



Full wwPDB NMR Structure Validation Report ⓘ

Oct 22, 2024 – 08:37 PM EDT

PDB ID : 2LAG
BMRB ID : 16677
Title : Structure of the 44 kDa complex of interferon-alpha2 with the extracellular part of IFNAR2 obtained by 2D-double difference NOESY
Authors : Nudelman, I.; Akabayov, S.R.; Scherf, T.; Anglister, J.
Deposited on : 2011-03-13

This is a Full wwPDB NMR Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.39

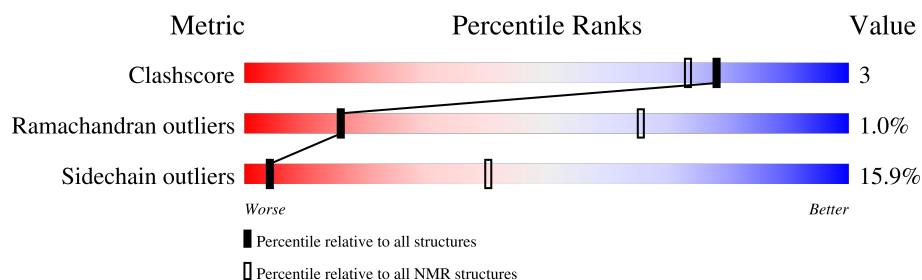
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 38%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	212	
2	A	165	

2 Ensemble composition and analysis

This entry contains 10 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	B:5-B:212, A:1-A:160 (368)	0.66	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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6052 atoms, of which 2993 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Interferon alpha/beta receptor 2.

Mol	Chain	Residues	Atoms						Trace
1	B	212	Total	C	H	N	O	S	0
			3356	1094	1647	270	335	10	

- Molecule 2 is a protein called Interferon alpha-2.

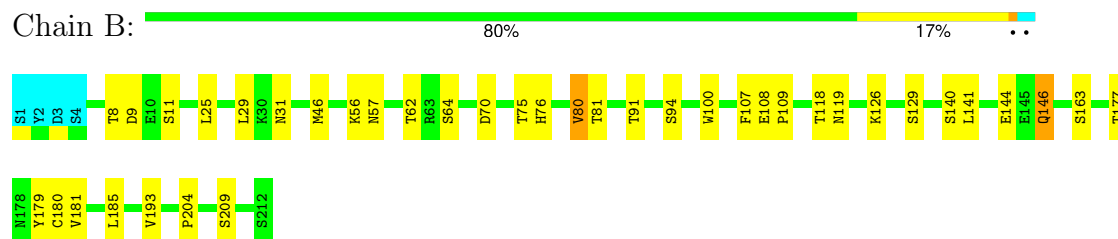
Mol	Chain	Residues	Atoms						Trace
2	A	165	Total	C	H	N	O	S	0
			2696	860	1346	227	254	9	

4 Residue-property plots

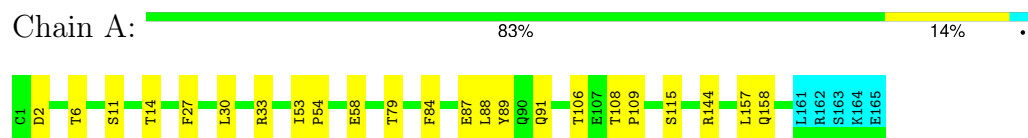
4.1 Average score per residue in the NMR ensemble

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: Interferon alpha/beta receptor 2



- Molecule 2: Interferon alpha-2

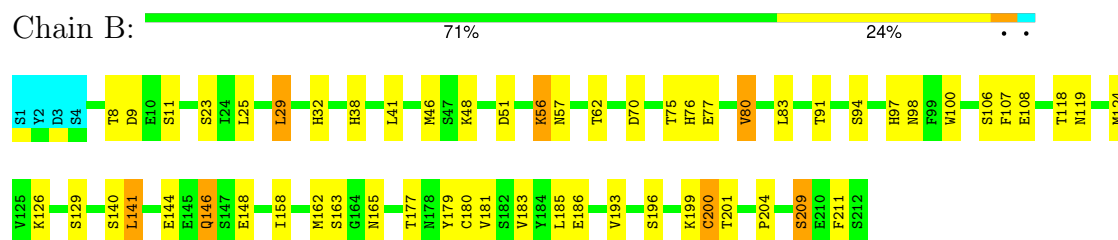


4.2 Scores per residue for each member of the ensemble

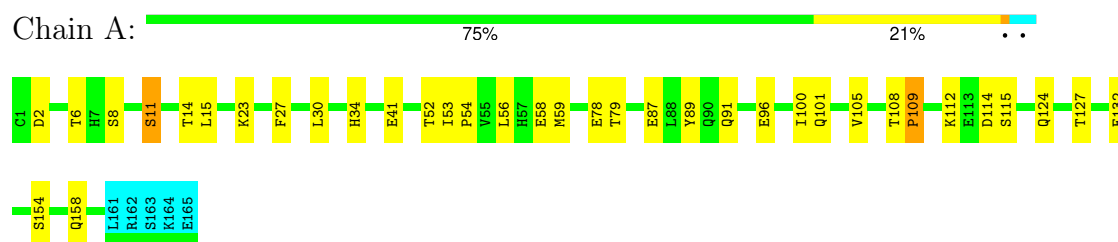
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Interferon alpha/beta receptor 2

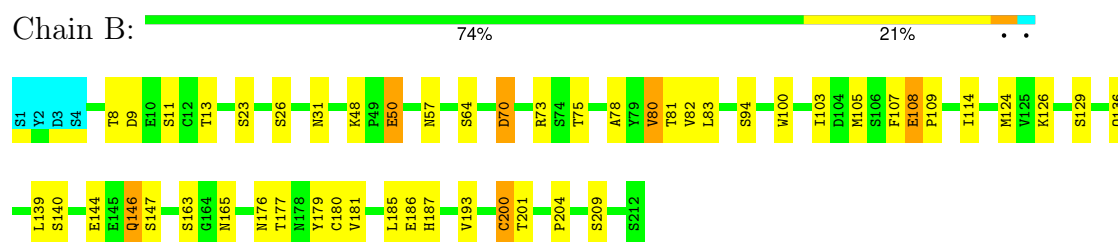


- Molecule 2: Interferon alpha-2

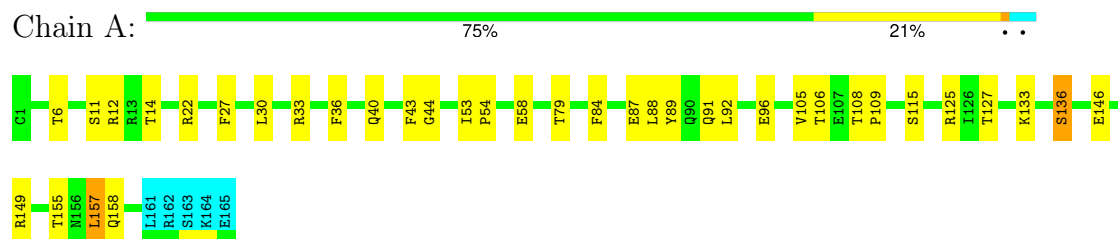


4.2.2 Score per residue for model 2

- Molecule 1: Interferon alpha/beta receptor 2

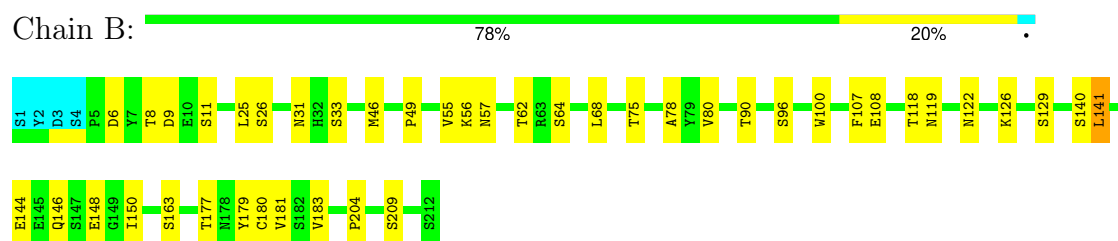


- Molecule 2: Interferon alpha-2

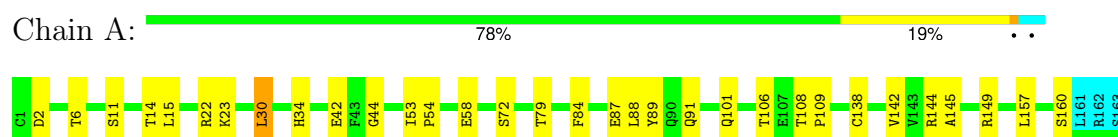


4.2.3 Score per residue for model 3

- Molecule 1: Interferon alpha/beta receptor 2



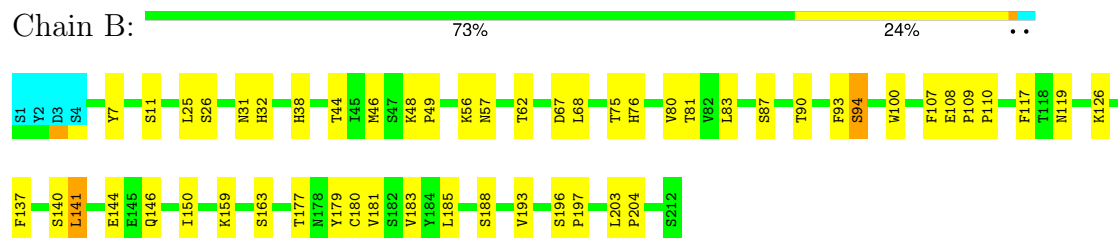
- Molecule 2: Interferon alpha-2



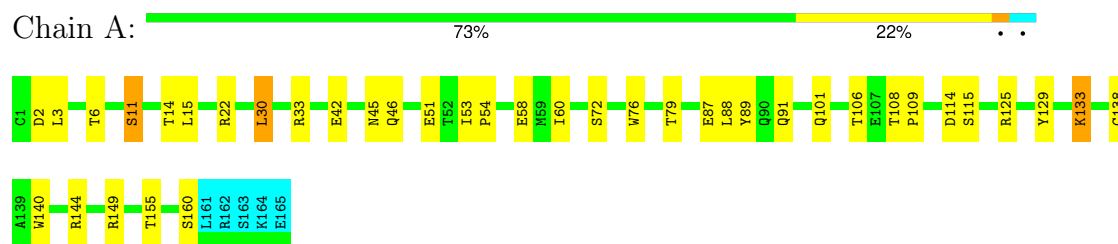
K164
E165

