

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

#### Apr 6, 2021 – 11:03 am BST

PDB ID	:	6Y2P
Title	:	Escherichia coli RnlA-RnlB Toxin-Antitoxin System.
Authors	:	Garcia-Rodriguez, G.; Talavera Perez, A.; Loris, R.
Deposited on	:	2020-02-17
Resolution	:	2.64  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 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 2.64 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	Whole archive	Similar resolution
	$(\# \mathbf{Entries})$	$(\# { m Entries}, { m resolution} \ { m range}({ m \AA}))$
$R_{free}$	130704	$1426 \ (2.66-2.62)$
Clashscore	141614	1472(2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	357	10%	23%	·
1	В	357	80%	18%	·
2	С	134	% • 77%	13%	10%
2	D	134	<sup>2%</sup> 80%	9% •	10%



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7002 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 mRNA endoribonuclease toxin LS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	355	Total 2728	C 1745	N 466	O 504	S 13	0	0	0
1	В	348	Total 2468	C 1566	N 426	O 465	S 11	0	0	0

• Molecule 2 is a protein called Antitoxin RnlB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	2 C	120	Total	С	Ν	Ο	S	0	0	0
		120	872	557	137	173	5	0		
0	П	120	Total	С	Ν	0	S	0	0	1
	2 D	120	907	579	147	176	5		0	1

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	124	ALA	-	expression tag	UNP P52130
С	125	ALA	-	expression tag	UNP P52130
С	126	ALA	-	expression tag	UNP P52130
С	127	LEU	-	expression tag	UNP P52130
С	128	GLU	-	expression tag	UNP P52130
С	129	HIS	-	expression tag	UNP P52130
С	130	HIS	-	expression tag	UNP P52130
С	131	HIS	-	expression tag	UNP P52130
С	132	HIS	-	expression tag	UNP P52130
С	133	HIS	-	expression tag	UNP P52130
С	134	HIS	-	expression tag	UNP P52130
D	124	ALA	-	expression tag	UNP P52130
D	125	ALA	-	expression tag	UNP P52130
D	126	ALA	-	expression tag	UNP P52130
D	127	LEU	-	expression tag	UNP P52130
D	128	GLU	-	expression tag	UNP P52130



Chain	Residue	Modelled	Actual	Comment	Reference
D	129	HIS	-	expression tag	UNP P52130
D	130	HIS	-	expression tag	UNP P52130
D	131	HIS	-	expression tag	UNP P52130
D	132	HIS	-	expression tag	UNP P52130
D	133	HIS	-	expression tag	UNP P52130
D	134	HIS	-	expression tag	UNP P52130

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	8	Total O 8 8	0	0
3	В	7	Total O 7 7	0	0
3	С	4	Total O 4 4	0	0
3	D	8	Total O 8 8	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.









## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	243.32Å $133.58$ Å $55.64$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $95.11^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	48.78 - 2.64	Depositor
	48.78 - 2.64	EDS
% Data completeness	99.1(48.78-2.64)	Depositor
(in resolution range)	99.2(48.78-2.64)	EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.43 (at 2.65 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
D D.	0.197 , $0.242$	Depositor
$\Pi, \Pi_{free}$	0.215 , $0.253$	DCC
$R_{free}$ test set	2584 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.7	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , $59.8$	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7002	wwPDB-VP
Average B, all atoms $(Å^2)$	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.04% 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)

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	0.54	0/2785	0.68	0/3790	
1	В	0.58	0/2517	0.70	0/3438	
2	С	0.47	0/887	0.65	0/1214	
2	D	0.56	0/922	0.71	0/1256	
All	All	0.55	0/7111	0.69	0/9698	

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	2728	0	2674	64	0
1	В	2468	0	2214	48	0
2	С	872	0	817	12	0
2	D	907	0	896	10	0
3	А	8	0	0	0	0
3	В	7	0	0	1	0
3	С	4	0	0	0	0
3	D	8	0	0	0	0
All	All	7002	0	6601	122	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 9.



