wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:27 PM GMT

PDB ID	:	1TR2
Title	:	Crystal structure of human full-length vinculin (residues 1-1066)
Authors	:	Borgon, R.A.; Vonrhein, C.; Bricogne, G.; Bois, P.R.; Izard, T.
Deposited on	:	2004-06-19
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

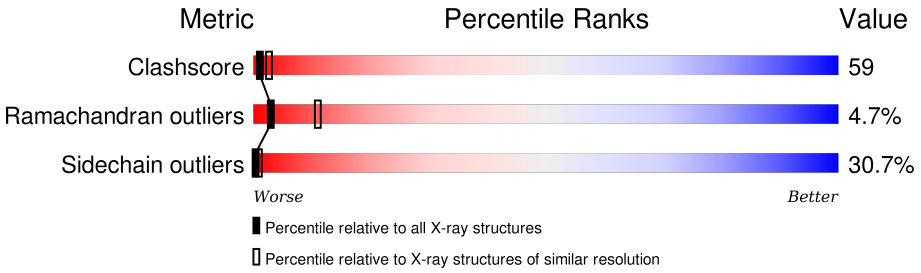
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1066	28% 48% 19%
1	B	1066	29% 48% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16033 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 VINCULIN ISOFORM 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1028	Total	C	N	O	S	Se	99	8	0
			7908	4876	1436	1550	10	36			
1	B	1029	Total	C	N	O	S	Se	117	7	0
			7907	4873	1438	1550	10	36			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	INITIATING METHIONINE	UNP P18206
A	26	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	74	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	94	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	154	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	168	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	171	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	174	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	190	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	195	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	209	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	237	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	266	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	327	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	331	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	350	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	377	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	533	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	534	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	587	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	591	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	698	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	709	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	741	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	748	MSE	MET	MODIFIED RESIDUE	UNP P18206

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Chain	Residue	Modelled	Actual	Comment	Reference
A	797	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	799	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	898	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	899	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	900	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	926	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	930	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	933	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	1005	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	1022	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	1031	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	1	MSE	MET	INITIATING METHIONINE	UNP P18206
B	26	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	74	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	94	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	154	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	168	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	171	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	174	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	190	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	195	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	209	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	237	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	266	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	327	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	331	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	350	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	377	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	533	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	534	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	587	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	591	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	698	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	709	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	741	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	748	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	797	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	799	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	898	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	899	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	900	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	926	MSE	MET	MODIFIED RESIDUE	UNP P18206

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Chain	Residue	Modelled	Actual	Comment	Reference
B	930	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	933	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	1005	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	1022	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	1031	MSE	MET	MODIFIED RESIDUE	UNP P18206

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	108	Total O 108 108	0	0
2	B	110	Total O 110 110	0	0

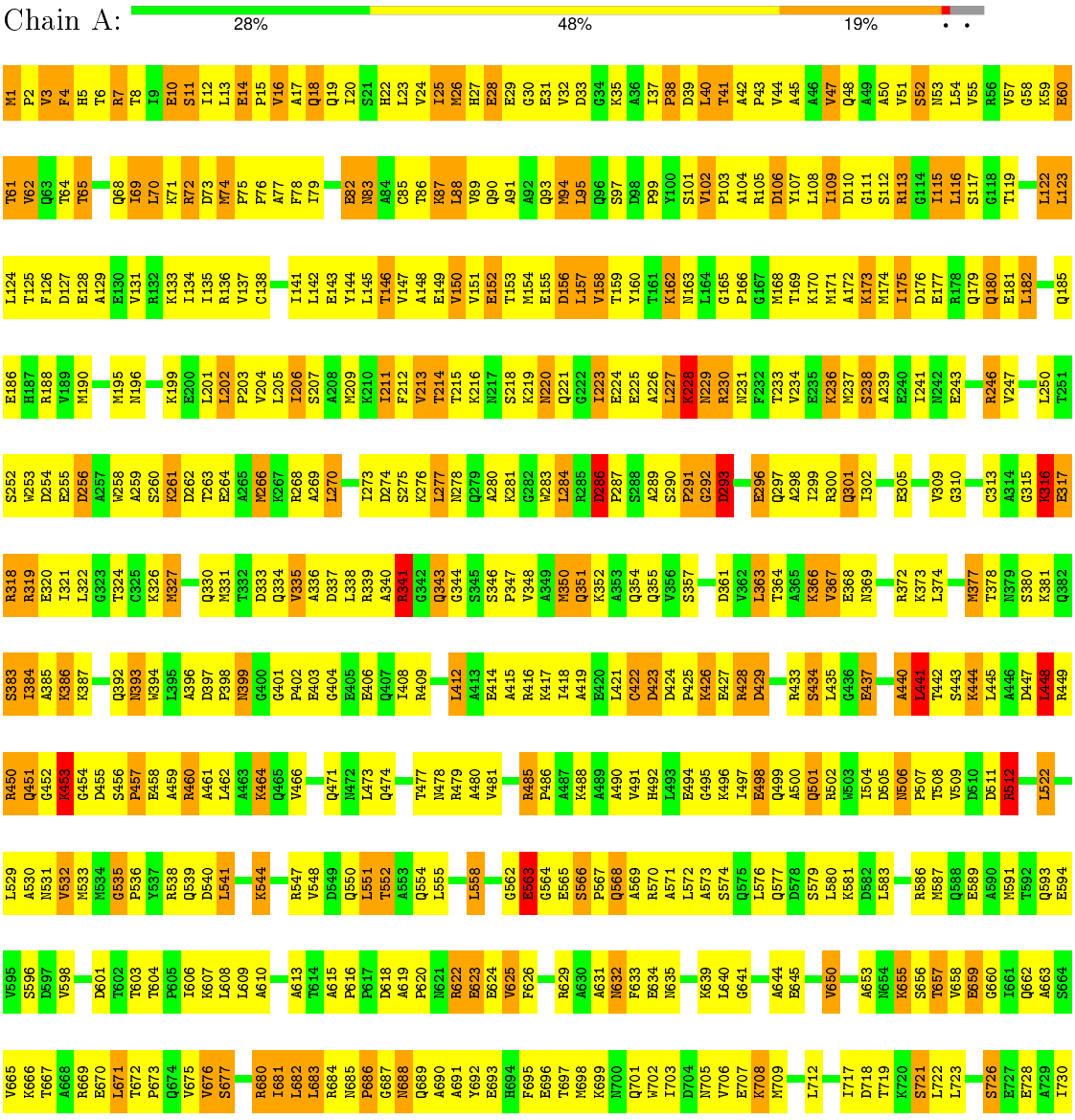
3 Residue-property plots (i)

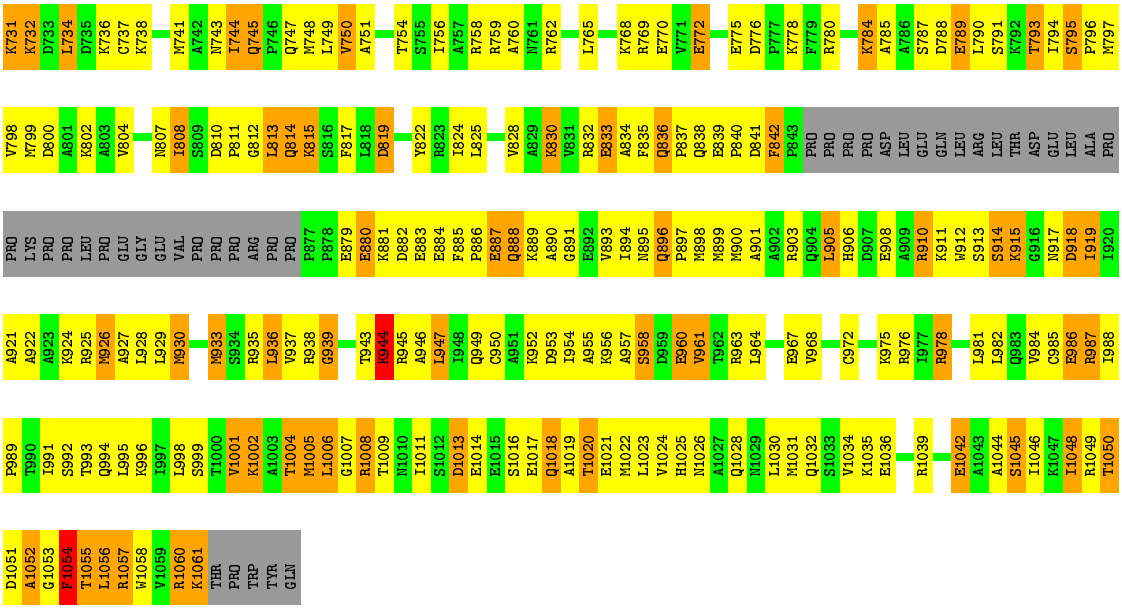
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: VINCULIN ISOFORM 1

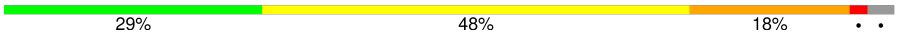
Chain A:

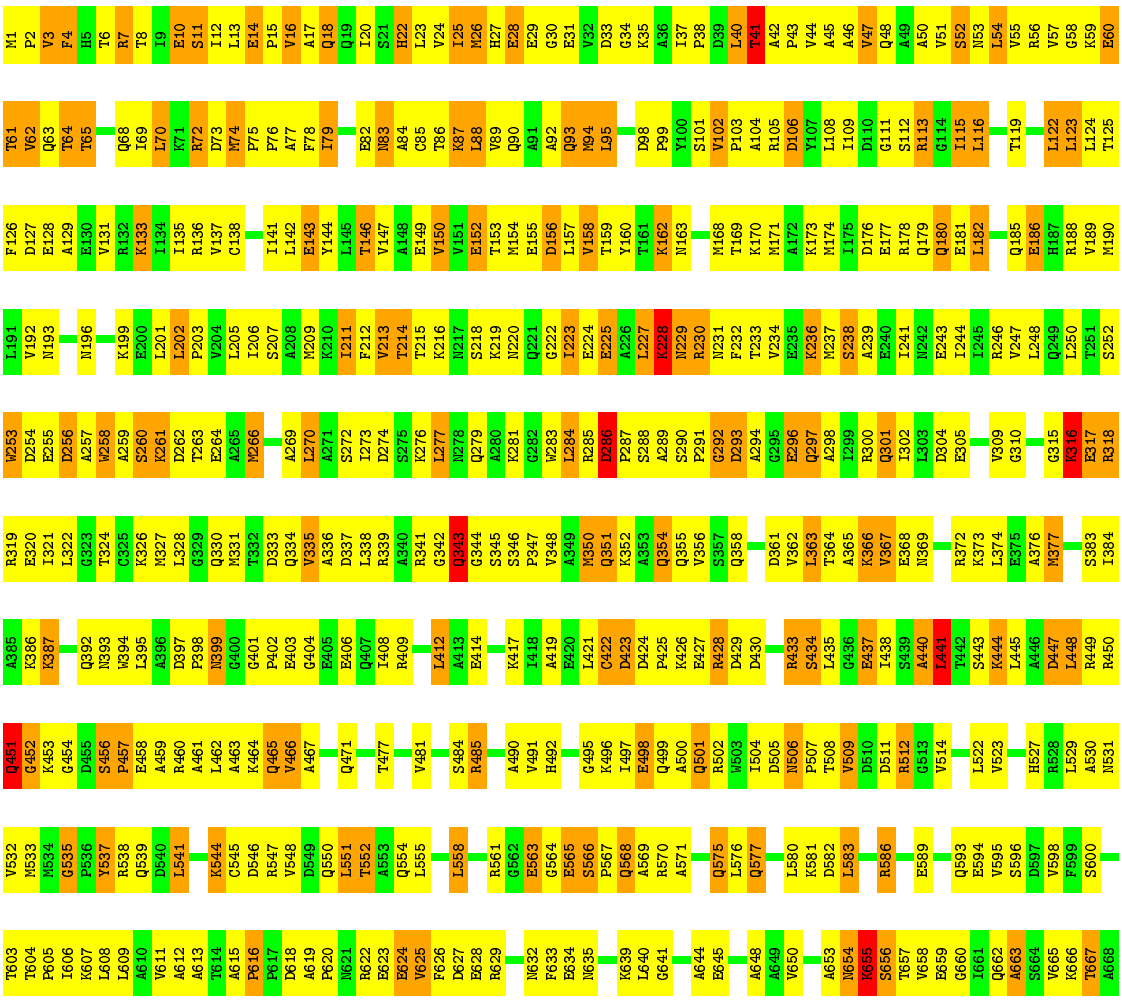


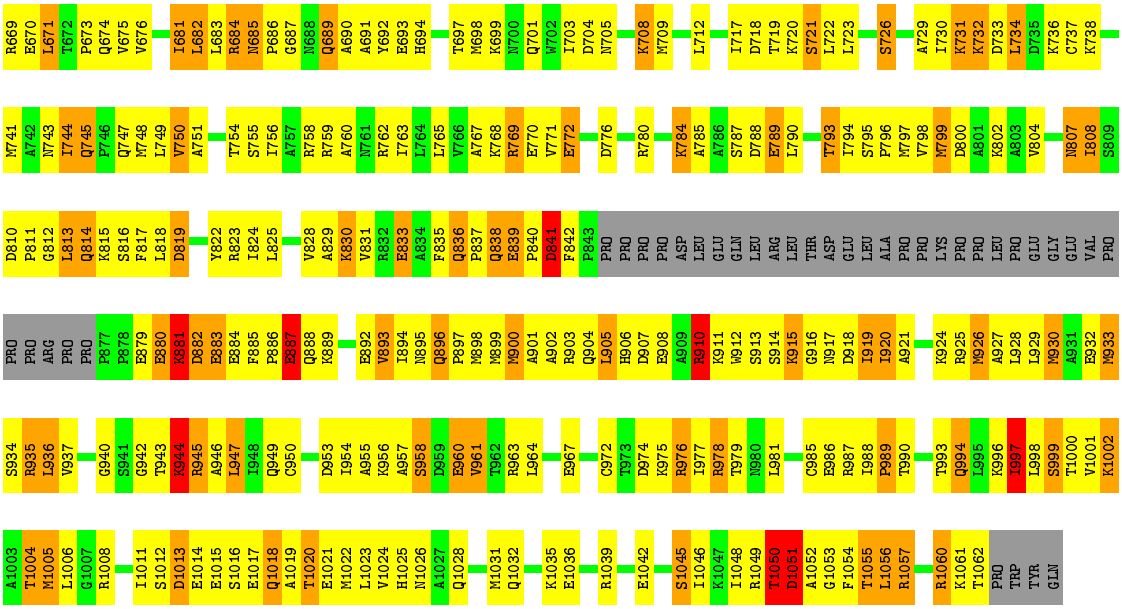


• Molecule 1: VINCULIN ISOFORM 1

Chain B:






R669 E670 L671 T672 P673 Q674 V675 V676 I681 L682 L683 R684 N685 P686 G687 N688 Q689 A690 A691 Y692 E693 H694 T697 M698 K699 N700 Q701 W702 I703 D704 N705 K708 M709 L712 I717 D718 T719 K720 S721 L722 L723 S726 A729 I730 K731 K732 D733 L734 D735 K736 C737 K738
M741 A742 N743 I744 Q745 P746 Q747 M748 L749 V750 A751 T754 S755 I756 A757 R758 R759 A760 N761 R762 I763 L764 L765 V766 A767 K768 R769 E770 V771 E772 D776 R780 K784 A785 A786 S787 D788 E789 L790 T793 I794 S795 P796 M797 V798 M799 D800 A801 K802 A803 V804 N807 I808 S809
D810 P811 G812 L813 Q814 K815 S816 F817 L818 D819 Y822 R823 I824 L825 V828 A829 K830 V831 R832 E833 A834 F835 Q836 P837 Q838 E839 P840 D841 F842 P843 PRO PRO PRO PRO ASP LEU GLU GLN LEU ARG LEU THR ASP GLU LEU ALA PRO PRO LYS PRO PRO LEU PRO GLU GLY GLU VAL PRO
PRO PRO ARG PRO PRO P877 P878 E879 E880 M881 D882 E883 E884 F885 P886 E887 Q888 K889 E892 V893 I894 N895 Q896 P897 M898 M899 N900 A901 A902 R903 Q904 L905 H906 D907 E908 A909 N910 K911 W912 S913 S914 K915 G916 N917 D918 I919 I920 A921 K924 R925 M926 A927 L928 L929 M930 A931 E932 M933
S934 R935 L936 V937 G940 S941 G942 T943 M944 R945 A946 L947 I948 Q949 C950 D953 I954 A955 K956 A957 S958 D959 E960 V961 T962 R963 L964 E967 G972 T973 D974 K975 R976 I977 R978 T979 N980 L981 C985 E986 R987 I988 P989 T990 T993 Q994 L995 K996 I997 L998 S999 T1000 V1001 K1002
A1003 T1004 M1005 L1006 G1007 R1008 I1011 S1012 D1013 E1014 E1015 S1016 E1017 Q1018 A1019 T1020 E1021 M1022 L1023 V1024 H1025 N1026 A1027 Q1028 M1031 Q1032 K1035 E1036 R1039 E1042 S1045 I1046 K1047 I1048 R1049 T1050 D1051 A1052 G1053 F1054 T1055 L1056 R1057 R1060 K1061 T1062 PRO TRP TYR GLN

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.74Å 154.08Å 108.95Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	56.86 – 2.90	Depositor
% Data completeness (in resolution range)	100.0 (56.86-2.90)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	BUSTER-TNT V. 1.1.1	Depositor
R, R_{free}	0.232 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16033	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.39	0/7994	0.61	2/10720 (0.0%)
1	B	0.38	0/7992	0.60	1/10717 (0.0%)
All	All	0.38	0/15986	0.61	3/21437 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1054	PHE	CB-CG-CD2	-10.78	113.25	120.80
1	A	1054	PHE	CB-CG-CD1	7.84	126.29	120.80
1	B	616	PRO	CA-N-CD	-5.02	104.48	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	7908	0	8065	912	0
1	B	7907	0	8072	958	0
2	A	108	0	0	12	0
2	B	110	0	0	12	0
All	All	16033	0	16137	1865	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 59.

The worst 5 of 1865 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:B:65:THR:HG21	1:B:70:LEU:HD22	1.21	1.18
1:A:74:MSE:HE3	1:A:122:LEU:HD21	1.18	1.18
1:B:913:SER:HB2	1:B:915:LYS:HG3	1.24	1.17
1:B:729:ALA:HA	1:B:732:LYS:HD3	1.24	1.16
1:B:215:THR:HG22	1:B:223:ILE:HG13	1.26	1.16

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	1032/1066 (97%)	849 (82%)	140 (14%)	43 (4%)	3 13
1	B	1032/1066 (97%)	849 (82%)	130 (13%)	53 (5%)	2 9
All	All	2064/2132 (97%)	1698 (82%)	270 (13%)	96 (5%)	3 11

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	402	PRO
1	A	441	LEU
1	A	453	LYS
1	A	686	PRO

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	850/842 (101%)	587 (69%)	263 (31%)	0 1
1	B	850/842 (101%)	590 (69%)	260 (31%)	0 1
All	All	1700/1684 (101%)	1177 (69%)	523 (31%)	0 1

5 of 523 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1002	LYS
1	B	83	ASN
1	B	944	LYS
1	A	1011	ILE
1	B	7	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	662	GLN
1	A	1025	HIS
1	B	895	ASN
1	A	701	GLN
1	A	904	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.