



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 2, 2020 – 08:59 pm BST

PDB ID : 6HJ7  
Title : The NMR structure of NRADD death domain  
Authors : Nadezhdin, K.D.; Mineev, K.S.; Goncharuk, S.A.; Arseniev, A.S.  
Deposited on : 2018-09-01

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with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

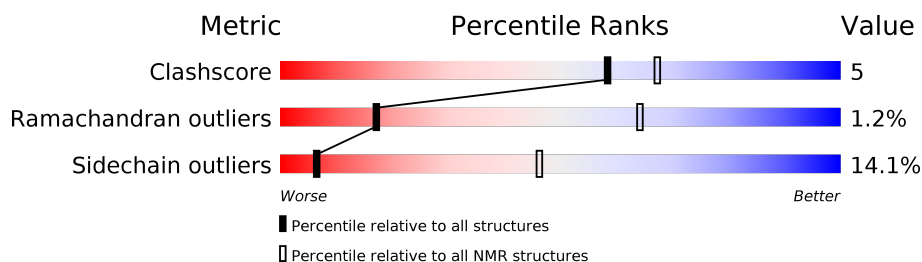
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 85%.

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	246	

## 2 Ensemble composition and analysis

This entry contains 20 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: *target function*.

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:155-A:237 (83)	0.88	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 2 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1549 atoms, of which 765 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Death domain-containing membrane protein NRADD.

Mol	Chain	Residues	Atoms						Trace
1	A	102	Total	C	H	N	O	S	0
			1549	487	765	137	154	6	

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8CJ26
A	2	HIS	-	expression tag	UNP Q8CJ26
A	3	HIS	-	expression tag	UNP Q8CJ26
A	4	HIS	-	expression tag	UNP Q8CJ26
A	5	HIS	-	expression tag	UNP Q8CJ26
A	6	HIS	-	expression tag	UNP Q8CJ26
A	7	HIS	-	expression tag	UNP Q8CJ26
A	8	GLY	-	expression tag	UNP Q8CJ26
A	9	SER	-	expression tag	UNP Q8CJ26
A	10	GLY	-	expression tag	UNP Q8CJ26
A	11	SER	-	expression tag	UNP Q8CJ26
A	12	GLY	-	expression tag	UNP Q8CJ26
A	13	LEU	-	expression tag	UNP Q8CJ26
A	14	VAL	-	expression tag	UNP Q8CJ26
A	15	PRO	-	expression tag	UNP Q8CJ26
A	16	ARG	-	expression tag	UNP Q8CJ26
A	17	GLY	-	expression tag	UNP Q8CJ26
A	18	SER	-	expression tag	UNP Q8CJ26
A	19	MET	-	expression tag	UNP Q8CJ26
A	20	LEU	-	expression tag	UNP Q8CJ26
A	21	TYR	-	expression tag	UNP Q8CJ26
A	22	ASN	-	expression tag	UNP Q8CJ26
A	23	VAL	-	expression tag	UNP Q8CJ26
A	24	SER	-	expression tag	UNP Q8CJ26
A	25	LYS	-	expression tag	UNP Q8CJ26
A	26	GLY	-	expression tag	UNP Q8CJ26
A	27	VAL	-	expression tag	UNP Q8CJ26
A	28	VAL	-	expression tag	UNP Q8CJ26
A	29	TYR	-	expression tag	UNP Q8CJ26
A	30	SER	-	expression tag	UNP Q8CJ26
A	31	ASP	-	expression tag	UNP Q8CJ26

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Chain	Residue	Modelled	Actual	Comment	Reference
A	32	THR	-	expression tag	UNP Q8CJ26
A	33	ALA	-	expression tag	UNP Q8CJ26
A	34	LEU	-	expression tag	UNP Q8CJ26
A	35	GLN	-	expression tag	UNP Q8CJ26
A	36	GLY	-	expression tag	UNP Q8CJ26
A	37	GLN	-	expression tag	UNP Q8CJ26
A	38	ASP	-	expression tag	UNP Q8CJ26
A	39	GLY	-	expression tag	UNP Q8CJ26
A	40	ASP	-	expression tag	UNP Q8CJ26
A	41	ARG	-	expression tag	UNP Q8CJ26
A	42	GLU	-	expression tag	UNP Q8CJ26
A	43	GLY	-	expression tag	UNP Q8CJ26
A	44	MET	-	expression tag	UNP Q8CJ26
A	45	TRP	-	expression tag	UNP Q8CJ26
A	46	VAL	-	expression tag	UNP Q8CJ26
A	47	GLY	-	expression tag	UNP Q8CJ26
A	48	ALA	-	expression tag	UNP Q8CJ26
A	49	GLY	-	expression tag	UNP Q8CJ26
A	50	GLY	-	expression tag	UNP Q8CJ26
A	51	ALA	-	expression tag	UNP Q8CJ26
A	52	LEU	-	expression tag	UNP Q8CJ26
A	53	ALA	-	expression tag	UNP Q8CJ26
A	54	PRO	-	expression tag	UNP Q8CJ26
A	55	ASN	-	expression tag	UNP Q8CJ26
A	56	THR	-	expression tag	UNP Q8CJ26
A	57	SER	-	expression tag	UNP Q8CJ26
A	58	SER	-	expression tag	UNP Q8CJ26
A	59	LEU	-	expression tag	UNP Q8CJ26
A	60	PHE	-	expression tag	UNP Q8CJ26
A	61	PRO	-	expression tag	UNP Q8CJ26
A	62	PRO	-	expression tag	UNP Q8CJ26
A	63	GLU	-	expression tag	UNP Q8CJ26
A	64	PRO	-	expression tag	UNP Q8CJ26
A	65	PRO	-	expression tag	UNP Q8CJ26
A	66	GLY	-	expression tag	UNP Q8CJ26
A	67	ALA	-	expression tag	UNP Q8CJ26
A	68	SER	-	expression tag	UNP Q8CJ26
A	69	SER	-	expression tag	UNP Q8CJ26
A	70	ASN	-	expression tag	UNP Q8CJ26
A	71	ILE	-	expression tag	UNP Q8CJ26
A	72	ILE	-	expression tag	UNP Q8CJ26
A	73	PRO	-	expression tag	UNP Q8CJ26