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:274:GLN:N	1:A:275:PRO:HD2	1.98	0.79
1:A:273:GLN:HB3	1:A:275:PRO:HD2	1.66	0.75
1:B:7:LYS:HA	1:B:69:THR:HG23	1.68	0.74
1:B:258:GLU:HB2	1:B:314:PHE:CE1	2.23	0.73
1:A:314:PHE:O	1:A:318:ARG:HB2	1.88	0.73
1:A:129:GLU:OE2	1:A:132:ARG:HD2	1.90	0.72
1:B:258:GLU:HG3	1:B:314:PHE:CZ	2.25	0.71
1:B:138:VAL:HA	1:B:153:SER:HA	1.72	0.70
1:B:191:LEU:HB3	1:B:192:ILE:HD12	1.75	0.69
1:B:216:ALA:HB3	1:B:352:LYS:HD2	1.75	0.68
1:A:115:VAL:HG22	1:A:181:LEU:HD12	1.75	0.68
2:C:45:THR:HA	2:C:68:MET:O	1.93	0.67
2:C:29:VAL:HA	2:C:32:ILE:HD12	1.77	0.67
1:A:184:LEU:HB3	1:A:187:LEU:HD13	1.77	0.65
2:C:112:PRO:HA	2:C:115:VAL:HG12	1.80	0.64
1:A:273:GLN:NE2	2:D:27:SER:O	2.31	0.64
1:B:179:ALA:HB1	1:B:185:GLN:HA	1.80	0.63
1:A:103:VAL:HG22	1:A:162:GLN:HB2	1.81	0.62
1:A:274:GLN:H	1:A:275:PRO:HD2	1.64	0.62
1:A:172:ARG:O	1:A:175:THR:HG22	1.99	0.62
1:A:175:THR:HG23	1:A:176:PHE:N	2.15	0.62
1:A:274:GLN:N	1:A:275:PRO:CD	2.62	0.62
1:B:43:GLY:HA2	1:B:62:TYR:HD2	1.65	0.61
1:A:12:VAL:HG23	1:A:15:ASN:HB2	1.83	0.60
2:C:86:VAL:HG13	2:C:91:LEU:HD11	1.82	0.60
1:B:195:GLU:HG2	1:B:198:LYS:HB2	1.83	0.60
1:B:258:GLU:HB2	1:B:314:PHE:HE1	1.66	0.59
2:C:62:ARG:HG2	2:C:63:PHE:CD2	2.36	0.59
1:A:66:GLY:HA3	1:A:148:ASP:HB3	1.84	0.59
1:A:129:GLU:CD	1:A:132:ARG:HD2	2.22	0.59
1:A:129:GLU:OE2	1:A:132:ARG:CD	2.51	0.58
1:A:280:THR:HG22	1:A:280:THR:O	2.04	0.58
1:A:88:LEU:O	1:A:91:THR:HB	2.03	0.57
1:A:324:MET:O	1:B:262:LYS:HE3	2.03	0.57
1:A:155:HIS:HB2	1:A:158:THR:OG1	2.05	0.57
1:B:139:TRP:N	1:B:152:VAL:O	2.25	0.56
1:A:13:ARG:CZ	1:A:62:TYR:HB3	2.35	0.56
1:A:190:VAL:HG11	1:B:190:VAL:HG11	1.87	0.56
1:A:252:PRO:HG2	1:A:253:GLU:OE1	2.06	0.56
1:B:136:THR:CB	1:B:155:HIS:HA	2.36	0.55

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:C:111:SER:OG	2:C:112:PRO:HD2	2.06	0.55	
2:D:2:PHE:HE2	2:D:4:ILE:HD11	1.71	0.55	
1:B:138:VAL:HG23	1:B:153:SER:OG	2.07	0.55	
1:A:104:LEU:HB2	1:A:107:PHE:HE2	1.70	0.55	
1:A:170:CYS:HA	1:A:173:VAL:HG12	1.89	0.54	
1:B:237:LYS:NZ	3:B:402:HOH:O	2.40	0.54	
2:D:4:ILE:HD12	2:D:4:ILE:H	1.73	0.53	
1:B:320:SER:HB3	1:B:332:ARG:HB3	1.90	0.53	
1:A:217:ASP:O	1:A:220:PRO:HD2	2.10	0.52	
1:A:237:LYS:NZ	1:A:249:LEU:O	2.40	0.52	
2:D:45:THR:HA	2:D:68:MET:O	2.10	0.52	
1:A:273:GLN:HA	1:A:273:GLN:OE1	2.10	0.51	
1:B:148:ASP:OD2	1:B:168:LEU:CB	2.59	0.50	
1:B:268:LEU:HD12	1:B:307:ILE:HD11	1.94	0.50	
1:B:137:VAL:O	1:B:154:LEU:N	2.44	0.50	
1:A:184:LEU:HA	1:B:186:GLY:HA3	1.94	0.50	
1:B:284:LYS:HD2	1:B:289:TYR:CZ	2.47	0.49	
1:A:11:LEU:HD23	1:A:92:ILE:HD11	1.95	0.49	
1:A:175:THR:CG2	1:A:176:PHE:N	2.76	0.49	
1:A:200:ASN:HB3	1:B:198:LYS:NZ	2.27	0.49	
1:B:88:LEU:O	1:B:91:THR:HG22	2.13	0.49	
2:D:112:PRO:O	2:D:116:ARG:HG2	2.12	0.49	
1:B:127:PHE:HA	1:B:141:ILE:HA	1.93	0.48	
1:B:289:TYR:O	1:B:308:SER:HB2	2.14	0.48	
1:A:86:ASP:O	1:A:90:GLU:HG3	2.14	0.48	
1:A:49:THR:OG1	1:A:55:LEU:HA	2.14	0.47	
1:A:258:GLU:HB2	1:A:314:PHE:CE1	2.49	0.47	
1:B:92:ILE:HD12	1:B:93:ASN:H	1.79	0.47	
1:A:7:LYS:HA	1:A:69:THR:HG23	1.97	0.47	
1:A:124:HIS:O	1:A:143:SER:HA	2.15	0.47	
1:A:65:ASP:HB3	1:A:166:ARG:HH11	1.80	0.46	
1:A:129:GLU:OE1	1:A:132:ARG:HD2	2.16	0.46	
2:D:48:ILE:HD11	2:D:68:MET:SD	2.55	0.46	
1:B:258:GLU:HG3	1:B:314:PHE:HZ	1.75	0.46	
2:C:112:PRO:O	2:C:115:VAL:HG12	2.16	0.46	
1:A:328:VAL:HB	1:B:223:HIS:CD2	2.50	0.46	
2:D:4:ILE:HD12	2:D:4:ILE:N	2.31	0.46	
1:A:179:ALA:HA	1:A:184:LEU:HB2	1.99	0.45	
2:C:91:LEU:HD23	2:C:91:LEU:HA	1.66	0.45	
1:A:241:PRO:HB3	1:B:201:ILE:HD12	1.99	0.45	
1:A:118:LEU:O	1:A:121:ASP:HB2	2.17	0.45	



