

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

#### Oct 24, 2024 – 10:47 AM EDT

PD	B ID	:	7HKO
	Title	:	Group deposition for crystallographic fragment screening of the NS5 RNA-
			dependent RNA polymerase from Dengue virus serotype 2 – Crystal structure
			of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 in
			complex with Z106579662 (DNV2_NS5A-x0376)
Aut	thors	:	Saini, M.; Chopra, A.; Aschenbrenner, J.C.; Marples, P.G.; Balcomb, B.H.;
			Fearon, D.; von Delft, F.; Ruiz, F.X.; Arnold, E.
Deposite	ed on	:	2024-10-15
Resolu	ution	:	1.82 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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.82 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	164625	9242 (1.84-1.80)
Clashscore	180529	1080 (1.82 - 1.82)
Ramachandran outliers	177936	1073 (1.82-1.82)
Sidechain outliers	177891	1073 (1.82-1.82)
RSRZ outliers	164620	9241 (1.84-1.80)

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		
			14%		
1	А	637	82%	9%	9%

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 criteria:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.39



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	А	1007	-	-	Х	-



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# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5268 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 Genome polyprotein.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	582	Total 4759	C 2999	N 853	0 873	S 34	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	264	GLY	-	expression tag	UNP Q91H74
А	265	PRO	-	expression tag	UNP $Q91H74$

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Zn 2 2	0	0

• Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
3	А	1	Total 12	C 6	N 1	0 4	S 1	0	0

• Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
4	Δ	1	Total	С	Ο	$\mathbf{S}$	0	0
4	Π	T	4	2	1	1	0	0
1	Δ	1	Total	С	Ο	$\mathbf{S}$	0	0
1 4	Π	T	4	2	1	1	0	0
4	Λ	1	Total	С	0	S	0	0
4	Л	L	4	2	1	1	0	0
4	Λ	1	Total	С	Ο	$\mathbf{S}$	0	0
4	А		4	2	1	1	0	0

• Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0

• Molecule 7 is [4-(propan-2-yl)piperazin-1-yl](thiophen-2-yl)methanone (three-letter code:



NUY) (formula:  $\mathrm{C}_{12}\mathrm{H}_{18}\mathrm{N}_{2}\mathrm{OS})$  (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
7	А	1	Total 16	C 12	N 2	0 1	S 1	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	446	Total O 446 446	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: Genome polyprotein



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	82.48Å 116.06Å 147.61Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	42.29 - 1.82	Depositor
	42.29 - 1.82	EDS
% Data completeness	98.9 (42.29-1.82)	Depositor
(in resolution range)	98.9 (42.29-1.82)	EDS
$R_{merge}$	0.22	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.07 (at 1.82 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
B B.	0.191 , $0.230$	Depositor
II, II, <i>free</i>	0.216 , $0.246$	DCC
$R_{free}$ test set	3292 reflections $(5.16%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	32.7	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 60.4	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5268	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.26% 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.

# 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: NUY, MES, DMS, PO4, PEG, ZN

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).

Mal	Chain	Bond	lengths	Bond angles		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.70	0/4865	0.80	0/6560	

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	273	ASN	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	А	4759	0	4668	30	0
2	А	2	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	12	0	13	0	0
4	А	16	0	24	2	0
5	А	10	0	0	4	0
6	А	7	0	10	0	0
7	А	16	0	0	0	0
8	А	446	0	0	6	2
All	All	5268	0	4715	32	2