4.2.4 Score per residue for model 4

- Molecule 1: Interferon alpha/beta receptor 2

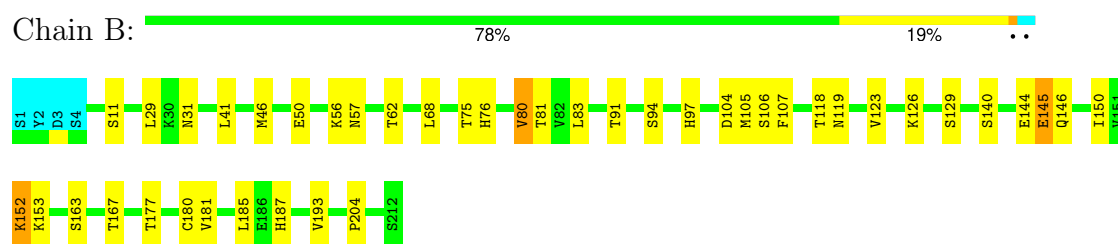


- Molecule 2: Interferon alpha-2

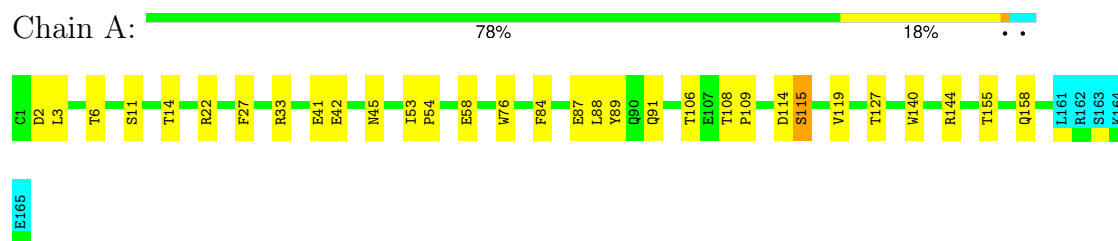


4.2.5 Score per residue for model 5

- Molecule 1: Interferon alpha/beta receptor 2

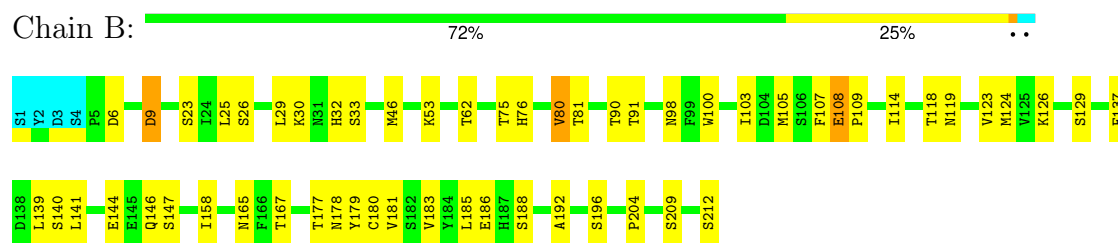


- Molecule 2: Interferon alpha-2

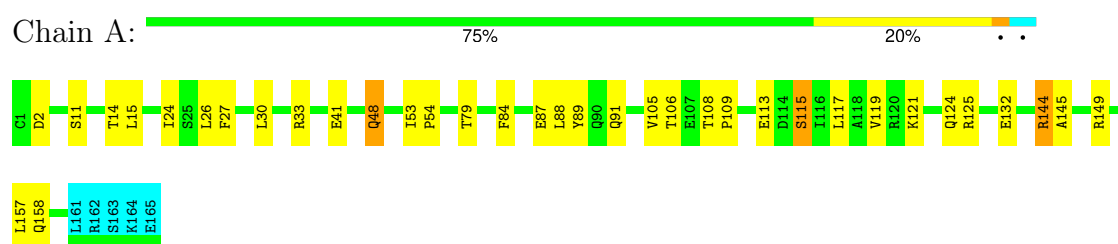


4.2.6 Score per residue for model 6

- Molecule 1: Interferon alpha/beta receptor 2

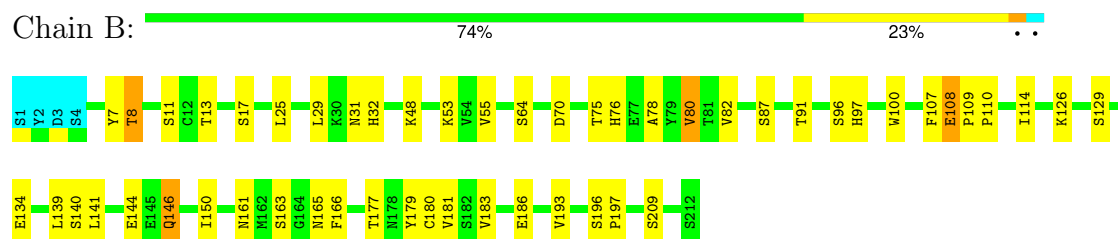


- Molecule 2: Interferon alpha-2

