



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 07:38 am BST

PDB ID : 1UX4
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 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 : 2.11
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) : 2.11

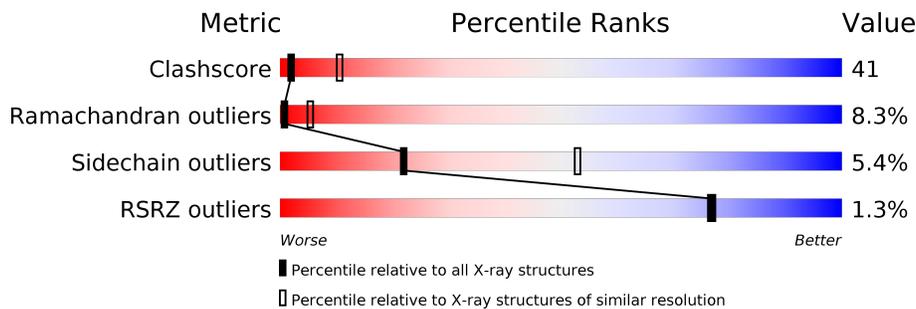
1 Overall quality at a glance

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	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	 2% 39% 53% 8%
1	B	410	 2% 38% 53% 8%

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
			Total	C	N	O	S			
1	A	410	3322	2119	555	638	10	204	0	0
1	B	410	3322	2119	555	638	10	197	0	0

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

K2584
Q2585
L2591
S2592
T2583
L2594
Q2595
R2596
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
L2642
E2643
Q2644
L2645
V2646
N2647
D2648
C2649
L2656
V2657
N2658
V2659
E2660
R2661
S2662
V2663
E2664
L2665
F2674
H2675
P2676
L2677
D2678
K2679
V2680
L2681
L2682
K2683
T2684
L2685
P2686
V2687
L2688
P2689
E2690
A2691
R2692
K2693
K2694
G2695
D2696
L2697
L2698
V2702
K2703
L2704
T2705
L2706
M2707
E2708
F2709
E2710
S2711
L2712
M2713
Y2716
D2719
D2722
K2723
F2724
A2725
K2726
L2727
S2728
F2729
F2730
K2731
K2732
F2733
A2734
D2735
F2736
L2737
Y2740
K2741
K2742
A2743
Q2744
M2747
E2751
E2752
E2753
E2754
R2755
L2756
Y2757
L2758
K2759
H2760
K2761
K2762
L2763
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 39.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	81.0 (20.00-3.30) 69.5 (39.96-3.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.12Å)	Xtrriage
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	Xtrriage
Anisotropy	1.149	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.186 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6644	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage'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	0.43	0/3382	0.67	1/4559 (0.0%)
1	B	0.43	0/3382	0.66	0/4559
All	All	0.43	0/6764	0.66	1/9118 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1545	LEU	CA-CB-CG	-5.17	103.40	115.30

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	248	0
1	B	3322	0	3340	262	0
All	All	6644	0	6680	509	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 41.

The worst 5 of 509 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:1528:ARG:HG3	1:A:1680:VAL:HG21	1.52	0.92
1:B:2552:VAL:O	1:B:2556:VAL:HG23	1.69	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%)	1	4
All	All	816/820 (100%)	552 (68%)	196 (24%)	68 (8%)	1	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%)	354 (95%)	19 (5%)	24	54
1	B	373/373 (100%)	352 (94%)	21 (6%)	21	52
All	All	746/746 (100%)	706 (95%)	40 (5%)	22	53

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1698	LEU
1	B	2418	ILE
1	B	2676	PRO
1	B	2380	GLU
1	B	2435	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1760	HIS
1	B	2457	GLN
1	B	2585	GLN
1	A	1644	GLN
1	A	1747	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

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	408/410 (99%)	-0.29	4 (0%) 82 82	14, 48, 170, 199	48 (11%)
1	B	410/410 (100%)	-0.31	7 (1%) 70 68	14, 52, 168, 199	49 (11%)
All	All	818/820 (99%)	-0.30	11 (1%) 77 77	14, 51, 170, 199	97 (11%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2361	LEU	5.3
1	B	2582	THR	3.9
1	A	1407	LEU	3.8
1	A	1361	LEU	3.0
1	B	2354	PRO	2.6

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 carbohydrates 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.