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Chain	Residue	Modelled	Actual	Comment	Reference
A	74	VAL	-	expression tag	UNP Q8CJ26
A	75	TYR	-	expression tag	UNP Q8CJ26
A	76	CYS	-	expression tag	UNP Q8CJ26
A	77	ALA	-	expression tag	UNP Q8CJ26
A	78	LEU	-	expression tag	UNP Q8CJ26
A	79	LEU	-	expression tag	UNP Q8CJ26
A	80	ALA	-	expression tag	UNP Q8CJ26
A	81	THR	-	expression tag	UNP Q8CJ26
A	82	VAL	-	expression tag	UNP Q8CJ26
A	83	ILE	-	expression tag	UNP Q8CJ26
A	84	LEU	-	expression tag	UNP Q8CJ26
A	85	GLY	-	expression tag	UNP Q8CJ26
A	86	LEU	-	expression tag	UNP Q8CJ26
A	87	LEU	-	expression tag	UNP Q8CJ26
A	88	ALA	-	expression tag	UNP Q8CJ26
A	89	TYR	-	expression tag	UNP Q8CJ26
A	90	VAL	-	expression tag	UNP Q8CJ26
A	91	ALA	-	expression tag	UNP Q8CJ26
A	92	PHE	-	expression tag	UNP Q8CJ26
A	93	LYS	-	expression tag	UNP Q8CJ26
A	94	CYS	-	expression tag	UNP Q8CJ26
A	95	TRP	-	expression tag	UNP Q8CJ26
A	96	ARG	-	expression tag	UNP Q8CJ26
A	97	SER	-	expression tag	UNP Q8CJ26
A	98	HIS	-	expression tag	UNP Q8CJ26
A	99	LYS	-	expression tag	UNP Q8CJ26
A	100	GLN	-	expression tag	UNP Q8CJ26
A	101	ARG	-	expression tag	UNP Q8CJ26
A	102	GLN	-	expression tag	UNP Q8CJ26
A	103	GLN	-	expression tag	UNP Q8CJ26
A	104	LEU	-	expression tag	UNP Q8CJ26
A	105	ALA	-	expression tag	UNP Q8CJ26
A	106	LYS	-	expression tag	UNP Q8CJ26
A	107	ALA	-	expression tag	UNP Q8CJ26
A	108	ARG	-	expression tag	UNP Q8CJ26
A	109	THR	-	expression tag	UNP Q8CJ26
A	110	VAL	-	expression tag	UNP Q8CJ26
A	111	GLU	-	expression tag	UNP Q8CJ26
A	112	LEU	-	expression tag	UNP Q8CJ26
A	113	GLY	-	expression tag	UNP Q8CJ26
A	114	ASP	-	expression tag	UNP Q8CJ26
A	115	PRO	-	expression tag	UNP Q8CJ26

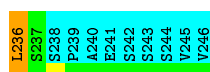
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Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ASP	-	expression tag	UNP Q8CJ26
A	117	ARG	-	expression tag	UNP Q8CJ26
A	118	ASP	-	expression tag	UNP Q8CJ26
A	119	GLN	-	expression tag	UNP Q8CJ26
A	120	ARG	-	expression tag	UNP Q8CJ26
A	121	ARG	-	expression tag	UNP Q8CJ26
A	122	GLY	-	expression tag	UNP Q8CJ26
A	123	ASP	-	expression tag	UNP Q8CJ26
A	124	SER	-	expression tag	UNP Q8CJ26
A	125	ASN	-	expression tag	UNP Q8CJ26
A	126	VAL	-	expression tag	UNP Q8CJ26
A	127	PHE	-	expression tag	UNP Q8CJ26
A	128	VAL	-	expression tag	UNP Q8CJ26
A	129	ASP	-	expression tag	UNP Q8CJ26
A	130	SER	-	expression tag	UNP Q8CJ26
A	131	PRO	-	expression tag	UNP Q8CJ26
A	132	PRO	-	expression tag	UNP Q8CJ26
A	133	SER	-	expression tag	UNP Q8CJ26
A	134	LEU	-	expression tag	UNP Q8CJ26
A	135	GLU	-	expression tag	UNP Q8CJ26
A	136	PRO	-	expression tag	UNP Q8CJ26
A	137	CYS	-	expression tag	UNP Q8CJ26
A	138	ILE	-	expression tag	UNP Q8CJ26
A	139	PRO	-	expression tag	UNP Q8CJ26
A	140	SER	-	expression tag	UNP Q8CJ26
A	141	GLN	-	expression tag	UNP Q8CJ26
A	142	GLY	-	expression tag	UNP Q8CJ26
A	143	PRO	-	expression tag	UNP Q8CJ26
A	144	HIS	-	expression tag	UNP Q8CJ26