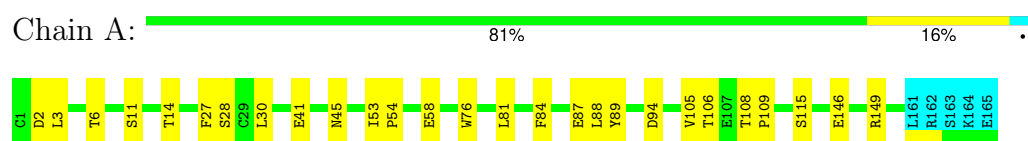


4.2.7 Score per residue for model 7

- Molecule 1: Interferon alpha/beta receptor 2



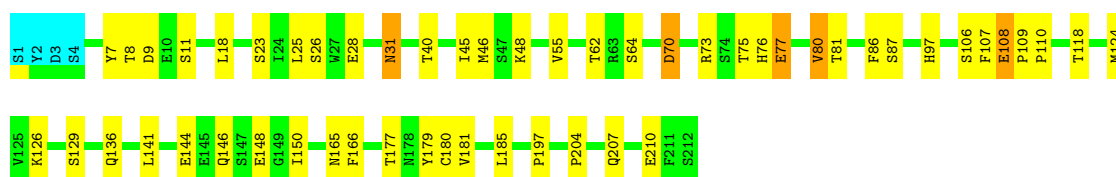
- Molecule 2: Interferon alpha-2



4.2.8 Score per residue for model 8

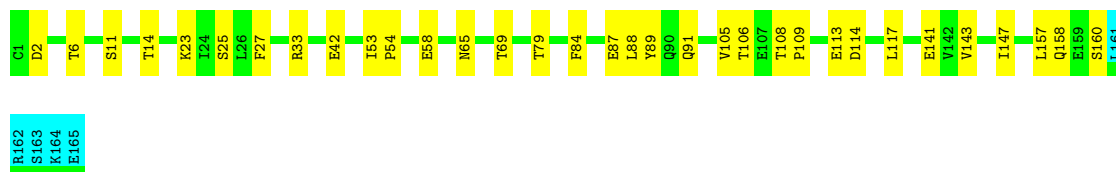
- Molecule 1: Interferon alpha/beta receptor 2





• Molecule 2: Interferon alpha-2

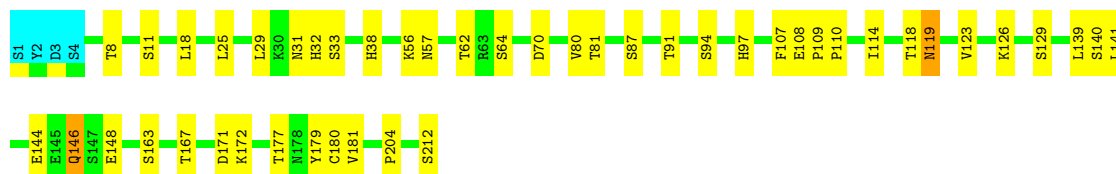
Chain A: 77% 20% .



4.2.9 Score per residue for model 9

• Molecule 1: Interferon alpha/beta receptor 2

Chain B: 76% 21% ..



• Molecule 2: Interferon alpha-2

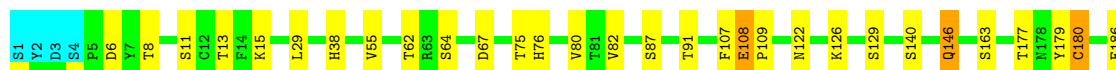
Chain A: 76% 21% .



4.2.10 Score per residue for model 10

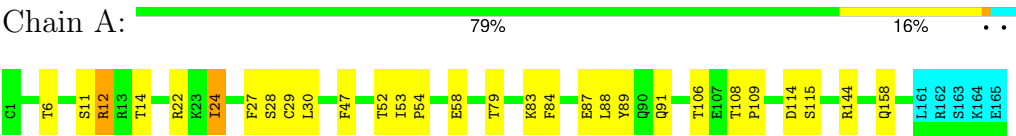
• Molecule 1: Interferon alpha/beta receptor 2

Chain B: 81% 16% ..





● Molecule 2: Interferon alpha-2



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 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
HADDOCK	refinement	

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)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	1950
Number of shifts mapped to atoms	1950
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	38%

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	B	1677	1624	1624	10±3
2	A	1307	1298	1299	8±2
All	All	29840	29220	29230	162

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:124:MET:SD	1:B:165:ASN:HB2	0.66	2.30	8	4
2:A:22:ARG:HA	2:A:144:ARG:NH2	0.66	2.05	4	2
2:A:11:SER:O	2:A:15:LEU:HG	0.61	1.96	4	2
1:B:146:GLN:O	1:B:179:TYR:HA	0.59	1.97	6	9
1:B:141:LEU:HD11	1:B:183:VAL:HG13	0.59	1.73	3	5
1:B:146:GLN:HA	1:B:150:ILE:O	0.53	2.03	4	5
1:B:179:TYR:CZ	1:B:201:THR:HB	0.53	2.39	2	2
2:A:113:GLU:O	2:A:117:LEU:HG	0.53	2.03	8	2
1:B:144:GLU:O	1:B:181:VAL:HA	0.52	2.05	7	9
2:A:54:PRO:HD3	2:A:105:VAL:CG1	0.51	2.36	8	5
1:B:109:PRO:N	1:B:110:PRO:HD2	0.51	2.20	7	4
1:B:187:HIS:CE1	2:A:12:ARG:HD2	0.50	2.41	10	2
2:A:84:PHE:O	2:A:88:LEU:HG	0.50	2.06	10	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:8:THR:O	1:B:32:HIS:HB2	0.50	2.06	7	1
1:B:123:VAL:O	1:B:167:THR:HA	0.49	2.08	5	3
1:B:46:MET:HB2	1:B:78:ALA:O	0.49	2.07	3	1
1:B:108:GLU:H	1:B:109:PRO:CD	0.48	2.20	6	4
2:A:133:LYS:HB3	2:A:136:SER:OG	0.48	2.08	2	1
2:A:53:ILE:N	2:A:54:PRO:HD2	0.48	2.24	6	10
2:A:41:GLU:O	2:A:45:ASN:HB2	0.48	2.09	5	2
2:A:22:ARG:HG2	2:A:23:LYS:N	0.48	2.24	3	1
1:B:83:LEU:O	1:B:94:SER:HA	0.47	2.09	2	4
1:B:78:ALA:HB2	1:B:100:TRP:CD1	0.47	2.43	2	2
1:B:114:ILE:HD13	1:B:181:VAL:HB	0.47	1.86	7	1
1:B:56:LYS:O	1:B:57:ASN:HB3	0.47	2.10	3	5
1:B:108:GLU:H	1:B:109:PRO:HD2	0.46	1.71	6	3
2:A:144:ARG:NH1	2:A:145:ALA:HA	0.46	2.25	6	2
2:A:52:THR:O	2:A:56:LEU:HG	0.46	2.10	1	1
2:A:48:GLN:HG3	2:A:157:LEU:HD12	0.46	1.86	6	1
1:B:46:MET:SD	2:A:149:ARG:HB2	0.46	2.51	4	1
