wwPDB NMR Structure Validation Summary Report (i)

Apr 27, 2016 – 04:55 AM BST

PDB ID	:	2VER
Title	:	STRUCTURAL MODEL FOR THE COMPLEX BETWEEN THE DR ADHESINS AND CARCINOEMBRYONIC ANTIGEN (CEA)
Authors	:	Korotkova, N.; Yang, Y.; Le Trong, I.; Cota, E.; Demeler, B.; Marchant, J.; Thomas, W.E.; Stenkamp, R.E.; Moseley, S.L.; Matthews, S.
Deposited on	:	2007-10-26

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:

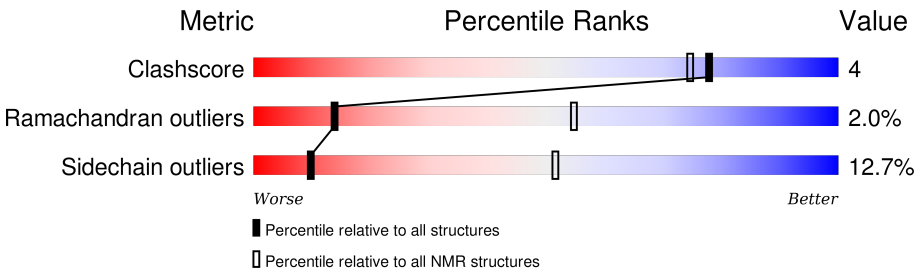
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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	143	73% 27% •
2	N	110	85% 14% •

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3942 atoms, of which 1949 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called AFIMBRIAL ADHESIN AFA-III.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	143	2139	677	1051	188	220	3	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	ASP	-	EXPRESSION TAG	UNP Q57254
A	125	ASN	-	EXPRESSION TAG	UNP Q57254
A	126	LYS	-	EXPRESSION TAG	UNP Q57254
A	127	GLN	-	EXPRESSION TAG	UNP Q57254
A	128	GLY	-	EXPRESSION TAG	UNP Q57254
A	129	PHE	-	EXPRESSION TAG	UNP Q57254
A	130	THR	-	EXPRESSION TAG	UNP Q57254
A	131	PRO	-	EXPRESSION TAG	UNP Q57254
A	132	SER	-	EXPRESSION TAG	UNP Q57254
A	133	GLY	-	EXPRESSION TAG	UNP Q57254
A	134	THR	-	EXPRESSION TAG	UNP Q57254
A	135	THR	-	EXPRESSION TAG	UNP Q57254
A	136	GLY	-	EXPRESSION TAG	UNP Q57254
A	137	THR	-	EXPRESSION TAG	UNP Q57254
A	138	THR	-	EXPRESSION TAG	UNP Q57254
A	139	LYS	-	EXPRESSION TAG	UNP Q57254
A	140	LEU	-	EXPRESSION TAG	UNP Q57254
A	141	THR	-	EXPRESSION TAG	UNP Q57254
A	142	VAL	-	EXPRESSION TAG	UNP Q57254
A	143	THR	-	EXPRESSION TAG	UNP Q57254

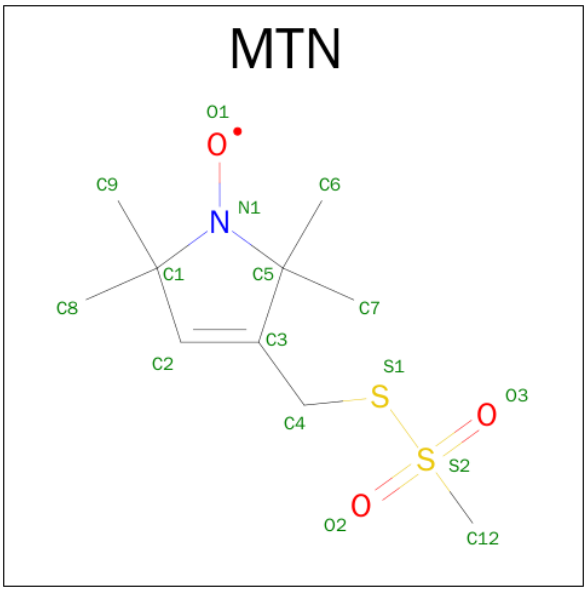
- Molecule 2 is a protein called ARCINOEMBRYONIC ANTIGEN-RELATED CELL ADHESION MOLECULE 5.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	N	110	1722	558	853	143	165	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	39	CYS	VAL	CONFLICT	UNP P06731
N	43	CYS	ARG	CONFLICT	UNP P06731
N	54	CYS	GLN	CONFLICT	UNP P06731

- Molecule 3 is S-[(1-OXYL-2,2,5,5-TETRAMETHYL-2,5-DIHYDRO-1H-PYRROL-3-YL)METHYL] METHANESULFONOTHIOATE (three-letter code: MTN) (formula: $C_{10}H_{18}NO_3S_2$).



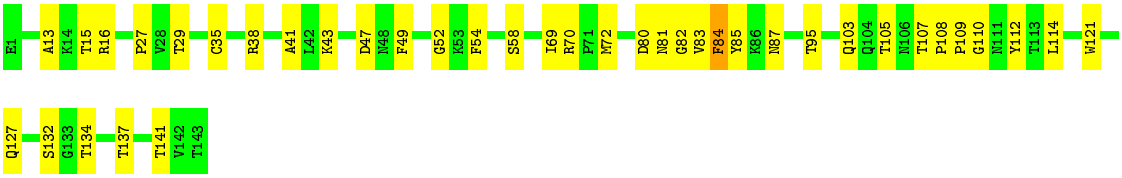
Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
3	N	1	27	9	15	1	1	1
			Total	C	H	N	O	S
3	N	1	27	9	15	1	1	1
			Total	C	H	N	O	S
3	N	1	27	9	15	1	1	1

4 Residue-property plots (i)

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: AFIMBRIAL ADHESIN AFA-III

Chain A:



- Molecule 2: ARCINOEMBRYONIC ANTIGEN-RELATED CELL ADHESION MOLECULE 5

Chain N:

5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 1 were deposited, based on the following criterion: *REPRESENTATIVE STRUCTURE*.

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

Software name	Classification	Version
CNS	refinement	
CNS	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)

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

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	1088	1051	1051	11
2	N	869	853	850	3
3	N	36	45	45	2
All	All	1993	1949	1946	14

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 4.

5 of 14 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:N:90:VAL:O	2:N:97:ASN:HA	0.67	1.90
2:N:83:THR:HG23	2:N:105:ARG:HA	0.63	1.69
1:A:13:ALA:HA	1:A:141:THR:O	0.61	1.95
1:A:80:ASP:HB3	1:A:83:VAL:O	0.51	2.05
1:A:70:ARG:HG2	1:A:84:PHE:CZ	0.51	2.40

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	141/143 (99%)	123 (87%)	15 (11%)	3 (2%)	13	53
2	N	108/110 (98%)	98 (91%)	8 (7%)	2 (2%)	14	56
All	All	249/253 (98%)	221 (89%)	23 (9%)	5 (2%)	14	55

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

Mol	Chain	Res	Type
1	A	82	GLY
1	A	108	PRO
2	N	98	GLU
2	N	41	GLY
1	A	110	GLY

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	117/117 (100%)	100 (85%)	17 (15%)	8	47
2	N	95/95 (100%)	85 (89%)	10 (11%)	13	57
All	All	212/212 (100%)	185 (87%)	27 (13%)	10	51

5 of 27 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	137	THR
1	A	69	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	95	THR
1	A	134	THR
1	A	105	THR

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)

3 ligands are 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
3	MTN	N	1111	2	10,12,16	1.07	0 (0%)
3	MTN	N	1112	2	10,12,16	1.09	0 (0%)
3	MTN	N	1113	2	10,12,16	1.08	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
3	MTN	N	1111	2	14,20,27	1.80	0 (0%)
3	MTN	N	1112	2	14,20,27	1.78	0 (0%)
3	MTN	N	1113	2	14,20,27	1.83	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
3	MTN	N	1111	2	-	0,0,25,29	0,1,1,1
3	MTN	N	1112	2	-	0,0,25,29	0,1,1,1
3	MTN	N	1113	2	-	0,0,25,29	0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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