



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 11:39 PM UTC

PDB ID : 1UX4 / pdb_00001ux4
Title : Crystal structures of a Formin Homology-2 domain reveal a tethered-dimer architecture
Authors : Xu, Y.; Moseley, J.B.; Sagot, I.; Poy, F.; Pellman, D.; Goode, B.L.; Eck, M.J.
Deposited on : 2004-02-19
Resolution : 3.30 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
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

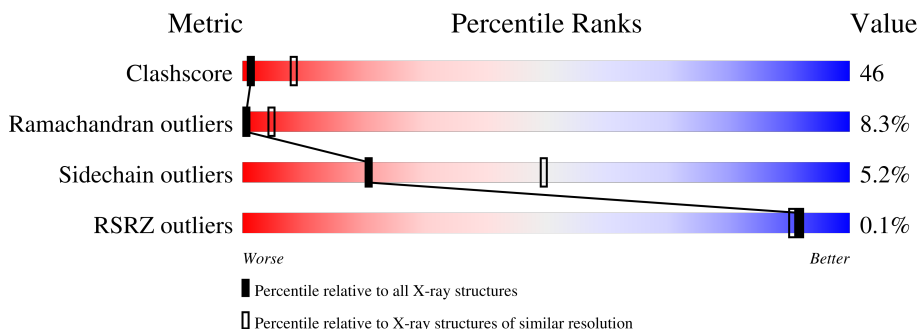
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	410	35% 55% 10%
1	B	410	33% 56% 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6644 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 BNI1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	204	0	0
			3322	2119	555	638	10			
1	B	410	Total	C	N	O	S	197	0	0
			3322	2119	555	638	10			

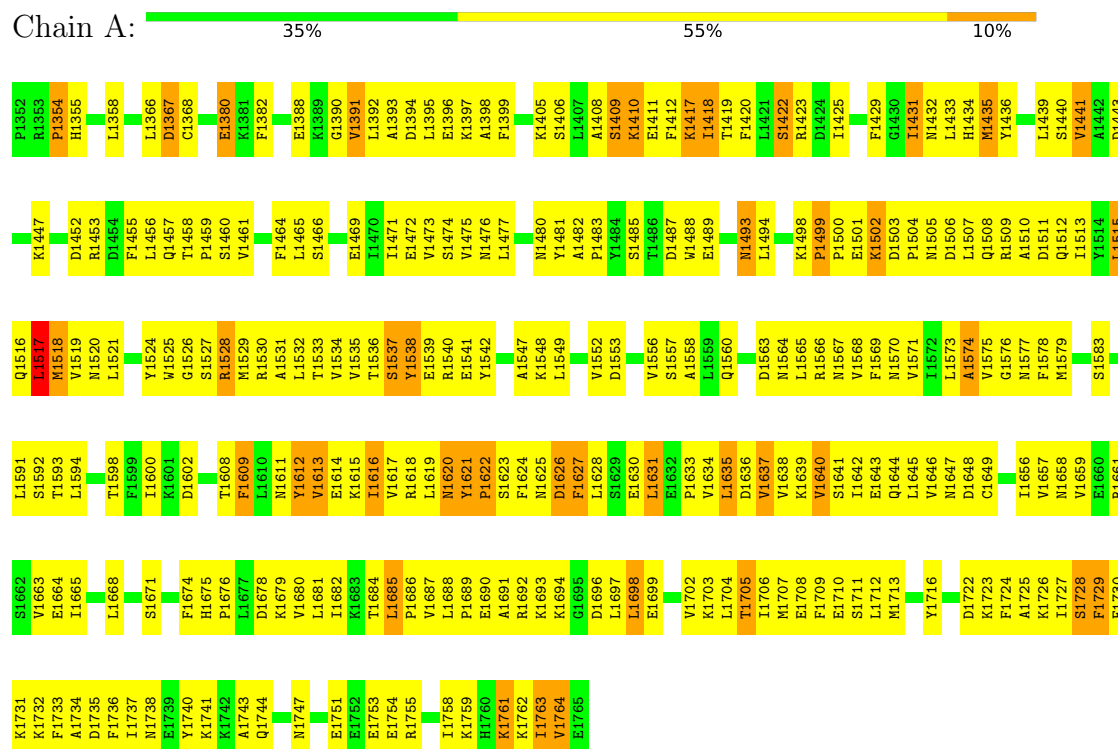
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1411	GLU	ARG	engineered mutation	UNP P41832
A	1412	PHE	LYS	engineered mutation	UNP P41832
B	2411	GLU	ARG	engineered mutation	UNP P41832
B	2412	PHE	LYS	engineered mutation	UNP P41832

