WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 1, 2014 – 04:03 AM GMT

PDB ID : 3D0A

Title : Human p53 core domain with hot spot mutation R249S and second site suppressor mutation H168R in sequence-specific complex with DNA

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Deposited on : 2008-05-01

Resolution : 1.80 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 1.80 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	Percentile Ranks	Value
Rfree		0.241
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		1.5%
RSRZ outliers		1.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
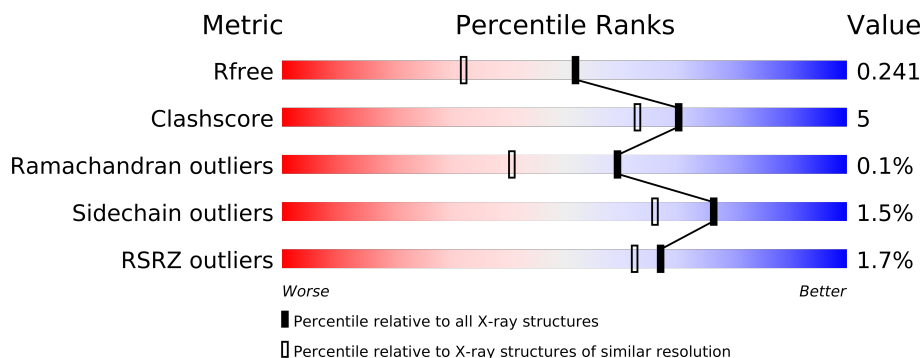
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	12	
1	F	12	
1	G	12	
1	H	12	
2	A	200	
2	B	200	
2	C	200	
2	D	200	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7857 atoms, of which 0 are hydrogen and 0 are deuterium.

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(*DCP*DGP*DGP*DGP*DCP*DAP*DTP* DGP*DCP*DCP*DCP*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	12	Total	C	N	O	P	0	0	0
			213	98	39	65	11			
1	F	11	Total	C	N	O	P	0	0	0
			216	102	44	59	11			
1	G	12	Total	C	N	O	P	0	0	0
			243	115	47	70	11			
1	H	12	Total	C	N	O	P	0	0	0
			227	107	47	63	10			

- Molecule 2 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	196	Total	C	N	O	S	0	11	0
			1577	974	288	295	20			
2	B	197	Total	C	N	O	S	0	11	0
			1550	957	282	292	19			
2	C	193	Total	C	N	O	S	0	12	0
			1554	963	277	294	20			
2	D	194	Total	C	N	O	S	0	7	0
			1522	946	272	284	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	ARG	HIS	ENGINEERED	UNP P04637
A	249	SER	ARG	ENGINEERED	UNP P04637
B	168	ARG	HIS	ENGINEERED	UNP P04637
B	249	SER	ARG	ENGINEERED	UNP P04637
C	168	ARG	HIS	ENGINEERED	UNP P04637
C	249	SER	ARG	ENGINEERED	UNP P04637
D	168	ARG	HIS	ENGINEERED	UNP P04637
D	249	SER	ARG	ENGINEERED	UNP P04637

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	213	Total 216	O 216	0	3
4	B	113	Total 113	O 113	0	0
4	C	219	Total 220	O 220	0	1
4	D	143	Total 143	O 143	0	0
4	E	24	Total 24	O 24	0	0
4	F	14	Total 14	O 14	0	0
4	G	12	Total 12	O 12	0	0
4	H	9	Total 9	O 9	0	0

3   Residue-property plots ⓘ

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: DNA (5'-D(*DCP*DGP*DGP*DGP*DCP*DAP*DTP*DGP*DCP*DCP*DCP*D G)-3')

Chain E:

• Molecule 1: DNA (5'-D(*DCP*DGP*DGP*DGP*DCP*DAP*DTP*DGP*DCP*DCP*DCP*D G)-3')

Chain F:

• Molecule 1: DNA (5'-D(*DCP*DGP*DGP*DGP*DCP*DAP*DTP*DGP*DCP*DCP*DCP*D G)-3')

Chain G:

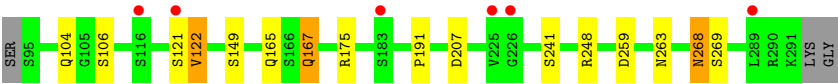• Molecule 1: DNA (5'-D(*DCP*DGP*DGP*DGP*DCP*DAP*DTP*DGP*DCP*DCP*DCP*D G)-3')

Chain H:
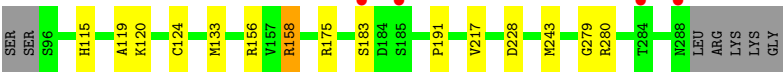
• Molecule 2: Cellular tumor antigen p53

Chain A:

• Molecule 2: Cellular tumor antigen p53

Chain B:

● Molecule 2: Cellular tumor antigen p53

Chain C:

● Molecule 2: Cellular tumor antigen p53

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.30Å 57.99Å 78.93Å 83.05° 88.11° 74.08°	Depositor
Resolution (Å)	17.76 – 1.80 17.82 – 1.79	Depositor EDS
% Data completeness (in resolution range)	96.6 (17.76-1.80) 96.5 (17.82-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.241 0.185 , 0.241	Depositor DCC
R_{free} test set	4181 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 83720 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7857	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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	E	1.11	0/236	1.92	8/362 (2.2%)
1	F	1.08	0/238	1.82	7/360 (1.9%)
1	G	1.03	0/272	1.71	5/418 (1.2%)
1	H	1.00	0/252	1.77	4/385 (1.0%)
2	A	0.76	1/1630 (0.1%)	0.78	1/2210 (0.0%)
2	B	0.53	0/1607	0.68	0/2179
2	C	0.78	0/1618	0.85	2/2194 (0.1%)
2	D	0.63	0/1568	0.69	0/2126
All	All	0.74	1/7421 (0.0%)	0.98	27/10234 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	135	CYS	CB-SG	5.01	1.90	1.82

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	6	DA	O4'-C1'-N9	-13.65	98.45	108.00
1	G	6	DA	O4'-C1'-N9	-10.62	100.57	108.00
1	E	6	DA	O4'-C1'-N9	-10.03	100.98	108.00
1	F	7	DT	O4'-C1'-N1	9.43	114.60	108.00
1	E	10	DC	P-O3'-C3'	7.91	129.19	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	213	0	112	1	0
1	F	216	0	113	1	0
1	G	243	0	135	3	0
1	H	227	0	120	1	0
2	A	1577	0	1521	17	0
2	B	1550	0	1491	13	0
2	C	1554	0	1520	11	0
2	D	1522	0	1466	18	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	216	0	0	6	0
4	B	113	0	0	4	0
4	C	220	0	0	3	0
4	D	143	0	0	1	0
4	E	24	0	0	0	0
4	F	14	0	0	0	0
4	G	12	0	0	0	0
4	H	9	0	0	0	0
All	All	7857	0	6478	63	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 63 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:133:MET:SD	2:D:141[A]:CYS:SG	2.38	1.20
2:A:103:TYR:OH	2:A:264:LEU:HB3	1.61	1.00
2:A:268[A]:ASN:ND2	4:A:506:HOH:O	1.90	0.98
2:C:115:HIS:HD2	4:C:586:HOH:O	1.61	0.83
2:A:103:TYR:HH	2:A:264:LEU:HB3	1.38	0.82

There are no symmetry-related clashes.

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	
2	A	205/200 (102%)	202 (98%)	3 (2%)	0	100	100
2	B	206/200 (103%)	200 (97%)	5 (2%)	1 (0%)	38	19
2	C	203/200 (102%)	198 (98%)	5 (2%)	0	100	100
2	D	199/200 (100%)	195 (98%)	4 (2%)	0	100	100
All	All	813/800 (102%)	795 (98%)	17 (2%)	1 (0%)	59	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	122	VAL

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	
2	A	180/179 (101%)	175 (97%)	5 (3%)	56	38
2	B	173/179 (97%)	169 (98%)	4 (2%)	63	46
2	C	181/179 (101%)	179 (99%)	2 (1%)	84	77
2	D	170/179 (95%)	168 (99%)	2 (1%)	82	74
All	All	704/716 (98%)	691 (98%)	13 (2%)	76	58

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	106	SER
2	B	149	SER
2	C	243	MET

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Mol	Chain	Res	Type
2	A	238[B]	CYS
2	C	183	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	167	GLN
2	D	247	ASN
2	B	268	ASN
2	B	104	GLN
2	B	247	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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(Å²)	Q<0.9
1	E	12/12 (100%)	0.07	1 (8%)	11	8	26, 35, 85, 86	0
1	F	11/12 (91%)	-0.14	0	100	100	27, 35, 62, 70	0
1	G	12/12 (100%)	0.01	0	100	100	27, 43, 58, 67	0
1	H	12/12 (100%)	0.10	1 (8%)	11	8	29, 41, 65, 72	0
2	A	196/200 (98%)	-0.29	0	100	100	14, 24, 40, 52	0
2	B	197/200 (98%)	0.05	6 (3%)	48	40	21, 34, 58, 72	0
2	C	193/200 (96%)	-0.22	4 (2%)	60	54	13, 25, 45, 63	2 (1%)
2	D	194/200 (97%)	-0.10	2 (1%)	79	76	18, 32, 51, 67	3 (1%)
All	All	827/848 (97%)	-0.13	14 (1%)	67	62	13, 29, 53, 86	5 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	226	GLY	3.9
2	B	183	SER	3.4
2	D	226	GLY	3.3
2	B	225	VAL	3.2
2	C	284	THR	3.1

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 ⓘ

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	C	1	1/1	0.04	-1.54	23,23,23,23	0
3	ZN	B	1	1/1	0.04	-2.08	26,26,26,26	0
3	ZN	A	1	1/1	0.05	-2.92	23,23,23,23	0
3	ZN	D	1	1/1	0.03	-4.05	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.