



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:46 PM UTC

PDB ID : 1KHJ / pdb_00001khj
Title : E. COLI ALKALINE PHOSPHATASE MUTANT (D153HD330N) MIMIC OF THE TRANSITION STATES WITH ALUMINIUM FLUORIDE
Authors : Le Du, M.H.; Lamoure, C.; Muller, B.H.; Bulgakov, O.V.; Lajeunesse, E.; Menez, A.; Boulain, J.C.
Deposited on : 2001-11-30
Resolution : 2.30 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

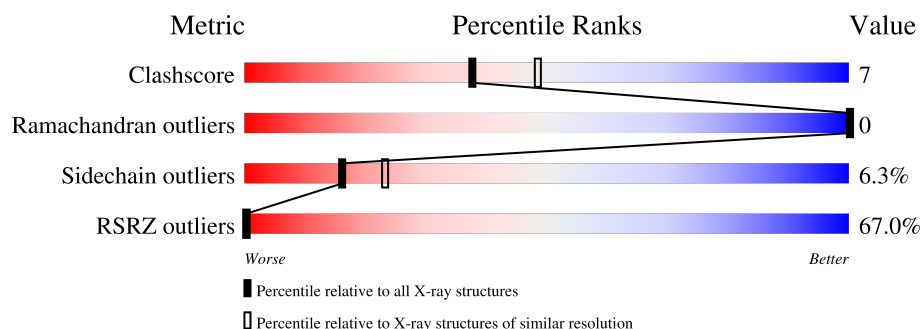
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	449	61% 78% 18% ..
1	B	449	71% 74% 23% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6967 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 Alkaline phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3258	2013	579	655	11			
1	B	444	Total	C	N	O	S	0	0	0
			3258	2013	579	655	11			

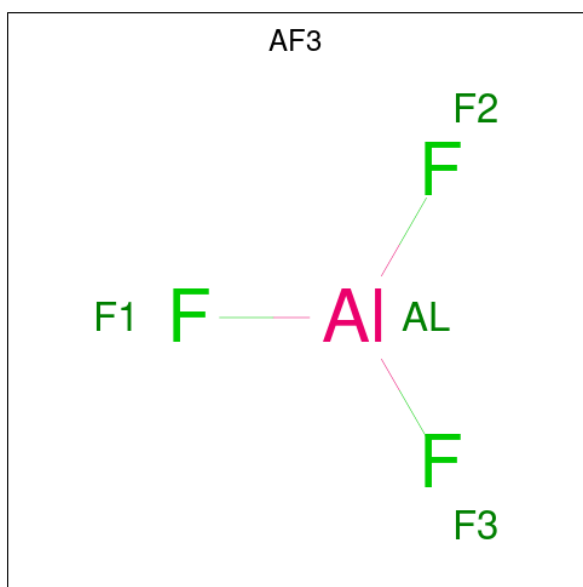
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ASN	ASP	conflict	UNP P00634
A	35	ASN	ASP	conflict	UNP P00634
A	153	HIS	ASP	engineered mutation	UNP P00634
A	176	GLN	GLU	conflict	UNP P00634
A	228	GLU	GLN	conflict	UNP P00634
A	230	GLU	GLN	conflict	UNP P00634
A	330	ASN	ASP	engineered mutation	UNP P00634
B	15	ASN	ASP	conflict	UNP P00634
B	35	ASN	ASP	conflict	UNP P00634
B	153	HIS	ASP	engineered mutation	UNP P00634
B	176	GLN	GLU	conflict	UNP P00634
B	228	GLU	GLN	conflict	UNP P00634
B	230	GLU	GLN	conflict	UNP P00634
B	330	ASN	ASP	engineered mutation	UNP P00634

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			4	1	3		
3	B	1	Total	Al	F	0	0
			4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	228	Total	O	0	0
			228	228		
4	B	211	Total	O	0	0
			211	211		

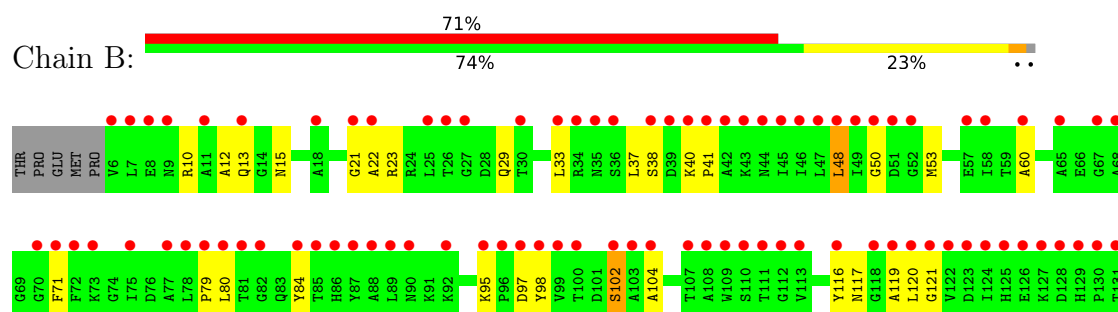
3 Residue-property plots [i](#)

