



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:45 PM UTC

PDB ID : 8DPX / pdb_00008dpx
BMRB ID : 31034
Title : Preligand association structure of DR5
Authors : Du, G.; Zhao, L.; Chou, J.J.
Deposited on : 2022-07-17

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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

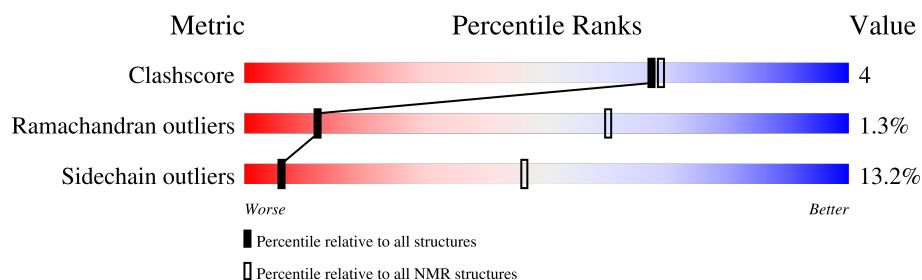
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 22%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	A	109	76% 18% 6%
1	B	109	73% 14% 13%
1	C	109	76% 12% 12%

2 Ensemble composition and analysis

This entry contains 15 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:79-A:181, B:79-B:145, B:153-B:180, C:79-C:145, C:152-C:180 (294)	0.42	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 6 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4809 atoms, of which 2289 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tumor necrosis factor receptor superfamily member 10B.

Mol	Chain	Residues	Atoms						Trace
1	A	109	Total	C	H	N	O	S	0
			1603	501	763	151	172	16	
1	B	109	Total	C	H	N	O	S	0
			1603	501	763	151	172	16	
1	C	109	Total	C	H	N	O	S	0
			1603	501	763	151	172	16	

There are 3 discrepancies between the modelled and reference sequences:

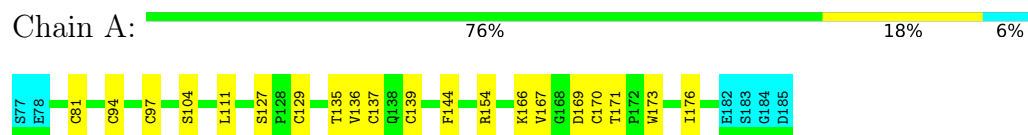
Chain	Residue	Modelled	Actual	Comment	Reference
A	185	ASP	-	expression tag	UNP O14763
B	185	ASP	-	expression tag	UNP O14763
C	185	ASP	-	expression tag	UNP O14763

4 Residue-property plots

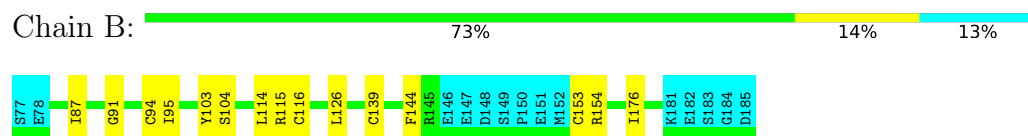
4.1 Average score per residue in the NMR ensemble

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.

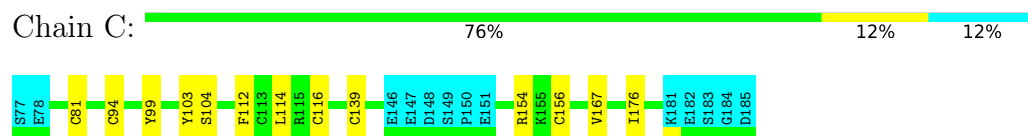
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



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- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

