

Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2024 – 11:41 AM EDT

PDB ID	:	7HKP
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 $Z1198279205$ (DNV2_NS5A-x0414)
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Deposited on	:	2024-10-15
Resolution	:	2.12 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-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	164625	7689 (2.14-2.10)
Clashscore	180529	8431 (2.14-2.10)
Ramachandran outliers	177936	8366 (2.14-2.10)
Sidechain outliers	177891	8367 (2.14-2.10)
RSRZ outliers	164620	7689 (2.14-2.10)

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			
			12%			
1	А	637	81%	10%	• 99	%

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	-
7	A1BDI	А	1010	-	-	-	Х



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2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5250 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: C₆H₁₃NO₄S).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
3	А	1	Total	С	Ν	0	\mathbf{S}	0	0
	11	T	12	6	1	4	1		0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	А	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 1	S 1	0	0
4	А	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 1	S 1	0	0
4	А	1	Total 4	С 2	0 1	S 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-fluoro-1 H-pyrazole (three-letter code: A1BDI) (formula: $\rm C_3H_3FN_2)$ (labeled



as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	А	1	Total 6	С 3	F 1	N 2	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	442	Total O 442 442	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	82.34Å 115.57Å 147.29Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	49.63 - 2.12	Depositor
Itesolution (A)	49.63 - 2.12	EDS
% Data completeness	99.6 (49.63-2.12)	Depositor
(in resolution range)	99.6 (49.63 - 2.12)	EDS
R_{merge}	0.44	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.04 (at 2.12 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R R.	0.202 , 0.270	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.235 , 0.275	DCC
R_{free} test set	2051 reflections $(5.10%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	39.8	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.36 , 69.7	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5250	wwPDB-VP
Average B, all atoms $(Å^2)$	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: A1BDI, MES, PO4, PEG, DMS, 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).

Mol	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.66	0/4865	0.79	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	А	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	36	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	12	0	18	2	0
5	А	10	0	0	3	0
6	А	7	0	10	0	0
7	А	6	0	0	0	0
8	А	442	0	0	7	2
All	All	5250	0	4709	38	2

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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 4.

All (38) 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	2.05	0.74
1:A:336:PRO:O	1:A:340:GLN:HG2	1.94	0.68
4:A:1004:DMS:H11	8:A:1293:HOH:O	1.94	0.67
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.56	0.64
1:A:511:GLY:N	8:A:1103:HOH:O	2.32	0.58
1:A:733:GLU:O	1:A:737:ARG:HG3	2.04	0.57
1:A:477:MET:SD	1:A:482:ARG:NH1	2.78	0.57
1:A:343:MET:HE3	8:A:1452:HOH:O	2.03	0.57
1:A:302:THR:OG1	1:A:360:ASP:OD1	2.23	0.57
1:A:562:LYS:O	1:A:566:GLU:HG3	2.04	0.56
4:A:1004:DMS:H13	8:A:1304:HOH:O	2.05	0.55
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.42	0.55
1:A:510:GLU:O	1:A:514:LYS:HG3	2.08	0.54
1:A:303:TRP:CD2	1:A:593:ILE:HD12	2.44	0.53
1:A:452:TYR:O	1:A:578:VAL:HA	2.09	0.53
1:A:745:GLY:N	8:A:1112:HOH:O	2.42	0.51
1:A:826:ASP:OD1	1:A:826:ASP:C	2.49	0.51
1:A:551:GLU:HG2	1:A:551:GLU:O	2.09	0.51
1:A:534:ASP:OD1	5:A:1007:PO4:O4	2.30	0.50
1:A:428:ASP:OD1	1:A:430:GLY:N	2.40	0.49
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.43	0.48
1:A:454:MET:HB3	1:A:580:VAL:HG13	1.94	0.48
1:A:431:PHE:O	1:A:434:LEU:HB2	2.15	0.47
1:A:411:ALA:HA	1:A:477:MET:O	2.16	0.46
1:A:764:LEU:HD12	1:A:764:LEU:HA	1.84	0.43
1:A:337:MET:HG2	8:A:1355:HOH:O	2.19	0.42
1:A:550:GLU:OE2	1:A:613:THR:OG1	2.27	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:400:THR:HG23	1:A:426:VAL:HG11	2.00	0.42
1:A:284:ILE:HD11	1:A:451:VAL:HG21	2.02	0.42
1:A:403:VAL:HG21	1:A:426:VAL:HG21	2.02	0.41
1:A:438:GLU:O	1:A:441:LEU:HB2	2.21	0.41
1:A:396:ARG:NH1	1:A:432:TRP:HB3	2.35	0.41
1:A:507:VAL:O	1:A:510:GLU:HG2	2.20	0.41
1:A:525:LYS:NZ	8:A:1134:HOH:O	2.52	0.41
1:A:528:GLY:O	1:A:668:LYS:HE3	2.21	0.41
1:A:582:ARG:O	1:A:588:THR:HA	2.20	0.41
1:A:576:LYS:NZ	1:A:597:ASP:O	2.51	0.40
1:A:695:GLU:HA	1:A:696:PRO:HD3	1.96	0.40

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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:1290:HOH:O	8:A:1449:HOH:O[2_545]	1.96	0.24
8:A:1115:HOH:O	8:A:1115:HOH:O[2_445]	2.04	0.16

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%)	540 (95%)	25~(4%)	3(0%)	25 22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	420	LYS
1	А	418	LYS
1	А	600	GLY



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

Mol	Chain	Analysed Rotameric		Outliers	Percentiles	
1	А	510/554~(92%)	495~(97%)	15 (3%)	37 40	

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	274	LEU
1	А	290	THR
1	А	297	ASP
1	А	356	LYS
1	А	359	VAL
1	А	396	ARG
1	А	426	VAL
1	А	446	LYS
1	А	482	ARG
1	А	580	VAL
1	А	589	VAL
1	А	631	SER
1	А	634	HIS
1	А	637	VAL
1	А	641	ILE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
1	А	417	ASN
1	А	513	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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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 Type Chain F		Dec	Tiple	Bo	Bond lengths			Bond angles		
	туре	Chain	nes	nes Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	DMS	А	1005	-	$3,\!3,\!3$	0.25	0	3,3,3	0.11	0
4	DMS	А	1006	-	3, 3, 3	0.21	0	3,3,3	0.25	0
5	PO4	А	1007	-	$4,\!4,\!4$	1.36	1 (25%)	$6,\!6,\!6$	0.65	0
5	PO4	А	1008	-	4,4,4	0.94	0	6,6,6	0.39	0
3	MES	А	1003	-	12,12,12	0.74	0	15, 16, 16	0.38	0
7	A1BDI	А	1010	-	$6,\!6,\!6$	0.70	0	1,7,7	0.30	0
6	PEG	А	1009	-	$6,\!6,\!6$	0.14	0	$5,\!5,\!5$	0.08	0
4	DMS	A	1004	-	$3,\!3,\!3$	0.20	0	3,3,3	0.19	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	MES	А	1003	-	-	3/6/14/14	0/1/1/1
7	A1BDI	А	1010	-	-	-	0/1/1/1
6	PEG	A	1009	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	А	1007	PO4	P-01	2.50	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	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
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 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	1007	PO4	3	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%)	1.17	74 (12%) 9 10	9, 50, 121, 164	20 (3%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	512	LEU	23.6
1	А	741	SER	20.6
1	А	763	SER	20.1
1	А	719	LYS	18.7
1	А	785	SER	18.6
1	А	801	HIS	18.3
1	А	551	GLU	18.0
1	А	853	LEU	17.7
1	А	851	ILE	17.7
1	А	850	LEU	17.3
1	А	838	TYR	16.9
1	А	774	LEU	16.7
1	А	864	GLN	16.1
1	А	886	MET	15.6
1	А	856	ARG	15.0
1	А	849	SER	14.8
1	А	888	ARG	13.6
1	А	770	ARG	12.7
1	А	705	GLN	9.2
1	А	750	GLU	4.6
1	А	407	ALA	4.4
1	А	355	PHE	3.9
1	А	317	ALA	3.9
1	А	745	GLY	3.7
1	А	413	PHE	3.6
1	А	600	GLY	3.5
1	А	799	ALA	3.1



Mol	Chain	Res	Type	RSRZ
1	А	846	TRP	3.0
1	А	294	TYR	2.9
1	А	299	PRO	2.9
1	А	794	THR	2.9
1	А	412	ILE	2.7
1	А	473	ALA	2.7
1	А	744	ALA	2.7
1	А	880	THR	2.7
1	А	565	ALA	2.6
1	А	298	HIS	2.6
1	А	286	GLN	2.6
1	А	288	HIS	2.6
1	А	887	LYS	2.5
1	A	403	VAL	2.5
1	A	793	THR	2.5
1	А	293	HIS	2.5
1	А	419	TRP	2.5
1	А	363	THR	2.5
1	А	800	THR	2.5
1	А	422	ALA	2.5
1	А	290	THR	2.5
1	А	358	LYS	2.4
1	А	431	PHE	2.4
1	А	475	TRP	2.3
1	А	281	ILE	2.3
1	А	411	ALA	2.3
1	A	308	SER	2.3
1	A	791	SER	2.3
1	А	284	ILE	2.3
1	A	274	LEU	2.3
1	A	589	VAL	2.3
1	A	409	LEU	2.3
1	A	359	VAL	2.2
1	A	406	ASN	2.2
1	A	634	HIS	2.2
1	A	534	ASP	2.2
1	A	410	GLY	2.2
1	A	314	THR	2.1
1	A	301	LYS	2.1
1	A	292	TRP	2.1
1	A	580	VAL	2.1
1	А	571	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	А	448	GLU	2.1
1	А	584	THR	2.1
1	А	742	GLN	2.1
1	А	311	THR	2.0
1	А	882	TYR	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
7	A1BDI	A	1010	6/6	0.44	0.57	44,45,46,47	6
5	PO4	А	1008	5/5	0.69	0.13	99,105,107,114	0
5	PO4	A	1007	5/5	0.84	0.12	50,58,75,81	0
4	DMS	A	1005	4/4	0.86	0.18	82,84,91,93	0
6	PEG	А	1009	7/7	0.87	0.15	80,86,88,89	0
3	MES	A	1003	12/12	0.87	0.36	760,771,796,796	12
4	DMS	А	1006	4/4	0.95	0.14	63,64,65,66	0
4	DMS	A	1004	4/4	0.96	0.18	58,60,62,62	0
2	ZN	А	1001	1/1	1.00	0.05	33,33,33,33	0
2	ZN	A	1002	1/1	1.00	0.03	$65,\!65,\!65,\!65$	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.

