



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 04:26 AM UTC

PDB ID : 2MHO / pdb_00002mho
BMRB ID : 19643
Title : Solution State Structure PSD-95 PDZ1 with 5HT2C Receptor peptide
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Deposited on : 2013-11-29

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

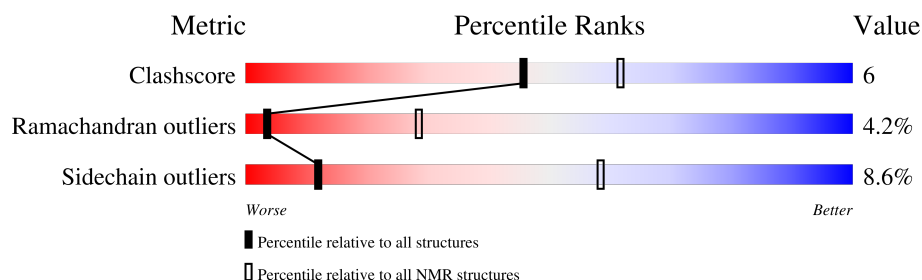
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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	99	
2	B	9	

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: *closest to the average*.

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:6-A:12, A:20-A:29, A:37-A:94, B:8-B:9 (77)	0.34	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 3 clusters and 5 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1630 atoms, of which 817 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Disks large homolog 4.

Mol	Chain	Residues	Atoms						Trace
1	A	99	Total	C	H	N	O	S	0
			1488	463	743	132	147	3	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P31016
A	2	ALA	-	expression tag	UNP P31016
A	3	MET	-	expression tag	UNP P31016

- Molecule 2 is a protein called peptide from 5-hydroxytryptamine receptor 2C.

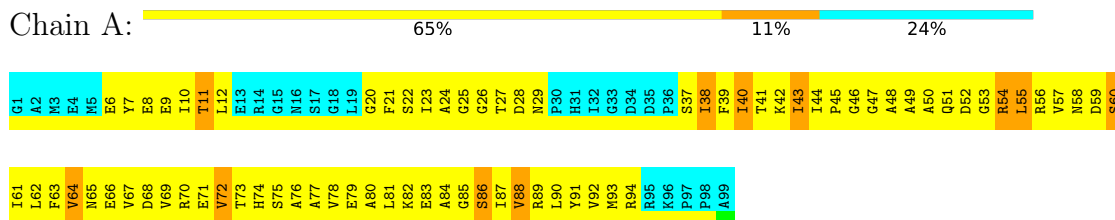
Mol	Chain	Residues	Atoms					Trace
2	B	9	Total	C	H	N	O	0
			142	41	74	12	15	

4 Residue-property plots [i](#)

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: Disks large homolog 4



- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

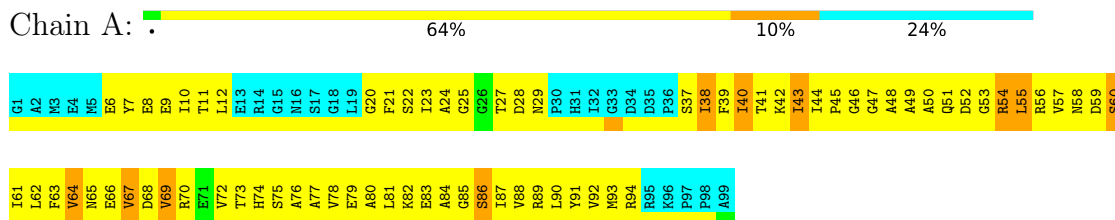


4.2 Scores per residue for each member of the ensemble

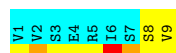
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Disks large homolog 4

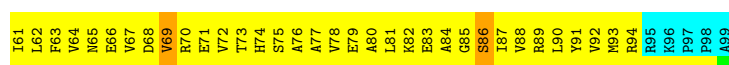
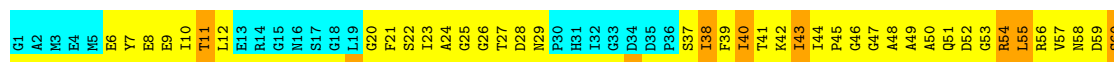
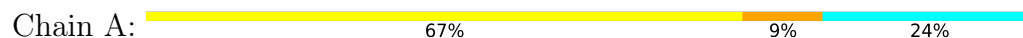


- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

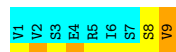


4.2.2 Score per residue for model 2

- Molecule 1: Disks large homolog 4

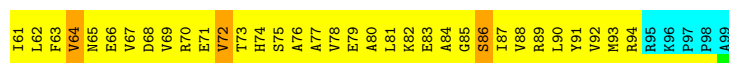
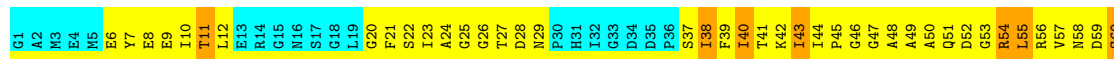


- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

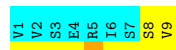


4.2.3 Score per residue for model 3

- Molecule 1: Disks large homolog 4



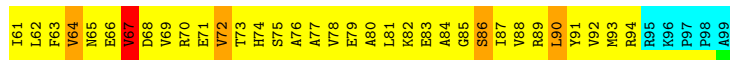
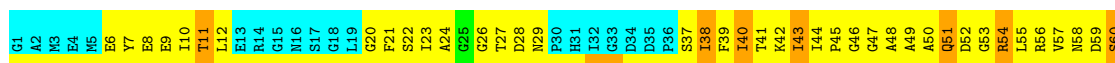
- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C



4.2.4 Score per residue for model 4

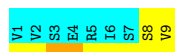
- Molecule 1: Disks large homolog 4





- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

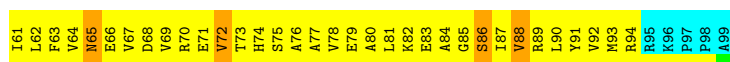
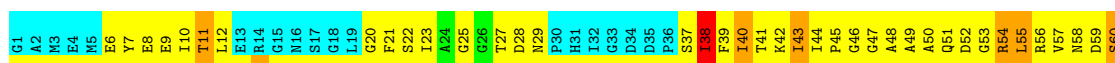
Chain B: 22% 78%



4.2.5 Score per residue for model 5

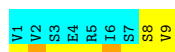
- Molecule 1: Disks large homolog 4

Chain A: 63% 10% 24%



- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

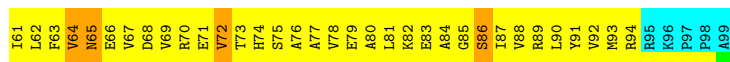
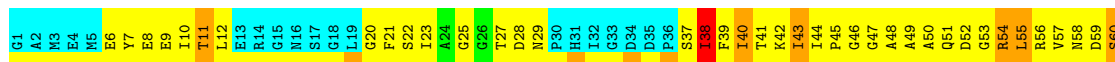
Chain B: 22% 78%



