wwPDB NMR Structure Validation Summary Report (i)

Apr 27, 2016 – 02:52 AM BST

PDB ID	:	2KH2
Title	:	Solution structure of a scFv-IL-1B complex
Authors	:	Wilkinson, I.C.; Hall, C.J.; Veverka, V.; Muskett, F.W.; Stephens, P.E.; Taylor, R.J.; Henry, A.J.; Carr, M.D.
Deposited on	:	2009-03-23

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:

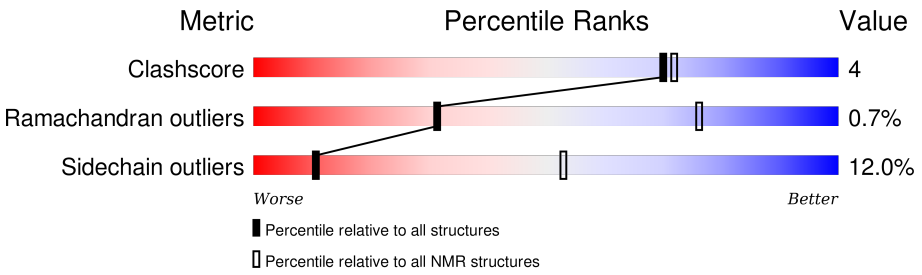
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	153	88% 12%
2	B	254	75% 17% 7%

2 Ensemble composition and analysis (i)

This entry contains 77 models. Model 1 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:1-A:153, B:1-B:110, B:129-B:254 (389)	0.56	1

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 11 clusters and 9 single-model clusters were found.

Cluster number	Models
1	1, 3, 7, 8, 15, 16, 17, 19, 20, 21, 24, 25, 29, 33, 42, 55, 58, 60
2	23, 31, 35, 37, 39, 40, 48, 56, 62, 66
3	45, 57, 64, 67, 68, 71, 74, 75, 77
4	5, 12, 30, 34, 43, 46, 59, 70, 72
5	6, 11, 22, 38, 54, 69
6	10, 14, 49, 53
7	36, 50, 61
8	2, 4, 41
9	47, 65
10	9, 27
11	44, 63
Single-model clusters	13; 18; 26; 28; 32; 51; 52; 73; 76

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6250 atoms, of which 3099 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Interleukin-1 beta.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	153	2457	773	1238	201	237	8	0

- Molecule 2 is a protein called scFv.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	254	3793	1208	1861	345	372	7	0

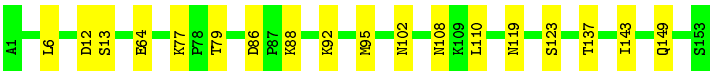
4 Residue-property plots (i)

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.

