wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2022 – 04:09 pm BST

PDB ID	:	6TM1
Title	:	Crystal structure of the DHR2 domain of DOCK10 in complex with RAC3
Authors	:	Barford, D.; Fan, D.; Cronin, N.; Yang, J.
Deposited on	:	2019-12-03
Resolution	:	3.71 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 (i) 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 (1)) were used in the production of this report:

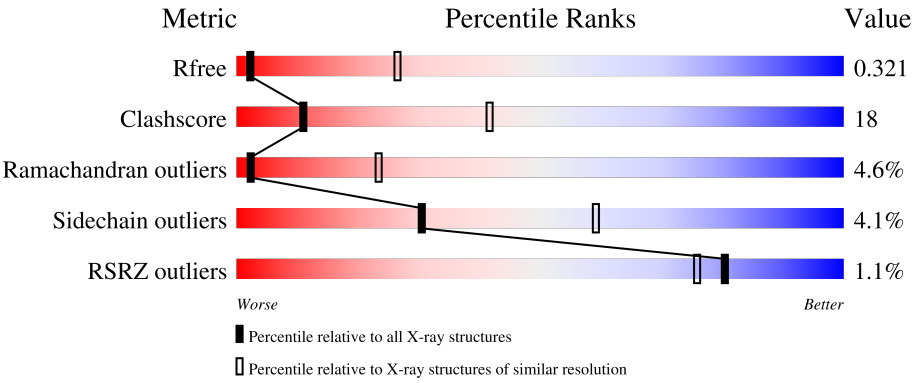
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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

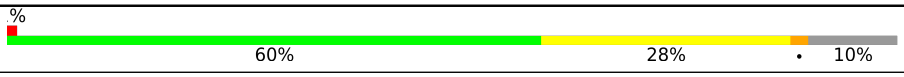
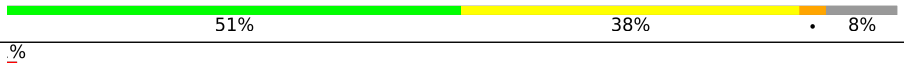
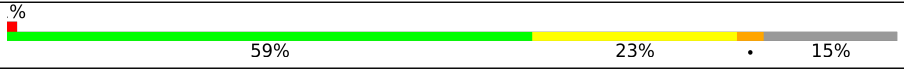
The reported resolution of this entry is 3.71 Å.

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}	130704	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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	B	457	
2	A	192	
3	C	458	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6775 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 Dedicator of cytokinesis protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	412	Total	C	N	O	S	0	0	0
			2969	1890	505	561	13			

- Molecule 2 is a protein called Ras-related C3 botulinum toxin substrate 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	177	Total	C	N	O	S	0	0	0
			1243	796	209	231	7			

- Molecule 3 is a protein called Dedicator of cytokinesis protein 10.

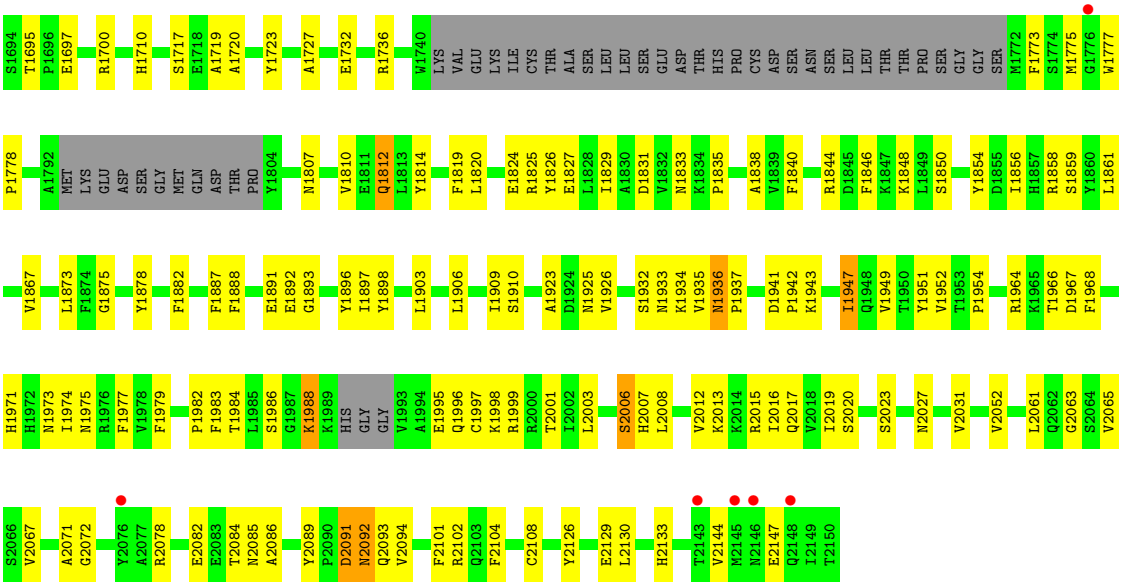
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	388	Total	C	N	O	S	0	0	0
			2563	1620	446	490	7			

