Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 08:56 AM EDT

PDB ID	:	2AXY
Title	:	Crystal Structure of KH1 domain of human Poly(C)-binding protein-2 with C-rich strand of human telomeric DNA
Authors	:	Du, Z.; Lee, J.K.; Tjhen, R.J.; Li, S.; Stroud, R.M.; James, T.L.
Deposited on	:	2005-09-06
Resolution	:	1.70 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

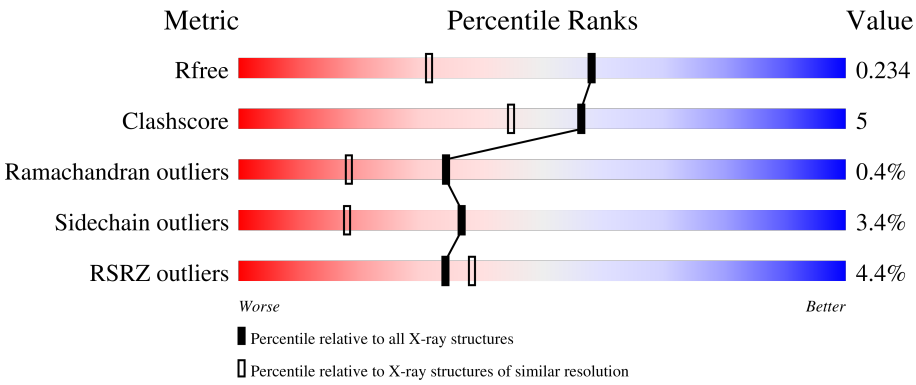
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	E	7	14% / 43% / 29% / 29%
1	F	7	14% / 57% / 14% / 29%
1	G	7	14% / 57% / 29% / 14%
1	H	7	14% / 43% / 14% / 29%
2	A	73	95% / . .

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Mol	Chain	Length	Quality of chain
2	B	73	3% 79% 16%
2	C	73	% 85% 11%
2	D	73	10% 88% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2850 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 DNA chain called C-rich strand of human telomeric dna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	7	137	67	26	38	6	0	0	0
1	F	5	95	47	16	28	4	0	0	0
1	G	6	116	57	21	33	5	0	0	0
1	H	5	96	47	19	26	4	0	0	0

- Molecule 2 is a protein called Poly(rC)-binding protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	A	72	550	346	98	102	1	3	0	0	0
2	B	71	542	340	95	103	1	3	0	0	0
2	C	72	550	346	98	102	1	3	0	0	0
2	D	71	542	340	95	103	1	3	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	LYS	-	CLONING ARTIFACT	UNP Q15366
A	20	MSE	MET	MODIFIED RESIDUE	UNP Q15366
A	39	MSE	MET	MODIFIED RESIDUE	UNP Q15366
A	74	MSE	MET	MODIFIED RESIDUE	UNP Q15366
B	10	LYS	-	CLONING ARTIFACT	UNP Q15366
B	20	MSE	MET	MODIFIED RESIDUE	UNP Q15366
B	39	MSE	MET	MODIFIED RESIDUE	UNP Q15366
B	74	MSE	MET	MODIFIED RESIDUE	UNP Q15366
C	10	LYS	-	CLONING ARTIFACT	UNP Q15366

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	MSE	MET	MODIFIED RESIDUE	UNP Q15366
C	39	MSE	MET	MODIFIED RESIDUE	UNP Q15366
C	74	MSE	MET	MODIFIED RESIDUE	UNP Q15366
D	10	LYS	-	CLONING ARTIFACT	UNP Q15366
D	20	MSE	MET	MODIFIED RESIDUE	UNP Q15366
D	39	MSE	MET	MODIFIED RESIDUE	UNP Q15366
D	74	MSE	MET	MODIFIED RESIDUE	UNP Q15366

- Molecule 3 is water.

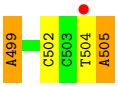
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	E	22	22	22	0	0
			Total	O		
3	F	7	7	7	0	0
			Total	O		
3	G	11	11	11	0	0
			Total	O		
3	H	5	5	5	0	0
			Total	O		
3	A	52	52	52	0	0
			Total	O		
3	B	34	34	34	0	0
			Total	O		
3	C	52	52	52	0	0
			Total	O		
3	D	39	39	39	0	0

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.

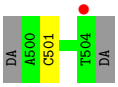
- Molecule 1: C-rich strand of human telomeric dna

Chain E:



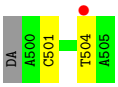
- Molecule 1: C-rich strand of human telomeric dna

Chain F:



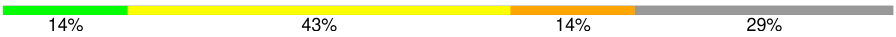
- Molecule 1: C-rich strand of human telomeric dna

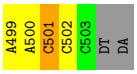
Chain G:



- Molecule 1: C-rich strand of human telomeric dna

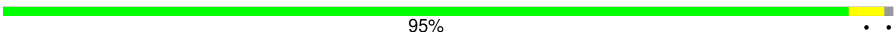
Chain H:





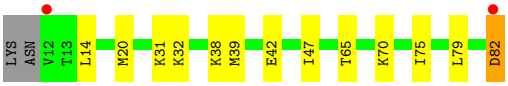
- Molecule 2: Poly(rC)-binding protein 2

Chain A:



- Molecule 2: Poly(rC)-binding protein 2

Chain B:

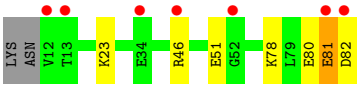


- Molecule 2: Poly(rC)-binding protein 2

Chain C:

- Molecule 2: Poly(rC)-binding protein 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	66.60Å 115.18Å 45.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 57.66 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-1.70) 99.3 (57.66-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.238 0.211 , 0.234	Depositor DCC
R_{free} test set	1991 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2850	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.23% 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	E	0.88	0/153	1.96	7/233 (3.0%)
1	F	1.10	0/105	1.46	1/159 (0.6%)
1	G	1.27	1/129 (0.8%)	1.96	4/196 (2.0%)
1	H	1.08	1/107 (0.9%)	1.51	2/162 (1.2%)
2	A	0.65	0/551	0.67	0/729
2	B	0.56	0/543	0.68	0/718
2	C	0.63	0/551	0.76	0/729
2	D	0.64	0/543	0.72	0/718
All	All	0.73	2/2682 (0.1%)	1.02	14/3644 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	504	DT	C5-C7	6.78	1.54	1.50
1	H	501	DC	C3'-O3'	5.07	1.50	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	501	DC	P-O3'-C3'	14.85	137.53	119.70
1	E	504	DT	O4'-C1'-N1	10.47	115.33	108.00
1	H	501	DC	O4'-C1'-N1	-7.89	102.48	108.00
1	G	501	DC	O4'-C1'-N1	-7.87	102.49	108.00
1	E	504	DT	C6-C5-C7	-6.57	118.96	122.90
1	E	504	DT	C1'-O4'-C4'	-6.41	103.69	110.10
1	E	499	DA	O4'-C1'-N9	6.27	112.39	108.00
1	E	502	DC	O4'-C1'-N1	5.91	112.13	108.00
1	G	501	DC	C4'-C3'-C2'	5.80	108.32	103.10
1	E	504	DT	P-O3'-C3'	5.72	126.56	119.70
1	E	505	DA	O4'-C1'-N9	5.64	111.95	108.00
1	G	501	DC	N1-C1'-C2'	5.54	123.14	112.60
1	F	501	DC	O4'-C1'-N1	-5.21	104.35	108.00
1	H	501	DC	N1-C1'-C2'	5.00	122.11	112.60

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	E	137	0	80	2	0
1	F	95	0	58	0	0
1	G	116	0	69	0	0
1	H	96	0	57	2	0
2	A	550	0	588	2	0
2	B	542	0	573	9	0
2	C	550	0	588	8	0
2	D	542	0	573	5	0
3	A	52	0	0	0	0
3	B	34	0	0	1	0
3	C	52	0	0	3	0
3	D	39	0	0	3	0
3	E	22	0	0	0	0
3	F	7	0	0	0	0
3	G	11	0	0	0	0
3	H	5	0	0	0	0
All	All	2850	0	2586	26	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.

All (26) 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)
2:B:39:MSE:HE2	2:B:47:ILE:HD13	1.74	0.70
2:C:20:MSE:SE	2:C:59:ILE:HD12	2.50	0.61
2:D:80:GLU:O	2:D:81:GLU:HB2	2.00	0.61
2:B:14:LEU:HD23	2:B:65:THR:HG23	1.83	0.59
2:D:46:ARG:HG2	3:D:117:HOH:O	2.01	0.59
2:B:20:MSE:HE1	2:B:79:LEU:HD11	1.85	0.58
2:B:70:LYS:HD3	3:B:98:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:66:ASN:ND2	3:C:132:HOH:O	2.39	0.55
2:D:78:LYS:HD3	2:D:82:ASP:HA	1.88	0.55
2:C:46:ARG:NH2	3:C:106:HOH:O	2.36	0.54
1:E:499:DA:H2	2:A:31:LYS:HE3	1.74	0.53
1:H:499:DA:H2'	1:H:500:DA:C8	2.43	0.53
2:B:38:LYS:O	2:B:42:GLU:HG2	2.11	0.50
2:C:64:PRO:HG2	2:C:66:ASN:HD21	1.78	0.49
2:D:46:ARG:HD2	3:D:83:HOH:O	2.13	0.48
2:C:53:ASN:ND2	3:C:88:HOH:O	2.47	0.47
2:B:39:MSE:HE1	2:B:75:ILE:HG13	1.96	0.47
1:H:501:DC:H2"	1:H:502:DC:OP2	2.16	0.46
1:E:505:DA:H5'	1:E:505:DA:H8	1.81	0.45
2:C:76:ILE:O	2:C:80:GLU:HG3	2.17	0.45
2:A:10:LYS:HD3	2:B:82:ASP:O	2.16	0.44
2:C:25:VAL:HG21	2:C:57:ARG:HB2	2.00	0.43
2:C:20:MSE:HE2	2:C:20:MSE:HB3	1.77	0.41
2:B:70:LYS:HE3	2:B:70:LYS:HB2	1.79	0.41
2:B:39:MSE:HE2	2:B:47:ILE:CD1	2.49	0.41
2:D:46:ARG:HG3	3:D:89:HOH:O	2.20	0.40

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
2	A	70/73 (96%)	69 (99%)	1 (1%)	0	100 100
2	B	69/73 (94%)	69 (100%)	0	0	100 100
2	C	70/73 (96%)	69 (99%)	1 (1%)	0	100 100
2	D	69/73 (94%)	68 (99%)	0	1 (1%)	11 2
All	All	278/292 (95%)	275 (99%)	2 (1%)	1 (0%)	34 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	81	GLU

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
2	A	60/58 (103%)	59 (98%)	1 (2%)	60 46
2	B	59/58 (102%)	56 (95%)	3 (5%)	24 8
2	C	60/58 (103%)	58 (97%)	2 (3%)	38 19
2	D	59/58 (102%)	57 (97%)	2 (3%)	37 18
All	All	238/232 (103%)	230 (97%)	8 (3%)	37 18

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	53	ASN
2	B	31	LYS
2	B	32	LYS
2	B	82	ASP
2	C	20	MSE
2	C	53	ASN
2	D	23	LYS
2	D	51	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	21	HIS
2	A	53	ASN
2	C	53	ASN
2	C	66	ASN
2	D	21	HIS

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	E	7/7 (100%)	0.88	1 (14%)	2	2	10, 12, 18, 26	0
1	F	5/7 (71%)	0.64	1 (20%)	1	0	10, 13, 15, 30	0
1	G	6/7 (85%)	0.30	1 (16%)	1	1	10, 11, 18, 20	0
1	H	5/7 (71%)	0.64	0	100	100	11, 12, 16, 18	0
2	A	69/73 (94%)	0.15	0	100	100	3, 9, 17, 20	0
2	B	68/73 (93%)	0.20	2 (2%)	51	56	4, 9, 17, 19	0
2	C	69/73 (94%)	0.10	1 (1%)	75	79	4, 9, 16, 24	0
2	D	68/73 (93%)	0.33	7 (10%)	6	7	4, 8, 18, 23	0
All	All	297/320 (92%)	0.23	13 (4%)	34	38	3, 9, 18, 30	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	82	ASP	5.4
2	B	12	VAL	4.9
2	D	12	VAL	3.5
1	E	504	DT	3.3
1	F	504	DT	3.2
2	B	82	ASP	3.1
2	D	52	GLY	3.0
2	D	81	GLU	2.6
2	C	81	GLU	2.3
1	G	504	DT	2.3
2	D	34	GLU	2.1
2	D	13	THR	2.1
2	D	46	ARG	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.