wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary 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:

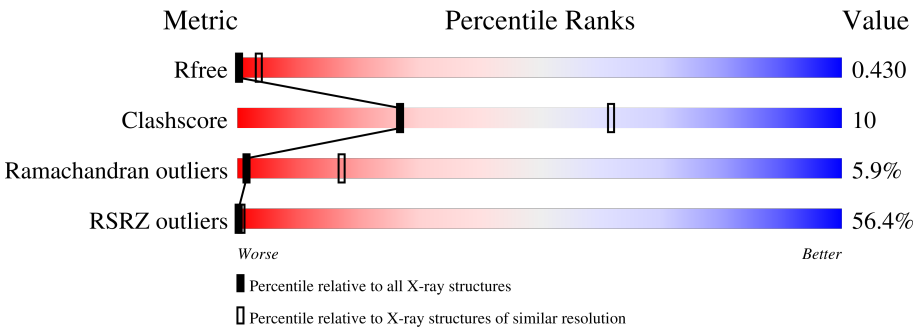
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

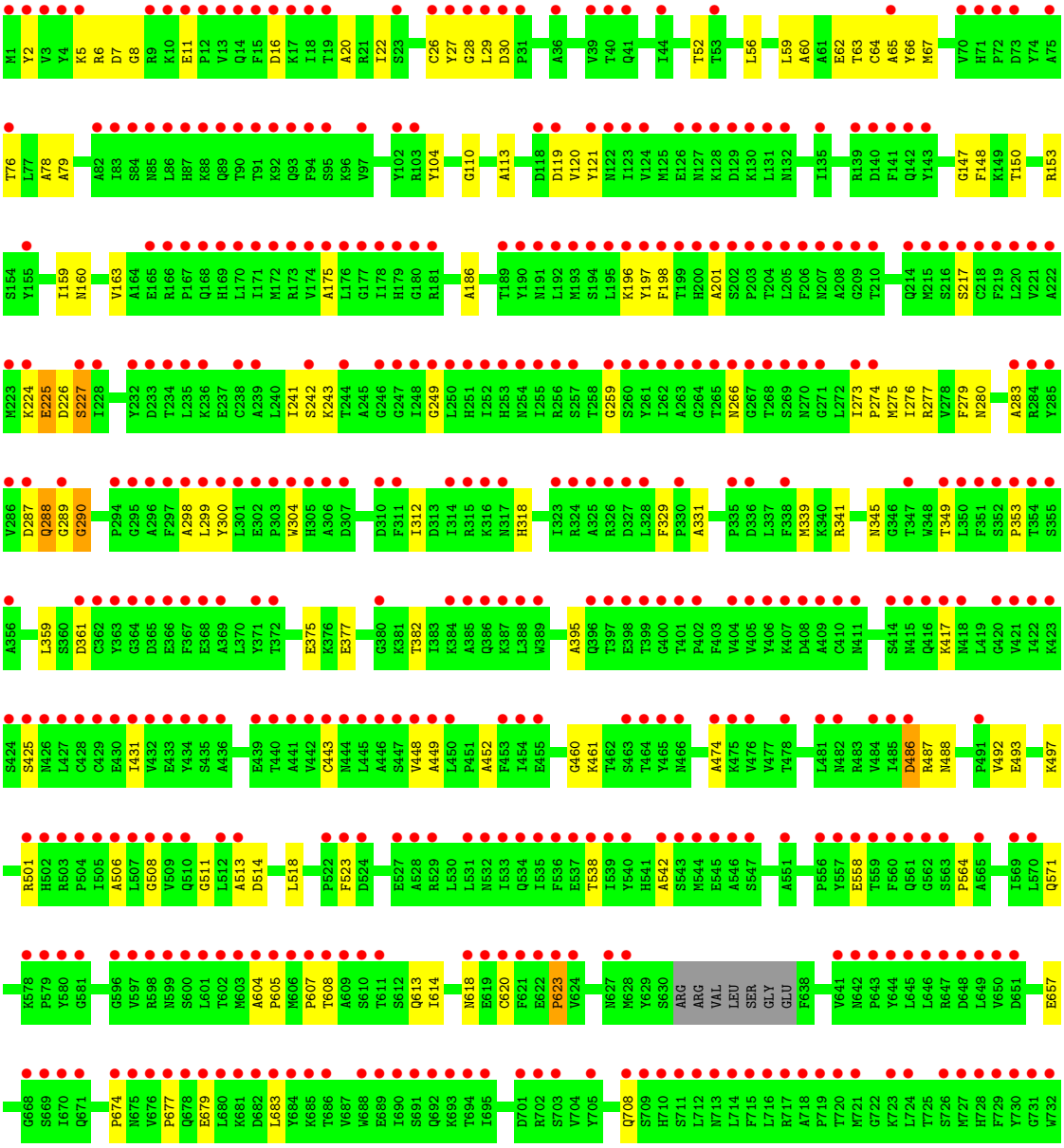
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	739	3649	2171	739	739	0	0	0
1	B	739	3649	2171	739	739	0	0	0
1	C	739	3649	2171	739	739	0	0	0
1	D	739	3649	2171	739	739	0	0	0

