

wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 10:11 AM EDT

PDB ID	:	1XK8
Title	:	Divalent cation tolerant protein CUTA from Homo sapiens O60888
Authors	:	Tempel, W.; Chen, L.; Liu, ZJ.; Lee, D.; Shah, A.; Dailey, T.A.; Mayer, M.R.;
		Arendall III, W.B.; Rose, J.P.; Dailey, H.A.; Richardson, J.S.; Richardson,
		D.C.; Wang, BC.; Southeast Collaboratory for Structural Genomics (SECSG)
Deposited on		
Resolution	:	2.70 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* 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:

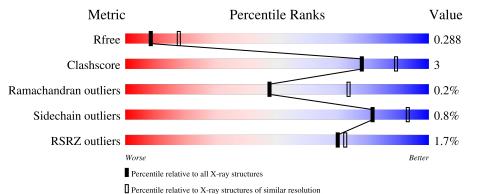
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.70 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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				
-		1.45	% •				
	A	147	65%	8%	27%		
-	D	1 4 5	% •				
	В	147	65%	7%	27%		
	a		% •				
	С	147	67%	5%	27%		
	- E		2%				
1	D	147	67%	6%	27%		
			2%				
	E	147	69%	•	27%		



Mol	Chain	Length	Quality of chair	n		
1	F	147	% • 65%	7%	·	27%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	С	203	-	-	-	Х



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4831 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		At	oms			ZeroOcc	AltConf	Trace
1	А	107	Total	С	Ν	Ο	S	0	0	0
	A	107	827	534	134	155	4	0	0	0
1	В	107	Total	С	Ν	0	S	0	0	0
	D	107	798	519	124	151	4	0	0	0
1	С	107	Total	С	Ν	0	S	0	0	0
	U	107	799	516	129	150	4	0	0	0
1	D	108	Total	С	Ν	0	S	0	0	0
	D	108	797	512	129	152	4	0	0	0
1	Е	107	Total	С	Ν	0	S	0	0	0
	Ľ	107	813	529	127	153	4	0	0	0
1	F	107	Total	С	Ν	0	S	0	0	0
	Г	107	794	515	121	154	4	0		U

• Molecule 1 is a protein called Divalent cation tolerant protein CUTA.

There are 66 discrepancies between the modelled and reference sequences:

Residue	Modelled	Actual	Comment	Reference
10	MET	-	expression tag	UNP O60888
11	GLY	-	expression tag	UNP O60888
12	GLY	-	expression tag	UNP O60888
13	SER	-	expression tag	UNP O60888
14	HIS	-	expression tag	UNP O60888
15	HIS	-	expression tag	UNP O60888
16	HIS	-	expression tag	UNP O60888
17	HIS	-	expression tag	UNP O60888
18	HIS	-	expression tag	UNP O60888
19	HIS	-	expression tag	UNP O60888
20	GLY	-	expression tag	UNP O60888
10	MET	-	expression tag	UNP O60888
11	GLY	-	expression tag	UNP O60888
12	GLY	-	expression tag	UNP O60888
13	SER	-	expression tag	UNP O60888
14	HIS	-	expression tag	UNP O60888
15	HIS	-	expression tag	UNP O60888
	$ \begin{array}{c} 10\\ 11\\ 12\\ 13\\ 14\\ 15\\ 16\\ 17\\ 18\\ 19\\ 20\\ 10\\ 11\\ 12\\ 13\\ 14\\ \end{array} $	10 MET 11 GLY 12 GLY 13 SER 14 HIS 15 HIS 16 HIS 17 HIS 18 HIS 20 GLY 10 MET 11 GLY 13 SER 14 HIS	10 MET - 11 GLY - 12 GLY - 13 SER - 14 HIS - 15 HIS - 16 HIS - 17 HIS - 18 HIS - 19 HIS - 10 MET - 11 GLY - 13 SER - 14 HIS -	10MET-expression tag11GLY-expression tag12GLY-expression tag13SER-expression tag14HIS-expression tag15HIS-expression tag16HIS-expression tag17HIS-expression tag18HIS-expression tag19HIS-expression tag10MET-expression tag11GLY-expression tag13SER-expression tag14HIS-expression tag