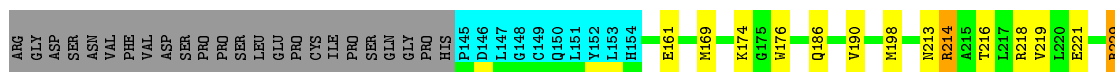






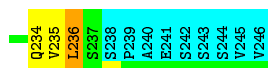
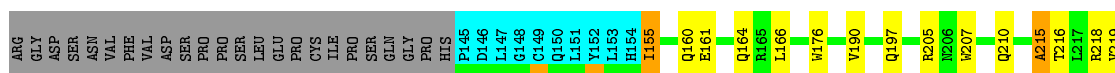
#### 4.2.2 Score per residue for model 2

- Molecule 1: Death domain-containing membrane protein NRADD



#### 4.2.3 Score per residue for model 3

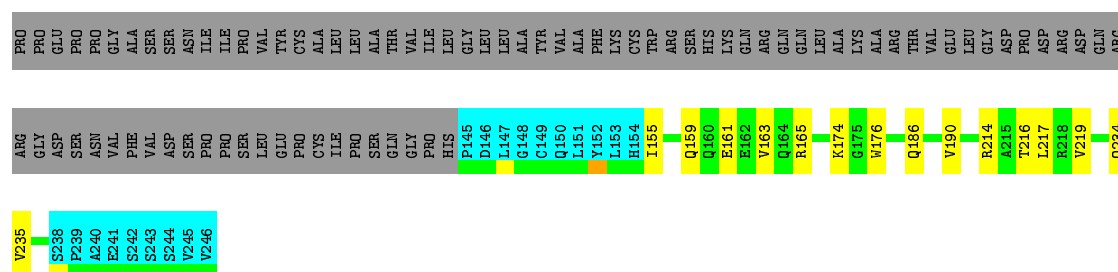
- Molecule 1: Death domain-containing membrane protein NRADD