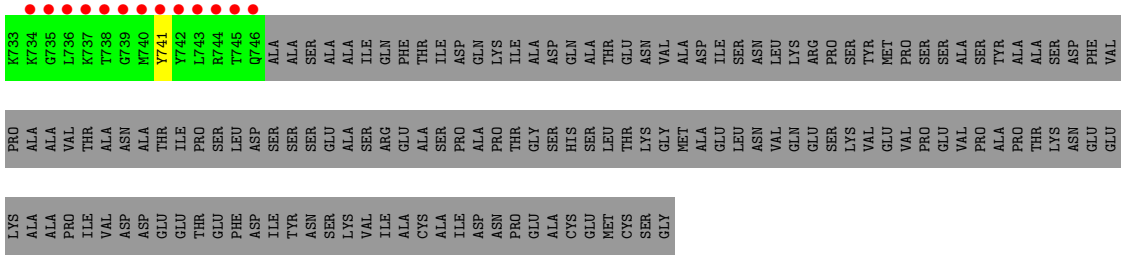
3 Residue-property plots (i)

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

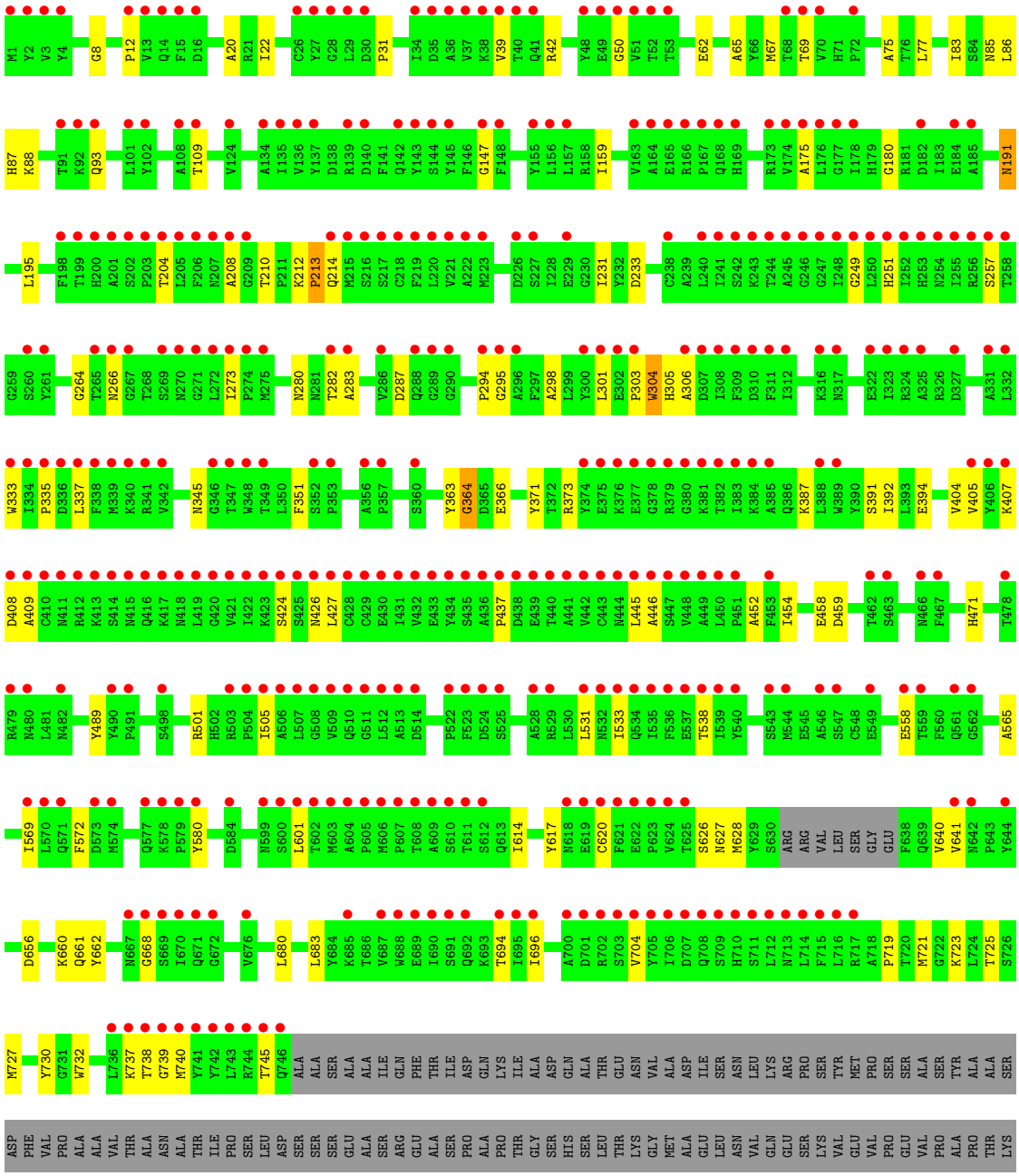
Chain A:





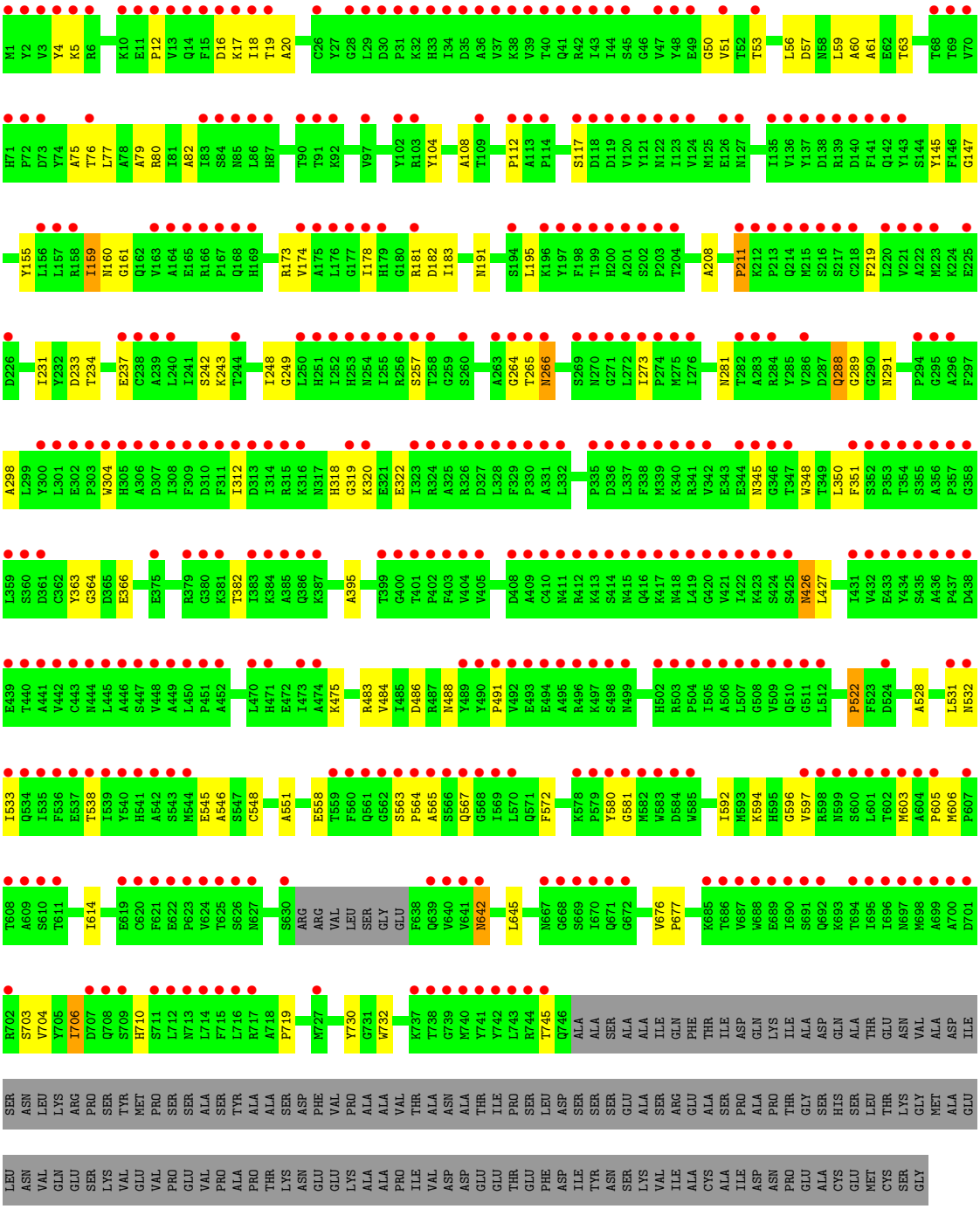
- Molecule 1: Ribonucleoside-diphosphate reductase large chain 1

Chain B:



• Molecule 1: Ribonucleoside-diphosphate reductase large chain 1

Chain C:



• Molecule 1: Ribonucleoside-diphosphate reductase large chain 1

Chain D:

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 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 VAL 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 ASP ALA THR ILE PRO SER LEU ASP 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 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 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.

The worst 5 of 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

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

5 of 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
1	A	486	ASP

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

The worst 5 of 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

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.