



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:30 PM UTC

PDB ID : 2HWX / pdb_00002hwx
Title : Structure of human SMG6 E1282C PIN domain mutant.
Authors : Glavan, F.; Behm-Ansmant, I.; Izaurralde, E.; Conti, E.
Deposited on : 2006-08-02
Resolution : 1.90 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

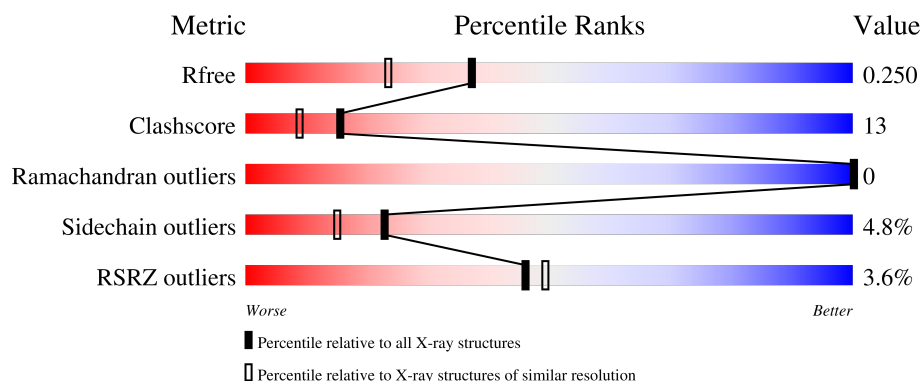
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	181	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1507 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 Telomerase-binding protein EST1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	32	2	0
			1329	840	238	243	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1282	CYS	GLU	engineered mutation	UNP Q86US8

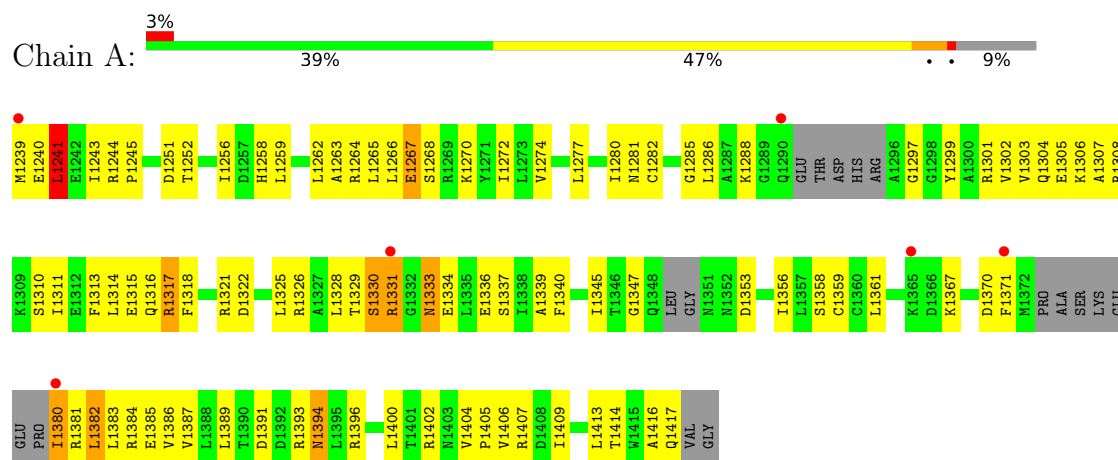
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	178	Total	O	0	0
			178	178		

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: Telomerase-binding protein EST1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.36Å 73.34Å 37.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-1.90) 99.4 (30.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.99 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.197 , 0.239 0.203 , 0.250	Depositor DCC
R_{free} test set	778 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 72.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	1507	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	A	2.29	81/1350 (6.0%)	1.23	0/1816

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1311	ILE	C-O	-9.14	1.13	1.24
1	A	1243	ILE	C-O	-8.61	1.14	1.24
1	A	1265	LEU	C-O	-7.98	1.14	1.24
1	A	1308	ARG	C-O	-7.68	1.15	1.24
1	A	1394	ASN	C-O	-7.63	1.15	1.24
1	A	1315	GLU	C-N	-7.60	1.23	1.33
1	A	1280	ILE	C-O	-7.50	1.15	1.24
1	A	1244	ARG	C-O	-7.48	1.15	1.24
1	A	1303	VAL	C-O	-7.47	1.15	1.24
1	A	1409	ILE	C-O	-7.47	1.18	1.24
1	A	1384	ARG	C-O	-7.46	1.15	1.24
1	A	1356	ILE	C-O	-7.36	1.15	1.24
1	A	1406	VAL	C-O	-7.26	1.16	1.24
1	A	1301	ARG	C-O	-7.21	1.15	1.24
1	A	1407	ARG	C-O	-7.20	1.15	1.23
1	A	1306	LYS	C-O	-7.17	1.15	1.24
1	A	1274	VAL	C-O	-7.13	1.16	1.24
1	A	1310	SER	C-O	-7.13	1.15	1.24
1	A	1262	LEU	C-O	-6.99	1.16	1.24
1	A	1353	ASP	C-O	-6.92	1.16	1.24
1	A	1409	ILE	CA-CB	-6.74	1.50	1.54
1	A	1241	LEU	C-O	-6.72	1.15	1.23
1	A	1334	GLU	C-N	-6.68	1.24	1.33
1	A	1359	CYS	C-O	-6.66	1.16	1.24
1	A	1405	PRO	C-O	-6.62	1.15	1.23
1	A	1282[A]	CYS	C-O	-6.58	1.16	1.24
1	A	1282[B]	CYS	C-O	-6.58	1.16	1.24
1	A	1387	VAL	C-O	-6.55	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1400	LEU	C-O	-6.50	1.16	1.24
1	A	1330	SER	C-O	-6.48	1.16	1.24
1	A	1286	LEU	C-O	-6.47	1.16	1.24
1	A	1307	ALA	C-O	-6.44	1.16	1.24
1	A	1252	THR	C-O	-6.34	1.16	1.24
1	A	1416	ALA	C-O	-6.30	1.16	1.24
1	A	1281	ASN	C-O	-6.29	1.16	1.24
1	A	1383	LEU	C-O	-6.23	1.16	1.24
1	A	1333	ASN	C-O	-6.20	1.16	1.24
1	A	1389	LEU	C-O	-6.18	1.16	1.24
1	A	1245	PRO	C-O	-6.15	1.16	1.23
1	A	1322	ASP	C-O	-6.14	1.16	1.24
1	A	1325	LEU	C-O	-6.10	1.16	1.24
1	A	1314	LEU	C-O	-6.09	1.17	1.24
1	A	1264	ARG	C-O	-6.07	1.17	1.24
1	A	1318	PHE	C-O	-5.97	1.17	1.24
1	A	1266	LEU	C-O	-5.94	1.17	1.24
1	A	1404	VAL	C-O	-5.92	1.17	1.24
1	A	1313	PHE	C-O	-5.86	1.17	1.24
1	A	1259	LEU	C-O	-5.84	1.17	1.24
1	A	1270	LYS	C-O	-5.80	1.16	1.24
1	A	1315	GLU	C-O	-5.80	1.17	1.24
1	A	1317	ARG	C-O	-5.80	1.17	1.24
1	A	1361	LEU	C-O	-5.77	1.16	1.24
1	A	1386	VAL	C-O	-5.76	1.18	1.24
1	A	1382	LEU	C-O	-5.72	1.17	1.24
1	A	1404	VAL	CA-C	5.65	1.58	1.53
1	A	1304	GLN	C-O	-5.61	1.17	1.24
1	A	1251	ASP	C-O	-5.59	1.16	1.23
1	A	1277	LEU	C-O	-5.58	1.17	1.24
1	A	1302	VAL	C-O	-5.46	1.18	1.24
1	A	1285	GLY	C-O	-5.45	1.17	1.23
1	A	1307	ALA	CA-CB	-5.42	1.44	1.53
1	A	1268	SER	C-O	-5.40	1.17	1.24
1	A	1358	SER	C-O	-5.36	1.17	1.24
1	A	1385	GLU	C-O	-5.31	1.16	1.24
1	A	1272	ILE	C-O	-5.30	1.18	1.24
1	A	1256	ILE	C-O	-5.29	1.18	1.24
1	A	1328	LEU	C-O	-5.28	1.17	1.24
1	A	1340	PHE	C-O	-5.28	1.17	1.24
1	A	1288	LYS	C-N	-5.25	1.24	1.33
1	A	1337	SER	C-O	-5.23	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1414	THR	C-O	-5.23	1.18	1.24
1	A	1396	ARG	C-O	-5.21	1.18	1.24
1	A	1339	ALA	C-O	-5.19	1.18	1.24
1	A	1299	TYR	C-O	-5.15	1.18	1.24
1	A	1416	ALA	CA-CB	-5.15	1.44	1.53
1	A	1305	GLU	C-O	-5.12	1.18	1.24
1	A	1402	ARG	C-O	-5.11	1.17	1.24
1	A	1297	GLY	C-O	-5.11	1.16	1.23
1	A	1413	LEU	C-O	-5.07	1.18	1.24
1	A	1326	ARG	C-O	-5.06	1.17	1.23
1	A	1267	GLU	C-O	-5.04	1.17	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	1329	0	1368	35	5
2	A	178	0	0	6	2
All	All	1507	0	1368	35	5

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 13.

