



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:35 PM GMT

PDB ID : 1KXT  
Title : Camelid VHH Domains in Complex with Porcine Pancreatic alpha-Amylase  
Authors : Desmyter, A.; Spinelli, S.; Payan, F.; Lauwereys, M.; Wyns, L.; Muyldermans, S.; Cambillau, C.  
Deposited on : 2002-02-01  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

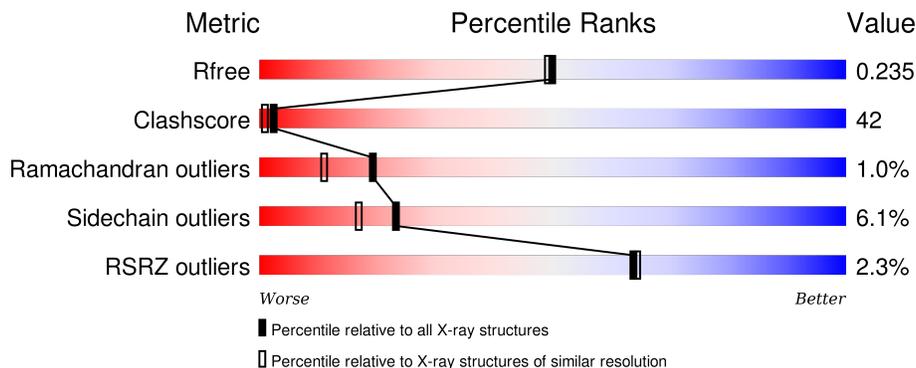
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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.



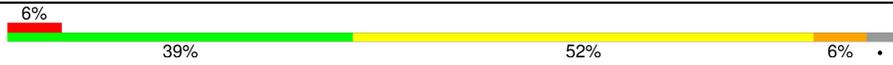
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	496	
1	C	496	
1	E	496	
2	B	127	
2	D	127	

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Mol	Chain	Length	Quality of chain
2	F	127	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment (6%), a green segment (39%), a large yellow segment (52%), and a small grey segment (6%).</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16172 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 ALPHA-AMYLASE, PANCREATIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	496	3910	2471	688	730	21	0	0	0
1	C	496	3910	2471	688	730	21	0	0	0
1	E	496	3910	2471	688	730	21	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	LYS	GLN	SEE REMARK 999	UNP P00690
A	310	SER	ALA	SEE REMARK 999	UNP P00690
A	323	ILE	VAL	SEE REMARK 999	UNP P00690
A	404	GLN	GLU	SEE REMARK 999	UNP P00690
C	243	LYS	GLN	SEE REMARK 999	UNP P00690
C	310	SER	ALA	SEE REMARK 999	UNP P00690
C	323	ILE	VAL	SEE REMARK 999	UNP P00690
C	404	GLN	GLU	SEE REMARK 999	UNP P00690
E	243	LYS	GLN	SEE REMARK 999	UNP P00690
E	310	SER	ALA	SEE REMARK 999	UNP P00690
E	323	ILE	VAL	SEE REMARK 999	UNP P00690
E	404	GLN	GLU	SEE REMARK 999	UNP P00690

- Molecule 2 is a protein called IMMUNOGLOBULIN VHH FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	123	903	560	158	179	6	0	0	0
2	D	123	903	560	158	179	6	0	0	0
2	F	123	903	560	158	179	6	0	0	0

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

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

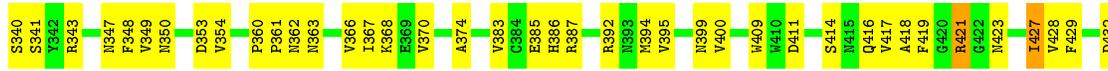
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0

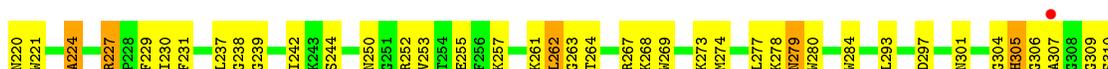
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	479	Total O 479 479	0	0
5	B	131	Total O 131 131	0	0
5	C	391	Total O 391 391	0	0
5	D	120	Total O 120 120	0	0
5	E	491	Total O 491 491	0	0
5	F	115	Total O 115 115	0	0

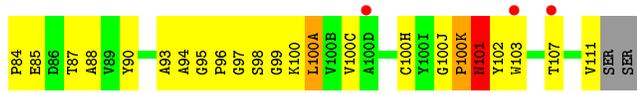




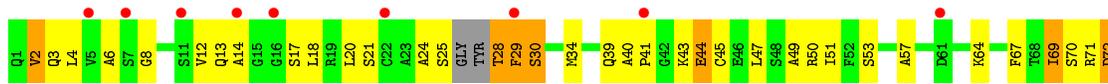
• Molecule 1: ALPHA-AMYLASE, PANCREATIC



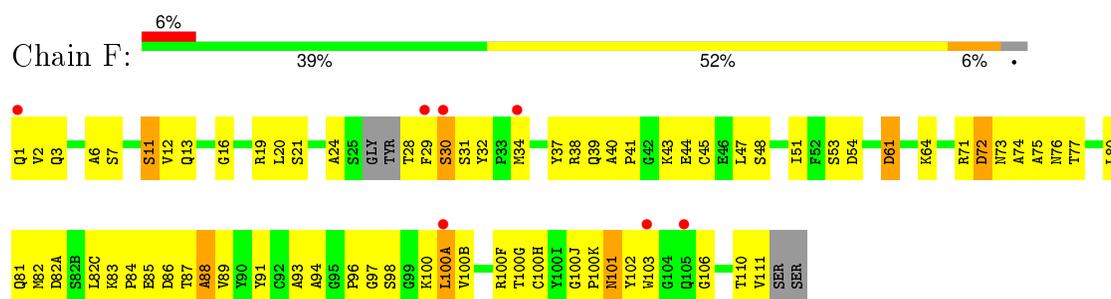
• Molecule 2: IMMUNOGLOBULIN VHH FRAGMENT



