wwPDB NMR Structure Validation Summary Report (i)

Apr 26, 2016 – 08:46 PM BST

PDB ID	:	2HQI
Title	:	NMR SOLUTION STRUCTURE OF THE OXIDIZED FORM OF MERP, 14 STRUCTURES
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Deposited on	:	1998-03-31

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:

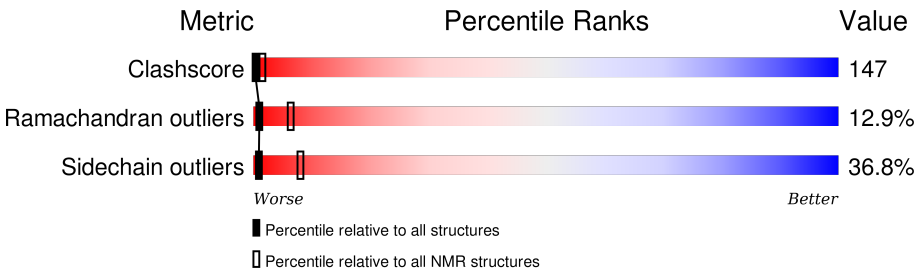
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	72	

2 Ensemble composition and analysis (i)

This entry contains 14 models. Model 4 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:3-A:72 (70)	0.36	4

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 and 1 single-model cluster was found.

Cluster number	Models
1	2, 3, 4, 5, 7, 8, 9, 14
2	1, 6, 10, 12, 13
Single-model clusters	11

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1072 atoms, of which 550 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MERCURIC TRANSPORT PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	72	1072	327	550	87	105	3	0

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: MERCURIC TRANSPORT PROTEIN

Chain A: 11% 61% 22%

A1 T2 Q3 T4 V5 T6 L7 A8 V9 P10 G11 M12 T13 C14 A15 A16 C17 P18 I19 T20 V21 K22 K23 A24 L25 S26 K27 V28 E29 G30 V31 S32 K33 V34 D35 V36 G37 F38 E39 K40 R41 E42 A43 V44 V45 T46 F47 D48 D49 T50 K51 A52 S53 V54 Q55 K56 L57 T58 K59 A60

T61 A62 Y66 P67 S68 S69 V70 K71 Q72

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

The representative model is number 4. Colouring as in section 4.1 above.

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 8% 58% 25% 6%

A1 T2 Q3 T4 V5 T6 L7 A8 V9 P10 G11 M12 T13 C14 A15 A16 C17 P18 I19 T20 V21 K22 K23 A24 L25 S26 K27 V28 E29 G30 V31 S32 K33 V34 D35 V36 G37 F38 E39 K40 R41 E42 A43 V44 V45 T46 F47 D48 D49 T50 K51 A52 S53 V54 Q55 K56 L57 T58 K59 A60

T61 A62 D63 Y66 P67 S68 S69 V70 K71 Q72

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *SA*.

Of the 20 calculated structures, 14 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
X-PLOR	refinement	3.8
X-PLOR	structure solution	

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	510	536	534	154±14
All	All	7140	7504	7476	2155

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 147.

5 of 702 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:VAL:CG2	1:A:43:ALA:HB2	1.00	1.87	9	7
1:A:24:ALA:O	1:A:28:VAL:HG23	1.00	1.56	10	6
1:A:57:LEU:O	1:A:61:THR:HG23	0.97	1.60	10	10
1:A:9:VAL:HG22	1:A:43:ALA:HB2	0.92	1.42	5	6
1:A:28:VAL:HG11	1:A:57:LEU:HA	0.91	1.42	14	3

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	69/72 (96%)	46±1 (67±2%)	14±2 (20±3%)	9±2 (13±2%)	1 6
All	All	966/1008 (96%)	647 (67%)	194 (20%)	125 (13%)	1 6

5 of 19 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	5	VAL	14
1	A	67	PRO	14
1	A	41	ARG	14
1	A	31	VAL	12
1	A	12	MET	11

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	57/58 (98%)	36±2 (63±4%)	21±2 (37±4%)	1 8
All	All	798/812 (98%)	504 (63%)	294 (37%)	1 8

5 of 47 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	38	PHE	14
1	A	66	TYR	13
1	A	32	SER	13
1	A	53	SER	13
1	A	20	THR	13

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