wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2KY6
Title	:	Structure of ARC92VBD/MED25ACID
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Deposited on	:	2010-05-14

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

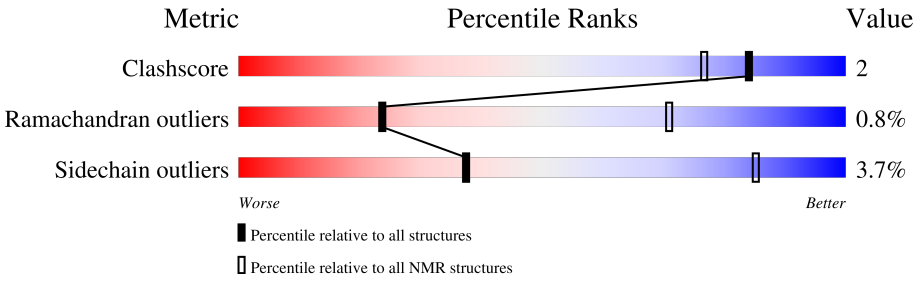
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	166	70% 7% 23%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 14 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:398-A:410, A:423-A:501, A:508-A:542 (127)	0.65	14

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 7 single-model clusters were found.

Cluster number	Models
1	4, 13, 14, 15, 16, 21, 22, 24
2	12, 17, 19
3	5, 18, 25
4	8, 10
5	6, 23
Single-model clusters	1; 2; 3; 7; 9; 11; 20

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2693 atoms, of which 1359 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	166	2693	855	1359	235	236	8	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	GLY	-	expression tag	UNP Q71SY5
A	389	GLU	-	expression tag	UNP Q71SY5
A	390	PHE	-	expression tag	UNP Q71SY5

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Mediator of RNA polymerase II transcription subunit 25

Chain A: 70% 7% 23%

G388 E389 F390 G391 Q392 Q393 S394 V395 S396 N397 E410 K411 P412 K413 P414 A415 S416 V417 D418 A419 N420 T421 K422 T441 W444 R469 M490 G493 H502 T503 A504 P505 C506 E507 K520 Q530 V534 N535 G536 Q539 N543 H544 K545 Q546 V547 Q548 Q549 Q550

K551 L552 E553

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

The representative model is number 14. Colouring as in section 4.1 above.

• Molecule 1: Mediator of RNA polymerase II transcription subunit 25

Chain A: 68% 8% 23%

G388 E389 F390 G391 Q392 Q393 S394 V395 S396 N397 E410 K411 P412 K413 P414 A415 S416 V417 D418 A419 N420 T421 K422 L427 P428 C429 T441 W444 F475 L483 R488 I489 M490 G493 H502 T503 A504 P505 C506 E507 Q530 V534 N535 G536 Q539 N543 H544

K545 Q546 V547 Q548 Q549 Q550 K551 L552 E553

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, molecular dynamics.*

Of the 50 calculated structures, 25 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CYANA	structure solution	3.0
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.2±0.5
All	All	0	4

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	469	ARG	Sidechain	3
1	A	425	ARG	Sidechain	1

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	1033	1067	1067	5±2
All	All	25825	26675	26675	122

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 2.

5 of 32 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:453:ILE:HD13	1:A:497:CYS:SG	0.80	2.17	20	1
1:A:536:GLY:O	1:A:539:GLN:HG2	0.58	1.98	6	13
1:A:441:THR:HA	1:A:444:TRP:CD1	0.58	2.34	3	16
1:A:429:CYS:HB3	1:A:475:PHE:CD1	0.57	2.35	24	4
1:A:469:ARG:NE	1:A:469:ARG:HA	0.56	2.16	7	5

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	127/166 (77%)	121±2 (95±1%)	5±2 (4±1%)	1±1 (1±1%)	24	71
All	All	3175/4150 (77%)	3022 (95%)	128 (4%)	25 (1%)	24	71

5 of 6 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	493	GLY	14
1	A	463	PRO	4
1	A	509	ARG	3
1	A	462	GLY	2
1	A	467	ASN	1

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	115/149 (77%)	111±1 (96±1%)	4±1 (4±1%)	37	85
All	All	2875/3725 (77%)	2769 (96%)	106 (4%)	37	85

5 of 21 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	490	MET	24
1	A	410	GLU	22
1	A	520	LYS	17
1	A	469	ARG	8
1	A	513	LEU	5

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 monosaccharides 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