4.2.6 Score per residue for model 6

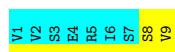
- Molecule 1: Disks large homolog 4

Chain A: 63% 10% 24%



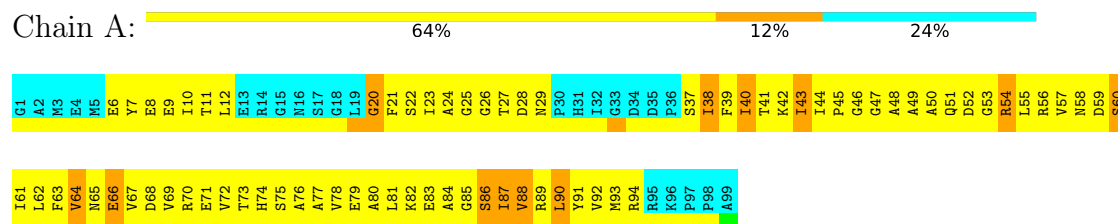
- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 22% 78%



4.2.7 Score per residue for model 7

- Molecule 1: Disks large homolog 4

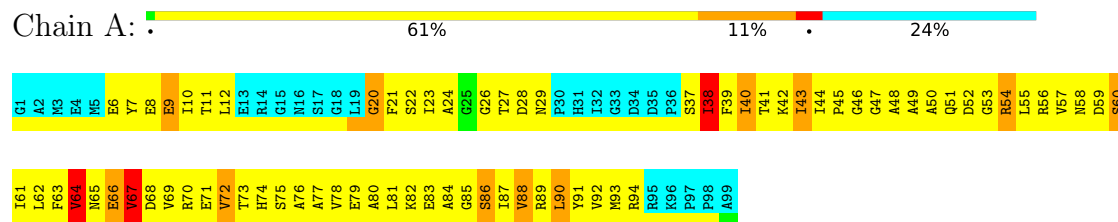


- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C



4.2.8 Score per residue for model 8

- Molecule 1: Disks large homolog 4

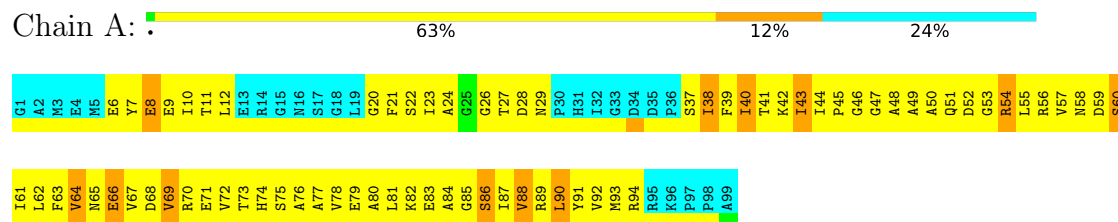


- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C



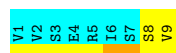
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Disks large homolog 4



- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

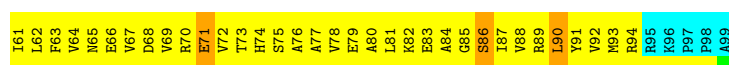
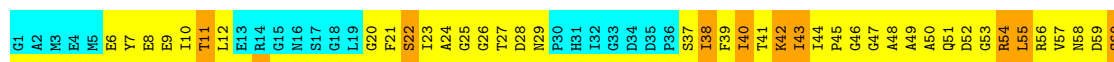
Chain B:  22% 78%



4.2.10 Score per residue for model 10

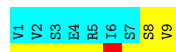
- Molecule 1: Disks large homolog 4

Chain A:  64% 12% 24%



- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

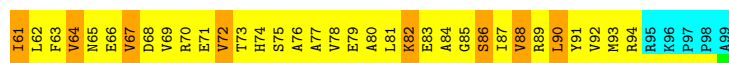
Chain B:  22% 78%



4.2.11 Score per residue for model 11

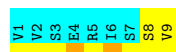
- Molecule 1: Disks large homolog 4

Chain A:  59% 16% 24%



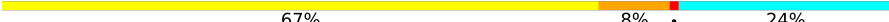
- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

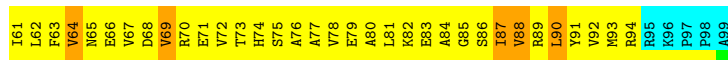
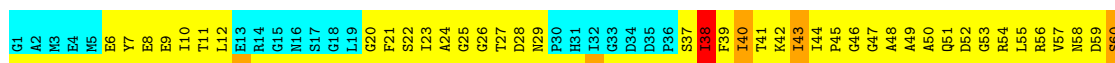
Chain B:  22% 78%



4.2.12 Score per residue for model 12

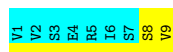
- Molecule 1: Disks large homolog 4

Chain A:  67% 8% 24%



- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

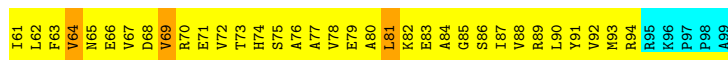
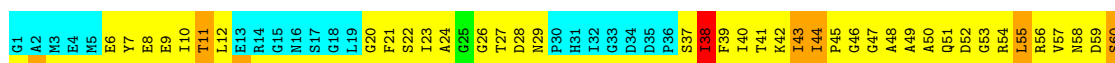
Chain B: 22% 78%



4.2.13 Score per residue for model 13

- Molecule 1: Disks large homolog 4

Chain A: 66% 8% 24%



- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

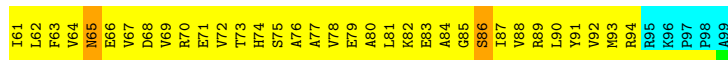
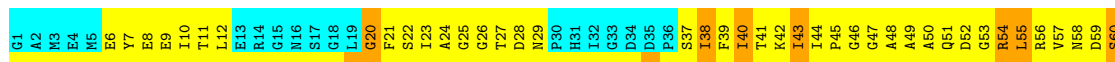
Chain B: 22% 78%



4.2.14 Score per residue for model 14

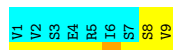
- Molecule 1: Disks large homolog 4

Chain A: 67% 9% 24%



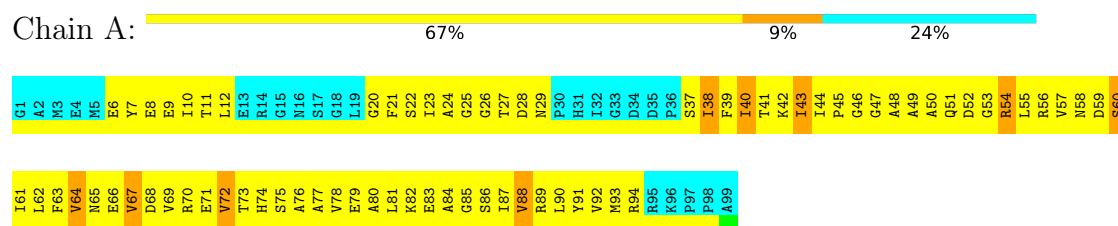
- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 22% 78%



