

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

Nov 15, 2023 – 12:16 AM JST

PDB ID : 6IK9

Title: HIV-1 reverse transcriptase with Q151M/G112S/D113A/Y115F/F116Y/F16

0L/I159L:DNA:dGTP ternary complex

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Deposited on : 2018-10-15

Resolution : 2.44 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
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 : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

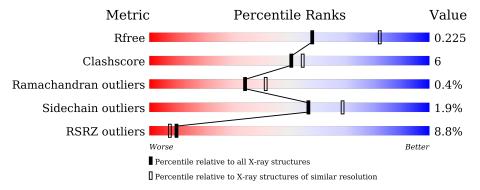
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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 >=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 <=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	557	83%	16%	
1	С	557	11%	10%	<b>%</b> ••
2	В	444	13% 75%	16% •	9%
2	D	444	5% 81%	10% •	9%
3	Е	38	66%	21% 5%	8%
3	F	38	66%	26%	8%



# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17566 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 HIV-1 reverse transcriptase p66 subunit.

$\mathbf{Mol}$	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	553	Total	С	N	О	S	0	0	0
	Λ	000	4494	2908	750	828	8	0		
1	С	553	Total	С	N	О	S	0	0	0
		999	4494	2908	750	828	8	0		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP D3XFN7
A	0	VAL	-	expression tag	UNP D3XFN7
A	112	SER	GLY	engineered mutation	UNP D3XFN7
A	113	ALA	ASP engineered mutation		UNP D3XFN7
A	115	PHE	TYR	engineered mutation	UNP D3XFN7
A	116	TYR	PHE	engineered mutation	UNP D3XFN7
A	151	MET	GLN	engineered mutation	UNP D3XFN7
A	159	LEU	ILE	engineered mutation	UNP D3XFN7
A	160	LEU	PHE	engineered mutation	UNP D3XFN7
A	162	SER	CYS	engineered mutation	UNP D3XFN7
A	280	SER	CYS	engineered mutation	UNP D3XFN7
С	-1	MET	-	expression tag	UNP D3XFN7
С	0	VAL	-	expression tag	UNP D3XFN7
С	112	SER	GLY	engineered mutation	UNP D3XFN7
С	113	ALA	ASP	engineered mutation	UNP D3XFN7
С	115	PHE	TYR	engineered mutation	UNP D3XFN7
С	116	TYR	PHE	engineered mutation	UNP D3XFN7
С	151	MET	GLN	engineered mutation	UNP D3XFN7
С	159	LEU	ILE	engineered mutation	UNP D3XFN7
С	160	LEU	PHE	engineered mutation	UNP D3XFN7
С	162	SER	CYS	engineered mutation	UNP D3XFN7
С	280	SER	CYS	engineered mutation	UNP D3XFN7

• Molecule 2 is a protein called HIV-1 reverse transcriptase p51 subunit.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	406	Total 3347	C 2178	N 557	O 606	S 6	0	0	0
2	D	406	Total 3347	C 2178		O 606	S 6	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

