Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2021 – 06:14 PM EDT

PDB ID	:	1TXD
Title	:	Crystal Structure of the DH/PH domains of Leukemia-associated RhoGEF
Authors	:	Kristelly, R.; Gao, G.; Tesmer, J.J.
Deposited on	:	2004-07-03
Resolution	:	2.13 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

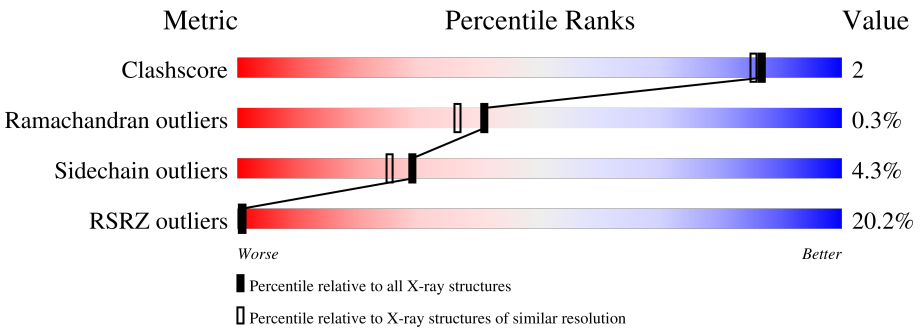
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

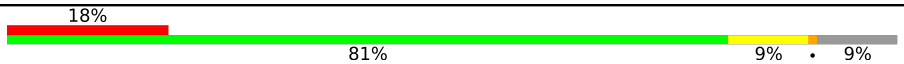
The reported resolution of this entry is 2.13 Å.

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	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 <=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	385	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2972 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 Rho guanine nucleotide exchange factor 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	352	2881	1822	514	533	12	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	764	GLY	THR	cloning artifact	UNP Q9NZN5
A	765	SER	ASP	cloning artifact	UNP Q9NZN5
A	973	PHE	TYR	engineered mutation	UNP Q9NZN5
A	1139	VAL	-	cloning artifact	UNP Q9NZN5
A	1140	ASP	-	cloning artifact	UNP Q9NZN5
A	1141	GLY	-	cloning artifact	UNP Q9NZN5
A	1142	GLY	-	cloning artifact	UNP Q9NZN5
A	1143	HIS	-	expression tag	UNP Q9NZN5
A	1144	HIS	-	expression tag	UNP Q9NZN5
A	1145	HIS	-	expression tag	UNP Q9NZN5
A	1146	HIS	-	expression tag	UNP Q9NZN5
A	1147	HIS	-	expression tag	UNP Q9NZN5
A	1148	HIS	-	expression tag	UNP Q9NZN5

- Molecule 2 is water.

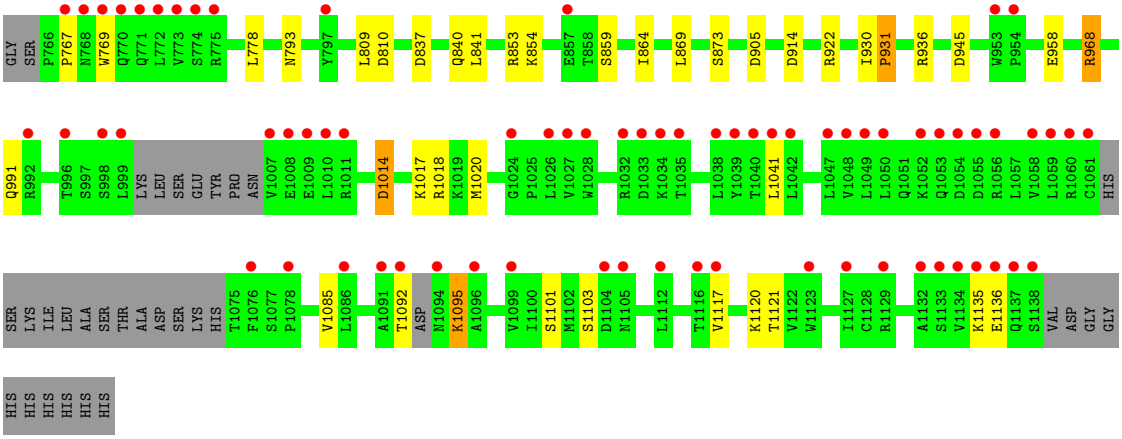
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	91	91	91	0	0

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: Rho guanine nucleotide exchange factor 12

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	193.61Å 45.86Å 74.73Å 90.00° 107.49° 90.00°	Depositor
Resolution (Å)	24.85 – 2.13 24.83 – 2.07	Depositor EDS
% Data completeness (in resolution range)	97.5 (24.85-2.13) 97.4 (24.83-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.235 , 0.274 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2972	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.77	1/2922 (0.0%)	0.89	9/3937 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	931	PRO	CG-CD	5.43	1.68	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	837	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	810	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	914	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	968	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	1014	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	936	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	968	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	922	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	905	ASP	CB-CG-OD1	5.06	122.86	118.30

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	2881	0	2972	12	0
2	A	91	0	0	0	0
All	All	2972	0	2972	12	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 2.

All (12) 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:769:TRP:CD1	1:A:793:ASN:ND2	2.61	0.68
1:A:1020:MET:HE2	1:A:1041:LEU:HD22	1.86	0.58
1:A:930:ILE:N	1:A:931:PRO:CD	2.67	0.57
1:A:1095:LYS:HG2	1:A:1117:VAL:HG22	1.91	0.53
1:A:869:LEU:O	1:A:873:SER:OG	2.24	0.53
1:A:841:LEU:C	1:A:841:LEU:HD23	2.30	0.51
1:A:945:ASP:OD2	1:A:968:ARG:NH2	2.44	0.50
1:A:1085:VAL:O	1:A:1135:LYS:NZ	2.45	0.48
1:A:793:ASN:OD1	1:A:853:ARG:NH2	2.46	0.48
1:A:991:GLN:NE2	1:A:1014:ASP:HA	2.30	0.47
1:A:809:LEU:HD23	1:A:809:LEU:HA	1.81	0.43
1:A:769:TRP:CZ3	1:A:778:LEU:HD11	2.55	0.42

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	344/385 (89%)	331 (96%)	12 (4%)	1 (0%)	41 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	767	PRO

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	326/354 (92%)	312 (96%)	14 (4%)	29 25

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	840	GLN
1	A	854	LYS
1	A	859	SER
1	A	864	ILE
1	A	958	GLU
1	A	1017	LYS
1	A	1018	ARG
1	A	1092	THR
1	A	1095	LYS
1	A	1101	SER
1	A	1103	SER
1	A	1120	LYS
1	A	1121	THR
1	A	1136	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1031	ASN
1	A	1094	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 monosaccharides 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	352/385 (91%)	1.05	71 (20%) 1 1	10, 31, 69, 83	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1138	SER	7.8
1	A	1034	LYS	6.9
1	A	1047	LEU	6.3
1	A	1033	ASP	6.3
1	A	1054	ASP	6.3
1	A	771	GLN	6.2
1	A	953	TRP	6.0
1	A	1048	VAL	5.9
1	A	1041	LEU	5.8
1	A	999	LEU	5.8
1	A	1040	THR	5.8
1	A	768	ASN	5.6
1	A	1104	ASP	5.6
1	A	772	LEU	5.4
1	A	1007	VAL	5.4
1	A	1135	LYS	5.3
1	A	769	TRP	5.3
1	A	770	GLN	5.2
1	A	1032	ARG	5.1
1	A	1112	LEU	5.1
1	A	1117	VAL	4.9
1	A	1137	GLN	4.7
1	A	1049	LEU	4.6
1	A	1055	ASP	4.5
1	A	1092	THR	4.5
1	A	1053	GLN	4.3
1	A	1011	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1136	GLU	4.2
1	A	1076	PHE	4.1
1	A	1134	VAL	4.1
1	A	1050	LEU	4.0
1	A	1008	GLU	3.9
1	A	1105	ASN	3.8
1	A	1035	THR	3.8
1	A	1010	LEU	3.6
1	A	1099	VAL	3.5
1	A	1039	TYR	3.5
1	A	1061	CYS	3.5
1	A	767	PRO	3.4
1	A	773	VAL	3.4
1	A	775	ARG	3.2
1	A	857	GLU	3.1
1	A	1009	GLU	3.0
1	A	1024	GLY	3.0
1	A	1052	LYS	3.0
1	A	1091	ALA	2.9
1	A	1056	ARG	2.9
1	A	954	PRO	2.9
1	A	1042	LEU	2.9
1	A	998	SER	2.9
1	A	1123	TRP	2.8
1	A	797	TYR	2.8
1	A	1026	LEU	2.7
1	A	1133	SER	2.6
1	A	1127	ILE	2.6
1	A	1094	ASN	2.6
1	A	1060	ARG	2.5
1	A	996	THR	2.5
1	A	1116	THR	2.4
1	A	1028	TRP	2.4
1	A	1078	PRO	2.4
1	A	1059	LEU	2.3
1	A	1096	ALA	2.3
1	A	1129	ARG	2.2
1	A	1086	LEU	2.1
1	A	1027	VAL	2.1
1	A	1058	VAL	2.1
1	A	992	ARG	2.0
1	A	1132	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1038	LEU	2.0
1	A	774	SER	2.0

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 monosaccharides 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.