Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:44 AM EDT

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

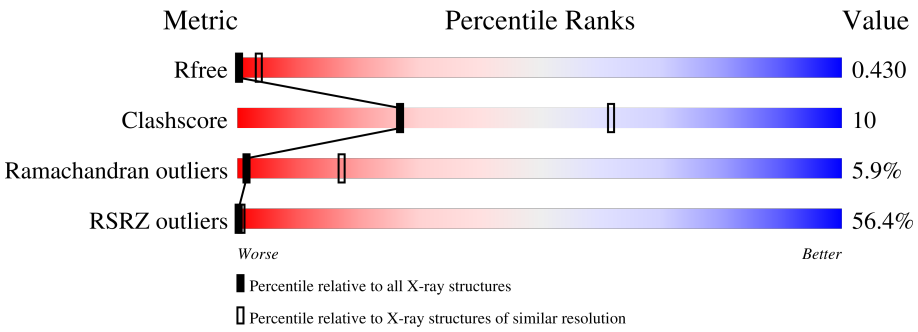
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 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	A	888	50%; 68%; 14%; • ; 17%
1	B	888	41%; 69%; 14%; 17%
1	C	888	45%; 69%; 13%; • ; 17%
1	D	888	52%; 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.

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

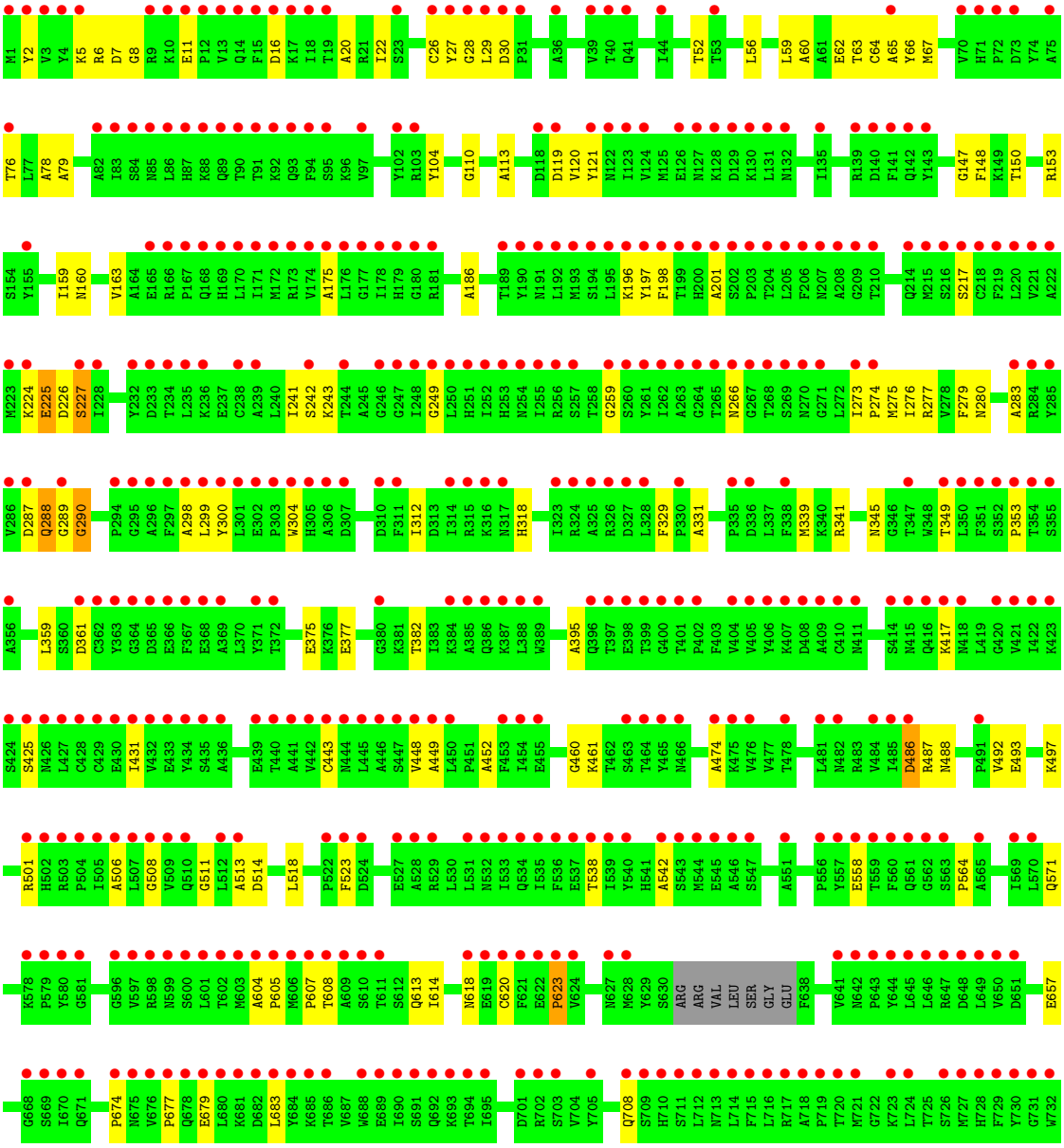
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	739	3649	2171	739	739	0	0	0
1	B	739	3649	2171	739	739	0	0	0
1	C	739	3649	2171	739	739	0	0	0
1	D	739	3649	2171	739	739	0	0	0

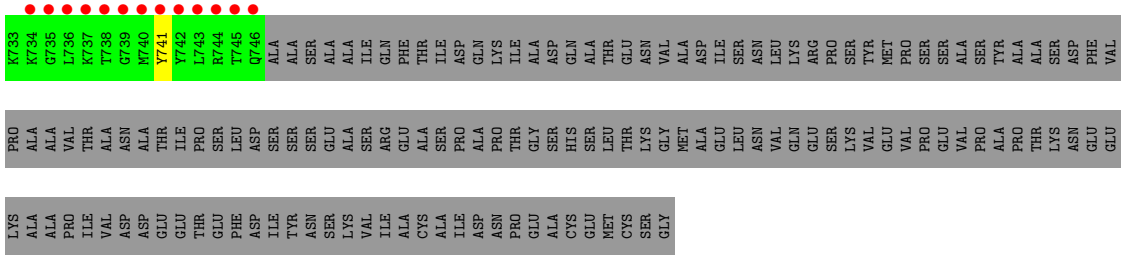
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ribonucleoside-diphosphate reductase large chain 1

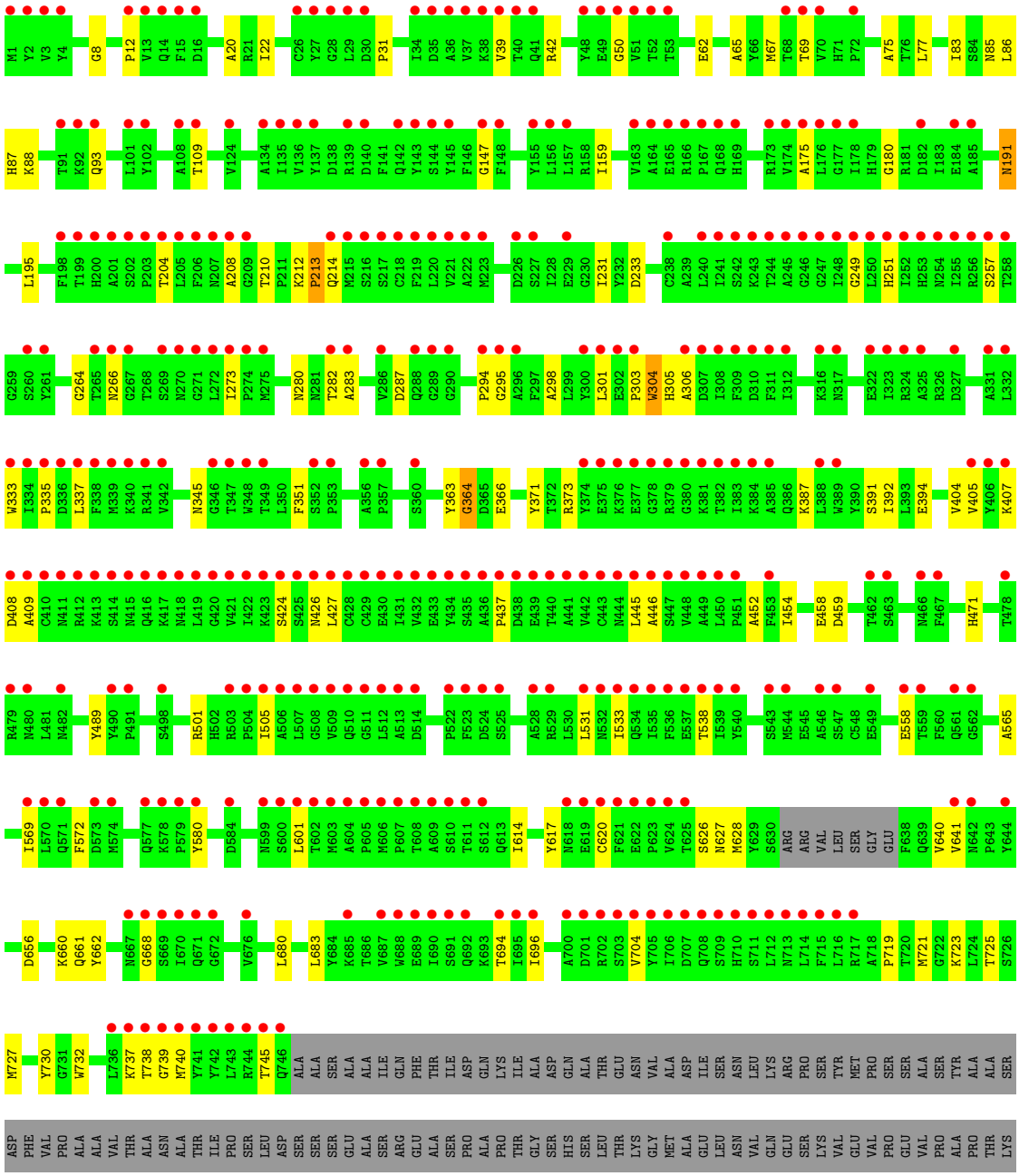
Chain A:

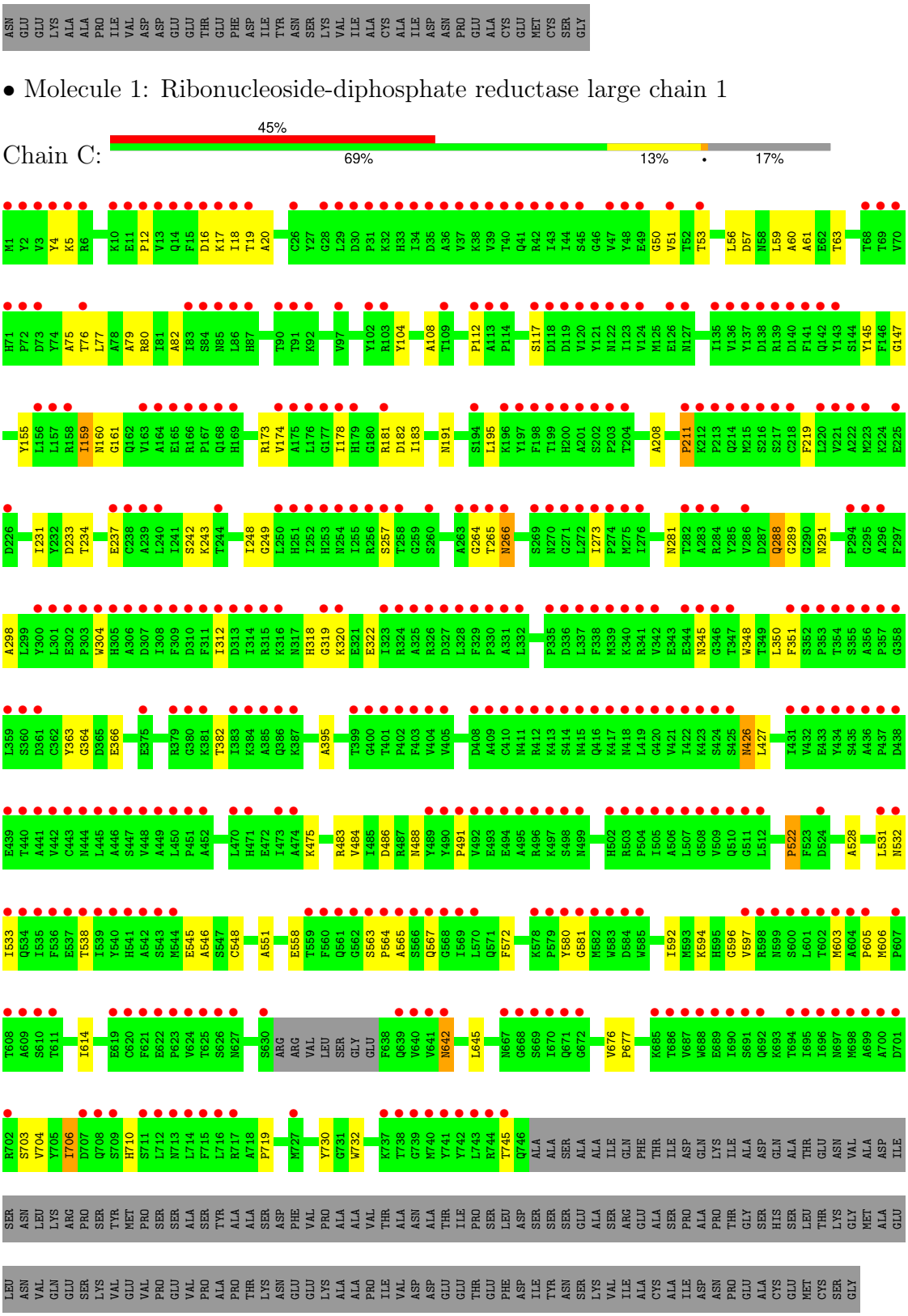


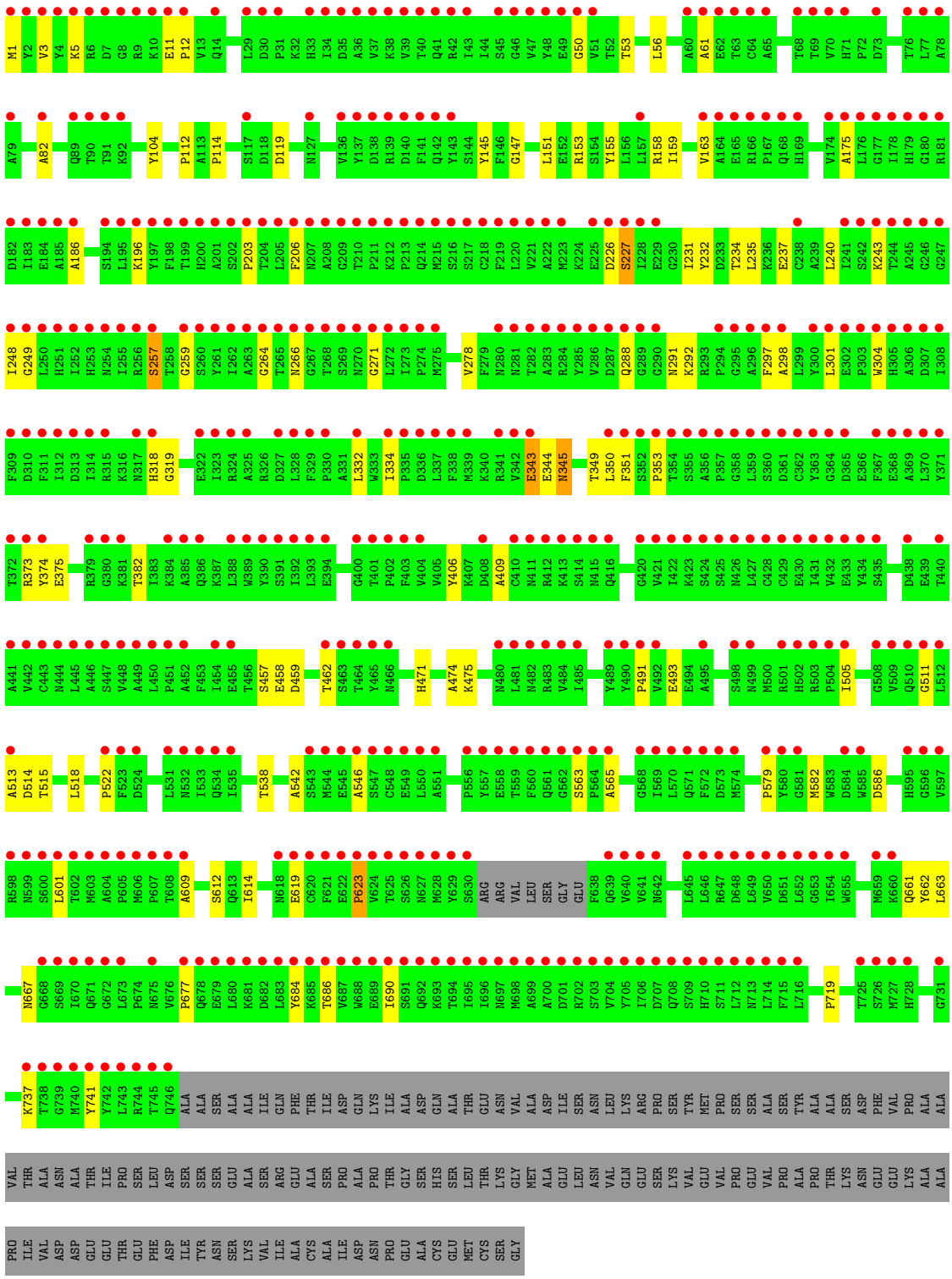


- Molecule 1: Ribonucleoside-diphosphate reductase large chain 1

Chain B:




ASN GLU GLU LYS ALA ALA PRO ILE VAL ASP ASP GLU GLU THR GLU PHE ASP ILE TYR ASN SER LYS VAL ILE ALA CYS ALA ILE ASP ASN PRO GLU ALA CYS GLU MET CYS SER GLY
• Molecule 1: Ribonucleoside-diphosphate reductase large chain 1
Chain C:
45%
69%
13%
17%
M1 Y2 V3 Y4 K5 R6 K10 E11 P12 V13 Q14 F15 D16 K17 I18 T19 A20 C26 Y27 G28 L29 D30 P31 K32 H33 I34 D35 A36 V37 K38 V39 T40 Q41 R42 I43 I44 S45 G46 V47 Y48 E49 G50 V51 T52 T53 L56 D57 N58 L59 A60 A61 E62 T63 T68 T69 V70
H71 P72 D73 Y74 A75 T76 L77 A78 A79 R80 I81 A82 I83 S84 N85 L86 H87 T90 T91 K92 V97 Y102 R103 Y104 A108 T109 P112 A113 P114 S117 D118 D119 V120 Y121 N122 I123 V124 M125 E126 N127 I135 V136 Y137 D138 R139 D140 F141 Q142 Y143 S144 Y145 F146 G147
Y155 L156 L157 R158 I159 N160 G161 Q162 V163 A164 E165 R166 P167 Q168 H169 R173 V174 A175 L176 G177 I178 H179 G180 R181 D182 I183 N191 S194 L195 K196 Y197 F198 T199 H200 A201 S202 P203 T204 A208 P211 K212 P213 Q214 M215 S216 S217 C218 F219 L220 V221 A222 M223 K224 E225
D226 I231 Y232 D233 T234 E237 C238 A239 L240 I241 S242 K243 T244 I248 G249 L250 H251 I252 H253 N254 I255 R256 S257 T258 G259 S260 A263 G264 T265 N266 S269 N270 G271 L272 I273 P274 M275 I276 N281 T282 A283 R284 Y285 V286 D287 Q288 G289 G290 N291 P294 G295 A296 F297
A298 L299 Y300 L301 E302 P303 W304 H305 A306 D307 I308 F309 D310 F311 I312 D313 I314 R315 K316 N317 H318 G319 K320 E321 E322 I323 R324 A325 R326 D327 L328 F329 P330 A331 L332 P335 D336 L337 F338 M339 K340 R341 V342 E343 E344 N345 G346 T347 W348 T349 L350 F351 S352 P353 T354 S355 A356 P357 G358
L359 S360 D361 C362 Y363 G364 D365 E366 E375 R379 G380 K381 T382 I383 K384 A385 Q386 K387 A395 T399 G400 T401 P402 F403 V404 V405 D408 A409 C410 N411 R412 K413 S414 N415 Q416 K417 N418 L419 G420 V421 I422 K423 S424 S425 N426 L427 I431 V432 E433 Y434 S435 A436 P437 D438
E439 T440 A441 V442 C443 N444 L445 A446 S447 V448 A449 L450 P451 A452 L470 H471 E472 I473 A474 K475 R483 V484 I485 D486 R487 N488 Y489 Y490 P491 V492 E493 E494 A495 R496 K497 S498 N499 H502 R503 P504 I505 A506 L507 G508 V509 Q510 G511 L512 P522 P523 D524 A528 L531 N532
I533 Q534 I535 F536 E537 T538 I539 Y540 H541 A542 S543 M544 E545 A546 S547 C548 A551 E558 T559 F560 Q561 G562 S563 P564 A565 S566 Q567 G568 I569 L570 Q571 F572 K578 F579 Y580 G581 M582 W583 D584 W585 I592 M593 K594 H595 G596 V597 R598 N599 S600 L601 T602 M603 A604 P605 M606 P607
T608 A609 S610 T611 I614 E619 G620 F621 E622 P623 V624 T625 S626 N627 S630 ARG ARG VAL LEU SER GLY GLU F638 Q639 V640 V641 N642 L645 M667 G668 S669 I670 Q671 G672 V676 P677 K685 T686 V687 W688 E689 I690 S691 Q692 K693 T694 I695 I696 N697 M698 A699 A700 D701
R702 S703 V704 Y705 I706 D707 Q708 S709 H710 S711 L712 N713 L714 F715 L716 R717 A718 P719 M727 Y730 G731 W732 K737 T738 G739 M740 Y741 Y742 L743 R744 T745 Q746 ALA ALA SER SER ALA ALA ILE GLN PHE THR ILE ASP GLN LYS ILE ALA ASP GLN ALA THR GLU ASN VAL ALA ASP ILE
SER ASN LEU LYS ARG PRO SER TYR MET PRO SER SER ALA SER TYR ALA ALA SER ASP PHE VAL PRO ALA ALA VAL THR ALA ASN ALA THR ILE PRO SER LEU ASP SER SER SER GLU ALA ALA SER ARG GLU ALA SER PRO ALA PRO THR GLY SER HIS SER LEU THR LYS GLY MET ALA GLU
LEU ASN VAL GLN GLU SER LYS VAL GLU VAL PRO GLU VAL PRO ALA PRO THR LYS ASN GLU GLU LYS ALA ALA PRO ILE VAL ASP ASP GLU GLU THR GLU PHE ASP ILE TYR ASN SER LYS VAL ILE ALA CYS ALA ILE ASP ASN PRO GLU ALA CYS GLU MET CYS SER GLY
• Molecule 1: Ribonucleoside-diphosphate reductase large chain 1
Chain D:
52%
71%
12%
17%


M1 Y2 V3 Y4 K5 R6 D7 G8 R9 K10 E11 P12 V13 Q14 L29 D30 P31 K32 H33 I34 D35 A36 V37 K38 V39 T40 Q41 R42 I43 I44 S45 G46 V47 Y48 E49 G50 V51 T52 T53 L56 A60 A61 E62 T63 C64 A65 T68 T69 V70 H71 P72 D73 T76 L77 A78
A79 A82 Q89 T90 T91 K92 Y104 P112 A113 P114 S117 D118 D119 N127 V136 Y137 D138 R139 D140 F141 Q142 Q143 S144 Y145 F146 G147 L151 E152 R153 S154 Y155 L156 L157 R158 I159 V163 A164 E165 R166 P167 Q168 H169 V174 A175 L176 G177 I178 H179 G180 R181
D182 I183 E184 A185 A186 S194 L195 K196 Y197 F198 T199 H200 A201 S202 P203 T204 L205 F206 N207 A208 G209 T210 P211 K212 P213 Q214 M215 S216 S217 C218 F219 L220 V221 A222 M223 K224 E225 D226 S227 I228 E229 G230 I231 Y232 D233 T234 L235 K236 E237 C238 A239 L240 I241 S242 K243 T244 A245 G246 G247
I248 G249 L250 H251 I252 H253 N254 I255 R256 S257 T258 G259 S260 Y261 I262 A263 G264 T265 N266 G267 T268 S269 N270 T210 G271 L272 I273 P274 M275 V278 F279 N280 N281 T282 A283 R284 Y285 V286 D287 Q288 G289 G290 N291 K292 R293 P294 G295 A296 F297 A298 L299 Y300 L301 E302 P303 W304 H305 A306 D307 I308
F309 D310 F311 I312 D313 I314 R315 K316 N317 H318 G319 E322 I323 R324 A325 R326 D327 L328 F329 P330 A331 L332 W333 I334 P335 D336 L337 F338 M339 K340 R341 V342 E343 E344 N345 T349 L350 F351 S352 P353 T354 S355 A356 P357 G358 L359 S360 D361 C362 Y363 G364 D365 E366 F367 E368 A369 L370 Y371
T372 R373 Y374 E375 R379 G380 K381 T382 I383 K384 A385 Q386 K387 I388 W389 Y390 S391 I392 L393 E394 G400 T401 P402 F403 V404 V405 Y406 K407 D408 A409 C410 N411 R412 K413 S414 N415 Q416 G420 V421 I422 K423 S424 S425 N426 L427 C428 C429 E430 I431 V432 E433 Y434 S435 D438 E439 T440
A441 V442 C443 N444 L445 A446 S447 V448 A449 L450 P451 A452 F453 I454 E455 T456 S457 E458 D459 T462 S463 T464 Y465 N466 H471 A474 K475 N480 I481 N482 R483 V484 I485 Y489 Y490 P491 V492 E493 E494 A495 S498 N499 M500 R501 H502 R503 P504 I505 G508 V509 Q510 G511 L512
A513 D514 T515 L518 P522 F523 D524 L531 N532 I533 Q534 I535 T538 A542 S543 M544 E545 A546 S547 C548 E549 L550 A551 P556 Y557 E558 T559 F560 Q561 G562 S563 P564 A565 G568 I569 L570 Q571 F572 D573 M574 P579 Y580 G581 M582 W583 D584 W585 D586 H595 G596 V597
R598 N599 S600 L601 T602 M603 A604 P605 M606 P607 T608 A609 S612 Q613 I614 N618 E619 C620 F621 E622 P623 V624 T625 S626 N627 M628 Y629 S630 ARG ARG VAL LEU SER GLY GLU F638 Q639 V640 V641 N642 L645 L646 R647 D648 L649 V650 D651 L652 G653 I654 W655 M659 K660 Q661 Y662 L663
N667 G668 S669 I670 Q671 G672 L673 P674 N675 V676 P677 Q678 E679 L680 K681 D682 L683 Y684 K685 T686 V687 W688 E689 I690 S691 Q692 K693 T694 I695 I696 N697 M698 A699 A700 D701 R702 S703 V704 Y705 I706 D707 Q708 S709 H710 S711 L712 N713 L714 F715 L716 P719 T725 S726 M727 H728 G731
K737 T738 G739 M740 Y741 Y742 L743 R744 T745 Q746 ALA ALA SER ALA ALA ILE GLN PHE THR ILE ASP GLN LYS ILE ALA ASP GLN ALA THR GLU ASN VAL ALA ASP ILE SER ASN LEU LYS LYS ARG PRO SER TYR MET PRO SER SER SER ALA SER TYR ALA ALA SER ASP PHE VAL PRO ALA ALA
VAL THR ALA ASN ASN ALA THR ILE PRO SER LEU ASP SER SER SER GLU ALA SER ARG GLU ALA SER PRO ALA PRO THR GLY SER HIS SER LEU THR LYS GLY MET ALA GLU LEU ASN VAL GLN GLN GLU SER LYS VAL GLU VAL PRO GLU VAL PRO ALA PRO THR LYS ASN ASN GLU GLU LYS ALA ALA
PRO ILE VAL ASP ASP GLU GLU THR GLU PHE ASP ILE TYR ASN SER LYS VAL ILE ALA CYS ALA ILE ASP ASN PRO GLU ALA CYS SER GLU MET CYS SER GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	166.51Å 166.51Å 381.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	192.45 – 6.61 36.56 – 6.61	Depositor EDS
% Data completeness (in resolution range)	87.8 (192.45-6.61) 88.3 (36.56-6.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 6.63Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.391 , 0.442 0.370 , 0.430	Depositor 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[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.52	0/3647	0.65	0/5075
1	B	0.52	0/3647	0.65	0/5075
1	C	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	A	3649	0	1652	61	0
1	B	3649	0	1652	55	0
1	C	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.