1:B:100:TRP:CZ3	2:A:15:LEU:HD13	0.46	2.46	4	3
1:B:80:VAL:HB	2:A:27:PHE:CE2	0.45	2.47	2	6
1:B:180:CYS:HA	1:B:199:LYS:O	0.45	2.11	1	2
2:A:44:GLY:HA2	2:A:157:LEU:HD11	0.45	1.89	9	3
1:B:145:GLU:OE1	1:B:152:LYS:HE2	0.45	2.11	5	1
1:B:70:ASP:OD1	1:B:73:ARG:HD3	0.44	2.13	2	2
1:B:171:ASP:O	1:B:172:LYS:HB2	0.44	2.12	9	1
2:A:109:PRO:O	2:A:112:LYS:HG2	0.44	2.12	1	1
2:A:60:ILE:HG23	2:A:88:LEU:HD22	0.44	1.88	4	1
1:B:136:GLN:NE2	2:A:160:SER:HA	0.44	2.27	8	1
1:B:82:VAL:HB	2:A:27:PHE:CD2	0.44	2.48	7	2
1:B:45:ILE:HB	1:B:77:GLU:OE2	0.44	2.13	8	1
1:B:31:ASN:N	1:B:31:ASN:HD22	0.44	2.11	8	1
1:B:104:ASP:O	1:B:105:MET:HB2	0.43	2.12	5	1
2:A:36:PHE:HA	2:A:125:ARG:NH1	0.43	2.28	2	2
1:B:179:TYR:O	1:B:200:CYS:HA	0.43	2.14	1	2
2:A:96:GLU:O	2:A:100:ILE:HG13	0.43	2.14	1	1
1:B:49:PRO:HB2	2:A:30:LEU:HD12	0.43	1.91	3	2
2:A:76:TRP:CH2	2:A:140:TRP:HB3	0.42	2.49	5	2
2:A:65:ASN:O	2:A:69:THR:HG23	0.42	2.13	8	1
1:B:100:TRP:CH2	2:A:15:LEU:HD22	0.42	2.49	6	1
2:A:41:GLU:HA	2:A:45:ASN:OD1	0.42	2.15	5	1
2:A:129:TYR:CZ	2:A:133:LYS:HE2	0.42	2.49	4	1
2:A:32:ASP:O	2:A:142:VAL:HG21	0.42	2.14	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:188:SER:HB3	2:A:12:ARG:O	0.42	2.14	10	1
2:A:92:LEU:O	2:A:96:GLU:HG2	0.42	2.14	2	1
2:A:45:ASN:O	2:A:46:GLN:HB2	0.42	2.15	4	1
2:A:24:ILE:HD12	2:A:29:CYS:SG	0.42	2.55	10	1
1:B:29:LEU:HD13	1:B:29:LEU:N	0.41	2.30	1	1
1:B:158:ILE:HG22	1:B:162:MET:HB2	0.41	1.92	1	1
2:A:76:TRP:HB2	2:A:81:LEU:HD11	0.41	1.93	7	1
2:A:56:LEU:HD22	2:A:154:SER:HB3	0.41	1.93	1	1
2:A:121:LYS:O	2:A:125:ARG:HG3	0.41	2.16	6	1
2:A:47:PHE:O	2:A:52:THR:HB	0.41	2.16	10	1
1:B:209:SER:HB2	1:B:211:PHE:CZ	0.41	2.51	1	1
2:A:115:SER:O	2:A:119:VAL:HG23	0.41	2.15	6	2
1:B:103:ILE:O	1:B:192:ALA:HB2	0.41	2.16	6	1
2:A:138:CYS:O	2:A:142:VAL:HG23	0.41	2.16	3	1
1:B:9:ASP:HA	1:B:30:LYS:O	0.40	2.16	6	1
1:B:82:VAL:HB	2:A:27:PHE:CE2	0.40	2.51	7	1
1:B:46:MET:SD	2:A:26:LEU:HD21	0.40	2.57	6	1
2:A:143:VAL:O	2:A:147:ILE:HG12	0.40	2.17	8	1
1:B:117:PHE:O	1:B:203:LEU:HB2	0.40	2.16	4	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	B	207/212 (98%)	174±4 (84±2%)	30±4 (15±2%)	3±1 (1±0%)	13	60
2	A	159/165 (96%)	145±2 (91±1%)	13±2 (8±1%)	1±0 (1±0%)	24	72
All	All	3660/3770 (97%)	3190 (87%)	433 (12%)	37 (1%)	16	65

