



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 08:58 PM UTC

PDB ID : 2K20 / pdb_00002k20
Title : Solution structure of Par-3 PDZ3 in complex with PTEN peptide
Authors : Feng, W.; Wu, H.; Chan, L.; Zhang, M.
Deposited on : 2008-03-18

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

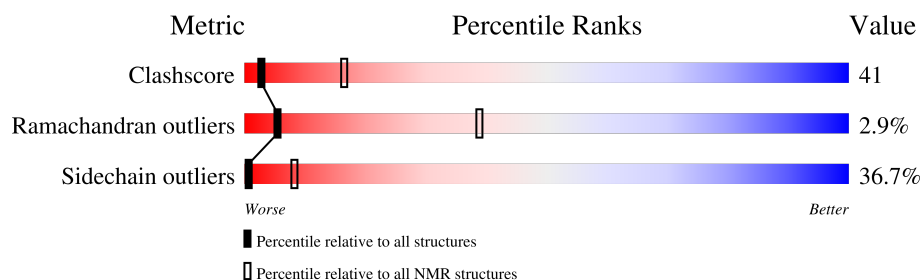
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	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	104	
2	B	11	

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:10-A:107, B:10-B:13 (102)	0.40	9

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 4 clusters and 7 single-model clusters were found.

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

3 Entry composition [i](#)

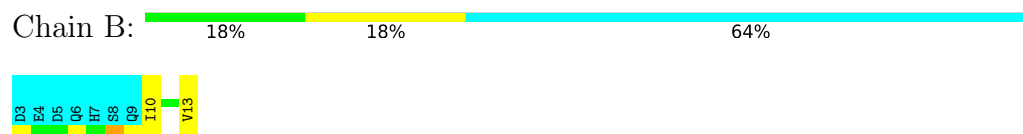
There are 2 unique types of molecules in this entry. The entry contains 1753 atoms, of which 884 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Partitioning-defective 3 homolog.

Mol	Chain	Residues	Atoms						Trace
1	A	104	Total	C	H	N	O	S	0
			1579	474	801	150	151	3	

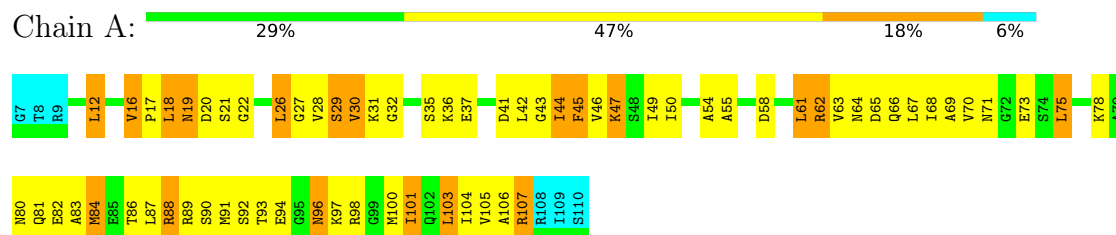
- Molecule 2 is a protein called Protein tyrosine phosphatase and tensin homolog.