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 3.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:664:ASP:OD1	5:A:1007:PO4:O4	1.88	0.91	
1:A:534:ASP:OD1	5:A:1007:PO4:O4	2.04	0.76	
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.57	0.62	
1:A:698:ARG:NH2	8:A:1105:HOH:O	2.32	0.61	
1:A:733:GLU:O	1:A:737:ARG:HG3	2.05	0.57	
1:A:510:GLU:O	1:A:514:LYS:HG3	2.07	0.55	
1:A:337:MET:HG2	8:A:1376:HOH:O	2.06	0.55	
1:A:411:ALA:HA	1:A:477:MET:O	2.07	0.54	
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.88	0.54	
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.48	0.54	
1:A:638:THR:HA	1:A:641:ILE:HG22	1.90	0.53	
1:A:582:ARG:O	1:A:588:THR:HA	2.08	0.53	
4:A:1004:DMS:C1	8:A:1237:HOH:O	2.57	0.52	
1:A:453:ASN:ND2	1:A:579:ARG:HD2	2.27	0.50	
4:A:1004:DMS:H11	8:A:1237:HOH:O	2.13	0.48	
1:A:701:ASN:ND2	8:A:1103:HOH:O	2.30	0.47	
1:A:438:GLU:O	1:A:441:LEU:HB2	2.15	0.47	
1:A:534:ASP:OD1	5:A:1007:PO4:P	2.73	0.47	
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.13	0.46	
1:A:428:ASP:OD1	1:A:430:GLY:N	2.49	0.46	
1:A:819:GLN:NE2	8:A:1110:HOH:O	2.40	0.44	
1:A:722:ARG:HB3	1:A:824:MET:SD	2.56	0.44	
1:A:579:ARG:HA	1:A:591:ASP:O	2.18	0.44	
1:A:277:ILE:HD12	1:A:281:ILE:HD11	2.01	0.43	
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.50	0.42	
1:A:475:TRP:CD1	1:A:475:TRP:N	2.88	0.42	
1:A:454:MET:HB3	1:A:580:VAL:HG13	2.01	0.41	



Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance} \ (\text{\AA}) \end{array}$	Clash overlap (Å)
1:A:528:GLY:O	1:A:668:LYS:HE3	2.20	0.41
1:A:580:VAL:HG21	1:A:593:ILE:HD11	2.02	0.41
1:A:638:THR:O	1:A:641:ILE:HG22	2.21	0.40
1:A:431:PHE:O	1:A:434:LEU:HB2	2.22	0.40
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1 Atom-2		Interatomic distance (Å)	Clash overlap (Å)
8:A:1107:HOH:O	8:A:1107:HOH:O[2_445]	1.66	0.54
8:A:1346:HOH:O	8:A:1421:HOH:O[2_545]	2.13	0.07

## 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	А	568/637~(89%)	543 (96%)	22~(4%)	3~(0%)	25 14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	410	GLY
1	А	420	LYS
1	А	291	SER

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Analysed Rotameric (		Percentiles	
1	А	510/554~(92%)	497~(98%)	13 (2%)	42 25	

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	274	LEU
1	А	355	PHE
1	А	356	LYS
1	А	358	LYS
1	А	365	GLU
1	А	375	LYS
1	А	423	ARG
1	А	426	VAL
1	А	429	SER
1	А	482	ARG
1	А	570	LYS
1	А	580	VAL
1	А	641	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	417	ASN
1	А	603	GLN
1	А	693	GLN
1	А	786	HIS
1	А	801	HIS

#### 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)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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).

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
	туре	Unain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MES	A	1003	-	12,12,12	0.70	0	15,16,16	0.29	0
4	DMS	А	1006	-	3,3,3	0.15	0	3,3,3	0.22	0
4	DMS	A	1010	-	3,3,3	0.30	0	3,3,3	0.05	0
5	PO4	А	1007	-	4,4,4	3.40	3 (75%)	$6,\!6,\!6$	0.84	0
5	PO4	А	1008	-	4,4,4	0.91	0	6,6,6	0.37	0
4	DMS	А	1005	-	3,3,3	0.25	0	3,3,3	0.08	0
4	DMS	А	1004	-	3,3,3	0.38	0	3,3,3	0.40	0
7	NUY	A	1011	-	16,17,17	0.55	0	18,23,23	0.87	1 (5%)
6	PEG	А	1009	-	6,6,6	0.10	0	$5,\!5,\!5$	0.13	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	NUY	А	1011	-	-	2/8/22/22	0/2/2/2
3	MES	А	1003	-	-	3/6/14/14	0/1/1/1
6	PEG	А	1009	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
5	А	1007	PO4	P-01	5.32	1.62	1.50
5	А	1007	PO4	P-04	-2.94	1.46	1.54



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	А	1007	PO4	P-O3	2.33	1.61	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	А	1011	NUY	C4-N1-C2	3.05	117.88	113.01

