

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7ZS6
Title	:	Crystal structure of Apis mellifera RidA
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Deposited on	:	2022-05-06
Resolution	:	1.31 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.31 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.



Matria	Whole archive	Similar resolution
wietric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	1667 (1.34-1.30)
Ramachandran outliers	138981	1615(1.34-1.30)
Sidechain outliers	138945	1615(1.34-1.30)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain		
1	AAA	140	79%	15%	• 5%
1	BBB	140	81%	14%	5%
1	CCC	140	77%	17%	• 5%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3991 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
		122	Total	С	Ν	0	\mathbf{S}	4	27	0
	100	1176	775	182	214	5	4			
1	BBB	122	Total	С	Ν	0	S	0	21	0
	100	1221	807	190	219	5	0	- 16	0	
1	CCC	122	Total	С	Ν	0	S	0	02	0
		199	1167	772	179	211	5	0	20	U

• Molecule 1 is a protein called Reactive intermediate deaminase A.

There are 9 discrepancies	between	the modelled	d and reference	e sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-2	GLY	-	expression tag	UNP A0A7M7GBQ0
AAA	-1	SER	-	expression tag	UNP A0A7M7GBQ0
AAA	0	HIS	-	expression tag	UNP A0A7M7GBQ0
BBB	-2	GLY	-	expression tag	UNP A0A7M7GBQ0
BBB	-1	SER	-	expression tag	UNP A0A7M7GBQ0
BBB	0	HIS	-	expression tag	UNP A0A7M7GBQ0
CCC	-2	GLY	-	expression tag	UNP A0A7M7GBQ0
CCC	-1	SER	-	expression tag	UNP A0A7M7GBQ0
CCC	0	HIS	-	expression tag	UNP A0A7M7GBQ0

• Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	BBB	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	O 2	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	Total Mg 1 1	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total Na 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	144	Total O 145 145	0	1
5	BBB	160	Total O 160 160	0	0
5	CCC	116	Total O 116 116	0	0



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. 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. 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.

Note EDS failed to run properly.

• Molecule 1: Reactive intermediate deaminase A





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	I 41 2 2	Depositor	
Cell constants	109.50Å 109.50Å 141.09Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	43.30 - 1.31	Depositor	
% Data completeness	99 / (/3 30-1 31)	Depositor	
(in resolution range)	55.4 (45.50-1.51)	Depositor	
R_{merge}	0.03	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.42 (at 1.31 \text{\AA})$	Xtriage	
Refinement program	REFMAC 5.8.0267	Depositor	
R, R_{free}	0.131 , 0.164	Depositor	
Wilson B-factor $(Å^2)$	18.7	Xtriage	
Anisotropy	0.121	Xtriage	
L-test for twinning ²	$ < L >=0.50, < L^2>=0.34$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	3991	wwPDB-VP	
Average B, all atoms $(Å^2)$	25.0	wwPDB-VP	

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.28% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: EDO, NA, MG

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	Bo	nd lengths	Bond angles		
INIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	AAA	0.89	3/1265~(0.2%)	1.03	2/1714~(0.1%)	
1	BBB	0.78	0/1315	0.97	3/1776~(0.2%)	
1	CCC	0.86	0/1246	1.02	3/1689~(0.2%)	
All	All	0.84	3/3826~(0.1%)	1.01	8/5179~(0.2%)	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	AAA	137	ILE	C-OXT	6.25	1.35	1.23
1	AAA	126[A]	GLU	CD-OE2	-5.66	1.19	1.25
1	AAA	126[B]	GLU	CD-OE2	-5.66	1.19	1.25

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	CCC	109	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	CCC	112	PHE	CB-CG-CD1	6.11	125.08	120.80
1	BBB	112	PHE	CB-CG-CD2	-5.79	116.75	120.80
1	BBB	112	PHE	CB-CG-CD1	5.61	124.73	120.80
1	BBB	58	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	AAA	16[A]	CYS	CB-CA-C	5.42	121.24	110.40
1	AAA	16[B]	CYS	CB-CA-C	5.42	121.24	110.40
1	CCC	112	PHE	CB-CG-CD2	-5.40	117.02	120.80

All (8) bond angle outliers are listed below:

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	AAA	1176	0	1296	23	0
1	BBB	1221	0	1348	19	0
1	CCC	1167	0	1268	21	0
2	BBB	4	0	6	2	0
3	BBB	1	0	0	0	0
4	BBB	1	0	0	0	0
5	AAA	145	0	0	2	0
5	BBB	160	0	0	4	0
5	CCC	116	0	0	3	0
All	All	3991	0	3918	53	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 7.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:CCC:58[A]:ARG:NH2	1:CCC:100[A]:GLU:OE2	1.90	1.04
1:BBB:74[A]:ASN:OD1	1:BBB:76[A]:ASN:OD1	1.82	0.96
1:AAA:22:PRO:HD2	1:CCC:95[B]:ASN:OD1	1.66	0.96
1:AAA:22:PRO:CD	1:CCC:95[B]:ASN:OD1	2.17	0.93
1:AAA:16[B]:CYS:SG	1:AAA:67[B]:ILE:HG13	2.12	0.90
1:CCC:41:ILE:HD11	1:CCC:119[B]:MET:HE1	1.59	0.85
1:BBB:79[B]:ILE:HD12	1:CCC:29[B]:VAL:HG21	1.64	0.80
1:BBB:16[B]:CYS:SG	1:BBB:67[B]:ILE:HG13	2.23	0.78
1:BBB:16[B]:CYS:SG	1:BBB:66:HIS:HB2	2.23	0.78
1:BBB:116[B]:LYS:HD3	5:BBB:735:HOH:O	1.87	0.75
1:BBB:137:ILE:OXT	5:BBB:601:HOH:O	2.04	0.73
1:BBB:49[B]:VAL:HG22	2:BBB:501:EDO:O2	1.92	0.70
1:AAA:79[B]:ILE:HD12	1:BBB:29[B]:VAL:HG21	1.78	0.64
1:AAA:80[B]:LYS:HB3	1:AAA:128[B]:ILE:HG22	1.79	0.63
1:AAA:80[B]:LYS:HZ1	1:BBB:126[B]:GLU:CD	2.02	0.63
1:AAA:51:GLY:O	5:AAA:202:HOH:O	2.15	0.63
1:CCC:45:THR:HG21	5:CCC:202:HOH:O	1.99	0.61
1:CCC:117[A]:LEU:HD23	1:CCC:124[A]:GLU:HB2	1.86	0.58

