Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2025 – 02:05 PM EDT

PDB ID	:	9CMB / pdb_00009cmb
Title	:	Human PU.1 ETS Domain (165-270) bound to d(AATAAAAGGAAGTGGG)
Authors	:	Poon, G.M.K.
Deposited on	:	2024-07-13
Resolution	:	2.15 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:

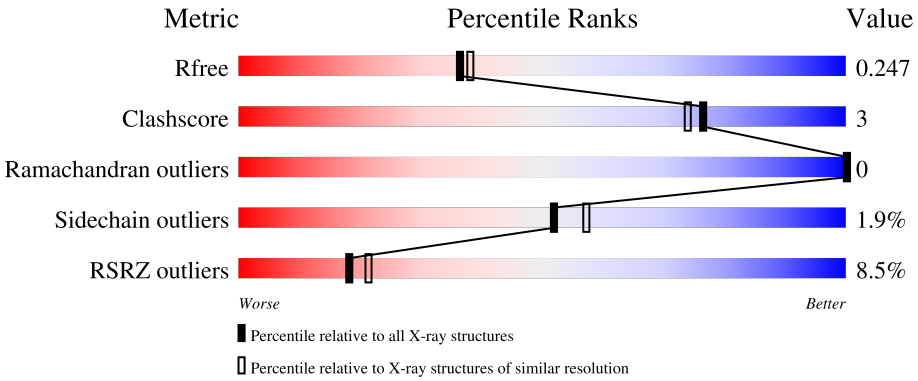
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.15 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}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	106	10% 79% 6% 14%
1	C	106	7% 76% 9% 14%
2	B	16	6% 88% 12%
2	D	16	6% 88% 12%
3	E	16	6% 94% 6%

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Mol	Chain	Length	Quality of chain
3	F	16	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5203 atoms, of which 2294 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 Transcription factor PU.1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	91	Total	C	H	N	O	S	17	1	0
			1539	487	782	139	128	3			
1	C	91	Total	C	H	N	O	S	14	1	0
			1539	487	782	139	128	3			

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*TP*AP*AP*AP*AP*GP*GP*AP*AP*GP*TP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	16	Total	C	H	N	O	P	0	0	0
			517	160	180	74	88	15			
2	D	16	Total	C	H	N	O	P	0	0	0
			517	160	180	74	88	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	16	Total	C	H	N	O	P	0	0	0
			497	154	184	44	100	15			
3	F	16	Total	C	H	N	O	P	0	0	0
			499	154	186	44	100	15			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

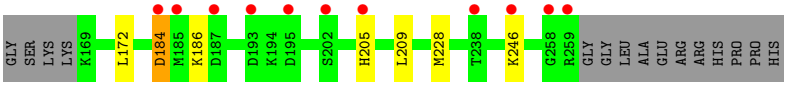
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	22	Total O 22 22	0	0
5	B	11	Total O 11 11	0	0
5	C	26	Total O 26 26	0	0
5	D	5	Total O 5 5	0	0
5	E	19	Total O 19 19	0	0
5	F	11	Total O 11 11	0	0

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.

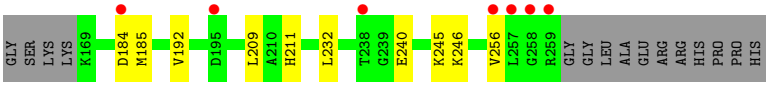
• Molecule 1: Transcription factor PU.1

Chain A:



• Molecule 1: Transcription factor PU.1

Chain C:

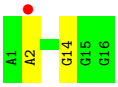


• Molecule 2: DNA (5'-D(*AP*AP*TP*AP*AP*AP*AP*GP*GP*AP*AP*GP*TP*GP*GP*G)-3')

Chain B:

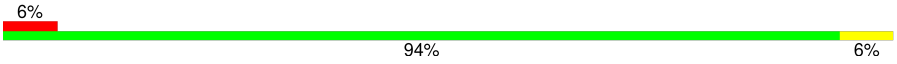
• Molecule 2: DNA (5'-D(*AP*AP*TP*AP*AP*AP*AP*GP*GP*AP*AP*GP*TP*GP*GP*G)-3')

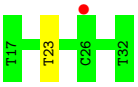
Chain D:



• Molecule 3: DNA (5'-D(*TP*CP*CP*CP*AP*CP*TP*TP*CP*CP*TP*TP*TP*TP*AP*T)-3')

Chain E:





• Molecule 3: DNA (5'-D(*TP*CP*CP*CP*AP*CP*TP*TP*CP*CP*TP*TP*TP*TP*AP*T)-3')

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	90.95Å 102.73Å 55.75Å 90.00° 111.65° 90.00°	Depositor
Resolution (Å)	28.91 – 2.15 28.91 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.91-2.15) 86.6 (28.91-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.233 , 0.246 0.234 , 0.247	Depositor DCC
R_{free} test set	23907 reflections (7.76%)	wwPDB-VP
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5203	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0258e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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

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	0.68	0/775	0.87	1/1030 (0.1%)
1	C	0.75	0/775	0.88	1/1030 (0.1%)
2	B	0.64	0/382	0.97	0/590
2	D	0.59	0/382	0.85	1/590 (0.2%)
3	E	0.72	0/346	0.95	1/530 (0.2%)
3	F	0.61	0/346	0.84	0/530
All	All	0.68	0/3006	0.89	4/4300 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	192	VAL	N-CA-C	-5.73	105.51	111.58
1	A	184	ASP	CA-CB-CG	5.71	118.31	112.60
3	E	23	DT	N1-C1'-C2'	5.15	121.22	113.50
2	D	2	DA	P-O3'-C3'	5.09	127.83	120.20

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	757	782	782	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	757	782	782	6	2
2	B	337	180	180	1	0
2	D	337	180	180	1	0
3	E	313	184	184	0	0
3	F	313	186	186	2	0
4	C	1	0	0	0	0
5	A	22	0	0	0	0
5	B	11	0	0	0	0
5	C	26	0	0	0	1
5	D	5	0	0	0	0
5	E	19	0	0	0	0
5	F	11	0	0	0	0
All	All	2909	2294	2294	13	4

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 3.

All (13) 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:172:LEU:HD11	1:A:228:MET:HE2	1.61	0.81
1:A:172:LEU:CD1	1:A:228:MET:HE2	2.19	0.72
1:C:209:LEU:HD23	1:C:209:LEU:C	2.31	0.56
1:A:209:LEU:C	1:A:209:LEU:HD23	2.31	0.55
1:C:240:GLU:HB3	1:C:256:VAL:HG21	1.96	0.47
1:C:209:LEU:HD23	1:C:209:LEU:O	2.15	0.46
1:C:185:MET:HE1	1:C:209:LEU:HA	1.98	0.46
2:B:1:DA:H2'	2:B:2:DA:C8	2.52	0.45
3:F:17:DT:H2'	3:F:18:DC:C5	2.53	0.43
3:F:17:DT:C2'	3:F:18:DC:C6	3.02	0.42
1:C:245:LYS:O	1:C:246:LYS:HD2	2.20	0.41
1:C:232:LEU:HD23	1:C:232:LEU:HA	1.93	0.41
2:D:14:DG:H2'	2:D:14:DG:N3	2.37	0.40

All (4) 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)
5:C:424:HOH:O	5:C:424:HOH:O[2_556]	2.08	0.12
1:A:205:HIS:NE2	1:A:205:HIS:NE2[2_655]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ASP:OD2	1:C:211:HIS:HE1[2_556]	1.57	0.03
1:C:184:ASP:OD2	1:C:211:HIS:CE1[2_556]	2.18	0.02

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	90/106 (85%)	89 (99%)	1 (1%)	0	100	100
1	C	90/106 (85%)	90 (100%)	0	0	100	100
All	All	180/212 (85%)	179 (99%)	1 (1%)	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	78/90 (87%)	75 (96%)	3 (4%)	28	27
1	C	78/90 (87%)	78 (100%)	0	100	100
All	All	156/180 (87%)	153 (98%)	3 (2%)	52	57

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	ASP

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Mol	Chain	Res	Type
1	A	186	LYS
1	A	246	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	HIS
1	C	211	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)

Of 1 ligands modelled in this entry, 1 is 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

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	A	91/106 (85%)	0.87	11 (12%) 10 12	22, 51, 77, 95	5 (5%)
1	C	91/106 (85%)	0.64	7 (7%) 21 25	21, 46, 76, 93	4 (4%)
2	B	16/16 (100%)	0.60	1 (6%) 27 33	39, 63, 89, 90	0
2	D	16/16 (100%)	0.72	1 (6%) 27 33	52, 62, 97, 98	0
3	E	16/16 (100%)	0.34	1 (6%) 27 33	37, 49, 85, 87	0
3	F	16/16 (100%)	0.39	0 100 100	40, 70, 95, 99	0
All	All	246/276 (89%)	0.69	21 (8%) 18 21	21, 51, 86, 99	9 (3%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	HIS	7.8
1	C	259	ARG	4.9
1	A	259	ARG	4.0
1	A	184	ASP	3.8
1	A	187	ASP	3.5
1	C	184	ASP	3.5
2	B	1	DA	3.1
3	E	26	DC	3.1
1	C	258	GLY	2.9
1	A	185	MET	2.6
1	A	195	ASP	2.6
1	A	258	GLY	2.5
2	D	2	DA	2.4
1	A	246	LYS	2.4
1	C	257	LEU	2.3
1	A	238	THR	2.3
1	A	193	ASP	2.2
1	C	195	ASP	2.2
1	C	256	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	202	SER	2.1
1	C	238	THR	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)

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
4	ZN	C	301	1/1	0.96	0.12	115,115,115,115	0

6.5 Other polymers (i)

There are no such residues in this entry.