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	109	PRO	10
1	B	108	GLU	9

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Mol	Chain	Res	Type	Models (Total)
1	B	204	PRO	8
1	B	197	PRO	3
1	B	119	ASN	2
1	B	106	SER	1
1	B	50	GLU	1
1	B	176	ASN	1
1	B	187	HIS	1
1	B	158	ILE	1

6.3.2 Protein sidechains ⓘ

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	B	197/201 (98%)	163±3 (83±2%)	34±3 (17±2%)	3	37
2	A	147/152 (97%)	126±3 (86±2%)	21±3 (14±2%)	5	44
All	All	3440/3530 (97%)	2893 (84%)	547 (16%)	4	40

All 144 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	B	80	VAL	10
1	B	107	PHE	10
1	B	126	LYS	10
1	B	177	THR	10
2	A	14	THR	10
2	A	87	GLU	10
2	A	89	TYR	10
2	A	108	THR	10
1	B	11	SER	9
1	B	75	THR	9
1	B	129	SER	9
1	B	140	SER	9
2	A	6	THR	9
2	A	11	SER	9
1	B	180	CYS	9
2	A	106	THR	9

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Mol	Chain	Res	Type	Models (Total)
1	B	62	THR	8
1	B	163	SER	8
2	A	2	ASP	8
2	A	30	LEU	8
2	A	58	GLU	8
2	A	91	GLN	8
2	A	115	SER	8
1	B	8	THR	7
1	B	25	LEU	7
1	B	76	HIS	7
2	A	79	THR	7
2	A	158	GLN	7
1	B	31	ASN	7
1	B	29	LEU	6
1	B	91	THR	6
1	B	118	THR	6
1	B	185	LEU	6
1	B	193	VAL	6
1	B	209	SER	6
1	B	64	SER	6
1	B	81	THR	6
2	A	33	ARG	6
1	B	9	ASP	5
1	B	48	LYS	5
1	B	70	ASP	5
1	B	97	HIS	5
1	B	119	ASN	5
1	B	141	LEU	5
1	B	146	GLN	5
1	B	186	GLU	5
1	B	196	SER	5
2	A	114	ASP	5
1	B	26	SER	5
2	A	42	GLU	5
1	B	87	SER	5
1	B	23	SER	4
1	B	32	HIS	4
1	B	38	HIS	4
1	B	148	GLU	4
2	A	127	THR	4
1	B	139	LEU	4
2	A	149	ARG	4

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Mol	Chain	Res	Type	Models (Total)
2	A	155	THR	4
1	B	55	VAL	4
1	B	46	MET	3
2	A	23	LYS	3
2	A	101	GLN	3
1	B	13	THR	3
1	B	114	ILE	3
1	B	6	ASP	3
1	B	33	SER	3
1	B	68	LEU	3
1	B	90	THR	3
2	A	160	SER	3
1	B	7	TYR	3
1	B	188	SER	3
2	A	3	LEU	3
2	A	28	SER	3
1	B	41	LEU	2
1	B	77	GLU	2
1	B	98	ASN	2
1	B	200	CYS	2
2	A	34	HIS	2
2	A	41	GLU	2
2	A	78	GLU	2
2	A	124	GLN	2
2	A	132	GLU	2
1	B	50	GLU	2
1	B	105	MET	2
1	B	147	SER	2
2	A	22	ARG	2
2	A	43	PHE	2
2	A	136	SER	2
2	A	146	GLU	2
2	A	157	LEU	2
1	B	96	SER	2
1	B	122	ASN	2
2	A	72	SER	2
1	B	67	ASP	2
1	B	94	SER	2
1	B	137	PHE	2
1	B	106	SER	2
1	B	53	LYS	2
1	B	212	SER	2

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Mol	Chain	Res	Type	Models (Total)
2	A	24	ILE	2
2	A	144	ARG	2
1	B	166	PHE	2
1	B	18	LEU	2
1	B	51	ASP	1
1	B	56	LYS	1
2	A	8	SER	1
2	A	59	MET	1
1	B	57	ASN	1
1	B	82	VAL	1
1	B	103	ILE	1
1	B	136	GLN	1
2	A	40	GLN	1
1	B	44	THR	1
1	B	93	PHE	1
1	B	159	LYS	1
2	A	51	GLU	1
2	A	125	ARG	1
2	A	133	LYS	1
2	A	138	CYS	1
1	B	145	GLU	1
1	B	152	LYS	1
1	B	153	LYS	1
1	B	178	ASN	1
2	A	48	GLN	1
1	B	17	SER	1
1	B	134	GLU	1
1	B	161	ASN	1
1	B	165	ASN	1
2	A	94	ASP	1
1	B	28	GLU	1
1	B	40	THR	1
1	B	86	PHE	1
1	B	207	GLN	1
1	B	210	GLU	1
2	A	25	SER	1
2	A	141	GLU	1
2	A	31	LYS	1
2	A	121	LYS	1
2	A	152	SER	1
1	B	15	LYS	1
1	B	203	LEU	1

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Mol	Chain	Res	Type	Models (Total)
2	A	12	ARG	1
2	A	83	LYS	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 oligosaccharides 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](#)

The completeness of assignment taking into account all chemical shift lists is 38% for the well-defined parts and 37% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned.str_1*

7.1.1 Bookkeeping [i](#)

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	533
Number of shifts mapped to atoms	533
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	115	-0.06 ± 0.37	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 10%, i.e. 519 atoms were assigned a chemical shift out of a possible 5098. 0 out of 59 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	211/1820 (12%)	99/732 (14%)	0/736 (0%)	112/352 (32%)
Sidechain	292/2809 (10%)	292/1825 (16%)	0/893 (0%)	0/91 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	16/469 (3%)	16/233 (7%)	0/220 (0%)	0/16 (0%)
Overall	519/5098 (10%)	407/2790 (15%)	0/1849 (0%)	112/459 (24%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 533 atoms were assigned a chemical shift out of a possible 5219. 0 out of 60 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	216/1865 (12%)	101/750 (13%)	0/754 (0%)	115/361 (32%)
Sidechain	301/2876 (10%)	301/1867 (16%)	0/914 (0%)	0/95 (0%)
Aromatic	16/478 (3%)	16/237 (7%)	0/225 (0%)	0/16 (0%)
Overall	533/5219 (10%)	418/2854 (15%)	0/1893 (0%)	115/472 (24%)