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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:CCC:58[A]:ARG:HH22	1:CCC:100[A]:GLU:CD	2.02	0.57
1:CCC:41:ILE:CD1	1:CCC:119[B]:MET:HE1	2.34	0.55
1:CCC:16[A]:CYS:SG	1:CCC:67[A]:ILE:HD11	2.46	0.55
1:AAA:5:LYS:HE3	1:AAA:7:ILE:HD11	1.88	0.55
1:AAA:16[B]:CYS:HB2	1:AAA:25[B]:GLN:NE2	2.23	0.54
1:AAA:80[B]:LYS:HB3	1:AAA:128[B]:ILE:CG2	2.37	0.54
1:AAA:22:PRO:CG	1:CCC:95[B]:ASN:OD1	2.56	0.54
1:AAA:95[B]:ASN:OD1	1:AAA:109:ARG:NH1	2.41	0.53
1:AAA:41:ILE:HD11	1:AAA:119[A]:MET:SD	2.49	0.53
1:AAA:6:THR:HG21	1:CCC:130[B]:ILE:HG21	1.92	0.52
1:AAA:29[A]:VAL:HG11	1:CCC:130[A]:ILE:HD11	1.92	0.52
1:AAA:16[B]:CYS:SG	1:AAA:66:HIS:HB2	2.52	0.50
1:BBB:18[A]:LYS:HE3	5:BBB:612:HOH:O	2.12	0.49
1:AAA:22:PRO:HD3	1:CCC:95[B]:ASN:HD21	1.77	0.48
1:CCC:62[B]:LEU:HD12	5:CCC:268:HOH:O	2.14	0.47
1:CCC:25:GLN:OE1	1:CCC:67[B]:ILE:HD12	2.15	0.47
1:CCC:19:PRO:HB3	1:CCC:23[B]:TYR:CE2	2.50	0.47
1:BBB:123[B]:LEU:C	1:BBB:123[B]:LEU:HD22	2.36	0.46
1:BBB:79[A]:ILE:HD11	1:BBB:130[A]:ILE:HG12	1.98	0.46
1:BBB:116[B]:LYS:HE3	1:BBB:116[B]:LYS:HB2	1.73	0.46
1:AAA:95[B]:ASN:ND2	5:AAA:204:HOH:O	2.49	0.45
1:BBB:46[A]:GLU:HG2	5:BBB:715:HOH:O	2.17	0.44
1:CCC:45:THR:O	1:CCC:46[B]:GLU:HG2	2.18	0.44
1:CCC:57:THR:HA	1:CCC:123[B]:LEU:HD11	1.98	0.43
1:AAA:12[B]:SER:HA	1:AAA:25[B]:GLN:OE1	2.17	0.43
1:BBB:49[B]:VAL:CG2	2:BBB:501:EDO:O2	2.64	0.43
1:AAA:137:ILE:HG13	1:BBB:9[B]:LYS:HG3	2.00	0.43
1:AAA:17:PRO:HG2	1:AAA:41:ILE:HB	2.01	0.42
1:AAA:61:LEU:HD23	1:AAA:61:LEU:HA	1.93	0.42
1:CCC:126[A]:GLU:HA	5:CCC:255:HOH:O	2.19	0.42
1:BBB:79[A]:ILE:CG1	1:BBB:130[A]:ILE:HG12	2.50	0.42
1:CCC:77:LYS:O	1:CCC:130[B]:ILE:HG13	2.21	0.41
1:BBB:70[B]:GLU:OE2	1:BBB:70[B]:GLU:HA	2.21	0.40

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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	AAA	158/140~(113%)	153~(97%)	5(3%)	0	100 100
1	BBB	163/140~(116%)	159~(98%)	4 (2%)	0	100 100
1	CCC	154/140~(110%)	150 (97%)	4 (3%)	0	100 100
All	All	475/420 (113%)	462 (97%)	13 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	AAA	141/119 (118%)	141 (100%)	0	100	100	
1	BBB	146/119~(123%)	146 (100%)	0	100	100	
1	CCC	136/119~(114%)	131 (96%)	5 (4%)	34	4	
All	All	423/357~(118%)	418 (99%)	5 (1%)	78	38	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	80	LYS
1	CCC	91[A]	PHE
1	CCC	91[B]	PHE
1	CCC	123[A]	LEU
1	CCC	123[B]	LEU



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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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).

Mal	ol Type Chain Res I		Tink	Link Bond lengths			Bond angles			
WIOI	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	EDO	BBB	501	-	3,3,3	1.59	1 (33%)	2,2,2	0.13	0

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
2	EDO	BBB	501	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	BBB	501	EDO	O2-C2	2.39	1.54	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	501	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	501	EDO	2	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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

