



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2HXG / pdb_00002hxg
Title : Crystal Structure of Mn²⁺ bound ECAI
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Deposited on : 2006-08-03
Resolution : 2.80 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 ⓘ 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

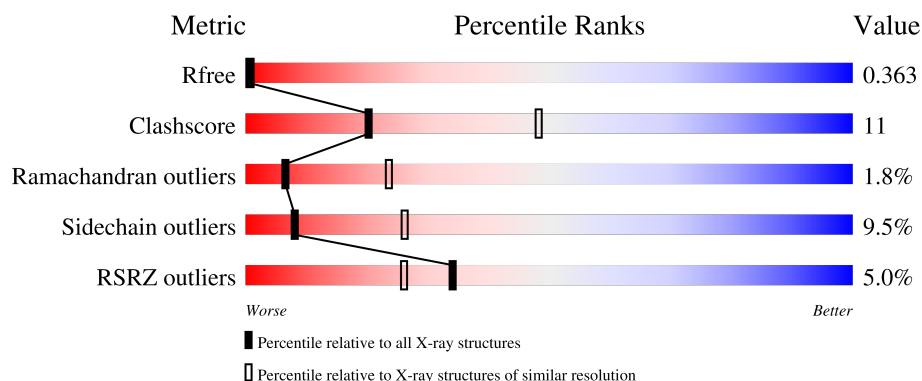
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	500	4% 76% 20% .
1	B	500	4% 74% 22% .
1	C	500	7% 72% 23% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11565 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 L-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3829	2431	669	705	24			
1	B	498	Total	C	N	O	S	0	0	0
			3895	2474	680	717	24			
1	C	498	Total	C	N	O	S	0	0	0
			3735	2353	650	708	24			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	PRO	ARG	SEE REMARK 999	UNP Q8FL89
B	72	PRO	ARG	SEE REMARK 999	UNP Q8FL89
C	72	PRO	ARG	SEE REMARK 999	UNP Q8FL89

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	37	Total	O	0	0
			37	37		

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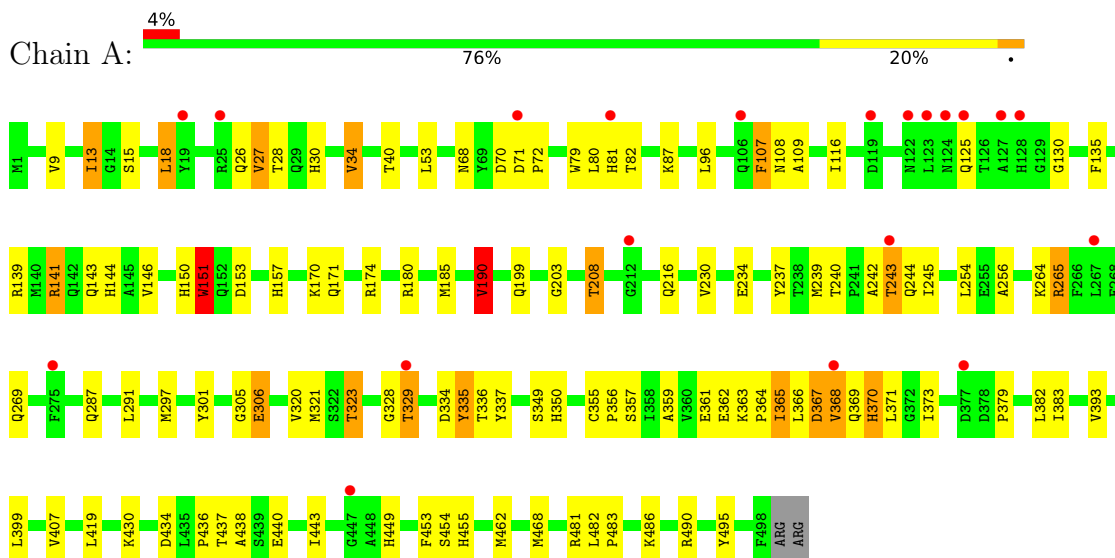
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	25	Total	O	0	0
			25	25		

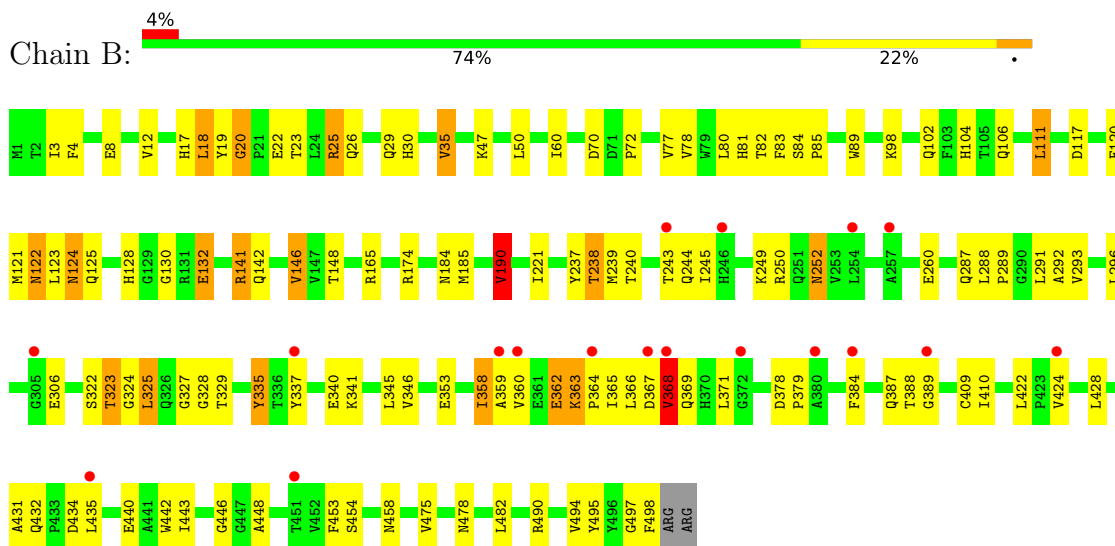
3 Residue-property plots [i](#)

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: L-arabinose isomerase



- Molecule 1: L-arabinose isomerase



- Molecule 1: L-arabinose isomerase



H1	T2	I3	F4	Y7	F11	V12	I13	H17	T23	T28	A31	V35	T40	E41	A42	K43	L44	P45	C46	K47	L53	R65	D70	D71	P72	V77	V78	W79	L80	H81	T82	F83	S84	P85	A86	H91	T94	K98	P99	L100	L101	Q102	F103	H104			
T105	Q106	F107	N108	A109	L111	P112	W113	D114	S115	I116	D117	M118	M121	N122	L123	N124	Q125	H128	G129	G130	R131	E132	F135	Q143	H144	A145	V146	H150	K154	Q155	A156	H157	V168	K177	V178	C179	R180	F181	M185	R186	E187	V188	T191	D192	K195	V206	
N207	T208	N219	S220	I221	Y233	E234	S235	C236	Y237	P241	A242	T243	Q244	I245	W246	G247	R249	R250	Q251	N252	A256	A257	G262	N263	K264	R265	F266	L267	E268	G271	F272	H273	A274	F275	T276	T277	T278	F279	L282	K286	Q287	L288	P289	G290	L291	Q294	N297
F303	A304	G305	E306	K310	R316	V320	T323	G327	G328	T329	S330	F339	N343	D344	L345	S349	H350	M351	L352	E353	I358	A359	V360	P364	V368	Q369	H370	L371	K376	L382	I383	F384	N385	T386	L399	C409	P416	L422	P423	V424	L428						
W429	K430	A431	Q432	L435	P436	I443	G446	G447	F453	A456	I476	R481	R490	E493	V494	Y495	Y496	G497	F498	ARG	ARG																										

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.87Å 116.87Å 215.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (20.00-2.80) 92.0 (20.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.229 , 0.288 0.317 , 0.363	Depositor DCC
R_{free} test set	1988 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11565	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.61	0/3922	0.84	1/5325 (0.0%)
1	B	0.62	0/3991	0.87	2/5424 (0.0%)
1	C	0.57	0/3826	0.85	5/5203 (0.1%)
All	All	0.60	0/11739	0.85	8/15952 (0.1%)

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
1	B	0	3
1	C	0	3
All	All	0	7

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	VAL	CB-CA-C	-7.47	102.25	112.04
1	A	190	VAL	CB-CA-C	-6.68	102.30	112.05
1	C	84	SER	CA-C-N	6.28	126.65	119.93
1	C	84	SER	C-N-CA	6.28	126.65	119.93
1	C	369	GLN	CA-C-N	5.74	132.03	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	PHE	Peptide
1	B	327	GLY	Peptide
1	B	362	GLU	Peptide
1	B	368	VAL	Peptide
1	C	46	CYS	Peptide

5.2 Too-close contacts

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	3829	0	3686	97	0
1	B	3895	0	3783	94	0
1	C	3735	0	3440	90	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	41	0	0	3	0
3	B	37	0	0	2	0
3	C	25	0	0	0	0
All	All	11565	0	10909	253	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 11.

The worst 5 of 253 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:180:ARG:HD2	1:C:195:LYS:HZ2	1.26	0.99
1:B:360:VAL:HG22	1:B:387:GLN:HG2	1.52	0.90
1:C:109:ALA:HB2	1:C:150:HIS:CG	2.12	0.85
1:A:364:PRO:HD2	1:A:383:ILE:O	1.80	0.79
1:C:180:ARG:HD2	1:C:195:LYS:NZ	1.97	0.79

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	496/500 (99%)	453 (91%)	36 (7%)	7 (1%)	9	30
1	B	496/500 (99%)	451 (91%)	41 (8%)	4 (1%)	16	44
1	C	496/500 (99%)	418 (84%)	62 (12%)	16 (3%)	3	11
All	All	1488/1500 (99%)	1322 (89%)	139 (9%)	27 (2%)	6	23

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	TRP
1	A	368	VAL
1	A	370	HIS
1	B	245	ILE
1	C	287	GLN

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	394/419 (94%)	359 (91%)	35 (9%)	9	29
1	B	410/419 (98%)	374 (91%)	36 (9%)	9	29
1	C	369/419 (88%)	329 (89%)	40 (11%)	6	21
All	All	1173/1257 (93%)	1062 (90%)	111 (10%)	8	26

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	250	ARG
1	C	498	PHE
1	C	28	THR
1	C	481	ARG
1	C	345	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	298	GLN
1	C	102	GLN
1	C	460	ASN
1	B	343	ASN
1	B	478	ASN

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 oligosaccharides 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, 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	498/500 (99%)	0.68	20 (4%) 42 33	42, 49, 55, 65	0
1	B	498/500 (99%)	0.63	18 (3%) 46 37	39, 47, 55, 71	0
1	C	498/500 (99%)	0.85	36 (7%) 21 16	36, 46, 53, 64	0
All	All	1494/1500 (99%)	0.72	74 (4%) 34 26	36, 47, 54, 71	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	246	HIS	3.9
1	A	123	LEU	3.8
1	B	424	VAL	3.6
1	C	237	TYR	3.6
1	B	384	PHE	3.5

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](#)

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, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	C	501	1/1	0.93	0.11	71,71,71,71	0
2	MN	B	501	1/1	0.96	0.04	50,50,50,50	0
2	MN	A	501	1/1	0.98	0.03	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.