

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7Z5H
Title	:	human Zn MATCAP
Authors	:	Bak, J.; Adamopoulos, A.; Heidebrecht, T.; Perrakis, A.
Deposited on	:	2022-03-09
Resolution	:	2.50 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
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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			
Metric	$(\# { m Entries})$	$(\# \text{Entries, resolution range}(\text{\AA}))$			
R_{free}	130704	4661 (2.50-2.50)			
Clashscore	141614	5346 (2.50-2.50)			
Ramachandran outliers	138981	5231 (2.50-2.50)			
Sidechain outliers	138945	5233 (2.50-2.50)			
RSRZ outliers	127900	4559 (2.50-2.50)			

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% 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	А	335	2% 9 4%	5%•
1	В	335	16%	6% •
1	С	335	5% 95%	• •
1	D	335	% • 94%	5%•



$7\mathrm{Z5H}$

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21714 atoms, of which 10703 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						AltConf	Trace
1	Δ	330	Total	С	Η	Ν	0	\mathbf{S}	77	0	0
1	Π	552	5408	1722	2686	495	491	14			0
1	В	330	Total	С	Η	Ν	Ο	\mathbf{S}	77	0	0
1	D	550	5376	1712	2671	493	486	14		0	U
1	С	330	Total	С	Η	Ν	0	\mathbf{S}	77	0	0
1	U	- 330	5376	1712	2671	493	486	14		0	0
1	П	221	Total	С	Н	Ν	0	S	77	0	0
	- 391	5389	1716	2675	494	490	14	11	0	U	

• Molecule 1 is a protein called Uncharacterized protein KIAA0895-like.

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	66	Total O 66 66	0	0
3	В	12	Total O 12 12	0	0
3	С	24	Total O 24 24	0	0
3	D	59	Total O 59 59	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 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: Uncharacterized protein KIAA0895-like





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	55.65Å 88.07 Å 165.58 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.77° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	47.08 - 2.50	Depositor
Resolution (A)	47.04 - 2.50	EDS
% Data completeness	99.9 (47.08-2.50)	Depositor
(in resolution range)	$100.0 \ (47.04-2.50)$	EDS
R _{merge}	0.17	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.75 (at 2.51 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
D D.	0.232 , 0.255	Depositor
Π, Π_{free}	0.237 , 0.259	DCC
R_{free} test set	2762 reflections $(4.97%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	39.5	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.40 , 49.0	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21714	wwPDB-VP
Average B, all atoms $(Å^2)$	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 22.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0116e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: ZN

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).

Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.35	0/2787	0.58	1/3771~(0.0%)	
1	В	0.32	0/2770	0.59	2/3749~(0.1%)	
1	С	0.32	0/2770	0.57	0/3749	
1	D	0.34	0/2779	0.57	0/3760	
All	All	0.33	0/11106	0.58	3/15029~(0.0%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	455	MET	CA-CB-CG	6.58	124.48	113.30
1	А	271	GLN	CA-CB-CG	5.14	124.71	113.40
1	В	436	ARG	NE-CZ-NH2	-5.07	117.76	120.30

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	А	2722	2686	2672	10	0
1	В	2705	2671	2657	15	0
1	С	2705	2671	2657	9	0
1	D	2714	2675	2661	9	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	А	66	0	0	0	0
3	В	12	0	0	0	0
3	С	24	0	0	0	0
3	D	59	0	0	0	0
All	All	11011	10703	10647	38	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 2.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 amo 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:208:PHE:O	1:B:212:THR:HG22	1.69	0.91
1:B:150:ARG:O	1:B:153:ASP:OD1	1.89	0.90
1:B:401:LEU:HD22	1:B:455:MET:HE3	1.79	0.65
1:B:401:LEU:HD22	1:B:455:MET:CE	2.26	0.65
1:C:163:ASN:ND2	1:C:349:SER:OG	2.34	0.61
1:A:171:PRO:O	1:B:305:ARG:NH1	2.36	0.59
1:A:296:PRO:HB2	1:A:306:TYR:CE2	2.39	0.57
1:A:363:ASP:OD2	1:A:366:VAL:HG23	2.04	0.57
1:B:325:LEU:O	1:B:450:GLN:OE1	2.27	0.52
1:D:340:TYR:OH	1:D:359:ARG:NH2	2.44	0.50
1:B:153:ASP:OD1	1:B:154:LYS:N	2.44	0.50
1:A:342:ILE:HD11	1:A:390:ASP:HB2	1.94	0.49
1:C:342:ILE:HD11	1:C:390:ASP:HB2	1.93	0.49
1:B:342:ILE:HD11	1:B:390:ASP:HB2	1.94	0.49
1:D:342:ILE:HD11	1:D:390:ASP:HB2	1.93	0.49
1:A:325:LEU:O	1:A:450:GLN:NE2	2.30	0.47
1:B:347:ARG:HB3	1:C:189:HIS:CE1	2.50	0.47
1:B:245:GLU:HG2	1:B:266:LEU:HD11	1.98	0.46
1:D:287:LEU:HA	1:D:290:VAL:HG22	1.97	0.46
1:A:245:GLU:HG2	1:A:266:LEU:HD11	1.98	0.45
1:C:307:GLY:HA3	1:D:173:PRO:HA	1.98	0.45
1:B:334:ARG:NH2	1:B:373:ARG:HH11	2.15	0.45
1:A:266:LEU:HD12	1:A:267:THR:N	2.32	0.45
1:B:266:LEU:HD12	1:B:267:THR:N	2.34	0.43
1:B:455:MET:HE2	1:B:455:MET:HB3	1.80	0.43



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-1 Atom-2		overlap (Å)
1:D:334:ARG:NH2	1:D:373:ARG:HH11	2.16	0.43
1:C:266:LEU:HD12	1:C:267:THR:N	2.34	0.42
1:D:266:LEU:HD12	1:D:267:THR:N	2.34	0.42
1:C:173:PRO:HA	1:D:307:GLY:HA3	2.02	0.42
1:C:334:ARG:NH2	1:C:373:ARG:HH11	2.17	0.42
1:A:256:GLU:O	1:A:259:ARG:HG2	2.20	0.42
1:A:296:PRO:CB	1:A:306:TYR:CE2	3.03	0.42
1:D:431:VAL:HG23	1:D:431:VAL:O	2.21	0.41
1:C:425:HIS:CE1	1:D:171:PRO:HB2	2.56	0.41
1:B:225:ILE:O	1:B:228:LYS:HG2	2.21	0.40
1:A:431:VAL:O	1:A:431:VAL:HG23	2.22	0.40
1:B:404:ARG:HD3	1:B:455:MET:HE1	2.03	0.40
1:C:431:VAL:HG23	1:C:431:VAL:O	2.21	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	Perce	entiles
1	А	330/335~(98%)	321~(97%)	9~(3%)	0	100	100
1	В	328/335~(98%)	319~(97%)	9(3%)	0	100	100
1	С	328/335~(98%)	318~(97%)	10 (3%)	0	100	100
1	D	329/335~(98%)	321 (98%)	8 (2%)	0	100	100
All	All	1315/1340~(98%)	1279 (97%)	36 (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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	288/291~(99%)	287 (100%)	1 (0%)	92	97
1	В	286/291~(98%)	286 (100%)	0	100	100
1	С	286/291~(98%)	286 (100%)	0	100	100
1	D	287/291~(99%)	284 (99%)	3 (1%)	76	90
All	All	1147/1164 (98%)	1143 (100%)	4 (0%)	92	97

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

Mol	Chain	Res	Type
1	А	265	ASN
1	D	232	LYS
1	D	355	GLN
1	D	433	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	242	GLN
1	А	265	ASN
1	В	189	HIS
1	В	242	GLN
1	В	329	GLN
1	В	450	GLN
1	С	157	GLN
1	С	163	ASN
1	С	189	HIS
1	С	292	ASN
1	С	298	HIS
1	D	157	GLN
1	D	189	HIS
1	D	292	ASN
1	D	298	HIS



Continued from previous page...

\mathbf{Mol}	Chain	\mathbf{Res}	Type
1	D	355	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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 (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, 95^{th} 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	А	332/335~(99%)	0.45	8 (2%) 59 62	32, 51, 78, 108	0
1	В	330/335~(98%)	1.08	53 (16%) 1 1	50, 74, 110, 131	0
1	С	330/335~(98%)	0.59	16 (4%) 30 32	44, 59, 92, 125	0
1	D	331/335~(98%)	0.40	3 (0%) 84 86	28, 48, 71, 106	0
All	All	1323/1340~(98%)	0.63	80 (6%) 21 22	28, 58, 98, 131	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	252	VAL	5.7
1	В	176	VAL	5.5
1	В	168	TYR	5.2
1	В	383	LEU	5.1
1	С	467	ARG	4.9
1	В	162	TYR	4.7
1	В	247	LEU	4.7
1	В	470	PRO	4.5
1	С	255	VAL	4.3
1	В	164	PRO	4.1
1	В	173	PRO	4.1
1	В	172	MET	3.9
1	С	465	LEU	3.8
1	В	149	ASP	3.8
1	С	258	SER	3.7
1	В	372	VAL	3.5
1	В	166	PHE	3.5
1	D	246	ASP	3.4
1	С	246	ASP	3.4
1	В	321	LEU	3.3
1	В	381	THR	3.3



7Z5H

Mol	Chain	Res	Type	RSRZ
1	В	463	ALA	3.3
1	В	467	ARG	3.3
1	В	468	LEU	3.2
1	В	148	MET	3.2
1	С	463	ALA	3.2
1	В	154	LYS	3.0
1	В	205	TYR	2.9
1	D	471	ASP	2.9
1	В	377	GLY	2.8
1	В	150	ARG	2.7
1	А	140	LEU	2.7
1	С	351	ARG	2.7
1	С	468	LEU	2.6
1	В	329	GLN	2.6
1	В	246	ASP	2.6
1	А	173	PRO	2.5
1	В	257	ASN	2.5
1	В	449	GLN	2.5
1	В	143	LEU	2.5
1	В	266	LEU	2.4
1	В	444	LEU	2.4
1	В	271	GLN	2.4
1	В	360	TYR	2.4
1	В	250	GLN	2.4
1	В	194	ILE	2.4
1	В	228	LYS	2.4
1	А	266	LEU	2.4
1	С	248	LEU	2.4
1	С	141	VAL	2.4
1	В	144	ARG	2.3
1	С	206	GLU	2.3
1	А	245	GLU	2.3
1	В	357	LEU	2.3
1	В	465	LEU	2.3
1	В	169	GLN	2.3
1	В	274	LEU	2.3
1	В	451	LEU	2.3
1	В	379	THR	2.2
1	А	141	VAL	2.2
1	В	160	TYR	2.2
1	В	152	ARG	2.2
1	В	177	LEU	2.2



Mol	Chain	Res	Type	RSRZ
1	В	460	LEU	2.2
1	В	469	LEU	2.2
1	В	219	LYS	2.2
1	А	174	THR	2.2
1	В	213	GLY	2.1
1	С	464	GLU	2.1
1	С	266	LEU	2.1
1	В	325	LEU	2.1
1	В	251	ALA	2.1
1	С	462	GLU	2.1
1	С	469	LEU	2.1
1	А	258	SER	2.1
1	В	380	ASP	2.1
1	D	444	LEU	2.1
1	В	159	HIS	2.0
1	С	328	LYS	2.0
1	А	347	ARG	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 monosaccharides 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, 95^{th} 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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
2	ZN	С	501	1/1	0.95	0.04	$57,\!57,\!57,\!57$	0
2	ZN	В	501	1/1	0.96	0.07	$55,\!55,\!55,\!55$	0
2	ZN	А	501	1/1	0.96	0.07	46,46,46,46	0
2	ZN	D	501	1/1	0.97	0.07	44,44,44,44	0

The following is a graphical depiction of the model fit to experimental electron density of all



instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.















6.5 Other polymers (i)

There are no such residues in this entry.