#### 4.2.4 Score per residue for model 4

- Molecule 1: Death domain-containing membrane protein NRADD

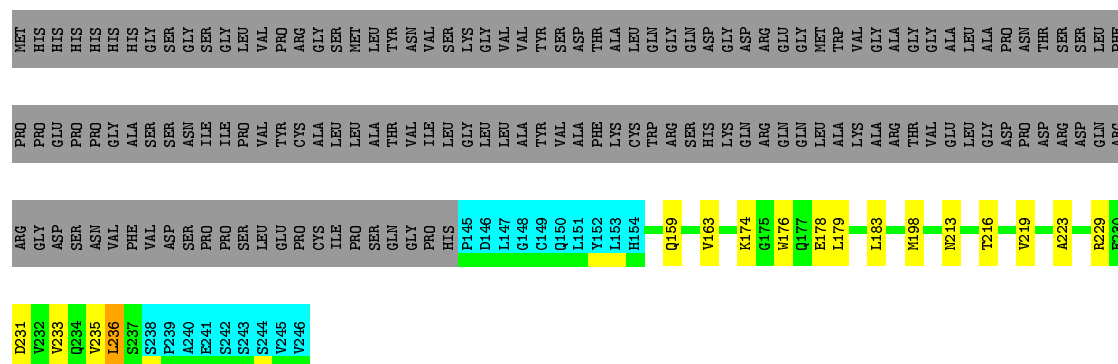




#### 4.2.5 Score per residue for model 5

- Molecule 1: Death domain-containing membrane protein NRADD

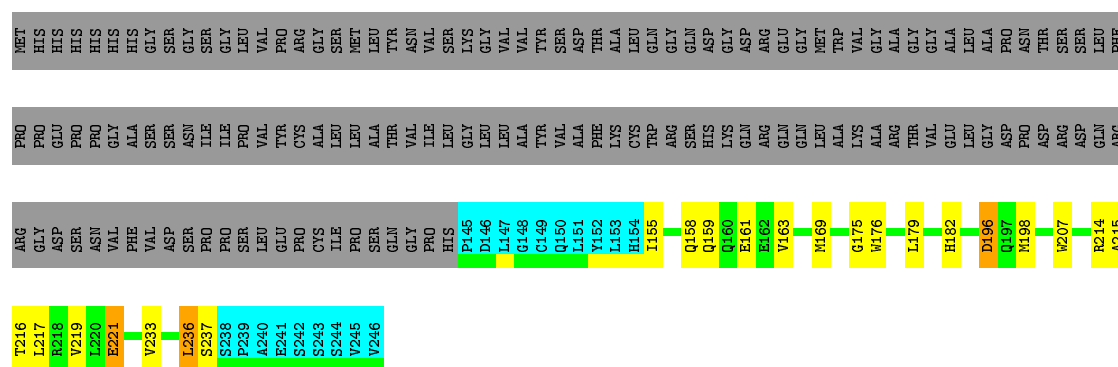
Chain A: 27% 7% 8% 59%



#### 4.2.6 Score per residue for model 6

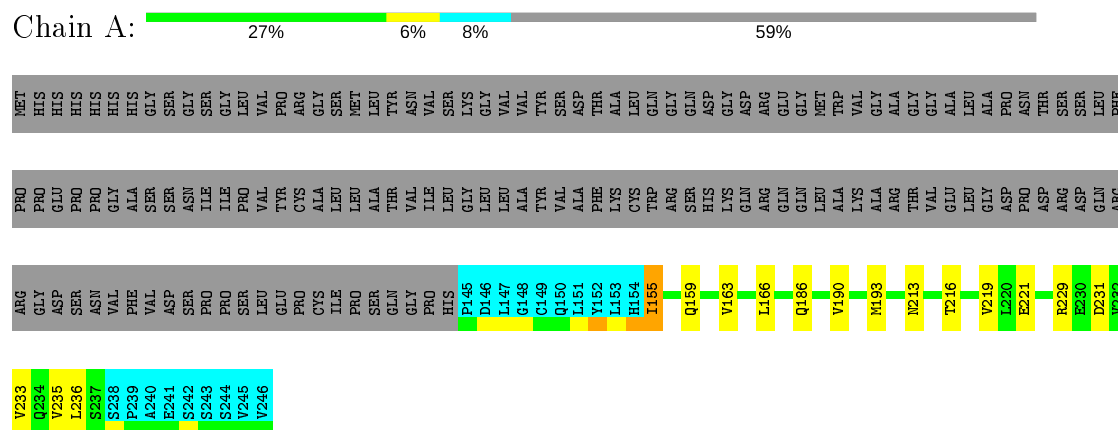
- Molecule 1: Death domain-containing membrane protein NRADD

Chain A: 25% 8% 8% 59%



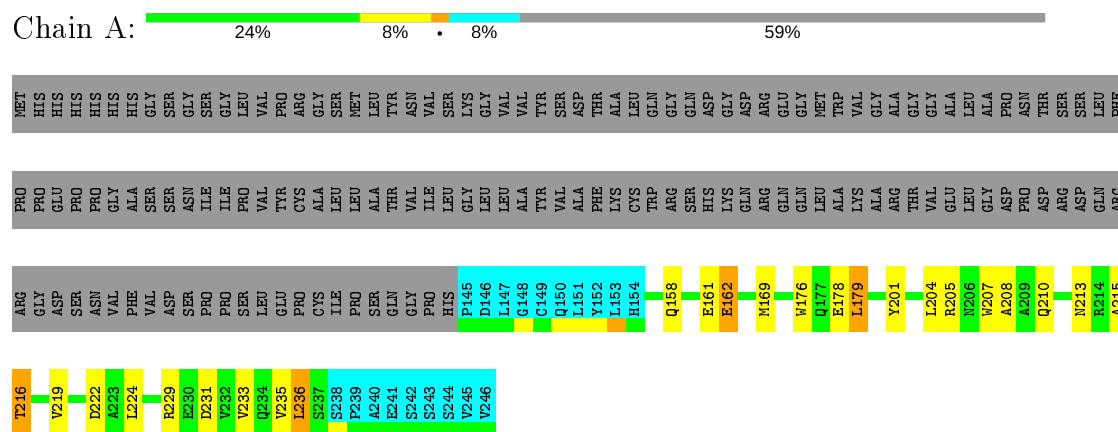
#### 4.2.7 Score per residue for model 7

- Molecule 1: Death domain-containing membrane protein NRADD



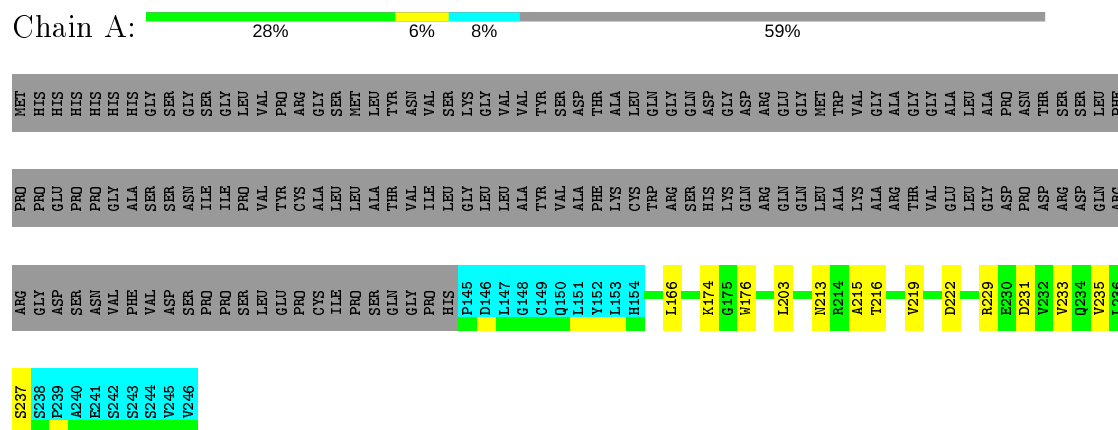
#### 4.2.8 Score per residue for model 8

- Molecule 1: Death domain-containing membrane protein NRADD



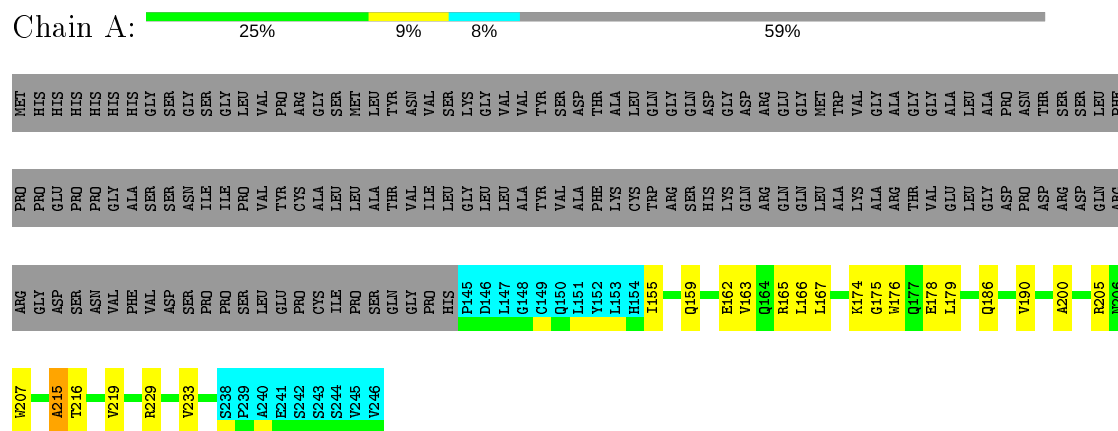
#### 4.2.9 Score per residue for model 9

- Molecule 1: Death domain-containing membrane protein NRADD



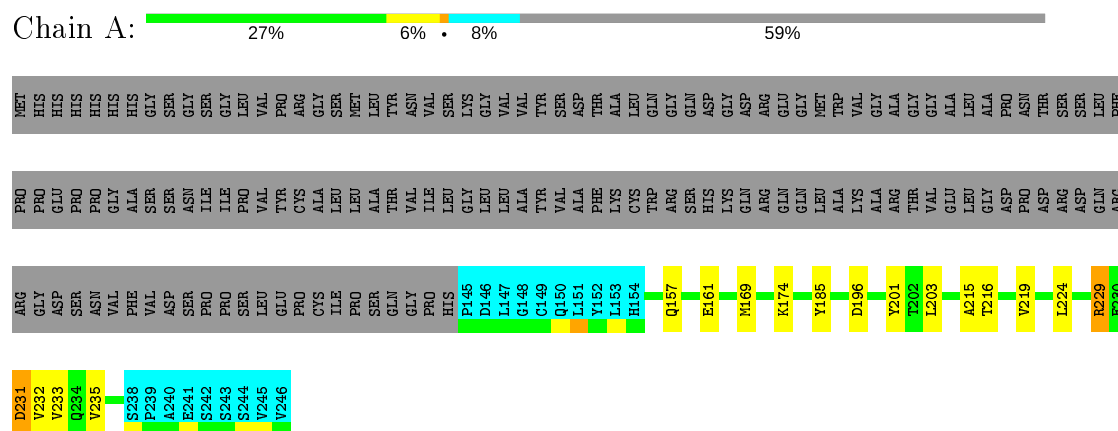
#### 4.2.10 Score per residue for model 10

- Molecule 1: Death domain-containing membrane protein NRADD



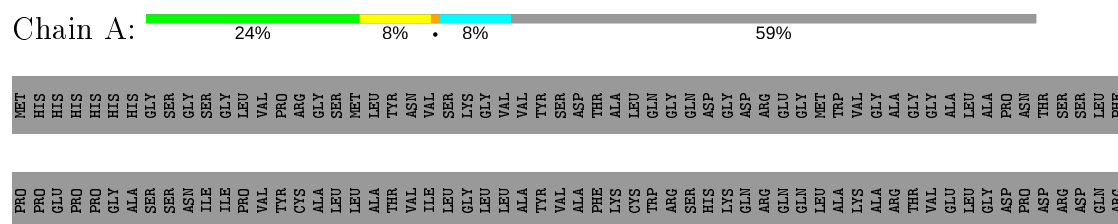
#### 4.2.11 Score per residue for model 11

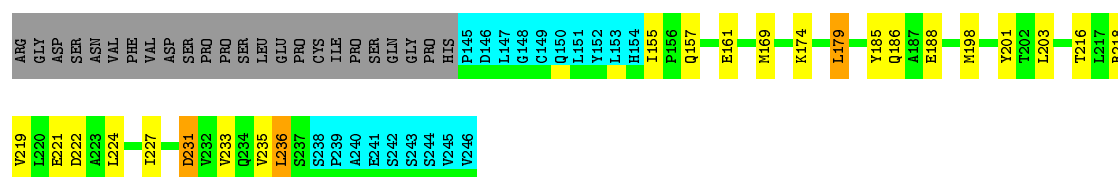
- Molecule 1: Death domain-containing membrane protein NRADD



#### 4.2.12 Score per residue for model 12

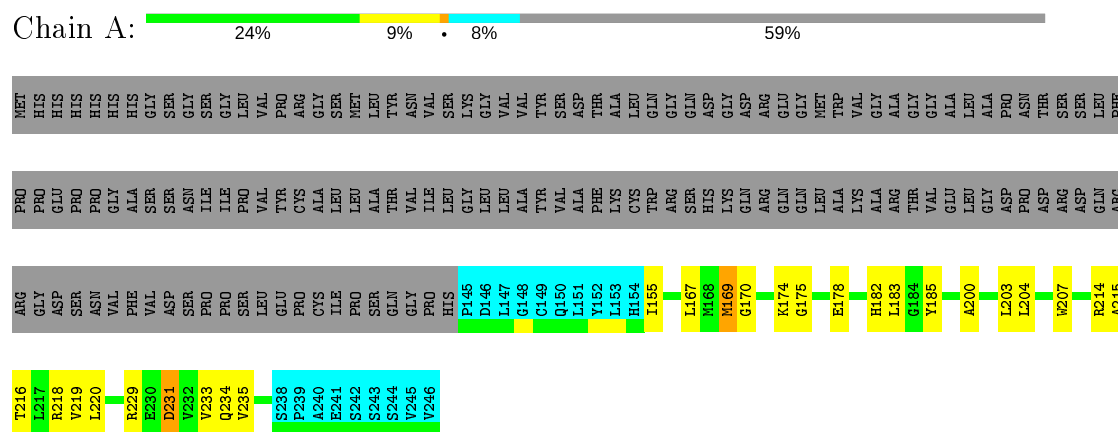
- Molecule 1: Death domain-containing membrane protein NRADD