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: Alkaline phosphatase



• Molecule 1: Alkaline phosphatase



N391	T392	K393	D394	V397	M398	V399	M400	S401	Y402	E406	E407	D408	S409	Q410	E411	H412	T413	G414	L417	R418	T419	A420	A421	Y422	G423	P424	H425	A426	A427	N428	V429	V430	G431	L432	T433	D434	Q435	T436	D437	L438	F439	Y440	T441	M442	K443	A444	A445	L446	G447	L448	K449								
S325	I326	D327	K328	Q329	N330	H331	A332	A333	N334	G337	G340	E341	T342	V343	D344	L345	D346	E347	A348	V349	Q350	R351	A352	L353	E354	F355	A356	K357	K358	E359	G360	N361	T362	L363	V364	I365	V366	T367	A368	D369	H370	A373	S374	Q375	I376	V377	A378	P379	A383	P384	G385	L386	T387	L390					
Q252	K253	P254	L255	L256	G257	L258	F259	A260	D261	G262	N263	V266	R267	W268	L269	G270	P271	K272	A273	T274	Y275	H276	G277	A283	V284	P288	N289	P290	Q291	R292	N293	A300	Q301	M302	T303	P304	K305	A306	I307	E308	L309	S310	S311	D312	A313	G316	F317	F318	L319	Q320	V321	E322	G323	A324					
T192	E193	Q194	L195	L196	N197	A198	A199	A200	D201	V202	T203	L204	G205	G206	G207	A208	K209	T210	F211	A212	E213	T214	A215	T216	K217	G218	E219	W220	Q221	G222	Y223	T224	L225	R226	E227	E228	A229	E230	A231	R232	G233	Y234	Q235	L236	V237	S238	D239	A240	A241	S242	L243	N244	S245	V246	T247	E248	A249	N250	Q251
I132	I133	E134	M135	A136	K137	A138	A139	G140	L141	A142	T143	G144	H145	V146	S147	T148	A149	E150	L151	Q152	H153	A154	T155	P156	A157	A158	L159	V160	A161	H162	V163	T164	S165	R166	K167	C168	Y169	G170	P171	S172	A173	T174	S175	Q176	K177	C178	P179	G180	A181	A182	L183	E184	K185	G186	G187	K188	G189	S190	I191

4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	163.51Å 163.51Å 138.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (10.00-2.30) 98.5 (10.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.27Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.180 , 0.223 0.391 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 28.7	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	0.76	EDS
Total number of atoms	6967	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AF3, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.69	0/3312	1.12	26/4496 (0.6%)
1	B	0.70	0/3312	1.10	23/4496 (0.5%)
All	All	0.69	0/6624	1.11	49/8992 (0.5%)

There are no bond length outliers.

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	ILE	N-CA-C	-9.50	100.93	110.62
1	A	324	ALA	N-CA-C	9.37	121.26	111.14
1	A	326	ILE	N-CA-C	-8.62	102.14	110.42
1	B	324	ALA	N-CA-C	7.78	119.83	111.36
1	A	373	ALA	N-CA-C	7.76	121.24	111.69

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	A	3258	0	3195	44	6
1	B	3258	0	3195	50	7
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	228	0	0	2	8
4	B	211	0	0	5	5
All	All	6967	0	6390	90	14

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.

The worst 5 of 90 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:A:334:ASN:HD22	1:A:337:GLY:H	1.35	0.73
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.72	0.69
1:A:253:LYS:HB2	1:A:253:LYS:NZ	2.08	0.68
1:B:182:ALA:HB1	1:B:184:GLU:OE1	1.93	0.67
1:B:38:SER:OG	1:B:40:LYS:HG2	1.96	0.66

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLU:OE1	4:B:1308:HOH:O[9_766]	1.47	0.73
1:B:95:LYS:CE	4:A:1376:HOH:O[9_766]	1.54	0.66
4:A:1118:HOH:O	4:A:1201:HOH:O[9_766]	1.66	0.54
4:A:1189:HOH:O	4:A:1189:HOH:O[9_766]	1.76	0.44
1:A:393:LYS:NZ	4:A:1290:HOH:O[9_766]	1.85	0.35

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	442/449 (98%)	434 (98%)	8 (2%)	0	100	100
1	B	442/449 (98%)	435 (98%)	7 (2%)	0	100	100
All	All	884/898 (98%)	869 (98%)	15 (2%)	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	A	332/340 (98%)	313 (94%)	19 (6%)	18	27
1	B	332/340 (98%)	309 (93%)	23 (7%)	14	20
All	All	664/680 (98%)	622 (94%)	42 (6%)	16	23

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	225	LEU
1	B	310	LEU
1	B	232	ARG
1	B	253	LYS
1	B	393	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	9	ASN
1	B	29	GLN
1	B	329	GLN
1	B	15	ASN
1	B	35	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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AF3	A	453	1,2,4	0,3,3	-	-	-		
3	AF3	B	453	1,2,4	0,3,3	-	-	-		

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 ⓘ

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	444/449 (98%)	2.42	275 (61%) 0 0	11, 21, 46, 72	0
1	B	444/449 (98%)	2.75	320 (72%) 0 0	10, 20, 46, 69	0
All	All	888/898 (98%)	2.58	595 (67%) 0 0	10, 20, 46, 72	0

The worst 5 of 595 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	GLY	6.4
1	B	138	ALA	6.3
1	A	6	VAL	6.2
1	A	431	GLY	6.0
1	B	165	SER	5.9

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
3	AF3	B	453	4/4	0.32	0.37	35,39,40,41	0
2	ZN	B	450	1/1	0.58	0.11	20,20,20,20	0
2	ZN	A	450	1/1	0.61	0.09	23,23,23,23	0
2	ZN	A	451	1/1	0.61	0.12	27,27,27,27	0
2	ZN	B	451	1/1	0.66	0.10	26,26,26,26	0
3	AF3	A	453	4/4	0.84	0.16	31,34,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.