



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 21, 2024 – 01:34 PM EDT

PDB ID : 1TR2
Title : Crystal structure of human full-length vinculin (residues 1-1066)
Authors : Borgon, R.A.; Vonnrhein, 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

<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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

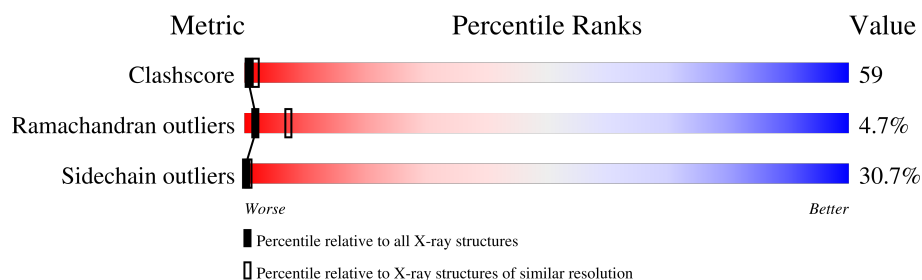
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

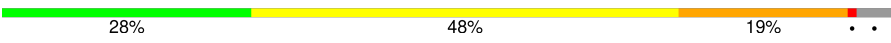
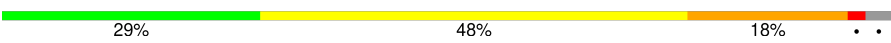
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (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 ≥ 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	 28% 48% 19% . .
1	B	1066	 29% 48% 18% . .

2 Entry composition

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
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B	377	MSE	MET	modified residue	UNP P18206
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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.

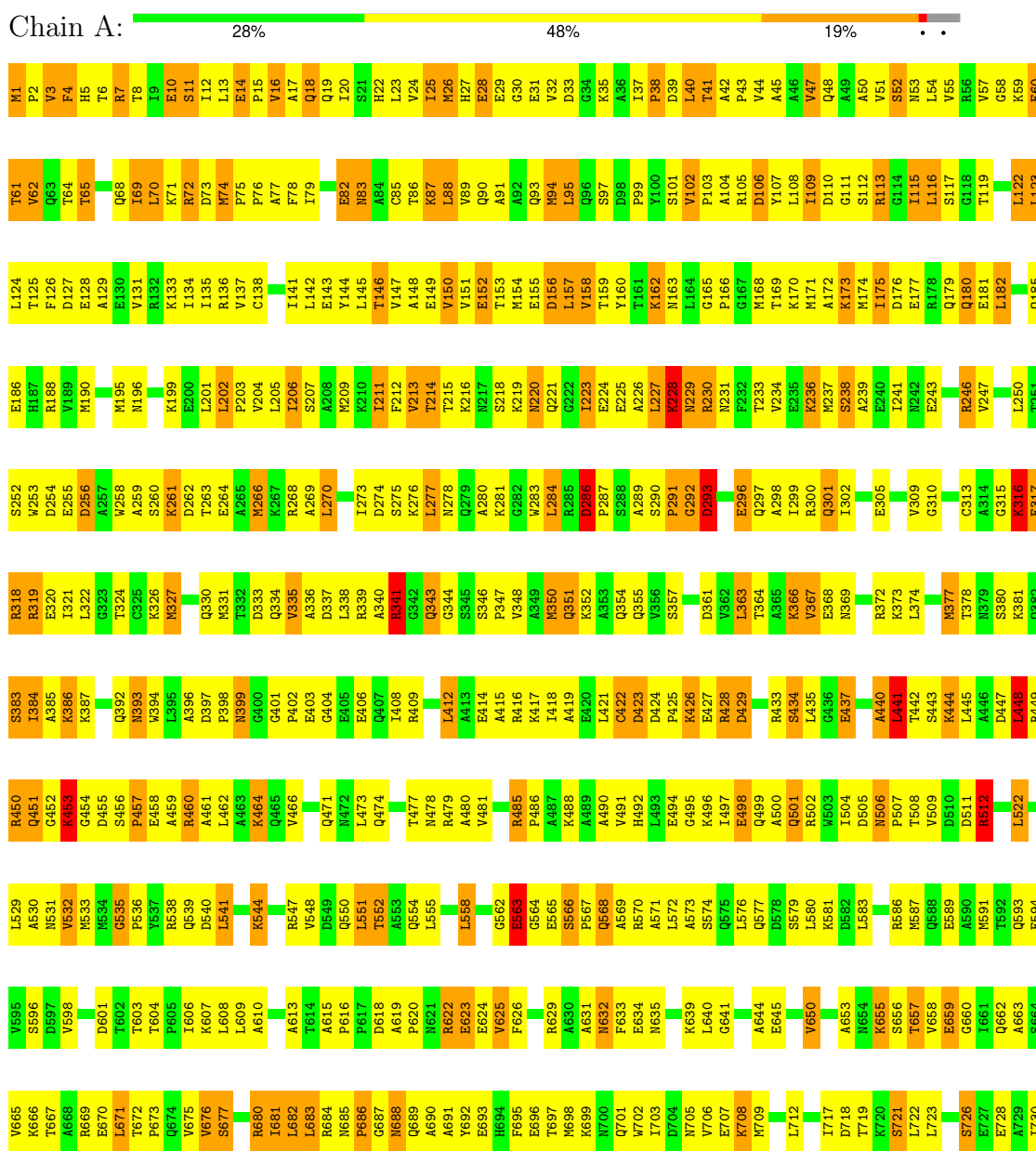
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	108	Total 108	O 108	0	0
2	B	110	Total 110	O 110	0	0

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



D1051	P889	A921	PR0	V798	K731
A1052	T990	A922	LYS	M799	K732
G1053	T991	A923	PRO	D800	D733
F1054	S992	K924	PRO	A801	L734
T1055	T993	R925	LEU	K802	D735
L1056	Q994	M826	PRO	A803	K736
R1057	L995	A927	GLU	V804	K737
W1058	K996	L928	GLY		K738
V1059	T997	L929		N807	
R1060	L998	M930	VAL	I808	M741
K1061	S999		PRO	S809	A742
THR	T1000	M833	PRO	D810	N743
PRO	V1001	S934	PRO	P811	I744
TRP	K1002	R935	ARG	G812	Q745
TYR	A1003	L936	PRO	L813	T746
GLN	T1004	V937	PRO	Q814	Q747
	M1005	R938		K815	M748
	L1006	G839	P877	S816	L749
	G1007		P878	F817	V750
	R1008	T943	E879	L818	A751
	T1009	R944	K881	D819	
	M1010	R945	D882		T754
	I1011	A946	E883	Y822	S755
	S1012	L947	E884	R823	I756
	D1013	L948	F885	I824	A757
	E1014	Q949	P886	L825	R758
	E1015	Q950	E887		R759
	S1016	A951	O158	V828	A760
	E1017	K952	K889	A829	N761
	Q1018	D953	A890	K830	R762
	A1019	L954	G891	E831	
	T1020	A955	E892	R832	L765
	E1021	R956	V993	E833	
	M1022	A957	I894	A834	K768
	L1023	S958	N895	F835	R769
	V1024	D959	Q896	Q836	E770
	H1025	E960	P897	P837	V771
	M1026	N961	M898	Q838	E772
	A1027	T962	M899	E839	
	Q1028	R963	M900	P840	E775
	N1029	L964	A901	D841	D776
	L1030		A902	F842	P777
	M1031	E967	R903	P843	K778
	Q1032	V968	Q904	PR0	F779
	S1033		L905	PR0	R780
	V1034	C972	H906	PR0	
	K1035		D907	PR0	K784
	E1036	K975	E908	ASP	A785
		R976	A909	LEU	A786
		I977	R910	GLU	R787
		R978	K911	GLN	D788
			W912	LEU	E789
			S913	ARG	L790
		L981	S914	LEU	S791
		L982	G915	THR	K792
		Q983	R916	ASP	T793
		V984	N917	GLU	I794
		C985	D918	LEU	S795
		E986	D918	GLU	P796
		R987	I919	ALA	M797
		T988	E920	PR0	

• Molecule 1: VINCULIN ISOFORM 1

Chain B: 29% 48% 18%

V532	Q451	A385	R319	W253	L191	F126	T61	M1
M533	K452	K386	E320	D254	V192	D127	V62	P2
M534	K453	K387	I321	E255	N193	E128	Q63	V3
G535	G454		L322	D256		A129	T64	F4
P536	D455	Q392	G323	A257	N196	E130	T65	H5
Y537	S456	N393	T324	W258		V131		T6
R538	P457	V394	C325	A259	K199	R132	Q68	R7
Q539	E458	L395	K326	S260		K133	T69	R8
D540	A459	A396	M327	D261	L201	I134	L70	I9
R460	R460	D397	L328	D262	L202	I135	K71	E10
A461	A461	P398	G329	T263	P203	R136	R72	S11
L462	L462	N399	Q330	E264	R204	V137	D73	I12
C545	A463	G400	N331	A265	L205	C138	M74	L13
D546	K464	G401	T332	S207	I206		P75	E14
R547	Q465	P402	D333	S207			P76	P15
V466	V466	E403	Q334	A208	V160	L142	A77	V16
D549	A467	G404	V335	L270	M209	E143	F78	A17
Q550		E405	A336	A271	K210	Y144	I79	Q18
L551	Q471	E406	D337	S272	I211	L145		Q19
T552	T477	Q407	L338	I273	F212	T146	E82	I20
A553		R408	R339	D274	V213	V147	N83	S21
Q554		R409	A340	S275	T214	A148	A84	H22
L555	V481		R341	K276	T215	E149	C85	L23
		L412	G342	L277	K216	V150	T86	V24
L558	S484	E413	Q343	N278	M217	E151	A87	I25
	R485	E414	G344	Q279	S218	E152	M26	G30
R561	A490	K417	S345	A280	K219	T153	V89	E31
E562	V491	V418	S346	K281	N220	M154	Q90	H27
G564	H492	A419	P347	G282	Q221	E155	A91	E28
E565		E420	V348	W283	G222	D156	A92	E29
S566	G495	L421	A349	L284	I223	L157	Q93	G30
P567	K496	C422	M350	R285	E224	V158	M94	E31
Q568	L497	D423	K352	D286	E225	T159	V32	D33
A569	E498	D424	A353	P287	A226	Y160	G34	G34
R570	Q499	P425	Q354	S288	L227	T161	D98	K35
A571	A500	K426	Q354	A289	K228	K162	P99	A36
	Q501	R428	V356	S290	N230	M163	Y100	I37
Q575	R502	E427	S357	P291	R231		S101	P38
L576	S503	D429	Q358	G292	F232	T169	V102	D39
Q577	L504	D430		A294	T233	K170	P103	L40
	D505		D361	G295	V234	M171	R105	F41
L580	N506	R433	V362	E296	E235	A172	D106	A42
K581	P507	L434	L363	Q297	K173	K173	P43	P43
D582	T508	L435	T364	A298	M237	M174	Y107	V44
L583	V509	G436	A365	L299	S238	I175	L108	A45
	D510	E437	K366	R300	A239	D176	I109	A46
R586	D511	L438	V367	Q301	E240	E177	D110	V47
	R512	E439	E368	I302	T241	R178	G111	Q48
E589	G513	A440	N369	L303	N242	Q179	S112	A49
	V514	L441	R372	D304	E243	Q180	R113	A50
Q593	L522	S443	K373	E305	T245	E181	G114	V51
E594	V523	K444	L374	V309	R246	L182	I115	S52
V595		L445	E375	G310	V247	Q185	L116	N53
S596	H527	L446	A376	G315	L248	E186	T119	L54
D597	R528	A447	M377		Q249	H187		V55
V598	L529	L448		G316	L250	R188	L122	V57
F599	A530	R449	S383	E317	T251	R189	L123	G58
S600	N521	R450	L384	R216	S252	V199	L124	K59
						A190	T125	E60

PRO	S934	A1003	D810	W741	R669	T603
	R935	T1004	PRO	A742	E670	T604
	L936	M1005	ARG	W743	L671	G605
	V937	L1006	PRO	T744	T672	I606
		G1007	PRO	Q745	P673	K607
	G940	R1008	K815	W746	Q674	L608
	S941	I1011	S816	Q747	V675	L609
	G942		E879	W748	V676	A610
	T943		E880	L818	L749	V611
	R944		PRO	D819	W750	A612
R945	E1014	D882	A751	L682	A613	
A946	E1015	E883	Y822	L683	T614	
L947	S1016	E884		T754	A615	
I948	E1017	F885		S755	N685	P616
Q949	Q1018	P886		I756	P686	P617
C950	E1019	S887	A757	G687	D618	
		Q888	R758	N688	A619	
T1020	E1020	K889	R759	Q689	P620	
D953	E1021	E892	A760	A690	N621	
L954	L1022		W761	A691	R622	
A955	L1023		R762	Y692	E623	
K956	V1024		K763	G693	E624	
A957	H1025	E893	I763	V694	V625	
S958	M1026	N895	L764	H694	F626	
D959	A1027	K896	L765	T697	D627	
E960	Q1028	P897	W766		M698	E628
V961	M1031	M898	A767		K699	R629
T962		K898	K768		N705	N632
R963	Q1032	N900	R769	Q701		F633
L964	E1036	P840	E770	W702		E634
E967		A901	V771	I703		D704
	Q972	L905	E772	W705	K639	L640
T973	R1039	H906	D776	K708	G641	
D974	E1042	D907	R780	W709	A644	
K975	S1045	E908		L712	E645	
R976		A909	K784	I717	A648	
I977	L1046	R910	A785	D718	A649	
K978	K1047	K911	A786	T719	V650	
T979	L1048	W912	S787	K720	A653	
N980	R1049	S913	D788	L722	N654	
L981	T1050	S914	E789	L734	K655	
		K915	L790	D733	S656	
C985	A1051	ARG	S726	T657	T657	
	D1052	LEU		S721	V658	
E986	L1052	THR	A729	I730	E659	
R987	G1053	G916	T793	K731	G660	
F1054	R987	N917	I794	W732	T661	
T1055	L1054	D918	T795	D733	Q662	
I988	L1055	T919	S795	L734	A663	
P989	L1056	I920	W796	D733	S664	
T990	R1057	A921	P797	K736	V665	
	T993	PRO	W797	C737	T667	
T994	K1061	PRO	W798	K738	A669	
L995	T1062	LYS	T799	A729		
K996	PRO	R925	D800	I730		
T997		M926	K731	K732		
L998	TRP	PRO	A801	T732		
S999	TYR	LEU	K802	D733		
T1000	GLN	PRO	A803	L734		
E1001	GLN	L928	W804	D733		
		L929	G803	L734		
A931		GLY	K807	V665		
E932		GLU	T808	T667		
W932		VAL	K738	A669		

4 Data and refinement statistics

Xtriage (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, 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 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 [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	0.39	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(°)	Ideal(°)
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 [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	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%)	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%)	587 (69%)	263 (31%)	0	0
1	B	850/842 (101%)	590 (69%)	260 (31%)	0	1
All	All	1700/1684 (101%)	1177 (69%)	523 (31%)	0	0

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

Mol	Chain	Res	Type
1	B	879	GLU
1	B	919	ILE
1	B	841	ASP
1	B	1057	ARG
1	A	814	GLN

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

Mol	Chain	Res	Type
1	B	351	GLN
1	B	807	ASN
1	B	472	ASN
1	B	593	GLN
1	B	888	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 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.