All (35) 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:1347:GLY:HA2	2:A:200:HOH:O	1.36	1.22
1:A:1267:GLU:OE1	2:A:124:HOH:O	1.72	1.07
1:A:1316:GLN:HE22	1:A:1317:ARG:HH21	1.02	0.98
1:A:1331:ARG:NH1	2:A:132:HOH:O	1.97	0.97
1:A:1331:ARG:H	1:A:1331:ARG:CD	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1240:GLU:CG	1:A:1381:ARG:HG2	2.03	0.87
1:A:1240:GLU:HG3	1:A:1381:ARG:HG2	1.62	0.82
1:A:1316:GLN:NE2	1:A:1317:ARG:HH21	1.81	0.77
1:A:1347:GLY:CA	2:A:200:HOH:O	2.12	0.72
1:A:1380:ILE:HG13	1:A:1380:ILE:O	1.89	0.71
1:A:1331:ARG:CD	1:A:1331:ARG:N	2.57	0.65
1:A:1316:GLN:HE22	1:A:1317:ARG:NH2	1.86	0.64
1:A:1239:MET:HE1	1:A:1371:PHE:HE2	1.65	0.61
1:A:1331:ARG:H	1:A:1331:ARG:HD2	1.63	0.60
1:A:1239:MET:HE1	1:A:1371:PHE:CE2	2.37	0.59
1:A:1331:ARG:H	1:A:1331:ARG:HD3	1.63	0.59
1:A:1371:PHE:HD2	1:A:1380:ILE:CD1	2.17	0.57
1:A:1239:MET:CE	1:A:1380:ILE:HD11	2.36	0.56
1:A:1394:ASN:ND2	2:A:171:HOH:O	2.36	0.56
1:A:1347:GLY:N	2:A:200:HOH:O	2.35	0.55
1:A:1371:PHE:CD2	1:A:1380:ILE:CD1	2.89	0.54
1:A:1371:PHE:HD2	1:A:1380:ILE:HD11	1.73	0.53
1:A:1330:SER:HB2	1:A:1331:ARG:HD2	1.90	0.53
1:A:1241:LEU:HD12	1:A:1382:LEU:HB3	1.93	0.50
1:A:1329:THR:HB	1:A:1331:ARG:HD3	1.93	0.49
1:A:1331:ARG:N	1:A:1331:ARG:HD2	2.25	0.49
1:A:1258:HIS:HE1	1:A:1391:ASP:OD2	1.95	0.49
1:A:1371:PHE:CD2	1:A:1380:ILE:HD13	2.48	0.48
1:A:1371:PHE:CD2	1:A:1380:ILE:HD11	2.50	0.47
1:A:1316:GLN:NE2	1:A:1317:ARG:HD2	2.30	0.46
1:A:1239:MET:HE3	1:A:1380:ILE:HD11	1.99	0.44
1:A:1239:MET:HE1	1:A:1380:ILE:HD11	1.98	0.44
1:A:1263:ALA:O	1:A:1267:GLU:HG3	2.19	0.42
1:A:1321:ARG:NH1	1:A:1336:GLU:OE1	2.53	0.42
1:A:1240:GLU:HG2	1:A:1381:ARG:HG2	1.96	0.41

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1394:ASN:OD1	2:A:152:HOH:O[2_655]	1.16	1.04
1:A:1367:LYS:NZ	2:A:178:HOH:O[4_457]	1.75	0.45
1:A:1240:GLU:OE1	1:A:1331:ARG:NE[1_554]	2.12	0.08
1:A:1240:GLU:OE2	1:A:1333:ASN:ND2[1_554]	2.13	0.07
1:A:1240:GLU:CB	1:A:1331:ARG:NH2[1_554]	2.16	0.04

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	159/181 (88%)	154 (97%)	5 (3%)	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	148/159 (93%)	141 (95%)	7 (5%)	23	15

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1241	LEU
1	A	1331	ARG
1	A	1345	ILE
1	A	1370	ASP
1	A	1380	ILE
1	A	1393	ARG
1	A	1417	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	A	1258	HIS

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Mol	Chain	Res	Type
1	A	1316	GLN
1	A	1352	ASN
1	A	1362	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 oligosaccharides 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	165/181 (91%)	0.17	6 (3%) 46 49	8, 12, 26, 34	10 (6%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1239	MET	3.8
1	A	1331	ARG	3.1
1	A	1380	ILE	2.6
1	A	1371	PHE	2.3
1	A	1365	LYS	2.2
1	A	1290	GLN	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 oligosaccharides 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.