	Continued from previous page						
Chain	Residue	Modelled	Actual	Comment	Reference		
В	16	HIS	-	expression tag	UNP O60888		
В	17	HIS	-	expression tag	UNP O60888		
В	18	HIS	-	expression tag	UNP O60888		
B	19	HIS	-	expression tag	UNP O60888		
В	20	GLY	-	expression tag	UNP O60888		
C	10	MET	-	expression tag	UNP O60888		
С	11	GLY	-	expression tag	UNP O60888		
С	12	GLY	-	expression tag	UNP O60888		
С	13	SER	-	expression tag	UNP O60888		
С	14	HIS	-	expression tag	UNP O60888		
С	15	HIS	-	expression tag	UNP 060888		
С	16	HIS	-	expression tag	UNP 060888		
С	17	HIS	-	expression tag	UNP O60888		
С	18	HIS	-	expression tag	UNP 060888		
С	19	HIS	-	expression tag	UNP 060888		
С	20	GLY	-	expression tag	UNP 060888		
D	10	MET	-	expression tag	UNP O60888		
D	11	GLY	-	expression tag	UNP O60888		
D	12	GLY	-	expression tag	UNP 060888		
D	13	SER	-	expression tag	UNP O60888		
D	14	HIS	-	expression tag	UNP 060888		
D	15	HIS	-	expression tag	UNP O60888		
D	16	HIS	-	expression tag	UNP 060888		
D	17	HIS	-	expression tag	UNP 060888		
D	18	HIS	-	expression tag	UNP O60888		
D	19	HIS	-	expression tag	UNP O60888		
D	20	GLY	-	expression tag	UNP O60888		
E	10	MET	-	expression tag	UNP O60888		
Е	11	GLY	-	expression tag	UNP O60888		
E	12	GLY	-	expression tag	UNP 060888		
E	13	SER	-	expression tag	UNP 060888		
E	14	HIS	-	expression tag	UNP O60888		
E	15	HIS	-	expression tag	UNP 060888		
E	16	HIS	-	expression tag	UNP O60888		
E	17	HIS	-	expression tag	UNP 060888		
E	18	HIS	-	expression tag	UNP O60888		
E	19	HIS	-	expression tag	UNP 060888		
E	20	GLY	-	expression tag	UNP 060888		
F	10	MET	-	expression tag	UNP O60888		
F	11	GLY	-	expression tag	UNP O60888		
F	12	GLY	-	expression tag	UNP O60888		
F	13	SER	-	expression tag	UNP O60888		



Continu					
Chain	Residue	Modelled	Actual	Comment	Reference
F	14	HIS	-	expression tag	UNP O60888
F	15	HIS	-	expression tag	UNP O60888
F	16	HIS	-	expression tag	UNP O60888
F	17	HIS	-	expression tag	UNP O60888
F	18	HIS	-	expression tag	UNP O60888
F	19	HIS	-	expression tag	UNP O60888
F	20	GLY	-	expression tag	UNP O60888

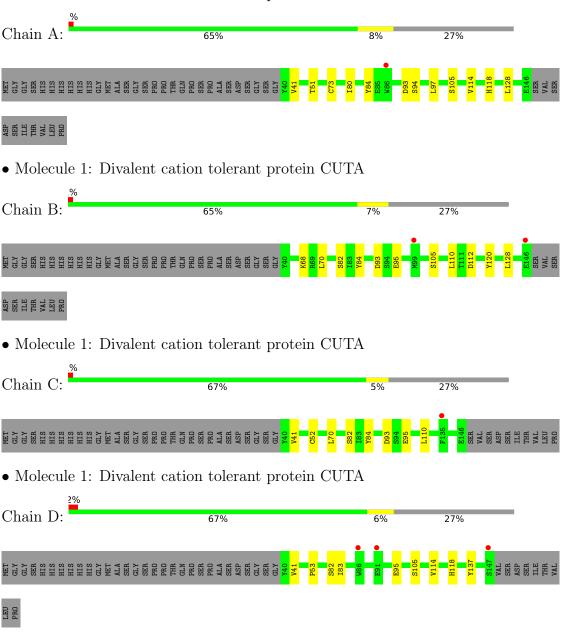
• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mo	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Na 1 1	0	0
2	С	2	Total Na 2 2	0	0



3 Residue-property plots (i)

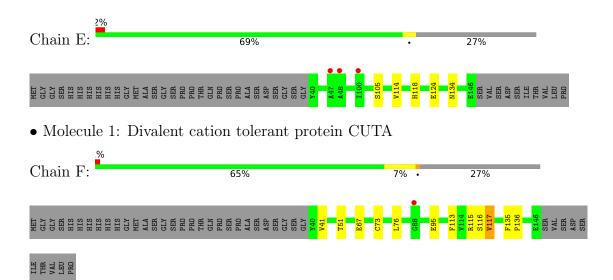
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Divalent cation tolerant protein CUTA

• Molecule 1: Divalent cation tolerant protein CUTA







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	70.16Å 89.52Å 125.85Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.67 - 2.70	Depositor
Resolution (A)	32.66 - 2.40	EDS
% Data completeness	100.0 (32.67-2.70)	Depositor
(in resolution range)	76.3(32.66-2.40)	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.04 (at 2.39 \text{\AA})$	Xtriage
Refinement program	REFMAC refmac_5.2.0005	Depositor
D D.	0.245 , 0.283	Depositor
R, R_{free}	0.248 , 0.288	DCC
R_{free} test set	1215 reflections (5.05%)	wwPDB-VP
Wilson B-factor $(Å^2)$	46.8	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32, 25.6	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4831	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.66% 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: NA

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	Mol Chain		nd lengths	Bond	angles
			RMSZ $\# Z > 5$		# Z > 5
1	А	0.64	1/845~(0.1%)	0.51	0/1157
1	В	0.64	0/816	0.52	0/1120
1	С	0.71	1/817~(0.1%)	0.56	0/1121
1	D	0.63	0/813	0.53	0/1112
1	Е	0.58	0/831	0.53	0/1137
1	F	0.75	1/812~(0.1%)	0.53	0/1117
All	All	0.66	3/4934~(0.1%)	0.53	0/6764

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	73	CYS	CB-SG	-5.42	1.73	1.81
1	F	73	CYS	CB-SG	-5.10	1.73	1.81
1	С	52	CYS	CB-SG	-5.08	1.73	1.81

There are no bond angle outliers.

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	827	0	822	6	0
1	В	798	0	771	7	0



	v	Non-H	1 0	H(added)	Clashes	Symm-Clashes
1	С	799	0	774	4	0
1	D	797	0	779	8	0
1	Е	813	0	800	4	0
1	F	794	0	755	8	0
2	А	1	0	0	0	0
2	С	2	0	0	0	0
All	All	4831	0	4701	28	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 3.

The worst 5 of 28 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:C:41:VAL:HG21	1:E:105:SER:HA	1.78	0.65
1:B:70:LEU:HD23	1:B:110:LEU:HA	1.78	0.65
1:B:105:SER:HA	1:F:41:VAL:HG21	1.85	0.57
1:F:116:SER:O	1:F:117:VAL:HB	2.03	0.57
1:A:84:TYR:OH	1:A:93:ASP:OD2	2.23	0.53

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	ntiles
1	А	105/147~(71%)	104 (99%)	1 (1%)	0	100	100
1	В	105/147~(71%)	104 (99%)	1 (1%)	0	100	100
1	С	105/147~(71%)	103 (98%)	2(2%)	0	100	100
1	D	106/147~(72%)	101 (95%)	5 (5%)	0	100	100
1	Е	105/147~(71%)	104 (99%)	1 (1%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	105/147~(71%)	103~(98%)	1 (1%)	1 (1%)	15 37
All	All	631/882~(72%)	619~(98%)	11 (2%)	1 (0%)	47 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	117	VAL

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	А	90/126~(71%)	88~(98%)	2(2%)	52 79
1	В	83/126~(66%)	82~(99%)	1 (1%)	71 88
1	С	84/126~(67%)	84 (100%)	0	100 100
1	D	85/126~(68%)	85 (100%)	0	100 100
1	Ε	86/126~(68%)	86 (100%)	0	100 100
1	F	83/126~(66%)	82~(99%)	1 (1%)	71 88
All	All	511/756~(68%)	507~(99%)	4 (1%)	81 93

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

Mol	Chain	Res	Type
1	А	51	THR
1	А	94	SER
1	В	112	ASP
1	F	67	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains 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, 3 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	107/147~(72%)	-0.06	1 (0%) 84 85	50, 54, 60, 66	0
1	В	107/147~(72%)	-0.14	2 (1%) 66 69	50, 54, 59, 61	0
1	С	107/147~(72%)	-0.09	1 (0%) 84 85	50, 54, 62, 64	0
1	D	108/147~(73%)	-0.04	3 (2%) 53 54	50, 54, 61, 64	0
1	Ε	107/147~(72%)	-0.06	3 (2%) 53 54	50, 54, 58, 59	0
1	F	107/147~(72%)	-0.07	1 (0%) 84 85	50, 54, 62, 67	0
All	All	643/882~(72%)	-0.08	11 (1%) 70 72	50, 54, 61, 67	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	147	SER	4.3
1	F	88	GLY	3.7
1	Е	47	ALA	3.0
1	D	91	GLU	2.7
1	В	146	GLU	2.4

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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	NA	С	203	1/1	0.73	0.63	$57,\!57,\!57,\!57$	0
2	NA	С	201	1/1	0.87	0.16	60,60,60,60	0
2	NA	А	202	1/1	0.90	0.55	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.