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:268:LEU:HD23	1:B:268:LEU:HA	1.81	0.45
2:C:29:VAL:HG22	2:C:73:ILE:HD12	1.98	0.45
1:B:299:LEU:HB2	1:B:304:ILE:HD11	1.99	0.45
1:A:217:ASP:N	1:A:217:ASP:OD1	2.43	0.45
2:D:5:THR:HG23	2:D:93:LYS:HG2	1.99	0.44
1:B:215:MET:O	1:B:352:LYS:HG3	2.18	0.44
1:B:137:VAL:N	1:B:154:LEU:O	2.47	0.44
1:B:8:ASN:HA	1:B:67:SER:HB3	1.99	0.44
1:A:29:TYR:CZ	1:A:80:LEU:HD11	2.52	0.44
1:A:193:ARG:HE	1:B:102:MET:HE3	1.82	0.44
1:A:174:PHE:CZ	1:A:178:LEU:HD12	2.53	0.44
1:A:193:ARG:HE	1:B:102:MET:CE	2.31	0.44
1:B:268:LEU:HD13	1:B:299:LEU:HD22	2.00	0.43
1:A:329:ASP:HB3	2:C:80:ILE:HD11	2.01	0.43
1:A:20:SER:O	1:A:24:ILE:HD12	2.17	0.43
1:A:278:PHE:HB3	1:A:311:TYR:CZ	2.53	0.43
1:A:212:GLN:HG3	1:A:219:TYR:CD2	2.53	0.43
1:B:256:THR:O	1:B:260:VAL:HG23	2.19	0.43
2:D:36:LEU:HD23	2:D:36:LEU:HA	1.79	0.43
1:B:152:VAL:HG13	1:B:163:ILE:HG22	2.01	0.42
1:A:272:VAL:HG21	1:A:278:PHE:CE1	2.54	0.42
1:A:324:MET:HG3	1:B:255:ARG:HG2	2.01	0.42
2:C:53:LEU:HD21	2:C:110:LEU:HD11	2.00	0.42
1:A:262:LYS:HG3	1:A:278:PHE:HZ	1.84	0.42
1:A:218:ALA:CB	1:A:352:LYS:HG3	2.50	0.42
2:C:65:THR:HG21	2:C:81:ILE:HD11	2.00	0.42
1:A:24:ILE:HG23	1:A:29:TYR:HB2	2.02	0.42
1:A:49:THR:HG22	1:A:50:ARG:O	2.19	0.42
1:A:113:LEU:N	1:A:114:PRO:HD2	2.35	0.42
1:A:283:ASP:OD1	1:A:292:LYS:NZ	2.53	0.42
1:B:211:LEU:HA	1:B:214:VAL:HG12	2.01	0.41
1:A:12:VAL:HG23	1:A:12:VAL:O	2.20	0.41
1:B:230:LEU:HD23	1:B:230:LEU:HA	1.73	0.41
1:B:209:THR:O	1:B:213:THR:HG23	2.20	0.41
1:A:352:LYS:O	1:A:356:ILE:HB	2.20	0.41
1:B:268:LEU:HD13	1:B:299:LEU:CD2	2.50	0.41
2:D:1:MET:CE	2:D:25:PRO:HA	2.51	0.41
1:A:274:GLN:H	1:A:275:PRO:CD	2.30	0.40
1:A:255:ARG:HG2	1:B:324:MET:HG3	2.02	0.40
1:B:93:ASN:HA	1:B:94:PRO:HD3	1.93	0.40
1:B:274:GLN:N	1:B:275:PRO:CD	2.84	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	$\mathbf{ntiles}$
1	А	353/357~(99%)	336~(95%)	17~(5%)	0	100	100
1	В	344/357~(96%)	320~(93%)	24 (7%)	0	100	100
2	С	118/134~(88%)	114 (97%)	4 (3%)	0	100	100
2	D	118/134~(88%)	115~(98%)	3(2%)	0	100	100
All	All	933/982~(95%)	885~(95%)	48 (5%)	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	$\mathbf{ntiles}$
1	А	286/309~(93%)	284~(99%)	2(1%)	84	91
1	В	217/309~(70%)	214~(99%)	3~(1%)	67	80
2	С	88/117~(75%)	88 (100%)	0	100	100
2	D	98/117~(84%)	97~(99%)	1 (1%)	76	86
All	All	689/852~(81%)	683~(99%)	6 (1%)	78	88

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



Mol	Chain	Res	Type
1	А	32	GLN
1	А	315	ASN
1	В	136	THR
1	В	294	GLN
1	В	326	THR
2	D	116	ARG

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)

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)

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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	$Q{<}0.9$
1	А	355/357~(99%)	0.58	35 (9%) 7 5	47, 90, 152, 188	0
1	В	348/357~(97%)	1.02	65 (18%) 1 1	42, 101, 197, 235	0
2	С	120/134~(89%)	0.08	1 (0%) 86 85	56, 94, 141, 170	0
2	D	120/134~(89%)	0.27	3 (2%) 57 53	47, 73, 116, 143	0
All	All	943/982~(96%)	0.64	104 (11%) 5 3	42, 89, 175, 235	0

All (104) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	В	51	PRO	8.1
1	В	62	TYR	6.7
1	В	54	ASN	5.7
1	В	48	PHE	5.6
1	В	173	VAL	5.5
1	В	85	ALA	5.3
1	В	56	ALA	5.2
1	В	57	THR	5.1
1	А	111	SER	5.1
1	В	46	VAL	4.8
1	А	48	PHE	4.7
1	А	176	PHE	4.7
1	В	34	ILE	4.5
1	В	58	VAL	4.2
1	В	50	ARG	4.2
1	В	87	HIS	4.2
1	В	76	ALA	4.2
1	A	139	TRP	4.2
1	А	110	THR	4.2
1	В	89	PHE	4.1
1	В	70	ILE	4.1



6	Y	2F	)

Mol	Chain	Res	Type	RSRZ
1	В	12	VAL	4.1
1	А	112	VAL	4.0
1	В	55	LEU	4.0
1	В	60	ILE	4.0
1	В	81	GLY	3.9
1	А	274	GLN	3.8
2	С	70	TYR	3.7
1	В	138	VAL	3.7
1	В	144	THR	3.6
1	А	154	LEU	3.6
1	В	38	PRO	3.5
1	А	80	LEU	3.5
1	В	117	GLU	3.5
1	В	59	ASP	3.5
1	В	88	LEU	3.5
1	А	135	HIS	3.4
1	В	72	TYR	3.4
1	В	49	THR	3.3
1	А	137	VAL	3.3
1	А	31	ILE	3.3
1	В	113	LEU	3.3
1	В	171	TYR	3.3
1	В	8	ASN	3.3
1	А	113	LEU	3.2
1	В	112	VAL	3.2
1	В	42	ALA	3.1
1	В	174	PHE	3.1
1	В	145	SER	3.1
2	D	10	SER	3.0
1	A	138	VAL	3.0
1	В	132	ARG	2.9
1	В	190	VAL	2.9
1	A	285	PRO	2.9
1	A	114	PRO	2.9
1	A	3	ILE	2.8
1	В	68	THR	2.8
1	В	108	VAL	2.8
1	В	142	ILE	2.8
1	A	38	PRO	2.8
1	В	143	SER	2.8
1	В	78	ARG	2.8
1	А	46	VAL	2.8



6Y2P
------

Mol	Chain	Res	Type	RSRZ
1	В	36	PRO	2.8
1	А	175	THR	2.7
1	В	52	GLY	2.7
1	А	136	THR	2.6
1	В	61	PHE	2.6
1	В	139	TRP	2.5
1	А	72	TYR	2.5
1	В	168	LEU	2.5
1	В	35	GLY	2.4
1	В	120	ALA	2.4
1	В	119	SER	2.4
1	В	15	ASN	2.4
1	В	247	CYS	2.4
1	А	32	GLN	2.3
1	В	93	ASN	2.3
1	А	44	LEU	2.3
2	D	44	THR	2.3
2	D	41	GLY	2.3
1	В	44	LEU	2.3
1	А	133	ASN	2.2
1	В	79	SER	2.2
1	А	134	ALA	2.2
1	А	186	GLY	2.2
1	А	278	PHE	2.2
1	А	279	GLY	2.2
1	В	148	ASP	2.2
1	В	82	GLN	2.1
1	A	29	TYR	2.1
1	А	40	SER	2.1
1	В	14	ALA	2.1
1	А	173	VAL	2.1
1	А	56	ALA	2.1
1	В	53	VAL	2.0
1	В	328	VAL	2.0
1	В	13	ARG	2.0
1	А	52	GLY	2.0
1	В	69	THR	2.0
1	В	248	MET	2.0
1	В	110	THR	2.0
1	В	146	TYR	2.0
1	А	30	SER	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.

### 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.

