



# wwPDB X-ray Structure Validation Summary Report

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PDB ID : 4LNV  
Title : Crystal Structure of TEP1s  
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Deposited on : 2013-07-12  
Resolution : 3.70 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

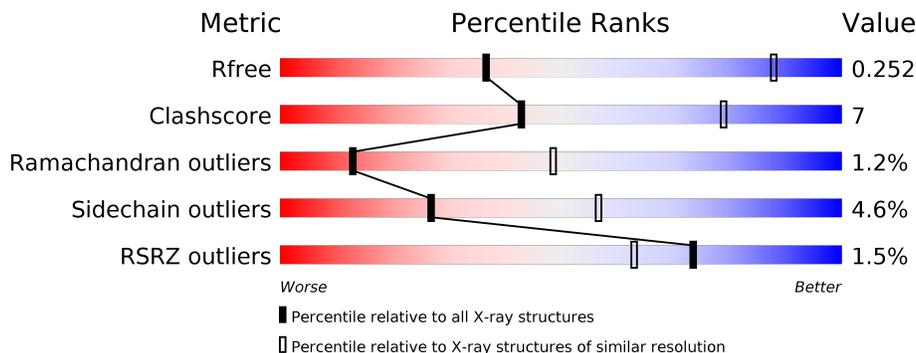
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	1323	<p>2% 79% 16% . .</p>
1	B	1323	<p>% 64% 15% . 20%</p>
1	C	1323	<p>% 79% 16% . .</p>
2	D	2	<p>100%</p>

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 27034 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 Thioester-containing protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1276	9704	6210	1583	1866	45	0	0	0
1	B	1063	7461	4750	1225	1454	32	0	0	0
1	C	1276	9631	6163	1573	1850	45	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

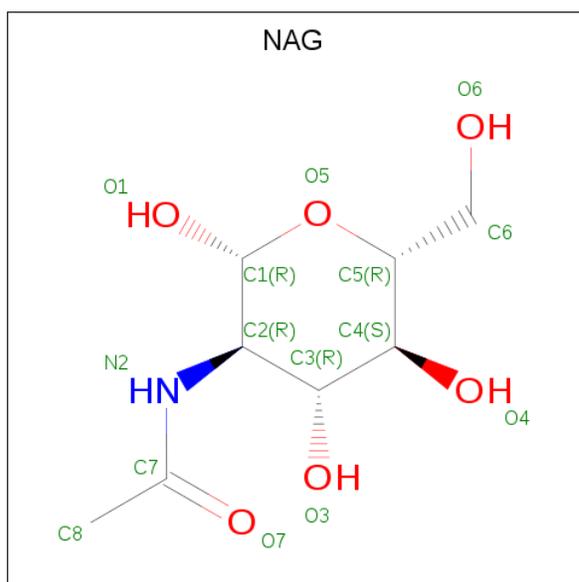
Chain	Residue	Modelled	Actual	Comment	Reference
A	1339	HIS	-	expression tag	UNP Q9GYW4
A	1340	HIS	-	expression tag	UNP Q9GYW4
A	1341	HIS	-	expression tag	UNP Q9GYW4
A	1342	HIS	-	expression tag	UNP Q9GYW4
A	1343	HIS	-	expression tag	UNP Q9GYW4
A	1344	HIS	-	expression tag	UNP Q9GYW4
B	1339	HIS	-	expression tag	UNP Q9GYW4
B	1340	HIS	-	expression tag	UNP Q9GYW4
B	1341	HIS	-	expression tag	UNP Q9GYW4
B	1342	HIS	-	expression tag	UNP Q9GYW4
B	1343	HIS	-	expression tag	UNP Q9GYW4
B	1344	HIS	-	expression tag	UNP Q9GYW4
C	1339	HIS	-	expression tag	UNP Q9GYW4
C	1340	HIS	-	expression tag	UNP Q9GYW4
C	1341	HIS	-	expression tag	UNP Q9GYW4
C	1342	HIS	-	expression tag	UNP Q9GYW4
C	1343	HIS	-	expression tag	UNP Q9GYW4
C	1344	HIS	-	expression tag	UNP Q9GYW4