• Molecule 2: IMMUNOGLOBULIN VHH FRAGMENT



• Molecule 2: IMMUNOGLOBULIN VHH FRAGMENT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.78Å 286.85Å 65.98Å 90.00° 93.73° 90.00°	Depositor
Resolution (Å)	19.95 – 2.00 39.50 – 2.00	Depositor EDS
% Data completeness (in resolution range)	50.1 (19.95-2.00) 50.2 (39.50-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.97 (at 2.00Å)	Xtrriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.203 , 0.236 0.203 , 0.235	Depositor DCC
$R_{free}$ test set	1655 reflections (2.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtrriage
Anisotropy	0.225	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Outliers	0 of 65792 reflections	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, CL

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	0.40	0/4020	0.65	0/5461
1	C	0.36	0/4020	0.63	1/5461 (0.0%)
1	E	0.39	0/4020	0.65	0/5461
2	B	0.40	0/921	0.66	1/1247 (0.1%)
2	D	0.36	0/921	0.65	1/1247 (0.1%)
2	F	0.40	0/921	0.67	0/1247
All	All	0.38	0/14823	0.65	3/20124 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	100(K)	PRO	N-CA-C	6.00	127.70	112.10
2	D	100(K)	PRO	N-CA-C	5.52	126.45	112.10
1	C	304	GLY	N-CA-C	5.02	125.66	113.10

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	3910	0	3693	317	0
1	C	3910	0	3693	290	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3910	0	3693	265	1
2	B	903	0	859	111	0
2	D	903	0	859	116	0
2	F	903	0	859	109	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	1	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	479	0	0	141	1
5	B	131	0	0	59	0
5	C	391	0	0	131	0
5	D	120	0	0	58	0
5	E	491	0	0	127	0
5	F	115	0	0	61	0
All	All	16172	0	13656	1193	1

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 42.

The worst 5 of 1193 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)
2:B:77:THR:HG22	5:B:205:HOH:O	1.37	1.24
1:E:185:LYS:HD2	5:E:4460:HOH:O	1.38	1.23
1:A:29:GLU:HG2	5:A:4430:HOH:O	1.34	1.22
1:C:278:LYS:HE2	5:C:4326:HOH:O	1.40	1.22
1:C:294:VAL:HB	5:C:4294:HOH:O	1.42	1.19

All (1) 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:E:460:ASN:OD1	5:A:4216:HOH:O[1_655]	2.14	0.06

## 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	494/496 (100%)	458 (93%)	31 (6%)	5 (1%)	19	11
1	C	494/496 (100%)	459 (93%)	33 (7%)	2 (0%)	39	33
1	E	494/496 (100%)	469 (95%)	22 (4%)	3 (1%)	30	22
2	B	119/127 (94%)	110 (92%)	7 (6%)	2 (2%)	11	4
2	D	119/127 (94%)	105 (88%)	9 (8%)	5 (4%)	3	1
2	F	119/127 (94%)	113 (95%)	4 (3%)	2 (2%)	11	4
All	All	1839/1869 (98%)	1714 (93%)	106 (6%)	19 (1%)	19	11

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASP
1	A	224	ALA
1	E	224	ALA
1	E	305	HIS
2	F	101	ASN

### 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	413/413 (100%)	385 (93%)	28 (7%)	20	13
1	C	413/413 (100%)	396 (96%)	17 (4%)	37	32
1	E	413/413 (100%)	396 (96%)	17 (4%)	37	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	92/95 (97%)	82 (89%)	10 (11%)	8	4
2	D	92/95 (97%)	80 (87%)	12 (13%)	5	2
2	F	92/95 (97%)	83 (90%)	9 (10%)	10	5
All	All	1515/1524 (99%)	1422 (94%)	93 (6%)	23	17

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	134	TRP
1	C	435	GLN
2	F	28	THR
1	C	165	LEU
1	C	279	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	299	HIS
1	C	435	GLN
1	E	435	GLN
1	C	347	ASN
1	C	373	ASN

### 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

Of 6 ligands modelled in this entry, 6 are 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

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	496/496 (100%)	-0.19	4 (0%) 87 88	4, 11, 20, 31	0
1	C	496/496 (100%)	0.01	5 (1%) 84 84	9, 18, 27, 33	0
1	E	496/496 (100%)	-0.17	3 (0%) 90 90	4, 11, 21, 34	0
2	B	123/127 (96%)	0.39	8 (6%) 22 23	9, 22, 31, 36	0
2	D	123/127 (96%)	0.82	15 (12%) 5 6	15, 28, 32, 35	0
2	F	123/127 (96%)	0.47	7 (5%) 27 29	11, 24, 32, 35	0
All	All	1857/1869 (99%)	0.02	42 (2%) 64 64	4, 15, 29, 36	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	29	PHE	5.5
1	C	134	TRP	4.9
2	F	103	TRP	4.7
2	D	103	TRP	4.5
1	A	305	HIS	4.3

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	E	4006	1/1	1.00	0.11	-0.77	21,21,21,21	0
4	CL	C	4004	1/1	0.99	0.14	-0.92	27,27,27,27	0
4	CL	A	4002	1/1	0.99	0.12	-1.20	22,22,22,22	0
3	CA	E	4005	1/1	0.98	0.07	-1.92	17,17,17,17	0
3	CA	A	4001	1/1	1.00	0.08	-1.92	16,16,16,16	0
3	CA	C	4003	1/1	0.99	0.07	-2.50	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.