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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
1:C:159:ILE:C	1:C:161:GLY:H	2.04	0.61
1:C:348:TRP:O	1:C:382:THR:HA	2.01	0.60
1:D:304:TRP:O	1:D:350:LEU:HA	2.01	0.60
1:A:2:TYR:HA	1:A:11:GLU:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ASP:O	1:C:20:ALA:HB2	2.02	0.59
1:C:174:VAL:HA	1:C:208:ALA:HB3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:GLU:O	1:D:345:ASN:N	2.42	0.52
1:A:508:GLY:HA3	1:A:605:PRO:HA	1.91	0.52
1:A:523:PHE:H	1:A:683:LEU:HA	1.74	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:A:52:THR:O	1:A:56:LEU:N	2.48	0.47
1:C:234:THR:HA	1:C:237:GLU:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:THR:HA	1:D:56:LEU: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:197:TYR:HA	1:A:452:ALA:HB1	1.97	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: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:64:CYS:CB	1:A:78:ALA:HB2	2.46	0.46
1:A:349:THR:HA	1:A:382:THR:HA	1.98	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:60:ALA:C	1:A:62:GLU:N	2.70	0.44
1:A:513:ALA:HB3	1:A:618:ASN:CB	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:SER:HA	1:A:431:ILE: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:59:LEU:O	1:C:63:THR:N	2.51	0.43
1:C:563:SER:O	1:C:565:ALA:N	2.52	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:79:ALA:HA	1:C:82:ALA:HB3	2.01	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: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:75:ALA:C	1:B:77:LEU:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:SER:HA	1:B:394:GLU:CB	2.50	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:83:ILE:C	1:B:85:ASN:H	2.25	0.40
1:B:680:LEU:HA	1:B:683:LEU:CB	2.51	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	Percentiles
1	A	735/888 (83%)	533 (72%)	157 (21%)	45 (6%)	1 17
1	B	735/888 (83%)	518 (70%)	180 (24%)	37 (5%)	2 20
1	C	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	A	225	GLU
1	A	227	SER
1	A	288	GLN
1	A	461	LYS

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Mol	Chain	Res	Type
1	A	486	ASP
1	A	677	PRO
1	B	501	ARG
1	B	719	PRO
1	C	5	LYS
1	C	145	TYR
1	C	291	ASN
1	C	318	HIS
1	C	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	A	120	VAL
1	A	290	GLY
1	A	487	ARG
1	A	558	GLU
1	A	613	GLN
1	A	623	PRO
1	A	674	PRO
1	B	159	ILE
1	B	364	GLY
1	B	452	ALA
1	C	108	ALA
1	C	159	ILE
1	C	182	ASP
1	C	288	GLN
1	C	319	GLY
1	C	364	GLY
1	C	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

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

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Mol	Chain	Res	Type
1	A	492	VAL
1	A	608	THR
1	A	657	GLU
1	B	8	GLY
1	B	12	PRO
1	B	191	ASN
1	B	266	ASN
1	B	304	TRP
1	B	458	GLU
1	B	580	TYR
1	B	656	ASP
1	B	737	LYS
1	C	76	THR
1	C	155	TYR
1	C	211	PRO
1	C	345	ASN
1	C	558	GLU
1	C	564	PRO
1	C	567	GLN
1	C	719	PRO
1	C	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	B	93	GLN
1	B	210	THR
1	B	273	ILE
1	B	387	LYS
1	B	459	ASP
1	B	558	GLU

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Mol	Chain	Res	Type
1	B	617	TYR
1	B	620	CYS
1	B	661	GLN
1	C	18	ILE
1	C	257	SER
1	C	264	GLY
1	C	351	PHE
1	C	538	THR
1	C	580	TYR
1	C	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	A	511	GLY
1	C	51	VAL
1	D	114	PRO
1	D	153	ARG
1	D	374	TYR
1	D	684	TYR
1	A	28	GLY
1	A	274	PRO
1	C	50	GLY
1	A	564	PRO
1	B	31	PRO
1	B	180	GLY
1	B	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	B	454	ILE
1	C	677	PRO
1	D	491	PRO
1	D	623	PRO
1	D	690	ILE
1	A	163	VAL
1	C	178	ILE

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 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, 95th 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			OWAB(Å^2)	Q<0.9
1	A	739/888 (83%)	3.15	441 (59%)	0	0	39, 81, 170, 183	0
1	B	739/888 (83%)	2.68	367 (49%)	0	1	52, 74, 175, 188	0
1	C	739/888 (83%)	2.93	396 (53%)	0	1	51, 73, 173, 194	0
1	D	739/888 (83%)	3.35	464 (62%)	0	0	58, 80, 175, 186	0
All	All	2956/3552 (83%)	3.03	1668 (56%)	0	1	39, 78, 173, 194	0

All (1668) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	ASN	18.1
1	D	711	SER	18.1
1	C	433	GLU	18.1
1	D	218	CYS	17.0
1	B	414	SER	16.9
1	B	510	GLN	16.5
1	C	415	ASN	16.4
1	D	596	GLY	15.8
1	B	220	LEU	15.0
1	A	605	PRO	14.8
1	D	217	SER	14.7
1	D	686	THR	14.5
1	D	219	PHE	14.5
1	A	14	GLN	14.5
1	B	416	GLN	14.4
1	A	441	ALA	14.3
1	B	433	GLU	14.3
1	C	215	MET	14.2
1	C	216	SER	14.0
1	C	686	THR	13.7
1	D	443	CYS	13.7

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Mol	Chain	Res	Type	RSRZ
1	A	557	TYR	13.5
1	C	442	VAL	13.5
1	D	216	SER	13.3
1	C	624	VAL	13.3
1	D	605	PRO	13.2
1	A	251	HIS	13.1
1	D	738	THR	13.0
1	C	435	SER	12.8
1	D	442	VAL	12.7
1	C	504	PRO	12.7
1	A	558	GLU	12.6
1	C	441	ALA	12.4
1	C	443	CYS	12.4
1	C	508	GLY	12.3
1	B	442	VAL	12.3
1	C	414	SER	12.2
1	D	256	ARG	12.2
1	D	685	LYS	12.0
1	A	254	ASN	12.0
1	D	220	LEU	12.0
1	B	509	VAL	12.0
1	D	710	HIS	11.9
1	D	623	PRO	11.8
1	B	36	ALA	11.8
1	C	537	GLU	11.8
1	B	254	ASN	11.7
1	D	433	GLU	11.6
1	C	416	GLN	11.5
1	B	219	PHE	11.4
1	B	14	GLN	11.4
1	A	692	GLN	11.3
1	A	623	PRO	11.3
1	D	689	GLU	11.3
1	B	379	ARG	11.2
1	D	286	VAL	11.1
1	A	715	PHE	11.1
1	B	136	VAL	11.0
1	C	444	ASN	11.0
1	D	255	ILE	10.9
1	C	625	THR	10.9
1	D	284	ARG	10.9
1	C	257	SER	10.8

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

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

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Mol	Chain	Res	Type	RSRZ
1	D	166	ARG	8.8
1	B	424	SER	8.8
1	D	432	VAL	8.8
1	A	600	SER	8.7
1	B	441	ALA	8.7
1	A	326	ARG	8.6
1	D	196	LYS	8.6
1	C	254	ASN	8.6
1	B	310	ASP	8.6
1	A	255	ILE	8.6
1	A	599	ASN	8.6
1	C	253	HIS	8.6
1	A	353	PRO	8.6
1	C	422	ILE	8.5
1	C	412	ARG	8.5
1	C	580	TYR	8.5
1	C	532	ASN	8.5
1	B	709	SER	8.5
1	B	135	ILE	8.5
1	D	624	VAL	8.4
1	D	289	GLY	8.4
1	C	600	SER	8.4
1	D	91	THR	8.4
1	B	418	ASN	8.4
1	B	1	MET	8.4
1	C	306	ALA	8.4
1	D	198	PHE	8.3
1	A	416	GLN	8.3
1	A	622	GLU	8.3
1	B	16	ASP	8.3
1	D	430	GLU	8.3
1	A	249	GLY	8.3
1	A	434	TYR	8.3
1	D	421	VAL	8.2
1	A	3	VAL	8.2
1	B	708	GLN	8.2
1	C	384	LYS	8.2
1	D	625	THR	8.2
1	A	504	PRO	8.2
1	A	739	GLY	8.2
1	A	714	LEU	8.2
1	C	533	ILE	8.2

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Mol	Chain	Res	Type	RSRZ
1	C	423	LYS	8.2
1	D	740	MET	8.2
1	D	226	ASP	8.1
1	D	741	TYR	8.1
1	A	93	GLN	8.1
1	D	202	SER	8.1
1	C	30	ASP	8.1
1	C	445	LEU	8.1
1	D	428	CYS	8.1
1	C	534	GLN	8.0
1	A	327	ASP	8.0
1	B	37	VAL	8.0
1	B	532	ASN	8.0
1	C	2	TYR	7.9
1	A	556	PRO	7.9
1	D	415	ASN	7.9
1	A	691	SER	7.9
1	A	260	SER	7.9
1	A	543	SER	7.9
1	B	247	GLY	7.9
1	A	440	THR	7.9
1	C	29	LEU	7.8
1	A	72	PRO	7.8
1	D	422	ILE	7.8
1	D	569	ILE	7.8
1	A	737	LYS	7.8
1	B	707	ASP	7.8
1	C	579	PRO	7.7
1	D	247	GLY	7.7
1	D	302	GLU	7.7
1	C	601	LEU	7.7
1	A	680	LEU	7.7
1	A	261	TYR	7.7
1	D	197	TYR	7.7
1	D	622	GLU	7.6
1	C	4	TYR	7.6
1	B	742	TYR	7.6
1	B	522	PRO	7.6
1	D	509	VAL	7.6
1	B	143	TYR	7.6
1	B	710	HIS	7.6
1	A	509	VAL	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	682	ASP	7.6
1	D	597	VAL	7.6
1	A	73	ASP	7.5
1	A	642	ASN	7.5
1	B	309	PHE	7.5
1	B	712	LEU	7.5
1	C	15	PHE	7.5
1	C	411	ASN	7.4
1	C	446	ALA	7.4
1	C	302	GLU	7.4
1	D	182	ASP	7.4
1	C	164	ALA	7.4
1	A	194	SER	7.4
1	C	507	LEU	7.4
1	C	536	PHE	7.4
1	D	503	ARG	7.3
1	C	270	ASN	7.3
1	D	451	PRO	7.3
1	C	538	THR	7.3
1	B	618	ASN	7.3
1	D	598	ARG	7.3
1	D	510	GLN	7.3
1	A	508	GLY	7.3
1	B	619	GLU	7.3
1	A	215	MET	7.3
1	B	435	SER	7.2
1	A	13	VAL	7.2
1	D	380	GLY	7.2
1	D	463	SER	7.2
1	A	424	SER	7.2
1	A	4	TYR	7.2
1	B	599	ASN	7.2
1	A	675	ASN	7.2
1	A	142	GLN	7.2
1	D	691	SER	7.1
1	A	253	HIS	7.1
1	B	252	ILE	7.1
1	A	647	ARG	7.1
1	D	50	GLY	7.1
1	D	414	SER	7.1
1	A	444	ASN	7.1
1	C	740	MET	7.1

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Mol	Chain	Res	Type	RSRZ
1	D	431	ILE	7.1
1	D	303	PRO	7.0
1	D	353	PRO	7.0
1	B	508	GLY	7.0
1	C	11	GLU	7.0
1	A	16	ASP	7.0
1	A	265	THR	7.0
1	D	265	THR	7.0
1	A	716	LEU	7.0
1	D	681	LYS	7.0
1	A	443	CYS	7.0
1	D	548	CYS	7.0
1	C	3	VAL	6.9
1	D	423	LYS	6.9
1	B	600	SER	6.9
1	B	534	GLN	6.9
1	C	535	ILE	6.9
1	C	688	TRP	6.9
1	C	1	MET	6.9
1	D	227	SER	6.9
1	B	208	ALA	6.9
1	A	709	SER	6.9
1	D	648	ASP	6.8
1	B	50	GLY	6.8
1	B	447	SER	6.8
1	C	715	PHE	6.8
1	C	424	SER	6.8
1	C	413	LYS	6.8
1	D	599	ASN	6.7
1	D	167	PRO	6.7
1	D	354	THR	6.7
1	A	743	LEU	6.7
1	D	695	ILE	6.7
1	C	418	ASN	6.7
1	D	684	TYR	6.7
1	A	252	ILE	6.7
1	B	30	ASP	6.7
1	C	271	GLY	6.7
1	A	30	ASP	6.7
1	C	352	SER	6.6
1	D	49	GLU	6.6
1	C	491	PRO	6.6

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Mol	Chain	Res	Type	RSRZ
1	D	327	ASP	6.6
1	A	604	ALA	6.6
1	D	682	ASP	6.6
1	A	668	GLY	6.6
1	D	491	PRO	6.6
1	B	431	ILE	6.6
1	B	378	GLY	6.6
1	D	715	PHE	6.5
1	A	207	ASN	6.5
1	A	92	LYS	6.5
1	D	296	ALA	6.5
1	D	524	ASP	6.5
1	C	578	LYS	6.5
1	B	51	VAL	6.4
1	D	705	TYR	6.4
1	C	691	SER	6.4
1	B	512	LEU	6.4
1	C	447	SER	6.4
1	D	693	LYS	6.4
1	C	540	TYR	6.4
1	C	564	PRO	6.4
1	C	140	ASP	6.4
1	A	643	PRO	6.4
1	C	303	PRO	6.4
1	A	607	PRO	6.3
1	B	426	ASN	6.3
1	D	413	LYS	6.3
1	D	212	LYS	6.3
1	A	12	PRO	6.3
1	A	601	LEU	6.3
1	B	511	GLY	6.3
1	B	249	GLY	6.3
1	D	564	PRO	6.3
1	B	714	LEU	6.3
1	D	140	ASP	6.3
1	C	713	ASN	6.3
1	A	580	TYR	6.2
1	A	728	HIS	6.2
1	C	218	CYS	6.2
1	A	683	LEU	6.2
1	D	626	SER	6.2
1	B	466	ASN	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	143	TYR	6.2
1	A	204	THR	6.2
1	D	288	GLN	6.2
1	A	303	PRO	6.2
1	A	466	ASN	6.2
1	D	692	GLN	6.2
1	D	708	GLN	6.2
1	D	600	SER	6.2
1	B	248	ILE	6.2
1	A	222	ALA	6.2
1	A	208	ALA	6.2
1	D	429	CYS	6.2
1	D	490	TYR	6.2
1	D	570	LEU	6.2
1	D	137	TYR	6.1
1	D	203	PRO	6.1
1	A	532	ASN	6.1
1	D	266	ASN	6.1
1	A	90	THR	6.1
1	B	165	GLU	6.1
1	A	127	ASN	6.1
1	D	508	GLY	6.1
1	C	252	ILE	6.1
1	C	340	LYS	6.1
1	A	315	ARG	6.1
1	A	717	ARG	6.1
1	C	581	GLY	6.1
1	A	425	SER	6.1
1	D	251	HIS	6.1
1	C	14	GLN	6.0
1	B	250	LEU	6.0
1	C	327	ASP	6.0
1	C	12	PRO	6.0
1	D	30	ASP	6.0
1	D	264	GLY	6.0
1	A	264	GLY	6.0
1	B	92	LYS	6.0
1	C	324	ARG	6.0
1	D	670	ILE	6.0
1	D	607	PRO	6.0
1	B	738	THR	6.0
1	C	420	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	175	ALA	6.0
1	D	139	ARG	5.9
1	B	535	ILE	5.9
1	C	668	GLY	5.9
1	D	34	ILE	5.9
1	B	624	VAL	5.9
1	C	539	ILE	5.9
1	B	311	PHE	5.9
1	A	263	ALA	5.9
1	A	579	PRO	5.9
1	B	603	MET	5.9
1	A	408	ASP	5.9
1	C	5	LYS	5.9
1	A	266	ASN	5.9
1	A	423	LYS	5.9
1	C	741	TYR	5.9
1	D	571	GLN	5.9
1	C	690	ILE	5.9
1	D	707	ASP	5.9
1	A	523	PHE	5.9
1	D	355	SER	5.9
1	A	620	CYS	5.8
1	C	608	THR	5.8
1	A	140	ASP	5.8
1	D	532	ASN	5.8
1	B	246	GLY	5.8
1	C	221	VAL	5.8
1	C	565	ALA	5.8
1	D	360	SER	5.8
1	A	684	TYR	5.8
1	D	213	PRO	5.8
1	A	296	ALA	5.8
1	B	579	PRO	5.8
1	A	300	TYR	5.8
1	A	730	TYR	5.8
1	B	207	ASN	5.8
1	A	286	VAL	5.8
1	D	649	LEU	5.8
1	A	727	MET	5.7
1	D	389	TRP	5.7
1	C	137	TYR	5.7
1	A	295	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	91	THR	5.7
1	C	410	CYS	5.7
1	C	307	ASP	5.7
1	D	164	ALA	5.7
1	B	611	THR	5.7
1	D	179	HIS	5.7
1	A	352	SER	5.7
1	C	165	GLU	5.7
1	C	274	PRO	5.7
1	B	669	SER	5.7
1	C	251	HIS	5.7
1	C	177	GLY	5.7
1	D	201	ALA	5.7
1	D	678	GLN	5.7
1	C	739	GLY	5.6
1	A	428	CYS	5.6
1	A	524	ASP	5.6
1	C	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	D	200	HIS	5.6
1	A	421	VAL	5.6
1	A	679	GLU	5.6
1	D	671	GLN	5.6
1	D	207	ASN	5.6
1	B	450	LEU	5.6
1	A	546	ALA	5.6
1	A	406	TYR	5.6
1	B	533	ILE	5.6
1	B	536	PHE	5.6
1	A	168	GLN	5.6
1	C	136	VAL	5.6
1	B	711	SER	5.6
1	C	255	ILE	5.6
1	D	357	PRO	5.5
1	C	212	LYS	5.5
1	C	495	ALA	5.5
1	C	503	ARG	5.5
1	D	601	LEU	5.5
1	C	493	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	2	TYR	5.5
1	B	381	LYS	5.5
1	D	737	LYS	5.5
1	C	339	MET	5.5
1	B	38	LYS	5.5
1	A	174	VAL	5.5
1	D	683	LEU	5.5
1	B	703	SER	5.5
1	C	142	GLN	5.5
1	A	173	ARG	5.5
1	C	449	ALA	5.5
1	A	85	ASN	5.4
1	A	534	GLN	5.4
1	D	204	THR	5.4
1	A	641	VAL	5.4
1	A	703	SER	5.4
1	C	338	PHE	5.4
1	D	669	SER	5.4
1	C	670	ILE	5.4
1	C	336	ASP	5.4
1	A	731	GLY	5.4
1	C	622	GLU	5.4
1	A	674	PRO	5.4
1	A	694	THR	5.4
1	A	533	ILE	5.4
1	D	679	GLU	5.4
1	B	140	ASP	5.4
1	C	716	LEU	5.4
1	C	305	HIS	5.4
1	A	448	VAL	5.4
1	B	295	GLY	5.3
1	A	446	ALA	5.3
1	B	2	TYR	5.3
1	B	251	HIS	5.3
1	A	433	GLU	5.3
1	C	641	VAL	5.3
1	D	745	THR	5.3
1	D	595	HIS	5.3
1	C	563	SER	5.3
1	A	646	LEU	5.3
1	D	136	VAL	5.3
1	D	484	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	542	ALA	5.3
1	C	33	HIS	5.3
1	C	492	VAL	5.3
1	B	35	ASP	5.3
1	B	621	PHE	5.3
1	C	610	SER	5.3
1	A	744	ARG	5.3
1	B	265	THR	5.3
1	B	200	HIS	5.3
1	C	258	THR	5.3
1	B	49	GLU	5.3
1	B	385	ALA	5.3
1	A	304	TRP	5.3
1	D	199	THR	5.3
1	B	412	ARG	5.2
1	C	402	PRO	5.2
1	A	400	GLY	5.2
1	A	598	ARG	5.2
1	C	439	GLU	5.2
1	C	345	ASN	5.2
1	A	420	GLY	5.2
1	D	604	ALA	5.2
1	A	71	HIS	5.2
1	A	171	ILE	5.2
1	C	351	PHE	5.2
1	B	199	THR	5.2
1	B	449	ALA	5.2
1	C	448	VAL	5.2
1	B	444	ASN	5.2
1	C	213	PRO	5.2
1	B	604	ALA	5.2
1	B	537	GLU	5.2
1	B	504	PRO	5.2
1	C	708	GLN	5.2
1	A	219	PHE	5.2
1	C	744	ARG	5.2
1	C	738	THR	5.1
1	A	544	MET	5.1
1	B	446	ALA	5.1
1	A	439	GLU	5.1
1	D	714	LEU	5.1
1	C	404	VAL	5.1

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

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Mol	Chain	Res	Type	RSRZ
1	A	285	TYR	4.9
1	B	222	ALA	4.9
1	A	485	ILE	4.9
1	D	425	SER	4.9
1	D	696	ILE	4.9
1	B	523	PHE	4.9
1	A	417	LYS	4.9
1	D	194	SER	4.9
1	B	434	TYR	4.9
1	D	410	CYS	4.9
1	B	28	GLY	4.9
1	A	407	LYS	4.9
1	A	648	ASP	4.9
1	C	619	GLU	4.9
1	A	745	THR	4.9
1	A	505	ILE	4.9
1	C	143	TYR	4.9
1	C	498	SER	4.9
1	A	214	GLN	4.9
1	A	742	TYR	4.9
1	B	102	TYR	4.9
1	D	568	GLY	4.9
1	A	693	LYS	4.9
1	B	451	PRO	4.9
1	A	736	LEU	4.9
1	A	172	MET	4.9
1	C	222	ALA	4.9
1	B	217	SER	4.8
1	A	608	THR	4.8
1	A	741	TYR	4.8
1	C	626	SER	4.8
1	A	645	LEU	4.8
1	B	384	LYS	4.8
1	D	627	ASN	4.8
1	B	524	ASP	4.8
1	A	94	PHE	4.8
1	B	216	SER	4.8
1	A	491	PRO	4.8
1	B	608	THR	4.8
1	A	426	ASN	4.8
1	C	36	ALA	4.8
1	A	202	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	138	ASP	4.8
1	B	289	GLY	4.8
1	A	203	PRO	4.8
1	C	353	PRO	4.8
1	D	447	SER	4.8
1	D	449	ALA	4.8
1	B	347	THR	4.8
1	A	267	GLY	4.7
1	A	529	ARG	4.7
1	D	260	SER	4.7
1	B	156	LEU	4.7
1	D	446	ALA	4.7
1	D	244	THR	4.7
1	B	174	VAL	4.7
1	C	10	LYS	4.7
1	B	440	THR	4.7
1	B	578	LYS	4.7
1	D	482	ASN	4.7
1	D	680	LEU	4.7
1	D	351	PHE	4.7
1	D	364	GLY	4.7
1	A	82	ALA	4.7
1	B	91	THR	4.7
1	A	298	ALA	4.7
1	C	141	PHE	4.7
1	A	740	MET	4.7
1	C	346	GLY	4.7
1	D	505	ILE	4.7
1	A	597	VAL	4.7
1	B	580	TYR	4.7
1	D	620	CYS	4.6
1	C	319	GLY	4.6
1	D	533	ILE	4.6
1	C	168	GLN	4.6
1	A	670	ILE	4.6
1	B	266	ASN	4.6
1	B	570	LEU	4.6
1	B	274	PRO	4.6
1	B	602	THR	4.6
1	A	5	LYS	4.6
1	B	144	SER	4.6
1	A	562	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	621	PHE	4.6
1	A	248	ILE	4.6
1	C	524	ASP	4.6
1	D	404	VAL	4.6
1	D	464	THR	4.6
1	C	330	PRO	4.6
1	C	360	SER	4.6
1	A	247	GLY	4.6
1	D	181	ARG	4.6
1	A	522	PRO	4.6
1	D	186	ALA	4.6
1	C	313	ASP	4.6
1	B	382	THR	4.6
1	D	175	ALA	4.6
1	C	499	ASN	4.6
1	A	669	SER	4.6
1	B	423	LYS	4.6
1	C	598	ARG	4.6
1	C	265	THR	4.5
1	A	169	HIS	4.5
1	A	644	TYR	4.5
1	A	432	VAL	4.5
1	D	252	ILE	4.5
1	A	510	GLN	4.5
1	A	351	PHE	4.5
1	D	325	ALA	4.5
1	C	225	GLU	4.5
1	D	40	THR	4.5
1	B	202	SER	4.5
1	C	490	TYR	4.5
1	A	447	SER	4.5
1	A	430	GLU	4.5
1	B	164	ALA	4.5
1	B	706	ILE	4.5
1	C	604	ALA	4.5
1	A	685	LYS	4.5
1	B	436	ALA	4.5
1	D	391	SER	4.5
1	D	744	ARG	4.5
1	A	627	ASN	4.5
1	C	200	HIS	4.5
1	C	269	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	650	VAL	4.4
1	C	124	VAL	4.4
1	A	455	GLU	4.4
1	D	249	GLY	4.4
1	A	422	ILE	4.4
1	A	688	TRP	4.4
1	A	746	GLN	4.4
1	D	556	PRO	4.4
1	C	198	PHE	4.4
1	D	257	SER	4.4
1	A	506	ALA	4.4
1	D	48	TYR	4.4
1	C	743	LEU	4.4
1	D	328	LEU	4.4
1	B	203	PRO	4.4
1	C	405	VAL	4.4
1	C	543	SER	4.4
1	A	561	GLN	4.3
1	A	349	THR	4.3
1	D	580	TYR	4.3
1	C	669	SER	4.3
1	B	741	TYR	4.3
1	A	122	ASN	4.3
1	A	87	HIS	4.3
1	A	123	ILE	4.3
1	B	109	THR	4.3
1	C	163	VAL	4.3
1	C	671	GLN	4.3
1	D	142	GLN	4.3
1	B	166	ARG	4.3
1	D	448	VAL	4.3
1	B	540	TYR	4.3
1	C	139	ARG	4.3
1	D	138	ASP	4.3
1	B	610	SER	4.3
1	C	603	MET	4.3
1	D	143	TYR	4.3
1	A	301	LEU	4.3
1	A	363	TYR	4.3
1	C	45	SER	4.3
1	C	314	ILE	4.3
1	D	5	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	204	THR	4.3
1	C	401	THR	4.3
1	D	426	ASN	4.2
1	C	13	VAL	4.2
1	C	294	PRO	4.2
1	C	308	ILE	4.2
1	A	535	ILE	4.2
1	D	445	LEU	4.2
1	D	3	VAL	4.2
1	C	304	TRP	4.2
1	A	365	ASP	4.2
1	D	69	THR	4.2
1	A	560	PHE	4.2
1	A	702	ARG	4.2
1	B	301	LEU	4.2
1	C	49	GLU	4.2
1	D	6	ARG	4.2
1	B	429	CYS	4.2
1	D	608	THR	4.2
1	B	513	ALA	4.2
1	B	245	ALA	4.2
1	D	301	LEU	4.2
1	D	209	GLY	4.2
1	A	86	LEU	4.2
1	C	35	ASP	4.2
1	A	268	THR	4.1
1	A	306	ALA	4.1
1	A	418	ASN	4.1
1	B	215	MET	4.1
1	A	578	LYS	4.1
1	A	502	HIS	4.1
1	B	155	TYR	4.1
1	D	317	ASN	4.1
1	A	720	THR	4.1
1	D	185	ALA	4.1
1	A	324	ARG	4.1
1	D	703	SER	4.1
1	B	214	GLN	4.1
1	D	701	ASP	4.1
1	D	704	VAL	4.1
1	B	168	GLN	4.1
1	A	217	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	183	ILE	4.1
1	A	91	THR	4.1
1	D	208	ALA	4.1
1	D	248	ILE	4.1
1	C	502	HIS	4.1
1	D	310	ASP	4.1
1	D	452	ALA	4.1
1	C	337	LEU	4.1
1	D	402	PRO	4.1
1	D	545	GLU	4.1
1	D	746	GLN	4.1
1	A	581	GLY	4.0
1	D	416	GLN	4.0
1	B	342	VAL	4.0
1	D	2	TYR	4.0
1	C	71	HIS	4.0
1	A	401	THR	4.0
1	A	651	ASP	4.0
1	D	263	ALA	4.0
1	D	650	VAL	4.0
1	B	335	PRO	4.0
1	C	438	ASP	4.0
1	D	308	ILE	4.0
1	A	128	LYS	4.0
1	D	311	PHE	4.0
1	B	375	GLU	4.0
1	D	450	LEU	4.0
1	A	233	ASP	4.0
1	A	537	GLU	4.0
1	A	371	TYR	4.0
1	C	642	ASN	4.0
1	D	39	VAL	4.0
1	D	677	PRO	3.9
1	B	137	TYR	3.9
1	C	607	PRO	3.9
1	C	609	ALA	3.9
1	A	126	GLU	3.9
1	B	409	ALA	3.9
1	D	250	LEU	3.9
1	D	269	SER	3.9
1	D	628	MET	3.9
1	A	619	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	341	ARG	3.9
1	C	157	LEU	3.9
1	A	454	ILE	3.9
1	B	271	GLY	3.9
1	C	127	ASN	3.9
1	B	383	ILE	3.9
1	A	29	LEU	3.9
1	D	697	ASN	3.9
1	C	379	ARG	3.9
1	A	399	THR	3.9
1	A	355	SER	3.9
1	B	360	SER	3.9
1	D	178	ILE	3.9
1	A	200	HIS	3.9
1	D	584	ASP	3.9
1	A	507	LEU	3.9
1	B	300	TYR	3.9
1	D	4	TYR	3.9
1	D	743	LEU	3.9
1	B	242	SER	3.9
1	B	272	LEU	3.9
1	B	420	GLY	3.9
1	A	198	PHE	3.9
1	A	732	TRP	3.9
1	B	430	GLU	3.9
1	D	180	GLY	3.9
1	B	303	PRO	3.9
1	B	348	TRP	3.8
1	D	573	ASP	3.8
1	D	565	ALA	3.8
1	B	260	SER	3.8
1	A	474	ALA	3.8
1	D	558	GLU	3.8
1	D	716	LEU	3.8
1	D	702	ARG	3.8
1	A	284	ARG	3.8
1	D	361	ASP	3.8
1	A	429	CYS	3.8
1	A	536	PHE	3.8
1	C	627	ASN	3.8
1	D	562	GLY	3.8
1	C	178	ILE	3.8

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

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

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

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Mol	Chain	Res	Type	RSRZ
1	A	380	GLY	3.5
1	C	102	TYR	3.5
1	B	286	VAL	3.5
1	D	262	ILE	3.5
1	A	387	LYS	3.5
1	A	385	ALA	3.5
1	D	706	ILE	3.5
1	D	11	GLU	3.4
1	D	61	ALA	3.4
1	A	170	LEU	3.4
1	D	312	ILE	3.4
1	B	3	VAL	3.4
1	A	199	THR	3.4
1	B	716	LEU	3.4
1	C	585	TRP	3.4
1	A	141	PHE	3.4
1	D	205	LEU	3.4
1	B	244	THR	3.4
1	C	117	SER	3.4
1	B	437	PRO	3.4
1	D	89	GLN	3.4
1	D	434	TYR	3.4
1	C	87	HIS	3.4
1	C	544	MET	3.4
1	C	640	VAL	3.4
1	D	305	HIS	3.4
1	A	484	VAL	3.4
1	D	394	GLU	3.4
1	B	507	LEU	3.4
1	A	323	ILE	3.4
1	B	559	THR	3.4
1	C	118	ASP	3.4
1	D	210	THR	3.4
1	B	717	ARG	3.4
1	B	609	ALA	3.4
1	B	167	PRO	3.4
1	A	350	LEU	3.4
1	B	529	ARG	3.4
1	D	243	LYS	3.4
1	A	528	ALA	3.4
1	C	70	VAL	3.4
1	C	329	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	167	PRO	3.4
1	D	223	MET	3.4
1	A	139	ARG	3.3
1	D	639	GLN	3.3
1	C	194	SER	3.3
1	C	570	LEU	3.3
1	A	677	PRO	3.3
1	D	313	ASP	3.3
1	C	103	ARG	3.3
1	B	324	ARG	3.3
1	B	491	PRO	3.3
1	C	531	LEU	3.3
1	D	222	ALA	3.3
1	D	660	LYS	3.3
1	A	28	GLY	3.3
1	C	109	THR	3.3
1	B	490	TYR	3.3
1	A	486	ASP	3.3
1	B	448	VAL	3.3
1	D	427	LEU	3.3
1	B	376	LYS	3.3
1	B	676	VAL	3.3
1	D	342	VAL	3.3
1	A	191	ASN	3.3
1	A	76	THR	3.3
1	C	387	LYS	3.3
1	B	577	GLN	3.3
1	D	385	ALA	3.3
1	D	211	PRO	3.3
1	D	498	SER	3.2
1	C	72	PRO	3.2
1	B	40	THR	3.2
1	D	47	VAL	3.2
1	C	354	THR	3.2
1	D	699	ALA	3.2
1	A	603	MET	3.2
1	A	307	ASP	3.2
1	D	31	PRO	3.2
1	D	127	ASN	3.2
1	D	36	ALA	3.2
1	D	169	HIS	3.2
1	C	707	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	397	THR	3.2
1	A	465	TYR	3.2
1	B	145	TYR	3.2
1	B	691	SER	3.2
1	D	45	SER	3.2
1	D	307	ASP	3.2
1	C	86	LEU	3.2
1	C	250	LEU	3.2
1	C	122	ASN	3.2
1	D	275	MET	3.2
1	D	309	PHE	3.2
1	C	700	ALA	3.2
1	A	338	PHE	3.2
1	D	362	CYS	3.2
1	B	205	LEU	3.2
1	D	92	LYS	3.2
1	D	728	HIS	3.2
1	A	624	VAL	3.2
1	B	641	VAL	3.2
1	A	328	LEU	3.2
1	B	744	ARG	3.2
1	C	332	LEU	3.2
1	B	70	VAL	3.2
1	B	201	ALA	3.2
1	C	431	ILE	3.2
1	A	234	THR	3.2
1	D	268	THR	3.2
1	B	337	LEU	3.2
1	D	79	ALA	3.2
1	A	177	GLY	3.2
1	A	189	THR	3.2
1	C	40	THR	3.2
1	D	71	HIS	3.2
1	D	298	ALA	3.2
1	B	270	ASN	3.1
1	A	192	LEU	3.1
1	A	410	CYS	3.1
1	D	78	ALA	3.1
1	B	584	ASP	3.1
1	A	396	GLN	3.1
1	A	102	TYR	3.1
1	B	671	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	274	PRO	3.1
1	C	701	ASP	3.1
1	B	445	LEU	3.1
1	C	34	ILE	3.1
1	A	726	SER	3.1
1	B	642	ASN	3.1
1	C	425	SER	3.1
1	D	534	GLN	3.1
1	D	9	ARG	3.1
1	C	497	LYS	3.1
1	D	523	PHE	3.1
1	D	358	GLY	3.1
1	C	685	LYS	3.1
1	D	141	PHE	3.1
1	D	70	VAL	3.1
1	B	478	THR	3.1
1	D	673	LEU	3.1
1	B	561	GLN	3.1
1	C	496	ARG	3.1
1	D	408	ASP	3.1
1	C	196	LYS	3.1
1	A	259	GLY	3.1
1	B	746	GLN	3.1
1	D	379	ARG	3.1
1	A	570	LEU	3.1
1	D	228	ILE	3.1
1	D	272	LEU	3.1
1	B	206	PHE	3.1
1	B	739	GLY	3.1
1	C	452	ALA	3.1
1	D	420	GLY	3.1
1	D	609	ALA	3.1
1	D	561	GLN	3.0
1	B	389	TRP	3.0
1	A	362	CYS	3.0
1	C	403	PHE	3.0
1	A	405	VAL	3.0
1	C	409	ALA	3.0
1	D	700	ALA	3.0
1	C	437	PRO	3.0
1	A	431	ILE	3.0
1	D	280	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	37	VAL	3.0
1	C	202	SER	3.0
1	D	338	PHE	3.0
1	B	198	PHE	3.0
1	C	559	THR	3.0
1	B	243	LYS	3.0
1	D	535	ILE	3.0
1	D	466	ASN	3.0
1	B	139	ARG	3.0
1	D	374	TYR	3.0
1	A	336	ASP	3.0
1	C	326	ARG	3.0
1	D	14	GLN	3.0
1	D	323	ILE	3.0
1	D	363	TYR	3.0
1	D	630	SER	3.0
1	C	309	PHE	3.0
1	D	271	GLY	3.0
1	D	401	THR	3.0
1	D	647	ARG	3.0
1	A	335	PRO	3.0
1	B	668	GLY	3.0
1	D	273	ILE	3.0
1	D	653	GLY	3.0
1	C	158	ARG	3.0
1	A	475	LYS	3.0
1	C	176	LEU	3.0
1	A	36	ALA	3.0
1	C	97	VAL	3.0
1	B	506	ALA	2.9
1	B	558	GLU	2.9
1	C	331	ALA	2.9
1	A	476	VAL	2.9
1	A	9	ARG	2.9
1	A	436	ALA	2.9
1	B	745	THR	2.9
1	D	440	THR	2.9
1	C	597	VAL	2.9
1	D	579	PRO	2.9
1	C	84	SER	2.9
1	C	126	GLU	2.9
1	A	180	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	539	ILE	2.9
1	B	689	GLU	2.9
1	C	711	SER	2.9
1	C	347	THR	2.9
1	B	419	LEU	2.9
1	B	4	TYR	2.9
1	A	181	ARG	2.9
1	A	297	PHE	2.9
1	D	659	MET	2.9
1	D	365	ASP	2.9
1	D	369	ALA	2.9
1	D	403	PHE	2.9
1	B	612	SER	2.9
1	D	229	GLU	2.9
1	B	26	CYS	2.9
1	A	132	ASN	2.9
1	D	373	ARG	2.9
1	A	227	SER	2.9
1	A	723	LYS	2.9
1	D	176	LEU	2.9
1	C	44	ILE	2.9
1	D	698	MET	2.9
1	D	335	PRO	2.9
1	D	386	GLN	2.9
1	A	135	ILE	2.9
1	D	324	ARG	2.9
1	C	156	LEU	2.9
1	D	370	LEU	2.9
1	D	438	ASP	2.9
1	B	240	LEU	2.8
1	D	73	ASP	2.8
1	C	114	PRO	2.8
1	B	39	VAL	2.8
1	B	574	MET	2.8
1	B	327	ASP	2.8
1	C	355	SER	2.8
1	C	709	SER	2.8
1	D	381	LYS	2.8
1	C	85	ASN	2.8
1	A	671	GLN	2.8
1	C	583	TRP	2.8
1	C	42	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	561	GLN	2.8
1	A	179	HIS	2.8
1	D	483	ARG	2.8
1	B	261	TYR	2.8
1	A	228	ILE	2.8
1	B	346	GLY	2.8
1	D	495	ALA	2.8
1	B	740	MET	2.8
1	D	117	SER	2.8
1	C	605	PRO	2.8
1	C	311	PHE	2.8
1	C	383	ILE	2.8
1	C	584	ASP	2.8
1	B	462	THR	2.8
1	B	688	TRP	2.8
1	B	108	ALA	2.8
1	A	372	THR	2.8
1	C	169	HIS	2.8
1	D	157	LEU	2.8
1	D	501	ARG	2.8
1	B	48	TYR	2.8
1	D	51	VAL	2.8
1	C	166	ARG	2.8
1	D	400	GLY	2.8
1	B	173	ARG	2.8
1	D	304	TRP	2.8
1	D	63	THR	2.8
1	D	727	MET	2.8
1	B	317	ASN	2.8
1	A	367	PHE	2.7
1	C	41	GLN	2.7
1	C	76	THR	2.7
1	D	543	SER	2.7
1	B	531	LEU	2.7
1	C	361	ASP	2.7
1	A	97	VAL	2.7
1	B	607	PRO	2.7
1	D	585	TRP	2.7
1	D	629	TYR	2.7
1	B	101	LEU	2.7
1	B	323	ILE	2.7
1	B	339	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	267	GLY	2.7
1	C	119	ASP	2.7
1	A	176	LEU	2.7
1	C	320	LYS	2.7
1	C	399	THR	2.7
1	D	7	ASP	2.7
1	D	581	GLY	2.7
1	D	513	ALA	2.7
1	B	338	PHE	2.7
1	D	651	ASP	2.7
1	C	386	GLN	2.7
1	B	147	GLY	2.7
1	C	283	ALA	2.7
1	D	174	VAL	2.7
1	D	270	ASN	2.7
1	D	480	ASN	2.7
1	A	721	MET	2.7
1	A	538	THR	2.7
1	A	453	PHE	2.7
1	A	701	ASP	2.7
1	A	196	LYS	2.7
1	A	314	ILE	2.7
1	B	405	VAL	2.7
1	B	306	ALA	2.6
1	A	27	TYR	2.6
1	C	358	GLY	2.6
1	A	398	GLU	2.6
1	D	462	THR	2.6
1	A	369	ALA	2.6
1	D	238	CYS	2.6
1	A	411	ASN	2.6
1	B	312	ILE	2.6
1	B	528	ALA	2.6
1	D	531	LEU	2.6
1	A	257	SER	2.6
1	D	435	SER	2.6
1	A	130	LYS	2.6
1	A	596	GLY	2.6
1	A	23	SER	2.6
1	C	237	GLU	2.6
1	B	388	LEU	2.6
1	B	142	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	734	LYS	2.6
1	A	206	PHE	2.6
1	C	408	ASP	2.6
1	C	244	THR	2.6
1	C	696	ILE	2.6
1	C	419	LEU	2.6
1	A	610	SER	2.6
1	B	182	ASP	2.6
1	D	368	GLU	2.6
1	C	211	PRO	2.6
1	D	42	ARG	2.6
1	B	410	CYS	2.6
1	D	241	ILE	2.6
1	A	84	SER	2.6
1	C	181	ARG	2.6
1	A	40	THR	2.6
1	A	129	ASP	2.6
1	A	686	THR	2.6
1	A	481	LEU	2.6
1	B	525	SER	2.5
1	A	70	VAL	2.5
1	D	489	TYR	2.5
1	B	702	ARG	2.5
1	C	121	TYR	2.5
1	C	471	HIS	2.5
1	B	294	PRO	2.5
1	B	736	LEU	2.5
1	B	357	PRO	2.5
1	A	501	ARG	2.5
1	A	565	ALA	2.5
1	C	356	ALA	2.5
1	C	639	GLN	2.5
1	D	640	VAL	2.5
1	C	310	ASP	2.5
1	C	672	GLY	2.5
1	D	393	LEU	2.5
1	B	27	TYR	2.5
1	A	310	ASP	2.5
1	D	572	PHE	2.5
1	A	232	TYR	2.5
1	A	719	PRO	2.5
1	A	649	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	512	LEU	2.5
1	D	287	ASP	2.5
1	B	157	LEU	2.5
1	B	482	ASN	2.5
1	A	235	LEU	2.5
1	C	470	LEU	2.5
1	A	735	GLY	2.5
1	C	282	THR	2.5
1	C	316	LYS	2.5
1	C	26	CYS	2.5
1	D	322	GLU	2.5
1	C	264	GLY	2.5
1	D	359	LEU	2.5
1	A	695	ILE	2.5
1	B	498	SER	2.5
1	C	6	ARG	2.5
1	C	566	SER	2.5
1	A	41	GLN	2.5
1	B	352	SER	2.5
1	A	273	ILE	2.5
1	D	62	GLU	2.5
1	B	185	ALA	2.5
1	C	630	SER	2.5
1	D	76	THR	2.5
1	B	503	ARG	2.5
1	B	332	LEU	2.5
1	B	41	GLN	2.4
1	B	316	LYS	2.4
1	D	314	ILE	2.4
1	B	282	THR	2.4
1	B	238	CYS	2.4
1	C	381	LYS	2.4
1	D	646	LEU	2.4
1	B	422	ILE	2.4
1	D	412	ARG	2.4
1	A	178	ILE	2.4
1	B	569	ILE	2.4
1	D	550	LEU	2.4
1	C	53	THR	2.4
1	D	38	LYS	2.4
1	A	269	SER	2.4
1	B	421	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	427	LEU	2.4
1	D	618	ASN	2.4
1	C	238	CYS	2.4
1	C	300	TYR	2.4
1	D	454	ILE	2.4
1	B	177	GLY	2.4
1	D	336	ASP	2.4
1	A	121	TYR	2.4
1	C	240	LEU	2.4
1	A	609	ALA	2.4
1	D	668	GLY	2.4
1	A	618	ASN	2.4
1	B	687	VAL	2.4
1	D	551	ALA	2.4
1	D	560	PHE	2.4
1	D	455	GLU	2.4
1	A	118	ASP	2.4
1	A	119	ASP	2.4
1	A	569	ILE	2.4
1	B	625	THR	2.4
1	C	113	ALA	2.4
1	C	68	THR	2.4
1	A	449	ALA	2.4
1	B	480	ASN	2.4
1	C	39	VAL	2.4
1	A	402	PRO	2.4
1	C	375	GLU	2.4
1	A	246	GLY	2.4
1	B	571	GLN	2.4
1	B	743	LEU	2.4
1	D	46	GLY	2.4
1	D	300	TYR	2.4
1	B	223	MET	2.4
1	D	339	MET	2.4
1	B	52	THR	2.4
1	D	330	PRO	2.4
1	B	547	SER	2.4
1	B	704	VAL	2.4
1	A	103	ARG	2.4
1	C	203	PRO	2.4
1	B	694	THR	2.3
1	D	12	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	68	THR	2.3
1	B	407	LYS	2.3
1	C	266	ASN	2.3
1	D	343	GLU	2.3
1	B	275	MET	2.3
1	D	294	PRO	2.3
1	A	563	SER	2.3
1	C	695	ILE	2.3
1	A	165	GLU	2.3
1	B	374	TYR	2.3
1	A	539	ILE	2.3
1	A	65	ALA	2.3
1	A	450	LEU	2.3
1	D	337	LEU	2.3
1	C	357	PRO	2.3
1	C	698	MET	2.3
1	C	286	VAL	2.3
1	A	366	GLU	2.3
1	C	43	ILE	2.3
1	D	549	GLU	2.3
1	B	163	VAL	2.3
1	A	89	GLN	2.3
1	C	542	ALA	2.3
1	C	112	PRO	2.3
1	D	259	GLY	2.3
1	D	306	ALA	2.3
1	B	439	GLU	2.3
1	A	294	PRO	2.3
1	A	131	LEU	2.3
1	D	619	GLU	2.3
1	C	511	GLY	2.3
1	B	467	PHE	2.3
1	A	190	TYR	2.3
1	A	271	GLY	2.3
1	A	540	TYR	2.3
1	A	299	LEU	2.3
1	D	725	THR	2.3
1	B	331	ALA	2.3
1	A	238	CYS	2.3
1	C	359	LEU	2.3
1	C	611	THR	2.3
1	A	155	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	37	VAL	2.3
1	B	283	ALA	2.3
1	D	367	PHE	2.3
1	B	93	GLN	2.2
1	C	560	PHE	2.2
1	D	522	PRO	2.2
1	B	227	SER	2.2
1	B	269	SER	2.2
1	C	179	HIS	2.2
1	D	33	HIS	2.2
1	C	263	ALA	2.2
1	A	463	SER	2.2
1	B	672	GLY	2.2
1	A	244	THR	2.2
1	B	549	GLU	2.2
1	D	603	MET	2.2
1	D	82	ALA	2.2
1	C	174	VAL	2.2
1	A	464	THR	2.2
1	B	72	PRO	2.2
1	A	270	ASN	2.2
1	B	169	HIS	2.2
1	C	135	ILE	2.2
1	C	197	TYR	2.2
1	D	654	ILE	2.2
1	B	562	GLY	2.2
1	A	404	VAL	2.2
1	A	482	ASN	2.2
1	D	29	LEU	2.2
1	D	652	LEU	2.2
1	B	700	ALA	2.2
1	D	184	GLU	2.2
1	B	178	ILE	2.2
1	B	325	ALA	2.2
1	D	731	GLY	2.2
1	C	90	THR	2.2
1	B	229	GLU	2.2
1	A	224	LYS	2.2
1	B	544	MET	2.2
1	D	60	ALA	2.2
1	D	64	CYS	2.2
1	A	274	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	184	GLU	2.2
1	C	47	VAL	2.2
1	C	204	THR	2.2
1	A	330	PRO	2.2
1	B	438	ASP	2.2
1	A	347	THR	2.2
1	A	689	GLU	2.2
1	B	696	ILE	2.2
1	C	51	VAL	2.2
1	A	551	ALA	2.2
1	B	546	ALA	2.2
1	D	371	TYR	2.2
1	B	479	ARG	2.2
1	B	148	PHE	2.2
1	B	322	GLU	2.2
1	B	644	TYR	2.2
1	D	350	LEU	2.2
1	B	34	ILE	2.2
1	A	628	MET	2.1
1	B	685	LYS	2.1
1	B	53	THR	2.1
1	A	26	CYS	2.1
1	D	43	ILE	2.1
1	D	341	ARG	2.1
1	D	675	ASN	2.1
1	A	678	GLN	2.1
1	B	356	ALA	2.1
1	B	68	THR	2.1
1	D	372	THR	2.1
1	C	276	ILE	2.1
1	D	645	LEU	2.1
1	A	361	ASP	2.1
1	B	543	SER	2.1
1	C	48	TYR	2.1
1	C	120	VAL	2.1
1	C	699	ALA	2.1
1	B	514	ASP	2.1
1	B	453	PHE	2.1
1	A	287	ASP	2.1
1	A	414	SER	2.1
1	C	541	HIS	2.1
1	C	260	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	726	SER	2.1
1	A	311	PHE	2.1
1	B	428	CYS	2.1
1	C	697	ASN	2.1
1	A	236	LYS	2.1
1	C	489	TYR	2.1
1	A	239	ALA	2.1
1	A	283	ALA	2.1
1	D	465	TYR	2.1
1	D	574	MET	2.1
1	A	39	VAL	2.1
1	A	388	LEU	2.1
1	A	724	LEU	2.1
1	C	175	ALA	2.1
1	C	239	ALA	2.1
1	B	692	GLN	2.1
1	D	77	LEU	2.1
1	B	241	ILE	2.1
1	D	334	ILE	2.1
1	A	718	ALA	2.1
1	D	329	PHE	2.1
1	D	492	VAL	2.1
1	C	344	GLU	2.1
1	A	197	TYR	2.1
1	D	332	LEU	2.1
1	A	289	GLY	2.0
1	B	290	GLY	2.0
1	D	655	TRP	2.0
1	B	340	LYS	2.0
1	A	44	ILE	2.0
1	D	8	GLY	2.0
1	A	53	THR	2.0
1	A	88	LYS	2.0
1	A	210	THR	2.0
1	B	69	THR	2.0
1	D	315	ARG	2.0
1	A	242	SER	2.0
1	B	695	ILE	2.0
1	D	35	ASP	2.0
1	A	611	THR	2.0
1	C	284	ARG	2.0
1	A	356	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	727	MET	2.0
1	C	667	ASN	2.0
1	D	384	LYS	2.0
1	B	258	THR	2.0
1	A	389	TRP	2.0
1	B	124	VAL	2.0
1	D	163	VAL	2.0
1	C	83	ILE	2.0
1	B	408	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 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.