wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2DLE
Title	:	Solution structure of the fourth fn3 domain of human receptor-type tyrosine-protein phosphatase eta
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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 (i) symbol.

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

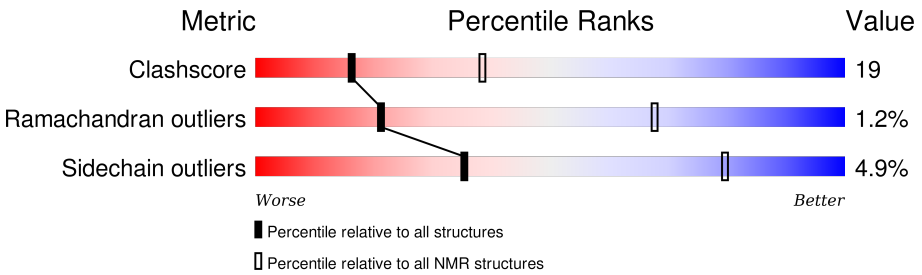
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	104	54% 20% • 25%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:9-A:31, A:39-A:47, A:51-A:96 (78)	0.20	16

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 3 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1491 atoms, of which 735 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Receptor-type tyrosine-protein phosphatase eta.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	104	1491	472	735	125	158	1	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP Q12913
A	2	SER	-	CLONING ARTIFACT	UNP Q12913
A	3	SER	-	CLONING ARTIFACT	UNP Q12913
A	4	GLY	-	CLONING ARTIFACT	UNP Q12913
A	5	SER	-	CLONING ARTIFACT	UNP Q12913
A	6	SER	-	CLONING ARTIFACT	UNP Q12913
A	7	GLY	-	CLONING ARTIFACT	UNP Q12913
A	99	SER	-	CLONING ARTIFACT	UNP Q12913
A	100	GLY	-	CLONING ARTIFACT	UNP Q12913
A	101	PRO	-	CLONING ARTIFACT	UNP Q12913
A	102	SER	-	CLONING ARTIFACT	UNP Q12913
A	103	SER	-	CLONING ARTIFACT	UNP Q12913
A	104	GLY	-	CLONING ARTIFACT	UNP Q12913

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: Receptor-type tyrosine-protein phosphatase eta

Chain A: 54% 20% • 25%

G1 S2 S3 G4 S5 S6 G7 A8 T15 A16 V17 S20 L24 T25 L26 I27 W28 S31 D32 N33 E34 S35 S36 S37 N38 Y39 T40 Y41 K42 I43 E48 T49 D50 L54 E58 P64 G65 L66 I74 T75 V76 L80 F89 L90 W97 P98 S99 G100

P101 S102 S103 G104

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

The representative model is number 16. Colouring as in section 4.1 above.

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 46% 27% • 25%

G1 S2 S3 G4 S5 S6 G7 A8 I9 A16 V17 N18 I19 S20 S23 L24 T25 L26 I27 W28 D32 N33 E34 S35 S36 S37 N38 Y39 T40 Y41 E48 T49 D50 L54 N55 E58 P59 I63 P64 G65 L66 R67 T75 V76 L80 G81 D82 I83 E84 F89

T94 P95 P96 V97 P98 S99 G100 P101 S102 S103 G104

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function,structures with the lowest energy,structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

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)

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	593	603	601	22±3
All	All	11860	12060	12020	444

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 19.

5 of 136 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:HD11	1:A:90:LEU:HD23	1.01	1.32	17	15
1:A:39:TYR:CD1	1:A:80:LEU:HD13	0.99	1.93	11	7
1:A:43:ILE:HG23	1:A:74:ILE:HG23	0.83	1.51	5	15
1:A:54:LEU:HD23	1:A:54:LEU:N	0.79	1.92	10	2
1:A:39:TYR:CE1	1:A:80:LEU:HD13	0.74	2.17	6	12

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	78/104 (75%)	71±1 (91±2%)	6±1 (7±2%)	1±1 (1±1%)	21 68
All	All	1560/2080 (75%)	1427 (91%)	115 (7%)	18 (1%)	21 68

All 4 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	81	GLY	10
1	A	31	SER	4
1	A	85	GLY	2
1	A	9	ILE	2

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	69/89 (78%)	66±1 (95±2%)	3±1 (5±2%)	35 79
All	All	1380/1780 (78%)	1313 (95%)	67 (5%)	35 79

5 of 19 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	24	LEU	20
1	A	40	THR	8
1	A	55	ASN	7
1	A	20	SER	5
1	A	17	VAL	3

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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