

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

#### Apr 20, 2021 – 12:03 pm BST

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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 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
$\mathrm{EDS}$	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	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)	:	2.18

# 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 3.45 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
	$(\# \mathbf{Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R <sub>free</sub>	130704	1291 (3.52-3.40)
Clashscore	141614	1372(3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)

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 ch	lain	
1	А	773	6% 70%	19%	10%
1	В	773	70%	20%	10%
2	С	65	2% 55%	34%	11%
2	D	65	55%	32%	12%



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14238 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 Telomerase reverse transcriptase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	693	Total 5725	$\mathrm{C}$ $3717$	N 961	O 1029	S 18	0	0	0
1	В	693	Total 5725	C 3717	N 961	O 1029	S 18	0	0	0

• Molecule 2 is a RNA chain called Chains: C,D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	C	65	Total	С	Ν	Ο	Р	0	0	0
		0.0	1394	623	254	452	65	0		0
0	П	65	Total	С	Ν	0	Р	0	0	0
		D 05	1394	623	254	452	65		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.

6% Chain A: 70% 19% 10% SER SER GLY GLY ASN PHE THR HIS THR THR A HERE AND ほいいやほほしほ A LEU LEU VS • Molecule 1: Telomerase reverse transcriptase 17% Chain B: 70% 20% 10%

• Molecule 1: Telomerase reverse transcriptase



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![](_page_4_Picture_4.jpeg)

## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	149.88Å $245.84$ Å $72.47$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$Paralution(\hat{\lambda})$	71.90 - 3.45	Depositor
Resolution (A)	71.90 - 3.45	EDS
% Data completeness	64.0 (71.90-3.45)	Depositor
(in resolution range)	64.0(71.90-3.45)	EDS
$R_{merge}$	0.11	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.56 (at 3.49 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R R.	0.248 , $0.301$	Depositor
$\Pi, \Pi_{free}$	0.248 , $0.301$	DCC
$\mathbf{R}_{free}$ test set	1097 reflections $(4.74\%)$	wwPDB-VP
Wilson B-factor ( $Å^2$ )	141.9	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 95.4	EDS
L-test for twinning <sup>2</sup>	$ L  > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14238	wwPDB-VP
Average B, all atoms $(Å^2)$	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.94% 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.

![](_page_5_Picture_8.jpeg)

<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.24	0/5843	0.41	0/7868
1	В	0.24	0/5843	0.41	0/7868
2	С	0.17	0/1561	0.73	0/2432
2	D	0.16	0/1559	0.72	0/2424
All	All	0.23	0/14806	0.50	0/20592

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	5725	0	5866	102	0
1	В	5725	0	5866	111	0
2	С	1394	0	699	18	0
2	D	1394	0	701	21	0
All	All	14238	0	13132	227	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 8.

All (227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

![](_page_6_Picture_16.jpeg)

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:428:ASN:N	1:B:429:LYS:HA	1.95	0.80
1:A:428:ASN:N	1:A:429:LYS:HA	1.97	0.78
1:B:171:ARG:NH2	1:B:347:ARG:O	2.16	0.78
2:D:1268:C:H42	2:D:1286:G:H1	1.29	0.78
1:A:490:ARG:NH1	1:A:769:SER:OG	2.19	0.76
1:A:490:ARG:NH2	1:A:767:ASP:OD2	2.22	0.73
1:B:159:ILE:HG22	1:B:293:LYS:HZ3	1.53	0.72
1:A:399:LEU:HD22	1:A:606:ASP:HB3	1.73	0.71
1:B:314:ALA:O	1:B:326:ARG:NH2	2.22	0.70
1:B:285:PHE:HE1	1:B:293:LYS:HE2	1.55	0.70
2:C:1304:A:H61	2:D:1305:U:H3	1.39	0.70
1:B:285:PHE:CE1	1:B:293:LYS:HE2	2.26	0.70
1:A:506:LEU:HB3	1:A:671:LEU:HB3	1.73	0.69
1:B:243:VAL:HG12	1:B:408:PRO:HB2	1.74	0.69
1:B:159:ILE:O	1:B:293:LYS:HB3	1.93	0.68
1:A:285:PHE:O	1:A:288:LEU:HG	1.93	0.68
1:A:603:GLN:HG3	1:A:633:LEU:HD12	1.73	0.68
1:A:542:ARG:HD3	1:A:544:TYR:HE2	1.57	0.68
1:B:256:VAL:HG21	1:B:286:LEU:HD11	1.76	0.68
1:B:512:GLU:HB3	1:B:515:ASP:HB2	1.74	0.68
1:A:466:ARG:NH1	1:A:475:SER:O	2.27	0.67
1:A:160:THR:O	1:A:343:LYS:NZ	2.27	0.66
1:A:770:PHE:HB2	1:A:772:VAL:HG22	1.77	0.66
1:A:517:LEU:HA	1:A:695:GLY:HA3	1.78	0.66
1:A:171:ARG:NH2	1:A:347:ARG:O	2.29	0.66
1:B:320:LYS:HE2	2:D:1292:A:H4'	1.76	0.65
1:A:320:LYS:HE2	2:C:1292:A:H4'	1.78	0.65
1:A:494:LEU:HD11	1:A:770:PHE:CZ	2.33	0.64
1:B:466:ARG:NH1	1:B:475:SER:O	2.31	0.63
1:B:161:LYS:HD2	1:B:288:LEU:HD12	1.81	0.63
1:A:165:LEU:HD23	1:A:352:ILE:HG22	1.80	0.63
1:B:738:LEU:HB3	1:B:739:VAL:HA	1.79	0.63
1:B:183:ILE:HG23	1:B:212:LEU:HD12	1.81	0.62
1:B:603:GLN:HG3	1:B:633:LEU:HD12	1.80	0.62
1:A:178:MET:O	1:A:344:ASN:ND2	2.33	0.62
1:A:738:LEU:HB3	1:A:739:VAL:HA	1.81	0.62
1:A:500:ILE:HD11	1:A:503:LEU:HD11	1.83	0.61
1:B:737:SER:HB3	1:B:739:VAL:HB	1.83	0.61
1:A:281:ARG:NH1	1:A:298:ASP:O	2.33	0.61
1:B:159:ILE:HG22	1:B:293:LYS:NZ	2.15	0.60
1:B:306:LYS:HE2	2:D:1320:G:H5'	1.82	0.60
1:B:542:ARG:HD3	1:B:544:TYR:HE2	1.65	0.60
		Continue	ed on next page

![](_page_7_Picture_4.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:288:LEU:HD22	1:B:292:GLU:O	2.02	0.60
1:A:173:PHE:HB3	1:A:225:ASP:HB3	1.83	0.60
1:B:241:ASN:ND2	1:B:244:SER:OG	2.35	0.60
1:B:399:LEU:HD22	1:B:606:ASP:HB3	1.84	0.59
1:A:256:VAL:HG21	1:A:286:LEU:HD11	1.83	0.59
1:A:737:SER:HB3	1:A:739:VAL:HB	1.84	0.59
1:A:167:ASN:O	1:A:368:GLN:NE2	2.28	0.59
1:B:500:ILE:HD11	1:B:503:LEU:HD11	1.84	0.59
1:B:724:THR:HG22	1:B:725:THR:HG23	1.83	0.59
1:A:506:LEU:HB2	1:A:679:TYR:CE1	2.38	0.58
1:B:422:ARG:NH2	1:B:429:LYS:O	2.36	0.58
1:B:281:ARG:NH1	1:B:298:ASP:O	2.37	0.58
1:B:375:TYR:HE2	1:B:611:VAL:HG13	1.70	0.57
1:A:171:ARG:HD3	1:A:176:PHE:CZ	2.38	0.57
1:B:512:GLU:HB2	1:B:516:ARG:HG3	1.86	0.57
1:A:820:THR:HG22	1:A:837:LEU:HD21	1.87	0.57
1:A:422:ARG:NH2	1:A:429:LYS:O	2.38	0.56
1:A:223:ARG:HG3	1:A:225:ASP:OD1	2.05	0.56
1:B:167:ASN:O	1:B:368:GLN:NE2	2.37	0.56
1:B:745:THR:HG22	1:B:747:LYS:H	1.70	0.56
1:A:314:ALA:O	1:A:326:ARG:NH2	2.38	0.56
1:A:183:ILE:HG23	1:A:212:LEU:HD12	1.86	0.56
1:B:508:PHE:HB3	1:B:703:THR:HG23	1.87	0.56
1:A:253:ILE:HD13	1:A:283:VAL:HG13	1.86	0.55
1:B:199:GLY:N	2:D:1269:U:OP1	2.35	0.55
1:A:382:TYR:CZ	1:A:415:VAL:HG21	2.42	0.55
1:B:285:PHE:O	1:B:288:LEU:HG	2.07	0.55
1:B:293:LYS:HZ1	1:B:343:LYS:HE3	1.72	0.55
1:B:253:ILE:HG12	1:B:286:LEU:HD12	1.89	0.54
2:C:1308:G:H2'	2:C:1309:A:H4'	1.88	0.54
1:A:225:ASP:OD1	1:A:226:ILE:N	2.41	0.54
1:B:382:TYR:CZ	1:B:415:VAL:HG21	2.43	0.54
1:A:512:GLU:HB3	1:A:515:ASP:HB2	1.90	0.54
1:A:164:VAL:HG12	1:A:352:ILE:HD13	1.89	0.53
1:A:730:LYS:HB3	1:A:779:ASN:HD21	1.73	0.53
1:B:530:PHE:CG	1:B:593:LYS:HD2	2.44	0.53
1:B:158:TYR:HD1	1:B:159:ILE:H	1.56	0.53
1:A:253:ILE:HG12	1:A:286:LEU:HD12	1.91	0.53
1:A:241:ASN:ND2	1:A:244:SER:OG	2.42	0.53
1:A:852:PHE:HD1	1:A:854:SER:H	1.57	0.53
1:A:713:PRO:O	1:A:724:THR:N	2.32	0.53

![](_page_8_Picture_6.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:731:ARG:NH2	1:B:762:GLU:OE1	2.43	0.52
1:A:731:ARG:NH2	1:A:762:GLU:OE1	2.43	0.51
1:B:510:MET:HB2	1:B:667:ASP:HB2	1.92	0.51
1:B:171:ARG:HD3	1:B:176:PHE:CZ	2.45	0.51
1:A:570:LEU:HD21	1:B:821:ILE:HG13	1.93	0.51
1:B:665:LEU:HD11	1:B:718:VAL:HG11	1.93	0.51
1:A:431:LEU:HD23	1:A:431:LEU:H	1.74	0.50
1:B:838:LEU:HD22	1:B:867:ILE:HG13	1.94	0.50
1:A:428:ASN:H	1:A:429:LYS:HA	1.76	0.50
2:D:1322:U:O2'	2:D:1324:G:O5'	2.22	0.49
1:A:493:LEU:HD23	1:A:500:ILE:HG13	1.94	0.49
1:B:770:PHE:HB2	1:B:772:VAL:HG22	1.95	0.49
1:B:539:TYR:OH	1:B:593:LYS:NZ	2.45	0.49
1:B:431:LEU:HD23	1:B:431:LEU:H	1.78	0.49
1:A:574:ARG:NH2	1:B:857:GLU:OE1	2.36	0.48
1:B:247:THR:OG1	1:B:350:TRP:NE1	2.46	0.48
1:B:519:GLN:HG2	1:B:625:ARG:O	2.13	0.48
1:A:512:GLU:HB2	1:A:516:ARG:HG3	1.95	0.48
2:C:1305:U:H3	2:D:1304:A:H61	1.60	0.48
2:D:1322:U:HO2'	2:D:1324:G:C5'	2.25	0.48
1:A:204:ARG:NH1	2:C:1267:G:O3'	2.47	0.48
1:B:253:ILE:HD13	1:B:283:VAL:HG13	1.96	0.48
1:B:428:ASN:H	1:B:429:LYS:HA	1.78	0.47
2:D:1291:A:H4'	2:D:1292:A:H5'	1.96	0.47
1:B:159:ILE:CG2	1:B:293:LYS:HZ3	2.23	0.47
1:A:471:SER:HA	1:A:654:TRP:CE2	2.49	0.47
1:B:317:ILE:HG22	2:D:1291:A:H61	1.79	0.47
1:B:852:PHE:HD1	1:B:854:SER:H	1.62	0.47
1:A:426:LEU:HB3	1:A:427:LEU:H	1.54	0.47
1:A:517:LEU:HD11	1:A:641:LEU:HD23	1.96	0.47
1:A:724:THR:HG22	1:A:725:THR:HG23	1.97	0.47
1:A:242:VAL:HG12	1:A:374:LEU:HD22	1.97	0.47
1:B:247:THR:HG1	1:B:350:TRP:HE1	1.63	0.47
1:B:160:THR:O	1:B:343:LYS:NZ	2.44	0.47
1:B:522:LEU:HD13	1:B:641:LEU:HB2	1.96	0.47
1:A:522:LEU:HD13	1:A:641:LEU:HB2	1.96	0.46
1:B:679:TYR:OH	1:B:705:VAL:HG23	2.15	0.46
1:A:351:TYR:N	1:A:366:PHE:O	2.35	0.46
1:B:267:ASP:OD1	1:B:267:ASP:N	2.46	0.46
1:A:506:LEU:HB2	1:A:679:TYR:HE1	1.80	0.46
1:A:677:ASN:O	1:A:681:GLN:HG3	2.14	0.46

![](_page_9_Picture_6.jpeg)

	Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlan (Å)			
1·B·165·LEU·HD23	1·B·352·ILE·HG22	1.97	0.46			
1:B:803:THB:OG1	2:D:1315:G:N2	2 49	0.46			
2·C·1302·A·C6	2·D·1299·A·H5"	2.51	0.46			
2:C:1322:U:HO2'	2:C:1324:G:C5'	2.34	0.46			
1:A:865:LEU:HD12	1:B:572:SER:HB3	1.97	0.46			
2:C:1317:U:H2'	2:C:1318:A:C8	2.50	0.46			
1:A:530:PHE:CG	1:A:593:LYS:HD2	2.50	0.46			
1:A:717:PHE:CD2	1:A:718:VAL:HG12	2.51	0.46			
1:A:426:LEU:O	1:A:427:LEU:HG	2.16	0.45			
1:A:572:SER:HB3	1:B:865:LEU:HD12	1.98	0.45			
1:A:204:ARG:HG3	2:C:1268:C:OP1	2.16	0.45			
1:A:675:ASP:HB3	1:A:678:ILE:HG22	1.98	0.45			
1:B:476:VAL:HG23	1:B:665:LEU:HD23	1.98	0.45			
1:B:797:SER:HA	1:B:800:LYS:HE2	1.98	0.45			
2:C:1300:A:H3'	2:D:1301:A:N6	2.32	0.45			
1:A:181:PRO:HG2	1:A:186:ILE:HD11	1.99	0.45			
1:A:657:LYS:HB2	1:A:660:PHE:HE1	1.81	0.45			
2:C:1291:A:H4'	2:C:1292:A:H5'	1.99	0.45			
1:A:446:TYR:O	1:A:450:VAL:HB	2.17	0.45			
1:A:267:ASP:OD1	1:A:267:ASP:N	2.48	0.45			
1:A:493:LEU:HD23	1:A:501:PRO:HD2	1.99	0.45			
1:A:785:ARG:NH2	1:A:844:ILE:HG12	2.32	0.45			
1:B:356:SER:HB2	1:B:414:ARG:NH1	2.32	0.45			
1:A:745:THR:HG22	1:A:747:LYS:H	1.82	0.44			
1:B:297:ASP:OD1	2:D:1294:A:O2'	2.35	0.44			
1:B:359:VAL:O	1:B:736:ILE:HD12	2.17	0.44			
1:A:601:ARG:NH2	1:A:606:ASP:OD1	2.51	0.44			
1:B:335:TRP:NE1	1:B:339:GLU:HG3	2.32	0.44			
1:B:428:ASN:N	1:B:429:LYS:CA	2.76	0.44			
1:A:243:VAL:O	1:A:246:LYS:HG2	2.18	0.44			
1:A:542:ARG:HB3	1:B:831:TRP:CE2	2.52	0.44			
1:B:178:MET:O	1:B:344:ASN:ND2	2.51	0.44			
1:B:431:LEU:O	1:B:432:GLU:HG2	2.18	0.44			
1:A:160:THR:HG22	1:A:293:LYS:HB3	1.99	0.44			
1:A:821:ILE:HG13	1:B:570:LEU:HD21	2.00	0.44			
1:B:166:TYR:HA	1:B:351:TYR:CZ	2.53	0.44			
1:B:173:PHE:HA	1:B:176:PHE:HD2	1.83	0.44			
1:A:171:ARG:NH2	1:A:368:GLN:HE21	2.16	0.44			
1:B:707:ASN:OD1	1:B:709:THR:OG1	2.34	0.44			
1:A:679:TYR:OH	1:A:705:VAL:HG23	2.18	0.43			
1:A:829:SER:O	1:B:460:LEU:HD11	2.18	0.43			

![](_page_10_Picture_6.jpeg)

		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:743:PHE:CZ	1:B:752:TYR:HB2	2.53	0.43	
1:A:740:THR:HG22	1:A:794:LYS:HD3	2.01	0.43	
1:A:784:LEU:HD23	1:A:844:ILE:HD12	1.99	0.43	
1:A:309:LYS:H	1:A:309:LYS:HG2	1.62	0.43	
1:B:493:LEU:HD23	1:B:500:ILE:HG13	2.01	0.43	
2:C:1270:U:H2'	2:C:1271:C:C6	2.54	0.43	
1:A:571:SER:O	1:A:572:SER:OG	2.35	0.43	
1:B:310:TRP:HZ3	1:B:329:PHE:HE2	1.65	0.43	
1:B:420:ILE:HD12	1:B:422:ARG:H	1.84	0.43	
1:A:168:SER:HA	1:A:368:GLN:CD	2.39	0.43	
1:A:761:LEU:HD11	1:A:766:LEU:HD21	2.01	0.43	
1:B:426:LEU:O	1:B:427:LEU:HG	2.19	0.43	
1:B:243:VAL:O	1:B:246:LYS:HG2	2.17	0.42	
1:A:229:ALA:O	1:A:233:GLY:HA2	2.19	0.42	
2:C:1307:G:N2	2:C:1310:A:OP1	2.51	0.42	
1:A:431:LEU:C	1:A:433:LEU:H	2.22	0.42	
2:C:1302:A:N6	2:D:1299:A:H5"	2.33	0.42	
1:A:831:TRP:HH2	1:B:569:ILE:HD13	1.84	0.42	
1:A:420:ILE:HD12	1:A:422:ARG:H	1.84	0.42	
1:B:390:MET:HG3	1:B:622:LYS:HG3	2.01	0.42	
1:B:611:VAL:HB	1:B:619:HIS:HB3	2.01	0.42	
2:C:1322:U:H4'	2:C:1324:G:OP1	2.19	0.42	
1:A:648:ASP:OD1	1:A:649:CYS:N	2.53	0.42	
1:A:806:CYS:SG	1:A:857:GLU:HB2	2.60	0.42	
1:A:292:GLU:HA	1:A:741:THR:HG21	2.02	0.42	
1:B:180:ARG:N	1:B:181:PRO:HD2	2.35	0.42	
2:C:1300:A:H3'	2:D:1301:A:H61	1.84	0.42	
1:B:163:ASN:HB2	1:B:343:LYS:NZ	2.35	0.41	
1:B:240:ALA:O	1:B:411:SER:OG	2.38	0.41	
2:C:1317:U:H2'	2:C:1318:A:H8	1.85	0.41	
1:A:310:TRP:HZ3	1:A:329:PHE:HE2	1.67	0.41	
1:B:431:LEU:C	1:B:433:LEU:H	2.23	0.41	
1:B:535:ASN:HA	1:B:593:LYS:HB3	2.02	0.41	
1:B:650:PHE:HE1	1:B:682:VAL:HG13	1.86	0.41	
1:B:505:ILE:HD11	1:B:724:THR:HG23	2.03	0.41	
2:D:1272:C:H1'	2:D:1282:G:H22	1.85	0.41	
1:A:585:LYS:HE2	1:A:585:LYS:HB3	1.89	0.41	
1:A:819:TYR:HA	1:A:822:VAL:HG22	2.03	0.41	
1:A:861:TRP:CD1	1:B:574:ARG:HG3	2.55	0.41	
1:A:664:ARG:HH21	1:A:666:VAL:HA	1.85	0.41	
1:B:471:SER:HA	1:B:654:TRP:CE2	2.55	0.41	

![](_page_11_Picture_6.jpeg)

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)	
2:D:1322:U:H4'	2:D:1324:G:OP1	2.21	0.41	
1:A:173:PHE:CB	1:A:225:ASP:HB3	2.49	0.41	
1:A:180:ARG:N	1:A:181:PRO:HD2	2.35	0.41	
1:B:161:LYS:HB3	1:B:291:ASN:HA	2.03	0.41	
1:B:163:ASN:HB2	1:B:343:LYS:HZ3	1.86	0.41	
1:B:319:SER:HB3	2:D:1266:G:H1'	2.02	0.41	
1:B:173:PHE:HB3	1:B:225:ASP:HB2	2.02	0.41	
2:D:1292:A:H2'	2:D:1293:U:C6	2.56	0.41	
1:B:471:SER:HB2	1:B:647:HIS:HA	2.02	0.40	
1:B:293:LYS:NZ	1:B:343:LYS:HE3	2.36	0.40	
2:D:1308:G:H2'	2:D:1309:A:H4'	2.03	0.40	
1:A:844:ILE:O	1:A:848:GLU:HG2	2.21	0.40	
1:B:212:LEU:O	1:B:216:ILE:HG13	2.21	0.40	
1:B:281:ARG:O	1:B:285:PHE:N	2.49	0.40	
1:B:300:PHE:HE1	1:B:330:LEU:HD23	1.87	0.40	
1:B:432:GLU:OE2	1:B:435:THR:HB	2.22	0.40	
1:B:446:TYR:O	1:B:450:VAL:HB	2.21	0.40	
1:B:648:ASP:OD1	1:B:649:CYS:N	2.55	0.40	
1:A:519:GLN:HG3	1:A:520:PRO:HD3	2.04	0.40	
1:B:249:ILE:HD11	1:B:286:LEU:HB3	2.04	0.40	
2:C:1267:G:N2	2:C:1289:U:H1'	2.37	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	Perce	ntiles
1	А	685/773~(89%)	639~(93%)	46 (7%)	0	100	100
1	В	685/773~(89%)	637 (93%)	48 (7%)	0	100	100
All	All	1370/1546~(89%)	1276~(93%)	94 (7%)	0	100	100

![](_page_12_Picture_11.jpeg)

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	entiles
1	А	649/723~(90%)	646~(100%)	3 (0%)	88	95
1	В	649/723~(90%)	646~(100%)	3~(0%)	88	95
All	All	1298/1446~(90%)	1292 (100%)	6 (0%)	88	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	665	LEU
1	А	830	ASP
1	А	852	PHE
1	В	830	ASP
1	В	836	GLU
1	В	852	PHE

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

Mol	Chain	Res	Type
1	А	241	ASN
1	В	241	ASN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	С	63/65~(96%)	17~(26%)	1(1%)
2	D	61/65~(93%)	16~(26%)	1 (1%)
All	All	124/130~(95%)	33~(26%)	2(1%)

All (33) RNA backbone outliers are listed below:

![](_page_13_Picture_15.jpeg)

$\mathbf{Mol}$	Chain	Res	Type
2	С	1264	А
2	С	1276	А
2	С	1279	G
2	С	1280	U
2	С	1282	G
2	С	1285	А
2	С	1292	А
2	С	1300	А
2	С	1301	А
2	С	1306	U
2	С	1307	G
2	С	1308	G
2	С	1309	А
2	С	1311	G
2	С	1315	G
2	С	1322	U
2	С	1324	G
2	D	1264	А
2	D	1276	А
2	D	1279	G
2	D	1280	U
2	D	1282	G
2	D	1285	А
2	D	1292	А
2	D	1300	А
2	D	1301	А
2	D	1307	G
2	D	1308	G
2	D	1309	A
2	D	1310	A
2	D	1311	G
2	D	1315	G
2	D	1324	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
2	С	1322	U
2	D	1322	U

### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

![](_page_14_Picture_8.jpeg)

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

There are no ligands in this entry.

#### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	2
1	А	1
1	В	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	174:SER	С	175:ARG	Ν	4.23
1	В	174:SER	С	175:ARG	Ν	4.10
1	D	1320:G	O3'	1321:U	Р	3.82
1	D	1305:U	O3'	1306:U	Р	3.26

![](_page_15_Picture_14.jpeg)

## 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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	693/773~(89%)	0.56	50 (7%) 15 17	71, 134, 212, 315	0
1	В	693/773~(89%)	0.95	130 (18%) 1 2	103, 171, 242, 329	0
2	С	65/65~(100%)	-0.17	1 (1%) 73 71	115, 170, 261, 328	0
2	D	65/65~(100%)	-0.47	2 (3%) 49 47	148, 211, 305, 392	0
All	All	1516/1676~(90%)	0.66	183 (12%) 4 6	71, 156, 240, 392	0

All (183) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	577	SER	10.8
1	В	205	TYR	8.6
1	В	394	ILE	8.5
1	А	565	HIS	7.0
1	В	577	SER	7.0
1	В	406	LEU	6.7
1	А	742	ASN	6.5
1	В	621	TYR	6.2
1	В	237	CYS	6.1
1	В	506	LEU	6.1
1	А	549	ALA	6.0
1	В	401	CYS	5.8
1	В	584	ASP	5.8
1	В	428	ASN	5.7
1	А	231	PHE	5.2
1	А	612	LYS	5.2
1	В	311	LEU	5.1
1	В	333	TYR	5.1
1	В	604	ILE	4.9
1	В	267	ASP	4.9
1	В	231	PHE	4.8

![](_page_16_Picture_10.jpeg)

6ZDU
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Mol	Chain	Res	Type	RSRZ
1	В	416	ILE	4.8
1	В	585	LYS	4.7
1	В	365	TYR	4.7
1	В	731	ARG	4.7
1	В	404	ILE	4.7
1	В	424	LEU	4.7
1	В	421	LYS	4.7
1	В	600	CYS	4.5
1	В	236	LYS	4.4
1	В	268	ALA	4.4
1	В	293	LYS	4.3
1	В	654	TRP	4.2
1	В	329	PHE	4.1
1	В	204	ARG	4.1
1	А	394	ILE	4.1
1	В	238	ASN	4.1
1	В	431	LEU	4.0
1	В	583	VAL	4.0
1	В	385	ASN	3.9
1	В	650	PHE	3.9
1	В	381	LYS	3.9
1	А	397	GLU	3.8
1	А	583	VAL	3.8
1	В	742	ASN	3.7
1	В	609	GLY	3.7
1	В	522	LEU	3.7
1	В	303	ILE	3.7
1	В	443	PHE	3.6
1	В	849	PHE	3.6
1	А	428	ASN	3.5
1	В	610	SER	3.5
1	В	349	PHE	3.4
1	В	341	LEU	3.4
1	В	209	LYS	3.4
1	А	179	ILE	3.4
1	В	370	LEU	3.3
1	В	663	VAL	3.3
1	В	436	LEU	3.3
1	В	310	TRP	3.3
1	В	262	LYS	3.3
1	А	430	LYS	3.3
1	A	283	VAL	3.3

![](_page_17_Picture_6.jpeg)

6ZDU
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Mol	Chain	Res	Type	RSRZ
1	В	622	LYS	3.3
1	В	296	MET	3.2
1	В	611	VAL	3.2
1	А	621	TYR	3.1
1	В	399	LEU	3.1
1	В	433	LEU	3.1
1	В	649	CYS	3.1
1	А	156	SER	3.1
1	В	397	GLU	3.1
1	А	608	VAL	3.1
1	В	313	ARG	3.0
1	В	266	LEU	3.0
1	А	834	ALA	3.0
1	А	544	TYR	3.0
1	А	611	VAL	3.0
1	В	390	MET	3.0
1	А	858	ILE	3.0
1	А	614	ALA	3.0
1	В	395	GLN	2.9
1	А	835	PRO	2.9
1	В	565	HIS	2.9
1	В	788	LEU	2.9
1	В	308	PHE	2.9
1	А	838	LEU	2.9
1	В	232	ILE	2.8
1	В	686	LEU	2.8
1	А	589	ILE	2.8
1	В	525	LYS	2.8
1	В	240	ALA	2.8
1	А	396	ARG	2.8
1	В	336	TRP	2.8
1	В	265	PRO	2.8
1	В	345	ILE	2.7
1	В	346	LEU	2.7
1	В	504	PHE	2.7
1	В	301	ARG	2.7
1	В	521	VAL	2.7
1	В	269	TRP	2.7
1	А	293	LYS	2.6
1	В	190	ILE	2.7
1	В	440	LYS	2.6
1	В	505	ILE	2.6

![](_page_18_Picture_6.jpeg)

6ZDU	
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Mol	Chain	Res	Type	RSRZ
1	А	548	ASP	2.6
1	А	574	ARG	2.6
1	В	662	PHE	2.6
1	В	286	LEU	2.6
1	В	300	PHE	2.6
1	В	549	ALA	2.6
1	В	305	LEU	2.6
1	В	196	LEU	2.6
1	А	546	GLN	2.5
1	В	338	PHE	2.5
1	В	264	LEU	2.5
1	В	411	SER	2.5
1	В	255	PHE	2.5
1	В	275	LYS	2.5
1	В	208	PHE	2.5
1	В	671	LEU	2.5
1	А	451	LEU	2.5
1	В	432	GLU	2.5
1	В	271	GLY	2.4
1	А	401	CYS	2.4
1	В	170	SER	2.4
1	В	278	ILE	2.4
1	В	418	VAL	2.4
1	В	239	PHE	2.4
1	В	612	LYS	2.4
1	В	291	ASN	2.4
1	А	759	LEU	2.4
1	В	287	LEU	2.4
1	B	679	TYR	2.4
1	В	458	LEU	2.4
1	В	302	GLY	2.4
1	B	646	VAL	2.4
1	В	792	LYS	2.4
1	В	337	LEU	2.4
1	В	155	VAL	2.3
1	В	630	GLY	2.3
1	A	867	ILE	2.3
1	A	584	ASP	2.3
1	В	373	GLU	2.3
1	В	507	LYS	2.3
1	A	291	ASN	2.3
1	В	867	ILE	2.3

![](_page_19_Picture_6.jpeg)

Mol	Chain	$\mathbf{Res}$	Type	$\mathbf{RSRZ}$
2	D	1310	A	2.3
1	А	308	PHE	2.3
1	В	274	ASN	2.3
1	А	399	LEU	2.3
1	А	738	LEU	2.3
1	В	720	LEU	2.3
1	В	277	ILE	2.3
1	А	628	PHE	2.3
1	В	283	VAL	2.3
1	В	455	GLY	2.3
2	D	1277	U	2.3
1	В	642	TYR	2.2
2	С	1310	А	2.2
1	В	292	GLU	2.2
1	В	619	HIS	2.2
1	А	392	SER	2.2
1	А	365	TYR	2.2
1	В	212	LEU	2.2
1	А	829	SER	2.2
1	В	405	LYS	2.2
1	А	666	VAL	2.1
1	А	613	ASP	2.1
1	А	349	PHE	2.1
1	А	609	GLY	2.1
1	В	462	LEU	2.1
1	В	641	LEU	2.1
1	B	403	LYS	2.1
1	A	633	LEU	2.1
1	B	249	ILE	2.1
1	В	474	ALA	2.1
1	В	186	ILE	2.1
1	В	589	ILE	2.1
1	А	509	ASP	2.0
1	A	167	ASN	2.0
1	В	685	ILE	2.0
1	A	841	ILE	2.0

Continued from previous page...

## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

![](_page_20_Picture_7.jpeg)

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.4 Ligands (i)

There are no ligands in this entry.

### 6.5 Other polymers (i)

There are no such residues in this entry.

![](_page_21_Picture_9.jpeg)