Mol	Chain	Residues	Atoms					Trace
2	B	11	Total	C	H	N	O	0
			174	53	83	16	22	

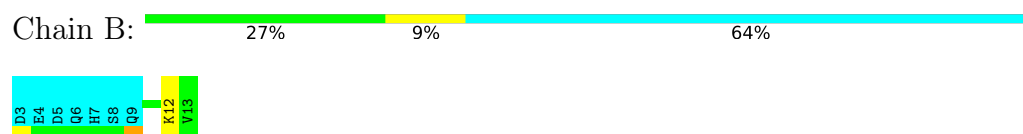


4.2.2 Score per residue for model 2

- Molecule 1: Partitioning-defective 3 homolog

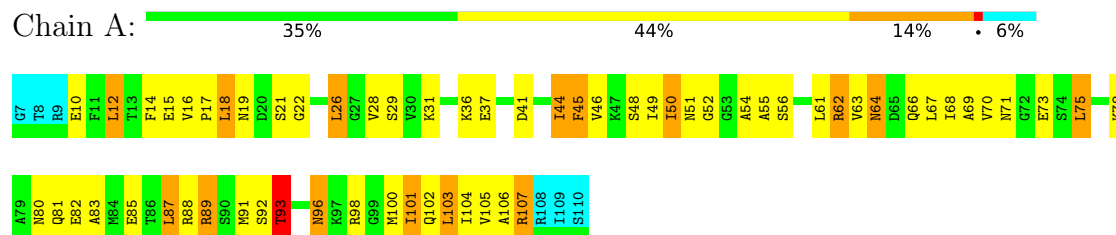


- Molecule 2: Protein tyrosine phosphatase and tensin homolog

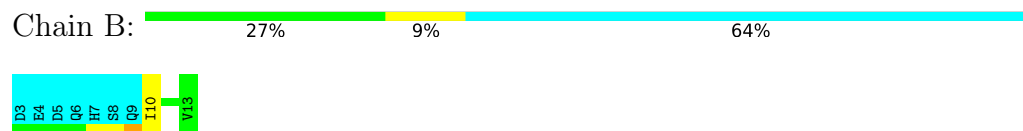


4.2.3 Score per residue for model 3

- Molecule 1: Partitioning-defective 3 homolog

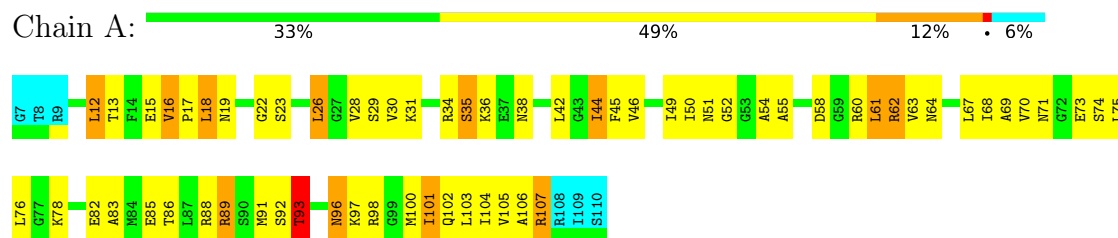


- Molecule 2: Protein tyrosine phosphatase and tensin homolog



4.2.4 Score per residue for model 4

- Molecule 1: Partitioning-defective 3 homolog

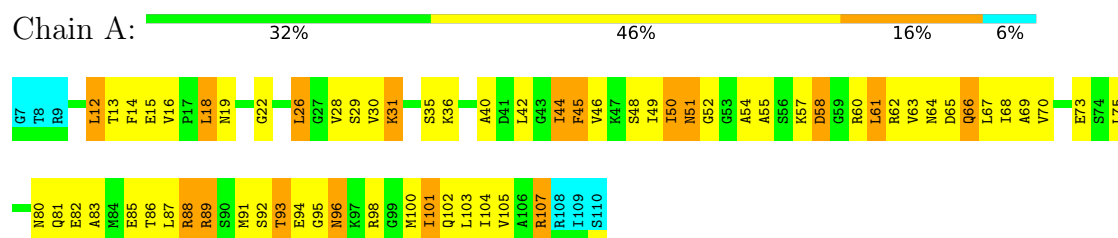


- Molecule 2: Protein tyrosine phosphatase and tensin homolog



4.2.5 Score per residue for model 5

- Molecule 1: Partitioning-defective 3 homolog

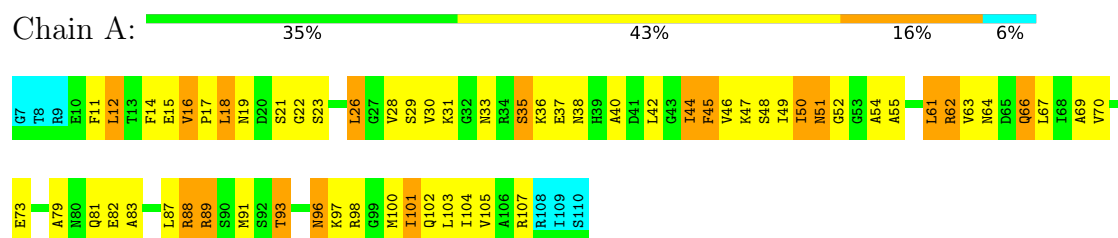


- Molecule 2: Protein tyrosine phosphatase and tensin homolog



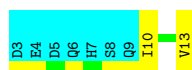
4.2.6 Score per residue for model 6

- Molecule 1: Partitioning-defective 3 homolog



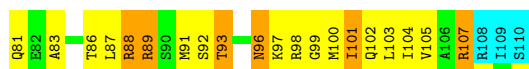
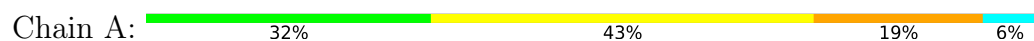
- Molecule 2: Protein tyrosine phosphatase and tensin homolog



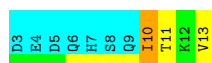


4.2.7 Score per residue for model 7

- Molecule 1: Partitioning-defective 3 homolog

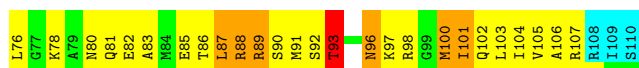
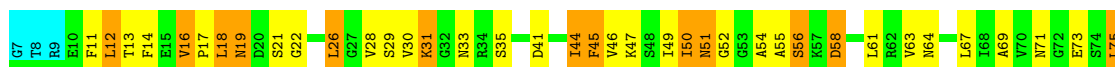


- Molecule 2: Protein tyrosine phosphatase and tensin homolog

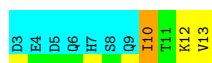


4.2.8 Score per residue for model 8

- Molecule 1: Partitioning-defective 3 homolog



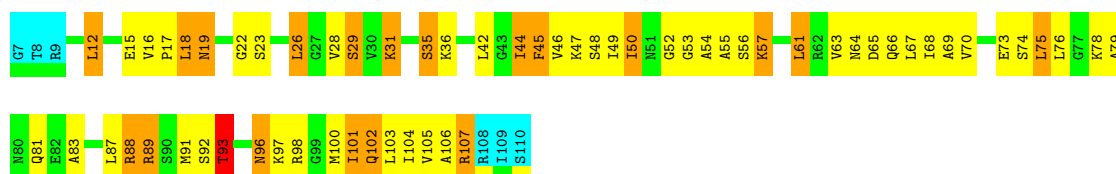
- Molecule 2: Protein tyrosine phosphatase and tensin homolog



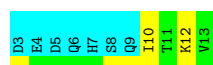
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Partitioning-defective 3 homolog





- Molecule 2: Protein tyrosine phosphatase and tensin homolog

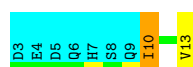


4.2.10 Score per residue for model 10

- Molecule 1: Partitioning-defective 3 homolog



- Molecule 2: Protein tyrosine phosphatase and tensin homolog



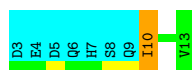
4.2.11 Score per residue for model 11

- Molecule 1: Partitioning-defective 3 homolog



- Molecule 2: Protein tyrosine phosphatase and tensin homolog

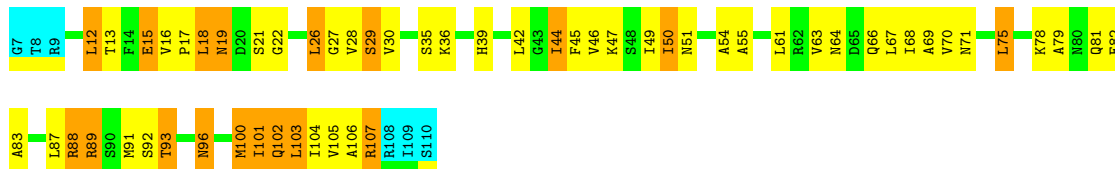




4.2.12 Score per residue for model 12

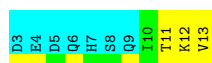
- Molecule 1: Partitioning-defective 3 homolog

Chain A: 39% 38% 17% 6%



- Molecule 2: Protein tyrosine phosphatase and tensin homolog

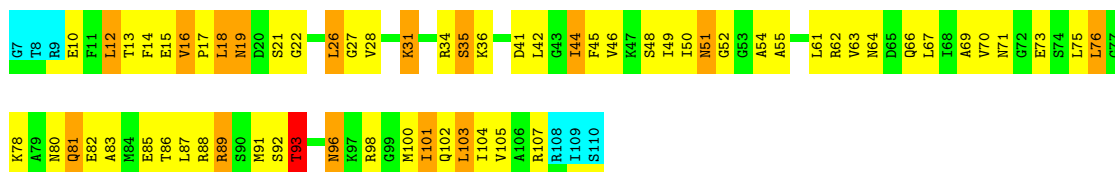
Chain B: 9% 27% 64%



4.2.13 Score per residue for model 13

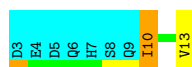
- Molecule 1: Partitioning-defective 3 homolog

Chain A: 33% 46% 14% 6%



- Molecule 2: Protein tyrosine phosphatase and tensin homolog

Chain B: 18% 9% 9% 64%



4.2.14 Score per residue for model 14

- Molecule 1: Partitioning-defective 3 homolog

Chain A: 30% 47% 17% 6%

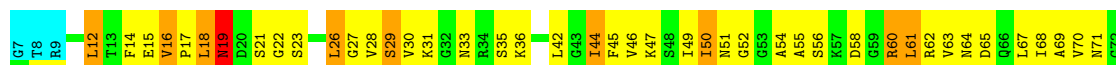


- Molecule 2: Protein tyrosine phosphatase and tensin homolog

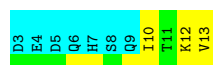


4.2.15 Score per residue for model 15

- Molecule 1: Partitioning-defective 3 homolog

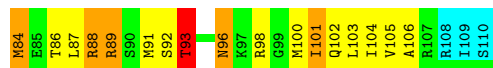
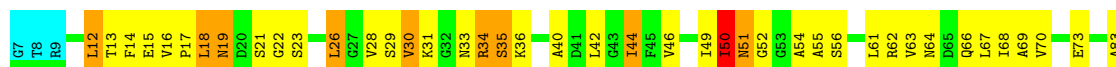


- Molecule 2: Protein tyrosine phosphatase and tensin homolog



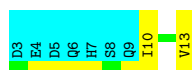
4.2.16 Score per residue for model 16

- Molecule 1: Partitioning-defective 3 homolog



- Molecule 2: Protein tyrosine phosphatase and tensin homolog





4.2.17 Score per residue for model 17

- Molecule 1: Partitioning-defective 3 homolog

Chain A: 34% 46% 14% 6%



- Molecule 2: Protein tyrosine phosphatase and tensin homolog

Chain B: 27% 9% 64%



4.2.18 Score per residue for model 18

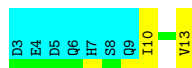
- Molecule 1: Partitioning-defective 3 homolog

Chain A: 40% 38% 16% 6%



- Molecule 2: Protein tyrosine phosphatase and tensin homolog

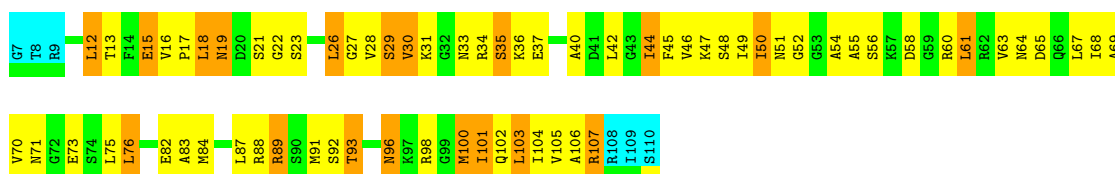
Chain B: 18% 18% 64%



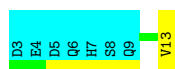
4.2.19 Score per residue for model 19

- Molecule 1: Partitioning-defective 3 homolog

Chain A: 29% 47% 18% 6%

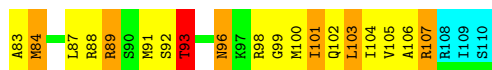


- Molecule 2: Protein tyrosine phosphatase and tensin homolog

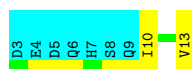


4.2.20 Score per residue for model 20

- Molecule 1: Partitioning-defective 3 homolog



- Molecule 2: Protein tyrosine phosphatase and tensin homolog



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 calculated structures, 20 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
CNS	structure solution	
CNS	refinement	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.29±0.00	0±0/736 (0.0± 0.0%)	0.68±0.02	1±0/985 (0.1± 0.0%)
2	B	0.37±0.02	0±0/31 (0.0± 0.0%)	0.71±0.04	0±0/39 (0.0± 0.0%)
All	All	0.30	0/15340 (0.0%)	0.68	12/20480 (0.1%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	16	VAL	N-CA-C	5.74	113.23	107.55	10	12

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	731	749	748	63±7
2	B	32	40	40	2±1
All	All	15260	15780	15760	1260

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 41.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:ILE:HD11	1:A:106:ALA:HB2	1.01	1.25	3	14
1:A:12:LEU:HD12	1:A:105:VAL:HG23	0.90	1.39	6	18
1:A:69:ALA:HB3	1:A:104:ILE:HD12	0.88	1.45	20	20
1:A:67:LEU:HD23	1:A:105:VAL:HG12	0.85	1.49	11	20
1:A:55:ALA:HB1	1:A:61:LEU:HD13	0.84	1.49	6	10
1:A:30:VAL:HG11	1:A:67:LEU:HD11	0.83	1.50	18	14
1:A:67:LEU:HD23	1:A:105:VAL:CG1	0.82	2.04	1	16
1:A:68:ILE:HD11	1:A:106:ALA:CB	0.82	2.03	10	12
1:A:33:ASN:ND2	1:A:42:LEU:HD12	0.81	1.90	15	3
1:A:18:LEU:HD22	1:A:26:LEU:CD1	0.79	2.07	14	20
1:A:26:LEU:HD22	1:A:91:MET:HE2	0.79	1.53	7	19
1:A:16:VAL:HG23	1:A:103:LEU:HD23	0.78	1.53	6	9
1:A:87:LEU:HD12	1:A:88:ARG:N	0.77	1.94	10	16
1:A:12:LEU:HD13	1:A:62:ARG:NH2	0.76	1.95	2	2
1:A:18:LEU:HD22	1:A:26:LEU:HD13	0.76	1.57	20	20
1:A:44:ILE:HG13	1:A:67:LEU:HD12	0.75	1.58	12	19
1:A:35:SER:HA	1:A:42:LEU:HD21	0.74	1.59	17	8
1:A:13:THR:HG23	1:A:102:GLN:OE1	0.74	1.83	7	8
1:A:35:SER:OG	1:A:42:LEU:HD21	0.74	1.83	18	2
1:A:16:VAL:HG13	1:A:58:ASP:OD1	0.73	1.81	14	2
1:A:12:LEU:HD22	1:A:62:ARG:NH2	0.73	1.99	4	1
1:A:101:ILE:HD11	1:A:103:LEU:HD11	0.73	1.61	4	9
1:A:12:LEU:CD1	1:A:105:VAL:HG23	0.71	2.16	6	4
1:A:12:LEU:HD11	1:A:107:ARG:HD2	0.71	1.62	3	2
1:A:44:ILE:CG1	1:A:67:LEU:HD12	0.70	2.16	4	12
1:A:79:ALA:HB3	1:A:81:GLN:OE1	0.70	1.86	10	1
1:A:17:PRO:O	1:A:54:ALA:HB1	0.70	1.85	10	19
1:A:67:LEU:HA	1:A:105:VAL:HG12	0.70	1.64	4	5
1:A:70:VAL:HG22	1:A:71:ASN:ND2	0.69	2.02	13	8
1:A:69:ALA:CB	1:A:104:ILE:HD12	0.69	2.18	11	15
1:A:35:SER:CA	1:A:42:LEU:HD21	0.69	2.18	7	8
1:A:18:LEU:HD11	1:A:96:ASN:HB2	0.68	1.64	16	17
1:A:28:VAL:HG12	1:A:49:ILE:HG23	0.68	1.66	10	19
1:A:16:VAL:HG21	1:A:61:LEU:HD11	0.68	1.65	20	11
1:A:16:VAL:CG2	1:A:61:LEU:HD11	0.67	2.19	3	10
1:A:87:LEU:HD11	2:B:13:VAL:HG11	0.67	1.64	6	4
1:A:46:VAL:O	1:A:63:VAL:HG13	0.67	1.90	6	20
1:A:68:ILE:CD1	1:A:106:ALA:HB2	0.65	2.15	3	5
1:A:69:ALA:HB3	1:A:104:ILE:CD1	0.64	2.23	19	8
1:A:28:VAL:HG13	1:A:55:ALA:HB3	0.64	1.70	10	10
1:A:70:VAL:HG22	1:A:71:ASN:HD22	0.64	1.53	19	10
1:A:88:ARG:CG	2:B:13:VAL:HG11	0.64	2.23	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:HD22	1:A:91:MET:CE	0.63	2.23	11	18
1:A:68:ILE:C	1:A:75:LEU:HD12	0.63	2.18	7	1
1:A:55:ALA:CB	1:A:61:LEU:HD13	0.63	2.22	6	13
1:A:18:LEU:HD12	1:A:22:GLY:HA2	0.63	1.71	19	20
1:A:67:LEU:HD13	1:A:87:LEU:HD22	0.62	1.70	11	8
1:A:89:ARG:O	1:A:93:THR:HB	0.62	1.94	12	17
1:A:49:ILE:HD13	1:A:61:LEU:HB3	0.62	1.69	6	14
1:A:21:SER:HB3	1:A:54:ALA:HB2	0.62	1.69	16	13
1:A:21:SER:CB	1:A:54:ALA:HB2	0.61	2.26	3	11
1:A:55:ALA:HB1	1:A:61:LEU:HD22	0.61	1.73	18	8
1:A:28:VAL:HG11	1:A:61:LEU:HD22	0.61	1.73	7	8
1:A:12:LEU:HD12	1:A:105:VAL:CG2	0.60	2.23	6	4
1:A:68:ILE:HG23	1:A:76:LEU:HD12	0.60	1.72	19	1
2:B:11:THR:HG22	2:B:13:VAL:HG13	0.60	1.73	12	3
1:A:70:VAL:HG23	1:A:103:LEU:CD1	0.59	2.27	16	4
1:A:44:ILE:HG21	1:A:84:MET:HB3	0.59	1.73	11	2
1:A:88:ARG:HG3	2:B:13:VAL:HG12	0.59	1.74	4	5
1:A:12:LEU:HD11	1:A:107:ARG:HG3	0.59	1.73	2	10
1:A:63:VAL:O	1:A:64:ASN:HB2	0.59	1.96	15	3
1:A:12:LEU:HD13	1:A:14:PHE:CZ	0.59	2.32	17	1
1:A:35:SER:HB2	1:A:40:ALA:HB3	0.59	1.73	16	2
1:A:55:ALA:HA	1:A:61:LEU:HD13	0.58	1.73	20	7
1:A:26:LEU:HB2	1:A:91:MET:HE2	0.58	1.75	8	4
1:A:75:LEU:HD22	1:A:83:ALA:HB1	0.58	1.73	7	5
1:A:88:ARG:HG3	2:B:13:VAL:HG11	0.58	1.75	10	5
1:A:70:VAL:HG11	1:A:87:LEU:HA	0.57	1.75	1	13
1:A:55:ALA:HB1	1:A:61:LEU:CD1	0.57	2.26	6	1
1:A:12:LEU:HD11	1:A:107:ARG:CG	0.57	2.29	18	10
1:A:67:LEU:HD13	1:A:87:LEU:HD13	0.57	1.76	3	2
1:A:69:ALA:HB3	1:A:104:ILE:HB	0.57	1.75	6	4
1:A:67:LEU:HD13	1:A:87:LEU:CD1	0.57	2.30	3	2
1:A:102:GLN:C	1:A:103:LEU:HD22	0.57	2.23	9	7
1:A:12:LEU:HD13	1:A:62:ARG:HH22	0.56	1.59	3	1
1:A:16:VAL:CG2	1:A:103:LEU:HD23	0.56	2.29	6	6
1:A:26:LEU:HD21	1:A:103:LEU:HD11	0.56	1.76	10	1
1:A:30:VAL:HG23	1:A:84:MET:SD	0.56	2.40	10	1
1:A:18:LEU:HB3	1:A:26:LEU:HD12	0.56	1.77	5	19
1:A:55:ALA:CA	1:A:61:LEU:HD13	0.56	2.30	20	13
1:A:28:VAL:HG13	1:A:55:ALA:CB	0.56	2.30	10	11
1:A:68:ILE:O	1:A:75:LEU:HD12	0.56	2.01	11	1
1:A:44:ILE:CG2	1:A:84:MET:HE2	0.56	2.31	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:LEU:HD22	1:A:103:LEU:N	0.56	2.15	15	5
1:A:44:ILE:HG12	1:A:67:LEU:HD12	0.56	1.78	4	1
1:A:73:GLU:OE1	1:A:86:THR:HG23	0.56	1.99	8	1
1:A:28:VAL:N	1:A:50:ILE:HD12	0.56	2.16	8	16
1:A:49:ILE:HG22	1:A:56:SER:OG	0.55	2.01	3	3
1:A:46:VAL:HG23	1:A:65:ASP:O	0.54	2.03	2	1
1:A:102:GLN:O	1:A:103:LEU:HD13	0.54	2.03	4	7
1:A:29:SER:O	1:A:47:LYS:N	0.53	2.42	2	10
1:A:70:VAL:HG23	1:A:103:LEU:HD13	0.53	1.80	16	2
1:A:65:ASP:OD2	1:A:105:VAL:HG21	0.53	2.03	2	3
1:A:87:LEU:HD12	1:A:87:LEU:C	0.53	2.28	14	14
1:A:44:ILE:CD1	1:A:83:ALA:HB3	0.53	2.33	11	19
1:A:28:VAL:CG1	1:A:49:ILE:HG23	0.53	2.34	10	3
1:A:67:LEU:HD13	1:A:87:LEU:CD2	0.53	2.34	1	7
1:A:101:ILE:HG12	1:A:103:LEU:HD21	0.52	1.81	9	4
2:B:13:VAL:O	2:B:13:VAL:HG23	0.52	2.04	14	4
1:A:11:PHE:CD1	1:A:106:ALA:HB2	0.51	2.41	8	1
1:A:35:SER:HB2	1:A:42:LEU:HD21	0.51	1.83	15	1
1:A:16:VAL:HG12	1:A:54:ALA:HB1	0.51	1.82	5	2
1:A:75:LEU:HD21	1:A:87:LEU:CD2	0.51	2.36	3	2
1:A:75:LEU:HB3	1:A:83:ALA:HB1	0.51	1.83	19	3
1:A:38:ASN:OD1	1:A:40:ALA:HB2	0.50	2.05	20	2
1:A:63:VAL:O	1:A:64:ASN:HB3	0.50	2.07	18	1
1:A:31:LYS:HB2	2:B:10:ILE:HD13	0.50	1.82	11	1
1:A:44:ILE:HD12	1:A:83:ALA:HB3	0.50	1.82	19	18
1:A:33:ASN:HD21	1:A:42:LEU:HD12	0.50	1.67	19	1
1:A:41:ASP:OD2	1:A:79:ALA:HB1	0.50	2.06	17	2
1:A:32:GLY:HA2	1:A:43:GLY:O	0.49	2.07	7	3
1:A:26:LEU:O	1:A:54:ALA:N	0.49	2.45	2	20
1:A:18:LEU:HD21	1:A:101:ILE:HG22	0.49	1.83	12	17
1:A:63:VAL:O	1:A:64:ASN:CB	0.49	2.61	18	17
1:A:16:VAL:CG2	1:A:103:LEU:HD13	0.48	2.39	10	1
1:A:70:VAL:HG23	1:A:101:ILE:HD11	0.48	1.85	10	2
1:A:31:LYS:HB3	2:B:10:ILE:HD13	0.48	1.85	14	5
1:A:70:VAL:HG23	1:A:101:ILE:CD1	0.48	2.38	10	1
1:A:35:SER:CB	1:A:42:LEU:HD21	0.48	2.38	13	3
1:A:12:LEU:HD12	1:A:105:VAL:O	0.47	2.09	4	1
1:A:49:ILE:CD1	1:A:61:LEU:HB3	0.47	2.38	20	9
1:A:34:ARG:O	1:A:35:SER:C	0.47	2.57	19	1
1:A:31:LYS:CB	2:B:10:ILE:HD13	0.47	2.39	7	5
1:A:35:SER:N	1:A:42:LEU:HD21	0.47	2.24	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LEU:HD22	1:A:83:ALA:HA	0.47	1.87	14	1
1:A:45:PHE:CD1	1:A:45:PHE:N	0.47	2.82	14	7
1:A:96:ASN:O	1:A:97:LYS:C	0.47	2.58	2	2
1:A:30:VAL:CG1	1:A:67:LEU:HD11	0.47	2.31	18	2
1:A:34:ARG:CD	1:A:35:SER:O	0.47	2.63	16	1
1:A:100:MET:HE3	1:A:100:MET:C	0.47	2.35	8	1
1:A:14:PHE:O	1:A:103:LEU:N	0.46	2.47	20	2
1:A:70:VAL:O	1:A:70:VAL:HG13	0.46	2.10	15	5
1:A:93:THR:O	1:A:97:LYS:HD3	0.46	2.10	7	4
1:A:16:VAL:HG21	1:A:103:LEU:HD13	0.46	1.86	10	1
1:A:46:VAL:HG11	1:A:49:ILE:CG1	0.46	2.40	10	2
1:A:45:PHE:CE2	1:A:66:GLN:NE2	0.46	2.83	18	4
1:A:17:PRO:HA	1:A:99:GLY:O	0.46	2.10	14	4
1:A:86:THR:O	1:A:89:ARG:HD3	0.46	2.10	14	2
1:A:44:ILE:HG21	1:A:84:MET:HE2	0.46	1.85	18	1
1:A:28:VAL:HG23	2:B:13:VAL:HG22	0.46	1.88	6	1
1:A:50:ILE:O	1:A:52:GLY:N	0.46	2.48	20	17
1:A:14:PHE:N	1:A:103:LEU:O	0.46	2.49	11	3
1:A:68:ILE:HD12	1:A:105:VAL:HA	0.46	1.86	5	1
1:A:33:ASN:OD1	1:A:33:ASN:N	0.46	2.48	6	1
1:A:79:ALA:HB3	1:A:81:GLN:HE21	0.46	1.70	6	3
1:A:33:ASN:ND2	1:A:45:PHE:CE1	0.45	2.84	7	3
1:A:16:VAL:HG22	1:A:61:LEU:HD11	0.45	1.84	3	2
1:A:90:SER:O	1:A:95:GLY:N	0.45	2.49	17	1
1:A:44:ILE:CD1	1:A:83:ALA:CB	0.45	2.95	12	16
1:A:18:LEU:CD2	1:A:101:ILE:CG2	0.45	2.94	18	17
1:A:12:LEU:HD11	1:A:107:ARG:CD	0.45	2.37	3	1
1:A:89:ARG:O	1:A:93:THR:HG22	0.45	2.11	17	2
1:A:29:SER:O	1:A:47:LYS:CB	0.45	2.65	2	1
1:A:12:LEU:HD13	1:A:62:ARG:HH21	0.45	1.72	6	1
1:A:91:MET:CB	1:A:101:ILE:HD13	0.45	2.41	7	3
1:A:14:PHE:CD2	1:A:61:LEU:CD2	0.45	3.00	10	1
1:A:26:LEU:CD2	1:A:91:MET:HE2	0.45	2.34	7	2
1:A:12:LEU:HD22	1:A:62:ARG:HH21	0.45	1.72	14	1
1:A:55:ALA:CB	1:A:61:LEU:HD22	0.45	2.42	18	1
1:A:16:VAL:HG11	1:A:26:LEU:HG	0.45	1.89	2	1
1:A:45:PHE:CE1	1:A:66:GLN:NE2	0.44	2.85	1	1
1:A:11:PHE:HE2	1:A:68:ILE:HG21	0.44	1.73	7	1
1:A:63:VAL:O	1:A:64:ASN:ND2	0.44	2.49	18	1
1:A:28:VAL:CG1	1:A:55:ALA:CB	0.44	2.95	5	12
1:A:16:VAL:CG2	1:A:103:LEU:CD1	0.44	2.96	12	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:GLY:O	1:A:50:ILE:N	0.44	2.50	2	6
1:A:94:GLU:HA	1:A:97:LYS:CG	0.44	2.43	2	1
1:A:13:THR:O	1:A:14:PHE:CD1	0.44	2.71	10	6
1:A:41:ASP:CB	1:A:80:ASN:ND2	0.44	2.81	8	4
1:A:68:ILE:HD11	1:A:106:ALA:HB3	0.43	1.90	4	1
1:A:69:ALA:HB3	1:A:104:ILE:HD13	0.43	1.89	19	1
1:A:70:VAL:HG11	1:A:87:LEU:CA	0.43	2.43	1	1
1:A:96:ASN:O	1:A:96:ASN:ND2	0.43	2.51	7	17
1:A:14:PHE:O	1:A:102:GLN:HA	0.43	2.13	6	2
1:A:44:ILE:HG21	1:A:84:MET:SD	0.43	2.53	10	2
1:A:33:ASN:OD1	1:A:42:LEU:HB2	0.43	2.14	19	1
1:A:18:LEU:O	1:A:19:ASN:C	0.43	2.61	14	15
1:A:71:ASN:ND2	1:A:90:SER:O	0.43	2.52	8	2
1:A:93:THR:O	1:A:97:LYS:CG	0.43	2.67	15	3
1:A:79:ALA:HB3	1:A:81:GLN:NE2	0.43	2.29	12	1
1:A:81:GLN:NE2	1:A:82:GLU:CG	0.43	2.81	13	1
1:A:89:ARG:HD3	1:A:90:SER:N	0.43	2.28	17	1
1:A:75:LEU:CD2	1:A:87:LEU:CD2	0.43	2.97	3	2
1:A:75:LEU:HD22	1:A:83:ALA:CA	0.43	2.43	14	1
1:A:95:GLY:HA3	1:A:101:ILE:HB	0.43	1.91	5	1
1:A:47:LYS:HD3	2:B:10:ILE:HD12	0.43	1.91	14	1
1:A:31:LYS:O	1:A:31:LYS:HG3	0.43	2.14	17	1
1:A:70:VAL:O	1:A:73:GLU:CG	0.43	2.67	18	2
1:A:67:LEU:CD1	1:A:87:LEU:HD22	0.43	2.44	20	1
1:A:27:GLY:C	1:A:50:ILE:HD12	0.42	2.39	7	4
1:A:40:ALA:O	1:A:42:LEU:HD23	0.42	2.13	19	1
1:A:46:VAL:O	1:A:63:VAL:CG1	0.42	2.66	15	3
1:A:75:LEU:HD13	1:A:83:ALA:HB1	0.42	1.90	4	1
1:A:79:ALA:HB1	1:A:81:GLN:OE1	0.42	2.14	9	1
1:A:17:PRO:O	1:A:54:ALA:CB	0.42	2.68	11	3
1:A:80:ASN:OD1	1:A:81:GLN:N	0.42	2.52	2	7
1:A:88:ARG:O	1:A:91:MET:HG2	0.42	2.15	15	2
1:A:70:VAL:CG2	1:A:101:ILE:CD1	0.42	2.98	10	2
1:A:18:LEU:HD12	1:A:22:GLY:CA	0.42	2.44	14	1
1:A:16:VAL:HG23	1:A:103:LEU:HD12	0.42	1.92	3	2
1:A:18:LEU:O	1:A:22:GLY:N	0.42	2.52	1	3
1:A:44:ILE:N	1:A:44:ILE:HD13	0.42	2.29	11	2
1:A:93:THR:HG23	1:A:94:GLU:HG2	0.41	1.92	17	2
1:A:81:GLN:HA	1:A:84:MET:HE3	0.41	1.92	20	1
1:A:50:ILE:O	1:A:56:SER:CB	0.41	2.68	14	1
1:A:95:GLY:O	1:A:100:MET:N	0.41	2.53	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:PHE:CD1	1:A:11:PHE:N	0.41	2.88	6	1
1:A:62:ARG:N	1:A:62:ARG:HD2	0.41	2.30	7	1
1:A:12:LEU:HD21	1:A:107:ARG:HD2	0.41	1.90	17	1
1:A:65:ASP:CG	1:A:105:VAL:HG21	0.41	2.41	19	1
1:A:11:PHE:CE2	1:A:68:ILE:HD13	0.41	2.50	1	2
1:A:66:GLN:O	1:A:105:VAL:HA	0.41	2.15	2	1
1:A:84:MET:HA	1:A:87:LEU:HD21	0.41	1.91	20	2
1:A:79:ALA:HB3	1:A:81:GLN:HE22	0.41	1.76	12	1
1:A:101:ILE:CD1	1:A:103:LEU:HD11	0.41	2.39	15	1
1:A:35:SER:CB	1:A:40:ALA:HB3	0.41	2.45	16	1
1:A:93:THR:O	1:A:97:LYS:HG3	0.41	2.16	1	1
1:A:12:LEU:N	1:A:105:VAL:O	0.41	2.53	15	2
1:A:18:LEU:C	1:A:20:ASP:N	0.41	2.79	2	1
1:A:27:GLY:O	1:A:28:VAL:CG1	0.41	2.68	2	4
1:A:17:PRO:CD	1:A:58:ASP:OD1	0.41	2.69	8	1
1:A:53:GLY:O	1:A:57:LYS:CG	0.41	2.68	9	1
1:A:87:LEU:O	1:A:91:MET:CG	0.41	2.68	20	1
1:A:26:LEU:CD2	1:A:91:MET:CE	0.41	2.98	20	2
1:A:43:GLY:O	1:A:45:PHE:CE1	0.41	2.73	14	1
1:A:58:ASP:OD1	1:A:60:ARG:NH2	0.41	2.54	15	2
1:A:28:VAL:CG2	2:B:13:VAL:CG2	0.41	2.98	6	1
1:A:15:GLU:HB3	1:A:100:MET:SD	0.41	2.56	12	3
1:A:67:LEU:CD1	1:A:87:LEU:CD2	0.41	2.99	1	2
1:A:75:LEU:HB3	1:A:83:ALA:CB	0.41	2.46	2	1
1:A:96:ASN:ND2	1:A:96:ASN:C	0.41	2.78	15	2
1:A:10:GLU:HG3	1:A:12:LEU:HD21	0.41	1.91	11	1
1:A:49:ILE:CD1	1:A:61:LEU:C	0.41	2.93	15	1
1:A:33:ASN:OD1	1:A:45:PHE:CE1	0.41	2.74	8	1
1:A:14:PHE:CZ	1:A:60:ARG:O	0.41	2.73	10	1
1:A:103:LEU:N	1:A:103:LEU:CD2	0.41	2.84	15	1
1:A:49:ILE:HD13	1:A:61:LEU:CB	0.41	2.46	18	1
1:A:26:LEU:O	1:A:55:ALA:N	0.41	2.52	20	1
1:A:89:ARG:O	1:A:93:THR:CG2	0.40	2.69	6	1
1:A:12:LEU:HD13	1:A:14:PHE:CE2	0.40	2.51	17	1
1:A:27:GLY:C	1:A:28:VAL:HG13	0.40	2.41	12	1
1:A:66:GLN:NE2	1:A:67:LEU:O	0.40	2.55	12	1
1:A:45:PHE:CE2	1:A:66:GLN:CD	0.40	2.99	17	1
1:A:58:ASP:CG	1:A:60:ARG:NE	0.40	2.80	10	1
1:A:28:VAL:CG1	1:A:55:ALA:HB3	0.40	2.46	4	1
1:A:84:MET:HA	1:A:87:LEU:CD2	0.40	2.47	11	1
1:A:44:ILE:HG21	1:A:84:MET:HG3	0.40	1.94	20	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	98/104 (94%)	82±2 (84±2%)	13±3 (13±3%)	3±1 (3±1%)	5	38
2	B	3/11 (27%)	3±0 (98±7%)	0±0 (2±7%)	0±0 (0±0%)	100	100
All	All	2020/2300 (88%)	1699 (84%)	262 (13%)	59 (3%)	5	39

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)
1	A	26	LEU	20
1	A	51	ASN	13
1	A	93	THR	8
1	A	76	LEU	5
1	A	50	ILE	4
1	A	46	VAL	3
1	A	64	ASN	2
1	A	19	ASN	2
1	A	39	HIS	1
1	A	35	SER	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	78/83 (94%)	49±3 (63±3%)	29±3 (37±3%)	1	8
2	B	4/11 (36%)	3±0 (71±12%)	1±0 (29±12%)	1	19
All	All	1640/1880 (87%)	1038 (63%)	602 (37%)	1	8

All 56 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	12	LEU	20
1	A	18	LEU	20
1	A	19	ASN	20
1	A	44	ILE	20
1	A	89	ARG	20
1	A	100	MET	20
1	A	101	ILE	20
1	A	93	THR	19
1	A	96	ASN	19
1	A	98	ARG	19
1	A	107	ARG	19
1	A	31	LYS	18
1	A	29	SER	17
1	A	36	LYS	17
1	A	92	SER	17
1	A	45	PHE	17
1	A	15	GLU	16
1	A	82	GLU	16
1	A	88	ARG	14
2	B	10	ILE	14
1	A	73	GLU	13
1	A	75	LEU	13
1	A	61	LEU	12
1	A	62	ARG	12
1	A	51	ASN	12
1	A	50	ILE	11
1	A	78	LYS	11
1	A	35	SER	11
1	A	66	GLN	10
1	A	85	GLU	10
1	A	103	LEU	10
1	A	34	ARG	9
2	B	12	LYS	9
1	A	86	THR	8
1	A	48	SER	8
1	A	102	GLN	8
1	A	23	SER	8
1	A	76	LEU	8
1	A	84	MET	7
1	A	58	ASP	6
1	A	37	GLU	6
1	A	30	VAL	5

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Mol	Chain	Res	Type	Models (Total)
1	A	56	SER	5
1	A	60	ARG	4
1	A	74	SER	4
1	A	65	ASP	4
1	A	81	GLN	3
1	A	47	LYS	2
1	A	10	GLU	2
1	A	87	LEU	2
1	A	57	LYS	2
1	A	38	ASN	1
1	A	21	SER	1
1	A	33	ASN	1
1	A	97	LYS	1
1	A	28	VAL	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

No chemical shift data were provided