

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

### May 15, 2020 - 12:30 am BST

PDB ID	:	3PAW
Title	:	Low resolution X-ray crystal structure of Yeast Rnr1p with dATP bound in
		the A-site
Authors	:	Fairman, J.W.; Wijerathna, S.R.; Dealwis, C.G.
Deposited on	:	2010-10-19
Resolution	:	6.61  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
$\mathrm{EDS}$	:	2.11
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)	:	2.11

# 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 6.61 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
$R_{free}$	130704	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
RSRZ outliers	127900	1002 (9.00-3.80)

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 on 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			
			50%			
1	А	888	68%	14%	·	17%
			41%			
1	В	888	69%	14%		17%
			45%			
1	С	888	69%	13%	•	17%
			52%			
1	D	888	71%	12%	•	17%



# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14596 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		Ator	ns		ZeroOcc	AltConf	Trace	
1 1	720	Total	С	Ν	Ο	0	0	0		
	A	109	3649	2171	739	739	0	0	0	
1	р	720	Total	С	Ν	Ο	0	0	0	
	D	139	3649	2171	739	739	0	0	0	
1	C	720	Total	С	Ν	Ο	0	0	0	
		109	3649	2171	739	739	0	0		
1 D	р	720	Total	С	Ν	Ο	0	0	0	
	D	109	3649	2171	739	739	0			

• Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Ribonucleoside-diphosphate reductase large chain 1



#### K733

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• Molecule 1: Ribonucleoside-diphosphate reductase large chain 1





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• Molecule 1: Ribonucleoside-diphosphate reductase large chain 1



• Molecule 1: Ribonucleoside-diphosphate reductase large chain 1

52%

Chain D:

17%



M1	Y2	V3	K5	R6	5 8 <u>9</u>	R9	E11	P12	V13	ų 14	L29	D30	P31 K30	H33	I34	D35	A30 V37	K38	V39	T40	R42	I 43	144 C 15	646 646	V47	Y48	<b>G</b> 50	V51	T52 T53		L56	A60	A61	E62 T63	C64	A65	T68	T69	• 02V	H/1 P72	D73	T76	L77 A78
A79		A82	<b>1</b> 89	06L	K92			P112	A113	F114	S117	D118	D119	N127		V136	113/ D138	R139	D140	F141	V143	S144	Y145 F146	6147		L151 F152	R153	S154	Y155 1.156	L157	R158	ACTT	V163	A164 •	R166	P167	ц168 Н169		V174		G177 •	H179	G180 R181
D182	I183	E184	A186	V 0 1 0	L195	K196	197 F198	T199	H200	A201	P203	T204	1205	N207	A208	G209	P211	K212	P213	Q214 M215	S216	S217	C218	r219 1220	V221	A222	K224	E225	D226 9227	1228	E229	6230 1231	Y232	D233	1235 1235	K236	E237	A239	1240	1241 S242	K243	12 45	G246 G247
I248	G249	L250	I252	H253	1255	R256	525/ T258	<mark>6259</mark>	S260	1262	A263	G264	T265	<b>G267</b>	T268	S269	6271	L272	1273	P274		V278	F279 N780	N280 N281	T282	A283	Y285	V286	D287	<b>G</b> 289	G290	K292	R293	P294	A296	F297	A298 L299	Y300	L301	E302	W304	A306	D307 • I308 •
F309	D310	F311	D313	1314 B215	K316	1317	H318 G319		E322	1323 R324	A325	R326	D327	F329	P330	A331	L332 W333	I334	P335	D336 1 337	F338	M339	K340 P241	K341 V342	E343	E344 N345		T3 <mark>49</mark>	L350	S352	P353	1354 S355	A356	P357	L359	S360	D361	Y363	G364	D305 E366	F367	A369	L370 • Y371 •
T372	R373	Y374	2	R379	K381	T382	1383 K384	A385	0386 1386	K38/	W389	¥390	5391 T307	1393	E394		G400 T401	P402	F403	V404 V405	Y406	K407	D408	6410	N411	R412 • K413 •	S414	N415	Q416	G420	V421	1422 K423	S424	S425	L427	C428	C429 E430	1431	V432	E433 Y434	S435	D438	E439 T440
A441	V442	C443 NAAA	L445	A 446	V 448	A 449	L450 P451	A452	F 453 7 45 4	1454 E455	T456	S457	E458 D450		T462	S 463	1404 Y465	N466		H471	A474	K475	MAGO	N480 L481 ●	N482	R483	1485		Y489	P491	V492	E494	A 495	0708	N499	M500	H502	R503	P504	COCT	G508	<b>q</b> 510	G511 L512
A513	D514	T515	L518		F523	D524	L531	N532	1533	4534 1535		T538	4540	S543	M544	E545	S547	C548	E549	L550	1004	P556	Y557	T559	F560	0,561 0,562	S563	P564	A565	G568	1569	L5/0	F572	D573 • M574 •	1	P579	1581 (581	M582	W583	U584 W585	D586	H595	G596 V597
R598	N5 99	S600	T602	M603	P605	M606	T608	A609		5012 0613	1614		N618	Ce20	F621	E622	V624	T625	S626	N627 M628	Y629	S630	ARG	VAL	LEU	SER GI V	GLU	F638	0639 V640	V641	N642	L645	<b>L646</b> ●	R647	• 6 <del>7</del> 91	V650	D651	G653	I654	CC QM	M659	0000 0661	Y662 L663
	N667	G668	1670	Q671	L673	P674	V676	P677	0678	1.680	K681	D682	L683	K685	<b>T686</b>	V687	MD 88	• 069I	S691	0692 К603	T694	I695	1696 ME07	M698	A699		R702	S703	V704	1706	D7 07	5709	H7 10	S711	N7 13	L714	F/15		P7 19	T725	S726	H7 28	G731
-	K737	T738	M740	Y741	L743	R744	1745 1746	ALA	ALA	ALA	ALA	TLE	DHF 0 LLN	王 王	ILE	ASP	U.YS	IIE	ALA	ASP	ALA	THR	GLU	VAL	ALA	ASP	SEE	ASN	LEU LYS	ARG	DRO	TYR	MET	DRQ ORFR	SER	ALA	TYR	ALA	ALA	ASP	PHE	PRO	ALA ALA
VAL	THR	ALA	ALA	THR	PRO	SER	ASP	SER	S E E E E E	SER.	ALA	SER	GIII	ALA	SER	PRO	PRO	E	GLY	SER	SER	LEU	THR	GLY	MET	ALA	LEU LEU	ASN	CAL	GLU	SER	VAL	GLU	VAL	GLU	VAL	ALA	PRO	THR	ASN	GLU	LYS	ALA ALA
PRO	ILE	VAL	ASP	GLU	THR	GLU	ASP	ILE	TYR	ASIN	LYS	VAL	ILE AT A	CYS	ALA	ILE	ASN	PRO	GLU	ALA	GLU	MET	CYS	GLY																			



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants	$166.51 \text{\AA}$ $166.51 \text{\AA}$ $381.70 \text{\AA}$	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	192.45 - 6.61	Depositor
Resolution (A)	36.56 - 6.61	$\mathrm{EDS}$
% Data completeness	87.8 (192.45-6.61)	Depositor
(in resolution range)	$88.3 \ (36.56\text{-}6.61)$	$\mathrm{EDS}$
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.82 (at 6.63 \text{\AA})$	Xtriage
Refinement program	REFMAC $5.5.0109$	Depositor
D D	0.391 , $0.442$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.370 , $0.430$	DCC
$R_{free}$ test set	469 reflections $(4.76\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	225.0	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 170.6	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.38, < L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.437 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.64	EDS
Total number of atoms	14596	wwPDB-VP
Average B, all atoms $(Å^2)$	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.88% 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.



 $<sup>^1 {\</sup>rm Intensities}$  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					
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5				
1	А	0.52	0/3647	0.65	0/5075				
1	В	0.52	0/3647	0.65	0/5075				
1	С	0.53	0/3647	0.66	0/5075				
1	D	0.53	0/3647	0.63	0/5075				
All	All	0.52	0/14588	0.65	0/20300				

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	3649	0	1652	61	0
1	В	3649	0	1652	55	0
1	С	3649	0	1652	58	0
1	D	3649	0	1652	44	0
All	All	14596	0	6608	217	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 10.

All (217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



1:C:159:ILE:C

1:C:348:TRP:O

1:D:304:TRP:O

1:A:2:TYR:HA

1:C:161:GLY:H

1:C:382:THR:HA

1:D:350:LEU:HA

1:A:11:GLU:O

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:147:GLY:HA3	1:A:614:ILE:HA	1.42	0.99
1:D:147:GLY:HA2	1:D:614:ILE:HA	1.48	0.95
1:C:603:MET:CB	1:C:706:ILE:HA	1.99	0.92
1:A:147:GLY:CA	1:A:614:ILE:HA	2.02	0.90
1:D:147:GLY:CA	1:D:614:ILE:HA	2.07	0.85
1:B:364:GLY:H	1:B:408:ASP:CB	1.94	0.81
1:D:343:GLU:C	1:D:345:ASN:H	1.84	0.79
1:A:513:ALA:HB2	1:A:623:PRO:HA	1.65	0.78
1:D:515:THR:HA	1:D:518:LEU:CB	2.14	0.77
1:C:57:ASP:HA	1:C:60:ALA:HB3	1.69	0.75
1:B:298:ALA:HB3	1:B:427:LEU:HA	1.70	0.74
1:C:147:GLY:CA	1:C:614:ILE:HA	2.18	0.73
1:D:158:ARG:HA	1:D:163:VAL:HA	1.70	0.72
1:B:660:LYS:C	1:B:662:TYR:H	1.92	0.71
1:D:175:ALA:HB1	1:D:186:ALA:HB1	1.73	0.71
1:C:147:GLY:HA3	1:C:614:ILE:O	1.89	0.71
1:C:147:GLY:HA3	1:C:614:ILE:HA	1.74	0.70
1:C:304:TRP:HA	1:C:350:LEU:HA	1.76	0.68
1:D:232:TYR:HA	1:D:235:LEU:CB	2.23	0.68
1:B:298:ALA:CB	1:B:427:LEU:HA	2.24	0.67
1:C:242:SER:O	1:C:288:GLN:HA	1.94	0.67
1:B:191:ASN:O	1:B:195:LEU:N	2.28	0.67
1:A:242:SER:O	1:A:288:GLN:HA	1.95	0.66
1:C:219:PHE:O	1:C:426:ASN:HA	1.96	0.66
1:D:349:THR:HA	1:D:382:THR:HA	1.77	0.66
1:C:75:ALA:C	1:C:77:LEU:H	2.00	0.64
1:D:151:LEU:HA	1:D:155:TYR:CB	2.27	0.64
1:D:474:ALA:HB3	1:D:542:ALA:CB	2.27	0.64
1:A:607:PRO:HA	1:A:620:CYS:CB	2.28	0.64
1:B:287:ASP:HA	1:B:294:PRO:HA	1.81	0.63
1:C:191:ASN:O	1:C:195:LEU:N	2.26	0.62
1:C:363:TYR:O	1:C:366:GLU:N	2.31	0.62
1:D:1:MET:O	1:D:12:PRO:HA	2.00	0.62
1:B:628:MET:HA	1:B:640:VAL:O	2.00	0.61
1:A:27:TYR:C	1:A:29:LEU:H	2.03	0.61
1:B:67:MET:C	1:B:69:THR:H	2.04	0.61
1:C:563:SER:C	1:C:565:ALA:H	2.04	0.61
1:D:3:VAL:N	1:D:11:GLU:O	2.34	0.61

Continued on next page...

0.61

0.60

0.60

0.59



2.04

2.01

2.01

2.03

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:174:VAL:HA	1:C:208:ALA:HB3	1.85	0.59
1:C:16:ASP:O	1:C:20:ALA:HB2	2.02	0.59
1:C:248:ILE:O	1:C:298:ALA:N	2.35	0.59
1:D:474:ALA:HB3	1:D:542:ALA:HB3	1.83	0.59
1:A:217:SER:N	1:A:443:CYS:O	2.35	0.59
1:A:198:PHE:CB	1:A:448:VAL:HA	2.32	0.58
1:A:119:ASP:C	1:A:121:TYR:H	2.07	0.58
1:B:627:ASN:N	1:B:668:GLY:HA3	2.18	0.58
1:C:484:VAL:O	1:C:488:ASN:CB	2.52	0.57
1:A:280:ASN:HA	1:A:283:ALA:HB3	1.84	0.57
1:C:147:GLY:HA3	1:C:614:ILE:CA	2.35	0.57
1:B:471:HIS:HA	1:B:538:THR:O	2.04	0.56
1:B:723:LYS:C	1:B:725:THR:H	2.09	0.56
1:C:563:SER:C	1:C:565:ALA:N	2.59	0.56
1:D:343:GLU:C	1:D:345:ASN:N	2.57	0.56
1:A:273:ILE:C	1:A:275:MET:H	2.09	0.56
1:C:312:ILE:O	1:C:395:ALA:HB1	2.05	0.56
1:B:20:ALA:C	1:B:22:ILE:H	2.08	0.56
1:C:605:PRO:O	1:C:710:HIS:HA	2.06	0.56
1:D:240:LEU:HA	1:D:243:LYS:CB	2.35	0.56
1:D:104:TYR:O	1:D:112:PRO:HA	2.06	0.56
1:A:226:ASP:O	1:A:227:SER:CB	2.55	0.55
1:A:514:ASP:O	1:A:518:LEU:CB	2.55	0.55
1:B:407:LYS:C	1:B:409:ALA:H	2.11	0.54
1:D:563:SER:O	1:D:565:ALA:N	2.37	0.54
1:B:249:GLY:HA3	1:B:426:ASN:C	2.27	0.54
1:A:65:ALA:C	1:A:67:MET:H	2.09	0.54
1:C:104:TYR:O	1:C:112:PRO:HA	2.08	0.53
1:A:298:ALA:HA	1:A:329:PHE:O	2.08	0.53
1:B:251:HIS:CB	1:B:424:SER:CB	2.87	0.53
1:C:548:CYS:HA	1:C:597:VAL:HA	1.90	0.53
1:D:612:SER:CB	1:D:619:GLU:HA	2.38	0.53
1:A:147:GLY:HA2	1:A:614:ILE:HA	1.88	0.53
1:B:86:LEU:C	1:B:88:LYS:H	2.12	0.53
1:C:57:ASP:O	1:C:61:ALA:N	2.36	0.53
1:A:249:GLY:HA2	1:A:298:ALA:O	2.09	0.53
1:B:660:LYS:C	1:B:662:TYR:N	2.62	0.52
1:C:545:GLU:HA	1:C:548:CYS:CB	2.39	0.52
1:A:175:ALA:HB1	1:A:186:ALA:O	2.10	0.52
1:C:147:GLY:HA3	1:C:614:ILE:C	2.29	0.52
1:D:257:SER:C	1:D:271:GLY:HA2	2.29	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:343:GLU:O	1:D:345:ASN:N	2.42	0.52
1:A:523:PHE:H	1:A:683:LEU:HA	1.74	0.52
1:A:508:GLY:HA3	1:A:605:PRO:HA	1.91	0.52
1:D:514:ASP:O	1:D:518:LEU:N	2.43	0.52
1:D:334:ILE:O	1:D:406:TYR:HA	2.10	0.52
1:A:197:TYR:HA	1:A:452:ALA:CB	2.40	0.52
1:B:304:TRP:O	1:B:351:PHE:N	2.42	0.52
1:D:513:ALA:HB2	1:D:623:PRO:HA	1.92	0.52
1:A:224:LYS:O	1:A:225:GLU:CB	2.58	0.51
1:C:572:PHE:N	1:C:704:VAL:O	2.43	0.51
1:C:249:GLY:HA2	1:C:298:ALA:O	2.10	0.51
1:C:243:LYS:HA	1:C:289:GLY:H	1.76	0.51
1:C:61:ALA:HB1	1:C:82:ALA:HB2	1.93	0.51
1:D:226:ASP:O	1:D:227:SER:CB	2.59	0.51
1:D:234:THR:HA	1:D:237:GLU:CB	2.41	0.50
1:C:17:LYS:C	1:C:19:THR:H	2.14	0.50
1:A:196:LYS:O	1:A:449:ALA:HB3	2.12	0.50
1:D:147:GLY:HA3	1:D:614:ILE:HA	1.91	0.50
1:B:363:TYR:O	1:B:366:GLU:N	2.40	0.50
1:B:725:THR:C	1:B:727:MET:H	2.16	0.49
1:C:298:ALA:HB3	1:C:427:LEU:HA	1.95	0.49
1:A:299:LEU:O	1:A:331:ALA:N	2.41	0.49
1:A:27:TYR:O	1:A:29:LEU:N	2.40	0.49
1:B:75:ALA:C	1:B:77:LEU:H	2.15	0.49
1:C:75:ALA:C	1:C:77:LEU:N	2.64	0.49
1:A:16:ASP:O	1:A:20:ALA:HB2	2.12	0.49
1:A:312:ILE:O	1:A:395:ALA:HB1	2.12	0.49
1:A:538:THR:O	1:A:542:ALA:N	2.46	0.49
1:C:117:SER:HA	1:C:211:PRO:HA	1.95	0.48
1:D:474:ALA:HB3	1:D:542:ALA:HB1	1.95	0.48
1:C:77:LEU:HA	1:C:80:ARG:CB	2.44	0.48
1:C:281:ASN:CB	1:D:278:VAL:HA	2.43	0.48
1:D:301:LEU:O	1:D:332:LEU:HA	2.13	0.48
1:D:61:ALA:CB	1:D:82:ALA:HB2	2.42	0.48
1:A:375:GLU:C	1:A:377:GLU:H	2.16	0.47
1:B:505:ILE:N	1:B:601:LEU:O	2.41	0.47
1:B:20:ALA:C	1:B:22:ILE:N	2.66	0.47
1:C:173:ARG:O	1:C:208:ALA:O	2.31	0.47
1:D:661:GLN:C	1:D:663:LEU:H	2.18	0.47
1:D:53:THR:HA	1:D:56:LEU:CB	2.45	0.47
1:A:52:THR:O	1:A:56:LEU:N	2.48	0.47



		Interatomic	Clash
Atom-1	Atom-2 distance (Å)		overlap (Å)
1:C:234:THR:HA	1:C:237:GLU:CB	2.45	0.47
1:C:53:THR:HA	1:C:56:LEU:CB	2.44	0.47
1:C:265:THR:O	1:C:266:ASN:CB	2.62	0.47
1:C:592:ILE:C	1:C:594:LYS:N	2.67	0.47
1:A:300:TYR:HA	1:A:331:ALA:O	2.14	0.47
1:B:257:SER:CB	1:B:306:ALA:HB3	2.45	0.47
1:D:505:ILE:O	1:D:601:LEU:O	2.33	0.47
1:B:301:LEU:O	1:B:333:TRP:N	2.47	0.46
1:A:279:PHE:O	1:A:283:ALA:N	2.46	0.46
1:A:359:LEU:C	1:A:361:ASP:H	2.18	0.46
1:A:197:TYR:HA	1:A:452:ALA:HB1	1.97	0.46
1:B:39:VAL:O	1:B:42:ARG:N	2.49	0.46
1:C:522:PRO:O	1:C:528:ALA:HB1	2.15	0.46
1:A:349:THR:HA	1:A:382:THR:HA	1.98	0.46
1:A:64:CYS:CB	1:A:78:ALA:HB2	2.46	0.46
1:B:231:ILE:C	1:B:233:ASP:H	2.17	0.46
1:A:339:MET:C	1:A:341:ARG:H	2.19	0.46
1:B:287:ASP:HA	1:B:294:PRO:CA	2.45	0.46
1:A:474:ALA:HB3	1:A:542:ALA:HB1	1.98	0.45
1:B:213:PRO:O	1:B:489:TYR:N	2.49	0.45
1:D:373:ARG:C	1:D:375:GLU:H	2.19	0.45
1:D:471:HIS:HA	1:D:542:ALA:HB2	1.98	0.45
1:B:404:VAL:O	1:B:739:GLY:N	2.49	0.45
1:B:572:PHE:N	1:B:704:VAL:O	2.49	0.45
1:B:721:MET:C	1:B:723:LYS:H	2.18	0.45
1:B:445:LEU:O	1:B:446:ALA:HB2	2.17	0.45
1:B:65:ALA:C	1:B:67:MET:H	2.20	0.45
1:C:181:ARG:O	1:C:183:ILE:N	2.49	0.45
1:B:694:THR:C	1:B:696:ILE:H	2.20	0.45
1:A:60:ALA:C	1:A:62:GLU:H	2.20	0.45
1:A:65:ALA:O	1:A:67:MET:N	2.50	0.45
1:B:67:MET:C	1:B:69:THR:N	2.69	0.45
1:C:592:ILE:HA	1:C:596:GLY:H	1.82	0.45
1:A:104:TYR:O	1:A:113:ALA:N	2.34	0.44
1:C:174:VAL:HA	1:C:208:ALA:CB	2.47	0.44
1:A:513:ALA:HB3	1:A:618:ASN:CB	2.47	0.44
1:A:60:ALA:C	1:A:62:GLU:N	2.70	0.44
1:C:231:ILE:C	1:C:233:ASP:H	2.21	0.44
1:D:249:GLY:HA2	1:D:298:ALA:H	1.81	0.44
1:A:59:LEU:O	1:A:63:THR:N	2.50	0.44
1:B:212:LYS:O	1:B:214:GLN:N	2.50	0.44



