

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

#### Feb 8, 2024 – 09:48 AM EST

PDB ID :	:	2HPI
Title :	:	Eubacterial and Eukaryotic Replicative DNA Polymerases are not Homolo-
		gous: X-ray Structure of DNA Polymerase III
Authors :	:	Bailey, S.; Wing, R.A.; Steitz, T.A.
Deposited on :	:	2006-07-17
Resolution :	:	3.00  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	:	4.02b-467
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	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:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	Δ	1000	3%		
1	A	1220	74%	18%	• 6%



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9155 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 DNA polymerase III alpha subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	1143	Total 9127	C 5820	N 1598	O 1681	S 28	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Mg 2 2	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total Cl 2 2	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	22	TotalO2222	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: DNA polymerase III alpha subunit



### 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	175.15Å 186.88Å 125.83Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$Resolution(\AA)$	20.00 - 3.00	Depositor
Resolution (A)	19.93 - 3.00	EDS
% Data completeness	97.5 (20.00-3.00)	Depositor
(in resolution range)	$97.5\ (19.93-3.00)$	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.27 (at 2.98 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
P. P.	0.222 , $0.275$	Depositor
$n, n_{free}$	0.221 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	100.1	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.26 , 116.0	EDS
L-test for $twinning^2$	$ < L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9155	wwPDB-VP
Average B, all atoms $(Å^2)$	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.93% 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: CL, MG, 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	0.37	0/9307	0.55	0/12562	

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	337	LEU	Mainchain

### 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	9127	0	9158	136	0
2	А	2	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	2	0	0	0	0
4	А	2	0	0	0	0
5	А	22	0	0	2	0
All	All	9155	0	9158	136	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 7.

All (136) 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:321:ARG:HH22	1:A:440:ASN:ND2	1.65	0.94	
1:A:1143:LYS:HA	1:A:1147:ARG:HB2	1.50	0.92	
1:A:321:ARG:HH22	1:A:440:ASN:HD21	1.11	0.92	
1:A:743:TYR:H	1:A:746:GLN:HE21	1.30	0.78	
1:A:1013:HIS:HD2	1:A:1015:VAL:H	1.30	0.78	
1:A:8:ALA:H	1:A:274:THR:HG21	1.49	0.77	
1:A:439:THR:HG21	5:A:1248:HOH:O	1.83	0.77	
1:A:667:VAL:HA	1:A:828:THR:HG21	1.69	0.74	
1:A:835:TYR:HB3	1:A:838:GLU:CG	2.18	0.74	
1:A:8:ALA:H	1:A:274:THR:CG2	2.01	0.73	
1:A:407:GLN:HG3	1:A:436:VAL:HG12	1.72	0.71	
1:A:660:SER:HB3	1:A:683:LYS:HD3	1.71	0.71	
1:A:835:TYR:HB3	1:A:838:GLU:HG2	1.74	0.69	
1:A:1159:LEU:HD11	1:A:1183:GLU:HG2	1.72	0.69	
1:A:1176:LEU:HD23	1:A:1179:VAL:HB	1.75	0.69	
1:A:602:THR:HG22	1:A:604:TYR:H	1.59	0.67	
1:A:840:MET:HA	1:A:840:MET:HE2	1.75	0.67	
1:A:951:ALA:HB2	1:A:993:LEU:HG	1.78	0.66	
1:A:77:ALA:O	1:A:129:ARG:NH2	2.28	0.66	
1:A:1019:PRO:O	1:A:1023:GLU:HG2	1.96	0.66	
1:A:1053:GLU:HB3	1:A:1068:PHE:HA	1.80	0.64	
1:A:662:GLY:HA3	1:A:680:ARG:HG3	1.82	0.62	
1:A:504:LEU:HD12	1:A:525:ILE:HD11	1.81	0.62	
1:A:1039:LEU:HB3	1:A:1040:PRO:HD2	1.82	0.61	
1:A:742:VAL:H	1:A:746:GLN:NE2	1.99	0.61	
1:A:170:LEU:HD21	1:A:205:LEU:HD21	1.83	0.60	
1:A:665:LYS:HB2	1:A:832:LYS:HZ1	1.65	0.60	
1:A:402:TYR:HE1	1:A:615:LEU:HD11	1.65	0.60	
1:A:186:LEU:HD21	1:A:245:PRO:HB2	1.85	0.59	
1:A:743:TYR:HB2	1:A:746:GLN:HG3	1.83	0.59	



	the pagetti	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:667:VAL:HA	1:A:828:THR:CG2	2.31	0.59	
1:A:447:GLY:H	1:A:815:LYS:NZ	2.00	0.59	
1:A:148:ALA:O	1:A:152:GLN:HB2	2.03	0.57	
1:A:406:VAL:HA	1:A:409:TYR:CE2	2.40	0.57	
1:A:591:PRO:HG2	1:A:603:GLN:HB2	1.86	0.56	
1:A:897:VAL:HG21	1:A:938:LEU:HD13	1.87	0.56	
1:A:402:TYR:HE1	1:A:615:LEU:CD1	2.19	0.56	
1:A:441:ILE:HD12	1:A:823:LEU:HD12	1.88	0.55	
1:A:1143:LYS:HG2	1:A:1147:ARG:HD2	1.88	0.55	
1:A:238:ASP:HB3	1:A:239:PRO:CA	2.36	0.55	
1:A:703:GLU:O	1:A:706:PRO:HD2	2.06	0.55	
1:A:407:GLN:HG3	1:A:436:VAL:CG1	2.36	0.54	
1:A:590:VAL:CG1	1:A:602:THR:HG23	2.38	0.54	
1:A:321:ARG:NH2	1:A:440:ASN:ND2	2.48	0.54	
1:A:15:GLN:HE21	1:A:25:LEU:HB2	1.74	0.53	
1:A:920:ASP:HA	1:A:923:LYS:HE2	1.90	0.53	
1:A:840:MET:HG2	1:A:861:ALA:HB2	1.91	0.53	
1:A:982:VAL:O	1:A:982:VAL:HG13	2.09	0.53	
1:A:399:PHE:N	1:A:400:PRO:CD	2.72	0.52	
1:A:788:ALA:HB1	1:A:793:VAL:HG23	1.90	0.52	
1:A:1039:LEU:HB3	1:A:1040:PRO:CD	2.39	0.52	
1:A:238:ASP:HB3	1:A:239:PRO:C	2.29	0.52	
1:A:239:PRO:O	1:A:240:GLU:CB	2.58	0.52	
1:A:862:ARG:HH22	1:A:1011:SER:H	1.57	0.52	
1:A:788:ALA:HB1	1:A:793:VAL:CG2	2.40	0.52	
1:A:549:MET:HG2	1:A:559:ILE:HD12	1.92	0.51	
1:A:439:THR:CG2	5:A:1248:HOH:O	2.50	0.51	
1:A:675:MET:O	1:A:679:VAL:HG23	2.10	0.51	
1:A:80:ARG:N	1:A:128:ASP:OD1	2.44	0.51	
1:A:447:GLY:H	1:A:815:LYS:HZ1	1.59	0.51	
1:A:727:GLU:OE2	1:A:731:ARG:NH1	2.43	0.50	
1:A:627:PHE:HA	1:A:846:VAL:HG21	1.93	0.50	
1:A:128:ASP:H	1:A:131:ILE:HG12	1.77	0.50	
1:A:1140:LEU:H	1:A:1143:LYS:HD2	1.77	0.50	
1:A:1181:VAL:HG11	1:A:1185:ALA:HB3	1.93	0.49	
1:A:473:ARG:NH1	1:A:477:ILE:HD11	2.26	0.49	
1:A:840:MET:HE2	1:A:843:LEU:HD12	1.94	0.49	
1:A:1039:LEU:HG	1:A:1040:PRO:HD3	1.95	0.49	
1:A:286:PRO:HA	1:A:290:LYS:HG3	1.95	0.49	
1:A:1029:ILE:HG12	1:A:1072:ASP:CG	2.33	0.49	
1:A:1039:LEU:CB	1:A:1040:PRO:CD	2.91	0.49	



	h h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1173:LEU:HD13	1:A:1202:ARG:HH22	1.78	0.49
1:A:367:LYS:O	1:A:368:ARG:HG2	2.13	0.48
1:A:1050:MET:O	1:A:1070:LEU:HA	2.13	0.48
1:A:181:ILE:HD13	1:A:266:TRP:CZ3	2.48	0.48
1:A:379:THR:HG23	1:A:382:ALA:H	1.79	0.48
1:A:521:LEU:HD21	1:A:548:GLU:HG2	1.95	0.48
1:A:1053:GLU:CB	1:A:1068:PHE:HA	2.44	0.48
1:A:425:GLY:H	1:A:817:HIS:CD2	2.32	0.48
1:A:1105:VAL:HG22	1:A:1113:VAL:HG22	1.96	0.47
1:A:590:VAL:HG11	1:A:602:THR:HG23	1.95	0.47
1:A:776:GLU:HG2	1:A:779:LYS:HD2	1.97	0.47
1:A:1140:LEU:HD12	1:A:1143:LYS:HE3	1.96	0.47
1:A:319:LEU:HD13	1:A:347:GLU:HG3	1.95	0.47
1:A:595:ASP:OD2	1:A:599:ARG:HD2	2.13	0.47
1:A:215:TYR:HB2	1:A:220:ASP:HB2	1.97	0.47
1:A:364:GLU:HA	1:A:367:LYS:HE2	1.96	0.47
1:A:402:TYR:CE2	1:A:462:PRO:HG2	2.50	0.46
1:A:236:LEU:O	1:A:241:ARG:NE	2.48	0.46
1:A:151:PRO:HB3	1:A:192:VAL:HG11	1.99	0.45
1:A:835:TYR:HB3	1:A:838:GLU:HG3	1.95	0.45
1:A:470:ASP:OD2	1:A:623:ARG:HA	2.16	0.45
1:A:1046:LEU:HA	1:A:1101:VAL:O	2.16	0.45
1:A:1036:VAL:HG13	1:A:1043:PRO:HG2	1.97	0.45
1:A:57:TYR:O	1:A:61:THR:HB	2.17	0.45
1:A:139:LEU:O	1:A:176:ARG:HD2	2.16	0.45
1:A:528:GLN:HB3	1:A:533:LYS:HE3	2.00	0.44
1:A:785:VAL:HG13	1:A:795:GLU:HB2	1.99	0.44
1:A:257:MET:HA	1:A:257:MET:HE2	1.99	0.44
1:A:570:ARG:HD3	1:A:570:ARG:HA	1.84	0.44
1:A:290:LYS:H	1:A:290:LYS:HG2	1.47	0.44
1:A:321:ARG:HG2	1:A:434:TYR:CE2	2.52	0.44
1:A:269:GLU:HB2	1:A:270:PRO:HD3	1.99	0.44
1:A:45:THR:HG22	1:A:70:GLY:HA3	1.99	0.44
1:A:800:ARG:O	1:A:803:ASP:HB2	2.17	0.44
1:A:1102:LEU:HD12	1:A:1119:TRP:HH2	1.83	0.43
1:A:838:GLU:CD	1:A:838:GLU:H	2.20	0.43
1:A:795:GLU:HA	1:A:798:ALA:HB3	2.00	0.43
1:A:443:PRO:O	1:A:446:PHE:O	2.36	0.43
1:A:226:VAL:HG21	1:A:561:VAL:HG11	2.01	0.42
1:A:1039:LEU:HG	1:A:1040:PRO:CD	2.50	0.42
1:A:1101:VAL:HG22	1:A:1118:VAL:HG22	2.00	0.42



A 4 1	A + 0	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:252:LYS:HB3	1:A:256:GLU:HB2	2.02	0.42	
1:A:431:LEU:HA	1:A:443:PRO:HG3	2.01	0.42	
1:A:252:LYS:HD2	1:A:257:MET:HE2	2.02	0.42	
1:A:752:SER:HA	1:A:757:TYR:HB2	2.01	0.42	
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.91	0.42	
1:A:402:TYR:CE1	1:A:615:LEU:CD1	3.01	0.42	
1:A:257:MET:HA	1:A:257:MET:CE	2.50	0.42	
1:A:915:PHE:HA	1:A:924:ARG:HH21	1.85	0.41	
1:A:594:ARG:HH11	1:A:594:ARG:HG3	1.84	0.41	
1:A:1014:PRO:HB2	1:A:1050:MET:CE	2.50	0.41	
1:A:1026:SER:HA	1:A:1202:ARG:NH2	2.34	0.41	
1:A:1036:VAL:O	1:A:1037:ARG:C	2.58	0.41	
1:A:1072:ASP:C	1:A:1074:THR:H	2.23	0.41	
1:A:252:LYS:HD2	1:A:257:MET:CE	2.50	0.41	
1:A:313:LEU:HB3	1:A:436:VAL:HG13	2.01	0.41	
1:A:1182:GLY:O	1:A:1183:GLU:HB2	2.21	0.41	
1:A:321:ARG:CG	1:A:434:TYR:CE2	3.04	0.41	
1:A:316:LEU:HD21	1:A:348:ARG:HA	2.02	0.41	
1:A:402:TYR:CE1	1:A:615:LEU:HD11	2.52	0.41	
1:A:602:THR:HG21	1:A:609:VAL:CG2	2.51	0.41	
1:A:1181:VAL:CG1	1:A:1185:ALA:HB3	2.51	0.41	
1:A:725:HIS:HD2	1:A:797:GLU:OE2	2.03	0.41	
1:A:27:ASP:HA	1:A:30:LYS:HG2	2.03	0.40	
1:A:1042:LYS:HG2	1:A:1106:GLU:HG2	2.03	0.40	

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 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	1123/1220~(92%)	1029~(92%)	78 (7%)	16 (1%)	11 43