4.2.15 Score per residue for model 15

- Molecule 1: Disks large homolog 4

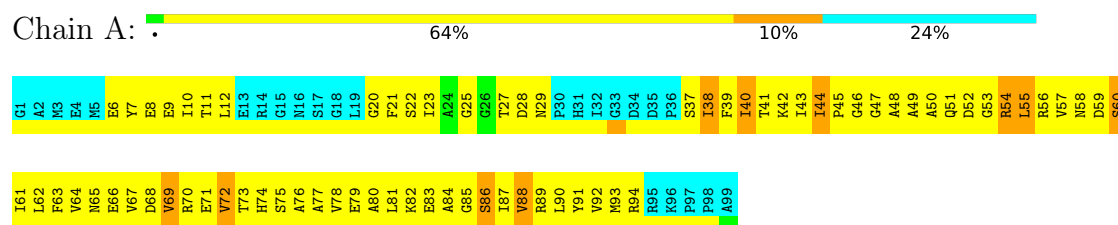


- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C



4.2.16 Score per residue for model 16

- Molecule 1: Disks large homolog 4

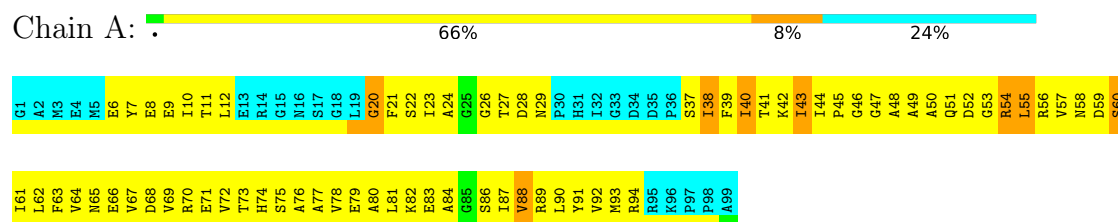


- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C



4.2.17 Score per residue for model 17

- Molecule 1: Disks large homolog 4

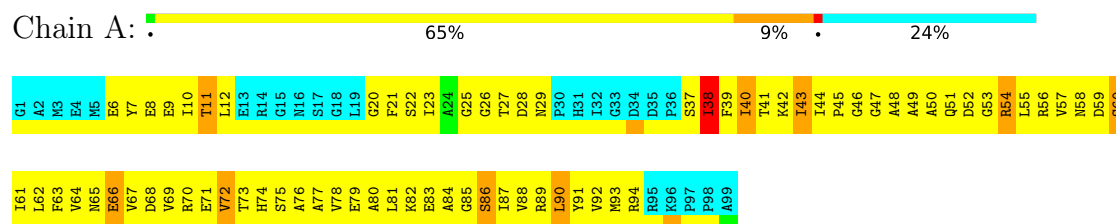


- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C



4.2.18 Score per residue for model 18

- Molecule 1: Disks large homolog 4

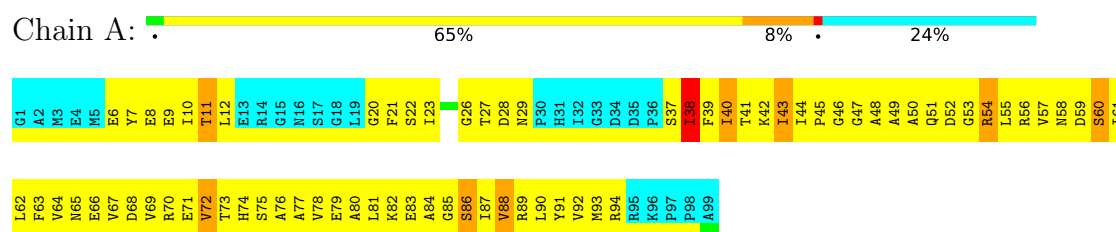


- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C



4.2.19 Score per residue for model 19

- Molecule 1: Disks large homolog 4



- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C



4.2.20 Score per residue for model 20

- Molecule 1: Disks large homolog 4





● Molecule 2: peptide from 5-hydroxytryptamine receptor 2C



5 Refinement protocol and experimental data overview

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

Of the 100 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	refinement	1.2
CNS	structure solution	1.2
CYANA	structure solution	2.1
CYANA	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	1051
Number of shifts mapped to atoms	1051
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

6 Model quality

6.1 Standard geometry

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	5.53±0.04	242±4/576 (42.0± 0.7%)	2.27±0.04	20±4/781 (2.5± 0.6%)
2	B	4.92±0.23	4±1/13 (34.6± 4.6%)	1.87±0.13	0±0/15 (0.0± 0.0%)
All	All	5.52	4927/11780 (41.8%)	2.26	395/15920 (2.5%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	44	ILE	CA-C	19.46	1.68	1.53	5	20
1	A	38	ILE	CA-CB	18.46	1.74	1.53	5	20
1	A	29	ASN	C-N	18.44	1.55	1.33	7	20
1	A	43	ILE	CA-CB	17.40	1.75	1.54	15	20
1	A	44	ILE	C-N	17.34	1.54	1.33	13	20
1	A	64	VAL	CA-CB	15.68	1.72	1.54	17	20
1	A	87	ILE	CA-CB	15.68	1.74	1.54	3	20
1	A	44	ILE	CA-CB	15.65	1.74	1.54	20	20
1	A	61	ILE	CA-CB	15.29	1.73	1.54	8	20
1	A	72	VAL	CA-CB	14.83	1.76	1.54	5	20
1	A	10	ILE	CA-CB	14.54	1.72	1.54	5	20
1	A	29	ASN	CA-C	14.14	1.68	1.52	9	20
1	A	88	VAL	CA-CB	13.99	1.71	1.54	3	20
1	A	57	VAL	N-CA	13.93	1.63	1.46	8	20
1	A	65	ASN	N-CA	13.54	1.62	1.46	4	20
1	A	40	ILE	CA-CB	13.50	1.71	1.54	11	20
1	A	78	VAL	CA-CB	13.22	1.71	1.54	12	20
1	A	54	ARG	N-CA	13.20	1.63	1.46	4	20
1	A	67	VAL	CA-CB	13.05	1.71	1.54	13	20
1	A	70	ARG	C-N	12.75	1.49	1.33	10	19
1	A	71	GLU	CA-CB	12.55	1.65	1.53	17	17
1	A	58	ASN	C-N	12.30	1.51	1.33	15	20
1	A	74	HIS	N-CA	12.17	1.60	1.46	16	20
1	A	78	VAL	N-CA	12.06	1.60	1.46	13	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	66	GLU	CA-C	11.76	1.67	1.52	15	20
1	A	65	ASN	CA-CB	11.57	1.69	1.53	11	20
1	A	79	GLU	N-CA	11.51	1.61	1.46	3	20
1	A	64	VAL	N-CA	11.50	1.59	1.46	19	20
1	A	84	ALA	N-CA	11.43	1.60	1.46	5	20
1	A	38	ILE	CA-C	11.33	1.66	1.52	12	20
1	A	59	ASP	C-N	11.12	1.49	1.33	5	20
2	B	8	SER	CA-C	11.01	1.64	1.53	15	20
1	A	41	THR	C-N	10.98	1.48	1.33	15	20
1	A	37	SER	C-N	10.97	1.46	1.33	3	20
1	A	60	SER	N-CA	10.95	1.60	1.46	1	20
1	A	70	ARG	N-CA	10.89	1.60	1.46	8	20
1	A	66	GLU	CA-CB	10.89	1.68	1.53	1	19
1	A	10	ILE	CA-C	10.73	1.65	1.52	2	20
1	A	92	VAL	CA-C	10.71	1.66	1.52	5	20
1	A	83	GLU	N-CA	10.60	1.60	1.46	10	19
1	A	70	ARG	CA-C	10.59	1.67	1.52	13	20
1	A	74	HIS	CA-C	10.54	1.66	1.52	1	20
1	A	90	LEU	CA-CB	10.43	1.68	1.53	7	20
1	A	66	GLU	N-CA	10.37	1.59	1.46	4	20
1	A	23	ILE	N-CA	10.34	1.58	1.46	8	20
1	A	78	VAL	CA-C	10.17	1.66	1.52	15	20
1	A	88	VAL	CA-C	10.15	1.64	1.52	2	20
1	A	20	GLY	C-N	10.14	1.46	1.33	11	20
1	A	92	VAL	CA-CB	10.13	1.70	1.54	16	20
1	A	93	MET	N-CA	10.05	1.58	1.46	5	20
1	A	69	VAL	CA-CB	10.04	1.66	1.54	12	20
1	A	58	ASN	CA-C	10.01	1.66	1.52	15	20
1	A	41	THR	CA-CB	9.95	1.70	1.53	4	20
1	A	75	SER	C-N	9.87	1.48	1.33	8	20
1	A	57	VAL	CA-C	9.87	1.66	1.52	7	20
1	A	21	PHE	CA-CB	9.86	1.68	1.53	16	20
1	A	82	LYS	C-N	9.85	1.47	1.33	12	20
1	A	93	MET	CA-CB	9.80	1.68	1.53	14	20
1	A	68	ASP	CA-CB	9.69	1.65	1.52	8	20
1	A	77	ALA	C-N	9.69	1.46	1.33	2	20
1	A	66	GLU	C-N	9.68	1.46	1.33	3	17
1	A	23	ILE	CA-CB	9.64	1.65	1.54	11	20
1	A	21	PHE	CA-C	9.64	1.64	1.52	11	20
1	A	65	ASN	CA-C	9.63	1.67	1.52	11	20
1	A	69	VAL	CA-C	9.55	1.64	1.53	12	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	50	ALA	C-N	9.51	1.45	1.33	7	20
1	A	61	ILE	CA-C	9.50	1.63	1.52	8	20
1	A	86	SER	C-N	9.49	1.45	1.33	17	20
1	A	89	ARG	CA-CB	9.46	1.66	1.53	15	20
1	A	52	ASP	C-N	9.42	1.47	1.33	20	20
1	A	62	LEU	C-N	9.42	1.45	1.33	11	20
2	B	8	SER	C-N	9.40	1.46	1.33	19	20
1	A	22	SER	C-N	9.39	1.45	1.33	4	20
1	A	73	THR	N-CA	9.37	1.58	1.45	4	20
1	A	76	ALA	C-N	9.34	1.47	1.33	8	20
1	A	73	THR	C-N	9.32	1.45	1.33	4	20
1	A	83	GLU	C-N	9.32	1.46	1.33	15	20
1	A	80	ALA	C-N	9.31	1.46	1.33	19	20
1	A	54	ARG	C-N	9.30	1.46	1.33	20	20
1	A	72	VAL	N-CA	9.27	1.57	1.46	8	20
1	A	86	SER	N-CA	9.24	1.58	1.46	10	19
1	A	72	VAL	CA-C	9.20	1.62	1.52	12	20
2	B	8	SER	N-CA	9.15	1.56	1.46	10	20
1	A	9	GLU	CA-CB	9.13	1.65	1.53	8	20
1	A	70	ARG	NE-CZ	9.11	1.43	1.33	1	20
1	A	56	ARG	NE-CZ	9.08	1.43	1.33	4	20
1	A	89	ARG	NE-CZ	9.08	1.43	1.33	5	20
1	A	74	HIS	C-N	9.04	1.46	1.34	10	20
1	A	11	THR	CA-CB	9.03	1.67	1.53	15	18
1	A	37	SER	N-CA	9.02	1.57	1.46	19	20
1	A	41	THR	N-CA	9.02	1.56	1.46	18	20
1	A	94	ARG	NE-CZ	9.02	1.43	1.33	1	20
1	A	46	GLY	C-N	9.00	1.44	1.33	4	20
1	A	75	SER	N-CA	8.99	1.57	1.46	4	20
1	A	92	VAL	N-CA	8.97	1.57	1.46	5	20
1	A	54	ARG	NE-CZ	8.97	1.43	1.33	4	20
1	A	42	LYS	CA-CB	8.84	1.66	1.53	16	18
1	A	7	TYR	N-CA	8.82	1.56	1.45	13	20
1	A	61	ILE	N-CA	8.81	1.56	1.46	7	20
1	A	49	ALA	C-N	8.80	1.45	1.33	20	20
1	A	6	GLU	CA-CB	8.79	1.65	1.53	12	20
1	A	10	ILE	N-CA	8.76	1.56	1.46	6	20
1	A	23	ILE	C-N	8.72	1.45	1.33	11	20
1	A	38	ILE	CB-CG1	8.64	1.70	1.53	7	20
1	A	65	ASN	C-N	8.62	1.46	1.33	15	16
1	A	89	ARG	N-CA	8.61	1.56	1.46	3	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	27	THR	N-CA	8.60	1.57	1.46	12	20
1	A	94	ARG	CA-C	8.60	1.63	1.52	19	17
1	A	94	ARG	CA-CB	8.58	1.66	1.53	14	11
1	A	51	GLN	C-N	8.53	1.46	1.33	18	20
1	A	23	ILE	CB-CG1	8.52	1.70	1.53	11	11
1	A	47	GLY	N-CA	8.51	1.53	1.44	5	20
1	A	53	GLY	C-N	8.49	1.45	1.33	4	20
1	A	41	THR	CA-C	8.46	1.62	1.52	17	6
1	A	59	ASP	N-CA	8.44	1.57	1.46	12	20
1	A	6	GLU	N-CA	8.44	1.56	1.46	14	20