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
3	А	1003	MES	C7-C8-S-O1S
3	А	1003	MES	C7-C8-S-O3S
6	А	1009	PEG	O2-C3-C4-O4
7	А	1011	NUY	C1-C2-N1-C4
7	А	1011	NUY	C3-C2-N1-C7
3	А	1003	MES	C7-C8-S-O2S
6	А	1009	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	1007	PO4	4	0
4	А	1004	DMS	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 sufficient 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>2	$OWAB(Å^2)$	Q<0.9
1	А	582/637~(91%)	1.07	91 (15%) 6 5	7, 41, 111, 167	21 (3%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	А	512	LEU	23.5	
1	А	741	SER	18.7	
1	А	801	HIS	18.7	
1	А	785	SER	18.6	
1	А	763	SER	18.4	
1	А	551	GLU	17.9	
1	А	698	ARG	17.9	
1	А	864	GLN	16.0	
1	А	800	THR	13.6	
1	А	514	LYS	10.3	
1	А	790	THR	10.1	
1	А	851	ILE	8.3	
1	А	887	LYS	8.1	
1	А	306	HIS	7.9	
1	А	852	GLY	7.5	
1	А	719	LYS	7.1	
1	А	799	ALA	7.0	
1	А	705	GLN	6.6	
1	А	841	LYS	6.5	
1	А	770	ARG	6.0	
1	А	589	VAL	5.1	
1	А	413	PHE	4.7	
1	А	412	ILE	4.5	
1	А	842	ARG	4.5	
1	А	407	ALA	4.4	
1	А	355	PHE	4.2	
1	А	475	TRP	4.0	



Mol	Chain	Res	Type	RSRZ
1	А	600	GLY	4.0
1	А	409	LEU	3.9
1	А	794	THR	3.9
1	А	845	GLN	3.9
1	А	584	THR	3.7
1	А	363	THR	3.6
1	А	317	ALA	3.5
1	А	292	TRP	3.4
1	А	293	HIS	3.4
1	А	745	GLY	3.3
1	А	473	ALA	3.3
1	А	637	VAL	3.2
1	А	298	HIS	3.2
1	A	359	VAL	3.1
1	А	422	ALA	3.1
1	А	419	TRP	3.0
1	А	410	GLY	3.0
1	А	284	ILE	2.9
1	А	356	LYS	2.9
1	А	793	THR	2.8
1	А	411	ALA	2.8
1	А	294	TYR	2.8
1	А	403	VAL	2.7
1	А	455	MET	2.7
1	А	880	THR	2.7
1	А	511	GLY	2.7
1	А	431	PHE	2.7
1	А	309	TYR	2.6
1	А	314	THR	2.6
1	А	344	THR	2.6
1	А	274	LEU	2.6
1	A	305	TYR	2.6
1	A	281	ILE	2.6
1	А	580	VAL	2.4
1	A	881	ASP	2.4
1	A	303	TRP	2.4
1	A	288	HIS	2.4
1	A	291	SER	2.4
1	A	361	THR	2.4
1	A	308	SER	2.3
1	A	408	ALA	2.3
1	А	565	ALA	2.3



Mol	Chain	Res	Type	RSRZ
1	А	290	THR	2.3
1	А	641	ILE	2.3
1	А	449	THR	2.3
1	А	474	ILE	2.2
1	А	299	PRO	2.2
1	А	426	VAL	2.2
1	А	882	TYR	2.2
1	А	583	PRO	2.2
1	А	744	ALA	2.2
1	А	558	GLU	2.2
1	А	588	THR	2.1
1	А	802	GLU	2.1
1	А	590	MET	2.1
1	А	534	ASP	2.1
1	А	889	PHE	2.1
1	А	472	ARG	2.1
1	А	592	ILE	2.0
1	А	593	ILE	2.0
1	А	476	TYR	2.0
1	А	528	GLY	2.0
1	А	418	LYS	2.0
1	А	791	SER	2.0

## 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)

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	$B-factors(Å^2)$	Q<0.9
4	DMS	А	1010	4/4	0.70	0.35	65,70,73,78	4



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PO4	А	1008	5/5	0.73	0.16	91,100,107,117	0
5	PO4	А	1007	5/5	0.79	0.13	38,41,48,60	0
7	NUY	А	1011	16/16	0.85	0.19	$39,\!43,\!45,\!48$	16
6	PEG	А	1009	7/7	0.87	0.15	70,71,75,78	0
3	MES	А	1003	12/12	0.87	0.36	783,832,839,839	12
4	DMS	А	1005	4/4	0.92	0.31	$68,\!77,\!79,\!79$	4
4	DMS	А	1006	4/4	0.95	0.11	57,61,61,66	0
4	DMS	А	1004	4/4	0.95	0.17	46,46,47,48	0
2	ZN	А	1002	1/1	0.99	0.03	$55,\!55,\!55,\!55$	0
2	ZN	А	1001	1/1	1.00	0.02	24,24,24,24	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.



## 6.5 Other polymers (i)

There are no such residues in this entry.

