

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

### Aug 1, 2022 – 10:05 AM EDT

PDB ID	:	8DT6
Title	:	Crystal Structure of DNA Polymerase III beta subunit from Elizabethkingia
		anophelis
Authors	:	Seattle Structural Genomics Center for Infectious Disease; Seattle Structural
		Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2022-07-25
Resolution	:	2.35  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
$\mathrm{EDS}$	:	2.29
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)	:	2.29

# 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 2.35 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.



Motrie	Whole archive	Similar resolution
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	$1211 \ (2.36-2.36)$
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	А	384	<sup>2%</sup> 87%	9% •
1	В	384	86%	10% •
1	С	384	% 92%	7% •
1	D	384	% 85%	11% •



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11930 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.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	Δ	371	Total	С	Ν	0	$\mathbf{S}$	0	1	0
	A	571	2801	1775	457	554	15	0	1	
1	В	371	Total	С	Ν	0	S	0	1	0
1	I D	371	2861	1813	471	562	15	0	1	0
1	C	201	Total	С	Ν	0	S	0	0	0
	301	2901	1834	480	572	15	0	0	0	
1 D	371	Total	С	Ν	0	S	0	1	0	
		2841	1796	463	567	15		L	U	

• Molecule 1 is a protein called Beta sliding clamp.

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	377	ALA	-	expression tag	UNP A0A077EHW1
А	378	GLY	-	expression tag	UNP A0A077EHW1
А	379	HIS	-	expression tag	UNP A0A077EHW1
А	380	HIS	-	expression tag	UNP A0A077EHW1
А	381	HIS	-	expression tag	UNP A0A077EHW1
А	382	HIS	-	expression tag	UNP A0A077EHW1
А	383	HIS	-	expression tag	UNP A0A077EHW1
А	384	HIS	-	expression tag	UNP A0A077EHW1
В	377	ALA	-	expression tag	UNP A0A077EHW1
В	378	GLY	-	expression tag	UNP A0A077EHW1
В	379	HIS	-	expression tag	UNP A0A077EHW1
В	380	HIS	-	expression tag	UNP A0A077EHW1
В	381	HIS	-	expression tag	UNP A0A077EHW1
В	382	HIS	-	expression tag	UNP A0A077EHW1
В	383	HIS	-	expression tag	UNP A0A077EHW1
В	384	HIS	-	expression tag	UNP A0A077EHW1
С	377	ALA	-	expression tag	UNP A0A077EHW1
С	378	GLY	-	expression tag	UNP A0A077EHW1
С	379	HIS	-	expression tag	UNP A0A077EHW1
С	380	HIS	-	expression tag	UNP A0A077EHW1
С	381	HIS	-	expression tag	UNP A0A077EHW1



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Chain	Residue	Modelled	Actual	Comment	Reference
С	382	HIS	-	expression tag	UNP A0A077EHW1
С	383	HIS	-	expression tag	UNP A0A077EHW1
С	384	HIS	-	expression tag	UNP A0A077EHW1
D	377	ALA	-	expression tag	UNP A0A077EHW1
D	378	GLY	-	expression tag	UNP A0A077EHW1
D	379	HIS	-	expression tag	UNP A0A077EHW1
D	380	HIS	-	expression tag	UNP A0A077EHW1
D	381	HIS	-	expression tag	UNP A0A077EHW1
D	382	HIS	-	expression tag	UNP A0A077EHW1
D	383	HIS	-	expression tag	UNP A0A077EHW1
D	384	HIS	-	expression tag	UNP A0A077EHW1

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• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Ca 1 1	0	0
2	В	2	Total Ca 2 2	0	0
2	С	3	Total Ca 3 3	0	0
2	D	3	Total Ca 3 3	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Cl 1 1	0	0
3	С	1	Total Cl 1 1	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues Atoms		ZeroOcc	AltConf
4	В	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

• Molecule 5 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	67	$\begin{array}{cc} \text{Total} & \text{O} \\ 67 & 67 \end{array}$	0	0
5	В	146	Total O 146 146	0	0
5	С	171	Total O 171 171	0	0
5	D	129	Total         O           129         129	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: Beta sliding clamp



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# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	92.41Å 88.01Å 100.24Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $95.75^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	40.26 - 2.35	Depositor
Resolution (A)	44.01 - 2.35	EDS
% Data completeness	99.8 (40.26-2.35)	Depositor
(in resolution range)	99.9 (44.01-2.35)	EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.93 (at 2.34 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
B B.	0.176 , $0.218$	Depositor
$n, n_{free}$	0.176 , $0.218$	DCC
$R_{free}$ test set	2024 reflections $(3.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	44.2	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , $40.3$	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11930	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 4.61% 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, CA, NA

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	
		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.37	0/2851	0.59	0/3879
1	В	0.40	0/2914	0.63	0/3959
1	С	0.43	0/2951	0.65	0/4010
1	D	0.40	0/2888	0.62	0/3925
All	All	0.40	0/11604	0.62	0/15773

There are no bond length outliers.

There are no bond angle outliers.

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	А	2801	0	2685	20	0
1	В	2861	0	2778	23	0
1	С	2901	0	2814	19	0
1	D	2841	0	2749	28	0
2	А	1	0	0	0	0
2	В	2	0	0	0	0
2	С	3	0	0	0	0
2	D	3	0	0	0	0
3	B	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	С	1	0	0	0	0
4	В	1	0	0	0	0
4	D	1	0	0	0	0
5	А	67	0	0	1	0
5	В	146	0	0	4	0
5	С	171	0	0	5	0
5	D	129	0	0	3	0
All	All	11930	0	11026	87	0

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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 (87) 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:C:179:HIS:ND1	5:C:503:HOH:O	2.27	0.68
1:D:141:GLU:OE2	5:D:501:HOH:O	2.12	0.68
1:A:180:ARG:NH1	1:A:331:GLU:OE1	2.26	0.67
1:B:108:ASP:OD2	5:B:501:HOH:O	2.14	0.64
1:C:1:MET:N	5:C:504:HOH:O	2.31	0.62
1:B:360:LEU:HD13	1:B:365:SER:HA	1.82	0.61
1:D:180:ARG:NH1	1:D:331:GLU:OE1	2.31	0.60
1:B:53:LEU:HD11	1:B:206:ILE:HG21	1.83	0.60
1:B:275:SER:HB2	1:B:283:ASN:OD1	2.04	0.58
1:C:21:ILE:HD13	1:C:71:ALA:CB	2.34	0.58
1:C:43:LYS:NZ	5:C:501:HOH:O	2.19	0.57
1:B:353:ILE:HG12	1:B:369:LEU:CD2	2.34	0.57
1:A:349:ASN:HA	1:A:374:ILE:HD11	1.87	0.56
1:D:53:LEU:HD11	1:D:206:ILE:HG21	1.88	0.56
1:B:379:HIS:HE1	5:C:560:HOH:O	1.89	0.55
1:B:292:ASN:HB3	1:B:313:CYS:O	2.07	0.55
1:B:34:LEU:HD21	1:B:66:ARG:NH2	2.23	0.54
1:B:41:ASN:ND2	5:B:513:HOH:O	2.40	0.53
1:C:155:LEU:HD11	1:C:177:ASP:HA	1.90	0.52
1:D:36:GLU:HG2	1:D:66:ARG:HG3	1.92	0.52
1:B:291:GLY:O	1:B:315:TYR:HB3	2.10	0.52
1:A:351:PRO:HA	1:A:372:PRO:HD3	1.92	0.52
1:A:100:LEU:HD23	1:A:113:ALA:HA	1.92	0.50
1:A:180:ARG:HD3	1:A:328:PHE:HB3	1.94	0.50
1:D:194:ASN:HD22	1:D:194:ASN:N	2.11	0.49
1:C:261:THR:HB	1:C:314:GLU:HB3	1.95	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:181:LEU:HB3	1:D:369:LEU:HB3	1.95	0.48
1:D:349:ASN:HA	1:D:374:ILE:HD11	1.94	0.48
1:D:260:LEU:HD23	1:D:343:MET:HE3	1.96	0.48
1:B:224:GLU:O	5:B:502:HOH:O	2.20	0.47
1:B:154:SER:O	1:C:286:ARG:NH1	2.48	0.47
1:A:2:LYS:HG3	1:A:89:VAL:HG22	1.97	0.46
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.69	0.46
1:D:7:SER:OG	1:D:82:GLY:O	2.29	0.46
1:A:278:SER:OG	1:A:283:ASN:OD1	2.29	0.46
1:C:163:LEU:HD11	1:C:196:GLU:HG3	1.97	0.46
1:D:165:GLN:HG2	1:D:196:GLU:HG3	1.97	0.46
1:A:101:LEU:HB2	1:A:114:LEU:HD21	1.97	0.46
1:D:66:ARG:NH1	5:D:504:HOH:O	2.34	0.46
1:D:258:ASN:HB3	1:D:315:TYR:OH	2.16	0.46
1:C:88:PHE:HB3	1:C:101:LEU:HD11	1.99	0.45
1:D:291:GLY:O	1:D:315:TYR:HB3	2.17	0.45
1:B:181:LEU:HB3	1:B:369:LEU:HB2	1.99	0.45
1:D:356:PRO:HG2	1:D:360:LEU:HD11	2.00	0.45
1:A:27:ARG:HA	1:A:28:PRO:HD3	1.87	0.44
1:D:87:THR:HB	1:D:104:LEU:HB2	1.99	0.44
1:B:187:LYS:HB2	1:B:363:ASN:HB3	2.00	0.44
1:D:155:LEU:O	1:D:157:PRO:HD3	2.18	0.44
1:D:165:GLN:HB2	1:D:172:ASN:HB3	1.99	0.44
1:B:101:LEU:HB2	1:B:114:LEU:HD21	1.99	0.44
1:C:351:PRO:HA	1:C:372:PRO:HD3	1.99	0.44
1:D:21:ILE:HD13	1:D:71:ALA:CB	2.48	0.44
1:A:149:ALA:HB3	1:A:175:SER:OG	2.19	0.43
1:B:145:ASN:HA	1:B:335:VAL:HG11	2.01	0.43
1:C:101:LEU:HB2	1:C:114:LEU:HD21	2.00	0.43
1:D:259:VAL:HG22	1:D:344:LYS:HG2	1.98	0.43
1:A:177:ASP:O	1:A:178:SER:OG	2.29	0.43
1:B:260:LEU:HD13	1:B:289:LEU:HD21	2.01	0.42
1:D:200:PRO:HG2	1:D:203:PRO:CG	2.48	0.42
1:C:165:GLN:O	1:C:171:ALA:HA	2.19	0.42
1:B:34:LEU:HB3	1:B:45:THR:HB	2.02	0.42
5:B:514:HOH:O	1:C:379:HIS:HE1	2.03	0.42
1:D:272:ARG:NH1	5:D:502:HOH:O	2.28	0.42
1:A:63:ASN:N	5:A:503:HOH:O	2.51	0.42
1:D:165:GLN:O	1:D:171:ALA:HA	2.19	0.42
1:C:360:LEU:HD13	1:C:365:SER:HA	2.02	0.41
1:A:88:PHE:HB3	1:A:101:LEU:HD11	2.02	0.41

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Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:165:GLN:HB2	1:C:172:ASN:HB2	2.02	0.41
1:D:329:LEU:HD12	1:D:329:LEU:HA	1.80	0.41
1:B:165:GLN:O	1:B:171:ALA:HA	2.20	0.41
1:C:29:ILE:HD12	1:C:29:ILE:HA	1.92	0.41
1:D:100:LEU:HD23	1:D:113:ALA:HA	2.01	0.41
1:B:353:ILE:HG12	1:B:369:LEU:HD21	2.00	0.41
1:D:180:ARG:HD3	1:D:328:PHE:HB3	2.03	0.41
1:D:204:LEU:HD23	1:D:204:LEU:HA	1.88	0.41
1:D:343:MET:HE2	1:D:343:MET:HB2	1.90	0.41
1:A:361:GLU:HG3	1:A:364:GLU:OE1	2.21	0.41
1:B:286:ARG:NH1	1:C:154:SER:O	2.51	0.40
1:D:332:MET:HG3	1:D:368:MET:SD	2.61	0.40
1:A:110:TYR:HB3	1:B:277:PHE:CE2	2.56	0.40
1:C:234:ASN:HB3	5:C:568:HOH:O	2.21	0.40
1:A:34:LEU:HB3	1:A:45:THR:HB	2.03	0.40
1:A:181:LEU:HB3	1:A:369:LEU:HB3	2.03	0.40
1:A:258:ASN:HB3	1:A:315:TYR:OH	2.21	0.40
1:A:342:THR:HG23	1:A:357:VAL:HG22	2.03	0.40
1:B:165:GLN:HB2	1:B:172:ASN:HB2	2.02	0.40
1:C:194:ASN:N	1:C:194:ASN:HD22	2.18	0.40

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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	Perce	entiles
1	А	368/384~(96%)	361~(98%)	7 (2%)	0	100	100
1	В	366/384~(95%)	360~(98%)	6 (2%)	0	100	100
1	С	379/384~(99%)	373~(98%)	6 (2%)	0	100	100
1	D	368/384~(96%)	360~(98%)	8 (2%)	0	100	100
All	All	1481/1536~(96%)	1454 (98%)	27 (2%)	0	100	100



There are no Ramachandran outliers to report.

#### 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	Perce	ntiles
1	А	305/345~(88%)	304 (100%)	1 (0%)	92	96
1	В	319/345~(92%)	313~(98%)	6(2%)	57	68
1	С	321/345~(93%)	318~(99%)	3 (1%)	78	87
1	D	317/345~(92%)	315~(99%)	2(1%)	86	93
All	All	1262/1380~(91%)	1250 (99%)	12 (1%)	76	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	343	MET
1	В	129	SER
1	В	150	THR
1	В	168	GLU
1	В	326	SER
1	В	343	MET
1	В	379	HIS
1	С	73	MET
1	С	343	MET
1	С	379	HIS
1	D	38	GLU
1	D	343	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 13 ligands modelled in this entry, 13 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,  $95^{th}$  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	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	371/384~(96%)	0.10	7 (1%) 66 76	44, 63, 97, 116	0
1	В	371/384~(96%)	-0.05	1 (0%) 94 97	33, 49, 74, 115	0
1	С	381/384~(99%)	-0.09	2 (0%) 91 95	32, 44, 76, 102	0
1	D	371/384~(96%)	-0.05	5 (1%) 77 84	34, 50, 78, 123	0
All	All	1494/1536~(97%)	-0.02	15 (1%) 82 88	32, 51, 86, 123	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	95	ASN	4.3
1	А	126	PHE	3.8
1	А	241	ILE	3.1
1	А	156	ARG	3.0
1	D	26	SER	2.9
1	D	153	ASP	2.9
1	А	283	ASN	2.9
1	D	155	LEU	2.7
1	А	124	PRO	2.6
1	D	154	SER	2.5
1	А	154	SER	2.4
1	D	25	GLN	2.4
1	А	226	MET	2.3
1	С	96	GLY	2.1
1	В	303	TYR	2.1

# 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	$B-factors(A^2)$	Q<0.9
2	CA	D	401	1/1	0.72	0.09	88,88,88,88	0
2	CA	А	401	1/1	0.83	0.11	93,93,93,93	0
4	NA	D	404	1/1	0.89	0.17	43,43,43,43	0
2	CA	В	402	1/1	0.91	0.06	92,92,92,92	0
2	CA	D	402	1/1	0.94	0.16	74, 74, 74, 74	0
2	CA	В	403	1/1	0.94	0.14	64,64,64,64	0
2	CA	С	403	1/1	0.95	0.03	80,80,80,80	0
2	CA	D	403	1/1	0.97	0.11	$55,\!55,\!55,\!55$	0
4	NA	В	404	1/1	0.97	0.15	44,44,44,44	0
2	CA	С	402	1/1	0.97	0.08	$53,\!53,\!53,\!53$	0
2	CA	С	404	1/1	0.98	0.08	36,36,36,36	0
3	CL	В	401	1/1	0.99	0.13	39,39,39,39	0
3	CL	С	401	1/1	1.00	0.11	37,37,37,37	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

