W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 20, 2024 – 10:07 PM JST

PDB ID	:	8YA8
Title	:	The crystal structure of human Rtel1 HHD2 domain
Authors	:	Chun, I.S.; Kim, M.S.
Deposited on	:	2024-02-08
Resolution	:	2.85 Å(reported)

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

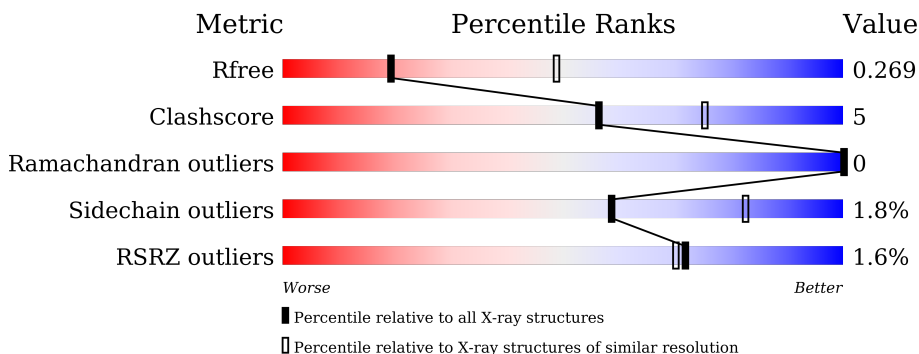|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.85 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	Percentile Ranks	Value
Rfree		0.269
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		1.8%
RSRZ outliers		1.6%

Worse / Better

▮ Percentile relative to all X-ray structures
❙ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	90	·% — 83% / 6% / 11%
1	B	90	79% / 10% / 11%
1	C	90	82% / 7% / 11%
1	D	90	·% — 79% / 11% / 10%
1	E	90	·% — 72% / 18% / 10%
1	F	90	6% — 80% / · / · / 12%

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Mol	Chain	Length	Quality of chain
1	G	90	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4365 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 Regulator of telomere elongation helicase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	S	0	0	0
			614	387	111	113	3			
1	B	80	Total	C	N	O	S	0	0	0
			619	390	112	114	3			
1	C	80	Total	C	N	O	S	0	0	0
			614	387	111	113	3			
1	D	81	Total	C	N	O	S	0	0	0
			623	392	113	115	3			
1	E	81	Total	C	N	O	S	0	0	0
			623	392	113	115	3			
1	F	79	Total	C	N	O	S	0	0	0
			610	385	110	112	3			
1	G	80	Total	C	N	O	S	0	0	0
			614	387	111	113	3			

- Molecule 2 is water.

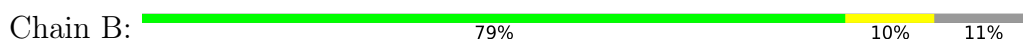| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	O	0	0
			6	6		
2	B	7	Total	O	0	0
			7	7		
2	C	13	Total	O	0	0
			13	13		
2	D	10	Total	O	0	0
			10	10		
2	E	8	Total	O	0	0
			8	8		
2	F	3	Total	O	0	0
			3	3		
2	G	1	Total	O	0	0
			1	1		

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.
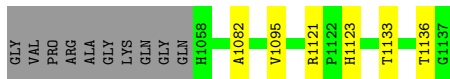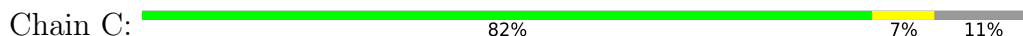
• Molecule 1: Regulator of telomere elongation helicase 1
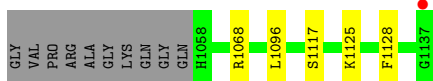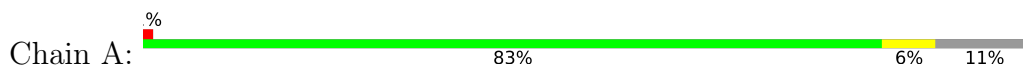
Chain A:

• Molecule 1: Regulator of telomere elongation helicase 1

Chain B:

• Molecule 1: Regulator of telomere elongation helicase 1

Chain C:

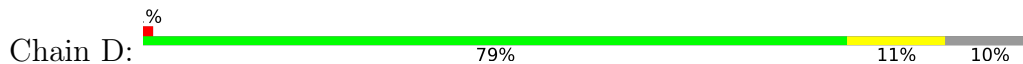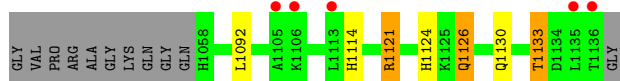• Molecule 1: Regulator of telomere elongation helicase 1

Chain D:

• Molecule 1: Regulator of telomere elongation helicase 1

Chain E:

• Molecule 1: Regulator of telomere elongation helicase 1

Chain F:

6%

80%

12%

GLY VAL PRO ARG ALA GLY LYS GLN GLY GLN H1058 L1092 A1105 K1106 L1113 H1114 R1121 H1124 K1125 Q1126 Q1130 T1133 D1134 L1135 T1136 GLY

• Molecule 1: Regulator of telomere elongation helicase 1

Chain G:

%

71%

17%

11%

GLY VAL PRO ARG ALA GLY LYS GLN GLY GLN H1058 A1059 V1060 L1064 Y1086 V1095 L1096 A1100 T1103 T1104 D1109 F1110 L1113 H1114 M1118 R1121 S1129 C1132 T1136 G1137
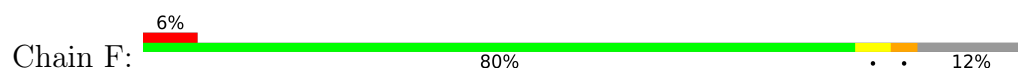
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.05Å 61.96Å 79.95Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	48.90 – 2.85 48.90 – 2.85	Depositor EDS
% Data completeness (in resolution range)	94.0 (48.90-2.85) 88.6 (48.90-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.239 , 0.268 0.239 , 0.269	Depositor DCC
R_{free} test set	722 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 29.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4365	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.29	0/626	0.52	0/848
1	B	0.35	0/631	0.51	0/855
1	C	0.30	0/626	0.51	0/848
1	D	0.34	0/635	0.58	0/860
1	E	0.34	0/635	0.54	0/860
1	F	0.34	0/622	0.56	0/843
1	G	0.31	0/626	0.51	0/848
All	All	0.32	0/4401	0.53	0/5962

There are no bond length outliers.

There are no bond angle outliers.

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	614	0	613	3	0
1	B	619	0	618	6	0
1	C	614	0	613	4	0
1	D	623	0	621	8	0
1	E	623	0	621	7	0
1	F	610	0	610	6	0
1	G	614	0	613	16	0
2	A	6	0	0	0	0
2	B	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	13	0	0	0	0
2	D	10	0	0	0	0
2	E	8	0	0	0	0
2	F	3	0	0	1	0
2	G	1	0	0	0	0
All	All	4365	0	4309	43	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 5.

The worst 5 of 43 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:G:1086:TYR:HB2	1:G:1095:VAL:HG11	1.69	0.74
1:D:1121:ARG:HD2	1:G:1129:SER:HB3	1.71	0.70
1:F:1092:LEU:HD22	1:F:1124:HIS:HB3	1.74	0.68
1:D:1123:HIS:HB3	1:G:1114:HIS:HB3	1.77	0.67
1:G:1103:THR:HG21	1:G:1113:LEU:HB2	1.78	0.65

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	78/90 (87%)	78 (100%)	0	0	100	100
1	B	78/90 (87%)	78 (100%)	0	0	100	100
1	C	78/90 (87%)	78 (100%)	0	0	100	100
1	D	79/90 (88%)	79 (100%)	0	0	100	100
1	E	79/90 (88%)	79 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	77/90 (86%)	76 (99%)	1 (1%)	0	100	100
1	G	78/90 (87%)	78 (100%)	0	0	100	100
All	All	547/630 (87%)	546 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	64/70 (91%)	64 (100%)	0	100	100
1	B	65/70 (93%)	65 (100%)	0	100	100
1	C	64/70 (91%)	64 (100%)	0	100	100
1	D	65/70 (93%)	65 (100%)	0	100	100
1	E	65/70 (93%)	61 (94%)	4 (6%)	18	43
1	F	64/70 (91%)	61 (95%)	3 (5%)	26	56
1	G	64/70 (91%)	63 (98%)	1 (2%)	62	84
All	All	451/490 (92%)	443 (98%)	8 (2%)	59	82

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	1136	THR
1	F	1133	THR
1	F	1121	ARG
1	E	1133	THR
1	F	1126	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1088	GLN
1	D	1114	HIS
1	G	1123	HIS
1	G	1124	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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, 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(Å²)	Q<0.9
1	A	80/90 (88%)	0.00	1 (1%)	77	76	32, 50, 68, 106	0
1	B	80/90 (88%)	-0.22	0	100	100	31, 42, 71, 86	0
1	C	80/90 (88%)	-0.19	0	100	100	32, 44, 68, 78	0
1	D	81/90 (90%)	-0.10	1 (1%)	79	78	30, 48, 75, 97	0
1	E	81/90 (90%)	0.01	1 (1%)	79	78	32, 58, 93, 114	0
1	F	79/90 (87%)	0.42	5 (6%)	20	15	37, 66, 115, 123	0
1	G	80/90 (88%)	0.00	1 (1%)	77	76	30, 58, 84, 99	0
All	All	561/630 (89%)	-0.01	9 (1%)	72	70	30, 51, 94, 123	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1137	GLY	4.0
1	F	1105	ALA	3.4
1	F	1106	LYS	3.3
1	F	1136	THR	3.2
1	A	1137	GLY	3.1

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 ⓘ

There are no such residues in this entry.