wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2021 – 03:51 AM EDT

PDB ID	:	1K25
Title	:	PBP2x from a Highly Penicillin-resistant Streptococcus pneumoniae Clinical Isolate
Authors	:	Dessen, A.; Mouz, N.; Hopkins, J.; Dideberg, O.
Deposited on	:	2001-09-26
Resolution	:	3.20 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 following versions of software and data (see references (1)) were used in the production of this report:

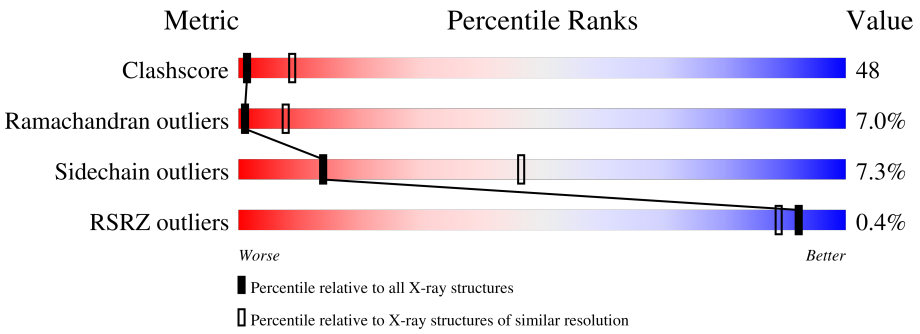
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.20 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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	685	28% 45% 7% • 19%
1	B	685	% 29% 48% 6% 16%
1	C	685	30% 42% 8% 20%
1	D	685	32% 43% 7% 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16786 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 low-affinity PENICILLIN-BINDING PROTEIN 2X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4161	2606	691	849	15	0	0	0
1	B	575	4311	2710	716	868	17	0	0	0
1	C	550	4114	2580	685	834	15	0	0	0
1	D	556	4179	2627	692	844	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	364	LEU	PHE	engineered mutation	UNP O34006
B	1364	LEU	PHE	engineered mutation	UNP O34006
C	2364	LEU	PHE	engineered mutation	UNP O34006
D	3364	LEU	PHE	engineered mutation	UNP O34006

- Molecule 2 is water.

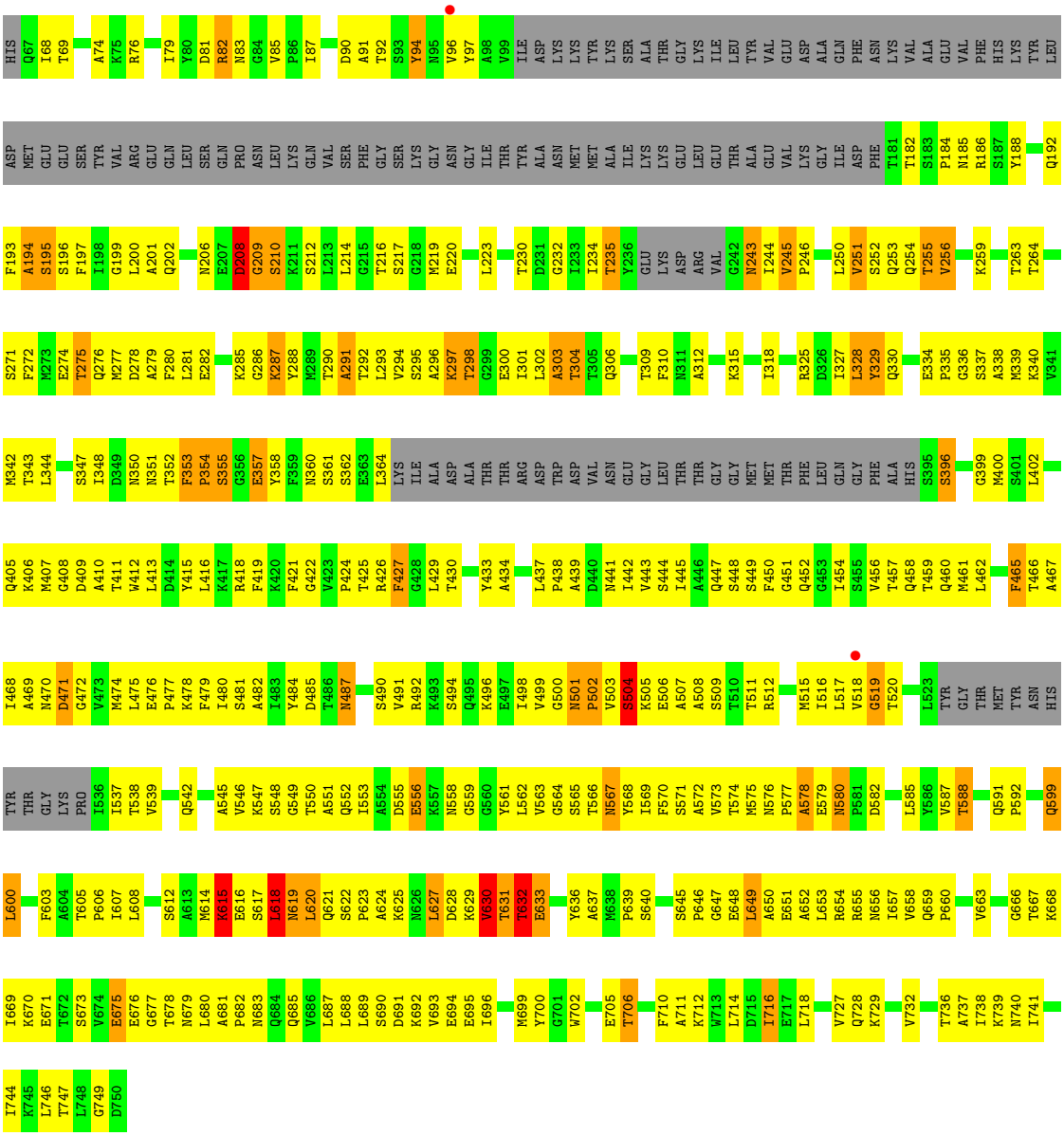
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	8	8	8	0	0
2	B	10	10	10	0	0
2	C	2	2	2	0	0
2	D	1	1	1	0	0

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.

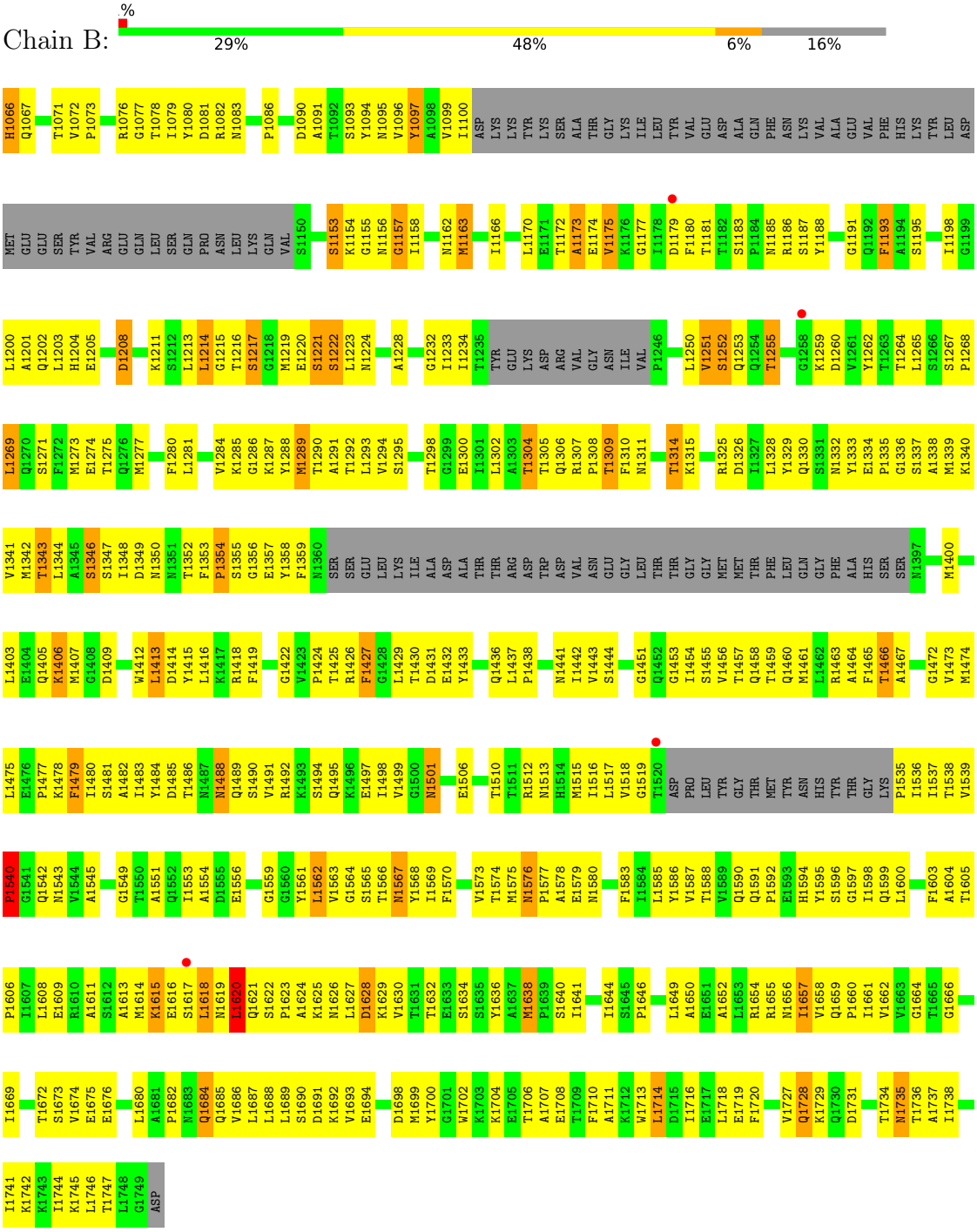
- Molecule 1: low-affinity PENICILLIN-BINDING PROTEIN 2X

Chain A: 28% 45% 7% • 19%



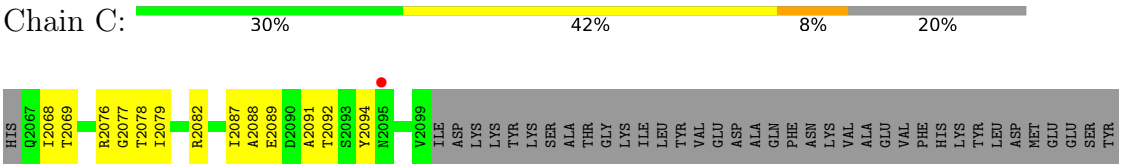
• Molecule 1: low-affinity PENICILLIN-BINDING PROTEIN 2X

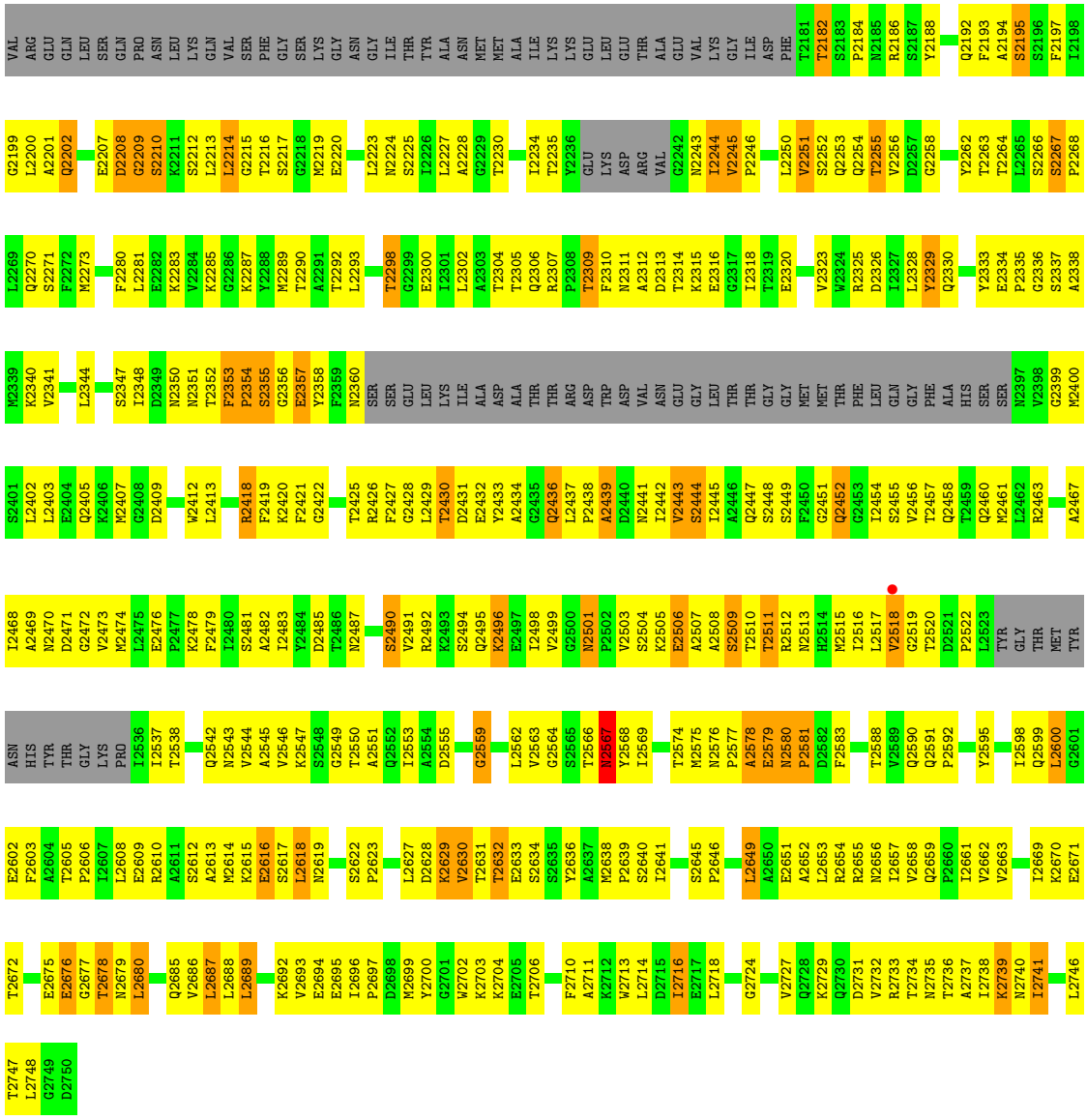
Chain B:



• Molecule 1: low-affinity PENICILLIN-BINDING PROTEIN 2X

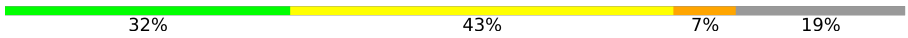
Chain C:

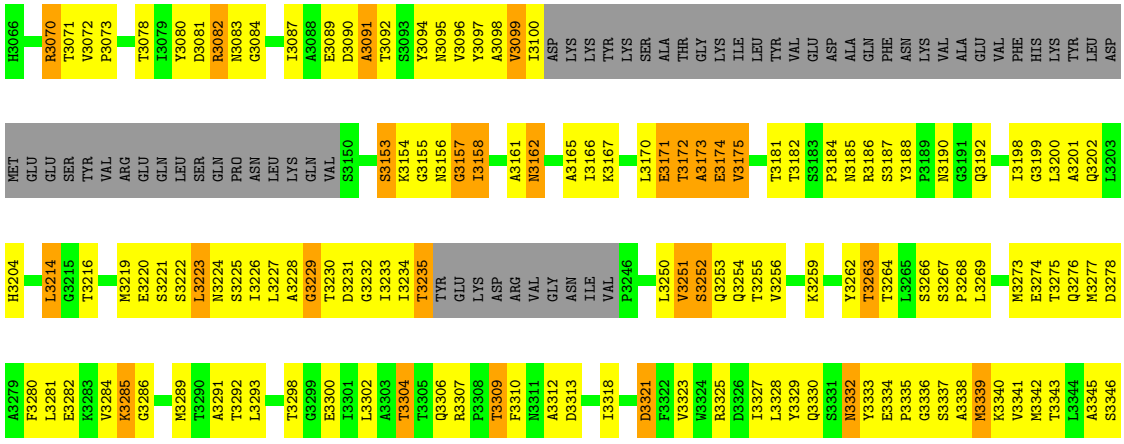


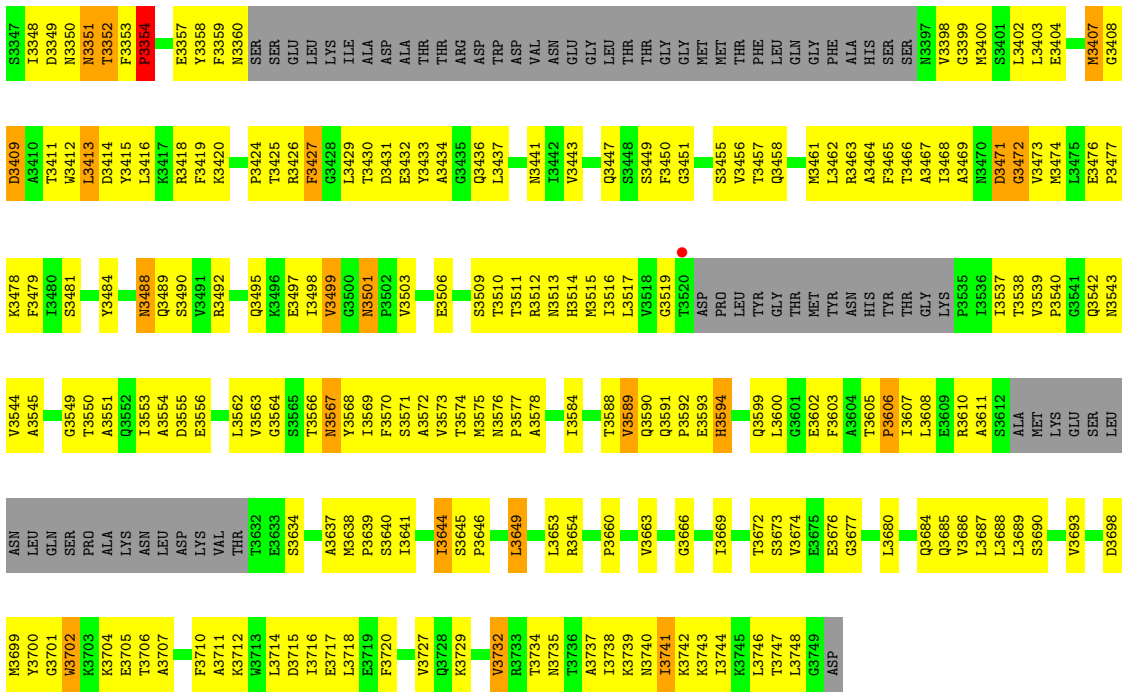


• Molecule 1: low-affinity PENICILLIN-BINDING PROTEIN 2X

Chain D:






S3347 I3348 D3349 N3350 N3351 T3352 F3353 P3354 E3357 Y3358 F3359 N3360 SER SER GLU LEU LYS ILE ALA ASP ALA THR THR ARG ASP TRP ASP VAL ASN GLU GLY LEU THR THR GLY GLY MET MET THR PHE LEU GLN GLY PHE ALA HIS SER SER N3397 V3398 G3399 M3400 S3401 L3402 L3403 E3404 M3407 G3408
D3409 A3410 T3411 W3412 L3413 D3414 Y3415 L3416 K3417 R3418 F3419 K3420 P3424 T3425 R3426 F3427 G3428 L3429 T3430 D3431 E3432 Y3433 A3434 G3435 Q3436 L3437 N3441 I3442 V3443 Q3447 S3448 S3449 F3450 G3451 S3455 V3456 T3457 Q3458 M3461 L3462 R3463 A3464 F3465 T3466 A3467 I3468 A3469 N3470 D3471 G3472 V3473 M3474 L3475 E3476 P3477
K3478 F3479 I3480 S3481 Y3484 N3488 Q3489 S3490 V3491 R3492 Q3495 K3496 E3497 I3498 V3499 G3500 N3501 P3502 V3503 E3506 S3509 T3510 T3511 R3512 N3513 H3514 M3515 I3516 L3517 V3518 G3519 T3520 ASP PRO LEU TYR GLY THR MET TYR ASN HIS TYR THR GLY LYS P3535 I3536 I3537 T3538 V3539 P3540 G3541 Q3542 N3543
V3544 A3545 G3549 T3550 A3551 Q3552 I3553 A3554 D3555 E3556 L3562 V3563 G3564 S3565 T3566 N3567 Y3568 I3569 F3570 S3571 A3572 V3573 T3574 M3575 N3576 P3577 A3578 I3584 T3588 V3589 Q3590 Q3591 P3592 E3593 H3594 Q3599 L3600 G3601 E3602 F3603 A3604 T3605 P3606 I3607 L3608 E3609 R3610 A3611 S3612 ALA MET LYS GLU SER LEU