	Clash			
Atom-1	Atom-2	distance $(Å)$	overlap(Å)	
1·A·425·SEB·HA	$1 \cdot A \cdot 431 \cdot ILE \cdot O$	2.17	0 44	
1:C:531:LEU:C	1:C:533:ILE:H	2.21	0.44	
1:D:457:SER:O	1:D:459:ASP:N	2.48	0.44	
1:B:335:PRO:C	1:B:337:LEU:H	2.20	0.44	
1:B:730:TYR:C	1:B:732:TRP:H	2.21	0.44	
1:A:486:ASP:O	1:A:488:ASN:N	2.51	0.44	
1:A:277:ARG:HA	1:A:280:ASN:CB	2.48	0.43	
1:D:538:THR:O	1:D:542:ALA:N	2.52	0.43	
1:A:287:ASP:O	1:A:290:GLY:N	2.52	0.43	
1:B:62:GLU:O	1:B:65:ALA:HB3	2.18	0.43	
1:C:159:ILE:C	1:C:161:GLY:N	2.72	0.43	
1:A:299:LEU:N	1:A:329:PHE:O	2.51	0.43	
1:A:506:ALA:CB	1:A:604:ALA:HB3	2.49	0.43	
1:B:392:ILE:C	1:B:394:GLU:H	2.22	0.43	
1:A:493:GLU:O	1:A:497:LYS:N	2.49	0.43	
1:B:531:LEU:C	1:B:533:ILE:H	2.22	0.43	
1:C:563:SER:O	1:C:565:ALA:N	2.52	0.43	
1:C:59:LEU:O	1:C:63:THR:N	2.51	0.43	
1:A:486:ASP:C	1:A:488:ASN:H	2.23	0.42	
1:C:703:SER:HA	1:C:706:ILE:CB	2.49	0.42	
1:A:22:ILE:O	1:A:26:CYS:N	2.53	0.42	
1:B:565:ALA:HA	1:B:569:ILE:O	2.19	0.42	
1:C:475:LYS:HA	1:C:546:ALA:HB2	2.01	0.42	
1:C:730:TYR:C	1:C:732:TRP:H	2.23	0.42	
1:C:79:ALA:HA	1:C:82:ALA:HB3	2.01	0.42	
1:D:406:TYR:CB	1:D:409:ALA:HB3	2.49	0.42	
1:A:65:ALA:C	1:A:67:MET:N	2.73	0.42	
1:C:483:ARG:HA	1:C:486:ASP:CB	2.49	0.42	
1:B:147:GLY:HA2	1:B:614:ILE:HA	2.01	0.42	
1:A:243:LYS:O	1:A:289:GLY:N	2.52	0.41	
1:B:283:ALA:HB1	1:B:295:GLY:O	2.19	0.41	
1:B:627:ASN:O	1:B:641:VAL:HA	2.20	0.41	
1:B:303:PRO:C	1:B:305:HIS:H	2.24	0.41	
1:C:642:ASN:CB	1:C:645:LEU:CB	2.98	0.41	
1:C:551:ALA:HB2	1:C:597:VAL:C	2.40	0.41	
1:D:231:ILE:O	1:D:235:LEU:N	2.54	0.41	
1:D:475:LYS:HA	1:D:546:ALA:HB2	2.02	0.41	
1:A:27:TYR:C	1:A:29:LEU:N	2.70	0.41	
1:A:287:ASP:O	1:A:289:GLY:N	2.53	0.41	
1:D:248:ILE:O	1:D:297:PHE:HA	2.20	0.41	
1:B:391:SER:HA	1:B:394:GLU:CB	2.50	0.41	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ALA:C	1:B:77:LEU:N	2.74	0.41
1:A:148:PHE:C	1:A:150:THR:N	2.75	0.41
1:A:76:THR:HA	1:A:79:ALA:HB3	2.02	0.40
1:A:5:LYS:C	1:A:7:ASP:H	2.24	0.40
1:B:280:ASN:C	1:B:282:THR:H	2.25	0.40
1:B:371:TYR:C	1:B:373:ARG:H	2.25	0.40
1:B:204:THR:O	1:B:208:ALA:HB2	2.21	0.40
1:B:405:VAL:HA	1:B:738:THR:HA	2.03	0.40
1:B:680:LEU:HA	1:B:683:LEU:CB	2.51	0.40
1:B:83:ILE:C	1:B:85:ASN:H	2.25	0.40
1:D:304:TRP:O	1:D:351:PHE:N	2.55	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	P	$\mathbf{erc}$	$\mathbf{entil}$	$\mathbf{es}$
1	А	735/888~(83%)	533~(72%)	157 (21%)	45~(6%)		1	17	
1	В	735/888~(83%)	518 (70%)	180 (24%)	37~(5%)		2	20	
1	С	735/888~(83%)	536~(73%)	154 (21%)	45~(6%)		1	17	
1	D	735/888~(83%)	542 (74%)	148 (20%)	45 (6%)		1	17	
All	All	2940/3552~(83%)	2129 (72%)	639 (22%)	172 (6%)		1	17	

All (172) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	225	GLU
1	А	227	SER
1	А	288	GLN
1	А	461	LYS



Mol	Chain	Res	Type
1	А	486	ASP
1	А	677	PRO
1	В	501	ARG
1	В	719	PRO
1	С	5	LYS
1	С	145	TYR
1	С	291	ASN
1	С	318	HIS
1	С	320	LYS
1	D	5	LYS
1	D	196	LYS
1	D	227	SER
1	D	291	ASN
1	D	667	ASN
1	D	677	PRO
1	А	120	VAL
1	А	290	GLY
1	А	487	ARG
1	А	558	GLU
1	А	613	GLN
1	А	623	PRO
1	А	674	PRO
1	В	159	ILE
1	В	364	GLY
1	В	452	ALA
1	С	108	ALA
1	С	159	ILE
1	С	182	ASP
1	С	288	GLN
1	С	319	GLY
1	С	364	GLY
1	С	491	PRO
1	C	706	ILE
1	D	159	ILE
1	D	206	PHE
1	D	288	GLN
1	D	318	HIS
1	D	319	GLY
1	D	343	GLU
1	D	344	GLU
1	D	522	PRO
1	D	719	PRO



Mol	Chain	Res	Type
1	А	6	ARG
1	А	8	GLY
1	А	66	TYR
1	А	201	ALA
1	А	259	GLY
1	А	353	PRO
1	А	501	ARG
1	А	679	GLU
1	А	708	GLN
1	А	741	TYR
1	В	50	GLY
1	В	87	HIS
1	В	109	THR
1	В	175	ALA
1	В	264	GLY
1	В	345	ASN
1	В	437	PRO
1	В	626	SER
1	В	740	MET
1	В	745	THR
1	С	4	TYR
1	С	12	PRO
1	С	160	ASN
1	С	266	ASN
1	С	273	ILE
1	С	322	GLU
1	С	426	ASN
1	С	522	PRO
1	С	532	ASN
1	C	581	GLY
1	С	606	MET
1	D	145	TYR
1	D	257	SER
1	D	266	ASN
1	D	345	ASN
1	D	462	THR
1	D	609	ALA
1	D	686	THR
1	А	153	ARG
1	А	159	ILE
1	А	304	TRP
1	А	318	HIS



Mol	Chain	Res	Type
1	А	492	VAL
1	А	608	THR
1	А	657	GLU
1	В	8	GLY
1	В	12	PRO
1	В	191	ASN
1	В	266	ASN
1	В	304	TRP
1	В	458	GLU
1	В	580	TYR
1	В	656	ASP
1	В	737	LYS
1	С	76	THR
1	С	155	TYR
1	С	211	PRO
1	С	345	ASN
1	С	558	GLU
1	С	564	PRO
1	С	567	GLN
1	С	719	PRO
1	С	745	THR
1	D	50	GLY
1	D	119	ASP
1	D	259	GLY
1	D	264	GLY
1	D	458	GLU
1	D	493	GLU
1	D	582	MET
1	D	586	ASP
1	D	662	TYR
1	D	741	TYR
1	A	110	GLY
1	A	160	ASN
1	A	345	ASN
1	A	460	GLY
1	A	571	GLN
1	В	93	GLN
1	В	210	THR
1	B	273	ILE
1	В	387	LYS
1	В	459	ASP
1	В	558	GLU



Mol	Chain	Res	Type
1	В	617	TYR
1	В	620	CYS
1	В	661	GLN
1	C	18	ILE
1	C	257	SER
1	С	264	GLY
1	С	351	PHE
1	С	538	THR
1	С	580	TYR
1	С	642	ASN
1	D	292	LYS
1	D	353	PRO
1	D	579	PRO
1	D	737	LYS
1	A	266	ASN
1	A	417	LYS
1	А	511	GLY
1	С	51	VAL
1	D	114	PRO
1	D	153	ARG
1	D	374	TYR
1	D	684	TYR
1	А	28	GLY
1	А	274	PRO
1	С	50	GLY
1	А	564	PRO
1	В	31	PRO
1	В	180	GLY
1	В	213	PRO
1	C	676	VAL
1	D	203	PRO
1	D	511	GLY
1	A	30	ASP
1	A	241	ILE
1	A	276	ILE
1	В	454	ILE
1	С	677	PRO
1	D	491	PRO
1	D	623	PRO
1	D	690	ILE
1	A	163	VAL
1	С	178	ILE

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#### 5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

#### 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 carbohydrates 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<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	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	739/888~(83%)	3.15	441 (59%) 0 0	39, 81, 170, 183	0
1	В	739/888~(83%)	2.69	368~(49%) 0 1	52, 74, 175, 188	0
1	С	739/888~(83%)	2.94	396~(53%) 0 1	51, 73, 173, 194	0
1	D	739/888~(83%)	3.36	464~(62%) 0 0	58, 80, 175, 186	0
All	All	2956/3552~(83%)	3.03	1669~(56%) 0 0	39, 78, 173, 194	0

All (1669) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	В	415	ASN	18.2
1	D	711	SER	18.2
1	С	433	GLU	18.1
1	D	218	CYS	17.0
1	В	414	SER	16.9
1	В	510	GLN	16.6
1	С	415	ASN	16.4
1	D	596	GLY	15.7
1	В	220	LEU	15.0
1	А	605	PRO	14.8
1	D	217	SER	14.7
1	А	14	GLN	14.5
1	D	686	THR	14.5
1	D	219	PHE	14.5
1	В	416	GLN	14.4
1	А	441	ALA	14.3
1	В	433	GLU	14.3
1	С	215	MET	14.2
1	С	216	SER	14.0
1	С	686	THR	13.7
1	D	443	CYS	13.7



3PA	W
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Mol	Chain	Res	Type	RSRZ
1	А	557	TYR	13.5
1	С	442	VAL	13.5
1	D	216	SER	13.3
1	С	624	VAL	13.3
1	D	605	PRO	13.2
1	А	251	HIS	13.1
1	D	738	THR	13.0
1	С	435	SER	12.8
1	D	442	VAL	12.7
1	С	504	PRO	12.7
1	А	558	GLU	12.6
1	С	441	ALA	12.4
1	С	443	CYS	12.4
1	С	508	GLY	12.4
1	В	442	VAL	12.3
1	D	256	ARG	12.2
1	С	414	SER	12.2
1	D	685	LYS	12.0
1	D	220	LEU	12.0
1	А	254	ASN	12.0
1	В	509	VAL	12.0
1	D	710	HIS	11.9
1	D	623	PRO	11.8
1	В	36	ALA	11.8
1	С	537	GLU	11.8
1	В	254	ASN	11.7
1	D	433	GLU	11.6
1	С	416	GLN	11.5
1	В	219	PHE	11.4
1	В	14	GLN	11.4
1	А	623	PRO	11.3
1	А	692	GLN	11.3
1	D	689	GLU	11.3
1	В	379	ARG	11.2
1	D	286	VAL	11.1
1	А	715	PHE	11.1
1	В	136	VAL	11.0
1	С	444	ASN	11.0
1	D	255	ILE	10.9
1	D	284	ARG	10.9
1	С	625	THR	10.9
1	С	257	SER	10.9



Mol	Chain	Res	Type	RSRZ
1	D	712	LEU	10.8
1	D	444	ASN	10.7
1	В	413	LYS	10.7
1	С	220	LEU	10.7
1	С	341	ARG	10.6
1	А	711	SER	10.6
1	А	221	VAL	10.5
1	С	599	ASN	10.5
1	С	417	LYS	10.4
1	А	15	PHE	10.4
1	А	442	VAL	10.4
1	В	620	CYS	10.4
1	С	385	ALA	10.3
1	D	687	VAL	10.3
1	A	559	THR	10.3
1	D	283	ALA	10.2
1	С	509	VAL	10.2
1	А	250	LEU	10.2
1	С	623	PRO	10.2
1	А	220	LEU	10.2
1	С	380	GLY	10.2
1	А	415	ASN	10.1
1	D	606	MET	10.1
1	В	218	CYS	10.1
1	С	214	GLN	10.1
1	D	441	ALA	10.1
1	С	440	THR	10.0
1	C	432	VAL	10.0
1	D	246	GLY	10.0
1	D	713	ASN	9.9
1	A	435	SER	9.9
1	А	681	LYS	9.9
1	D	709	SER	9.9
1	D	688	TRP	9.9
1	D	254	ASN	9.9
1	В	29	LEU	9.9
1	В	425	SER	9.9
1	А	325	ALA	9.9
1	В	443	CYS	9.9
1	В	713	ASN	9.8
1	В	432	VAL	9.8
1	D	690	ILE	9.8



Mol	Chain	Res	Type	RSRZ
1	В	256	ARG	9.8
1	D	739	GLY	9.8
1	С	506	ALA	9.7
1	С	434	TYR	9.7
1	В	417	LYS	9.7
1	D	90	THR	9.6
1	С	510	GLN	9.6
1	D	547	SER	9.6
1	А	710	HIS	9.6
1	D	215	MET	9.6
1	А	713	ASN	9.5
1	В	380	GLY	9.5
1	В	253	HIS	9.5
1	D	282	THR	9.5
1	В	715	PHE	9.4
1	С	687	VAL	9.4
1	D	694	THR	9.4
1	А	302	GLU	9.3
1	В	255	ILE	9.3
1	D	285	TYR	9.3
1	В	623	PRO	9.3
1	D	504	PRO	9.3
1	А	738	THR	9.3
1	С	505	ILE	9.3
1	В	302	GLU	9.2
1	D	165	GLU	9.2
1	D	221	VAL	9.2
1	С	256	ARG	9.1
1	D	295	GLY	9.1
1	С	16	ASP	9.1
1	С	494	GLU	9.1
1	В	15	PHE	9.1
1	В	622	GLU	9.1
1	D	352	SER	9.0
1	D	214	GLN	9.0
1	С	712	LEU	9.0
1	А	712	LEU	9.0
1	А	1	MET	9.0
1	D	253	HIS	8.9
1	С	602	THR	8.9
1	С	421	VAL	8.8
1	А	606	MET	8.8



Mol	Chain	Res	Type	RSRZ
1	В	424	SER	8.8
1	D	166	ARG	8.8
1	D	432	VAL	8.8
1	А	600	SER	8.7
1	В	441	ALA	8.7
1	D	196	LYS	8.7
1	А	326	ARG	8.6
1	В	310	ASP	8.6
1	С	254	ASN	8.6
1	А	255	ILE	8.6
1	А	599	ASN	8.6
1	С	253	HIS	8.6
1	А	353	PRO	8.6
1	С	422	ILE	8.5
1	С	580	TYR	8.5
1	С	412	ARG	8.5
1	С	532	ASN	8.5
1	В	709	SER	8.5
1	D	624	VAL	8.5
1	В	135	ILE	8.5
1	D	289	GLY	8.4
1	С	600	SER	8.4
1	В	418	ASN	8.4
1	D	91	THR	8.4
1	В	1	MET	8.4
1	С	306	ALA	8.4
1	А	416	GLN	8.3
1	D	198	PHE	8.3
1	А	622	GLU	8.3
1	A	249	GLY	8.3
1	D	430	GLU	8.3
1	А	434	TYR	8.3
1	В	16	ASP	8.3
1	A	3	VAL	8.2
1	D	421	VAL	8.2
1	В	708	GLN	8.2
1	С	384	LYS	8.2
1	D	625	THR	8.2
1	А	504	PRO	8.2
1	A	739	GLY	8.2
1	A	714	LEU	8.2
1	С	423	LYS	8.2



Mol	Chain	Res	Type	RSRZ
1	С	533	ILE	8.2
1	D	740	MET	8.2
1	D	226	ASP	8.1
1	D	741	TYR	8.1
1	А	93	GLN	8.1
1	D	202	SER	8.1
1	С	30	ASP	8.1
1	D	428	CYS	8.1
1	С	445	LEU	8.1
1	С	534	GLN	8.0
1	В	37	VAL	8.0
1	А	327	ASP	8.0
1	В	532	ASN	8.0
1	С	2	TYR	7.9
1	А	556	PRO	7.9
1	D	415	ASN	7.9
1	А	691	SER	7.9
1	А	543	SER	7.9
1	А	440	THR	7.9
1	А	260	SER	7.9
1	В	247	GLY	7.9
1	С	29	LEU	7.8
1	А	72	PRO	7.8
1	D	569	ILE	7.8
1	D	422	ILE	7.8
1	А	737	LYS	7.8
1	В	707	ASP	7.8
1	С	579	PRO	7.7
1	D	247	GLY	7.7
1	D	302	GLU	7.7
1	С	601	LEU	7.7
1	A	680	LEU	7.7
1	А	261	TYR	7.7
1	D	197	TYR	7.7
1	D	622	GLU	7.6
1	В	742	TYR	7.6
1	С	4	TYR	7.6
1	В	522	PRO	7.6
1	D	509	VAL	7.6
1	В	143	TYR	7.6
1	В	710	HIS	7.6
1	А	509	VAL	7.6



Mol	Chain	Res	Type	RSRZ
1	А	682	ASP	7.6
1	D	597	VAL	7.6
1	А	642	ASN	7.5
1	А	73	ASP	7.5
1	В	309	PHE	7.5
1	В	712	LEU	7.5
1	С	15	PHE	7.5
1	С	411	ASN	7.4
1	С	302	GLU	7.4
1	С	446	ALA	7.4
1	D	182	ASP	7.4
1	С	164	ALA	7.4
1	С	507	LEU	7.4
1	А	194	SER	7.4
1	С	536	PHE	7.4
1	D	503	ARG	7.3
1	С	270	ASN	7.3
1	D	451	PRO	7.3
1	В	618	ASN	7.3
1	С	538	THR	7.3
1	В	619	GLU	7.3
1	D	598	ARG	7.3
1	D	510	GLN	7.3
1	А	508	GLY	7.3
1	А	215	MET	7.3
1	А	13	VAL	7.3
1	В	435	SER	7.2
1	D	463	SER	7.2
1	А	424	SER	7.2
1	D	380	GLY	7.2
1	А	4	TYR	7.2
1	В	599	ASN	7.2
1	A	142	GLN	7.2
1	A	675	ASN	7.2
1	D	691	SER	7.2
1	А	253	HIS	7.1
1	В	252	ILE	7.1
1	А	647	ARG	7.1
1	D	414	SER	7.1
1	А	444	ASN	7.1
1	D	50	GLY	7.1
1	D	431	ILE	7.1



Mol	Chain	Res	Type	RSRZ
1	С	740	MET	7.1
1	D	353	PRO	7.1
1	D	303	PRO	7.1
1	A	16	ASP	7.0
1	В	508	GLY	7.0
1	С	11	GLU	7.0
1	А	265	THR	7.0
1	D	265	THR	7.0
1	А	716	LEU	7.0
1	D	681	LYS	7.0
1	А	443	CYS	7.0
1	D	548	CYS	7.0
1	В	600	SER	6.9
1	D	423	LYS	6.9
1	В	534	GLN	6.9
1	С	3	VAL	6.9
1	С	688	TRP	6.9
1	С	535	ILE	6.9
1	С	1	MET	6.9
1	D	227	SER	6.9
1	В	208	ALA	6.9
1	А	709	SER	6.9
1	D	648	ASP	6.8
1	В	50	GLY	6.8
1	В	447	SER	6.8
1	С	424	SER	6.8
1	С	715	PHE	6.8
1	С	413	LYS	6.8
1	D	167	PRO	6.7
1	D	599	ASN	6.7
1	D	354	THR	6.7
1	С	418	ASN	6.7
1	D	695	ILE	6.7
1	А	743	LEU	6.7
1	D	684	TYR	6.7
1	А	252	ILE	6.7
1	С	271	GLY	6.7
1	В	30	ASP	6.7
1	А	30	ASP	6.6
1	С	491	PRO	6.6
1	С	352	SER	6.6
1	D	49	GLU	6.6



Mol	Chain	Res	Type	RSRZ
1	D	327	ASP	6.6
1	А	604	ALA	6.6
1	D	491	PRO	6.6
1	D	682	ASP	6.6
1	А	668	GLY	6.6
1	В	431	ILE	6.6
1	D	715	PHE	6.6
1	А	207	ASN	6.6
1	В	378	GLY	6.6
1	А	92	LYS	6.5
1	D	296	ALA	6.5
1	D	524	ASP	6.5
1	С	578	LYS	6.5
1	В	51	VAL	6.5
1	D	705	TYR	6.4
1	С	691	SER	6.4
1	В	512	LEU	6.4
1	С	447	SER	6.4
1	D	693	LYS	6.4
1	С	540	TYR	6.4
1	С	140	ASP	6.4
1	С	564	PRO	6.4
1	А	643	PRO	6.4
1	А	607	PRO	6.4
1	С	303	PRO	6.4
1	В	426	ASN	6.3
1	D	413	LYS	6.3
1	В	511	GLY	6.3
1	А	12	PRO	6.3
1	D	212	LYS	6.3
1	А	601	LEU	6.3
1	В	249	GLY	6.3
1	D	564	PRO	6.3
1	В	714	LEU	6.3
1	С	713	ASN	6.3
1	D	140	ASP	6.3
1	A	580	TYR	6.2
1	А	728	HIS	6.2
1	С	218	CYS	6.2
1	D	626	SER	6.2
1	А	683	LEU	6.2
1	А	143	TYR	6.2



Mol	Chain	Res	Type	RSRZ
1	А	204	THR	6.2
1	В	466	ASN	6.2
1	D	288	GLN	6.2
1	А	303	PRO	6.2
1	D	708	GLN	6.2
1	D	692	GLN	6.2
1	А	466	ASN	6.2
1	А	208	ALA	6.2
1	А	222	ALA	6.2
1	D	429	CYS	6.2
1	D	600	SER	6.2
1	В	248	ILE	6.2
1	D	490	TYR	6.2
1	D	570	LEU	6.2
1	D	203	PRO	6.1
1	D	137	TYR	6.1
1	А	532	ASN	6.1
1	В	165	GLU	6.1
1	А	90	THR	6.1
1	D	266	ASN	6.1
1	С	252	ILE	6.1
1	С	340	LYS	6.1
1	D	508	GLY	6.1
1	А	127	ASN	6.1
1	С	581	GLY	6.1
1	А	315	ARG	6.1
1	А	717	ARG	6.1
1	С	14	GLN	6.1
1	А	425	SER	6.1
1	D	251	HIS	6.1
1	В	250	LEU	6.1
1	С	327	ASP	6.0
1	D	264	GLY	6.0
1	С	12	PRO	6.0
1	D	30	ASP	6.0
1	В	92	LYS	6.0
1	А	264	GLY	6.0
1	D	670	ILE	6.0
1	С	420	GLY	6.0
1	С	324	ARG	6.0
1	D	607	PRO	6.0
1	В	738	THR	6.0



Mol	Chain	Res	Type	RSRZ
1	С	668	GLY	6.0
1	В	535	ILE	6.0
1	В	175	ALA	6.0
1	D	139	ARG	5.9
1	В	624	VAL	5.9
1	С	539	ILE	5.9
1	В	311	PHE	5.9
1	D	34	ILE	5.9
1	А	579	PRO	5.9
1	В	603	MET	5.9
1	А	263	ALA	5.9
1	А	266	ASN	5.9
1	А	408	ASP	5.9
1	А	423	LYS	5.9
1	D	571	GLN	5.9
1	С	690	ILE	5.9
1	С	741	TYR	5.9
1	D	707	ASP	5.9
1	С	5	LYS	5.9
1	А	523	PHE	5.9
1	А	620	CYS	5.9
1	D	355	SER	5.9
1	А	140	ASP	5.8
1	С	608	THR	5.8
1	D	532	ASN	5.8
1	С	565	ALA	5.8
1	С	221	VAL	5.8
1	D	360	SER	5.8
1	А	684	TYR	5.8
1	В	246	GLY	5.8
1	D	213	PRO	5.8
1	A	296	ALA	5.8
1	A	300	TYR	5.8
1	A	730	TYR	5.8
1	В	207	ASN	5.8
1	В	579	PRO	5.8
1	А	286	VAL	5.8
1	D	649	LEU	5.8
1	A	727	MET	5.8
1	A	295	GLY	5.7
1	С	91	THR	5.7
1	С	137	TYR	5.7



Mol	Chain	Res	Type	RSRZ
1	D	389	TRP	5.7
1	С	410	CYS	5.7
1	С	307	ASP	5.7
1	D	179	HIS	5.7
1	D	164	ALA	5.7
1	С	165	GLU	5.7
1	В	611	THR	5.7
1	А	352	SER	5.7
1	С	274	PRO	5.7
1	С	251	HIS	5.7
1	В	669	SER	5.7
1	С	177	GLY	5.7
1	D	201	ALA	5.7
1	A	428	CYS	5.7
1	A	524	ASP	5.7
1	С	739	GLY	5.6
1	D	678	GLN	5.6
1	С	436	ALA	5.6
1	A	256	ARG	5.6
1	A	262	ILE	5.6
1	A	676	VAL	5.6
1	D	511	GLY	5.6
1	A	421	VAL	5.6
1	D	200	HIS	5.6
1	D	671	GLN	5.6
1	A	546	ALA	5.6
1	B	450	LEU	5.6
1	D	207	ASN	5.6
1	A	679	GLU	5.6
1	C	136	VAL	5.6
1	A	406	TYR	5.6
1	A	168	GLN	5.6
1	B	533	ILE	5.6
1	C	255	ILE	5.6
1	B	536	PHE	5.6
1	D	357	PRO	5.6
1	B	711	SER.	5.6
1	 C	212	LYS	5.6
1	Č	495	ALA	5.5
1	Č	493	GLU	5.5
1	D	601	LEU	5.5
1	B	381	LYS	5.5



Mol	Chain	Res	Type	RSRZ
1	С	503	ARG	5.5
1	А	2	TYR	5.5
1	D	737	LYS	5.5
1	С	339	MET	5.5
1	В	38	LYS	5.5
1	D	683	LEU	5.5
1	А	174	VAL	5.5
1	С	142	GLN	5.5
1	В	703	SER	5.5
1	С	449	ALA	5.5
1	А	173	ARG	5.5
1	А	85	ASN	5.5
1	А	534	GLN	5.4
1	А	641	VAL	5.4
1	D	204	THR	5.4
1	D	669	SER	5.4
1	С	338	PHE	5.4
1	С	336	ASP	5.4
1	А	703	SER	5.4
1	А	731	GLY	5.4
1	С	670	ILE	5.4
1	С	622	GLU	5.4
1	А	694	THR	5.4
1	А	533	ILE	5.4
1	А	674	PRO	5.4
1	С	716	LEU	5.4
1	С	305	HIS	5.4
1	В	140	ASP	5.4
1	D	679	GLU	5.4
1	В	251	HIS	5.4
1	A	448	VAL	5.4
1	В	295	GLY	5.4
1	D	745	THR	5.4
1	В	2	TYR	5.4
1	A	433	GLU	5.3
1	A	446	ALA	5.3
1	C	641	VAL	5.3
1	A	646	LEU	5.3
1	A	542	ALA	5.3
1	C	563	SER	5.3
1	D	484	VAL	5.3
1	D	595	HIS	5.3



Mol	Chain	Res	Type	RSRZ
1	С	492	VAL	5.3
1	D	136	VAL	5.3
1	В	35	ASP	5.3
1	С	33	HIS	5.3
1	В	621	PHE	5.3
1	А	744	ARG	5.3
1	В	265	THR	5.3
1	С	610	SER	5.3
1	В	200	HIS	5.3
1	В	385	ALA	5.3
1	С	258	THR	5.3
1	В	49	GLU	5.3
1	В	412	ARG	5.3
1	А	304	TRP	5.3
1	D	199	THR	5.2
1	C	402	PRO	5.2
1	А	400	GLY	5.2
1	С	439	GLU	5.2
1	С	345	ASN	5.2
1	А	598	ARG	5.2
1	А	420	GLY	5.2
1	В	449	ALA	5.2
1	D	604	ALA	5.2
1	В	199	THR	5.2
1	А	171	ILE	5.2
1	С	351	PHE	5.2
1	С	448	VAL	5.2
1	А	71	HIS	5.2
1	С	213	PRO	5.2
1	В	604	ALA	5.2
1	В	444	ASN	5.2
1	В	537	GLU	5.2
1	C	708	GLN	5.2
1	С	744	ARG	5.2
1	В	504	PRO	5.2
1	А	219	PHE	5.2
1	В	446	ALA	5.2
1	А	544	MET	5.1
1	А	439	GLU	5.1
1	D	714	LEU	5.1
1	С	738	THR	5.1
1	С	404	VAL	5.1



Mol	Chain	Res	Type	RSRZ
1	D	742	TYR	5.1
1	С	689	GLU	5.1
1	В	13	VAL	5.1
1	А	445	LEU	5.1
1	D	245	ALA	5.1
1	С	328	LEU	5.1
1	А	503	ARG	5.1
1	А	602	THR	5.1
1	В	538	THR	5.1
1	D	195	LEU	5.1
1	С	31	PRO	5.1
1	С	272	LEU	5.1
1	А	216	SER	5.1
1	С	692	GLN	5.1
1	А	354	THR	5.1
1	В	605	PRO	5.1
1	А	218	CYS	5.1
1	D	168	GLN	5.1
1	В	273	ILE	5.0
1	С	315	ARG	5.0
1	С	273	ILE	5.0
1	D	621	PHE	5.0
1	В	221	VAL	5.0
1	А	223	MET	5.0
1	С	199	THR	5.0
1	В	670	ILE	5.0
1	А	10	LYS	5.0
1	С	620	CYS	5.0
1	А	512	LEU	5.0
1	С	295	GLY	5.0
1	D	424	SER	5.0
1	D	356	ALA	5.0
1	D	672	GLY	5.0
1	A	513	ALA	5.0
1	С	296	ALA	5.0
1	C	450	LEU	5.0
1	A	11	GLU	5.0
1	A	364	GLY	5.0
1	D	502	HIS	4.9
1	С	28	GLY	4.9
1	С	217	SER	4.9
1	А	193	MET	4.9



Mol	Chain	Res	Type	RSRZ
1	В	222	ALA	4.9
1	А	285	TYR	4.9
1	D	425	SER	4.9
1	D	696	ILE	4.9
1	А	417	LYS	4.9
1	С	619	GLU	4.9
1	А	485	ILE	4.9
1	В	523	PHE	4.9
1	D	194	SER	4.9
1	А	407	LYS	4.9
1	В	28	GLY	4.9
1	А	648	ASP	4.9
1	В	434	TYR	4.9
1	D	410	CYS	4.9
1	А	505	ILE	4.9
1	А	745	THR	4.9
1	С	143	TYR	4.9
1	В	102	TYR	4.9
1	С	498	SER	4.9
1	А	736	LEU	4.9
1	А	214	GLN	4.9
1	А	742	TYR	4.9
1	С	222	ALA	4.9
1	D	568	GLY	4.9
1	А	693	LYS	4.9
1	А	172	MET	4.9
1	В	451	PRO	4.9
1	А	608	THR	4.8
1	С	626	SER	4.8
1	В	217	SER	4.8
1	А	741	TYR	4.8
1	А	645	LEU	4.8
1	В	384	LYS	4.8
1	D	627	ASN	4.8
1	В	524	ASP	4.8
1	А	202	SER	4.8
1	А	491	PRO	4.8
1	А	94	PHE	4.8
1	А	426	ASN	4.8
1	В	216	SER	4.8
1	С	138	ASP	4.8
1	В	347	THR	4.8



Mol	Chain	Res	Type	RSRZ
1	В	608	THR	4.8
1	А	203	PRO	4.8
1	С	36	ALA	4.8
1	В	289	GLY	4.8
1	С	353	PRO	4.8
1	В	156	LEU	4.8
1	D	447	SER	4.8
1	А	267	GLY	4.8
1	D	449	ALA	4.7
1	А	529	ARG	4.7
1	D	260	SER	4.7
1	D	446	ALA	4.7
1	D	244	THR	4.7
1	В	174	VAL	4.7
1	C	10	LYS	4.7
1	В	440	THR	4.7
1	В	578	LYS	4.7
1	D	351	PHE	4.7
1	D	364	GLY	4.7
1	D	482	ASN	4.7
1	А	82	ALA	4.7
1	В	91	THR	4.7
1	D	680	LEU	4.7
1	А	298	ALA	4.7
1	С	141	PHE	4.7
1	С	346	GLY	4.7
1	D	505	ILE	4.7
1	А	740	MET	4.7
1	А	597	VAL	4.7
1	В	580	TYR	4.7
1	D	620	CYS	4.6
1	C	168	GLN	4.6
1	C	319	GLY	4.6
1	D	533	ILE	4.6
1	В	266	ASN	4.6
1	A	670	ILE	4.6
1	В	274	PRO	4.6
1	A	562	GLY	4.6
1	B	602	THR	4.6
1	B	144	SER	4.6
1	В	570	LEU	4.6
1	A	248	ILE	4.6