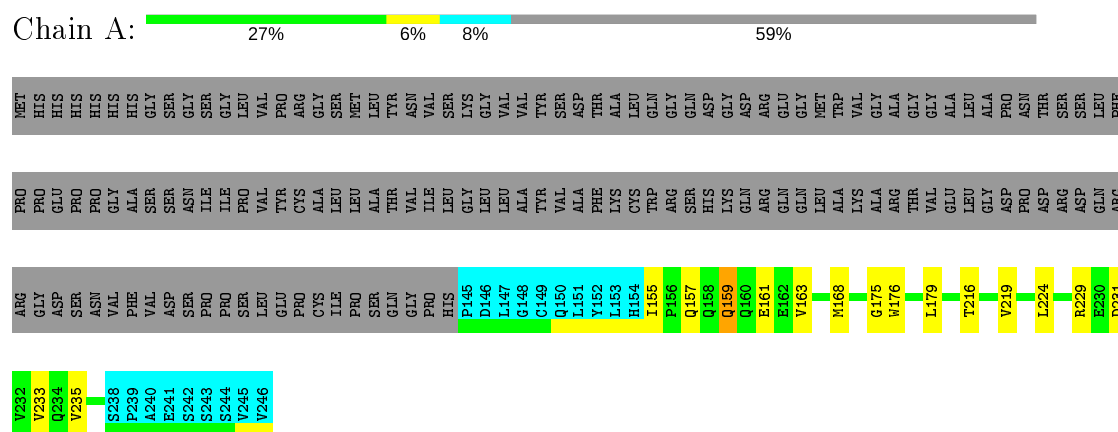
#### 4.2.13 Score per residue for model 13

- Molecule 1: Death domain-containing membrane protein NRADD



#### 4.2.14 Score per residue for model 14 (medoid)

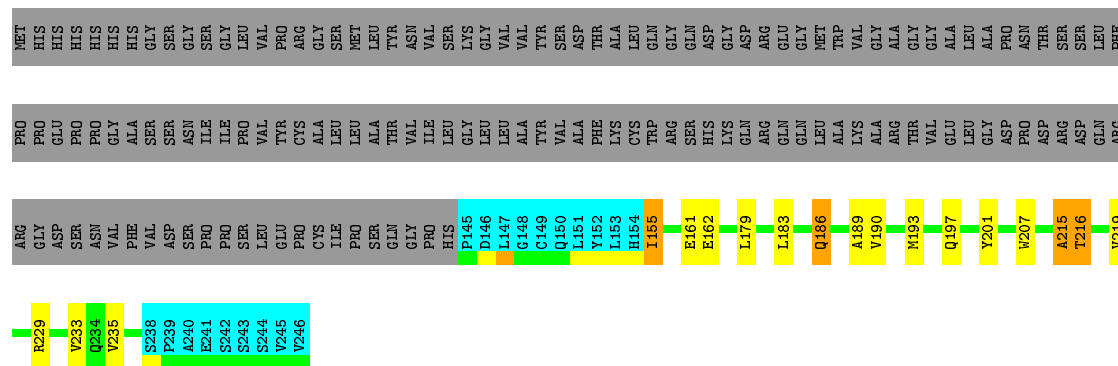
- Molecule 1: Death domain-containing membrane protein NRADD