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: Dedicator of cytokinesis protein 10

Chain B:

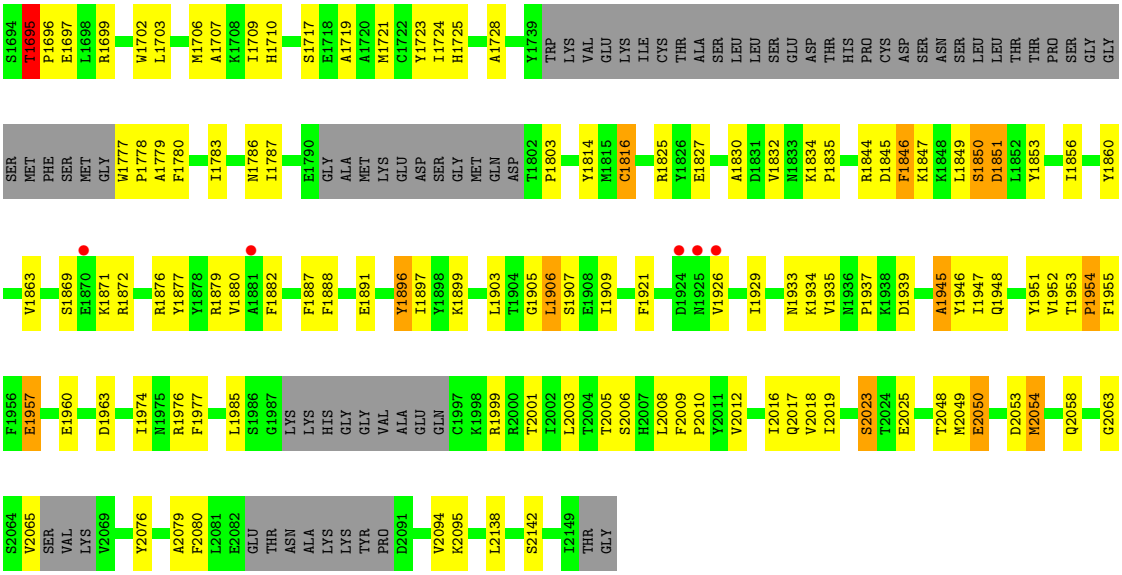


• Molecule 2: Ras-related C3 botulinum toxin substrate 3

Chain A:

• Molecule 3: Dedicator of cytokinesis protein 10

Chain C:


S1694 T1695 P1696 E1697 L1698 R1699 W1702 L1703 M1706 A1707 K1708 I1709 H1710 S1717 E1718 A1719 A1720 M1721 C1722 Y1723 I1724 H1725 A1728 Y1739 TRP LYS VAL GLU LYS ILE CYS THR ALA SER LEU LEU SER GLU ASP THR HIS PRO CYS ASP SER ASN SER LEU LEU THR THR PRO SER GLY GLY
SER MET PHE SER MET GLY W1777 P1778 A1779 F1780 I1783 N1786 I1787 E1790 GLY ALA MET LYS GLU ASP SER GLY MET GLN ASP T1802 P1803 Y1814 M1815 C1816 R1825 Y1826 E1827 A1830 D1831 V1832 N1833 K1834 P1835 R1844 D1845 F1846 K1847 K1848 L1849 S1850 D1851 L1852 Y1853 I1856 Y1860
V1863 S1869 E1870 K1871 R1872 R1876 Y1877 Y1878 R1879 V1880 A1881 F1882 F1887 F1888 E1891 Y1896 I1897 Y1898 K1899 L1903 T1904 G1905 L1906 S1907 E1908 I1909 F1921 D1924 N1925 V1926 I1929 N1933 K1934 V1935 N1936 P1937 K1938 D1939 A1945 Y1946 I1947 Q1948 Y1951 V1952 T1953 P1954 F1955
F1956 E1957 E1960 D1963 I1974 N1975 R1976 F1977 L1985 S1986 G1987 LYS LYS HIS GLY GLY VAL ALA GLU GLN C1997 K1998 R1999 R2000 T2001 I2002 L2003 T2004 T2005 S2006 H2007 L2008 F2009 P2010 Y2011 V2012 I2016 Q2017 V2018 I2019 S2023 T2024 E2025 T2048 M2049 E2050 D2053 M2054 Q2058 G2063
S2064 V2065 SER VAL LYS V2069 Y2076 A2079 F2080 L2081 E2082 GLU THR ASN ALA LYS LYS TYR PRO D2091 V2094 K2095 L2138 S2142 I2149 THR GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	110.08Å 128.46Å 215.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 3.71 29.60 – 3.71	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.60-3.71) 96.5 (29.60-3.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 3.75Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.260 , 0.321 0.260 , 0.321	Depositor DCC
R_{free} test set	797 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	152.9	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6775	wwPDB-VP
Average B, all atoms (Å^2)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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

5.1 Standard geometry

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	B	0.29	0/3028	0.50	0/4133
2	A	0.27	0/1273	0.55	1/1753 (0.1%)
3	C	0.27	0/2606	0.49	0/3586
All	All	0.28	0/6907	0.51	1/9472 (0.0%)

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
3	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	79	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	1695	THR	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	B	2969	0	2562	100	0
2	A	1243	0	1117	58	0
3	C	2563	0	1997	74	0
All	All	6775	0	5676	225	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 18.

The worst 5 of 225 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:1973:ASN:HB3	1:B:2008:LEU:HD23	1.26	1.17
1:B:1973:ASN:HB3	1:B:2008:LEU:CD2	1.99	0.91
3:C:2054:MET:O	3:C:2058:GLN:OE1	1.93	0.86
2:A:93:VAL:HA	2:A:97:TRP:HD1	1.39	0.85
1:B:2091:ASP:O	1:B:2093:GLN:N	2.11	0.83

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	B	404/457 (88%)	341 (84%)	49 (12%)	14 (4%)	3 30
2	A	175/192 (91%)	148 (85%)	18 (10%)	9 (5%)	2 22
3	C	376/458 (82%)	310 (82%)	45 (12%)	21 (6%)	2 20
All	All	955/1107 (86%)	799 (84%)	112 (12%)	44 (5%)	2 23

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1934	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1936	ASN
1	B	2019	ILE
1	B	2092	ASN
2	A	36	VAL

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	B	259/411 (63%)	246 (95%)	13 (5%)	24	55
2	A	114/167 (68%)	112 (98%)	2 (2%)	59	77
3	C	184/411 (45%)	176 (96%)	8 (4%)	29	58
All	All	557/989 (56%)	534 (96%)	23 (4%)	30	59

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	157	CYS
3	C	1850	SER
3	C	1816	CYS
3	C	1851	ASP
1	B	1932	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	2127	GLN

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	B	412/457 (90%)	-0.22	6 (1%) 73 68	98, 151, 204, 230	0
2	A	177/192 (92%)	-0.33	0 100 100	110, 152, 189, 207	0
3	C	388/458 (84%)	-0.42	5 (1%) 77 72	96, 143, 181, 225	0
All	All	977/1107 (88%)	-0.32	11 (1%) 80 76	96, 147, 197, 230	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1925	ASN	3.4
3	C	1926	VAL	3.1
1	B	2146	ASN	3.0
3	C	1924	ASP	2.9
1	B	1776	GLY	2.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.