ASN LEU GLN SER PRO ALA LYS ASN LEU ASP LYS VAL THR T3632 E3633 S3634 A3637 M3638 P3639 S3640 I3641 I3644 S3645 P3646 L3649 L3653 R3654 P3660 V3663 G3666 I3669 T3672 S3673 V3674 E3675 E3676 G3677 L3680 Q3684 Q3685 V3686 L3687 L3688 L3689 S3690 V3693 D3698
M3699 Y3700 G3701 W3702 K3703 K3704 E3705 T3706 A3707 F3710 A3711 K3712 W3713 L3714 D3715 I3716 E3717 L3718 E3719 F3720 V3727 Q3728 K3729 V3732 R3733 T3734 N3735 I3736 A3737 I3738 K3739 N3740 I3741 K3742 K3743 I3744 K3745 L3746 T3747 L3748 G3749 ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	146.56Å 146.56Å 132.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 3.20 24.94 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.0 (19.90-3.20) 89.0 (24.94-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 3.23Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.235 , 0.312 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 4.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.428 for -h,-k,l 0.148 for h,-h-k,-l 0.147 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	16786	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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	0.46	0/4229	0.77	4/5747 (0.1%)
1	B	0.44	0/4383	0.74	0/5951
1	C	0.47	0/4182	0.75	1/5684 (0.0%)
1	D	0.45	0/4248	0.75	1/5766 (0.0%)
All	All	0.46	0/17042	0.75	6/23148 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	630	VAL	N-CA-C	10.02	138.05	111.00
1	A	630	VAL	CB-CA-C	-9.35	93.64	111.40
1	A	630	VAL	CA-C-N	-5.79	104.46	117.20
1	A	632	THR	N-CA-C	-5.13	97.16	111.00
1	D	3437	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	2329	TYR	Sidechain

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	4161	0	4017	420	0
1	B	4311	0	4182	430	0
1	C	4114	0	3962	380	0
1	D	4179	0	4052	362	0
2	A	8	0	0	1	0
2	B	10	0	0	5	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
All	All	16786	0	16213	1581	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 48.

The worst 5 of 1581 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:629:LYS:O	1:A:630:VAL:HG13	1.43	1.18
1:A:618:LEU:HD23	1:A:618:LEU:H	1.04	1.11
1:D:3672:THR:HG22	1:D:3674:VAL:H	1.07	1.09
1:D:3590:GLN:HG2	1:D:3591:GLN:HG3	1.35	1.08
1:C:2714:LEU:HD13	1:C:2738:ILE:HD11	1.34	1.04

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	546/685 (80%)	401 (73%)	105 (19%)	40 (7%)	1 7
1	B	565/685 (82%)	431 (76%)	99 (18%)	35 (6%)	1 11
1	C	540/685 (79%)	390 (72%)	106 (20%)	44 (8%)	1 5
1	D	544/685 (79%)	430 (79%)	80 (15%)	34 (6%)	1 10
All	All	2195/2740 (80%)	1652 (75%)	390 (18%)	153 (7%)	1 8

5 of 153 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	194	ALA
1	A	209	GLY
1	A	251	VAL
1	A	252	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	449/583 (77%)	413 (92%)	36 (8%)	12 42
1	B	461/583 (79%)	429 (93%)	32 (7%)	15 49
1	C	439/583 (75%)	403 (92%)	36 (8%)	11 41
1	D	448/583 (77%)	421 (94%)	27 (6%)	19 54
All	All	1797/2332 (77%)	1666 (93%)	131 (7%)	14 46

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3321	ASP
1	D	3427	PHE
1	D	3732	VAL
1	B	1304	THR
1	B	1289	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2470	ASN
1	C	2656	ASN
1	D	3580	ASN
1	C	2501	ASN
1	C	2580	ASN

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	556/685 (81%)	-0.26	2 (0%)	92	89	3, 26, 59, 100	0
1	B	575/685 (83%)	-0.23	4 (0%)	87	81	7, 29, 62, 81	0
1	C	550/685 (80%)	-0.26	2 (0%)	92	89	4, 27, 58, 99	0
1	D	556/685 (81%)	-0.25	1 (0%)	95	94	7, 30, 56, 88	0
All	All	2237/2740 (81%)	-0.25	9 (0%)	92	89	3, 28, 59, 100	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3520	THR	3.5
1	B	1520	THR	3.4
1	A	518	VAL	3.0
1	B	1179	ASP	2.7
1	C	2518	VAL	2.6

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.