Mol	Chain	Res	Type
1	А	774	VAL
1	А	1039	LEU
1	А	1176	LEU
1	А	290	LYS
1	А	291	MET
1	А	570	ARG
1	А	792	GLY
1	А	975	LEU
1	А	976	VAL
1	А	1177	ARG
1	А	53	ALA
1	А	238	ASP
1	А	736	GLU
1	А	977	GLY
1	А	1193	GLY
1	А	399	PHE

All (16) Ramachandran outliers are listed below:

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

Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	А	949/1009~(94%)	886~(93%)	63~(7%)	16	49

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	6	LYS
1	А	61	THR
1	А	75	VAL
1	А	85	ARG
1	А	132	LEU
1	А	165	ARG
1	А	207	MET
1	А	211	ASN
1	А	215	TYR



Mol	Chain	Res	Type
1	A	222	ARG
1	A	235	THR
1	A	253	THR
1	A	274	THR
1	A	271 276	GLU
1	A	290	
1	A	300	LEU
1	A	305	THR
1	A	319	LEU
1	A	321	ABG
1	Δ	326	ILE
1	Δ	368	ARG
1	Δ	407	GLN
1	Δ	49/	ARC
1	Δ	424	THR
1	Δ	409	
1		440	LEU
1		444	ABC
1		402	
1	A	403	IFU
1	A	490 510	CLU
1	A	519	GLU I FII
1	A	540	
1	A	580	VAL TUD
1	A	007	
1	A	010	LIS
1	A	017 C22	MEI
1	A	022 625	LEU
	A	625 670	
1	A	070	LEU
1	A	672	SER
	A	707	THR
1	A	719	SER
1	A	736	GLU
1	A	786	ARG
1	A	795	GLU
1	A	823	LEU
1	A	840	MET
1	А	903	ARG
1	А	927	GLU
1	А	958	GLU
1	A	997	THR
1	А	1018	TYR



Mol	Chain	Res	Type
1	А	1027	CYS
1	А	1028	THR
1	А	1032	LEU
1	А	1045	VAL
1	А	1046	LEU
1	А	1074	THR
1	А	1095	GLU
1	А	1096	ASP
1	А	1104	GLU
1	А	1169	PHE
1	А	1184	GLU
1	А	1192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	9	HIS
1	А	15	GLN
1	А	440	ASN
1	А	575	HIS
1	А	715	GLN
1	А	725	HIS
1	А	746	GLN
1	А	814	ASN
1	А	817	HIS
1	А	1013	HIS
1	А	1155	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 monosaccharides in this entry.



### 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis. There are no bond length outliers. There are no bond angle outliers. There are no chirality outliers. There are no torsion outliers. There are no ring outliers. No monomer is involved in short contacts.

### 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<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		$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	А	1143/1220~(93%)	0.05	38 (3%) 46	20	103, 126, 144, 167	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	А	1116	GLN	5.7	
1	А	571	HIS	4.5	
1	А	775	GLU	4.3	
1	А	85	ARG	4.1	
1	А	1094	LYS	3.9	
1	А	1195	ARG	3.9	
1	А	531	LYS	3.2	
1	А	459	VAL	3.1	
1	А	553	GLU	3.0	
1	А	324	ASP	3.0	
1	А	64	GLY	2.9	
1	А	530	GLY	2.9	
1	А	1080	VAL	2.9	
1	А	297	ARG	2.8	
1	А	974	GLY	2.8	
1	А	596	GLN	2.7	
1	А	1048	SER	2.7	
1	А	6	LYS	2.7	
1	А	364	GLU	2.6	
1	А	911	ARG	2.6	
1	А	811	TYR	2.5	
1	А	916	LYS	2.5	
1	А	91	GLY	2.4	
1	А	520	GLU	2.4	
1	А	377	GLU	2.3	
1	А	242	TRP	2.3	
1	А	912	GLY	2.3	



Mol	Chain	Res	Type	RSRZ
1	А	39	ASP	2.3
1	А	973	SER	2.3
1	А	969	GLU	2.2
1	А	773	ARG	2.2
1	А	515	HIS	2.2
1	А	527	VAL	2.1
1	А	63	MET	2.1
1	А	975	LEU	2.1
1	A	359	GLU	2.0
1	А	1160	PRO	2.0
1	А	914	PRO	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	CL	А	1225	1/1	0.79	0.12	118,118,118,118	0
3	MG	А	1223	1/1	0.85	0.17	125,125,125,125	0
4	CL	А	1226	1/1	0.90	0.35	112,112,112,112	0
3	MG	А	1224	1/1	0.95	0.14	83,83,83,83	0
2	ZN	А	1222	1/1	0.97	0.10	102,102,102,102	0
2	ZN	А	1221	1/1	0.99	0.11	96,96,96,96	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

