Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2016 – 07:48 PM EST

PDB ID	:	5GKP
Title	:	Crystal structure of the EndoG worm homologue CPS-6 H148A/F122A in complex with DNA
Authors	:	Lin, J.L.; Yuan, H.S.
Deposited on	:	2016-07-05
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/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:

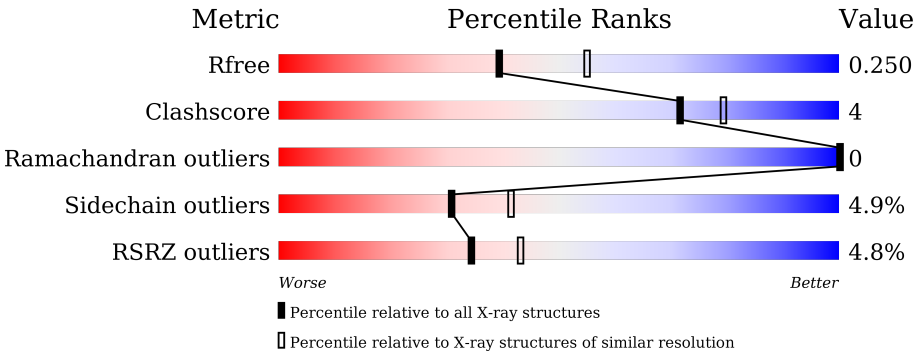
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 2.30 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))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	252	4%, 86%, 7%, •, 7%
1	B	252	4%, 83%, 11%, •, 5%
2	C	8	13%, 25%, 38%, 38%
2	D	8	25%, 13%, 38%, 13%, 38%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7955 atoms, of which 3784 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 Endonuclease G, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	235	3701	1203	1819	327	344	8	0	0	0
1	B	239	3788	1226	1870	334	350	8	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	MET	-	expression tag	UNP Q95NM6
A	55	HIS	-	expression tag	UNP Q95NM6
A	56	HIS	-	expression tag	UNP Q95NM6
A	57	HIS	-	expression tag	UNP Q95NM6
A	58	HIS	-	expression tag	UNP Q95NM6
A	59	HIS	-	expression tag	UNP Q95NM6
A	60	HIS	-	expression tag	UNP Q95NM6
A	61	GLY	-	expression tag	UNP Q95NM6
A	62	SER	-	expression tag	UNP Q95NM6
A	122	ALA	PHE	engineered mutation	UNP Q95NM6
A	148	ALA	HIS	engineered mutation	UNP Q95NM6
B	54	MET	-	expression tag	UNP Q95NM6
B	55	HIS	-	expression tag	UNP Q95NM6
B	56	HIS	-	expression tag	UNP Q95NM6
B	57	HIS	-	expression tag	UNP Q95NM6
B	58	HIS	-	expression tag	UNP Q95NM6
B	59	HIS	-	expression tag	UNP Q95NM6
B	60	HIS	-	expression tag	UNP Q95NM6
B	61	GLY	-	expression tag	UNP Q95NM6
B	62	SER	-	expression tag	UNP Q95NM6
B	122	ALA	PHE	engineered mutation	UNP Q95NM6
B	148	ALA	HIS	engineered mutation	UNP Q95NM6

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	C	5	145	50	48	10	33	4	0	0	0
2	D	5	144	50	47	10	33	4	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	B	1	1	1	0	0
3	A	1	1	1	0	0

- Molecule 4 is water.

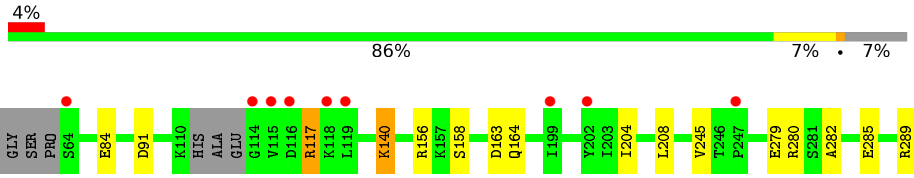
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	72	72	72	0	0
4	B	99	99	99	0	0
4	C	1	1	1	0	0
4	D	3	3	3	0	0

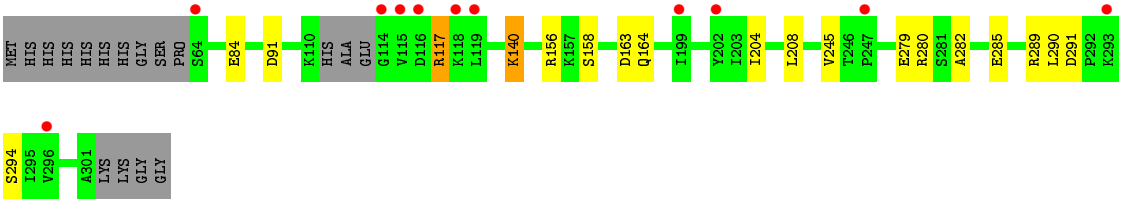
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Endonuclease G, mitochondrial

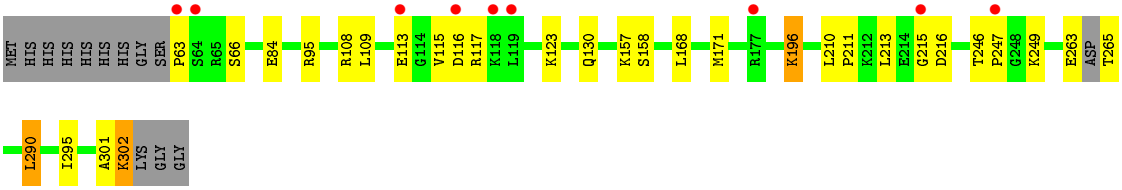
Chain A:





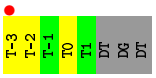
- Molecule 1: Endonuclease G, mitochondrial

Chain B:



- Molecule 2: DNA (5'-D(*TP*TP*TP*TP*T)-3')

Chain C:



- Molecule 2: DNA (5'-D(*TP*TP*TP*TP*T)-3')

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.67Å 72.56Å 127.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.78 – 2.30 19.78 – 2.27	Depositor EDS
% Data completeness (in resolution range)	92.6 (19.78-2.30) 92.6 (19.78-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.173 , 0.253 0.172 , 0.250	Depositor DCC
R_{free} test set	1890 reflections (8.26%)	DCC
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.5	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	0.95	EDS
Total number of atoms	7955	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.10% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.65	0/1927	0.68	1/2602 (0.0%)
1	B	0.68	0/1965	0.75	2/2652 (0.1%)
2	C	1.55	1/106 (0.9%)	1.55	0/162
2	D	1.57	0/106	1.41	1/162 (0.6%)
All	All	0.74	1/4104 (0.0%)	0.78	4/5578 (0.1%)

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
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	0	DT	C1'-N1	5.36	1.56	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	216	ASP	N-CA-C	-6.37	93.81	111.00
1	B	216	ASP	C-N-CA	6.21	135.33	122.30
1	A	91	ASP	CB-CG-OD2	5.32	123.09	118.30
2	D	1	DT	N3-C4-O4	5.29	123.07	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	215	GLY	Peptide

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	1882	1819	1865	8	0
1	B	1918	1870	1904	17	0
2	C	97	48	62	6	0
2	D	97	47	62	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	72	0	0	0	0
4	B	99	0	0	1	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
All	All	4171	3784	3893	34	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 4.