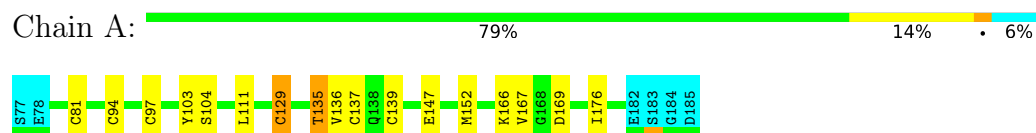


4.2 Scores per residue for each member of the ensemble

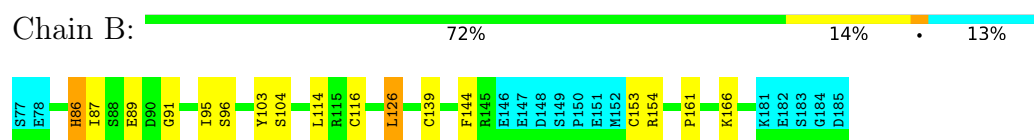
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

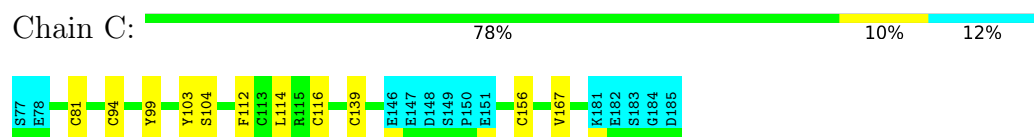
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



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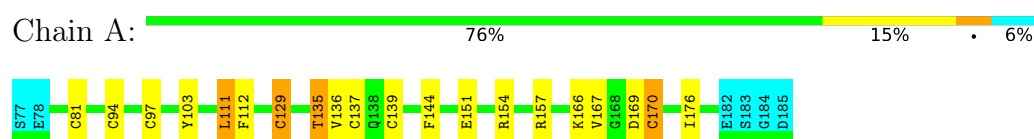


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

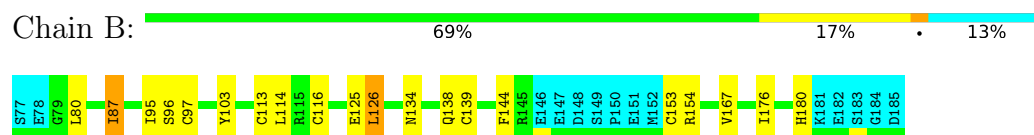


4.2.2 Score per residue for model 2

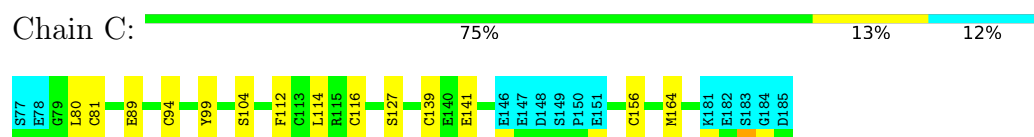
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



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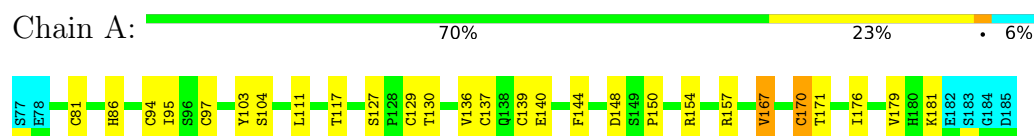


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

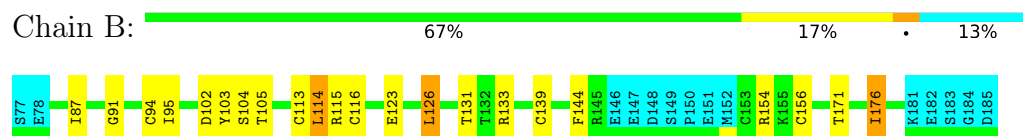


4.2.3 Score per residue for model 3

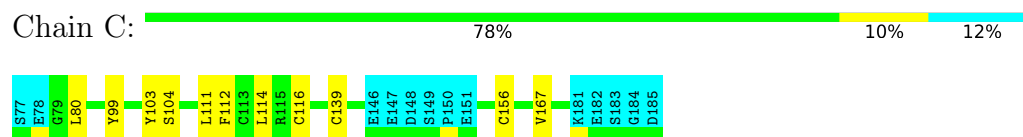
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

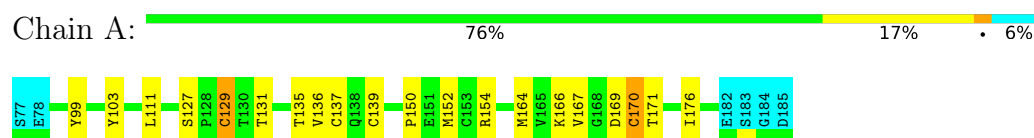


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

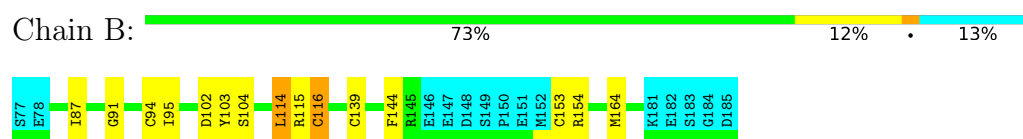


4.2.4 Score per residue for model 4

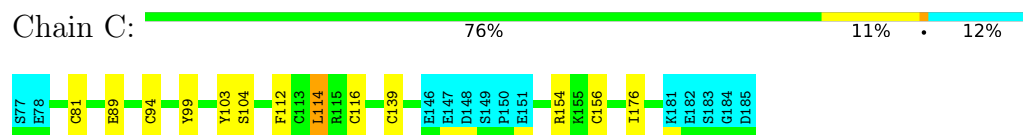
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

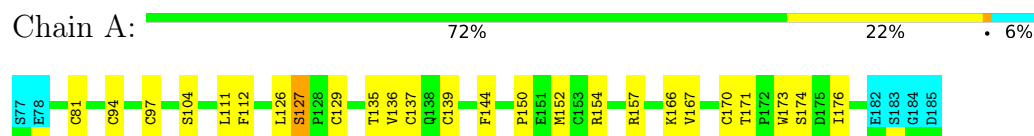


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



4.2.5 Score per residue for model 5

- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B





- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain C: 



4.2.6 Score per residue for model 6

- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain A: 



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain B: 



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain C: 



4.2.7 Score per residue for model 7

- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain A: 

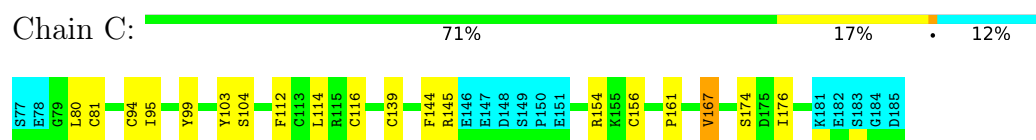


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain B: 

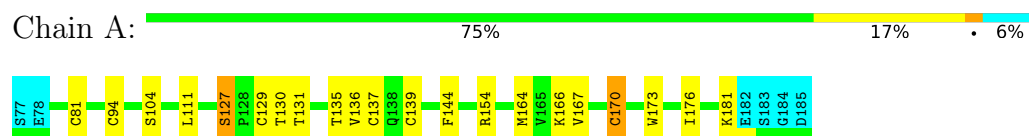


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

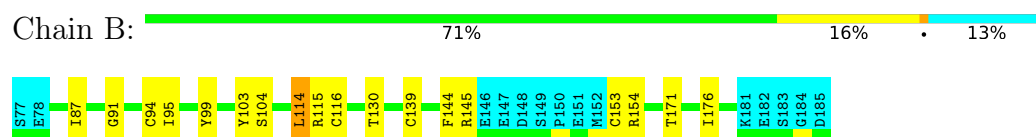


4.2.8 Score per residue for model 8

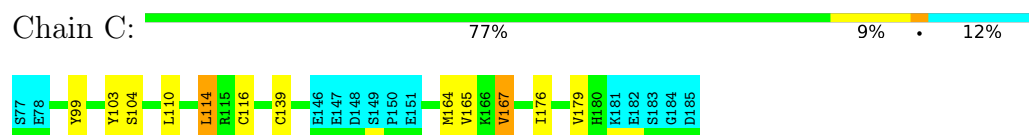
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

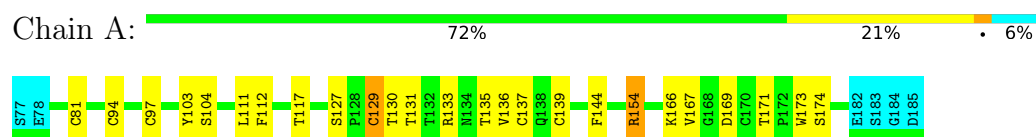


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

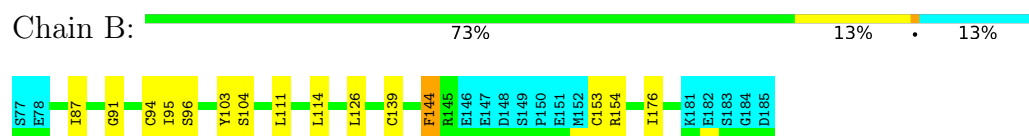


4.2.9 Score per residue for model 9

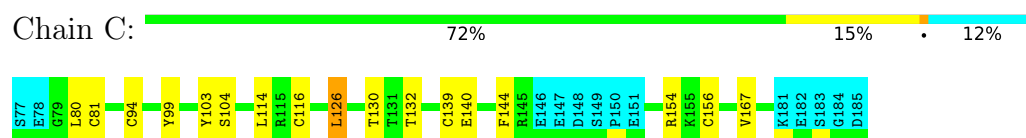
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



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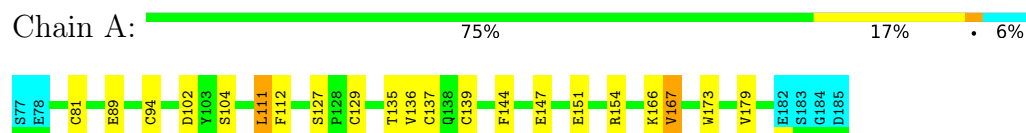


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

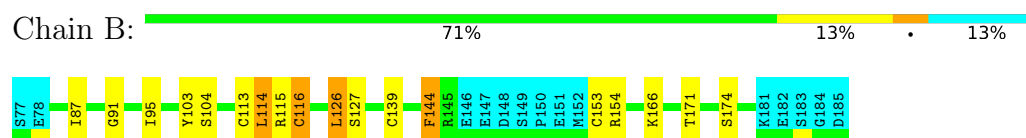


4.2.10 Score per residue for model 10

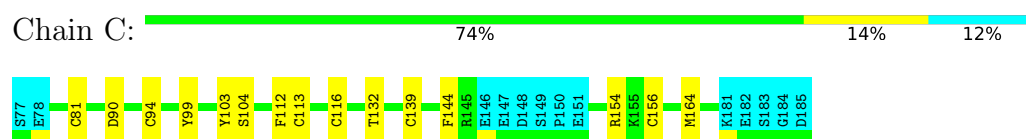
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

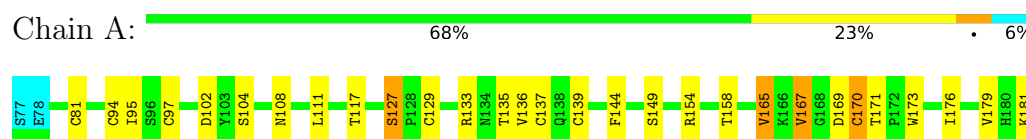


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

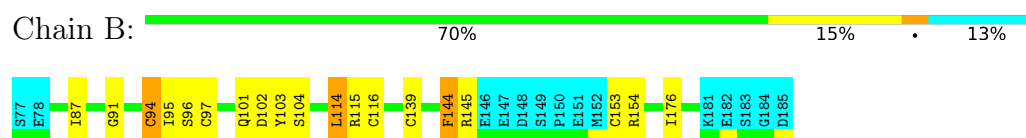


4.2.11 Score per residue for model 11

- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

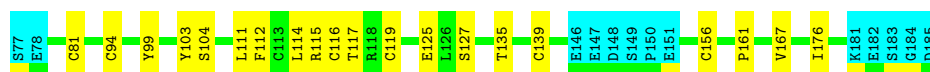


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

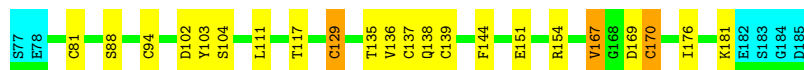




4.2.12 Score per residue for model 12

- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain A: 74% 17% 6%



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain B: 73% 14% 13%



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain C: 71% 17% 12%



4.2.13 Score per residue for model 13

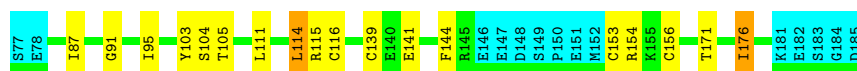
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain A: 74% 19% 6%



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain B: 71% 15% 13%



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain C: 74% 14% 12%



4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain A:  71% 23% 6%



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain B:  69% 18% 13%



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

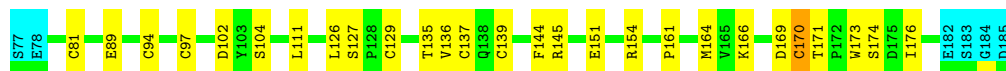
Chain C:  72% 17% 12%



4.2.15 Score per residue for model 15

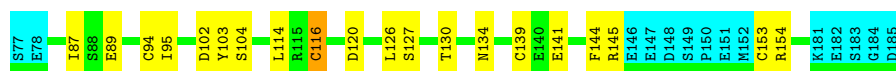
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain A:  70% 24% 6%



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain B:  69% 17% 13%



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain C:  72% 16% 12%



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 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
X-PLOR NIH	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	1
Total number of shifts	831
Number of shifts mapped to atoms	831
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	22%

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	A	799	732	728	8±2
1	B	734	676	672	8±1
1	C	742	685	681	3±2
All	All	34125	31395	31215	250