Mol	Chain	Res	Type	RSRZ
1	А	5	LYS	4.6
1	А	621	PHE	4.6
1	А	247	GLY	4.6
1	D	181	ARG	4.6
1	D	464	THR	4.6
1	С	524	ASP	4.6
1	D	404	VAL	4.6
1	В	382	THR	4.6
1	D	186	ALA	4.6
1	А	522	PRO	4.6
1	С	330	PRO	4.6
1	С	360	SER	4.6
1	D	175	ALA	4.6
1	С	499	ASN	4.6
1	А	669	SER	4.6
1	С	313	ASP	4.6
1	В	423	LYS	4.6
1	С	598	ARG	4.6
1	А	169	HIS	4.5
1	А	644	TYR	4.5
1	А	432	VAL	4.5
1	С	265	THR	4.5
1	D	252	ILE	4.5
1	А	510	GLN	4.5
1	А	351	PHE	4.5
1	С	490	TYR	4.5
1	D	325	ALA	4.5
1	С	225	GLU	4.5
1	D	40	THR	4.5
1	В	202	SER	4.5
1	В	164	ALA	4.5
1	А	447	SER	4.5
1	А	430	GLU	4.5
1	В	706	ILE	4.5
1	С	604	ALA	4.5
1	А	685	LYS	4.5
1	D	744	ARG	4.5
1	В	436	ALA	4.5
1	D	391	SER	4.5
1	А	627	ASN	4.5
1	С	200	HIS	4.5
1	А	650	VAL	4.5



Mol	Chain	Res	Type	RSRZ
1	С	269	SER	4.5
1	D	249	GLY	4.5
1	А	422	ILE	4.4
1	А	455	GLU	4.4
1	С	124	VAL	4.4
1	А	688	TRP	4.4
1	А	746	GLN	4.4
1	D	556	PRO	4.4
1	D	257	SER	4.4
1	С	198	PHE	4.4
1	А	506	ALA	4.4
1	D	48	TYR	4.4
1	С	743	LEU	4.4
1	D	328	LEU	4.4
1	В	203	PRO	4.4
1	С	405	VAL	4.4
1	А	561	GLN	4.4
1	С	543	SER	4.4
1	А	349	THR	4.3
1	С	669	SER	4.3
1	D	580	TYR	4.3
1	В	741	TYR	4.3
1	С	163	VAL	4.3
1	А	87	HIS	4.3
1	А	122	ASN	4.3
1	D	142	GLN	4.3
1	В	166	ARG	4.3
1	В	109	THR	4.3
1	С	671	GLN	4.3
1	А	123	ILE	4.3
1	В	540	TYR	4.3
1	С	139	ARG	4.3
1	C	603	MET	4.3
1	D	138	ASP	4.3
1	D	448	VAL	4.3
1	А	301	LEU	4.3
1	D	143	TYR	4.3
1	В	610	SER	4.3
1	D	5	LYS	4.3
1	С	45	SER	4.3
1	D	426	ASN	4.3
1	А	363	TYR	4.3



JF AW	3PAW

Mol	Chain	Res	Type	RSRZ
1	В	204	THR	4.3
1	С	294	PRO	4.3
1	С	314	ILE	4.3
1	С	401	THR	4.3
1	С	13	VAL	4.3
1	С	308	ILE	4.2
1	D	3	VAL	4.2
1	А	365	ASP	4.2
1	С	304	TRP	4.2
1	D	445	LEU	4.2
1	А	535	ILE	4.2
1	А	560	PHE	4.2
1	D	69	THR	4.2
1	А	702	ARG	4.2
1	В	301	LEU	4.2
1	С	49	GLU	4.2
1	D	6	ARG	4.2
1	В	513	ALA	4.2
1	D	608	THR	4.2
1	В	429	CYS	4.2
1	D	301	LEU	4.2
1	А	86	LEU	4.2
1	В	245	ALA	4.2
1	D	209	GLY	4.1
1	А	306	ALA	4.1
1	В	155	TYR	4.1
1	А	418	ASN	4.1
1	С	35	ASP	4.1
1	А	268	THR	4.1
1	В	215	MET	4.1
1	А	578	LYS	4.1
1	А	502	HIS	4.1
1	D	185	ALA	4.1
1	D	703	SER	4.1
1	D	704	VAL	4.1
1	D	701	ASP	4.1
1	А	324	ARG	4.1
1	В	168	GLN	4.1
1	D	183	ILE	4.1
1	D	317	ASN	4.1
1	А	91	THR	4.1
1	А	720	THR	4.1



Mol	Chain	Res	Type	RSRZ
1	В	214	GLN	4.1
1	D	208	ALA	4.1
1	D	248	ILE	4.1
1	А	217	SER	4.1
1	D	452	ALA	4.1
1	С	502	HIS	4.1
1	D	746	GLN	4.1
1	С	337	LEU	4.1
1	D	310	ASP	4.1
1	D	402	PRO	4.1
1	D	545	GLU	4.1
1	В	342	VAL	4.0
1	D	416	GLN	4.0
1	А	581	GLY	4.0
1	D	2	TYR	4.0
1	С	71	HIS	4.0
1	А	401	THR	4.0
1	А	651	ASP	4.0
1	D	650	VAL	4.0
1	С	438	ASP	4.0
1	D	263	ALA	4.0
1	D	308	ILE	4.0
1	В	335	PRO	4.0
1	А	233	ASP	4.0
1	А	128	LYS	4.0
1	D	450	LEU	4.0
1	D	311	PHE	4.0
1	В	375	GLU	4.0
1	А	537	GLU	4.0
1	C	642	ASN	4.0
1	D	39	VAL	4.0
1	A	371	TYR	3.9
1	A	619	GLU	3.9
1	С	607	PRO	3.9
1	C	609	ALA	3.9
1	D	250	LEU	3.9
1	D	677	PRO	3.9
1	В	137	TYR	3.9
1	В	341	ARG	3.9
1	D	628	MET	3.9
1	В	409	ALA	3.9
1	D	269	SER	3.9



Mol	Chain	Res	Type	RSRZ
1	А	126	GLU	3.9
1	С	157	LEU	3.9
1	А	454	ILE	3.9
1	В	271	GLY	3.9
1	В	383	ILE	3.9
1	С	127	ASN	3.9
1	D	697	ASN	3.9
1	D	584	ASP	3.9
1	В	360	SER	3.9
1	А	29	LEU	3.9
1	А	399	THR	3.9
1	D	4	TYR	3.9
1	D	178	ILE	3.9
1	А	200	HIS	3.9
1	А	507	LEU	3.9
1	В	300	TYR	3.9
1	А	355	SER	3.9
1	В	272	LEU	3.9
1	С	379	ARG	3.9
1	В	420	GLY	3.9
1	D	743	LEU	3.9
1	А	732	TRP	3.9
1	В	242	SER	3.9
1	D	180	GLY	3.9
1	А	198	PHE	3.9
1	В	348	TRP	3.9
1	В	303	PRO	3.9
1	В	430	GLU	3.9
1	D	573	ASP	3.9
1	D	716	LEU	3.9
1	D	565	ALA	3.8
1	A	474	ALA	3.8
1	B	260	SER	3.8
1	D	558	GLU	3.8
1	D	702	ARG	3.8
1	A	284	ARG	3.8
1	C	627	ASN	3.8
1	А	429	CYS	3.8
1	D	361	ASP	3.8
1	А	536	PHE	3.8
1	D	562	GLY	3.8
1	А	209	GLY	3.8



Mol	Chain	Res	Type	RSRZ
1	С	178	ILE	3.8
1	А	201	ALA	3.8
1	С	167	PRO	3.8
1	D	177	GLY	3.8
1	D	392	ILE	3.8
1	D	485	ILE	3.8
1	А	729	PHE	3.8
1	С	621	PHE	3.8
1	С	325	ALA	3.8
1	В	737	LYS	3.8
1	А	705	TYR	3.8
1	В	406	TYR	3.8
1	В	296	ALA	3.8
1	С	226	ASP	3.8
1	А	18	ILE	3.7
1	А	317	ASN	3.8
1	С	92	LYS	3.8
1	С	400	GLY	3.8
1	D	559	THR	3.7
1	А	427	LEU	3.7
1	В	209	GLY	3.7
1	А	95	SER	3.7
1	С	201	ALA	3.7
1	В	308	ILE	3.7
1	D	1	MET	3.7
1	С	714	LEU	3.7
1	D	290	GLY	3.7
1	А	386	GLN	3.7
1	С	312	ILE	3.7
1	В	705	TYR	3.7
1	В	176	LEU	3.7
1	В	257	SER	3.7
1	В	690	ILE	3.7
1	D	390	TYR	3.7
1	В	463	SER	3.7
1	С	335	PRO	3.7
1	D	499	ASN	3.7
1	А	124	VAL	3.7
1	В	134	ALA	3.7
1	A	83	ILE	3.7
1	С	717	ARG	3.7
1	В	12	PRO	3.7



Mol	Chain	Res	Type	RSRZ
1	D	297	PHE	3.7
1	С	568	GLY	3.7
1	А	316	LYS	3.7
1	С	17	LYS	3.7
1	С	745	THR	3.7
1	D	642	ASN	3.6
1	С	275	MET	3.6
1	D	225	GLU	3.6
1	D	544	MET	3.6
1	А	31	PRO	3.6
1	С	451	PRO	3.6
1	А	17	LYS	3.6
1	В	601	LEU	3.6
1	D	388	LEU	3.6
1	В	333	TRP	3.6
1	D	242	SER	3.6
1	С	223	MET	3.6
1	С	323	ILE	3.6
1	А	195	LEU	3.6
1	D	641	VAL	3.6
1	В	288	GLN	3.6
1	D	267	GLY	3.6
1	С	702	ARG	3.6
1	А	409	ALA	3.6
1	D	65	ALA	3.6
1	А	305	HIS	3.6
1	А	175	ALA	3.6
1	В	349	THR	3.6
1	С	567	GLN	3.6
1	В	667	ASN	3.6
1	В	307	ASP	3.6
1	С	19	THR	3.6
1	С	474	ALA	3.6
1	С	562	GLY	3.6
1	С	73	ASP	3.6
1	A	478	THR	3.6
1	В	336	ASP	3.6
1	D	41	GLN	3.6
1	В	606	MET	3.6
1	А	708	GLN	3.6
1	А	368	GLU	3.6
1	А	531	LEU	3.6



Mol	Chain	Res	Type	RSRZ
1	В	411	ASN	3.6
1	С	301	LEU	3.6
1	D	411	ASN	3.6
1	В	353	PRO	3.6
1	С	569	ILE	3.6
1	С	342	VAL	3.6
1	С	737	LYS	3.6
1	D	318	HIS	3.6
1	А	690	ILE	3.6
1	С	473	ILE	3.6
1	С	694	THR	3.6
1	В	377	GLU	3.5
1	D	10	LYS	3.5
1	A	75	ALA	3.5
1	А	205	LEU	3.5
1	В	573	ASP	3.5
1	С	32	LYS	3.5
1	D	563	SER	3.5
1	А	384	LYS	3.5
1	D	261	TYR	3.5
1	А	545	GLU	3.5
1	В	226	ASP	3.5
1	С	123	ILE	3.5
1	С	38	LYS	3.5
1	D	481	LEU	3.5
1	D	546	ALA	3.5
1	А	547	SER	3.5
1	D	512	LEU	3.5
1	D	602	THR	3.5
1	В	334	ILE	3.5
1	D	206	PHE	3.5
1	C	69	THR	3.5
1	C	582	MET	3.5
1	D	281	ASN	3.5
1	В	701	ASP	3.5
1	В	505	ILE	3.5
1	С	18	ILE	3.5
1	A	527	GLU	3.5
1	C	742	TYR	3.5
1	A	166	ARG	3.5
1	A	19	THR	3.5
1	D	557	TYR	3.5



Mol	Chain	Res	Type	RSRZ
1	D	11	GLU	3.5
1	А	380	GLY	3.5
1	С	102	TYR	3.5
1	В	286	VAL	3.5
1	А	385	ALA	3.5
1	D	706	ILE	3.5
1	А	387	LYS	3.5
1	D	262	ILE	3.5
1	А	170	LEU	3.5
1	В	3	VAL	3.4
1	D	61	ALA	3.4
1	D	312	ILE	3.4
1	В	716	LEU	3.4
1	А	199	THR	3.4
1	А	141	PHE	3.4
1	C	585	TRP	3.4
1	D	205	LEU	3.4
1	С	117	SER	3.4
1	В	437	PRO	3.4
1	В	244	THR	3.4
1	С	640	VAL	3.4
1	С	87	HIS	3.4
1	D	89	GLN	3.4
1	D	305	HIS	3.4
1	D	434	TYR	3.4
1	С	544	MET	3.4
1	В	507	LEU	3.4
1	В	559	THR	3.4
1	А	484	VAL	3.4
1	D	394	GLU	3.4
1	A	323	ILE	3.4
1	В	717	ARG	3.4
1	D	210	THR	3.4
1	В	167	PRO	3.4
1	С	118	ASP	3.4
1	А	350	LEU	3.4
1	В	529	ARG	3.4
1	D	243	LYS	3.4
1	А	528	ALA	3.4
1	В	609	ALA	3.4
1	С	70	VAL	3.4
1	D	223	MET	3.4



Mol	Chain	Res	Type	RSRZ
1	А	167	PRO	3.4
1	А	139	ARG	3.4
1	С	194	SER	3.3
1	С	329	PHE	3.3
1	А	677	PRO	3.3
1	D	639	GLN	3.3
1	С	570	LEU	3.3
1	D	313	ASP	3.3
1	В	324	ARG	3.3
1	С	103	ARG	3.3
1	В	491	PRO	3.3
1	С	531	LEU	3.3
1	D	222	ALA	3.3
1	А	28	GLY	3.3
1	D	660	LYS	3.3
1	D	427	LEU	3.3
1	В	490	TYR	3.3
1	В	448	VAL	3.3
1	С	109	THR	3.3
1	А	486	ASP	3.3
1	В	376	LYS	3.3
1	D	342	VAL	3.3
1	В	676	VAL	3.3
1	А	191	ASN	3.3
1	С	387	LYS	3.3
1	D	385	ALA	3.3
1	А	76	THR	3.3
1	В	577	GLN	3.3
1	D	211	PRO	3.3
1	D	498	SER	3.3
1	B	40	THR	3.2
1	C	72	PRO	3.2
1	D	699	ALA	3.2
1	А	603	MET	3.2
1	D	47	VAL	3.2
1	C	354	THR	3.2
1	A	307	ASP	3.2
1	D	127	ASN	3.2
1	В	691	SER	3.2
1	С	707	ASP	3.2
1	D	31	PRO	3.2
1	D	36	ALA	3.2



Mol	Chain	Res	Type	RSRZ
1	D	169	HIS	3.2
1	D	307	ASP	3.2
1	С	86	LEU	3.2
1	С	250	LEU	3.2
1	А	465	TYR	3.2
1	В	145	TYR	3.2
1	D	45	SER	3.2
1	А	397	THR	3.2
1	D	275	MET	3.2
1	D	309	PHE	3.2
1	С	122	ASN	3.2
1	А	338	PHE	3.2
1	D	362	CYS	3.2
1	В	205	LEU	3.2
1	С	700	ALA	3.2
1	А	624	VAL	3.2
1	В	744	ARG	3.2
1	А	328	LEU	3.2
1	В	70	VAL	3.2
1	В	201	ALA	3.2
1	В	641	VAL	3.2
1	С	332	LEU	3.2
1	D	92	LYS	3.2
1	D	728	HIS	3.2
1	D	79	ALA	3.2
1	А	234	THR	3.2
1	В	337	LEU	3.2
1	С	431	ILE	3.2
1	D	268	THR	3.2
1	D	298	ALA	3.2
1	A	177	GLY	3.2
1	A	189	THR	3.2
1	A	410	CYS	3.2
1	В	270	ASN	3.2
1	С	40	THR	3.2
1	D	71	HIS	3.2
1	А	192	LEU	3.1
1	D	78	ALA	3.1
1	В	584	ASP	3.1
1	А	396	GLN	3.1
1	А	102	TYR	3.1
1	D	9	ARG	3.1



Mol	Chain	Res	Type	RSRZ
1	В	445	LEU	3.1
1	А	726	SER	3.1
1	В	671	GLN	3.1
1	С	701	ASP	3.1
1	D	274	PRO	3.1
1	В	642	ASN	3.1
1	С	425	SER	3.1
1	D	534	GLN	3.1
1	С	497	LYS	3.1
1	D	358	GLY	3.1
1	С	34	ILE	3.1
1	D	523	PHE	3.1
1	С	685	LYS	3.1
1	D	141	PHE	3.1
1	С	496	ARG	3.1
1	D	673	LEU	3.1
1	В	478	THR	3.1
1	В	561	GLN	3.1
1	D	408	ASP	3.1
1	D	70	VAL	3.1
1	С	196	LYS	3.1
1	А	259	GLY	3.1
1	В	746	GLN	3.1
1	В	206	PHE	3.1
1	D	228	ILE	3.1
1	D	272	LEU	3.1
1	С	452	ALA	3.1
1	D	420	GLY	3.1
1	D	561	GLN	3.1
1	D	609	ALA	3.1
1	А	570	LEU	3.1
1	В	389	TRP	3.1
1	В	739	GLY	3.1
1	D	379	ARG	3.1
1	C	403	PHE	3.1
1	A	362	CYS	3.0
1	A	405	VAL	3.0
1	D	280	ASN	3.0
1	D	700	ALA	3.0
1	С	437	PRO	3.0
1	A	431	ILE	3.0
1	С	409	ALA	3.0



Mol	Chain	Res	Type	RSRZ
1	С	37	VAL	3.0
1	С	202	SER	3.0
1	В	198	PHE	3.0
1	D	338	PHE	3.0
1	С	559	THR	3.0
1	D	14	GLN	3.0
1	В	243	LYS	3.0
1	D	535	ILE	3.0
1	D	466	ASN	3.0
1	В	139	ARG	3.0
1	А	336	ASP	3.0
1	D	323	ILE	3.0
1	С	309	PHE	3.0
1	D	363	TYR	3.0
1	D	374	TYR	3.0
1	D	630	SER	3.0
1	D	653	GLY	3.0
1	С	158	ARG	3.0
1	С	326	ARG	3.0
1	А	335	PRO	3.0
1	В	668	GLY	3.0
1	D	271	GLY	3.0
1	D	401	THR	3.0
1	D	647	ARG	3.0
1	А	475	LYS	3.0
1	D	273	ILE	3.0
1	А	9	ARG	3.0
1	С	97	VAL	3.0
1	В	558	GLU	3.0
1	C	176	LEU	3.0
1	В	506	ALA	3.0
1	А	36	ALA	3.0
1	С	331	ALA	3.0
1	А	436	ALA	2.9
1	А	476	VAL	2.9
1	В	745	THR	2.9
1	D	440	THR	2.9
1	В	689	GLU	2.9
1	C	84	SER	2.9
1	А	180	GLY	2.9
1	С	597	VAL	2.9
1	D	579	PRO	2.9



Mol	Chain	Res	Type	RSRZ
1	С	126	GLU	2.9
1	В	539	ILE	2.9
1	С	711	SER	2.9
1	В	419	LEU	2.9
1	С	347	THR	2.9
1	А	297	PHE	2.9
1	В	4	TYR	2.9
1	А	181	ARG	2.9
1	В	612	SER	2.9
1	D	365	ASP	2.9
1	D	659	MET	2.9
1	D	229	GLU	2.9
1	D	369	ALA	2.9
1	D	403	PHE	2.9
1	В	26	CYS	2.9
1	D	176	LEU	2.9
1	А	227	SER	2.9
1	А	132	ASN	2.9
1	А	723	LYS	2.9
1	С	44	ILE	2.9
1	D	373	ARG	2.9
1	D	698	MET	2.9
1	D	335	PRO	2.9
1	D	386	GLN	2.9
1	D	324	ARG	2.9
1	С	156	LEU	2.9
1	D	438	ASP	2.9
1	А	135	ILE	2.9
1	D	370	LEU	2.9
1	В	240	LEU	2.9
1	С	114	PRO	2.9
1	В	39	VAL	2.8
1	В	574	MET	2.8
1	D	73	ASP	2.8
1	C	85	ASN	2.8
1	В	327	ASP	2.8
1	С	583	TRP	2.8
1	C	709	SER	2.8
1	A	671	GLN	2.8
1	А	179	HIS	2.8
1	D	381	LYS	2.8
1	С	355	SER	2.8



Mol	Chain	Res	Type	RSRZ
1	С	561	GLN	2.8
1	В	346	GLY	2.8
1	С	42	ARG	2.8
1	D	483	ARG	2.8
1	А	228	ILE	2.8
1	В	261	TYR	2.8
1	D	495	ALA	2.8
1	В	688	TRP	2.8
1	В	740	MET	2.8
1	С	311	PHE	2.8
1	С	584	ASP	2.8
1	С	383	ILE	2.8
1	D	117	SER	2.8
1	С	169	HIS	2.8
1	C	605	PRO	2.8
1	В	108	ALA	2.8
1	В	462	THR	2.8
1	D	157	LEU	2.8
1	А	372	THR	2.8
1	С	166	ARG	2.8
1	D	501	ARG	2.8
1	В	48	TYR	2.8
1	В	173	ARG	2.8
1	D	51	VAL	2.8
1	D	304	TRP	2.8
1	D	400	GLY	2.8
1	D	727	MET	2.8
1	D	63	THR	2.8
1	A	367	PHE	2.8
1	В	531	LEU	2.8
1	В	317	ASN	2.7
1	C	41	GLN	2.7
1	C	76	THR	2.7
1	D	543	SER	2.7
1	С	361	ASP	2.7
1	В	101	LEU	2.7
1	D	585	TRP	2.7
1	A	97	VAL	2.7
1	В	323	ILE	2.7
1	В	267	GLY	2.7
1	В	607	PRO	2.7
1	D	629	TYR	2.7



Mol	Chain	Res	Type	RSRZ
1	В	339	MET	2.7
1	С	320	LYS	2.7
1	D	7	ASP	2.7
1	А	176	LEU	2.7
1	С	119	ASP	2.7
1	С	399	THR	2.7
1	D	513	ALA	2.7
1	В	338	PHE	2.7
1	D	581	GLY	2.7
1	С	386	GLN	2.7
1	В	147	GLY	2.7
1	С	283	ALA	2.7
1	D	174	VAL	2.7
1	D	270	ASN	2.7
1	D	480	ASN	2.7
1	D	651	ASP	2.7
1	А	538	THR	2.7
1	А	721	MET	2.7
1	А	701	ASP	2.7
1	А	453	PHE	2.7
1	А	196	LYS	2.7
1	В	405	VAL	2.7
1	В	306	ALA	2.7
1	А	314	ILE	2.7
1	С	358	GLY	2.6
1	А	398	GLU	2.6
1	D	462	THR	2.6
1	А	27	TYR	2.6
1	А	411	ASN	2.6
1	В	528	ALA	2.6
1	D	238	CYS	2.6
1	A	369	ALA	2.6
1	D	531	LEU	2.6
1	D	435	SER	2.6
1	А	734	LYS	2.6
1	В	312	ILE	2.6
1	В	388	LEU	2.6
1	A	596	GLY	2.6
1	A	257	SER	2.6
1	C	237	GLU	2.6
1	A	206	PHE	2.6
1	A	130	LYS	2.6