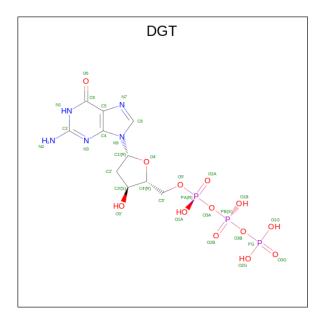
ChainResidueModelledActualCommentReferB-15MET-expression tagUNP FB-14ALA-expression tagUNP FB-13HIS-expression tagUNP FB-12HIS-expression tagUNP FB-11HIS-expression tagUNP FB-9HIS-expression tagUNP FB-8HIS-expression tagUNP FB-7ALA-expression tagUNP FB-6LEU-expression tagUNP F	P12497 P12497 P12497 P12497 P12497 P12497 P12497
B -14 ALA - expression tag UNP F B -13 HIS - expression tag UNP F B -12 HIS - expression tag UNP F B -11 HIS - expression tag UNP F B -10 HIS - expression tag UNP F B -9 HIS - expression tag UNP F B -8 HIS - expression tag UNP F B -7 ALA - expression tag UNP F B -6 LEU - expression tag UNP F	P12497 P12497 P12497 P12497 P12497 P12497 P12497
B         -13         HIS         -         expression tag         UNP F           B         -12         HIS         -         expression tag         UNP F           B         -11         HIS         -         expression tag         UNP F           B         -10         HIS         -         expression tag         UNP F           B         -9         HIS         -         expression tag         UNP F           B         -8         HIS         -         expression tag         UNP F           B         -7         ALA         -         expression tag         UNP F           B         -6         LEU         -         expression tag         UNP F	P12497 P12497 P12497 P12497 P12497 P12497
B         -12         HIS         -         expression tag         UNP F           B         -11         HIS         -         expression tag         UNP F           B         -10         HIS         -         expression tag         UNP F           B         -9         HIS         -         expression tag         UNP F           B         -8         HIS         -         expression tag         UNP F           B         -7         ALA         -         expression tag         UNP F           B         -6         LEU         -         expression tag         UNP F	P12497 P12497 P12497 P12497 P12497
B -11 HIS - expression tag UNP F B -10 HIS - expression tag UNP F B -9 HIS - expression tag UNP F B -8 HIS - expression tag UNP F B -7 ALA - expression tag UNP F B -6 LEU - expression tag UNP F	P12497 P12497 P12497 P12497
B -10 HIS - expression tag UNP F B -9 HIS - expression tag UNP F B -8 HIS - expression tag UNP F B -7 ALA - expression tag UNP F B -6 LEU - expression tag UNP F	P12497 P12497 P12497
B -9 HIS - expression tag UNP F B -8 HIS - expression tag UNP F B -7 ALA - expression tag UNP F B -6 LEU - expression tag UNP F	P12497 P12497
B -8 HIS - expression tag UNP F B -7 ALA - expression tag UNP F B -6 LEU - expression tag UNP F	P12497
B -7 ALA - expression tag UNP F B -6 LEU - expression tag UNP F	
B -6 LEU - expression tag UNP F	P12497
1 0	
D E CHI LIND I	P12497
B -5 GLU - expression tag UNP F	P12497
B -4 VAL - expression tag UNP F	P12497
B -3 LEU - expression tag UNP F	P12497
B -2 PHE - expression tag UNP F	P12497
B -1 GLN - expression tag UNP F	P12497
B 0 GLY - expression tag UNP F	P12497
B 162 SER CYS engineered mutation UNP F	P12497
B 280 SER CYS engineered mutation UNP F	P12497
D -15 MET - expression tag UNP F	P12497
D -14 ALA - expression tag UNP F	P12497
D -13 HIS - expression tag UNP F	P12497
D -12 HIS - expression tag UNP F	P12497
D -11 HIS - expression tag UNP F	P12497
D -10 HIS - expression tag UNP F	P12497
D -9 HIS - expression tag UNP F	P12497
D -8 HIS - expression tag UNP F	P12497
D -7 ALA - expression tag UNP F	P12497
D -6 LEU - expression tag UNP F	12497
D -5 GLU - expression tag UNP F	12497
D -4 VAL - expression tag UNP F	
D -3 LEU - expression tag UNP F	212497
D -2 PHE - expression tag UNP F	P12497
D -1 GLN - expression tag UNP F	212497
D 0 GLY - expression tag UNP F	212497
D 162 SER CYS engineered mutation UNP F	110105
D 280 SER CYS engineered mutation UNP F	12497



•	Molecule 3	is	a DNA	chain	called	DNA	/RNA	(38-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	2 F	35	Total	С	N	О	Р	0	0	0
3	15		718	339	128	216	35	U		
2	Б	20	Total	С	N	О	Р	0	0	0
3	Г	F 38	777	369	140	231	37		U	U

• Molecule 4 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



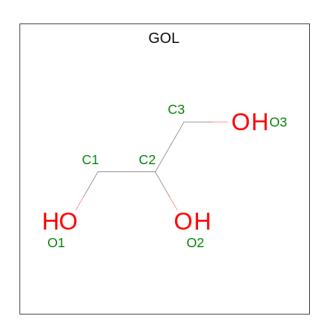
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	Λ	1	Total	С	N	О	Р	0	0	
4	4 A	1	31	10	5	13	3	U	0	
4	Г	1	Total	С	N	О	Р	0	0	
4 F	Г	1	31	10	5	13	3	U		

