



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 08:49 am GMT

PDB ID : 4A46
Title : Crosstalk between Cu(I) and Zn(II) homeostasis
Authors : Badarau, A.; Basle, A.; Firbank, S.J.; Denninson, C.
Deposited on : 2011-10-07
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 : 4.02b-467
Xtrriage (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) : 2.36

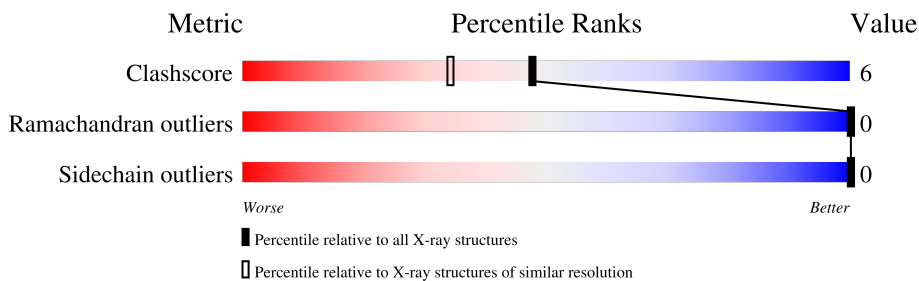
1 Overall quality at a glance

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))
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1937 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 SSR2857 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	63	455	277	76	100	2	0	0	0
1	B	63	448	276	75	95	2	0	1	0
1	C	63	459	283	76	98	2	0	2	0
1	D	63	442	273	72	95	2	0	1	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	45	Total O 45 45	0	0
5	B	26	Total O 26 26	0	0
5	C	40	Total O 40 40	0	0
5	D	16	Total O 16 16	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	30.71Å 41.99Å 45.24Å 83.34° 89.52° 75.28°	Depositor
Resolution (Å)	44.92 – 1.85	Depositor
% Data completeness (in resolution range)	91.5 (44.92-1.85)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.86Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.192 , 0.243	Depositor
Wilson B-factor (Å ²)	20.7	Xtrriage
Anisotropy	0.133	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1937	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.84% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN, CL

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	0.73	0/456	0.82	1/621 (0.2%)
1	B	0.58	0/452	0.69	0/617
1	C	0.68	0/466	0.74	0/634
1	D	0.54	0/446	0.72	0/610
All	All	0.64	0/1820	0.74	1/2482 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ASP	CB-CG-OD1	5.51	123.26	118.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	455	0	452	4	0
1	B	448	0	449	11	0
1	C	459	0	466	2	0
1	D	442	0	438	5	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	45	0	0	1	0
5	B	26	0	0	0	0
5	C	40	0	0	0	0
5	D	16	0	0	0	0
All	All	1937	0	1805	22	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 6.

All (22) 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:2:THR:HG21	1:B:42:THR:CG2	2.13	0.79
1:D:10[A]:ILE:HG22	1:D:36:LEU:CD2	2.18	0.74
1:B:2:THR:HG21	1:B:42:THR:HG22	1.70	0.73
1:B:10[B]:ILE:HG22	1:B:36:LEU:CD2	2.19	0.73
1:D:10[A]:ILE:HG23	1:D:15:CYS:HB3	1.70	0.72
1:D:10[A]:ILE:HD11	1:D:19:VAL:HG21	1.72	0.71
1:D:10[A]:ILE:HG22	1:D:36:LEU:HD23	1.84	0.59
1:A:50:GLU:OE1	1:A:53:ARG:NH1	2.39	0.53
1:B:2:THR:HG21	1:B:42:THR:HG23	1.92	0.52
1:B:10[B]:ILE:HD11	1:B:19:VAL:HG21	1.92	0.51
1:B:7:VAL:O	1:B:10[A]:ILE:HG12	2.10	0.51
1:A:4:GLN:NE2	5:A:2001:HOH:O	1.96	0.47
1:A:49:GLU:OE2	1:A:53:ARG:NH2	2.36	0.47
1:D:10[A]:ILE:CD1	1:D:19:VAL:HG21	2.42	0.47
1:B:3:ILE:HD12	1:B:3:ILE:N	2.30	0.46
1:B:45:SER:OG	1:B:46:ALA:N	2.50	0.44
1:C:2:THR:HG22	1:C:44[B]:THR:HG22	2.00	0.43
1:A:7:VAL:HB	1:A:10:ILE:HD12	2.02	0.42
1:B:36:LEU:HD23	1:B:36:LEU:HA	1.90	0.42
1:B:10[B]:ILE:CG2	1:B:36:LEU:CD2	2.95	0.41
1:C:12:CYS:O	1:C:15:CYS:HB2	2.21	0.41
1:B:2:THR:CG2	1:B:42:THR:CG2	2.93	0.41

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	61/63 (97%)	61 (100%)	0	0	100	100
1	B	62/63 (98%)	61 (98%)	1 (2%)	0	100	100
1	C	63/63 (100%)	63 (100%)	0	0	100	100
1	D	62/63 (98%)	60 (97%)	2 (3%)	0	100	100
All	All	248/252 (98%)	245 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	49/50 (98%)	49 (100%)	0	100	100
1	B	47/50 (94%)	47 (100%)	0	100	100
1	C	49/50 (98%)	49 (100%)	0	100	100
1	D	46/50 (92%)	46 (100%)	0	100	100
All	All	191/200 (96%)	191 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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