1	A	64	VAL	C-N	8.43	1.44	1.33	19	20
1	A	94	ARG	N-CA	8.42	1.56	1.46	14	20
1	A	21	PHE	C-N	8.41	1.45	1.33	7	20
1	A	11	THR	CA-C	8.38	1.62	1.52	3	13
1	A	56	ARG	CA-CB	8.38	1.67	1.53	15	13
1	A	40	ILE	CA-C	8.37	1.62	1.52	13	20
1	A	44	ILE	N-CA	8.37	1.55	1.46	5	20
1	A	84	ALA	CA-C	8.29	1.64	1.52	1	20
1	A	71	GLU	CA-C	8.26	1.63	1.53	6	16
1	A	7	TYR	C-N	8.26	1.45	1.33	13	20
1	A	83	GLU	CA-C	8.25	1.64	1.52	15	3
1	A	79	GLU	C-N	8.24	1.45	1.34	7	19
1	A	80	ALA	CA-C	8.23	1.64	1.52	14	20
1	A	40	ILE	N-CA	8.21	1.56	1.46	5	20
1	A	27	THR	C-N	8.18	1.45	1.33	2	20
1	A	37	SER	CA-C	8.16	1.63	1.52	19	20
1	A	49	ALA	N-CA	8.15	1.56	1.46	18	20
1	A	38	ILE	N-CA	8.14	1.55	1.46	3	20
1	A	39	PHE	CA-CB	8.12	1.68	1.53	12	19
1	A	75	SER	CA-C	8.10	1.63	1.52	2	20
1	A	93	MET	CA-C	8.10	1.62	1.52	2	20
1	A	11	THR	N-CA	8.05	1.55	1.46	6	20
1	A	63	PHE	C-N	8.04	1.43	1.33	4	18
1	A	12	LEU	C-N	8.04	1.44	1.33	3	20
1	A	39	PHE	CA-C	8.03	1.62	1.52	19	20
1	A	43	ILE	C-N	8.00	1.42	1.33	2	20
1	A	21	PHE	N-CA	8.00	1.57	1.45	16	18
1	A	39	PHE	N-CA	7.99	1.56	1.45	12	20
1	A	55	LEU	CA-CB	7.99	1.65	1.53	19	20
1	A	67	VAL	CA-C	7.98	1.62	1.52	1	4
1	A	12	LEU	CA-CB	7.98	1.67	1.53	16	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	56	ARG	CA-C	7.95	1.62	1.52	4	20
1	A	43	ILE	CA-C	7.93	1.62	1.52	16	20
1	A	76	ALA	CA-C	7.91	1.63	1.52	11	20
1	A	55	LEU	CA-C	7.91	1.62	1.52	13	20
1	A	69	VAL	N-CA	7.89	1.56	1.46	20	18
1	A	10	ILE	C-N	7.85	1.43	1.33	6	20
1	A	56	ARG	C-N	7.83	1.43	1.34	13	20
1	A	8	GLU	N-CA	7.79	1.55	1.46	17	20
1	A	48	ALA	C-N	7.79	1.45	1.33	14	20
1	A	61	ILE	C-N	7.77	1.43	1.33	12	20
1	A	89	ARG	CA-C	7.77	1.61	1.52	14	18
1	A	91	TYR	C-O	7.76	1.32	1.24	1	20
2	B	9	VAL	CA-CB	7.73	1.75	1.54	19	20
1	A	71	GLU	N-CA	7.72	1.56	1.46	13	2
1	A	62	LEU	CA-CB	7.69	1.66	1.53	2	20
1	A	8	GLU	CA-C	7.67	1.61	1.52	19	14
1	A	78	VAL	C-N	7.65	1.44	1.33	6	20
1	A	92	VAL	C-N	7.63	1.43	1.33	5	20
1	A	54	ARG	CA-CB	7.62	1.66	1.53	12	20
1	A	45	PRO	N-CA	7.59	1.57	1.47	13	20
1	A	91	TYR	CA-CB	7.58	1.64	1.53	10	20
1	A	74	HIS	CA-CB	7.58	1.65	1.53	7	20
1	A	81	LEU	N-CA	7.49	1.55	1.46	4	15
1	A	57	VAL	CA-CB	7.49	1.65	1.54	15	20
1	A	48	ALA	CA-C	7.47	1.62	1.52	18	20
1	A	29	ASN	CA-CB	7.46	1.63	1.53	19	20
1	A	85	GLY	C-N	7.46	1.44	1.33	2	19
1	A	45	PRO	CA-C	7.45	1.64	1.52	16	20
1	A	39	PHE	C-O	7.45	1.33	1.23	12	9
1	A	69	VAL	C-N	7.38	1.43	1.34	18	18
1	A	28	ASP	CA-C	7.34	1.62	1.52	1	20
1	A	52	ASP	CA-C	7.33	1.62	1.52	13	20
1	A	74	HIS	CB-CG	7.30	1.60	1.50	6	20
1	A	49	ALA	CA-C	7.28	1.62	1.52	20	20
1	A	28	ASP	C-N	7.27	1.45	1.33	9	20
1	A	73	THR	CA-C	7.24	1.62	1.53	13	20
1	A	84	ALA	C-N	7.22	1.43	1.34	14	20
1	A	64	VAL	C-O	-7.22	1.16	1.24	8	16
1	A	51	GLN	CA-C	7.21	1.61	1.53	18	20
1	A	82	LYS	N-CA	7.20	1.55	1.46	10	20
1	A	28	ASP	CA-CB	7.19	1.64	1.53	4	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	54	ARG	CA-C	7.14	1.62	1.52	13	20
1	A	60	SER	CA-C	7.14	1.62	1.52	18	20
1	A	38	ILE	C-N	7.13	1.43	1.33	12	20
1	A	63	PHE	N-CA	7.13	1.54	1.46	4	20
1	A	63	PHE	CA-CB	7.12	1.64	1.53	11	17
1	A	87	ILE	CB-CG1	7.08	1.67	1.53	10	20
1	A	50	ALA	CA-C	7.01	1.62	1.52	1	20
1	A	77	ALA	CA-C	7.00	1.62	1.52	12	20
1	A	25	GLY	N-CA	6.97	1.51	1.45	3	11
1	A	68	ASP	C-N	6.96	1.41	1.34	15	9
1	A	56	ARG	N-CA	6.95	1.54	1.45	5	20
1	A	22	SER	N-CA	6.93	1.54	1.45	17	19
1	A	58	ASN	CA-CB	6.93	1.65	1.53	13	19
1	A	48	ALA	N-CA	6.92	1.55	1.46	19	20
1	A	79	GLU	CA-C	6.86	1.62	1.52	15	14
1	A	45	PRO	C-N	6.85	1.43	1.33	16	20
1	A	39	PHE	C-N	6.83	1.46	1.33	13	8
1	A	12	LEU	N-CA	6.82	1.54	1.45	3	16
1	A	43	ILE	CB-CG1	6.80	1.67	1.53	5	20
1	A	53	GLY	N-CA	6.79	1.55	1.45	9	20
1	A	12	LEU	CA-C	6.79	1.61	1.52	5	5
1	A	8	GLU	CA-CB	6.78	1.66	1.53	3	14
1	A	93	MET	C-N	6.78	1.43	1.33	19	20
1	A	42	LYS	C-N	6.75	1.41	1.33	17	20
1	A	94	ARG	C-N	6.73	1.43	1.33	5	18
1	A	90	LEU	N-CA	6.69	1.54	1.46	3	20
1	A	72	VAL	C-N	6.67	1.42	1.33	12	15
1	A	28	ASP	N-CA	6.66	1.54	1.46	17	20
1	A	52	ASP	N-CA	6.65	1.54	1.46	18	19
1	A	82	LYS	CA-C	6.65	1.61	1.52	17	19
1	A	42	LYS	CA-C	6.63	1.60	1.52	9	15
1	A	68	ASP	CA-C	6.63	1.61	1.52	11	8
1	A	9	GLU	CA-C	6.63	1.61	1.52	11	20
1	A	20	GLY	N-CA	6.62	1.54	1.45	3	7
1	A	81	LEU	C-N	6.62	1.43	1.33	13	19
1	A	74	HIS	C-O	6.59	1.31	1.24	1	8
1	A	9	GLU	C-N	6.58	1.42	1.33	11	19
1	A	40	ILE	CB-CG1	6.57	1.66	1.53	7	20
1	A	67	VAL	N-CA	6.57	1.53	1.46	13	7
1	A	51	GLN	N-CA	6.56	1.54	1.46	11	20
1	A	70	ARG	CD-NE	6.55	1.55	1.46	3	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	54	ARG	CD-NE	6.54	1.55	1.46	17	7
1	A	6	GLU	CA-C	6.53	1.60	1.52	1	9
1	A	76	ALA	N-CA	6.51	1.54	1.46	10	15
1	A	71	GLU	C-N	6.49	1.42	1.33	5	18
1	A	89	ARG	CD-NE	6.49	1.55	1.46	13	1
2	B	8	SER	CA-CB	6.44	1.63	1.53	1	6
1	A	94	ARG	CD-NE	6.44	1.55	1.46	5	7
1	A	90	LEU	CA-C	6.43	1.60	1.52	20	18
1	A	81	LEU	CA-CB	6.43	1.63	1.53	13	13
1	A	9	GLU	N-CA	6.42	1.54	1.46	19	17
1	A	29	ASN	N-CA	6.42	1.53	1.46	4	13
1	A	73	THR	CA-CB	6.39	1.63	1.53	3	20
1	A	70	ARG	CA-CB	6.39	1.64	1.53	9	8
1	A	24	ALA	N-CA	6.37	1.53	1.46	12	7
1	A	67	VAL	C-N	6.34	1.42	1.33	2	19
1	A	87	ILE	N-CA	6.34	1.54	1.46	13	17
1	A	77	ALA	N-CA	6.28	1.54	1.46	11	20
1	A	50	ALA	N-CA	6.17	1.54	1.46	20	20
1	A	88	VAL	N-CA	6.14	1.54	1.46	13	14
1	A	25	GLY	C-N	6.12	1.42	1.33	5	10
1	A	59	ASP	CA-C	6.11	1.60	1.52	15	10
1	A	11	THR	C-N	6.10	1.42	1.33	10	19
1	A	22	SER	CA-C	6.10	1.59	1.52	11	8
1	A	91	TYR	C-N	6.09	1.41	1.33	9	20
1	A	89	ARG	C-N	6.08	1.42	1.33	11	14
1	A	26	GLY	C-N	6.08	1.41	1.33	13	16
1	A	86	SER	CA-CB	6.08	1.63	1.53	19	9
1	A	90	LEU	C-N	6.08	1.42	1.33	2	20
1	A	55	LEU	N-CA	6.06	1.53	1.46	20	3
1	A	82	LYS	CA-CB	6.06	1.63	1.53	6	3
1	A	61	ILE	CB-CG1	6.02	1.65	1.53	1	20
1	A	47	GLY	C-N	5.95	1.42	1.33	11	20
1	A	7	TYR	CA-CB	5.94	1.62	1.53	17	18
1	A	6	GLU	C-N	5.93	1.41	1.33	9	16
1	A	60	SER	C-N	5.91	1.42	1.33	9	12
1	A	8	GLU	C-N	5.88	1.43	1.33	19	20
1	A	27	THR	CA-C	5.84	1.59	1.52	8	20
1	A	80	ALA	N-CA	5.77	1.53	1.46	13	8
1	A	62	LEU	N-CA	5.76	1.53	1.46	19	13
1	A	55	LEU	C-N	5.74	1.41	1.33	19	4
1	A	71	GLU	C-O	5.72	1.28	1.23	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	81	LEU	CB-CG	5.69	1.64	1.53	10	6
1	A	45	PRO	N-CD	5.66	1.55	1.47	16	20
1	A	51	GLN	CA-CB	5.63	1.61	1.53	13	16
1	A	81	LEU	CA-C	5.60	1.60	1.52	14	9
1	A	12	LEU	CB-CG	5.60	1.64	1.53	20	5
1	A	27	THR	CA-CB	5.52	1.62	1.53	1	19
1	A	87	ILE	C-N	5.52	1.40	1.33	15	6
1	A	24	ALA	CA-C	5.50	1.59	1.52	17	7
1	A	87	ILE	CA-C	5.49	1.59	1.52	10	3
1	A	86	SER	CA-C	5.45	1.60	1.52	19	5
2	B	9	VAL	CA-C	5.44	1.64	1.52	19	1
1	A	43	ILE	N-CA	5.36	1.52	1.46	9	4
1	A	24	ALA	CA-CB	5.32	1.61	1.53	12	1
2	B	9	VAL	N-CA	5.31	1.56	1.46	19	3
1	A	25	GLY	C-O	5.24	1.28	1.23	12	1
1	A	60	SER	CA-CB	5.20	1.62	1.53	7	6
1	A	26	GLY	N-CA	5.12	1.52	1.45	13	1
1	A	37	SER	CA-CB	5.09	1.61	1.53	6	3
1	A	7	TYR	CA-C	5.07	1.58	1.52	11	1
1	A	24	ALA	C-N	5.06	1.39	1.33	1	1
1	A	10	ILE	CB-CG1	5.04	1.63	1.53	6	1
1	A	21	PHE	CB-CG	5.03	1.62	1.50	16	2
1	A	88	VAL	C-N	5.03	1.40	1.33	14	2
1	A	91	TYR	N-CA	5.02	1.52	1.46	20	1
1	A	67	VAL	C-O	5.01	1.30	1.23	19	1
1	A	83	GLU	C-O	5.01	1.30	1.24	3	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	39	PHE	CA-CB-CG	13.09	126.89	113.80	1	20
1	A	88	VAL	CA-CB-CG2	10.05	127.48	110.40	19	8
1	A	88	VAL	CA-CB-CG1	9.76	126.99	110.40	16	3
1	A	23	ILE	N-CA-C	8.99	120.69	108.11	3	20
1	A	64	VAL	CA-CB-CG1	8.84	125.43	110.40	8	6
1	A	74	HIS	CA-CB-CG	8.62	122.42	113.80	4	20
1	A	21	PHE	CA-CB-CG	8.37	122.17	113.80	16	20
1	A	69	VAL	CA-CB-CG1	7.79	123.64	110.40	9	6
1	A	83	GLU	N-CA-C	7.75	119.80	111.36	7	16
1	A	69	VAL	CB-CA-C	7.68	121.02	112.19	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	58	ASN	CA-CB-CG	7.67	120.27	112.60	10	8
1	A	68	ASP	CA-CB-CG	7.47	120.07	112.60	14	20
1	A	28	ASP	CA-CB-CG	7.35	119.95	112.60	7	3
1	A	65	ASN	CA-C-N	7.34	132.67	120.70	10	13
1	A	65	ASN	C-N-CA	7.34	132.67	120.70	10	13
1	A	67	VAL	CA-CB-CG1	7.31	122.83	110.40	4	3
1	A	57	VAL	CA-CB-CG1	7.15	122.56	110.40	14	14
1	A	64	VAL	N-CA-CB	6.92	120.96	111.41	7	9
1	A	72	VAL	CA-CB-CG2	6.80	121.97	110.40	16	6
1	A	23	ILE	CA-CB-CG1	6.78	121.92	110.40	11	20
1	A	83	GLU	N-CA-CB	-6.47	100.33	110.30	15	1
1	A	67	VAL	CA-CB-CG2	6.35	121.19	110.40	13	11
1	A	78	VAL	CA-C-N	6.31	129.37	120.28	12	6
1	A	78	VAL	C-N-CA	6.31	129.37	120.28	12	6
1	A	38	ILE	CA-CB-CG1	6.17	120.89	110.40	12	19
1	A	73	THR	CA-C-N	6.06	129.21	120.79	13	7
1	A	73	THR	C-N-CA	6.06	129.21	120.79	13	7
1	A	20	GLY	CA-C-N	6.04	131.70	120.95	16	1
1	A	20	GLY	C-N-CA	6.04	131.70	120.95	16	1
1	A	74	HIS	CA-C-N	5.91	128.20	120.28	5	6
1	A	74	HIS	C-N-CA	5.91	128.20	120.28	5	6
1	A	56	ARG	CA-C-N	5.90	129.79	120.47	20	14
1	A	56	ARG	C-N-CA	5.90	129.79	120.47	20	14
1	A	88	VAL	CB-CA-C	5.82	119.24	110.63	11	1
1	A	69	VAL	CA-C-N	5.74	128.76	120.38	7	8
1	A	69	VAL	C-N-CA	5.74	128.76	120.38	7	8
1	A	65	ASN	CA-CB-CG	5.71	118.31	112.60	19	7
1	A	43	ILE	CA-C-N	5.45	128.75	121.23	16	1
1	A	43	ILE	C-N-CA	5.45	128.75	121.23	16	1
1	A	23	ILE	N-CA-CB	5.45	118.72	111.64	16	1
1	A	29	ASN	CB-CA-C	5.40	115.30	110.44	19	1
1	A	64	VAL	CA-CB-CG2	5.38	119.54	110.40	1	4
1	A	83	GLU	CA-CB-CG	5.29	124.68	114.10	15	1
1	A	85	GLY	N-CA-C	5.29	119.98	113.79	6	2
1	A	44	ILE	CB-CA-C	5.22	115.79	110.94	7	2
1	A	42	LYS	CA-CB-CG	5.21	124.53	114.10	17	4
1	A	77	ALA	CA-C-N	5.21	127.82	120.42	4	6
1	A	77	ALA	C-N-CA	5.21	127.82	120.42	4	6
1	A	79	GLU	CA-C-N	5.20	128.21	120.31	12	1
1	A	79	GLU	C-N-CA	5.20	128.21	120.31	12	1
1	A	55	LEU	N-CA-C	5.18	117.74	109.96	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	ASN	CA-CB-CG	5.11	117.71	112.60	14	1
1	A	47	GLY	CA-C-N	5.11	129.31	120.58	7	1
1	A	47	GLY	C-N-CA	5.11	129.31	120.58	7	1
1	A	68	ASP	CA-C-N	5.10	128.79	121.55	2	1
1	A	68	ASP	C-N-CA	5.10	128.79	121.55	2	1
1	A	94	ARG	CA-C-N	5.08	128.09	120.87	12	1
1	A	94	ARG	C-N-CA	5.08	128.09	120.87	12	1
1	A	64	VAL	N-CA-C	5.05	115.18	108.11	12	1
1	A	27	THR	N-CA-CB	5.04	117.70	110.40	6	1
1	A	70	ARG	N-CA-C	5.03	118.19	111.75	20	1

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	569	573	572	7±3
2	B	14	14	14	1±1
All	All	11660	11740	11720	144

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:ILE:CA	1:A:43:ILE:CB	1.65	1.75	18	19
1:A:87:ILE:CA	1:A:87:ILE:CB	1.62	1.74	12	2
1:A:38:ILE:CB	1:A:38:ILE:CA	1.62	1.74	5	7
1:A:72:VAL:CA	1:A:72:VAL:CB	1.59	1.76	3	10
1:A:44:ILE:CA	1:A:44:ILE:CB	1.57	1.74	13	2
2:B:9:VAL:CA	2:B:9:VAL:CB	1.56	1.74	7	3
1:A:72:VAL:CA	1:A:72:VAL:HB	0.75	2.06	16	10
1:A:38:ILE:CA	1:A:38:ILE:HB	0.74	2.07	13	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:ILE:CA	1:A:43:ILE:HB	0.71	2.11	11	19
1:A:64:VAL:O	1:A:67:VAL:HB	0.63	1.93	4	1
2:B:9:VAL:CA	2:B:9:VAL:CG1	0.61	2.74	7	3
1:A:44:ILE:CA	1:A:44:ILE:HB	0.60	2.10	16	2
1:A:87:ILE:CA	1:A:87:ILE:HB	0.59	2.13	7	2
1:A:38:ILE:CA	1:A:38:ILE:CG2	0.56	2.77	12	7
1:A:72:VAL:CB	1:A:72:VAL:C	0.55	2.76	4	10
1:A:72:VAL:CA	1:A:72:VAL:CG1	0.55	2.78	4	10
2:B:9:VAL:CA	2:B:9:VAL:CG2	0.55	2.79	19	3
2:B:9:VAL:CA	2:B:9:VAL:HB	0.53	2.15	20	2
1:A:44:ILE:CB	1:A:44:ILE:N	0.53	2.68	16	1
1:A:38:ILE:CB	1:A:38:ILE:C	0.47	2.81	13	7
1:A:44:ILE:CA	1:A:44:ILE:CG1	0.45	2.83	13	1
1:A:44:ILE:CA	1:A:44:ILE:CG2	0.44	2.83	16	2
1:A:64:VAL:O	1:A:67:VAL:HG22	0.44	2.13	15	3
1:A:87:ILE:CA	1:A:87:ILE:CG1	0.42	2.87	12	1
1:A:64:VAL:O	1:A:67:VAL:HG12	0.42	2.15	8	1
1:A:87:ILE:CA	1:A:87:ILE:CG2	0.41	2.86	7	1
1:A:22:SER:HB2	1:A:42:LYS:HB3	0.41	1.92	10	1
1:A:43:ILE:CA	1:A:43:ILE:CG1	0.41	2.87	17	3
1:A:87:ILE:CB	1:A:87:ILE:C	0.41	2.80	12	1
1:A:61:ILE:HG21	1:A:64:VAL:HG23	0.40	1.94	11	1
1:A:43:ILE:CB	1:A:43:ILE:C	0.40	2.83	14	2

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	75/99 (76%)	66±1 (88±2%)	6±1 (8±2%)	3±1 (4±1%)	3	28
2	B	1/9 (11%)	1±0 (80±40%)	0±0 (20±40%)	0±0 (0±0%)	100	100
All	All	1520/2160 (70%)	1333 (88%)	123 (8%)	64 (4%)	3	28

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	60	SER	20
1	A	54	ARG	18
1	A	86	SER	15
1	A	20	GLY	5
1	A	65	ASN	3
1	A	66	GLU	3

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	60/78 (77%)	55±1 (91±2%)	5±1 (9±2%)	11	58
2	B	2/9 (22%)	2±0 (98±11%)	0±0 (2±11%)	42	88
All	All	1240/1740 (71%)	1133 (91%)	107 (9%)	12	58

All 19 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	38	ILE	20
1	A	40	ILE	19
1	A	55	LEU	11
1	A	88	VAL	11
1	A	11	THR	10
1	A	90	LEU	9
1	A	64	VAL	8
1	A	69	VAL	6
1	A	67	VAL	3
2	B	9	VAL	1
1	A	51	GLN	1
1	A	9	GLU	1
1	A	66	GLU	1
1	A	8	GLU	1
1	A	71	GLU	1
1	A	23	ILE	1
1	A	82	LYS	1
1	A	81	LEU	1
1	A	12	LEU	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 80% for the well-defined parts and 74% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	992
Number of shifts mapped to atoms	992
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
$^{13}\text{C}_\alpha$	95	0.16 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	84	-0.05 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	90	0.07 ± 0.67	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 79%, i.e. 807 atoms were assigned a chemical shift out of a possible 1028. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	301/390 (77%)	154/160 (96%)	74/154 (48%)	73/76 (96%)
Sidechain	464/582 (80%)	319/382 (84%)	145/179 (81%)	0/21 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	42/56 (75%)	21/27 (78%)	21/27 (78%)	0/2 (0%)
Overall	807/1028 (79%)	494/569 (87%)	240/360 (67%)	73/99 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 992 atoms were assigned a chemical shift out of a possible 1425. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	381/541 (70%)	196/222 (88%)	95/216 (44%)	90/103 (87%)
Sidechain	565/820 (69%)	387/536 (72%)	178/252 (71%)	0/32 (0%)
Aromatic	46/64 (72%)	23/31 (74%)	23/29 (79%)	0/4 (0%)
Overall	992/1425 (70%)	606/789 (77%)	296/497 (60%)	90/139 (65%)

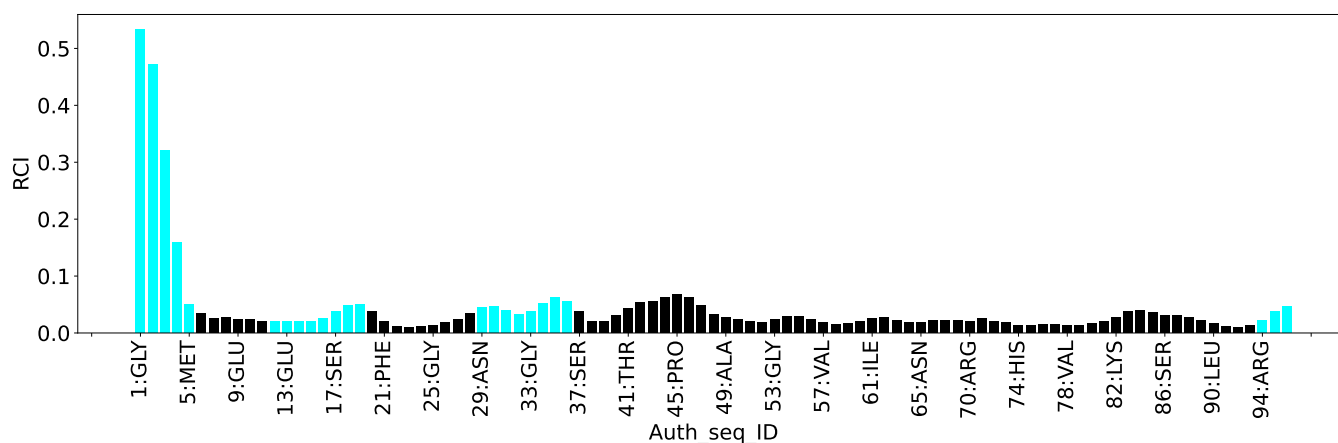
7.1.4 Statistically unusual chemical shifts [i](#)

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	59
Number of shifts mapped to atoms	59
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

7.2.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 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 1%, i.e. 13 atoms were assigned a chemical shift out of a possible 1028. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	4/390 (1%)	4/160 (2%)	0/154 (0%)	0/76 (0%)
Sidechain	9/582 (2%)	9/382 (2%)	0/179 (0%)	0/21 (0%)
Aromatic	0/56 (0%)	0/27 (0%)	0/27 (0%)	0/2 (0%)
Overall	13/1028 (1%)	13/569 (2%)	0/360 (0%)	0/99 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 59 atoms were assigned a chemical shift out of a possible 1425. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	14/541 (3%)	14/222 (6%)	0/216 (0%)	0/103 (0%)
Sidechain	45/820 (5%)	45/536 (8%)	0/252 (0%)	0/32 (0%)
Aromatic	0/64 (0%)	0/31 (0%)	0/29 (0%)	0/4 (0%)
Overall	59/1425 (4%)	59/789 (7%)	0/497 (0%)	0/139 (0%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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:

