wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1MW4
Title	:	Solution structure of the human Grb7-SH2 domain in complex with a 10 amino acid peptide pY1139
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Deposited on	:	2002-09-27

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 (i) symbol.

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

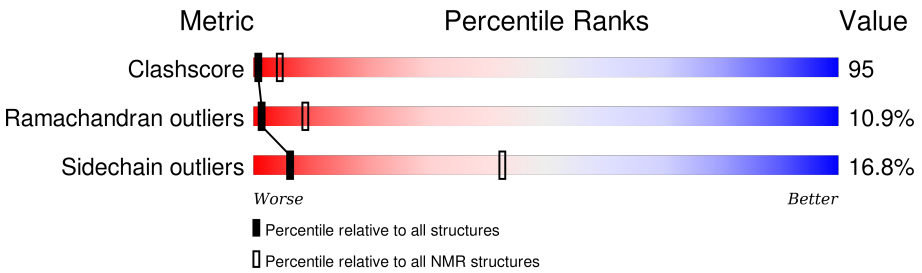
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	120	15% 60% 15% 10%
2	B	10	30% 30% 40%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 5 as representative, based on the following criterion: *closest to the average*.

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:13-A:120, B:1138-B:1138, B:1140-B:1144 (114)	0.58	9

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 7, 9
2	1, 2, 6, 8, 10

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2066 atoms, of which 1018 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Growth factor receptor-bound protein 7.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	120	1913	605	952	180	171	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP Q14451
A	2	SER	-	CLONING ARTIFACT	UNP Q14451

- Molecule 2 is a protein called Receptor protein-tyrosine kinase erbB-2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	10	153	52	66	13	21	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1139	PTR	TYR	MODIFIED RESIDUE	UNP P04626

4 Residue-property plots (i)

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: Growth factor receptor-bound protein 7

Chain A: 15% 60% 15% 10%

G1 S2 P3 A4 S5 G6 T7 S8 L9 S10 A11 A12 I13 H14 L18 W19 F20 H21 G22 R23 I24 S25 R26 E27 E28 S29 Q30 R31 L32 I33 Q36 G37 L38 V39 D40 G41 L42 F43 L44 V45 R46 E47 S48 Q49 R50 N51 P52 Q53 G54 F55 V56 L57 S58 L59 C60 H61 L62 Q63

K64 V65 K66 H67 Y68 L69 I70 L71 F72 S73 E74 R78 L79 Y80 F81 S82 N83 D84 D85 G86 Q87 T88 R89 F90 T91 D92 L93 L94 Q95 L96 V97 E98 F99 H100 Q101 L102 N103 R104 G105 I106 L107 P108 C109 L110 L111 R112 H113 C114 C115 T116 R117 V118 A119 L120

- Molecule 2: Receptor protein-tyrosine kinase erbB-2

Chain B: 30% 30% 40%

P1135 Q1136 P1137 E1138 Y1139 V1140 N1141 Q1142 P1143 D1144

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

The representative model is number 9. Colouring as in section 4.1 above.

- Molecule 1: Growth factor receptor-bound protein 7

Chain A: 23% 48% 18% • 10%

G1 S2 P3 A4 S5 G6 T7 S8 L9 S10 A11 A12 I13 H14 Q17 L18 W19 F20 H21 G22 R23 I24 S25 R26 S29 Q30 I33 L38 V39 D40 G41 L42 F43 L44 V45 R46 E47 S48 Q49 R50 N51 P52 Q53 G54 F55 V56 L57 S58 L59 C60 H61 L62 Q63 K64 V65 K66

H67 Y68 L69 I70 L71 F72 S73 R78 L79 Y80 F81 S82 M83 Q87 T88 R89 F90 T91 D92 L93 L94 Q95 L96 F99 H100 Q101 L102 N103 R104 G105 I106 L107 P108 C109 L110 L111 R112 H113 C114 C115 T116 R117 V118 A119 L120

- Molecule 2: Receptor protein-tyrosine kinase erbB-2

Chain B: 10% 20% 30% 40%

P1135
Q1136
P1137
E1138
Y1139
V1140
N1141
Q1142
P1143
D1144

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with favorable non-bond energy*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

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 (i)

6.1 Standard geometry (i)

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

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 (i)

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	892	884	898	168±12
2	B	48	38	40	24±6
All	All	9400	9220	9380	1777

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 95.

5 of 793 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:LEU:HD13	1:A:69:LEU:O	1.19	1.34	1	5
1:A:59:LEU:HD13	1:A:106:ILE:HG22	1.07	1.09	8	3
1:A:69:LEU:O	1:A:69:LEU:HD13	1.07	1.50	7	4
1:A:55:PHE:O	1:A:69:LEU:HA	1.06	1.48	9	9
1:A:70:ILE:HD12	2:B:1141:ASN:HB2	0.98	1.36	2	6

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	107/120 (89%)	66±2 (62±2%)	31±4 (29±3%)	10±2 (10±2%)	2 11
2	B	5/10 (50%)	1±2 (22±30%)	2±2 (38±33%)	2±1 (40±20%)	0 0
All	All	1120/1300 (86%)	674 (60%)	324 (29%)	122 (11%)	1 9

5 of 26 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	108	PRO	10
1	A	89	ARG	10
1	A	25	SER	9
1	A	107	LEU	9
1	A	105	GLY	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	99/106 (93%)	83±3 (84±3%)	16±3 (16±3%)	6 43
2	B	6/9 (67%)	5±1 (77±13%)	1±1 (23±13%)	3 29
All	All	1050/1150 (91%)	874 (83%)	176 (17%)	6 42

5 of 46 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)
1	A	69	LEU	10
1	A	111	LEU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	26	ARG	10
1	A	62	LEU	9
1	A	56	VAL	9

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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
2	PTR	B	1139	2	13,16,17	0.95±0.02	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
2	PTR	B	1139	2	19,22,24	2.55±0.04	2±0 (10±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
2	PTR	B	1139	2	-	0±0,9,11,13	0±0,1,1,1

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	1139	PTR	O3P-P-OH	6.18	85.78	105.47	9	10
2	B	1139	PTR	O2P-P-OH	5.74	87.18	105.47	1	10

There are no chirality outliers.

There are no torsion outliers.

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 (i)

No chemical shift data were provided