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	С	1	Total Mg 1 1	0	0

 $\bullet$  Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $\mathrm{C_3H_8O_3}).$ 





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total C O 6 3 3	0	0
6	В	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

#### • Molecule 7 is water.

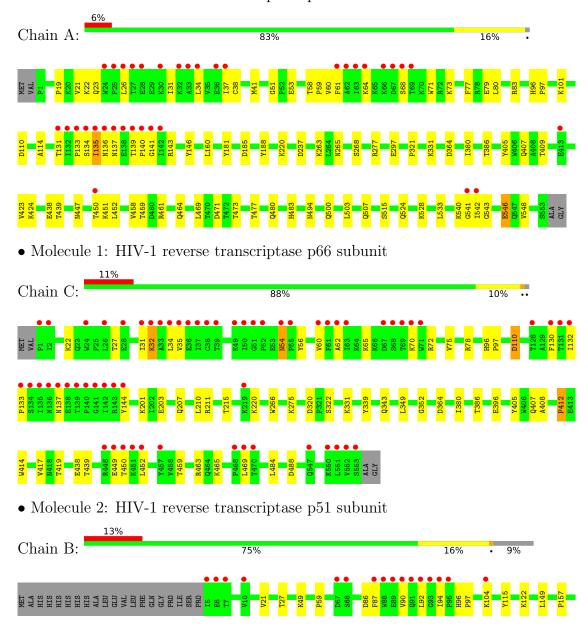
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	71	Total O 71 71	0	0
7	В	48	Total O 48 48	0	0
7	E	21	Total O 21 21	0	0
7	С	75	Total O 75 75	0	0
7	D	68	Total O 68 68	0	0
7	F	18	Total O 18 18	0	0



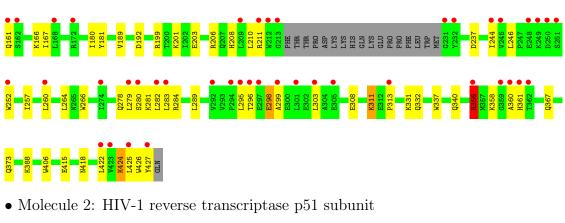
# 3 Residue-property plots (i)

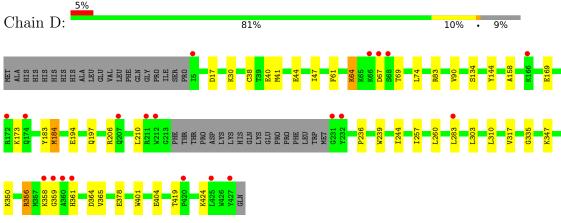
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HIV-1 reverse transcriptase p66 subunit









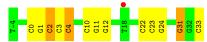
• Molecule 3: DNA/RNA (38-MER)

Chain E: 66% 21% 5% 8%



• Molecule 3: DNA/RNA (38-MER)

Chain F: 66% 26% 8%





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	284.87Å 284.87Å 95.89Å	Donogiton
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	48.74 - 2.44	Depositor
resolution (A)	48.74 - 2.43	EDS
% Data completeness	99.9 (48.74-2.44)	Depositor
(in resolution range)	99.9 (48.74-2.43)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.36  (at  2.42Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
$R, R_{free}$	0.186 , $0.225$	Depositor
it, it free	0.186 , $0.225$	DCC
$R_{free}$ test set	5558 reflections $(5.12%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.9	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	$0.35\;,50.8$	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17566	wwPDB-VP
Average B, all atoms $(\mathring{A}^2)$	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  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.

## 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: DGT, OMC, MG, GOL

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	Bond lengths		ond angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.37	0/4611	0.52	$1/6262 \ (0.0\%)$
1	С	0.34	0/4611	0.49	0/6262
2	В	0.34	0/3441	0.51	0/4673
2	D	0.38	0/3441	0.49	0/4673
3	Е	0.80	0/756	0.95	1/1165 (0.1%)
3	F	0.68	0/823	0.94	1/1269 (0.1%)
All	All	0.41	0/17683	0.56	3/24304 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	A	68	SER	C-N-CA	-5.61	107.68	121.70
3	F	31	DG	C4'-C3'-C2'	-5.19	98.43	103.10
3	Ε	31	DG	O4'-C4'-C3'	-5.10	102.46	104.50

There are no chirality outliers.

There are no planarity outliers.

### 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	4494	0	4558	66	0
1	С	4494	0	4558	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	3347	0	3379	55	0
2	D	3347	0	3379	31	0
3	Ε	718	0	397	7	0
3	F	777	0	432	10	0
4	A	31	0	12	3	0
4	F	31	0	12	2	0
5	A	1	0	0	0	0
5	С	1	0	0	0	0
6	В	12	0	16	1	0
6	D	12	0	16	0	0
7	A	71	0	0	2	0
7	В	48	0	0	1	0
7	С	75	0	0	0	0
7	D	68	0	0	1	0
7	Ε	21	0	0	0	0
7	F	18	0	0	1	0
All	All	17566	0	16759	195	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 6.

The worst 5 of 195 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.43	0.98
2:D:356:ARG:NH1	2:D:361:HIS:CG	2.35	0.94
2:D:356:ARG:HH11	2:D:361:HIS:HB2	1.33	0.92
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.19	0.91
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.01	0.91

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 r	number of residu	ies for which	the backbone	conformation	was
analysed, and the total number of	residues.				

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percer	ntiles
1	A	551/557 (99%)	532 (97%)	17 (3%)	2 (0%)	34	41
1	С	551/557 (99%)	533 (97%)	16 (3%)	2 (0%)	34	41
2	В	402/444 (90%)	382 (95%)	18 (4%)	2 (0%)	29	34
2	D	402/444 (90%)	387 (96%)	14 (4%)	1 (0%)	47	57
All	All	1906/2002 (95%)	1834 (96%)	65 (3%)	7 (0%)	34	41

#### 5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	137	ASN
1	A	135	ILE
2	В	356	ARG
2	В	313	PRO
2	D	424	LYS

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Percentil	les
1	A	492/494~(100%)	484 (98%)	8 (2%)	62 74	
1	С	$492/494 \ (100\%)$	486 (99%)	6 (1%)	71 81	
2	В	365/400~(91%)	352 (96%)	13 (4%)	35 46	
2	D	365/400~(91%)	360 (99%)	5 (1%)	67 78	
All	All	$1714/1788 \ (96\%)$	1682 (98%)	32 (2%)	57 69	

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	67	ASP
2	D	134	SER
2	В	280	SER

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Mol	Chain	Res	Type
2	В	237	ASP
2	D	184	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	182	GLN
2	D	407	GLN
2	В	367	GLN
2	В	418	ASN
1	С	54	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)

4 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	Trino	Chain	Res	Link	Во	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMC	Е	2	3	19,22,23	2.80	8 (42%)	26,31,34	0.83	1 (3%)
3	OMC	F	4	3	19,22,23	3.06	8 (42%)	26,31,34	0.73	0
3	OMC	F	2	3	19,22,23	2.89	8 (42%)	26,31,34	0.80	0
3	OMC	Е	4	3	19,22,23	2.90	8 (42%)	26,31,34	0.67	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	OMC	Е	2	3	-	1/9/27/28	0/2/2/2
3	OMC	F	4	3	-	0/9/27/28	0/2/2/2
3	OMC	F	2	3	-	0/9/27/28	0/2/2/2
3	OMC	Е	4	3	-	0/9/27/28	0/2/2/2

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
3	F	4	OMC	C2-N3	6.44	1.49	1.36
3	Е	4	OMC	C2-N3	6.14	1.48	1.36
3	F	4	OMC	C6-C5	6.06	1.49	1.35
3	Е	4	OMC	C6-C5	5.86	1.48	1.35
3	F	2	OMC	C6-C5	5.83	1.48	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$	
3	Ε	2	OMC	O2-C2-N3	-2.06	118.98	122.33	

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Е	2	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Е	2	OMC	1	0
3	F	4	OMC	1	0
3	F	2	OMC	1	0
3	Е	4	OMC	2	0

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



### 5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	Tuno	Chain	Res	Link	В	ond leng	$\operatorname{gths}$	Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
4	DGT	A	601	5	26,33,33	3.23	14 (53%)	32,52,52	1.60	6 (18%)
6	GOL	В	701	-	5,5,5	1.05	0	5,5,5	1.04	0
6	GOL	D	602	-	5,5,5	1.07	0	5,5,5	0.98	0
6	GOL	D	601	-	5,5,5	1.25	0	5,5,5	0.98	0
4	DGT	F	701	5	26,33,33	3.27	14 (53%)	32,52,52	1.94	11 (34%)
6	GOL	В	702	-	5,5,5	1.27	0	5,5,5	0.90	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
4	DGT	A	601	5	-	4/18/34/34	0/3/3/3
6	GOL	В	701	-	-	2/4/4/4	-
6	GOL	D	602	-	-	0/4/4/4	-
6	GOL	D	601	-	-	4/4/4/4	-
4	DGT	F	701	5	-	7/18/34/34	0/3/3/3
6	GOL	В	702	-	-	3/4/4/4	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
4	F	701	DGT	C2'-C3'	-8.41	1.30	1.52
4	A	601	DGT	C2'-C3'	-7.61	1.32	1.52
4	F	701	DGT	O4'-C1'	-6.27	1.28	1.42
4	A	601	DGT	O4'-C4'	5.53	1.57	1.45
4	A	601	DGT	O4'-C1'	-5.13	1.30	1.42

The worst 5 of 17 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
4	F	701	DGT	C2-N1-C6	-4.40	116.99	125.10
4	F	701	DGT	C5-C6-N1	4.29	121.52	113.95
4	F	701	DGT	PA-O3A-PB	-3.72	120.07	132.83
4	A	601	DGT	PB-O3B-PG	-3.67	120.23	132.83
4	A	601	DGT	C5-C6-N1	3.65	120.40	113.95

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	701	DGT	C5'-O5'-PA-O1A
4	F	701	DGT	C5'-O5'-PA-O2A
6	В	701	GOL	C1-C2-C3-O3
6	D	601	GOL	O1-C1-C2-C3
6	D	601	GOL	C1-C2-C3-O3

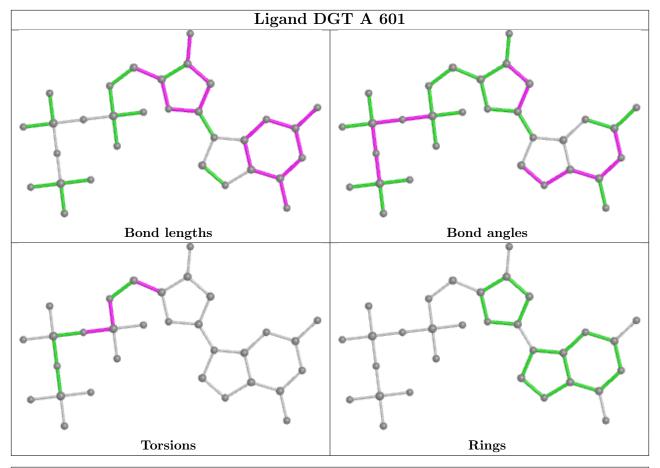
There are no ring outliers.

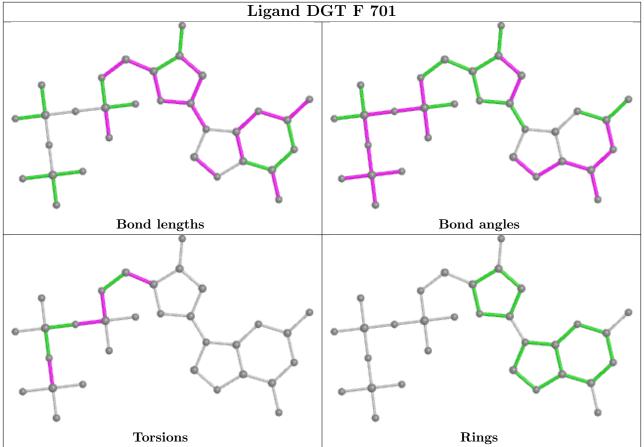
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	DGT	3	0
6	В	701	GOL	1	0
4	F	701	DGT	2	0

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.









## 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,  $95^{th}$  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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	553/557 (99%)	0.35	35 (6%) 20 16	33, 60, 109, 164	0
1	С	553/557 (99%)	0.53	60 (10%) 5 4	35, 63, 113, 157	0
2	В	406/444 (91%)	0.71	58 (14%) 2 1	36, 73, 135, 177	0
2	D	406/444 (91%)	0.24	20 (4%) 29 27	33, 57, 98, 157	0
3	E	33/38~(86%)	-0.16	0 100 100	37, 58, 91, 128	0
3	F	36/38 (94%)	0.12	1 (2%) 53 49	40, 68, 121, 153	0
All	All	1987/2078 (95%)	0.44	174 (8%) 10 7	33, 62, 119, 177	0

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	9.5
2	В	301	LEU	8.9
2	В	88	TRP	8.8
1	С	140	PRO	7.8
2	D	67	ASP	7.7

### 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	OMC	Ε	2	21/22	0.97	0.20	31,40,44,58	0
3	OMC	F	2	21/22	0.97	0.18	49,53,62,70	0
3	OMC	Ε	4	21/22	0.98	0.20	27,39,43,48	0
3	OMC	F	4	21/22	0.98	0.19	34,40,46,53	0



### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 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,  $95^{th}$  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.

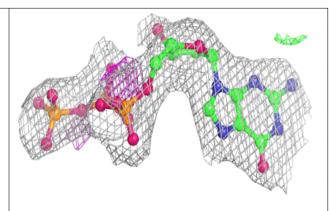
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	MG	С	601	1/1	0.71	0.21	97,97,97,97	0
6	GOL	В	701	6/6	0.86	0.28	65,71,73,74	0
5	MG	A	602	1/1	0.87	0.22	60,60,60,60	1
4	DGT	F	701	31/31	0.90	0.16	59,80,115,118	0
6	GOL	D	601	6/6	0.90	0.20	52,61,62,63	0
4	DGT	A	601	31/31	0.91	0.18	57,80,119,120	0
6	GOL	D	602	6/6	0.91	0.21	40,52,55,57	0
6	GOL	В	702	6/6	0.94	0.27	46,57,62,75	0

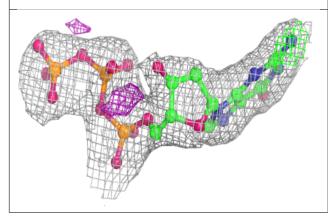
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

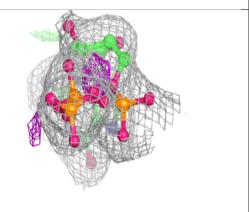


#### Electron density around DGT F 701:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

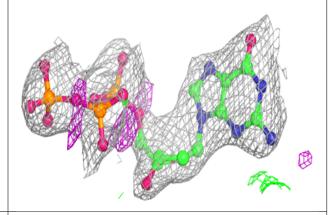


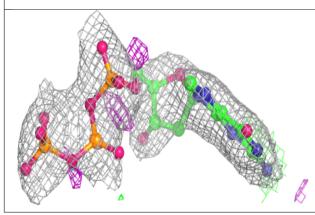


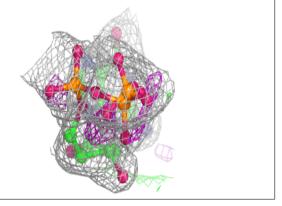


#### Electron density around DGT A 601:

 $2mF_o$ -DF<sub>c</sub> (at 0.7 rmsd) in gray  $mF_o$ -DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)









# 6.5 Other polymers (i)

There are no such residues in this entry.

