wwPDB X-ray Structure Validation Summary Report (i)

Feb 5, 2024 – 08:17 AM EST

PDB ID	:	1TUP
Title	:	TUMOR SUPPRESSOR P53 COMPLEXED WITH DNA
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Deposited on	:	1995-07-11
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

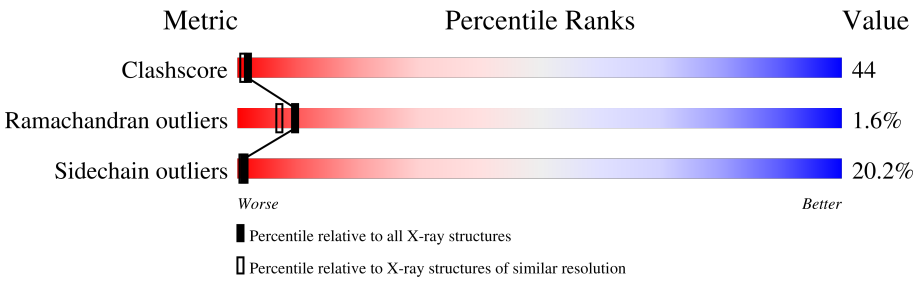
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	21	10% 29% 62%
2	F	21	48% 52%
3	A	219	49% 29% 11% • 11%
3	B	219	34% 41% 12% • 11%
3	C	219	26% 41% 18% • 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5828 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 DNA (5'-D(*TP*TP*TP*CP*CP*TP*AP*GP*AP*CP*TP*TP*GP*CP*CP*CP*A P*AP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	21	420	204	69	127	20	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	21	435	208	86	121	20	0	0	0

- Molecule 3 is a protein called PROTEIN (P53 TUMOR SUPPRESSOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	196	1535	945	283	291	16	0	0	0
3	B	194	1522	939	281	286	16	0	0	0
3	C	195	1529	942	282	289	16	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	E	22	22	22	0	0
			Total	O		
5	F	14	14	14	0	0
			Total	O		
5	A	198	198	198	0	0
			Total	O		
5	B	70	70	70	0	0
			Total	O		
5	C	80	80	80	0	0

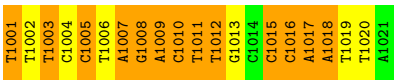
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: DNA (5'-D(*TP*TP*TP*CP*CP*TP*AP*GP*AP*CP*TP*TP*GP*CP*CP*CP*A P*AP*TP*TP*A)-3')

Chain E: 10% 29% 62%

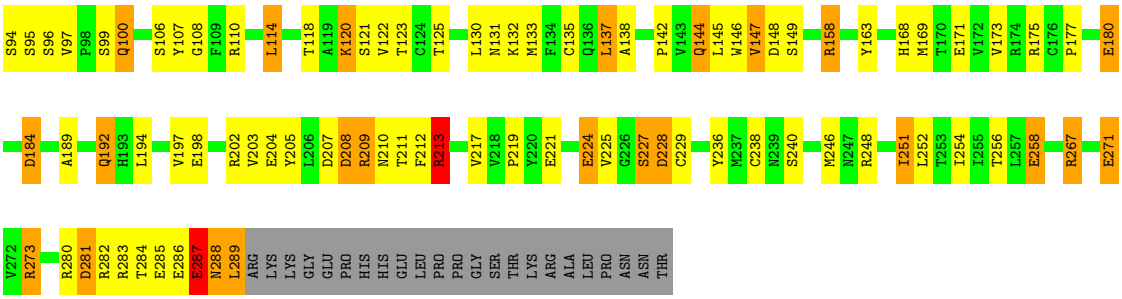


• Molecule 2: DNA (5'-D(*AP*TP*AP*AP*TP*TP*GP*GP*GP*CP*AP*AP*GP*TP*CP*TP *A P*GP*GP*AP*A)-3')

Chain F: 48% 52%

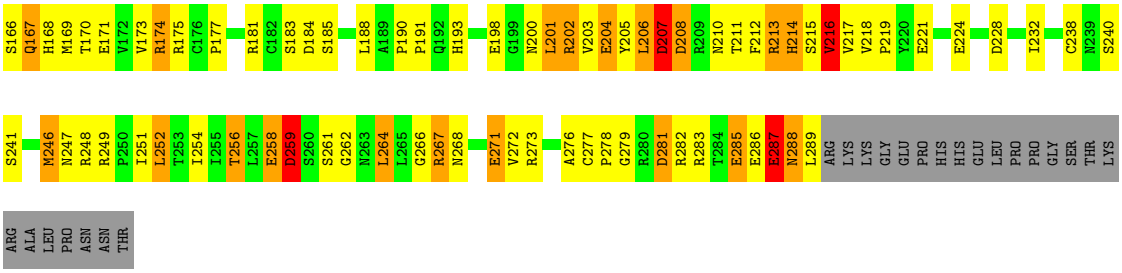
• Molecule 3: PROTEIN (P53 TUMOR SUPPRESSOR)

Chain A: 49% 29% 11% • 11%



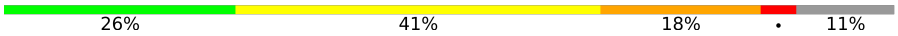
• Molecule 3: PROTEIN (P53 TUMOR SUPPRESSOR)

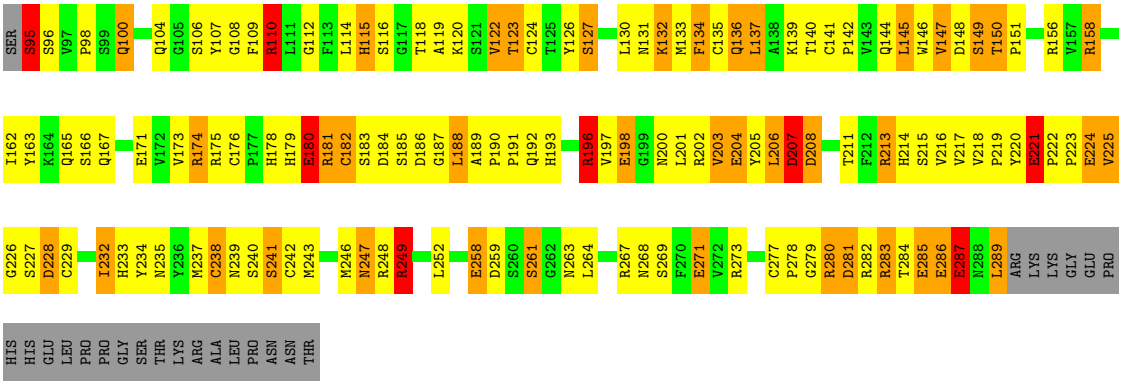
Chain B: 34% 41% 12% • 11%



• Molecule 3: PROTEIN (P53 TUMOR SUPPRESSOR)

Chain C:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.50Å 67.90Å 108.80Å 90.00° 105.50° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR, TNT	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5828	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

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: 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	E	1.05	0/468	1.84	17/719 (2.4%)
2	F	1.13	1/490 (0.2%)	1.93	21/756 (2.8%)
3	A	0.86	11/1570 (0.7%)	1.38	20/2129 (0.9%)
3	B	0.87	7/1557 (0.4%)	1.44	23/2112 (1.1%)
3	C	0.86	9/1564 (0.6%)	1.51	30/2121 (1.4%)
All	All	0.90	28/5649 (0.5%)	1.54	111/7837 (1.4%)

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
3	A	1	0
3	C	1	0
All	All	2	0

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	271	GLU	CD-OE1	6.37	1.32	1.25
3	C	204	GLU	CD-OE2	6.30	1.32	1.25
3	C	287	GLU	CD-OE2	6.27	1.32	1.25
3	A	224	GLU	CD-OE2	6.06	1.32	1.25
3	B	287	GLU	CD-OE2	6.03	1.32	1.25

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1003	DT	O4'-C1'-N1	13.37	117.36	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1015	DC	P-O3'-C3'	10.91	132.79	119.70
3	C	267	ARG	NE-CZ-NH1	10.88	125.74	120.30
3	A	158	ARG	NE-CZ-NH2	-10.08	115.26	120.30
2	F	1107	DG	P-O3'-C3'	9.96	131.65	119.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	211	THR	CB
3	C	247	ASN	CA

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	420	0	241	51	0
2	F	435	0	238	40	0
3	A	1535	0	1490	74	0
3	B	1522	0	1477	129	0
3	C	1529	0	1485	169	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	198	0	0	15	0
5	B	70	0	0	7	0
5	C	80	0	0	14	1
5	E	22	0	0	1	0
5	F	14	0	0	3	0
All	All	5828	0	4931	448	1

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 44.

The worst 5 of 448 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:F:1113:DG:H2"	2:F:1114:DT:H5"	1.33	1.08
3:B:166:SER:HB2	3:C:114:LEU:HD21	1.29	1.07
3:A:211:THR:HG23	3:A:213:ARG:HB2	1.40	1.03
1:E:1004:DC:H2'	1:E:1005:DC:C6	1.99	0.97
3:C:119:ALA:HB3	3:C:122:VAL:HG13	1.45	0.96

All (1) 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:2313:HOH:O	5:C:2313:HOH:O[2_657]	1.91	0.29

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
3	A	194/219 (89%)	189 (97%)	4 (2%)	1 (0%)	29 31
3	B	192/219 (88%)	171 (89%)	17 (9%)	4 (2%)	7 4
3	C	193/219 (88%)	167 (86%)	22 (11%)	4 (2%)	7 4
All	All	579/657 (88%)	527 (91%)	43 (7%)	9 (2%)	9 7

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	225	VAL
3	C	187	GLY
3	C	225	VAL
3	B	106	SER
3	B	201	LEU

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
3	A	176/196 (90%)	146 (83%)	30 (17%)	2 1
3	B	173/196 (88%)	147 (85%)	26 (15%)	3 2
3	C	175/196 (89%)	125 (71%)	50 (29%)	0 0
All	All	524/588 (89%)	418 (80%)	106 (20%)	1 1

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	100	GLN
3	C	149	SER
3	C	261	SER
3	C	115	HIS
3	C	134	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	115	HIS
3	C	193	HIS
3	C	214	HIS
3	C	178	HIS
3	B	131	ASN

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)

Of 3 ligands modelled in this entry, 3 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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.