All (34) 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:117:ARG:NH1	2:D:-2:DT:OP2	1.99	0.95
1:B:117:ARG:HH12	2:D:-3:DT:H3'	1.33	0.92
1:B:117:ARG:HH12	2:D:-3:DT:C3'	1.99	0.75
1:A:117:ARG:HH12	2:C:-2:DT:P	2.15	0.69
1:B:117:ARG:O	1:B:117:ARG:HG2	1.96	0.65
2:D:-3:DT:H2"	2:D:-2:DT:C5'	2.27	0.64
2:D:-3:DT:H2"	2:D:-2:DT:H5"	1.79	0.63
1:B:263:GLU:O	1:B:265:THR:N	2.32	0.62
1:A:117:ARG:NH1	2:C:-2:DT:OP2	2.33	0.61
1:B:63:PRO:N	1:B:66:SER:HG	1.99	0.60
2:C:-3:DT:H4'	2:C:-2:DT:OP1	2.02	0.58
1:A:117:ARG:NH1	2:C:-3:DT:O3'	2.36	0.58
2:D:-2:DT:C5'	2:D:-2:DT:H6	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLU:OE1	1:B:158:SER:OG	2.27	0.52
2:D:0:DT:H2"	2:D:1:DT:H4'	1.94	0.50
1:B:246:THR:HB	1:B:247:PRO:HD2	1.95	0.48
1:A:117:ARG:NH1	2:C:-2:DT:P	2.86	0.48
2:C:-3:DT:O5'	2:C:-3:DT:H2'	2.14	0.48
1:A:140:LYS:HB2	1:A:140:LYS:NZ	2.29	0.48
1:B:95:ARG:NH1	4:B:504:HOH:O	2.47	0.47
1:A:208:LEU:HD21	1:A:282:ALA:HB2	1.97	0.47
2:D:-2:DT:C6	2:D:-2:DT:C5'	2.98	0.46
1:B:117:ARG:NH1	2:D:-3:DT:H3'	2.16	0.46
1:B:108:ARG:HA	1:B:157:LYS:HE3	1.97	0.45
1:B:210:LEU:HA	1:B:211:PRO:HD3	1.89	0.42
2:D:-3:DT:H5"	2:D:-3:DT:C6	2.53	0.42
2:D:-3:DT:H5"	2:D:-3:DT:H6	1.84	0.42
1:A:84:GLU:HB2	1:A:164:GLN:OE1	2.19	0.42
1:B:115:VAL:HG12	1:B:116:ASP:N	2.34	0.42
1:A:290:LEU:HG	1:A:291:ASP:N	2.36	0.41
1:B:168:LEU:HD23	1:B:171:MET:HG3	2.01	0.41
1:B:109:LEU:HD13	1:B:196:LYS:HE2	2.02	0.41
1:B:290:LEU:CD1	1:B:295:ILE:HD11	2.51	0.41
1:B:301:ALA:O	1:B:302:LYS:HB3	2.21	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	
1	A	231/252 (92%)	224 (97%)	7 (3%)	0	100	100
1	B	235/252 (93%)	225 (96%)	10 (4%)	0	100	100
All	All	466/504 (92%)	449 (96%)	17 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	203/217 (94%)	191 (94%)	12 (6%)	24	32
1	B	207/217 (95%)	199 (96%)	8 (4%)	39	53
All	All	410/434 (94%)	390 (95%)	20 (5%)	31	41

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ARG
1	A	140	LYS
1	A	156	ARG
1	A	158	SER
1	A	163	ASP
1	A	204	ILE
1	A	245	VAL
1	A	279	GLU
1	A	280	ARG
1	A	285	GLU
1	A	289	ARG
1	A	294	SER
1	B	113	GLU
1	B	123	LYS
1	B	130	GLN
1	B	196	LYS
1	B	213	LEU
1	B	249	LYS
1	B	290	LEU
1	B	302	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	235/252 (93%)	0.07	11 (4%)	35	44	17, 34, 63, 85	0
1	B	239/252 (94%)	-0.07	9 (3%)	44	53	16, 28, 56, 78	0
2	C	5/8 (62%)	1.13	1 (20%)	1	2	44, 54, 57, 64	0
2	D	5/8 (62%)	1.18	2 (40%)	0	0	43, 45, 59, 89	0
All	All	484/520 (93%)	0.03	23 (4%)	34	43	16, 32, 62, 89	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	63	PRO	5.3
1	B	215	GLY	4.9
1	A	119	LEU	4.8
1	B	119	LEU	4.6
2	D	-3	DT	4.3
1	A	115	VAL	3.9
1	B	118	LYS	3.9
1	A	64	SER	3.8
2	C	-3	DT	3.7
1	B	113	GLU	3.1
1	A	116	ASP	3.1
1	B	177	ARG	2.9
1	B	247	PRO	2.8
1	A	293	LYS	2.8
1	A	118	LYS	2.6
1	B	116	ASP	2.5
1	B	64	SER	2.4
2	D	1	DT	2.4
1	A	247	PRO	2.3
1	A	114	GLY	2.3
1	A	296	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	199	ILE	2.1
1	A	202	TYR	2.1

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	A	401	1/1	0.98	0.14	-0.40	32,32,32,32	0
3	MG	B	401	1/1	0.99	0.12	-0.60	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.