



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:29 PM UTC

PDB ID : 3S5K / pdb_00003s5k
Title : Crystal structures of falcilysin, a M16 metalloprotease from the malaria parasite *Plasmodium falciparum*
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Deposited on : 2011-05-23
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

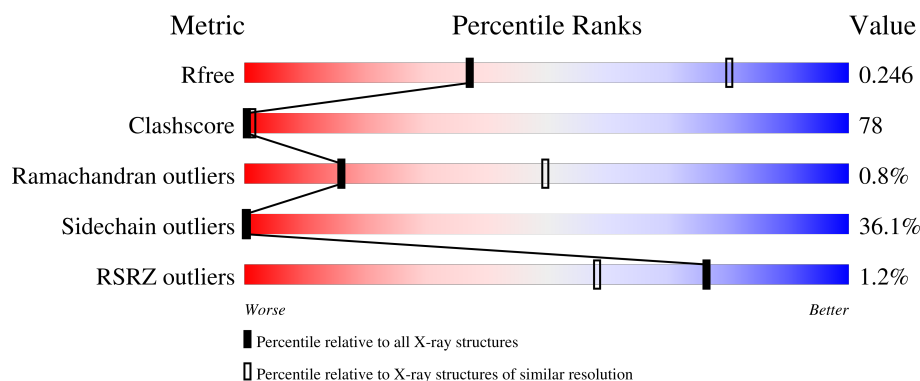
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 $\leq 5\%$. 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	1193	14% 36% 30% 8% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8741 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 Falcilysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1053	Total	C	N	O	S	0	0	0
			8674	5577	1418	1653	26			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

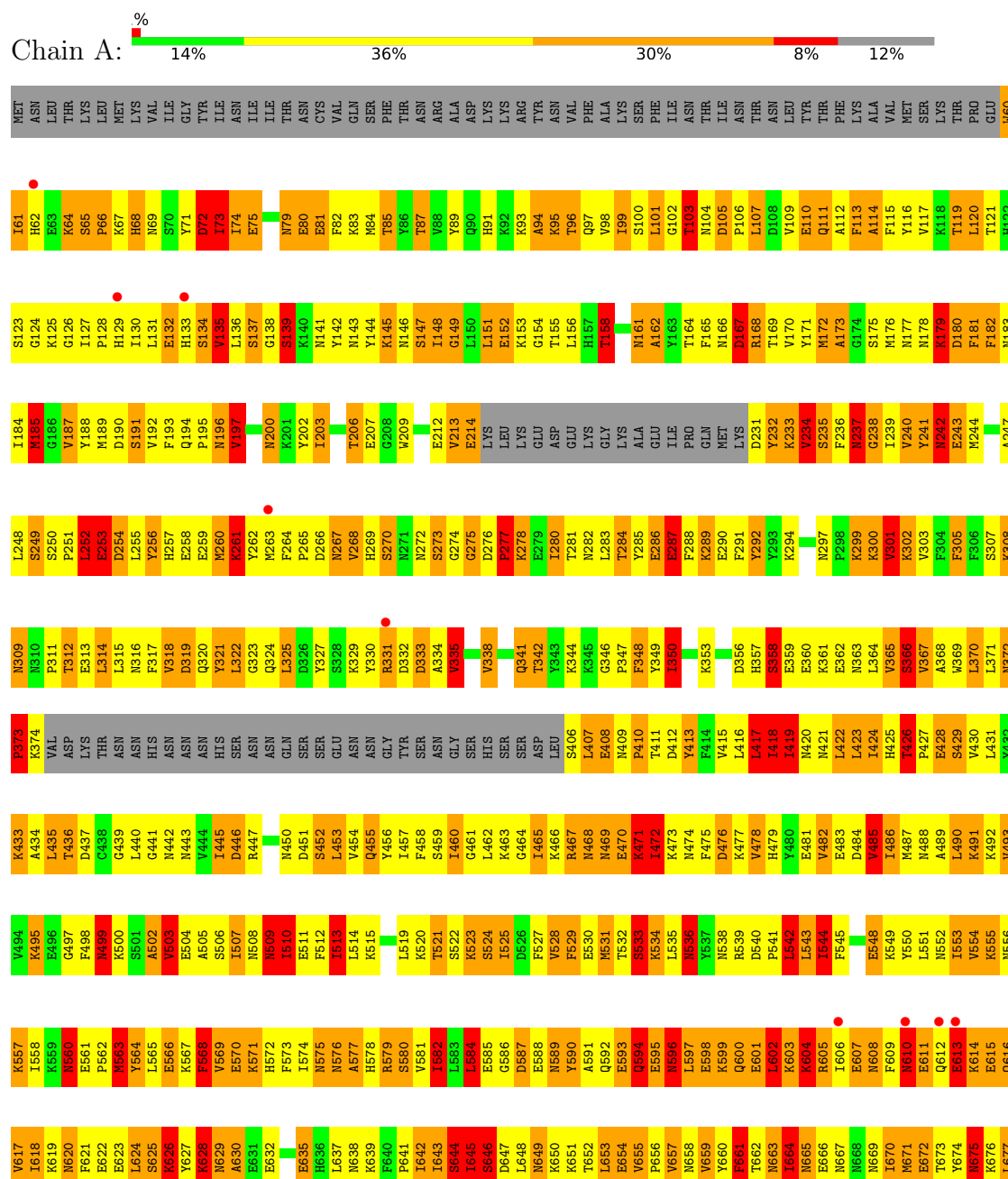
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		

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 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: Falcilysin



E1174	K1110	Y1049	K988	K927	K366	H802	L739	K678
K1175	F1111	G1050	L989	A928	G867	L803	V740	T679
A1176	R1112	F1051	F990	Y929	Y868	N804	V741	M690
N1177	R1113	F1052	D991	A869	A869	N804	L742	E681
E1178	G1114	A1053	E992	Y931	A870	T806	Q743	H692
Y1179	T1115	D1054	E993	S932	L871	K808	F744	M683
I1180	E1116	T1085	K994	Y933	H872	F745	V745	L684
A1181	L1117	E1086	Y995	T934	K873	F746	F746	K685
N1182	S1118	Y1057	S935	S935	H874	S747	S747	D696
V1183	K1119	D1058	K997	D936	H875	A811	L748	N687
D1184	L1120	G1059	E998	Y937	K876	Q812	D749	M688
G1185	S1121	S1060	F999	Q938	L879	A813	H750	D689
E1186	F1122	V1061	A939	A939	H860	L834	L751	V690
F1187	L1123	V1062	L940	L940	S881	F815	T752	F691
K1188	R1124	F1063	K941	K941	K882	H816	V753	L692
K1189	L1125	L1064	H942	H942	H883	L817		K693
V1190	T1126	S1065	L943	L943	H883	L817	L756	K694
L1191	S1127	A1066	F944	F944	Y884	M819	A757	Y695
I1192	N1128	R1067	Y945	Y945	A885	H820	Y758	V696
E1193	Q1132	P1068	A946	A946	H886	V821	L759	L697
		P1069	S947	S947	N887	L822	N760	K698
		N1070	N948	N948	L888	S823	ASN	ASN
	V1135	L1071	E949	E949	Y890	C826	ASP	ASP
E1136	F1137	E1072	S950	S950	G891	K763	LYS	LYS
R1138	K1139	K1073	L951	L951	Y892	T764	HIS	HIS
K1139	R1140	L1075	E953	E953	E893	L765	ASN	ASN
R1140	T1141	A1076	F1016	F1016	N894	L766	THR	THR
T1141		T1077	Y955	Y955	H895	E768	ASN	ASN
M1142		F1078	S956	S956	L896	N769	ASN	ASN
N1143	T1143	R1079	Y957	Y957	K897	K770	ASN	ASN
T1144	K1145	E1080	F958	F958	L998	T771	ASN	ASN
K1146	K1146	S1081	E959	E959	Q899		ASN	ASN
E1147	K1147	A1082	E960	E960	K838	R774	ASN	ASN
D1148	D1148	K1083	N961	N961	E839	S775	ASN	ASN
F1149	F1149	G1084	D962	D962	S840	S776	ASN	ASN
		L1085	K963	K963	D841	E777	MET	MET
		R1086	Y964	Y964	F842	D778	ASP	ASP
		K1087	T1026	T1026	S843	F779	TYR	TYR
F1152	A1153	M1088	T1027	T1027	K846	V780	SER	SER
D1154	D1154		V1028	V1028	K847	L781	PHE	PHE
L1155	L1155		I1029	I1029	D908	L782	THR	THR
L1156	L1156		Y1030	Y1030	F909	R783	E720	E720
E1157	E1157	M1092	A1031	A1031	K910	E784	T721	T721
S1158	S1158	T1093	L1032	L1032	T911	D850	K722	K722
K1159	K1159	N1095	K1034	K1034	E912	L851	Y723	Y723
V1160	V1160	D1096	N1035	N1035	E913	L852	E724	E724
N1161	N1161	L1097	S1036	S1036	N914	K853	G725	G725
E1162	E1162	L1098	Y1037	Y1037	J915	R854	N726	N726
F1163	F1163	R1099	L1038	L1038	L916	K855	V727	V727
E1164	E1164	Y1100	W1039	W1039	V917	L856	F728	F728
K1165	K1165	T1101	D1040	D1040	R918	N857	I729	I729
N1166	N1166	I1102	T1041	T1041	G979	C858		
T1167	T1167	N1103	V1042	V1042	Y980	H859	A795	A795
V1168	V1168	T1104	R1043	R1043	N921	K860	L796	L796
T1169	T1169	T1105	G1044	G1044	K922	T861	Y797	Y797
T1170	T1170	G1106	L1045	L1045	T923	T862	F735	F735
T1171	T1171	T1107	N1046	N1046	F924	F863	K799	K799
T1172	T1172	I1108	S986	S986	N925	S864	D800	D800
K1173	K1173	D1109	A1048	A1048	K926	E865	T737	T737
							G738	G738

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.78Å 105.29Å 114.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.83 – 3.20 42.83 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.83-3.20) 99.9 (42.83-3.20)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.210 , 0.316 0.222 , 0.246	Depositor DCC
R_{free} test set	1075 reflections (4.11%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 84.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8741	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	2.25	221/8849 (2.5%)	1.66	231/11918 (1.9%)

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	A	0	1

The worst 5 of 221 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	821	VAL	CA-CB	-9.20	1.41	1.55
1	A	148	ILE	CA-CB	-8.46	1.44	1.54
1	A	502	ALA	CA-CB	-8.42	1.39	1.53
1	A	510	ILE	CA-CB	-8.05	1.45	1.54
1	A	888	ILE	CA-CB	-7.89	1.45	1.54

The worst 5 of 231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	786	ASN	N-CA-C	14.01	126.63	111.36
1	A	181	PHE	N-CA-C	-13.21	96.89	111.28
1	A	292	TYR	N-CA-C	-12.59	97.24	110.97
1	A	646	SER	N-CA-C	-12.20	97.50	112.38
1	A	915	ILE	CB-CA-C	-11.86	96.80	111.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	560	ASN	Peptide

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	8674	0	8613	1346	2
2	A	1	0	0	0	0
3	A	66	0	0	7	0
All	All	8741	0	8613	1346	2

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 78.

The worst 5 of 1346 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:263:MET:CE	1:A:457:ILE:HD12	1.14	1.54
1:A:263:MET:CE	1:A:457:ILE:CD1	1.80	1.53
1:A:610:ASN:C	1:A:613:GLU:CG	1.75	1.47
1:A:232:TYR:HB2	1:A:614:LYS:NZ	1.30	1.45
1:A:151:LEU:O	1:A:155:THR:CG2	1.67	1.42

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ASN:ND2	1:A:988:LYS:CG[2_554]	1.98	0.22
1:A:538:ASN:O	1:A:679:THR:OG1[2_654]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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	1043/1193 (87%)	998 (96%)	37 (4%)	8 (1%)	16	50

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	VAL
1	A	610	ASN
1	A	613	GLU
1	A	1128	ASN
1	A	373	PRO

5.3.2 Protein sidechains

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	972/1104 (88%)	621 (64%)	351 (36%)	0	0

5 of 351 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	781	ILE
1	A	959	GLU
1	A	806	THR
1	A	873	LYS
1	A	1014	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	880	ASN
1	A	1177	ASN
1	A	894	ASN
1	A	953	ASN
1	A	324	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1053/1193 (88%)	0.08	13 (1%) 76 58	9, 32, 70, 128	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	ASN	4.9
1	A	612	GLN	4.3
1	A	908	ASP	3.9
1	A	1145	LYS	3.7
1	A	263	MET	3.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	1194	1/1	0.65	0.20	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.