



Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2026 – 10:20 AM JST

PDB ID : 9WGQ / pdb_00009wgq
Title : Crystal structure of OcKAI2d6 from Orobanche cumana
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Deposited on : 2025-08-25
Resolution : 1.85 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

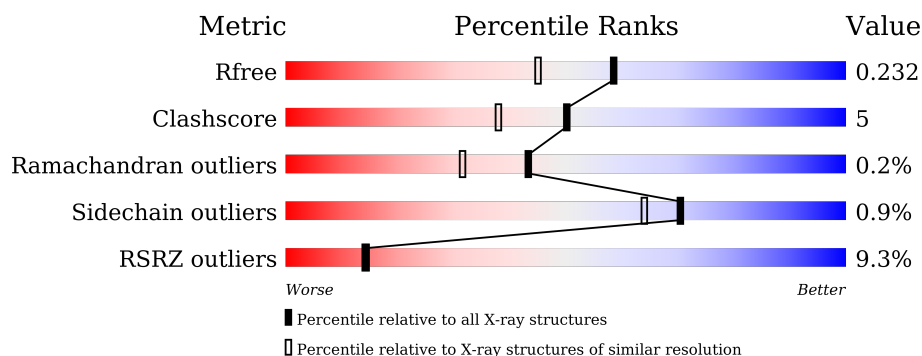
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	276	<div> <div>8%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	B	276	<div> <div>11%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4319 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/beta-hydrolases superfamily protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2073	1304	359	392	18			
1	B	267	Total	C	N	O	S	0	0	0
			2053	1293	356	387	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A9E9EMW1
A	2	PRO	-	expression tag	UNP A0A9E9EMW1
A	3	LEU	-	expression tag	UNP A0A9E9EMW1
A	4	GLY	-	expression tag	UNP A0A9E9EMW1
A	5	SER	-	expression tag	UNP A0A9E9EMW1
B	1	GLY	-	expression tag	UNP A0A9E9EMW1
B	2	PRO	-	expression tag	UNP A0A9E9EMW1
B	3	LEU	-	expression tag	UNP A0A9E9EMW1
B	4	GLY	-	expression tag	UNP A0A9E9EMW1
B	5	SER	-	expression tag	UNP A0A9E9EMW1

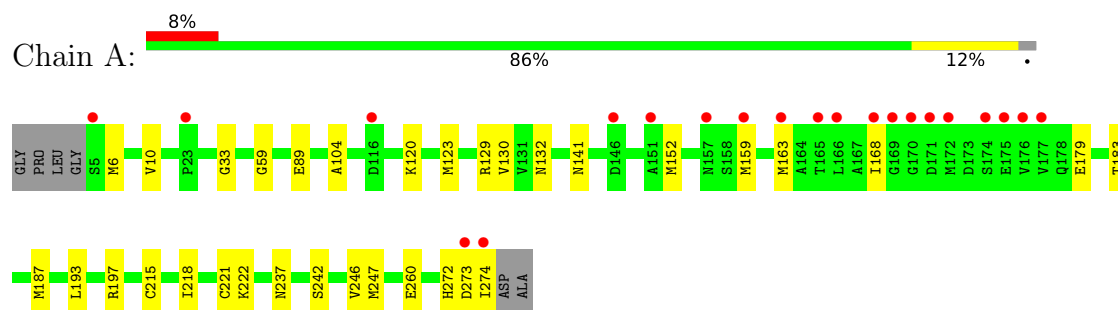
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	121	Total	O	0	0
			121	121		
2	B	72	Total	O	0	0
			72	72		

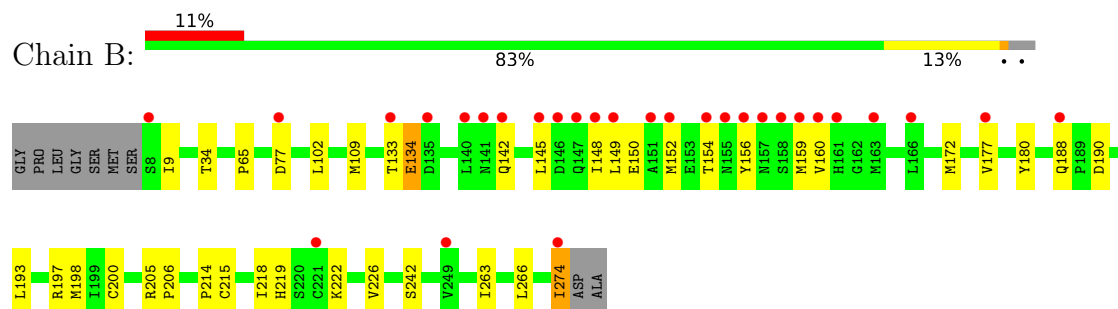
3 Residue-property plots

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: Alpha/beta-hydrolases superfamily protein



- Molecule 1: Alpha/beta-hydrolases superfamily protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	36.90Å 122.34Å 123.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.73 – 1.85 38.73 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.73-1.85) 100.0 (38.73-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.195 , 0.229 0.197 , 0.232	Depositor DCC
R_{free} test set	2348 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4319	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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](#)

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	0.37	0/2118	0.57	0/2883
1	B	0.32	0/2098	0.52	0/2857
All	All	0.34	0/4216	0.54	0/5740

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ARG	Sidechain

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	2073	0	2033	19	0
1	B	2053	0	2014	25	0
2	A	121	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	72	0	0	0	0
All	All	4319	0	4047	43	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 5.

All (43) 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:PRO:HB3	1:B:188:GLN:OE1	1.82	0.80
1:B:152:MET:HG2	1:B:159:MET:HE3	1.66	0.76
1:B:214:PRO:CB	1:B:274:ILE:HD13	2.25	0.67
1:A:218:ILE:HG22	1:A:247:MET:HE2	1.78	0.65
1:A:246:VAL:O	1:B:222:LYS:HE3	1.98	0.64
1:A:179:GLU:O	1:A:183:THR:HG23	1.99	0.62
1:B:188:GLN:HG2	1:B:190:ASP:OD1	2.03	0.57
1:A:120:LYS:NZ	1:A:272:HIS:O	2.38	0.57
1:A:273:ASP:O	1:A:274:ILE:HB	2.06	0.56
1:B:145:LEU:HD21	1:B:200:CYS:SG	2.46	0.55
1:B:142:GLN:HE22	1:B:145:LEU:HD12	1.72	0.54
1:B:9:ILE:H	1:B:9:ILE:HD12	1.72	0.54
1:A:6:MET:HA	1:A:6:MET:HE2	1.90	0.54
1:B:77:ASP:OD1	1:B:109:MET:HE3	2.09	0.53
1:B:156:TYR:O	1:B:160:VAL:HG23	2.10	0.52
1:B:149:LEU:HD21	1:B:200:CYS:SG	2.50	0.52
1:A:104:ALA:HB1	1:A:123:MET:HG2	1.91	0.51
1:A:10:VAL:HG21	1:A:89:GLU:HG3	1.93	0.51
1:B:150:GLU:O	1:B:154:THR:HG23	2.10	0.51
1:B:219:HIS:HE1	1:B:226:VAL:O	1.92	0.51
1:B:218:ILE:HD13	1:B:266:LEU:HD23	1.92	0.51
1:B:193:LEU:O	1:B:197:ARG:HG3	2.12	0.49
1:A:33:GLY:HA2	1:A:187:MET:SD	2.52	0.49
1:A:221:CYS:SG	1:A:222:LYS:NZ	2.86	0.49
1:B:9:ILE:HD12	1:B:9:ILE:N	2.29	0.48
1:A:193:LEU:O	1:A:197:ARG:HG3	2.14	0.47
1:B:102:LEU:CD1	1:B:198:MET:HE1	2.44	0.47
1:A:237:ASN:OD1	2:A:301:HOH:O	2.21	0.44
1:B:205:ARG:HB2	1:B:206:PRO:HD3	2.00	0.44
1:A:152:MET:HE3	1:A:159:MET:HE3	2.00	0.44
1:A:159:MET:SD	1:A:163:MET:HE2	2.58	0.44
1:B:142:GLN:NE2	1:B:145:LEU:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:MET:HA	1:B:177:VAL:HG11	2.00	0.43
1:A:132:ASN:HD22	1:A:141:ASN:ND2	2.17	0.43
1:A:260:GLU:H	1:A:260:GLU:CD	2.21	0.42
1:B:148:ILE:O	1:B:152:MET:HG3	2.19	0.42
1:B:34:THR:HG23	1:B:180:TYR:HE1	1.84	0.41
1:B:172:MET:HE3	1:B:172:MET:HB3	1.84	0.41
1:A:59:GLY:O	1:A:187:MET:HE3	2.20	0.41
1:B:215:CYS:O	1:B:242:SER:HA	2.21	0.41
1:A:215:CYS:O	1:A:242:SER:HA	2.21	0.41
1:A:152:MET:HE3	1:A:159:MET:CE	2.51	0.41
1:B:133:THR:O	1:B:134:GLU:C	2.64	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	A	268/276 (97%)	262 (98%)	6 (2%)	0	100	100
1	B	265/276 (96%)	256 (97%)	8 (3%)	1 (0%)	30	17
All	All	533/552 (97%)	518 (97%)	14 (3%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	GLU

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	231/234 (99%)	229 (99%)	2 (1%)	70	64
1	B	228/234 (97%)	226 (99%)	2 (1%)	70	64
All	All	459/468 (98%)	455 (99%)	4 (1%)	70	64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	VAL
1	A	168	ILE
1	B	263	ILE
1	B	274	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	81	ASN
1	A	119	HIS
1	A	141	ASN
1	A	142	GLN
1	A	157	ASN
1	A	186	ASN
1	A	235	HIS
1	B	36	GLN
1	B	142	GLN
1	B	219	HIS
1	B	237	ASN

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 [i](#)

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

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	270/276 (97%)	0.38	21 (7%)	19 20	25, 34, 60, 115	0
1	B	267/276 (96%)	0.61	29 (10%)	10 10	29, 41, 103, 127	0
All	All	537/552 (97%)	0.49	50 (9%)	14 14	25, 38, 79, 127	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	ILE	6.2
1	B	149	LEU	5.8
1	B	145	LEU	5.2
1	A	274	ILE	5.0
1	A	170	GLY	4.6
1	A	166	LEU	4.4
1	B	156	TYR	4.3
1	A	171	ASP	4.3
1	A	172	MET	3.9
1	B	148	ILE	3.8
1	A	175	GLU	3.7
1	B	141	ASN	3.7
1	B	154	THR	3.6
1	A	163	MET	3.5
1	B	159	MET	3.4
1	A	169	GLY	3.3
1	A	165	THR	3.1
1	B	155	ASN	3.0
1	B	151	ALA	3.0
1	B	157	ASN	2.8
1	B	8	SER	2.8
1	B	152	MET	2.7
1	B	163	MET	2.7
1	A	273	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	249	VAL	2.6
1	A	174	SER	2.6
1	B	133	THR	2.6
1	A	151	ALA	2.5
1	B	140	LEU	2.5
1	B	161	HIS	2.5
1	A	168	ILE	2.4
1	A	177	VAL	2.4
1	B	160	VAL	2.4
1	A	23	PRO	2.3
1	B	177	VAL	2.3
1	B	221	CYS	2.3
1	A	157	ASN	2.2
1	B	158	SER	2.2
1	A	159	MET	2.2
1	A	146	ASP	2.2
1	A	116	ASP	2.2
1	A	5	SER	2.1
1	B	166	LEU	2.1
1	B	146	ASP	2.1
1	B	77	ASP	2.1
1	B	135	ASP	2.1
1	B	147	GLN	2.0
1	B	188	GLN	2.0
1	B	142	GLN	2.0
1	A	176	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.