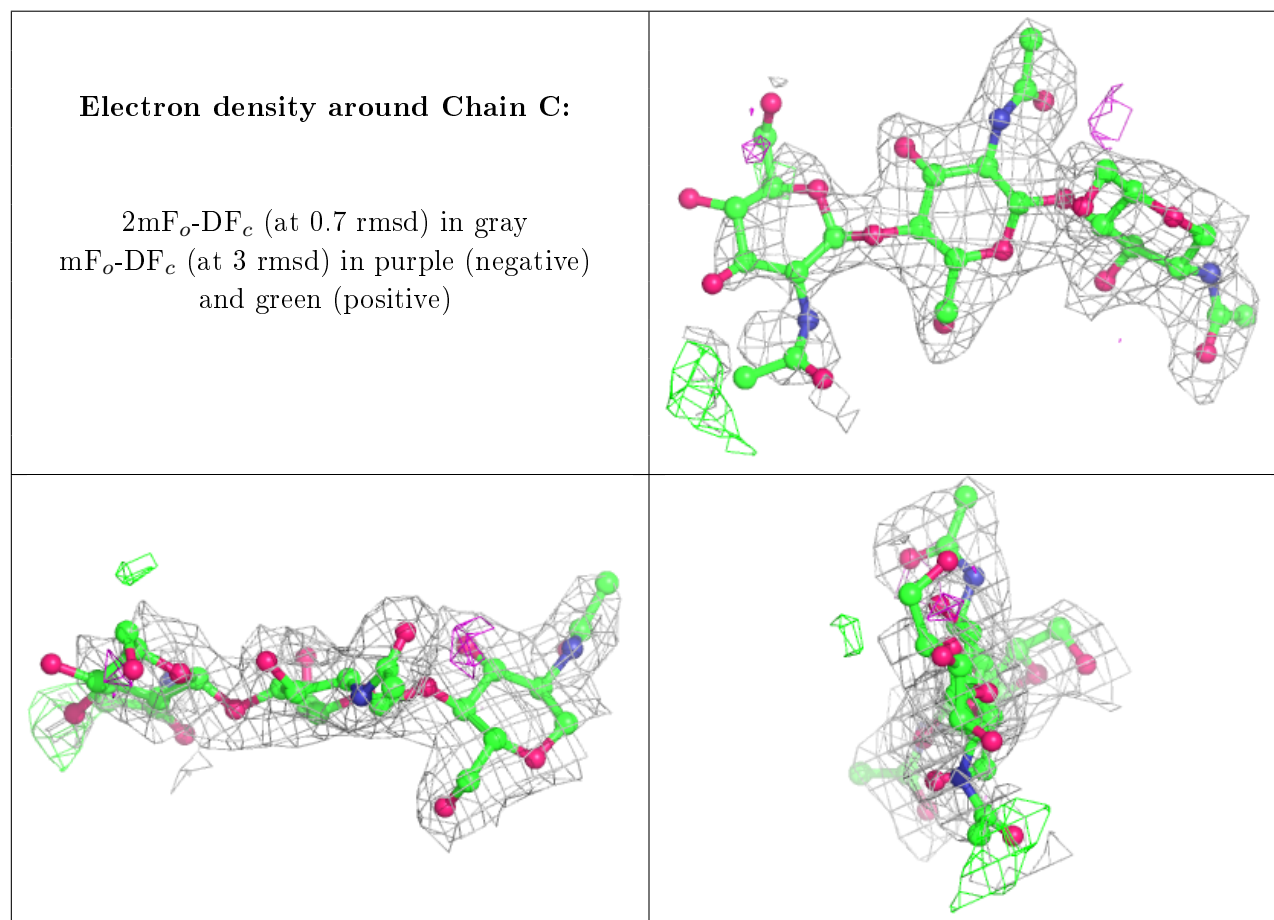
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPQ	B	470	14/15	0.82	0.21	40,53,55,56	0
1	TPQ	A	470	14/15	0.85	0.18	40,50,52,52	0

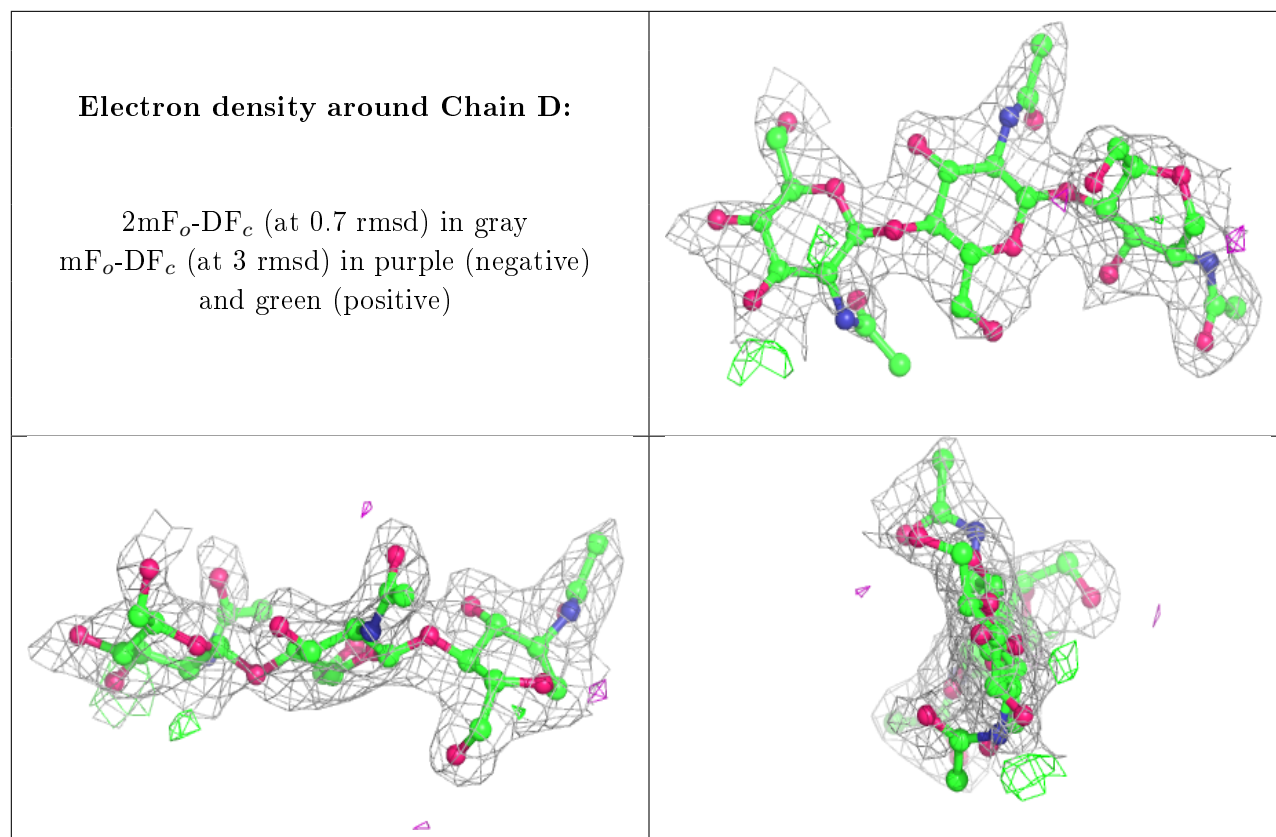
### 6.3 Carbohydrates [i](#)

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	NAG	C	3	14/15	0.68	0.47	63,70,73,74	0
2	NAG	D	3	14/15	0.69	0.41	61,64,66,67	0
2	NAG	C	2	14/15	0.89	0.15	28,44,49,55	0
2	NAG	D	2	14/15	0.91	0.22	35,42,49,55	0
2	NAG	C	1	14/15	0.93	0.13	29,30,32,36	0
2	NAG	D	1	14/15	0.94	0.12	29,31,35,35	0

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





## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	B	804	14/15	0.70	0.50	57,60,62,63	0
3	NAG	A	803	14/15	0.77	0.42	48,49,51,52	0
3	NAG	A	804	14/15	0.80	0.53	64,67,67,68	0
6	CL	A	904	1/1	0.94	0.08	32,32,32,32	0
6	CL	B	1904	1/1	0.98	0.09	32,32,32,32	0
6	CL	B	1905	1/1	0.98	0.10	25,25,25,25	0
5	CA	A	903	1/1	0.98	0.03	19,19,19,19	0
5	CA	A	902	1/1	0.99	0.10	18,18,18,18	0
4	CU	B	901	1/1	0.99	0.07	23,23,23,23	0
5	CA	B	1902	1/1	0.99	0.06	23,23,23,23	0
5	CA	B	1903	1/1	0.99	0.05	23,23,23,23	0
4	CU	A	901	1/1	1.00	0.08	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.