#### 4.2.15 Score per residue for model 15

- Molecule 1: Death domain-containing membrane protein NRADD

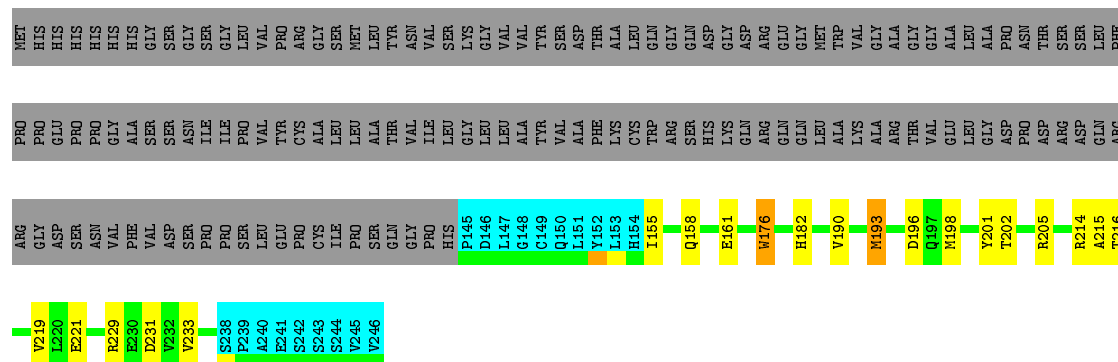




#### 4.2.16 Score per residue for model 16

- Molecule 1: Death domain-containing membrane protein NRADD

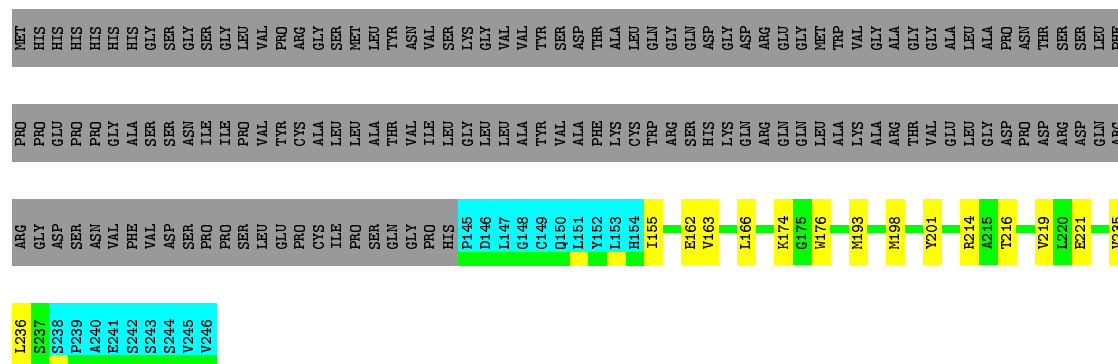
Chain A: 26% 7% 8% 59%



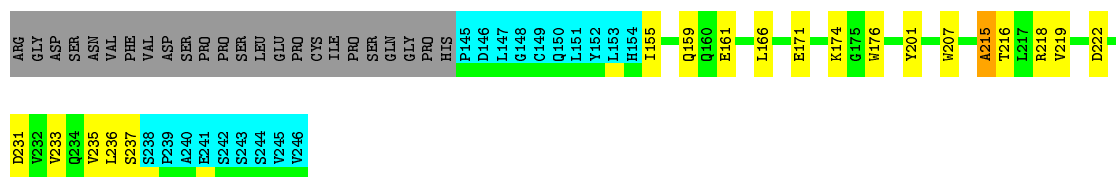
#### 4.2.17 Score per residue for model 17

- Molecule 1: Death domain-containing membrane protein NRADD

Chain A: 28% 6% 8% 59%









## 5 Refinement protocol and experimental data overview

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

Of the 2000 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	
CYANA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1903
Number of shifts mapped to atoms	1903
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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 ⓘ

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	645	633	633	6±2
All	All	12900	12660	12660	125

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:231:ASP:O	1:A:235:VAL:HG23	0.62	1.94	12	8
1:A:233:VAL:O	1:A:236:LEU:HD23	0.61	1.96	12	1
1:A:221:GLU:OE2	1:A:233:VAL:HG22	0.60	1.97	6	2
1:A:179:LEU:HD21	1:A:224:LEU:HD13	0.60	1.73	19	1
1:A:216:THR:O	1:A:219:VAL:HG12	0.60	1.96	13	20
1:A:214:ARG:O	1:A:216:THR:HG23	0.60	1.96	6	3
1:A:207:TRP:CD1	1:A:215:ALA:HB1	0.58	2.33	19	5
1:A:224:LEU:HD21	1:A:232:VAL:HG11	0.58	1.75	11	1
1:A:176:TRP:CH2	1:A:190:VAL:HG22	0.58	2.34	3	1
1:A:179:LEU:HD21	1:A:224:LEU:HD12	0.57	1.74	14	1
1:A:229:ARG:O	1:A:233:VAL:HG23	0.57	1.99	14	14
1:A:162:GLU:OE2	1:A:235:VAL:HG11	0.56	2.00	8	1
1:A:204:LEU:HD11	1:A:220:LEU:CD2	0.55	2.32	13	1
1:A:185:TYR:CZ	1:A:203:LEU:HD11	0.55	2.37	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:236:LEU:HD12	1:A:236:LEU:O	0.53	2.03	8	2
1:A:207:TRP:NE1	1:A:215:ALA:HB1	0.53	2.19	6	3
1:A:166:LEU:HD21	1:A:235:VAL:CG1	0.53	2.33	19	1
1:A:167:LEU:HD13	1:A:200:ALA:CB	0.53	2.33	13	1
1:A:155:ILE:HG21	1:A:217:LEU:HD11	0.53	1.81	4	1
1:A:166:LEU:HD21	1:A:235:VAL:HG11	0.51	1.80	19	3
1:A:224:LEU:CD2	1:A:232:VAL:HG11	0.51	2.35	11	1
1:A:236:LEU:O	1:A:236:LEU:HD12	0.51	2.04	1	2
1:A:186:GLN:O	1:A:190:VAL:HG12	0.51	2.04	18	5
1:A:163:VAL:HG22	1:A:236:LEU:HD21	0.51	1.83	17	1
1:A:159:GLN:O	1:A:163:VAL:HG23	0.51	2.06	5	6
1:A:183:LEU:HD13	1:A:185:TYR:CE2	0.51	2.41	13	1
1:A:204:LEU:HD11	1:A:220:LEU:HD22	0.50	1.83	13	1
1:A:155:ILE:O	1:A:155:ILE:HD12	0.49	2.08	4	1
1:A:204:LEU:HD23	1:A:207:TRP:CE3	0.49	2.43	8	1
1:A:179:LEU:HD11	1:A:224:LEU:CD1	0.49	2.38	12	2
1:A:193:MET:CB	1:A:202:THR:HG21	0.49	2.38	16	1
1:A:162:GLU:OE1	1:A:166:LEU:HD12	0.48	2.08	10	1
1:A:179:LEU:HD12	1:A:227:ILE:HG13	0.47	1.87	12	1
1:A:155:ILE:HD13	1:A:155:ILE:N	0.47	2.25	7	1
1:A:236:LEU:HD23	1:A:237:SER:N	0.46	2.25	6	1
1:A:185:TYR:OH	1:A:203:LEU:HD11	0.46	2.11	11	1
1:A:166:LEU:HD11	1:A:235:VAL:HG11	0.46	1.88	3	3
1:A:185:TYR:CE2	1:A:203:LEU:HD11	0.45	2.47	12	1
1:A:179:LEU:HD11	1:A:224:LEU:HD12	0.44	1.88	8	1
1:A:176:TRP:CZ3	1:A:190:VAL:HG23	0.44	2.47	16	1
1:A:166:LEU:CD1	1:A:235:VAL:HG21	0.44	2.42	7	1
1:A:207:TRP:CD1	1:A:207:TRP:C	0.44	2.90	8	1
1:A:167:LEU:HD12	1:A:200:ALA:HB2	0.43	1.90	10	1
1:A:186:GLN:H	1:A:189:ALA:HB3	0.43	1.73	15	1
1:A:163:VAL:HG22	1:A:236:LEU:HD13	0.43	1.90	5	1
1:A:179:LEU:O	1:A:183:LEU:HD12	0.43	2.14	15	1
1:A:190:VAL:HG23	1:A:193:MET:CE	0.43	2.43	15	1
1:A:155:ILE:N	1:A:155:ILE:HD13	0.43	2.29	15	2
1:A:175:GLY:O	1:A:179:LEU:HD12	0.43	2.14	10	1
1:A:221:GLU:OE1	1:A:233:VAL:HG22	0.42	2.14	7	1
1:A:169:MET:O	1:A:170:GLY:C	0.42	2.56	13	1
1:A:193:MET:CE	1:A:203:LEU:HD13	0.42	2.44	18	1
1:A:207:TRP:HE1	1:A:215:ALA:HB1	0.42	1.74	20	1
1:A:176:TRP:HZ3	1:A:190:VAL:HG23	0.42	1.75	18	1
1:A:166:LEU:HD21	1:A:235:VAL:CB	0.41	2.45	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:LEU:HD21	1:A:223:ALA:HB1	0.41	1.92	5	1
1:A:229:ARG:HB3	1:A:232:VAL:HG22	0.41	1.91	11	1
1:A:163:VAL:CG2	1:A:236:LEU:HD21	0.41	2.45	17	1
1:A:185:TYR:CE2	1:A:203:LEU:HD21	0.41	2.51	13	1
1:A:203:LEU:O	1:A:203:LEU:HD12	0.40	2.17	9	1

## 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	83/246 (34%)	75±2 (91±3%)	7±2 (8±2%)	1±1 (1±1%)	17	64
All	All	1660/4920 (34%)	1506 (91%)	134 (8%)	20 (1%)	17	64

All 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	215	ALA	9
1	A	175	GLY	4
1	A	197	GLN	3
1	A	196	ASP	2
1	A	195	CYS	1
1	A	174	LYS	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	65/199 (33%)	56±3 (86±4%)	9±3 (14±4%)	6	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1300/3980 (33%)	1117 (86%)	183 (14%)	6 46

All 40 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	176	TRP	13
1	A	161	GLU	13
1	A	174	LYS	12
1	A	236	LEU	9
1	A	201	TYR	9
1	A	155	ILE	8
1	A	231	ASP	8
1	A	169	MET	7
1	A	222	ASP	6
1	A	198	MET	6
1	A	193	MET	6
1	A	218	ARG	5
1	A	213	ASN	5
1	A	205	ARG	5
1	A	179	LEU	4
1	A	229	ARG	4
1	A	178	GLU	4
1	A	234	GLN	4
1	A	186	GLN	4
1	A	159	GLN	4
1	A	214	ARG	4
1	A	235	VAL	4
1	A	221	GLU	4
1	A	162	GLU	3
1	A	157	GLN	3
1	A	158	GLN	3
1	A	160	GLN	3
1	A	182	HIS	3
1	A	210	GLN	3
1	A	237	SER	2
1	A	196	ASP	2
1	A	216	THR	2
1	A	165	ARG	2
1	A	168	MET	2
1	A	164	GLN	2
1	A	171	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	211	GLU	1
1	A	188	GLU	1
1	A	190	VAL	1
1	A	195	CYS	1

### 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

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 85% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *starch\_output*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1903
Number of shifts mapped to atoms	1903
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	174	$0.16 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	151	$0.81 \pm 0.13$	Should be applied
$^{13}\text{C}'$	170	$0.16 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	161	$0.37 \pm 0.27$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 85%, i.e. 854 atoms were assigned a chemical shift out of a possible 1008. 16 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	399/409 (98%)	160/163 (98%)	161/166 (97%)	78/80 (98%)
Sidechain	425/552 (77%)	257/321 (80%)	162/203 (80%)	6/28 (21%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	30/47 (64%)	17/24 (71%)	11/20 (55%)	2/3 (67%)
Overall	854/1008 (85%)	434/508 (85%)	334/389 (86%)	86/111 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1034 atoms were assigned a chemical shift out of a possible 1215. 21 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	489/500 (98%)	196/199 (98%)	198/204 (97%)	95/97 (98%)
Sidechain	509/653 (78%)	307/381 (81%)	195/243 (80%)	7/29 (24%)
Aromatic	36/62 (58%)	21/32 (66%)	13/26 (50%)	2/4 (50%)
Overall	1034/1215 (85%)	524/612 (86%)	406/473 (86%)	104/130 (80%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	216	THR	CB	59.33	78.10 – 61.30	-6.2
1	A	171	GLU	CG	29.29	42.24 – 29.94	-5.5

#### 7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



