



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1JSP
Title : NMR Structure of CBP Bromodomain in complex with p53 peptide
Authors : He, Y.; Mujtaba, S.; Zeng, L.; Yan, S.; Zhou, M.-M.
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This is a wwPDB NMR 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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

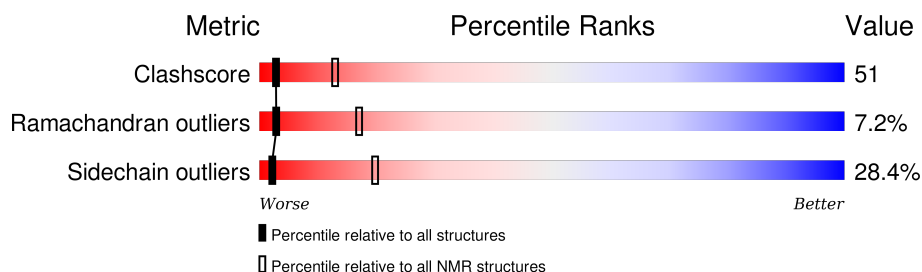
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	20	
2	B	121	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:383-A:384, B:1081- B:1197 (119)	0.65	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 6, 11, 18, 20
2	2, 4, 8, 10, 19
3	7, 14, 17
4	5, 9, 12
5	13, 16
Single-model clusters	15

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2375 atoms, of which 1192 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called tumor protein p53.

Mol	Chain	Residues	Atoms						Trace
1	A	20	Total	C	H	N	O	S	0
			354	105	186	34	28	1	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	ALY	LYS	MODIFIED RESIDUE	UNP P04637

- Molecule 2 is a protein called CREB-BINDING PROTEIN.

Mol	Chain	Residues	Atoms						Trace
2	B	121	Total	C	H	N	O	S	0
			2021	655	1006	169	185	6	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1077	GLY	-	CLONING ARTIFACT	UNP Q92793
B	1078	SER	-	CLONING ARTIFACT	UNP Q92793
B	1079	HIS	-	CLONING ARTIFACT	UNP Q92793
B	1080	MET	-	CLONING ARTIFACT	UNP Q92793

4 Residue-property plots

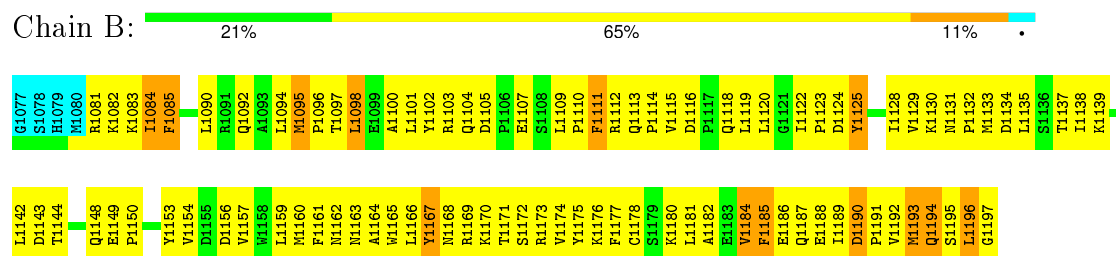
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: tumor protein p53



- Molecule 2: CREB-BINDING PROTEIN



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: tumor protein p53



- Molecule 2: CREB-BINDING PROTEIN



L1142		Q1146	Y1147	Q1148	E1149	P1150	M1151	Q1152	Y1153	V1154	D1155	D1156	V1157	M1158	L1159	M1160	F1161	N1162	M1163	A1164	M1165	L1166	Y1167	N1168	R1169	K1170	T1171	S1172	R1173	V1174	Y1175	K1176	F1177	C1178	S1179	K1180	L1181		V1184	F1185	E1186	Q1187	E1188	I1189	D1190	P1191	V1192	M1193	Q1194	S1195	L1196	G1197							
G1077	S1078	H1079	M1080	R1081	K1082	K1083	I1084	F1085		L1090	R1091	Q1092	A1093	L1094	M1095	P1096	T1097	L1098	E1099	A1100	L1101	Y1102	R1103	Q1104	D1105	P1106	E1107	L1109	S1108	P1110	F1111	R1112	Q1113	P1114	V1115	D1116	P1117	Q1118	L1119	L1120	G1121	I1122	P1123	D1124	Y1125	F1126	D1127	I1128	V1129		M1133	D1134	L1135	S1136	T1137	I1138	K1139	R1140	K1141

5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry simulated annealing*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	structure solution	3.1
X-PLOR	refinement	3.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	16	20	20	3±3
2	B	987	980	980	102±9
All	All	20060	20000	20000	2048

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 51.

5 of 811 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:1098:LEU:HD21	2:B:1142:LEU:HD23	1.08	1.21	3	4
2:B:1098:LEU:HD11	2:B:1142:LEU:HD13	1.07	1.27	14	5
2:B:1098:LEU:HD21	2:B:1142:LEU:HD21	1.05	1.26	5	1
2:B:1098:LEU:HD21	2:B:1142:LEU:HD13	1.04	1.12	19	2
2:B:1122:ILE:HD11	2:B:1128:ILE:HD11	0.99	1.31	4	8

6.3 Torsion angles [i](#)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	2/20 (10%)	1±1 (50±27%)	1±1 (45±31%)	0±0 (5±15%)	5	26
2	B	116/121 (96%)	87±4 (75±3%)	21±3 (18±3%)	8±2 (7±2%)	3	17
All	All	2360/2820 (84%)	1750 (74%)	439 (19%)	171 (7%)	3	17

5 of 42 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	1085	PHE	20
2	B	1104	GLN	12
2	B	1196	LEU	10
2	B	1114	PRO	9
2	B	1176	LYS	8

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	2/18 (11%)	1±1 (52±33%)	1±1 (48±33%)	0	1
2	B	110/113 (97%)	79±4 (72±3%)	31±4 (28±3%)	2	20
All	All	2240/2620 (85%)	1604 (72%)	636 (28%)	2	20

5 of 92 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	1185	PHE	19
2	B	1085	PHE	18

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Mol	Chain	Res	Type	Models (Total)
2	B	1095	MET	17
2	B	1190	ASP	16
2	B	1111	PHE	15

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	ALY	A	382	1	9,11,12	0.92±0.06	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	ALY	A	382	1	10,12,14	1.36±0.08	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	A	382	1	-	2±0,8,10,12	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	382	ALY	OH-CH-NZ-CE	20
1	A	382	ALY	CH3-CH-NZ-CE	20

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided