



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:09 PM UTC

PDB ID : 8AEH / pdb_00008aeh
Title : X-ray structure of Canis familiaris Odorant Binding Protein 1
Authors : Schwartz, M.; Briand, L.
Deposited on : 2022-07-13
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 4-5-2 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

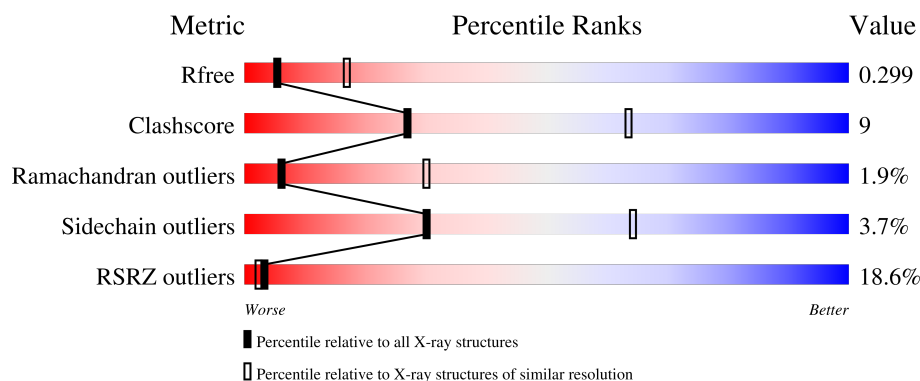
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 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	AA1	169	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 853 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 Major allergen Can f 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA1	118	Total	C	N	O	S	0	0	0
			852	547	136	163	6			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA1	6	MET	-	initiating methionine	UNP O18873
AA1	7	ARG	-	expression tag	UNP O18873
AA1	8	GLY	-	expression tag	UNP O18873
AA1	9	SER	-	expression tag	UNP O18873
AA1	10	HIS	-	expression tag	UNP O18873
AA1	11	HIS	-	expression tag	UNP O18873
AA1	12	HIS	-	expression tag	UNP O18873
AA1	13	HIS	-	expression tag	UNP O18873
AA1	14	HIS	-	expression tag	UNP O18873
AA1	15	HIS	-	expression tag	UNP O18873
AA1	16	THR	-	expression tag	UNP O18873
AA1	17	ASP	-	expression tag	UNP O18873
AA1	18	PRO	-	expression tag	UNP O18873

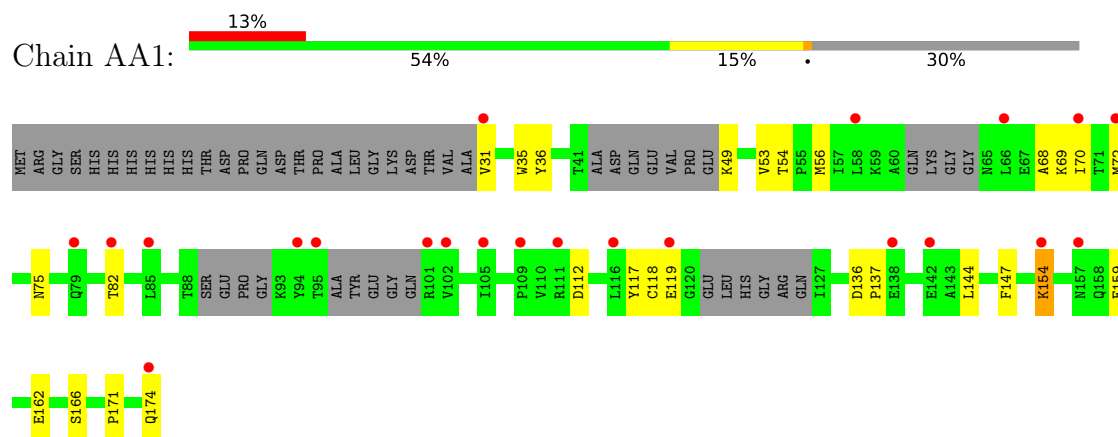
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AA1	1	Total	Ca	0	0
			1	1		

3 Residue-property plots [i](#)

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: Major allergen Can f 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.22Å 88.22Å 37.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.11 – 3.00 44.11 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.11-3.00) 100.0 (44.11-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.13 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.285 , 0.301 0.288 , 0.299	Depositor DCC
R_{free} test set	148 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.876	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	853	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% 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

5.1 Standard geometry

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

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	AA1	0.47	0/860	0.80	0/1154

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	AA1	852	0	785	15	0
2	AA1	1	0	0	0	0
All	All	853	0	785	15	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 9.

All (15) 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:AA1:69:LYS:HG2	1:AA1:82:THR:HG22	1.56	0.87
1:AA1:70:ILE:HD12	1:AA1:72:MET:HE3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA1:144:LEU:HD11	1:AA1:162:GLU:CD	2.18	0.69
1:AA1:70:ILE:CD1	1:AA1:72:MET:HE3	2.36	0.54
1:AA1:53:VAL:HG23	1:AA1:72:MET:HG2	1.89	0.53
1:AA1:49:LYS:NZ	1:AA1:75:ASN:HD21	2.14	0.46
1:AA1:56:MET:HE2	1:AA1:68:ALA:HB1	1.98	0.46
1:AA1:49:LYS:HD2	1:AA1:49:LYS:HA	1.79	0.45
1:AA1:154:LYS:HD3	1:AA1:154:LYS:HA	1.68	0.43
1:AA1:171:PRO:HB2	1:AA1:174:GLN:CB	2.48	0.42
1:AA1:36:TYR:CZ	1:AA1:137:PRO:HG3	2.54	0.42
1:AA1:54:THR:HA	1:AA1:166:SER:O	2.20	0.41
1:AA1:31:VAL:HA	1:AA1:35:TRP:HZ2	1.86	0.41
1:AA1:117:TYR:OH	1:AA1:119:GLU:OE2	2.24	0.41
1:AA1:144:LEU:O	1:AA1:147:PHE:N	2.54	0.40

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	AA1	106/169 (63%)	95 (90%)	9 (8%)	2 (2%)	6	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA1	159	GLU
1	AA1	112	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	AA1	81/144 (56%)	78 (96%)	3 (4%)	30	64

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA1	118	CYS
1	AA1	136	ASP
1	AA1	154	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	AA1	118/169 (69%)	1.11	22 (18%) 3 2	39, 60, 89, 100	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA1	142	GLU	5.4
1	AA1	85	LEU	4.2
1	AA1	70	ILE	3.8
1	AA1	102	VAL	3.4
1	AA1	174	GLN	3.4
1	AA1	66	LEU	3.1
1	AA1	95	THR	3.0
1	AA1	101	ARG	2.9
1	AA1	94	TYR	2.7
1	AA1	138	GLU	2.6
1	AA1	111	ARG	2.6
1	AA1	157	ASN	2.6
1	AA1	154	LYS	2.6
1	AA1	79	GLN	2.5
1	AA1	31	VAL	2.5
1	AA1	105	ILE	2.2
1	AA1	72	MET	2.2
1	AA1	58	LEU	2.2
1	AA1	82	THR	2.2
1	AA1	109	PRO	2.1
1	AA1	119	GLU	2.1
1	AA1	116	LEU	2.0

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($\text{\AA}^2$)	Q<0.9
2	CA	AA1	201	1/1	0.90	0.15	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.