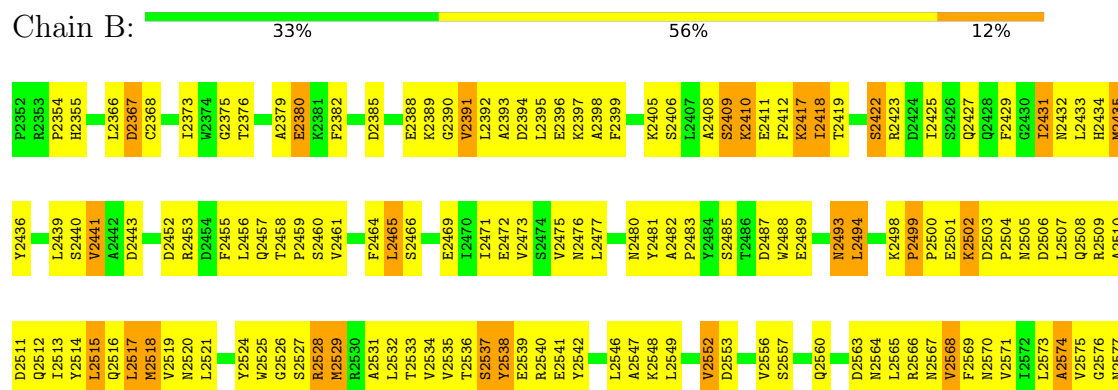
3 Residue-property plots

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: BNI1 PROTEIN



• Molecule 1: BNI1 PROTEIN



F2578	M2579	N2580	D2581	T2582	S2583	K2584	Q2585	L2591	S2592	T2593	L2594	Q2595	R2596	L2597	T2598	F2599	L2600	K2601	D2602	T2608	F2609	L2610	N2611	Y2612	V2613	E2614	K2615	L2616	V2617	R2618	L2619	N2620	Y2621	P2622	S2623	F2624	N2625	D2626	F2627	L2628	S2629	E2630	L2631	E2632	P2633	V2634	L2635	D2636	V2637	V2638	K2639	V2640	S2641	T2642	E2643	Q2644	L2645
V2646	N2647	D2648	C2649	K2650	L2656	V2657	N2658	V2659	E2660	R2661	S2662	V2663	E2664	I2665	L2668	S2671	F2674	H2675	P2676	L2677	D2678	K2679	V2680	L2681	I2682	K2683	T2684	L2685	P2686	V2687	L2688	P2689	E2690	A2691	R2692	K2693	K2694	G2695	D2696	L2697	L2698	E2699	D2700	E2701	V2702	K2703	L2704	T2705	I2706	M2707	E2708	F2709	E2710	S2711	L2712		
M2713	Y2716	D2719	D2722	K2723	F2724	A2725	K2726	I2727	S2728	F2729	F2730	K2731	K2732	F2733	A2734	D2735	F2736	I2737	Y2740	K2741	K2742	A2743	Q2744	N2747	E2751	E2752	E2753	E2754	R2755	L2756	Y2757	I2758	K2759	H2760	K2761	K2762	I2763	V2764	E2765																		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.10Å 172.20Å 120.60Å 90.00° 112.30° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	81.0 (20.00-3.30) 75.2 (20.00-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.289 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	1.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 115.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.186 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6644	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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](#)

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	0.54	0/3382	1.04	21/4559 (0.5%)
1	B	0.54	0/3382	1.02	19/4559 (0.4%)
All	All	0.54	0/6764	1.03	40/9118 (0.4%)

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1754	GLU	N-CA-C	-9.60	102.79	112.97
1	A	1759	LYS	N-CA-C	-9.43	100.67	113.30
1	B	2757	TYR	N-CA-C	-8.51	103.49	114.04
1	A	1593	THR	N-CA-C	7.31	120.18	111.33
1	B	2423	ARG	N-CA-C	-7.17	103.46	111.71

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	3322	0	3340	272	0
1	B	3322	0	3340	291	0
All	All	6644	0	6680	562	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 46.

The worst 5 of 562 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:2504:PRO:HA	1:B:2507:LEU:HD23	1.44	0.98
1:B:2528:ARG:HG3	1:B:2680:VAL:HG21	1.46	0.97
1:A:1504:PRO:HA	1:A:1507:LEU:HD23	1.44	0.96
1:A:1713:MET:HE1	1:A:1726:LYS:HA	1.48	0.96
1:B:2713:MET:HE1	1:B:2726:LYS:HA	1.51	0.92

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	408/410 (100%)	280 (69%)	97 (24%)	31 (8%)	1	6
1	B	408/410 (100%)	272 (67%)	99 (24%)	37 (9%)	0	3
All	All	816/820 (100%)	552 (68%)	196 (24%)	68 (8%)	0	5

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1354	PRO
1	A	1367	ASP
1	A	1409	SER
1	A	1417	LYS
1	A	1432	ASN

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	373/373 (100%)	355 (95%)	18 (5%)	23	52
1	B	373/373 (100%)	352 (94%)	21 (6%)	19	47
All	All	746/746 (100%)	707 (95%)	39 (5%)	21	49

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2529	MET
1	B	2698	LEU
1	B	2620	ASN
1	B	2637	VAL
1	B	2712	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2567	ASN
1	B	2585	GLN
1	B	2747	ASN
1	B	2620	ASN
1	B	2580	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	408/410 (99%)	-1.30	0 100 100	14, 44, 134, 199	48 (11%)
1	B	410/410 (100%)	-1.28	1 (0%) 91 86	12, 47, 149, 199	49 (11%)
All	All	818/820 (99%)	-1.29	1 (0%) 92 90	12, 45, 144, 199	97 (11%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2582	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.