



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2025 – 02:31 pm BST

PDB ID : 9GPA / pdb\_00009gpa  
Title : ManDH5- a beta-D-Mannanase of GH5 family from Dictyoglomus thermophilum  
Authors : Sivron, Y.; Romano, A.; Shoham, Y.; Shoham, G.  
Deposited on : 2024-09-07  
Resolution : 1.50 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 : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

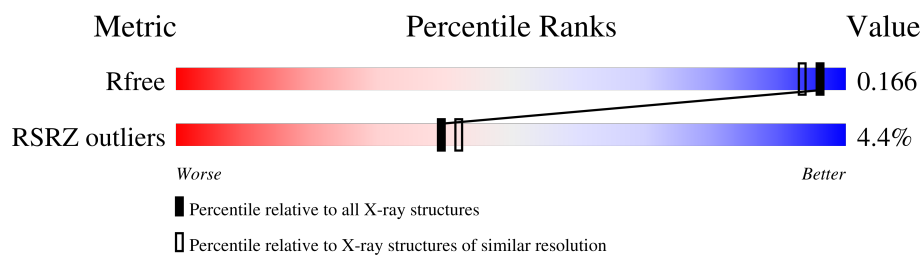
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	164625	3717 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

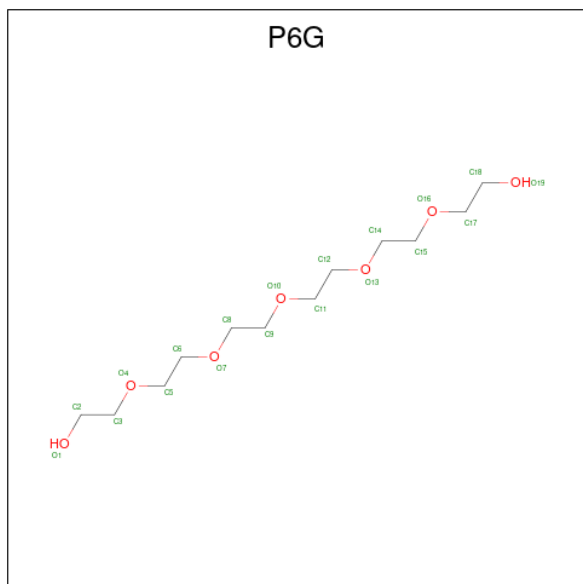
There are 8 unique types of molecules in this entry. The entry contains 9944 atoms, of which 4693 are hydrogens and 0 are deuteriums.

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 DUF5060 domain-containing protein.

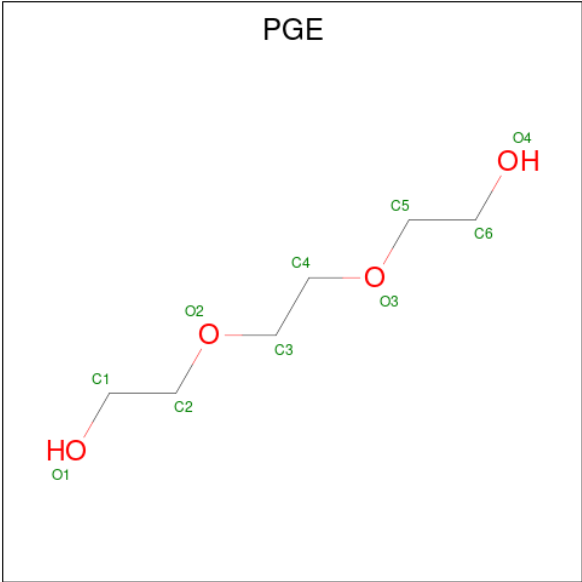
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	564	Total	C	H	N	O	S	0	4	0
			9256	3107	4537	750	853	9			

- Molecule 2 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



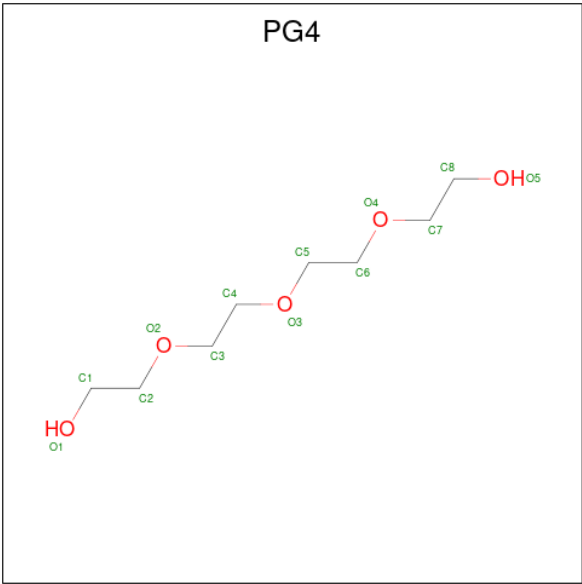
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			45	12	26	7		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



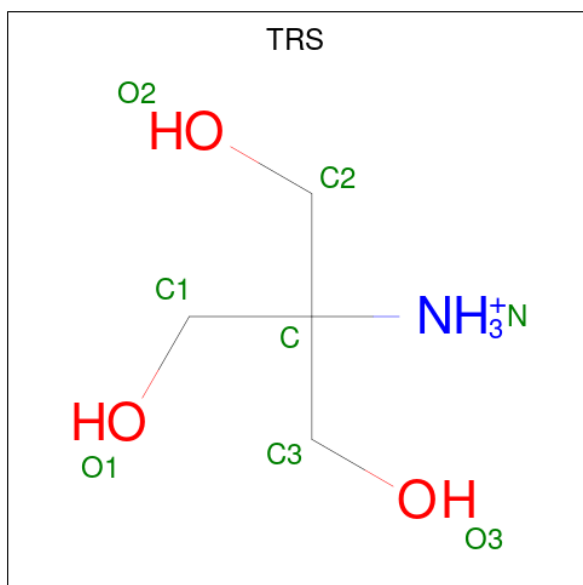
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



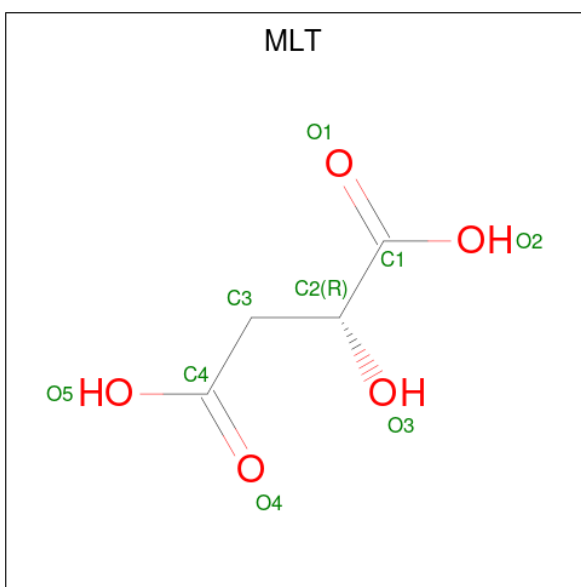
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			31	8	18	5		
4	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula:  $C_4H_{12}NO_3$ ).



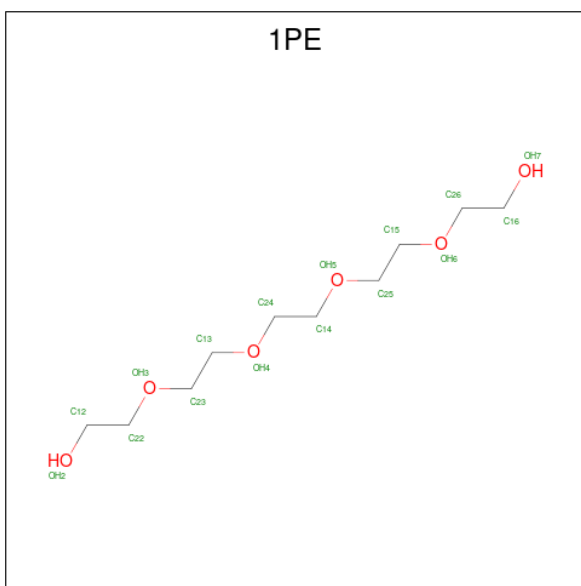
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

- Molecule 6 is D-MALATE (CCD ID: MLT) (formula:  $C_4H_6O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			13	4	4	5		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	413	Total 414	O 414	0	1

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### 3 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.65Å 99.26Å 153.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 1.50 49.63 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.63-1.50) 99.9 (49.63-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.14.3228_000	Depositor
R, $R_{free}$	0.144 , 0.161 0.151 , 0.166	Depositor DCC
$R_{free}$ test set	5961 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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.



## 4 Model quality [i](#)

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

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

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### 4.3 Torsion angles [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

10 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	$\# Z  > 2$
7	1PE	A	610	-	15,15,15	0.57	0	14,14,14	0.38	0
3	PGE	A	604	-	9,9,9	0.30	0	8,8,8	0.41	0
3	PGE	A	605	-	9,9,9	0.33	0	8,8,8	0.30	0
3	PGE	A	602	-	9,9,9	0.38	0	8,8,8	0.50	0
2	P6G	A	601	-	18,18,18	0.56	0	17,17,17	0.59	0
6	MLT	A	609	-	8,8,8	1.06	0	10,10,10	1.50	2 (20%)
4	PG4	A	606	-	12,12,12	0.51	0	11,11,11	0.53	0
4	PG4	A	607	-	12,12,12	0.53	0	11,11,11	0.45	0
5	TRS	A	608	-	7,7,7	0.71	0	9,9,9	2.22	3 (33%)
3	PGE	A	603	-	9,9,9	0.29	0	8,8,8	0.43	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
7	1PE	A	610	-	-	8/13/13/13	-
3	PGE	A	604	-	-	3/7/7/7	-
3	PGE	A	605	-	-	4/7/7/7	-
3	PGE	A	602	-	-	3/7/7/7	-
2	P6G	A	601	-	-	4/16/16/16	-
6	MLT	A	609	-	-	3/8/8/8	-
4	PG4	A	606	-	-	5/10/10/10	-
4	PG4	A	607	-	-	1/10/10/10	-
5	TRS	A	608	-	-	1/9/9/9	-
3	PGE	A	603	-	-	0/7/7/7	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	608	TRS	C3-C-C1	-3.93	98.63	110.81
5	A	608	TRS	C2-C-N	3.29	117.79	107.98
6	A	609	MLT	O2-C1-C2	3.25	119.86	112.72
5	A	608	TRS	C1-C-N	3.13	117.33	107.98

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	609	MLT	O2-C1-O1	-2.12	119.28	124.09

There are no chirality outliers.

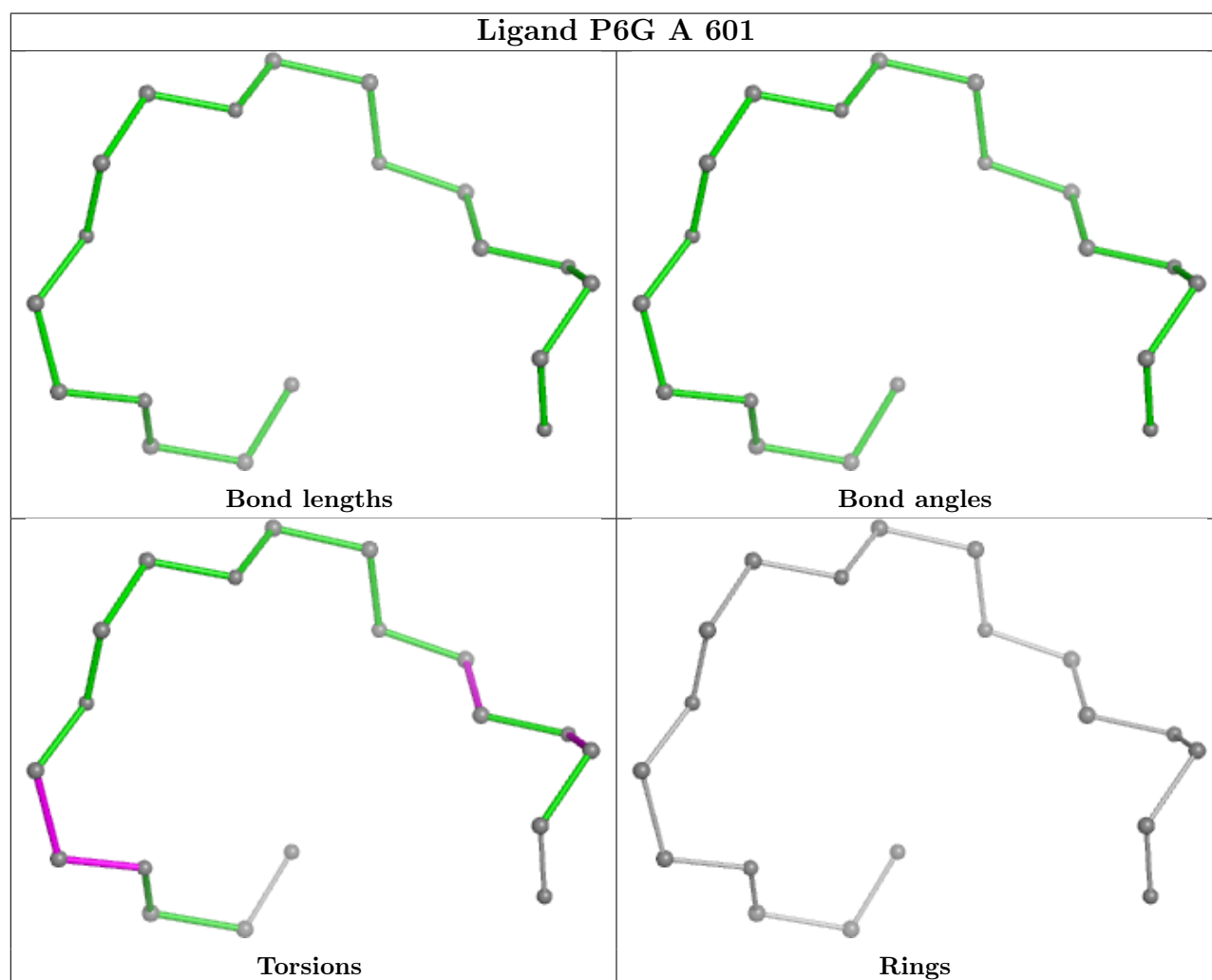
All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	609	MLT	O1-C1-C2-O3
6	A	609	MLT	O2-C1-C2-O3
7	A	610	1PE	OH5-C14-C24-OH4
7	A	610	1PE	OH4-C13-C23-OH3
4	A	606	PG4	O2-C3-C4-O3
7	A	610	1PE	OH6-C15-C25-OH5
3	A	605	PGE	O3-C5-C6-O4
4	A	606	PG4	O1-C1-C2-O2
7	A	610	1PE	OH7-C16-C26-OH6
3	A	605	PGE	O1-C1-C2-O2
4	A	606	PG4	O4-C7-C8-O5
4	A	607	PG4	O3-C5-C6-O4
3	A	602	PGE	O3-C5-C6-O4
2	A	601	P6G	O4-C5-C6-O7
3	A	605	PGE	O2-C3-C4-O3
2	A	601	P6G	C18-C17-O16-C15
3	A	604	PGE	C4-C3-O2-C2
7	A	610	1PE	C23-C13-OH4-C24
7	A	610	1PE	C25-C15-OH6-C26
7	A	610	1PE	C16-C26-OH6-C15
4	A	606	PG4	C4-C3-O2-C2
3	A	604	PGE	C1-C2-O2-C3
7	A	610	1PE	C24-C14-OH5-C25
3	A	605	PGE	C4-C3-O2-C2
3	A	602	PGE	C1-C2-O2-C3
2	A	601	P6G	C6-C5-O4-C3
3	A	604	PGE	O1-C1-C2-O2
4	A	606	PG4	C5-C6-O4-C7
2	A	601	P6G	O13-C14-C15-O16
5	A	608	TRS	C2-C-C3-O3
3	A	602	PGE	O1-C1-C2-O2
6	A	609	MLT	O2-C1-C2-C3

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 4.7 Other polymers ⓘ

There are no such residues in this entry.

## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 Protein, DNA and RNA chains ⓘ

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	564/568 (99%)	-0.17	25 (4%)	39 42	13, 24, 47, 86	4 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	ASP	4.8
1	A	403	TRP	4.7
1	A	565	GLY	4.3
1	A	564	LEU	4.2
1	A	474	ASN	3.8
1	A	508	MET	3.7
1	A	510	SER	3.6
1	A	521	ILE	3.6
1	A	511	SER	3.1
1	A	507	ASN	2.9
1	A	466	THR	2.9
1	A	77	ASN	2.8
1	A	563	LEU	2.8
1	A	470	PHE	2.7
1	A	400	ASN	2.6
1	A	502	LYS	2.4
1	A	467	ASN	2.4
1	A	475	ARG	2.4
1	A	520	LEU	2.3
1	A	524	PRO	2.2
1	A	541	LEU	2.2
1	A	469	LYS	2.2
1	A	486	LYS	2.2
1	A	544	ASP	2.1
1	A	514	LEU	2.0

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

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

## 5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.4 Ligands ⓘ

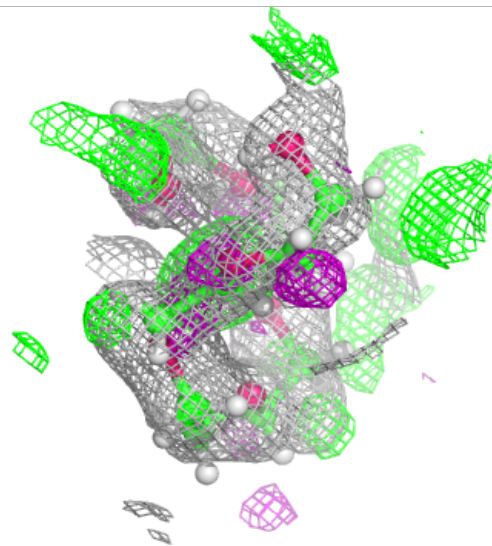
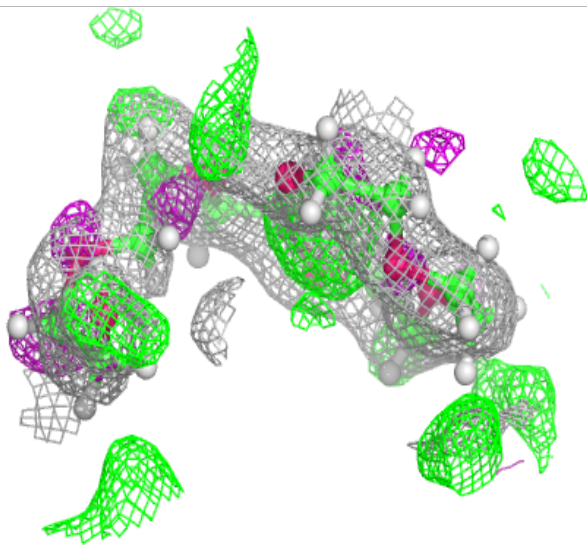
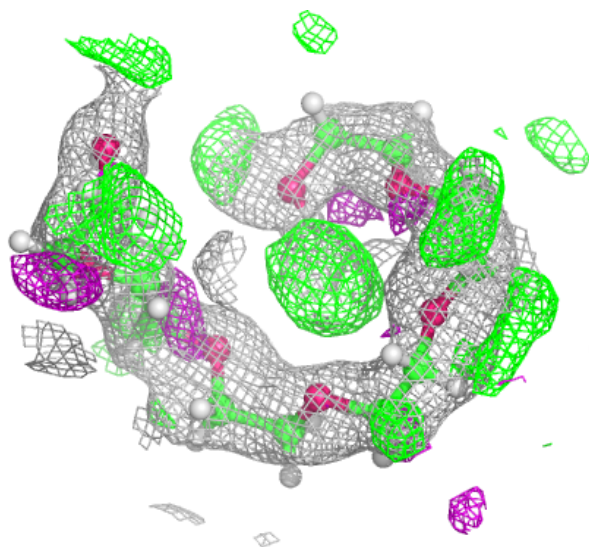
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	PGE	A	605	10/10	0.75	0.20	45,54,56,57	0
6	MLT	A	609	9/9	0.76	0.17	54,55,66,66	0
4	PG4	A	606	13/13	0.82	0.17	43,52,56,57	0
7	1PE	A	610	16/16	0.83	0.17	48,58,60,61	0
2	P6G	A	601	19/19	0.85	0.14	32,41,49,50	0
3	PGE	A	602	10/10	0.86	0.14	45,56,60,60	0
3	PGE	A	604	10/10	0.90	0.12	41,50,55,57	0
4	PG4	A	607	13/13	0.90	0.12	36,46,57,59	0
3	PGE	A	603	10/10	0.94	0.08	33,40,45,48	0
5	TRS	A	608	8/8	0.96	0.07	17,23,27,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around P6G A 601:**

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



## 5.5 Other polymers [i](#)

There are no such residues in this entry.