



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:09 PM UTC

PDB ID : 1TR2 / pdb\_00001tr2  
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](mailto: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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

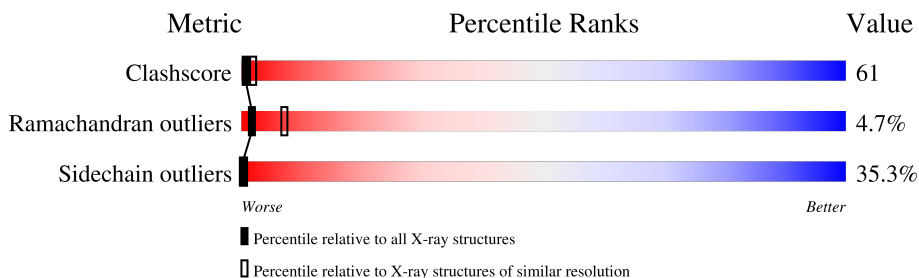
# 1 Overall quality at a glance

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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1066	 27% 46% 22% . .
1	B	1066	 27% 44% 23% . .

## 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
			Total	C	N	O	S	Se			
1	A	1028	7908	4876	1436	1550	10	36	99	8	0
1	B	1029	7907	4873	1438	1550	10	36	117	7	0

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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.

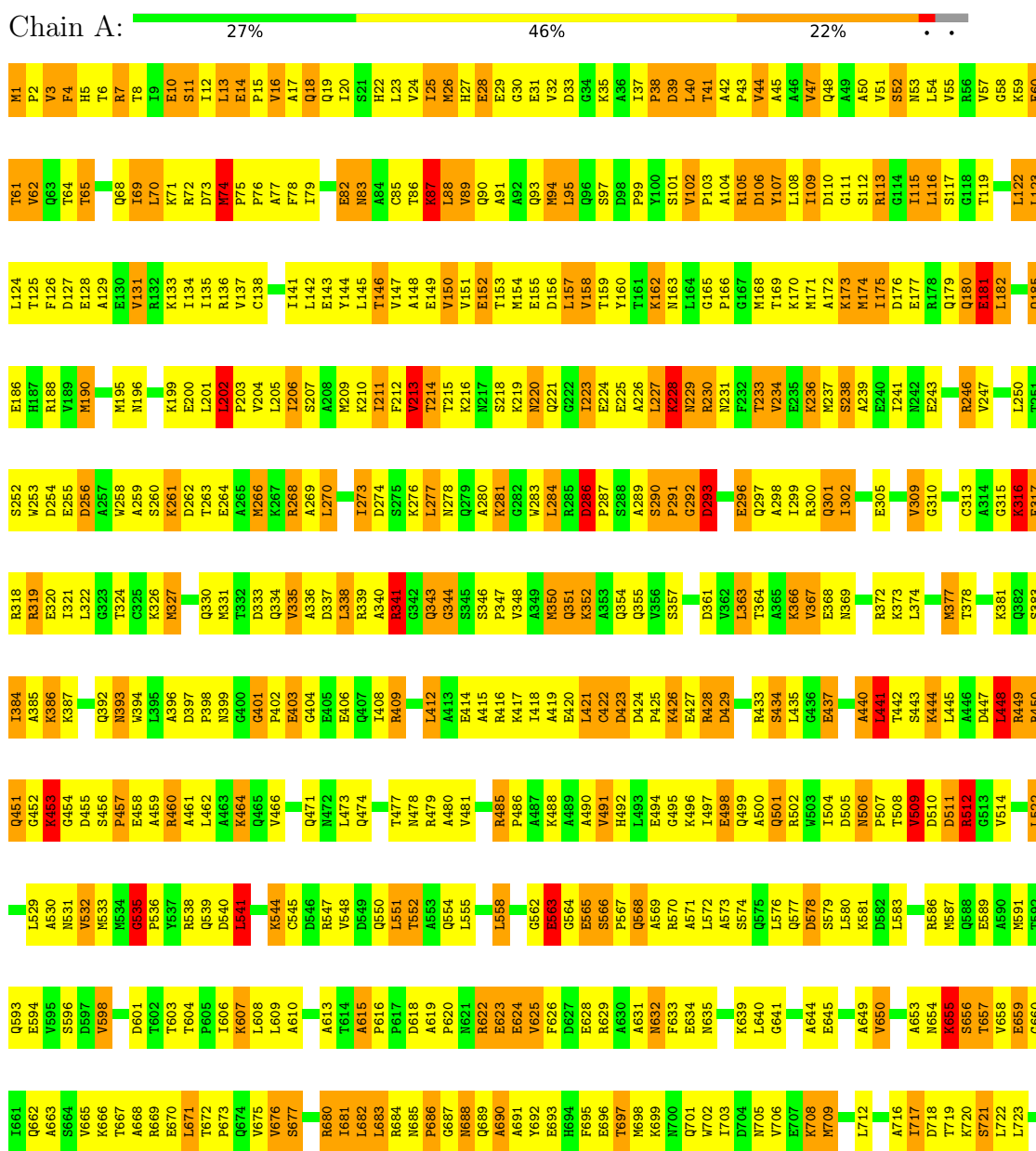
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	108	Total O 108 108	0	0
2	B	110	Total O 110 110	0	0

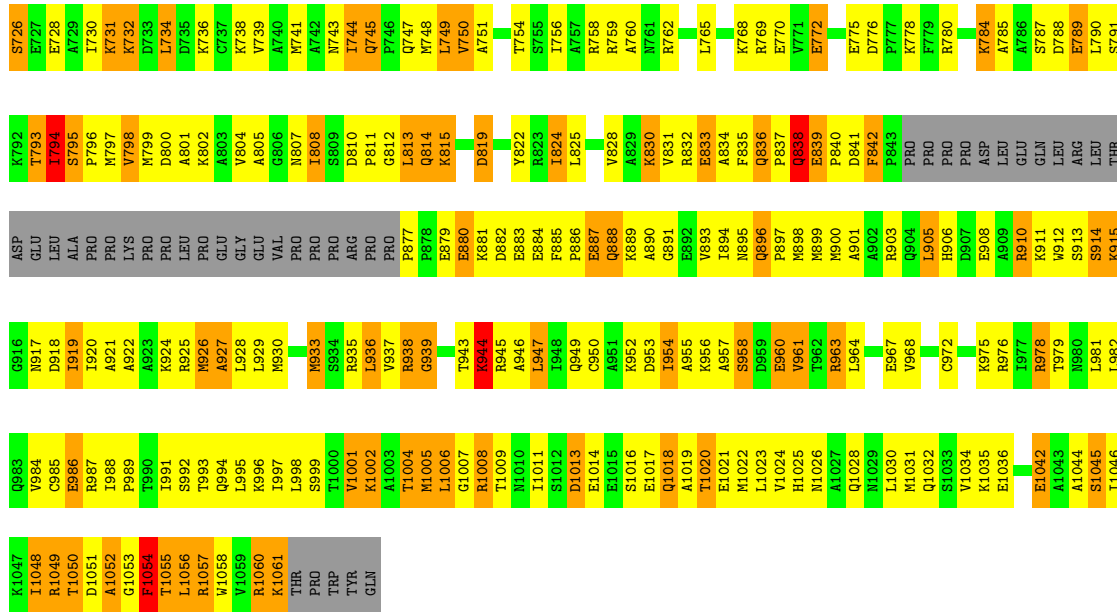
### 3 Residue-property plots

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. 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. 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.

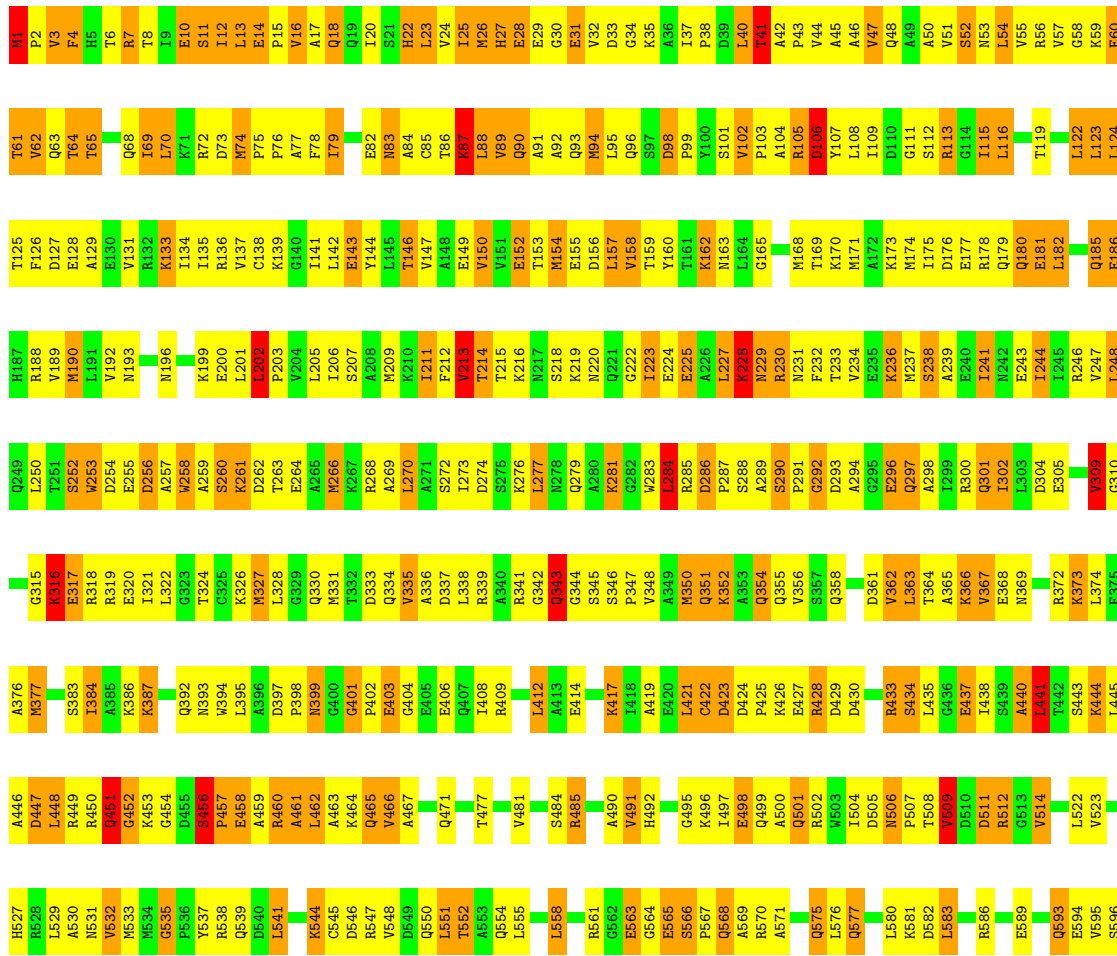
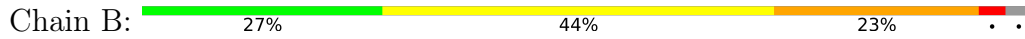
Note EDS was not executed.

- Molecule 1: VINCULIN ISOFORM 1





● Molecule 1: VINCULIN ISOFORM 1



TRP	L995	R925	D800	D733	D597
TYR	K996	M926	A801	L734	V598
GLN	I997	A927	K802	D735	F599
	L998	L928	A803	K736	S600
	S999	L929	V804	K737	T603
	T1000	M930	N807	K738	T604
	V1001	A931	I808	V739	P605
	K1002	E932	S809	A740	P606
	A1003	M933	D810	M741	K607
	T1004	S934	P811	A742	P673
	M1005	R935	P812	N743	L608
	L1006	L936	A812	I744	L609
	G1007	V937	L813	Q745	A610
	R1008	G940	Q814	F746	V611
	I1011	S941	K815	Q747	A612
	S1012	G942	S816	M748	A613
	D1013	T943	F817	L749	T614
	E1014	K944	L818	V750	A615
	E1015	R945	D819	A751	P616
	S1016	A946	Y822	T754	F617
	E1017	L947	R823	S755	D618
	Q1018	I948	I824	I756	A619
	A1019	Q949	L825	A757	P620
	T1020	C950	V828	R758	R622
	E1021	D953	K829	R759	E623
	M1022	I954	A830	A760	E624
	L1023	A955	V831	R762	V625
	V1024	K956	R832	I763	F626
	H1025	A957	E833	L764	D627
	M1026	S958	F835	L765	E628
	A1027	D959	P836	V766	R629
	Q1028	E960	P837	A767	M632
	M1031	V961	M838	K768	F633
	Q1032	T962	M839	R769	E634
	K1035	R963	M900	E770	M635
	E1036	L964	A901	V771	K639
	E1042	E967	A902	E772	L640
	S1045	C972	R903	D776	G641
	I1046	T973	L905	D777	A644
	K1047	D974	H906	R780	E645
	I1048	K975	D907	K784	A648
	R1049	R976	E908	A785	A649
	R1050	R977	A909	A786	V650
	D1051	R978	K911	S787	D718
	A1052	L981	W912	D788	T719
	G1053	C985	S913	E789	K720
	F1054	E986	S914	L790	S721
	T1055	R987	K915	S791	L722
	L1056	I988	G916	K792	S656
	R1057	P989	N917	T793	T657
	R1060	T990	D918	I794	V658
	K1061	T993	I919	S795	E659
	T1062	Q994	I920	P796	G660
	PRO		A921	V797	I661
			K924	M799	Q662
					A663

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 1.1.1	Depositor
R, $R_{free}$	0.232 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	16033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

## 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	0.51	0/7994	1.06	42/10720 (0.4%)
1	B	0.51	0/7992	1.05	53/10717 (0.5%)
All	All	0.51	0/15986	1.05	95/21437 (0.4%)

There are no bond length outliers.

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	675	VAL	N-CA-C	-11.51	102.53	111.62
1	A	794	ILE	N-CA-C	11.27	121.02	110.42
1	A	107	TYR	N-CA-C	-9.30	101.36	112.89
1	A	615	ALA	CA-C-N	9.29	129.95	120.38
1	A	615	ALA	C-N-CA	9.29	129.95	120.38

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	7908	0	8065	937	0
1	B	7907	0	8072	979	0
2	A	108	0	0	12	0
2	B	110	0	0	12	0
All	All	16033	0	16137	1911	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 61.

The worst 5 of 1911 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%)	2	9
1	B	1032/1066 (97%)	849 (82%)	130 (13%)	53 (5%)	1	6
All	All	2064/2132 (97%)	1698 (82%)	270 (13%)	96 (5%)	2	7

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%)	557 (66%)	293 (34%)	0	0
1	B	850/842 (101%)	543 (64%)	307 (36%)	0	0
All	All	1700/1684 (101%)	1100 (65%)	600 (35%)	0	0

5 of 600 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	566	SER
1	B	994	GLN
1	B	625	VAL
1	B	565	GLU
1	B	787	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	93	GLN
1	B	471	GLN
1	B	1026	ASN
1	B	895	ASN
1	B	179	GLN

### 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 oligosaccharides 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.