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:VAL:HG13	1:B:95:ILE:CG1	0.70	2.16	4	5
1:A:171:THR:HG21	1:B:102:ASP:OD1	0.66	1.89	7	3
1:B:99:TYR:CD1	1:B:130:THR:HG23	0.65	2.27	8	1
1:B:99:TYR:CE1	1:B:130:THR:HG22	0.61	2.30	7	1
1:A:127:SER:OG	1:A:136:VAL:HG23	0.60	1.96	15	1
1:A:136:VAL:HG13	1:B:95:ILE:HG23	0.60	1.73	2	10
1:A:171:THR:HG21	1:B:102:ASP:OD2	0.59	1.96	15	4
1:A:165:VAL:HG23	1:A:179:VAL:O	0.59	1.95	11	1
1:B:87:ILE:HD11	1:B:91:GLY:O	0.59	1.97	11	9
1:B:111:LEU:O	1:B:111:LEU:HD22	0.56	1.99	5	1
1:B:94:CYS:C	1:B:95:ILE:HD12	0.56	2.24	9	7
1:A:170:CYS:SG	1:A:176:ILE:HG23	0.54	2.42	8	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:VAL:HG13	1:B:95:ILE:HG13	0.54	1.79	9	4
1:B:87:ILE:HD13	1:B:87:ILE:O	0.53	2.02	2	1
1:A:127:SER:O	1:A:135:THR:HG23	0.53	2.04	11	4
1:B:126:LEU:O	1:B:126:LEU:HD13	0.52	2.05	3	5
1:A:136:VAL:HG13	1:B:95:ILE:CG2	0.51	2.35	11	11
1:A:152:MET:HE2	1:A:154:ARG:NH1	0.51	2.21	4	2
1:A:126:LEU:HD11	1:A:138:GLN:OE1	0.51	2.05	6	1
1:A:167:VAL:HG21	1:A:179:VAL:HG23	0.50	1.84	3	4
1:A:158:THR:OG1	1:C:117:THR:HG23	0.50	2.07	11	1
1:B:130:THR:HG22	1:B:133:ARG:HB2	0.50	1.83	14	1
1:B:130:THR:HG23	1:B:132:THR:H	0.49	1.67	14	1
1:B:176:ILE:HD12	1:B:176:ILE:C	0.48	2.34	9	1
1:A:126:LEU:HD12	1:A:136:VAL:HG11	0.48	1.85	6	2
1:B:86:HIS:C	1:B:86:HIS:CD2	0.48	2.92	12	1
1:C:176:ILE:HD12	1:C:176:ILE:C	0.48	2.34	5	6
1:A:136:VAL:CG1	1:B:95:ILE:HG23	0.47	2.37	2	9
1:B:144:PHE:N	1:B:154:ARG:O	0.47	2.48	10	15
1:A:164:MET:O	1:C:114:LEU:HD21	0.47	2.10	6	3
1:B:99:TYR:CE1	1:B:130:THR:HG23	0.47	2.44	8	1
1:C:95:ILE:HD12	1:C:95:ILE:N	0.47	2.25	14	4
1:B:111:LEU:HD22	1:B:111:LEU:C	0.46	2.36	5	1
1:A:95:ILE:HD12	1:A:95:ILE:N	0.46	2.26	7	4
1:A:152:MET:HE2	1:A:154:ARG:HD3	0.45	1.87	5	1
1:A:176:ILE:C	1:A:176:ILE:HD12	0.45	2.36	1	1
1:B:86:HIS:CD2	1:B:86:HIS:C	0.45	2.95	1	1
1:A:167:VAL:HG21	1:A:179:VAL:CG2	0.45	2.40	3	2
1:A:127:SER:O	1:A:135:THR:HA	0.45	2.11	5	3
1:C:126:LEU:HD13	1:C:138:GLN:OE1	0.45	2.12	14	1
1:A:111:LEU:N	1:A:111:LEU:HD12	0.45	2.27	1	7
1:B:111:LEU:C	1:B:111:LEU:HD12	0.44	2.37	9	1
1:A:111:LEU:HD11	1:A:112:PHE:CZ	0.44	2.47	7	3
1:B:114:LEU:HD13	1:B:115:ARG:O	0.44	2.13	10	6
1:B:156:CYS:SG	1:B:176:ILE:HG23	0.44	2.53	3	2
1:C:130:THR:HG23	1:C:132:THR:H	0.44	1.72	9	1
1:C:111:LEU:HD12	1:C:111:LEU:N	0.44	2.28	11	4
1:C:103:TYR:C	1:C:103:TYR:CD2	0.44	2.96	7	9
1:A:111:LEU:HD12	1:A:111:LEU:H	0.44	1.73	3	3
1:A:111:LEU:HD11	1:A:112:PHE:CE1	0.43	2.47	5	2
1:B:167:VAL:O	1:B:167:VAL:HG22	0.43	2.13	6	1
1:B:103:TYR:CD2	1:B:103:TYR:C	0.43	2.96	10	15
1:C:126:LEU:HD13	1:C:126:LEU:O	0.43	2.12	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:THR:HG22	1:A:131:THR:N	0.43	2.28	13	3
1:A:144:PHE:N	1:A:154:ARG:O	0.43	2.52	5	12
1:C:125:GLU:OE2	1:C:135:THR:HG21	0.43	2.13	11	1
1:A:111:LEU:HD12	1:A:111:LEU:N	0.43	2.29	3	1
1:A:136:VAL:HG13	1:B:95:ILE:HG12	0.43	1.89	4	1
1:C:144:PHE:N	1:C:154:ARG:O	0.42	2.51	7	7
1:C:103:TYR:CD1	1:C:103:TYR:C	0.42	2.97	10	3
1:C:176:ILE:HD13	1:C:176:ILE:O	0.42	2.14	6	1
1:A:103:TYR:CE1	1:A:129:CYS:SG	0.42	3.13	12	6
1:A:99:TYR:CE2	1:A:131:THR:HG22	0.42	2.50	4	1
1:B:99:TYR:CZ	1:B:130:THR:HG22	0.42	2.49	7	1
1:B:103:TYR:CD1	1:B:116:CYS:SG	0.42	3.13	15	4
1:C:103:TYR:CD2	1:C:103:TYR:C	0.42	2.97	5	1
1:C:170:CYS:HB2	1:C:176:ILE:HG22	0.41	1.92	6	1
1:C:167:VAL:HG21	1:C:179:VAL:HG21	0.41	1.93	8	1
1:A:129:CYS:SG	1:A:135:THR:OG1	0.41	2.79	2	3
1:C:111:LEU:HD12	1:C:111:LEU:H	0.41	1.75	3	1
1:B:114:LEU:HD13	1:B:115:ARG:N	0.40	2.32	7	1
1:C:80:LEU:HD12	1:C:80:LEU:N	0.40	2.31	7	1
1:C:167:VAL:O	1:C:167:VAL:HG22	0.40	2.17	7	1
1:B:80:LEU:N	1:B:80:LEU:HD12	0.40	2.32	2	1
1:A:103:TYR:CD1	1:A:130:THR:C	0.40	3.00	3	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	103/109 (94%)	90±1 (88±1%)	11±1 (10±1%)	2±1 (2±1%)	8	48
1	B	95/109 (87%)	87±1 (91±1%)	8±1 (8±1%)	0±0 (0±1%)	26	74
1	C	96/109 (88%)	89±1 (92±1%)	6±1 (6±1%)	1±1 (1±1%)	12	60
All	All	4410/4905 (90%)	3989 (90%)	364 (8%)	57 (1%)	12	60

All 12 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	167	VAL	13
1	C	167	VAL	10
1	A	151	GLU	7
1	C	161	PRO	7
1	A	181	LYS	6
1	A	150	PRO	4
1	B	167	VAL	3
1	B	161	PRO	2
1	B	79	GLY	2
1	A	79	GLY	1
1	C	79	GLY	1
1	A	161	PRO	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	A	94/99 (95%)	80±3 (85±3%)	14±3 (15±3%)	5	43
1	B	86/99 (87%)	76±2 (88±3%)	10±2 (12±3%)	7	49
1	C	87/99 (88%)	76±2 (87±2%)	11±2 (13±2%)	6	48
All	All	4005/4455 (90%)	3478 (87%)	527 (13%)	6	46

All 117 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	129	CYS	15
1	A	137	CYS	15
1	A	139	CYS	15
1	B	114	LEU	15
1	B	139	CYS	15
1	C	99	TYR	15
1	C	104	SER	15
1	C	116	CYS	15
1	B	104	SER	14
1	B	116	CYS	14
1	B	153	CYS	14

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Mol	Chain	Res	Type	Models (Total)
1	C	114	LEU	14
1	C	139	CYS	14
1	A	81	CYS	13
1	A	94	CYS	13
1	A	104	SER	13
1	C	156	CYS	13
1	A	166	LYS	11
1	C	81	CYS	11
1	C	94	CYS	11
1	C	112	PHE	11
1	A	170	CYS	11
1	A	97	CYS	10
1	A	173	TRP	9
1	A	135	THR	8
1	A	169	ASP	8
1	B	126	LEU	8
1	A	127	SER	8
1	B	176	ILE	7
1	A	111	LEU	5
1	B	113	CYS	5
1	A	117	THR	5
1	B	171	THR	5
1	A	174	SER	5
1	A	102	ASP	5
1	B	96	SER	4
1	B	166	LYS	4
1	B	87	ILE	4
1	B	97	CYS	4
1	C	164	MET	4
1	A	171	THR	4
1	C	152	MET	4
1	A	147	GLU	3
1	B	89	GLU	3
1	A	157	ARG	3
1	C	80	LEU	3
1	C	127	SER	3
1	B	111	LEU	3
1	C	174	SER	3
1	B	145	ARG	3
1	B	144	PHE	3
1	A	152	MET	2
1	B	125	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	B	134	ASN	2
1	C	89	GLU	2
1	C	141	GLU	2
1	A	140	GLU	2
1	B	105	THR	2
1	C	154	ARG	2
1	A	126	LEU	2
1	A	167	VAL	2
1	C	176	ILE	2
1	A	149	SER	2
1	A	154	ARG	2
1	B	115	ARG	2
1	A	133	ARG	2
1	C	126	LEU	2
1	A	89	GLU	2
1	B	127	SER	2
1	C	90	ASP	2
1	C	132	THR	2
1	B	141	GLU	2
1	B	86	HIS	1
1	B	138	GLN	1
1	B	180	HIS	1
1	A	86	HIS	1
1	A	148	ASP	1
1	A	181	LYS	1
1	B	123	GLU	1
1	B	131	THR	1
1	B	133	ARG	1
1	B	164	MET	1
1	A	176	ILE	1
1	B	80	LEU	1
1	B	90	ASP	1
1	C	98	LYS	1
1	A	106	HIS	1
1	A	146	GLU	1
1	B	132	THR	1
1	C	138	GLN	1
1	B	107	TRP	1
1	C	145	ARG	1
1	C	103	TYR	1
1	A	112	PHE	1
1	C	140	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	B	174	SER	1
1	C	113	CYS	1
1	A	108	ASN	1
1	A	165	VAL	1
1	B	94	CYS	1
1	B	101	GLN	1
1	C	115	ARG	1
1	C	119	CYS	1
1	A	88	SER	1
1	A	138	GLN	1
1	B	88	SER	1
1	C	88	SER	1
1	C	106	HIS	1
1	C	117	THR	1
1	C	175	ASP	1
1	C	153	CYS	1
1	A	90	ASP	1
1	C	125	GLU	1
1	A	145	ARG	1
1	A	164	MET	1
1	B	120	ASP	1
1	B	130	THR	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

The completeness of assignment taking into account all chemical shift lists is 22% for the well-defined parts and 20% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *bmr.b.txt*

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	831
Number of shifts mapped to atoms	831
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	102	0.68 ± 0.09	Should be applied
$^{13}\text{C}_\beta$	93	0.36 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}'$	101	-0.07 ± 0.11	None needed (< 0.5 ppm)
^{15}N	95	0.04 ± 0.36	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 22%, i.e. 817 atoms were assigned a chemical shift out of a possible 3737. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	479/1465 (33%)	188/599 (31%)	198/588 (34%)	93/278 (33%)
Sidechain	334/1990 (17%)	192/1274 (15%)	142/622 (23%)	0/94 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	4/282 (1%)	2/138 (1%)	0/114 (0%)	2/30 (7%)
Overall	817/3737 (22%)	382/2011 (19%)	340/1324 (26%)	95/402 (24%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 20%, i.e. 831 atoms were assigned a chemical shift out of a possible 4083. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	488/1629 (30%)	190/666 (29%)	203/654 (31%)	95/309 (31%)
Sidechain	339/2172 (16%)	194/1383 (14%)	145/693 (21%)	0/96 (0%)
Aromatic	4/282 (1%)	2/138 (1%)	0/114 (0%)	2/30 (7%)
Overall	831/4083 (20%)	386/2187 (18%)	348/1461 (24%)	97/435 (22%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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:

