

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 3, 2023 – 08:27 AM EDT

PDB ID	:	6PW3
Title	:	LARP1 DM15 FYRE (F844Y, R847E) mutant bound to m7GpppG dinu-
		cleotide (capG)
Authors	:	Lahr, R.M.; Berman, A.J.
Deposited on	:	2019-07-22
Resolution	:	2.34  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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\hbox{-}RAY\,DIFFRACTION$ 

The reported resolution of this entry is 2.34 Å.

There are no overall percentile quality scores available for this entry.

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



#### 6 PW3

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9780 atoms, of which 4593 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.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	1 C	140	Total	С	Η	Ν	0	$\mathbf{S}$	0	1	0
	U	145	2482	843	1186	222	227	4			0
1	Δ	144	Total	С	Η	Ν	0	S	0	2	0
1	Л	144	2408	817	1151	213	223	4	0		
1	Р	140	Total	С	Η	Ν	0	S	0	0	0
1	D	140	2362	798	1141	203	216	4	0	0	U
1	D	1.49	Total	С	Η	Ν	0	S	0	0	0
	D	140	2245	785	1034	205	217	4	0		0

• Molecule 1 is a protein called La-related protein 1.

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	785	GLY	-	expression tag	UNP Q6PKG0
С	786	HIS	-	expression tag	UNP Q6PKG0
С	787	SER	-	expression tag	UNP Q6PKG0
С	788	GLY	-	expression tag	UNP Q6PKG0
С	789	GLY	-	expression tag	UNP Q6PKG0
С	790	GLY	-	expression tag	UNP Q6PKG0
С	791	GLY	-	expression tag	UNP Q6PKG0
С	792	GLY	-	expression tag	UNP Q6PKG0
С	793	GLY	-	expression tag	UNP Q6PKG0
С	794	HIS	-	expression tag	UNP Q6PKG0
С	795	MET	-	expression tag	UNP Q6PKG0
С	844	TYR	PHE	engineered mutation	UNP Q6PKG0
С	847	GLU	ARG	engineered mutation	UNP Q6PKG0
А	785	GLY	-	expression tag	UNP Q6PKG0
А	786	HIS	-	expression tag	UNP Q6PKG0
А	787	SER	-	expression tag	UNP Q6PKG0
А	788	GLY	-	expression tag	UNP Q6PKG0
А	789	GLY	-	expression tag	UNP Q6PKG0
А	790	GLY	-	expression tag	UNP Q6PKG0
А	791	GLY	-	expression tag	UNP Q6PKG0
А	792	GLY	-	expression tag	UNP Q6PKG0



Chain	Residue	Modelled	Actual	Comment	Reference
А	793	GLY	-	expression tag	UNP Q6PKG0
А	794	HIS	-	expression tag	UNP Q6PKG0
А	795	MET	-	expression tag	UNP Q6PKG0
А	844	TYR	PHE	engineered mutation	UNP Q6PKG0
А	847	GLU	ARG	engineered mutation	UNP Q6PKG0
В	785	GLY	-	expression tag	UNP Q6PKG0
В	786	HIS	-	expression tag	UNP Q6PKG0
В	787	SER	-	expression tag	UNP Q6PKG0
В	788	GLY	-	expression tag	UNP Q6PKG0
В	789	GLY	-	expression tag	UNP Q6PKG0
В	790	GLY	-	expression tag	UNP Q6PKG0
В	791	GLY	-	expression tag	UNP Q6PKG0
В	792	GLY	-	expression tag	UNP Q6PKG0
В	793	GLY	-	expression tag	UNP Q6PKG0
В	794	HIS	-	expression tag	UNP Q6PKG0
В	795	MET	-	expression tag	UNP Q6PKG0
В	844	TYR	PHE	engineered mutation	UNP Q6PKG0
В	847	GLU	ARG	engineered mutation	UNP Q6PKG0
D	785	GLY	-	expression tag	UNP Q6PKG0
D	786	HIS	-	expression tag	UNP Q6PKG0
D	787	SER	-	expression tag	UNP Q6PKG0
D	788	GLY	-	expression tag	UNP Q6PKG0
D	789	GLY	-	expression tag	UNP Q6PKG0
D	790	GLY	-	expression tag	UNP Q6PKG0
D	791	GLY	-	expression tag	UNP Q6PKG0
D	792	GLY	-	expression tag	UNP Q6PKG0
D	793	GLY	-	expression tag	UNP Q6PKG0
D	794	HIS	-	expression tag	UNP Q6PKG0
D	795	MET	-	expression tag	UNP Q6PKG0
D	844	TYR	PHE	engineered mutation	UNP Q6PKG0
D	847	GLU	ARG	engineered mutation	UNP Q6PKG0

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• Molecule 2 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-GUANOSINE (three-letter code: GTG) (formula:  $C_{21}H_{30}N_{10}O_{18}P_3$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	2 C	1	Total	С	Η	Ν	Ο	Р	0	1
	1	158	42	54	20	36	6	0	1	
9	2 B	1	Total	С	Η	Ν	Ο	Р	0	0
		1	79	21	27	10	18	3	0	U

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	12	Total         O           12         12	0	0
4	А	15	Total         O           15         15	0	0
4	В	11	Total         O           11         11	0	0
4	D	7	Total O 7 7	0	0

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



# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	58.58Å 87.36Å 72.89Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $93.37^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	29.24 - 2.34	Depositor
% Data completeness	94.5(29.24-2.34)	Depositor
(in resolution range)	54.5 (25.24-2.54)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.86 (at 2.34 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
$R, R_{free}$	0.221 , $0.267$	Depositor
Wilson B-factor $(Å^2)$	54.3	Xtriage
Anisotropy	0.409	Xtriage
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9780	wwPDB-VP
Average B, all atoms $(Å^2)$	74.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.85% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 4 Model quality (i)

## 4.1 Standard geometry (i)

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

### 4.2 Too-close contacts (i)

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

### 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 monosaccharides in this entry.

## 4.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is 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



Mal Truna	Chain	<b>D</b>	т. 1	B	ond leng	$_{ m gths}$	Bond angles			
IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	GTG	С	1001[B]	-	46,57,57	4.00	28 (60%)	47,90,90	1.59	11 (23%)
2	GTG	С	1001[A]	-	46,57,57	4.02	28 (60%)	47,90,90	1.46	9 (19%)
2	GTG	В	1001	-	46,57,57	4.01	28 (60%)	47,90,90	1.51	9 (19%)

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).

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	GTG	С	1001[B]	-	-	10/24/64/64	0/6/6/6
2	GTG	С	1001[A]	-	-	13/24/64/64	0/6/6/6
2	GTG	В	1001	-	-	9/24/64/64	0/6/6/6

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	1001[A]	GTG	C2D-C3D	-10.72	1.24	1.53
2	В	1001	GTG	C2D-C3D	-10.65	1.24	1.53
2	С	1001[B]	GTG	C2D-C3D	-10.64	1.24	1.53
2	В	1001	GTG	C2D-C1D	8.88	1.67	1.53
2	С	1001[A]	GTG	C2D-C1D	8.80	1.67	1.53
2	С	1001[B]	GTG	C2D-C1D	8.73	1.67	1.53
2	В	1001	GTG	C3E-C4E	-8.45	1.31	1.53
2	С	1001[A]	GTG	C3E-C4E	-8.43	1.31	1.53
2	С	1001[B]	GTG	C3E-C4E	-8.24	1.31	1.53
2	В	1001	GTG	O4E-C4E	7.68	1.62	1.45
2	С	1001[A]	GTG	O4E-C4E	7.61	1.62	1.45
2	С	1001[B]	GTG	O4E-C4E	7.57	1.61	1.45
2	С	1001[A]	GTG	O4E-C1E	-7.51	1.30	1.41
2	С	1001[B]	GTG	O4D-C1D	-7.20	1.31	1.41
2	В	1001	GTG	O4D-C1D	-7.20	1.31	1.41
2	В	1001	GTG	O4E-C1E	-7.10	1.31	1.41
2	С	1001[B]	GTG	O4E-C1E	-7.10	1.31	1.41
2	С	1001[A]	GTG	O4D-C1D	-6.98	1.31	1.41
2	С	1001[B]	GTG	C2A-N3A	5.53	1.46	1.33
2	С	1001[A]	GTG	C2A-N3A	5.52	1.46	1.33



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1001	GTG	C2A-N3A	5.52	1.46	1.33
2	С	1001[A]	GTG	C2B-N3B	5.49	1.46	1.33
2	С	1001[B]	GTG	C2B-N3B	5.49	1.46	1.33
2	В	1001	GTG	C2B-N3B	5.49	1.46	1.33
2	С	1001[B]	GTG	C4B-N3B	5.27	1.50	1.37
2	С	1001[A]	GTG	C4B-N3B	5.23	1.50	1.37
2	В	1001	GTG	C4B-N3B	5.19	1.50	1.37
2	С	1001[B]	GTG	C4A-N3A	5.13	1.49	1.37
2	В	1001	GTG	C4A-N3A	5.13	1.49	1.37
2	С	1001[A]	GTG	C4A-N3A	5.12	1.49	1.37
2	С	1001[B]	GTG	C2B-N2B	4.82	1.45	1.34
2	С	1001[A]	GTG	C2B-N2B	4.81	1.45	1.34
2	В	1001	GTG	C2B-N2B	4.81	1.45	1.34
2	С	1001[B]	GTG	C2A-N2A	4.77	1.45	1.34
2	С	1001[A]	GTG	C2A-N2A	4.74	1.45	1.34
2	В	1001	GTG	C2A-N2A	4.74	1.45	1.34
2	В	1001	GTG	C5D-C4D	-3.95	1.39	1.51
2	С	1001[B]	GTG	C5D-C4D	-3.88	1.39	1.51
2	С	1001[A]	GTG	C5D-C4D	-3.81	1.39	1.51
2	В	1001	GTG	C6A-N1A	3.78	1.43	1.37
2	С	1001[B]	GTG	C6A-N1A	3.76	1.43	1.37
2	С	1001[A]	GTG	C6A-N1A	3.75	1.43	1.37
2	В	1001	GTG	C6B-N1B	3.71	1.43	1.37
2	С	1001[A]	GTG	C6B-N1B	3.70	1.43	1.37
2	С	1001[B]	GTG	C6B-N1B	3.61	1.43	1.37
2	С	1001[B]	GTG	O3D-C3D	3.35	1.50	1.43
2	В	1001	GTG	O3D-C3D	3.32	1.50	1.43
2	С	1001[A]	GTG	O3D-C3D	3.31	1.50	1.43
2	С	1001[B]	GTG	C5A-C6A	3.26	1.53	1.45
2	В	1001	GTG	C5A-C6A	3.26	1.53	1.45
2	С	1001[A]	GTG	C5A-C6A	3.23	1.53	1.45
2	С	1001[B]	GTG	C5B-C6B	3.21	1.53	1.47
2	В	1001	GTG	C5B-C6B	3.21	1.53	1.47
2	С	1001[B]	GTG	C3D-C4D	3.18	1.61	1.53
2	С	1001[A]	GTG	C5B-C6B	3.17	1.53	1.47
2	В	1001	GTG	$\overline{\text{C3D-C4D}}$	3.12	1.61	1.53
2	С	1001[A]	GTG	C3D-C4D	3.11	1.60	1.53
2	С	1001[B]	GTG	O3E-C3E	2.96	1.49	1.43
2	В	1001	GTG	O3E-C3E	2.95	1.49	1.43
2	С	1001[A]	GTG	O3E-C3E	2.94	1.49	1.43
2	С	1001[B]	GTG	O2E-C2E	-2.92	1.36	1.43
2	В	1001	GTG	O2E-C2E	-2.86	1.36	1.43

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/lol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	1001[A]	GTG	O2E-C2E	-2.85	1.36	1.43
2	С	1001[B]	GTG	C2A-N1A	2.77	1.44	1.37
2	В	1001	GTG	C2A-N1A	2.75	1.44	1.37
2	С	1001[A]	GTG	C2A-N1A	2.75	1.44	1.37
2	В	1001	GTG	C2B-N1B	2.71	1.44	1.37
2	С	1001[A]	GTG	C2B-N1B	2.70	1.44	1.37
2	С	1001[A]	GTG	O4D-C4D	2.68	1.51	1.45
2	С	1001[B]	GTG	O4D-C4D	2.67	1.51	1.45
2	С	1001[B]	GTG	C2B-N1B	2.58	1.44	1.37
2	В	1001	GTG	O4D-C4D	2.51	1.50	1.45
2	В	1001	GTG	O2D-C2D	2.32	1.48	1.43
2	С	1001[B]	GTG	O2D-C2D	2.30	1.48	1.43
2	В	1001	GTG	C5B-C4B	-2.30	1.37	1.43
2	С	1001[A]	GTG	O2D-C2D	2.28	1.48	1.43
2	С	1001[A]	GTG	C5B-C4B	-2.28	1.37	1.43
2	В	1001	GTG	O6A-C6A	-2.22	1.18	1.23
2	С	1001[A]	GTG	O6A-C6A	-2.21	1.18	1.23
2	С	1001[B]	GTG	O6A-C6A	-2.20	1.18	1.23
2	С	1001[B]	GTG	O6B-C6B	-2.17	1.18	1.23
2	В	1001	GTG	O6B-C6B	-2.17	1.18	1.23
2	С	1001[A]	GTG	O6B-C6B	-2.16	1.18	1.23
2	С	1001[B]	GTG	C5B-C4B	-2.14	1.37	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1001	GTG	C3D-C2D-C1D	4.16	107.24	100.98
2	С	1001[B]	GTG	C3D-C2D-C1D	3.89	106.84	100.98
2	С	1001[B]	GTG	C5B-C6B-N1B	3.67	120.43	113.95
2	В	1001	GTG	C5B-C6B-N1B	3.47	120.08	113.95
2	С	1001[A]	GTG	C5B-C6B-N1B	3.43	120.01	113.95
2	С	1001[B]	GTG	C3E-C2E-C1E	3.30	105.94	100.98
2	С	1001[B]	GTG	C2B-N1B-C6B	-3.29	119.04	125.10
2	В	1001	GTG	PB-O3A-PA	-3.18	121.92	132.83
2	С	1001[A]	GTG	C3D-C2D-C1D	3.08	105.62	100.98
2	В	1001	GTG	C2B-N1B-C6B	-3.05	119.48	125.10
2	С	1001[A]	GTG	C3E-C2E-C1E	3.01	105.51	100.98
2	В	1001	GTG	C2A-N1A-C6A	-2.98	119.61	125.10
2	С	1001[A]	GTG	C2A-N1A-C6A	-2.97	119.63	125.10
2	С	1001[B]	GTG	C2A-N1A-C6A	-2.95	119.66	125.10
2	С	1001[A]	GTG	C2B-N1B-C6B	-2.94	119.69	125.10
2	В	1001	GTG	C8B-N7B-C5B	2.90	108.51	102.99

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	1001[A]	GTG	C8B-N7B-C5B	2.85	108.43	102.99
2	В	1001	GTG	PG-O3B-PB	-2.84	123.08	132.83
2	С	1001[B]	GTG	C8B-N7B-C5B	2.75	108.23	102.99
2	С	1001[A]	GTG	PG-O3B-PB	-2.71	123.54	132.83
2	В	1001	GTG	C3E-C2E-C1E	2.67	105.00	100.98
2	С	1001[B]	GTG	PG-O3B-PB	-2.64	123.75	132.83
2	С	1001[A]	GTG	PB-O3A-PA	-2.56	124.06	132.83
2	С	1001[B]	GTG	PB-O3A-PA	-2.55	124.08	132.83
2	С	1001[B]	GTG	O6B-C6B-C5B	-2.34	119.79	124.37
2	С	1001[B]	GTG	O4E-C1E-C2E	-2.26	103.62	106.93
2	С	1001[A]	GTG	O6B-C6B-C5B	-2.22	120.03	124.37
2	В	1001	GTG	O6B-C6B-C5B	-2.20	120.07	124.37
2	С	1001[B]	GTG	C2E-C3E-C4E	2.18	106.88	102.64

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There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	1001[A]	GTG	C5D-O5D-PA-O1A
2	С	1001[A]	GTG	C5E-O5E-PG-O1G
2	С	1001[A]	GTG	C5E-O5E-PG-O2G
2	С	1001[B]	GTG	C5D-O5D-PA-O2A
2	С	1001[B]	GTG	C5D-O5D-PA-O3A
2	С	1001[B]	GTG	C5E-O5E-PG-O3B
2	С	1001[B]	GTG	C5E-O5E-PG-O2G
2	С	1001[B]	GTG	O4E-C4E-C5E-O5E
2	С	1001[B]	GTG	C3E-C4E-C5E-O5E
2	В	1001	GTG	C5D-O5D-PA-O3A
2	В	1001	GTG	C3D-C4D-C5D-O5D
2	В	1001	GTG	O4D-C4D-C5D-O5D
2	В	1001	GTG	C4D-C5D-O5D-PA
2	С	1001[A]	GTG	C5D-O5D-PA-O3A
2	С	1001[A]	GTG	O4D-C4D-C5D-O5D
2	С	1001[B]	GTG	PB-O3A-PA-O2A
2	С	1001[A]	GTG	C5D-O5D-PA-O2A
2	С	1001[B]	GTG	C5D-O5D-PA-O1A
2	С	1001[B]	GTG	C5E-O5E-PG-O1G
2	В	1001	GTG	C5D-O5D-PA-O1A
2	С	1001[B]	GTG	C4E-C5E-O5E-PG
2	С	1001[A]	GTG	PB-O3A-PA-O2A
2	В	1001	GTG	PB-O3B-PG-O2G
2	С	1001[A]	GTG	C4D-C5D-O5D-PA



Mol	Chain	Res	Type	Atoms
2	В	1001	GTG	C4E-C5E-O5E-PG
2	С	1001[A]	GTG	PG-O3B-PB-O3A
2	В	1001	GTG	O4E-C4E-C5E-O5E
2	В	1001	GTG	C3E-C4E-C5E-O5E
2	С	1001[A]	GTG	C5E-O5E-PG-O3B
2	С	1001[A]	GTG	PB-O3A-PA-O1A
2	С	1001[A]	GTG	PG-O3B-PB-O2B
2	С	1001[A]	GTG	O4E-C4E-C5E-O5E

Continued from previous page...

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 then 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 (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 5 Fit of model and data (i)

## 5.1 Protein, DNA and RNA chains (i)

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

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

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

### 5.3 Carbohydrates (i)

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

## 5.4 Ligands (i)

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

### 5.5 Other polymers (i)

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