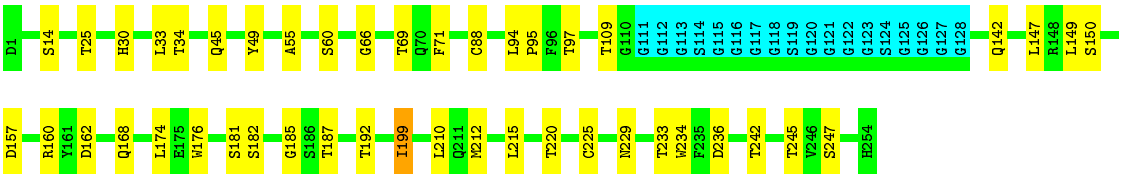
- Molecule 1: Interleukin-1 beta

Chain A: 88% 12%



- Molecule 2: scFv

Chain B: 75% 17% 7%

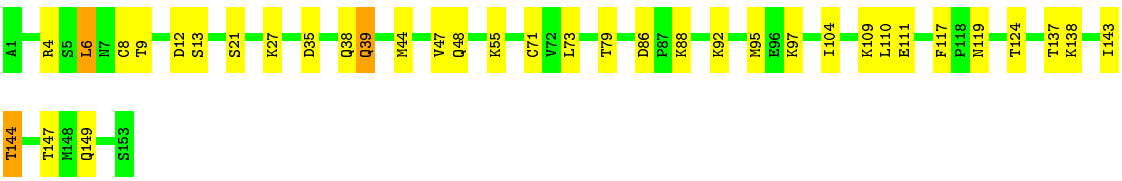


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

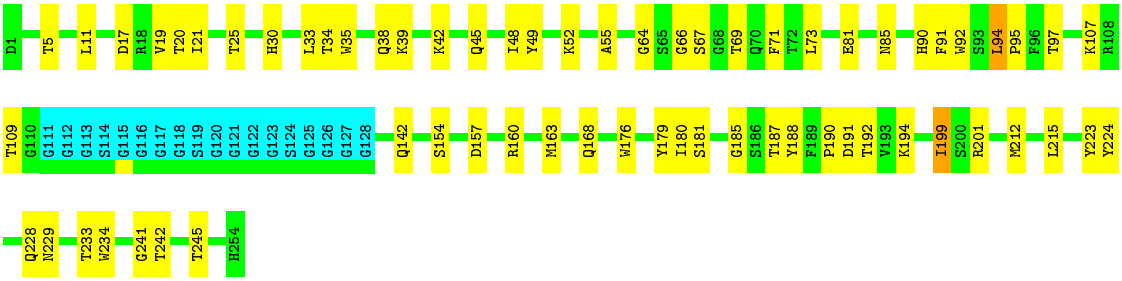
- Molecule 1: Interleukin-1 beta

Chain A: 76% 22% •



- Molecule 2: scFv

Chain B: 67% 25% • 7%


D1
T5
L11
D17
R18
V19
T20
I21
T25
H30
L33
T34
W35
Q38
K39
K42
Q45
I48
Y49
K52
A55
G64
S65
G66
S67
G68
T69
Q70
F71
I72
L73
E81
N85
H90
F91
W92
S93
L94
P95
F96
T97
K107
R108
T109
G110
G111
G112
G113
S114
G115
G116
G117
G118
S119
G120
G121
G122
G123
S124
G125
G126
G127
G128
Q142
S154
D157
R160
M163
Q168
W176
Y179
I180
S181
G185
S186
T187
Y188
F189
P190
D191
T192
V193
K194
I199
S200
R201
M212
L215
Y223
Y224
Q228
N229
T233
W234
G241
T242
T245
H254

5 Refinement protocol and experimental data overview (i)

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

Of the 77 calculated structures, 77 were deposited, based on the following criterion: *all calculated structures submitted.*

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

Software name	Classification	Version
Haddock	structure solution	2.0
Haddock	refinement	2.0

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.

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	0.1±0.5	0.0±0.0
2	B	0.0±0.2	0.0±0.0
All	All	8	0

There are no bond-length outliers.

There are no bond-angle outliers.

5 of 8 unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	76	SER	CA	1
1	A	58	VAL	CA	1
1	A	59	ALA	CA	1
1	A	1	ALA	CA	1
1	A	4	ARG	CA	1

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	1219	1238	1218	9±3
2	B	1854	1801	1773	20±5
All	All	236621	234003	230307	2095

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 432 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:94:LEU:HG	2:B:95:PRO:HA	0.94	1.36	58	32
1:A:12:ASP:HB2	1:A:143:ILE:HG21	0.84	1.48	55	51
1:A:108:ASN:HB3	2:B:185:GLY:HA3	0.83	1.49	23	10
2:B:142:GLN:HG2	2:B:248:SER:HA	0.81	1.49	54	5
2:B:168:GLN:HB2	2:B:174:LEU:HG	0.80	1.54	31	9

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	151/153 (99%)	142±2 (94±2%)	9±2 (6±2%)	1±1 (1±1%)	38	79
2	B	234/254 (92%)	217±3 (93±1%)	15±3 (6±1%)	2±1 (1±0%)	29	74
All	All	29645/31339 (95%)	27623 (93%)	1820 (6%)	202 (1%)	31	76

5 of 35 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	229	ASN	42
2	B	30	HIS	29
2	B	185	GLY	27
1	A	106	ILE	15
1	A	21	SER	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	140/140 (100%)	128±3 (91±2%)	12±3 (9±2%)	18 63
2	B	200/203 (99%)	171±4 (86±2%)	29±4 (14±2%)	8 48
All	All	26180/26411 (99%)	23050 (88%)	3130 (12%)	11 53

5 of 197 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)
2	B	199	ILE	73
2	B	192	THR	73
2	B	97	THR	73
2	B	33	LEU	72
2	B	234	TRP	70

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