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	2	28	16	2	10	0	0	0

- 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
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0

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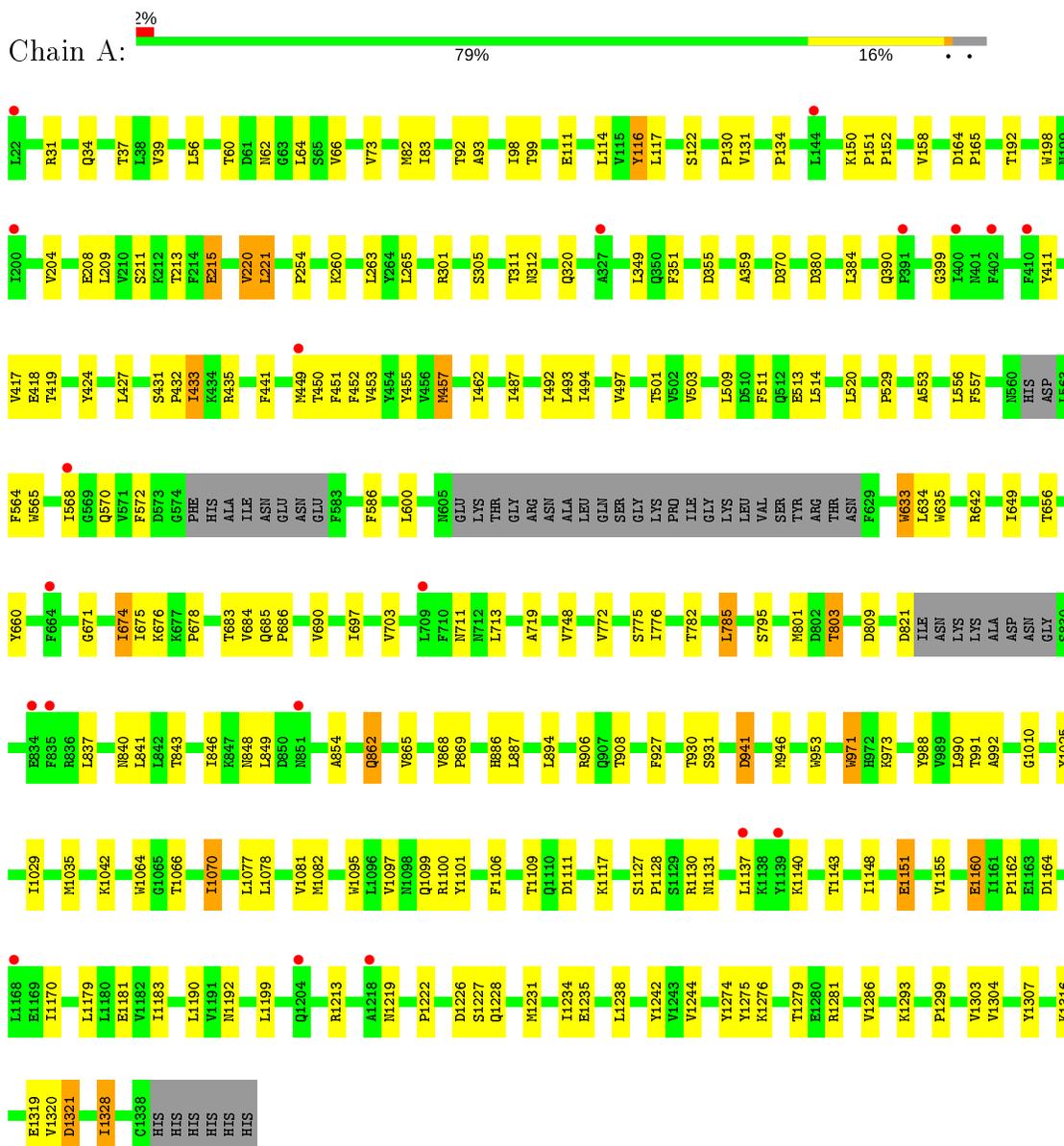
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>ZeroOcc</b>	<b>AltConf</b>
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

### 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: Thioester-containing protein I



- Molecule 1: Thioester-containing protein I





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	196.47Å 196.47Å 225.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 3.70 49.12 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.12-3.70) 99.7 (49.12-3.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.89	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 3.67Å)	Xtriage
Refinement program	REFMAC refmac_5.7.0025	Depositor
R, $R_{free}$	0.237 , 0.276 0.215 , 0.252	Depositor DCC
$R_{free}$ test set	4584 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	147.0	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 111.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.196 for h,-k,-l	Xtriage
Reported twinning fraction	0.504 for H, K, L 0.496 for K, H, -L	Depositor
Outliers	2 of 90746 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	27034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1834e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

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

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

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	0.41	6/9902 (0.1%)	0.53	0/13515
1	B	0.42	3/7592 (0.0%)	0.52	0/10410
1	C	0.40	2/9825 (0.0%)	0.52	0/13417
All	All	0.41	11/27319 (0.0%)	0.53	0/37342

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	TRP	CD2-CE2	5.30	1.47	1.41
1	A	198	TRP	CD2-CE2	5.27	1.47	1.41
1	A	971	TRP	CD2-CE2	5.24	1.47	1.41
1	B	971	TRP	CD2-CE2	5.24	1.47	1.41
1	C	953	TRP	CD2-CE2	5.08	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1064	TRP	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9704	0	9100	130	0
1	B	7461	0	6369	101	0
1	C	9631	0	8983	126	0
2	D	28	0	25	0	0
3	A	98	0	91	0	0
3	B	14	0	13	0	0
3	C	98	0	91	3	0
All	All	27034	0	24672	352	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 7.

The worst 5 of 352 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:C:1402:NAG:H4	3:C:1403:NAG:H5	1.59	0.84
1:A:62:ASN:HB3	1:B:970:VAL:HG23	1.63	0.79
1:C:862:GLN:HA	1:C:1109:THR:HG21	1.64	0.79
1:A:1100:ARG:HG2	1:A:1106:PHE:HE1	1.48	0.77
1:A:1100:ARG:HG2	1:A:1106:PHE:CE1	2.20	0.77

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	1266/1323 (96%)	1154 (91%)	101 (8%)	11 (1%)	17 54
1	B	1011/1323 (76%)	898 (89%)	94 (9%)	19 (2%)	8 40
1	C	1266/1323 (96%)	1157 (91%)	97 (8%)	12 (1%)	17 54
All	All	3543/3969 (89%)	3209 (91%)	292 (8%)	42 (1%)	13 48

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	642	ARG
1	A	1160	GLU
1	C	642	ARG
1	C	1160	GLU
1	A	418	GLU

### 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	997/1177 (85%)	957 (96%)	40 (4%)	31 60
1	B	670/1177 (57%)	627 (94%)	43 (6%)	17 48
1	C	979/1177 (83%)	940 (96%)	39 (4%)	31 60
All	All	2646/3531 (75%)	2524 (95%)	122 (5%)	27 57

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	815	THR
1	B	963	ARG
1	C	1042	LYS
1	B	859	CYS
1	B	889	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1039	HIS
1	B	1098	ASN
1	C	320	GLN
1	A	1228	GLN
1	A	1324	ASN

### 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$
2	NAG	D	1	1,2	14,14,15	0.71	0	17,19,21	1.83	4 (23%)
2	NAG	D	2	2	14,14,15	0.45	0	17,19,21	0.95	1 (5%)

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	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C2-N2-C7	4.53	129.35	122.90
2	D	1	NAG	O5-C1-C2	-3.26	106.13	111.29
2	D	1	NAG	C4-C3-C2	3.03	115.46	111.02
2	D	1	NAG	C3-C4-C5	2.44	114.59	110.24
2	D	2	NAG	C1-O5-C5	2.43	115.48	112.19

There are no chirality outliers.

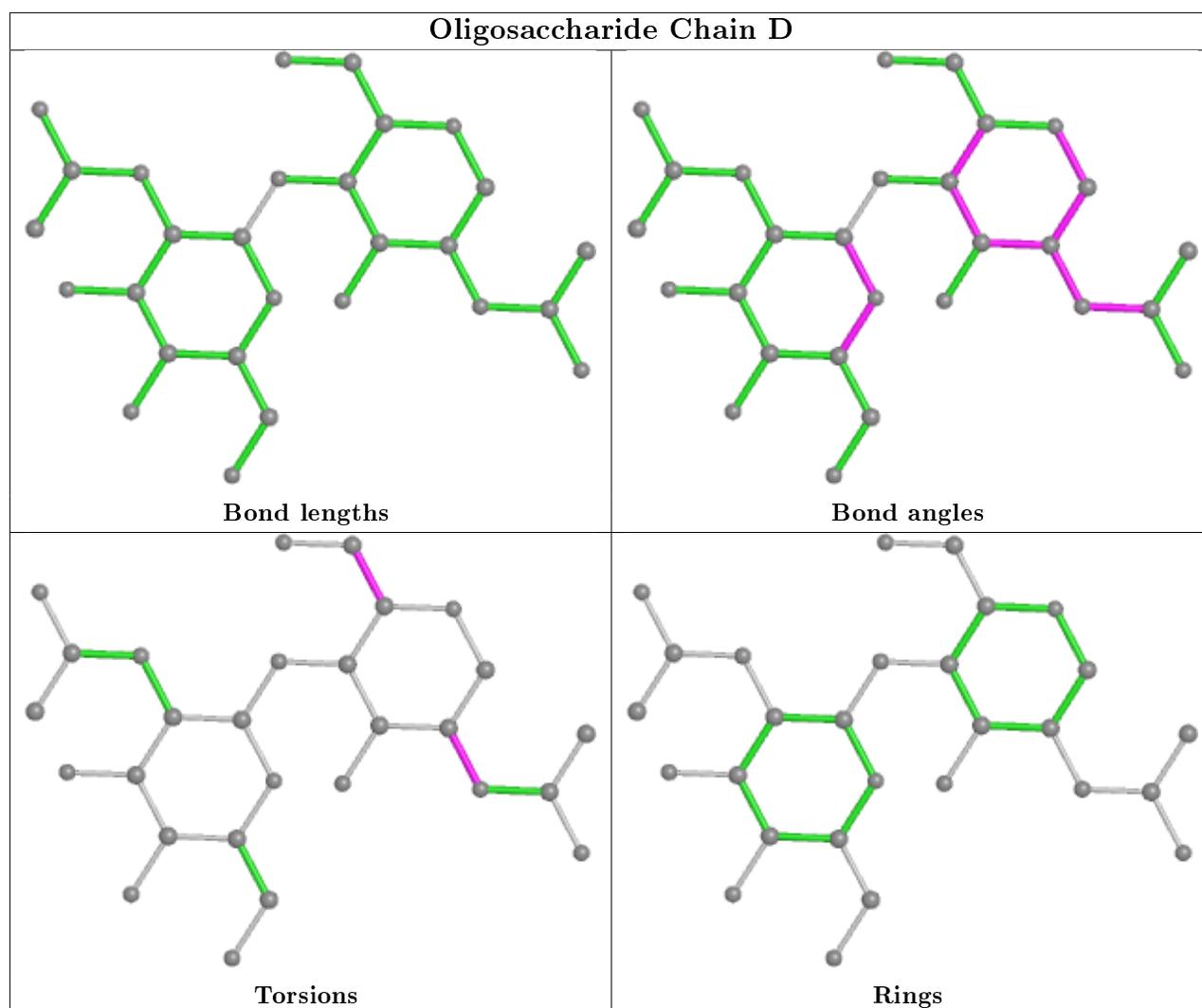
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7

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](#)

15 ligands 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	NAG	C	1405	1	14,14,15	0.49	0	17,19,21	1.13	1 (5%)
3	NAG	A	2003	1	14,14,15	0.48	0	17,19,21	0.87	0
3	NAG	A	2004	-	14,14,15	0.45	0	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1401	1	14,14,15	0.51	0	17,19,21	1.16	1 (5%)
3	NAG	C	1406	1	14,14,15	0.29	0	17,19,21	0.62	0
3	NAG	C	1402	1	14,14,15	0.49	0	17,19,21	0.69	0
3	NAG	A	2002	1	14,14,15	0.50	0	17,19,21	0.87	0
3	NAG	C	1403	-	14,14,15	0.48	0	17,19,21	1.63	4 (23%)
3	NAG	A	2005	1	14,14,15	0.62	0	17,19,21	2.28	5 (29%)
3	NAG	B	1401	1	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
3	NAG	A	2001	1	14,14,15	0.53	0	17,19,21	1.12	1 (5%)
3	NAG	C	1404	1	14,14,15	0.48	0	17,19,21	0.93	1 (5%)
3	NAG	C	1407	1	14,14,15	0.59	0	17,19,21	1.36	3 (17%)
3	NAG	A	2009	1	14,14,15	0.80	1 (7%)	17,19,21	1.65	4 (23%)
3	NAG	A	2008	1	14,14,15	0.43	0	17,19,21	2.54	3 (17%)

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	C	1405	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2003	1	-	1/6/23/26	0/1/1/1
3	NAG	A	2004	-	-	1/6/23/26	0/1/1/1
3	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1406	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1403	-	-	2/6/23/26	0/1/1/1
3	NAG	A	2005	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1407	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2009	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2008	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2009	NAG	C1-C2	2.20	1.55	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	2008	NAG	C1-O5-C5	9.60	125.20	112.19
3	A	2005	NAG	C1-O5-C5	6.21	120.61	112.19
3	A	2009	NAG	C4-C3-C2	4.56	117.70	111.02
3	A	2005	NAG	C2-N2-C7	4.47	129.27	122.90
3	C	1403	NAG	C1-O5-C5	4.12	117.77	112.19

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1401	NAG	C4-C5-C6-O6
3	B	1401	NAG	O5-C5-C6-O6
3	C	1402	NAG	C4-C5-C6-O6
3	A	2005	NAG	O5-C5-C6-O6
3	A	2008	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1406	NAG	1	0
3	C	1402	NAG	2	0
3	C	1403	NAG	2	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	1276/1323 (96%)	0.07	20 (1%) 72 61	113, 151, 175, 200	0
1	B	1063/1323 (80%)	0.04	17 (1%) 72 61	125, 165, 200, 200	0
1	C	1276/1323 (96%)	0.01	17 (1%) 77 67	123, 160, 191, 200	0
All	All	3615/3969 (91%)	0.04	54 (1%) 73 63	113, 157, 194, 200	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	PRO	3.0
1	C	660	TYR	3.0
1	A	410	PHE	2.9
1	B	84	ASN	2.8
1	B	241	VAL	2.8

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

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

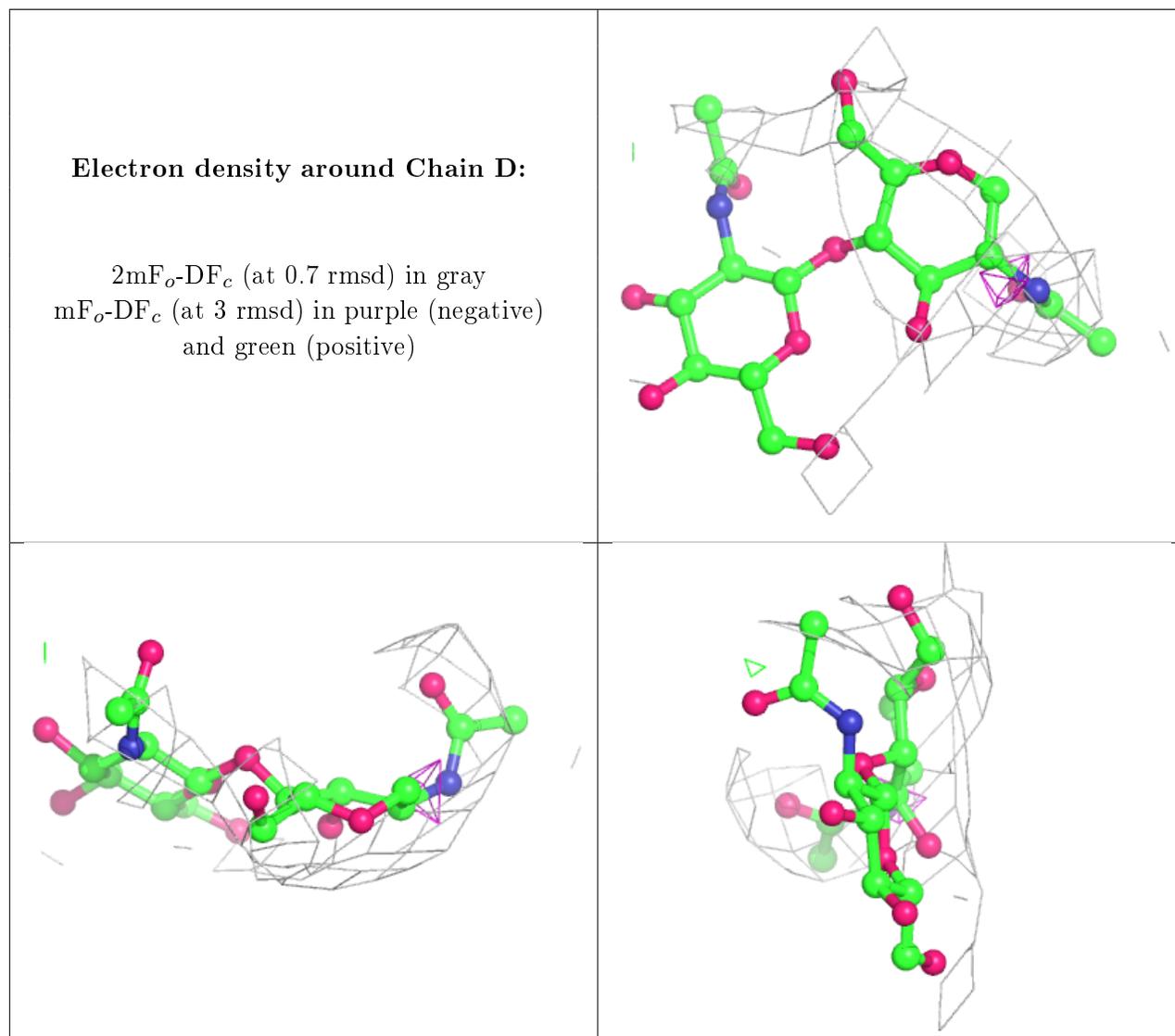
### 6.3 Carbohydrates [i](#)

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
2	NAG	D	1	14/15	0.87	0.28	167,168,169,170	0
2	NAG	D	2	14/15	0.92	0.12	169,171,172,173	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. 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
3	NAG	C	1401	14/15	0.76	0.26	166,167,168,168	0
3	NAG	A	2008	14/15	0.78	0.27	152,152,152,153	0
3	NAG	C	1407	14/15	0.79	0.24	168,169,169,169	0
3	NAG	A	2005	14/15	0.80	0.22	170,172,173,173	0
3	NAG	A	2009	14/15	0.81	0.22	166,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	1401	14/15	0.81	0.14	175,176,176,176	0
3	NAG	C	1406	14/15	0.82	0.22	174,175,176,176	0
3	NAG	C	1404	14/15	0.84	0.18	173,174,175,175	0
3	NAG	C	1405	14/15	0.84	0.16	162,163,163,164	0
3	NAG	A	2002	14/15	0.84	0.20	156,157,158,158	0
3	NAG	A	2001	14/15	0.84	0.20	165,168,168,169	0
3	NAG	A	2003	14/15	0.86	0.15	160,160,161,162	0
3	NAG	A	2004	14/15	0.87	0.13	177,177,178,178	0
3	NAG	C	1403	14/15	0.90	0.13	183,185,185,185	0
3	NAG	C	1402	14/15	0.91	0.14	166,166,167,168	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.