7.1.4 Statistically unusual chemical shifts [i](#)

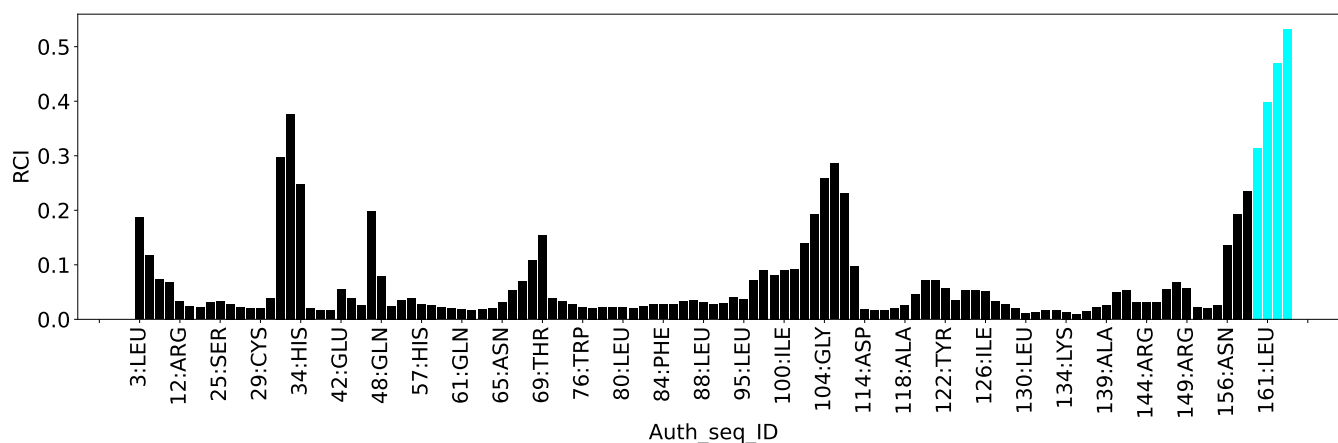
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	140	TRP	H	17.32	4.48 – 12.05	12.0
1	A	116	ILE	H	1.96	4.90 – 11.63	-9.4
1	A	131	LYS	HG2	-0.75	0.13 – 2.61	-8.5
1	A	75	ALA	HB1	-0.41	0.14 – 2.58	-7.2
1	A	75	ALA	HB2	-0.41	0.14 – 2.58	-7.2
1	A	75	ALA	HB3	-0.41	0.14 – 2.58	-7.2
1	A	104	GLY	H	12.35	5.23 – 11.42	6.5
1	A	133	LYS	HD3	0.38	0.54 – 2.65	-5.8

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

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned.str_2*

7.2.1 Bookkeeping [i](#)

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	1417
Number of shifts mapped to atoms	1417
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	170	-0.45 ± 0.32	None needed (< 0.5 ppm)

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 28%, i.e. 1407 atoms were assigned a chemical shift out of a possible 5098. 0 out of 59 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	525/1820 (29%)	357/732 (49%)	0/736 (0%)	168/352 (48%)
Sidechain	814/2809 (29%)	814/1825 (45%)	0/893 (0%)	0/91 (0%)
Aromatic	68/469 (14%)	68/233 (29%)	0/220 (0%)	0/16 (0%)
Overall	1407/5098 (28%)	1239/2790 (44%)	0/1849 (0%)	168/459 (37%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 27%, i.e. 1417 atoms were assigned a chemical shift out of a possible 5219. 0 out of 60 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	531/1865 (28%)	361/750 (48%)	0/754 (0%)	170/361 (47%)
Sidechain	818/2876 (28%)	818/1867 (44%)	0/914 (0%)	0/95 (0%)
Aromatic	68/478 (14%)	68/237 (29%)	0/225 (0%)	0/16 (0%)
Overall	1417/5219 (27%)	1247/2854 (44%)	0/1893 (0%)	170/472 (36%)

7.2.4 Statistically unusual chemical shifts [i](#)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	68	LEU	HD21	-0.86	-0.65 – 2.13	-5.8
2	B	68	LEU	HD22	-0.86	-0.65 – 2.13	-5.8
2	B	68	LEU	HD23	-0.86	-0.65 – 2.13	-5.8

7.2.5 Random Coil Index (RCI) plots [i](#)

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B:

