



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:13 am GMT

PDB ID : 1XF1
Title : Structure of C5a peptidase- a key virulence factor from Streptococcus
Authors : Brown, C.K.; Gu, Z.Y.; Cleary, P.P.; Matsuka, Y.; Olmstead, S.; Ohlendorf, D.H.; Earhart, C.A.
Deposited on : 2004-09-13
Resolution : 1.90 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

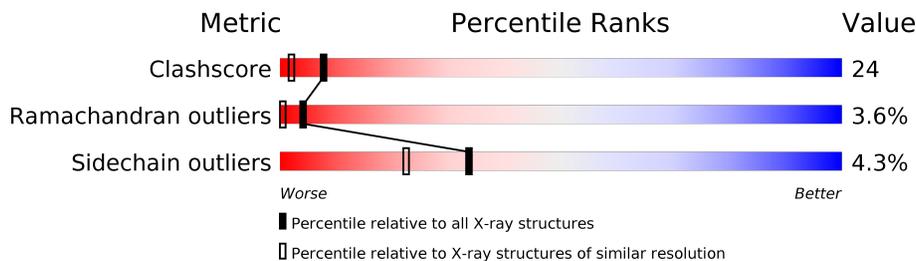
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	926	
1	B	926	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15509 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 C5a peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	926	7182	4510	1211	1445	16	0	0	0
1	B	926	7182	4510	1211	1445	16	4	0	0

There are 38 discrepancies between the modelled and reference sequences:

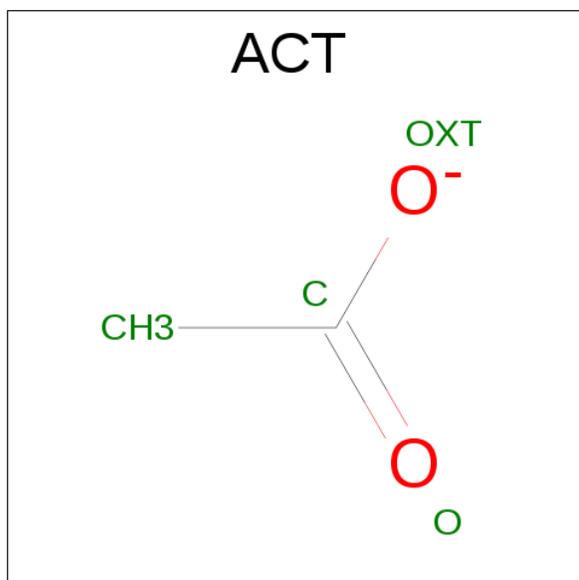
Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	227	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	259	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	353	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	433	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	513	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	522	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	536	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	550	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	585	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	648	THR	ALA	SEE REMARK 999	UNP P15926
A	680	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	697	THR	LYS	SEE REMARK 999	UNP P15926
A	702	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	794	PHE	LEU	SEE REMARK 999	UNP P15926
A	969	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	996	MSE	THR	ENGINEERED	UNP P15926
A	1005	MSE	MET	MODIFIED RESIDUE	UNP P15926
A	1015	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	219	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	227	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	259	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	353	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	433	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	513	MSE	MET	MODIFIED RESIDUE	UNP P15926

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Chain	Residue	Modelled	Actual	Comment	Reference
B	522	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	536	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	550	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	585	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	648	THR	ALA	SEE REMARK 999	UNP P15926
B	680	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	697	THR	LYS	SEE REMARK 999	UNP P15926
B	702	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	794	PHE	LEU	SEE REMARK 999	UNP P15926
B	969	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	996	MSE	THR	ENGINEERED	UNP P15926
B	1005	MSE	MET	MODIFIED RESIDUE	UNP P15926
B	1015	MSE	MET	MODIFIED RESIDUE	UNP P15926

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

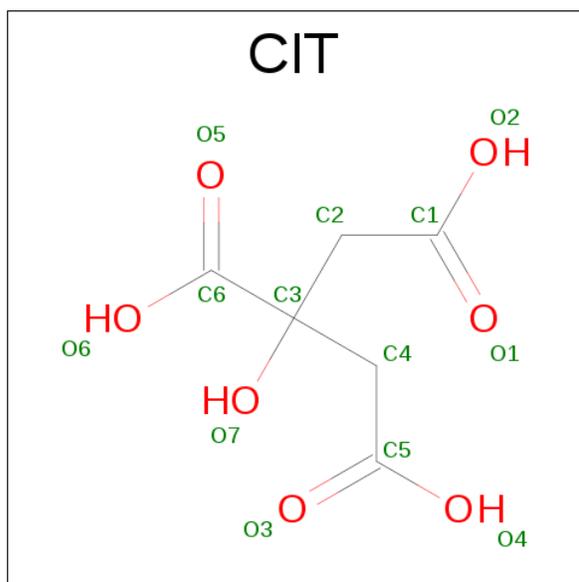


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	A	1	Total C O 13 6 7	0	0
4	A	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	544	Total O 544 544	0	0
5	B	513	Total O 513 513	0	0

M1015	R887	A760	L653	L542	G253
M1018	W888	K772	T654	A545	A254
I1019	K893	K775	P655	K546	K255
T1020	D894	E776	P656	K451	V256
K1026	V898	G777	N658	K452	M259
E1029	Y903	V778	S659	T453	M263
G1030	T910	N780	Q662	F456	A264
H1031	P911	I781	V663	N457	A265
	P912	E782	T664	K381	L266
	S913	D783	V665	D383	L271
	P932	I784	P666	K384	P272
	E933	E785	L667	K385	D273
	F940	S786	R671	G386	E274
	S941	G796	Q679	I388	T275
	T942	T797	Q679	A389	F279
	E943	F798	F685	I391	K283
	D944	Q801	R691	S476	V287
	R945	H806	Q694	W477	F398
	R946	I809	D695	I485	K399
	K952	Y818	K698	P492	D400
	P953	E699	E699	G493	K406
	K954	E700	E700	Q494	K407
	T955	R829	I704	D495	V328
	P958	Q833	P705	I496	Y331
	V959	F834	F706	V500	L337
	Y960	Q835	I707	N503	T338
	R961	F838	F713	K504	V341
	R963	N844	I723	R513	R342
	I964	V849	Y724	S514	V343
	A965	K852	G729	A515	K344
	M969	K852	H734	P516	A346
	P974	W858	E735	M522	D347
	Y978	T859	A736	G523	Q348
	D984	S860	N737	L524	K353
	E991	V862	S738	K527	P354
	E994	N869	D739	E621	V355
	T995	L874	A740	L622	L356
	M996	L878	K741	Y623	S357
	E997	L878	D742	E530	T358
	G998	R882	Q743	T531	K359
	A999	F883	L744	Y533	R360
	Y1010	K884	D745	A639	F361
	D1014	E885	L749	L640	S439
		K885	W749	V644	R440
		T886	N757	Q651	P363
			F758	K652	K365
			T759		K366
					A366
					Y367
					D368
					L446

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, α , β , γ	114.70Å 75.11Å 132.39Å 90.00° 104.95° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	15509	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACT, CIT

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	0.34	0/7312	0.63	0/9884
1	B	0.33	0/7312	0.61	0/9884
All	All	0.33	0/14624	0.62	0/19768

There are no bond length outliers.

There are no bond angle outliers.

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	7182	0	7004	319	0
1	B	7182	0	7005	384	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	39	0	15	0	0
4	B	39	0	15	2	0
5	A	544	0	0	34	0
5	B	513	0	0	23	0
All	All	15509	0	14045	688	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 24.

The worst 5 of 688 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:778:VAL:HG21	1:A:784:ILE:HD11	1.40	1.03
1:A:210:LYS:HA	1:A:337:LEU:HD12	1.40	1.03
1:B:343:VAL:HG12	1:B:454:ILE:HG22	1.41	1.02
1:A:465:THR:HG23	1:A:468:GLY:H	1.23	1.01
1:B:465:THR:HG23	1:B:468:GLY:H	1.25	1.00

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	924/926 (100%)	830 (90%)	64 (7%)	30 (3%)	5 0
1	B	924/926 (100%)	818 (88%)	70 (8%)	36 (4%)	3 0
All	All	1848/1852 (100%)	1648 (89%)	134 (7%)	66 (4%)	4 0

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	GLU
1	A	140	TRP
1	A	145	LYS
1	A	172	ASN
1	A	184	ASP

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	771/760 (101%)	736 (96%)	35 (4%)	32	21
1	B	771/760 (101%)	739 (96%)	32 (4%)	34	23
All	All	1542/1520 (101%)	1475 (96%)	67 (4%)	33	22

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	926	ILE
1	B	145	LYS
1	B	785	GLU
1	A	960	TYR
1	A	1026	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	982	ASN
1	B	241	ASN
1	B	835	GLN
1	B	136	ASN
1	B	349	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	A	1101	-	3,12,12	1.82	1 (33%)	3,17,17	5.03	3 (100%)
4	CIT	A	1103	-	3,12,12	1.78	1 (33%)	3,17,17	3.86	2 (66%)
4	CIT	A	1105	-	3,12,12	1.65	0	3,17,17	4.21	2 (66%)
2	ACT	A	1107	-	1,3,3	0.31	0	0,3,3	0.00	-
4	CIT	B	1102	-	3,12,12	1.57	1 (33%)	3,17,17	4.69	3 (100%)
4	CIT	B	1104	-	3,12,12	1.72	1 (33%)	3,17,17	3.95	2 (66%)
4	CIT	B	1106	-	3,12,12	1.62	0	3,17,17	4.51	3 (100%)
2	ACT	B	1108	-	1,3,3	0.56	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	A	1101	-	-	0/6/16/16	0/0/0/0
4	CIT	A	1103	-	-	0/6/16/16	0/0/0/0
4	CIT	A	1105	-	-	0/6/16/16	0/0/0/0
2	ACT	A	1107	-	-	0/0/0/0	0/0/0/0
4	CIT	B	1102	-	-	0/6/16/16	0/0/0/0
4	CIT	B	1104	-	-	0/6/16/16	0/0/0/0
4	CIT	B	1106	-	-	0/6/16/16	0/0/0/0
2	ACT	B	1108	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1103	CIT	C4-C3	-2.31	1.51	1.54
4	B	1104	CIT	C4-C3	-2.17	1.51	1.54
4	B	1102	CIT	O7-C3	2.08	1.46	1.43
4	A	1101	CIT	O7-C3	2.37	1.46	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1106	CIT	C3-C4-C5	2.91	119.50	114.95
4	A	1105	CIT	C3-C2-C1	3.24	120.02	114.95
4	B	1106	CIT	C3-C2-C1	3.36	120.20	114.95
4	B	1104	CIT	C3-C2-C1	3.43	120.31	114.95
4	B	1102	CIT	C3-C4-C5	3.85	120.97	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1104	CIT	1	0
4	B	1106	CIT	1	0

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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.