JF AW	3PAW

Mol	Chain	Res	Type	RSRZ
1	В	142	GLN	2.6
1	С	408	ASP	2.6
1	А	610	SER	2.6
1	С	244	THR	2.6
1	С	419	LEU	2.6
1	С	211	PRO	2.6
1	В	182	ASP	2.6
1	А	23	SER	2.6
1	С	696	ILE	2.6
1	D	241	ILE	2.6
1	D	368	GLU	2.6
1	D	42	ARG	2.6
1	В	410	CYS	2.6
1	А	84	SER	2.6
1	А	686	THR	2.6
1	С	181	ARG	2.6
1	В	525	SER	2.6
1	А	40	THR	2.6
1	А	129	ASP	2.6
1	А	481	LEU	2.6
1	D	489	TYR	2.6
1	А	70	VAL	2.5
1	С	471	HIS	2.5
1	В	294	PRO	2.5
1	В	702	ARG	2.5
1	В	736	LEU	2.5
1	С	639	GLN	2.5
1	А	501	ARG	2.5
1	А	565	ALA	2.5
1	С	121	TYR	2.5
1	С	310	ASP	2.5
1	В	357	PRO	2.5
1	А	232	TYR	2.5
1	С	672	GLY	2.5
1	С	356	ALA	2.5
1	С	512	LEU	2.5
1	D	572	PHE	2.5
1	А	310	ASP	2.5
1	D	640	VAL	2.5
1	В	157	LEU	2.5
1	A	649	LEU	2.5
1	D	393	LEU	2.5



Mol	Chain	Res	Type	RSRZ
1	В	27	TYR	2.5
1	А	735	GLY	2.5
1	D	287	ASP	2.5
1	А	719	PRO	2.5
1	А	235	LEU	2.5
1	С	470	LEU	2.5
1	В	482	ASN	2.5
1	С	282	THR	2.5
1	D	322	GLU	2.5
1	С	264	GLY	2.5
1	А	695	ILE	2.5
1	С	26	CYS	2.5
1	D	359	LEU	2.5
1	В	498	SER	2.5
1	С	630	SER	2.5
1	С	316	LYS	2.5
1	С	566	SER	2.5
1	А	41	GLN	2.5
1	В	185	ALA	2.5
1	В	352	SER	2.5
1	В	503	ARG	2.5
1	В	332	LEU	2.5
1	А	273	ILE	2.5
1	В	282	THR	2.5
1	D	76	THR	2.5
1	В	41	GLN	2.5
1	D	62	GLU	2.5
1	С	6	ARG	2.5
1	С	381	LYS	2.4
1	D	314	ILE	2.4
1	В	238	CYS	2.4
1	В	316	LYS	2.4
1	D	412	ARG	2.4
1	D	646	LEU	2.4
1	А	178	ILE	2.4
1	В	422	ILE	2.4
1	В	569	ILE	2.4
1	D	550	LEU	2.4
1	С	53	THR	2.4
1	С	300	TYR	2.4
1	В	421	VAL	2.4
1	D	454	ILE	2.4



JF AW	3PAW

Mol	Chain	Res	Type	RSRZ
1	D	618	ASN	2.4
1	С	238	CYS	2.4
1	D	38	LYS	2.4
1	D	336	ASP	2.4
1	А	269	SER	2.4
1	А	609	ALA	2.4
1	В	427	LEU	2.4
1	В	687	VAL	2.4
1	С	240	LEU	2.4
1	А	618	ASN	2.4
1	В	177	GLY	2.4
1	D	668	GLY	2.4
1	А	121	TYR	2.4
1	В	625	THR	2.4
1	D	560	PHE	2.4
1	D	455	GLU	2.4
1	А	118	ASP	2.4
1	А	119	ASP	2.4
1	С	113	ALA	2.4
1	D	551	ALA	2.4
1	С	68	THR	2.4
1	А	569	ILE	2.4
1	А	402	PRO	2.4
1	В	223	MET	2.4
1	А	449	ALA	2.4
1	А	246	GLY	2.4
1	В	480	ASN	2.4
1	В	571	GLN	2.4
1	D	300	TYR	2.4
1	С	375	GLU	2.4
1	С	39	VAL	2.4
1	D	46	GLY	2.4
1	D	339	MET	2.4
1	В	743	LEU	2.4
1	В	52	THR	2.4
1	С	203	PRO	2.4
1	D	12	PRO	2.4
1	D	330	PRO	2.4
1	В	547	SER	2.4
1	В	694	THR	2.4
1	В	704	VAL	2.4
1	A	103	ARG	2.3



Mol	Chain	Res	Type	RSRZ
1	В	407	LYS	2.3
1	D	343	GLU	2.3
1	D	294	PRO	2.3
1	А	563	SER	2.3
1	В	275	MET	2.3
1	С	266	ASN	2.3
1	D	68	THR	2.3
1	А	165	GLU	2.3
1	А	539	ILE	2.3
1	С	695	ILE	2.3
1	В	374	TYR	2.3
1	D	337	LEU	2.3
1	С	357	PRO	2.3
1	А	65	ALA	2.3
1	А	450	LEU	2.3
1	С	698	MET	2.3
1	В	163	VAL	2.3
1	С	286	VAL	2.3
1	А	366	GLU	2.3
1	D	549	GLU	2.3
1	С	542	ALA	2.3
1	D	306	ALA	2.3
1	А	294	PRO	2.3
1	С	112	PRO	2.3
1	А	89	GLN	2.3
1	С	43	ILE	2.3
1	С	511	GLY	2.3
1	D	259	GLY	2.3
1	В	439	GLU	2.3
1	D	619	GLU	2.3
1	В	467	PHE	2.3
1	А	131	LEU	2.3
1	А	540	TYR	2.3
1	А	190	TYR	2.3
1	А	271	GLY	2.3
1	А	299	LEU	2.3
1	В	331	ALA	2.3
1	А	155	TYR	2.3
1	D	725	THR	2.3
1	А	238	CYS	2.3
1	С	359	LEU	2.3
1	В	283	ALA	2.3



Mol	Chain	Res	Type	RSRZ
1	С	611	THR	2.3
1	D	367	PHE	2.3
1	С	560	PHE	2.3
1	D	37	VAL	2.3
1	D	522	PRO	2.3
1	В	269	SER	2.2
1	В	93	GLN	2.2
1	С	263	ALA	2.2
1	D	603	MET	2.2
1	С	179	HIS	2.2
1	А	244	THR	2.2
1	А	463	SER	2.2
1	В	227	SER	2.2
1	D	82	ALA	2.2
1	В	672	GLY	2.2
1	D	33	HIS	2.2
1	В	549	GLU	2.2
1	С	174	VAL	2.2
1	С	135	ILE	2.2
1	В	169	HIS	2.2
1	А	464	THR	2.2
1	В	72	PRO	2.2
1	С	197	TYR	2.2
1	D	654	ILE	2.2
1	D	184	GLU	2.2
1	В	562	GLY	2.2
1	А	270	ASN	2.2
1	D	652	LEU	2.2
1	А	482	ASN	2.2
1	А	404	VAL	2.2
1	D	29	LEU	2.2
1	В	178	ILE	2.2
1	В	700	ALA	2.2
1	С	90	THR	2.2
1	D	731	GLY	2.2
1	А	224	LYS	2.2
1	В	325	ALA	2.2
1	С	204	THR	2.2
1	В	544	MET	2.2
1	В	184	GLU	2.2
1	В	229	GLU	2.2
1	D	64	CYS	2.2



Mol	Chain	Res	Type	RSRZ
1	А	330	PRO	2.2
1	А	689	GLU	2.2
1	В	696	ILE	2.2
1	С	47	VAL	2.2
1	D	60	ALA	2.2
1	А	274	PRO	2.2
1	В	438	ASP	2.2
1	С	51	VAL	2.2
1	В	148	PHE	2.2
1	В	546	ALA	2.2
1	В	322	GLU	2.2
1	В	479	ARG	2.2
1	А	347	THR	2.2
1	А	551	ALA	2.2
1	В	644	TYR	2.2
1	D	371	TYR	2.2
1	D	350	LEU	2.2
1	В	34	ILE	2.2
1	D	341	ARG	2.1
1	А	628	MET	2.1
1	В	53	THR	2.1
1	В	685	LYS	2.1
1	А	678	GLN	2.1
1	D	43	ILE	2.1
1	D	675	ASN	2.1
1	В	68	THR	2.1
1	С	276	ILE	2.1
1	С	48	TYR	2.1
1	В	356	ALA	2.1
1	A	26	CYS	2.1
1	A	361	ASP	2.1
1	В	543	SER	2.1
1	D	372	THR	2.1
1	D	645	LEU	2.1
1	A	414	SER	2.1
1	B	$51\overline{4}$	ASP	2.1
1	C	120	VAL	2.1
1	С	699	ALA	2.1
1	A	287	ASP	2.1
1	В	453	PHE	2.1
1	C	541	HIS	2.1
1	D	726	SER	2.1



Mol	Chain	Res	Type	RSRZ
1	С	489	TYR	2.1
1	А	311	PHE	2.1
1	С	260	SER	2.1
1	А	236	LYS	2.1
1	А	283	ALA	2.1
1	С	697	ASN	2.1
1	D	465	TYR	2.1
1	В	692	GLN	2.1
1	D	574	MET	2.1
1	А	239	ALA	2.1
1	С	239	ALA	2.1
1	В	428	CYS	2.1
1	А	39	VAL	2.1
1	А	388	LEU	2.1
1	А	724	LEU	2.1
1	С	175	ALA	2.1
1	D	334	ILE	2.1
1	D	77	LEU	2.1
1	В	241	ILE	2.1
1	D	329	PHE	2.1
1	D	8	GLY	2.1
1	D	492	VAL	2.1
1	А	718	ALA	2.1
1	С	344	GLU	2.1
1	А	289	GLY	2.1
1	D	332	LEU	2.1
1	D	655	TRP	2.1
1	А	197	TYR	2.1
1	В	290	GLY	2.1
1	A	210	THR	2.0
1	В	340	LYS	2.0
1	А	88	LYS	2.0
1	A	611	THR	2.0
1	А	44	ILE	2.0
1	A	242	SER	2.0
1	В	695	ILE	2.0
1	А	53	THR	2.0
1	В	69	THR	2.0
1	D	315	ARG	2.0
1	С	284	ARG	2.0
1	С	727	MET	2.0
1	А	356	ALA	2.0



		-	1 0	
Mol	Chain	Res	Type	RSRZ
1	С	667	ASN	2.0
1	D	35	ASP	2.0
1	В	258	THR	2.0
1	D	384	LYS	2.0
1	D	163	VAL	2.0
1	А	389	TRP	2.0
1	В	408	ASP	2.0
1	С	83	ILE	2.0
1	В	124	VAL	2.0
1	В	486	ASP	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 carbohydrates 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.

