



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:23 PM UTC

PDB ID : 1ROU / pdb_00001rou
Title : STRUCTURE OF FKBP59-I, THE N-TERMINAL DOMAIN OF A 59 KDA
FK506-BINDING PROTEIN, NMR, 22 STRUCTURES
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Baulieu, E.-E.; Mispelter, J.
Deposited on : 1996-06-14

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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

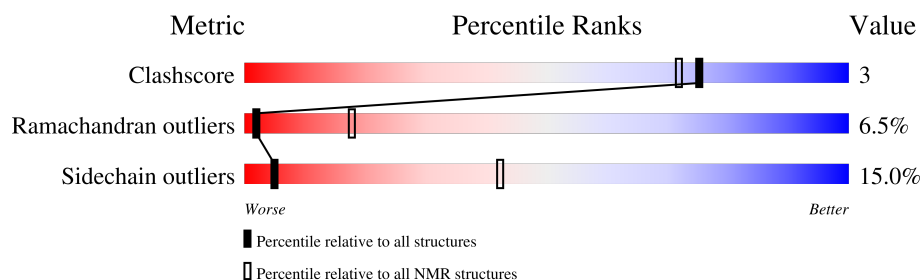
1 Overall quality at a glance

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	149	32% 37% • 7% 21%

2 Ensemble composition and analysis

This entry contains 22 models. Model 3 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:31-A:138 (108)	1.19	3

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 6 single-model clusters were found.

Cluster number	Models
1	3, 4, 6, 10, 12, 19
2	1, 8, 9, 11, 20
3	13, 15, 17
4	7, 16
Single-model clusters	2; 5; 14; 18; 21; 22

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1832 atoms, of which 918 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FKBP59-I.

Mol	Chain	Residues	Atoms						Trace
1	A	118	Total	C	H	N	O	S	0
			1832	589	918	148	173	4	

There are 2 discrepancies between the modelled and reference sequences:

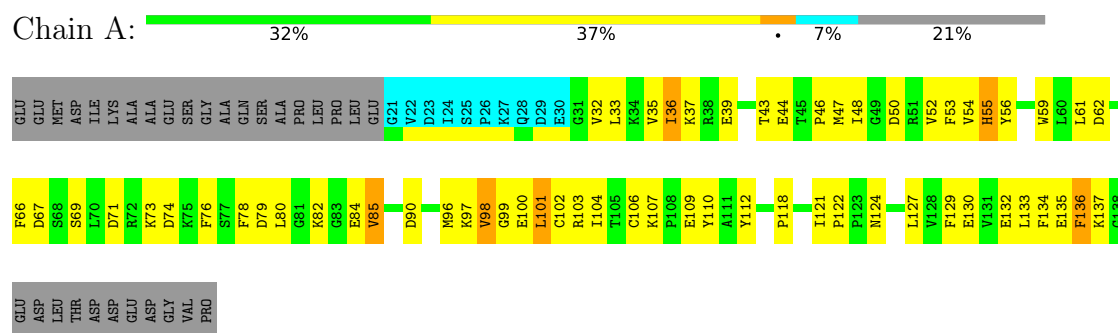
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ASP	-	insertion	UNP P27124
A	5	ILE	-	insertion	UNP P27124

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: FKBP59-I

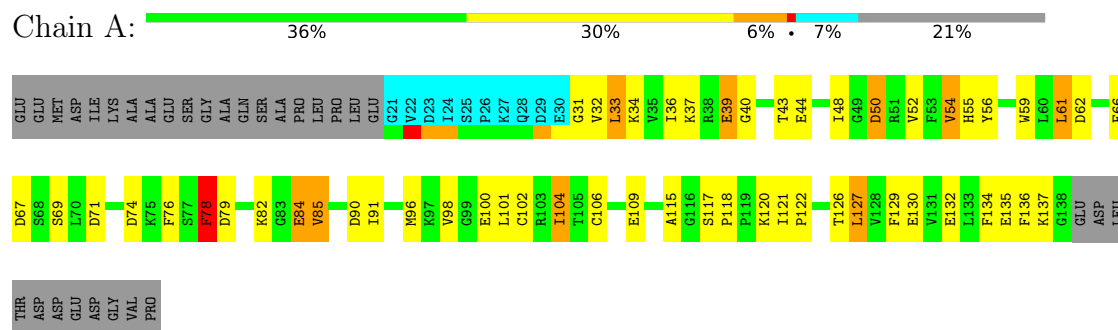


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

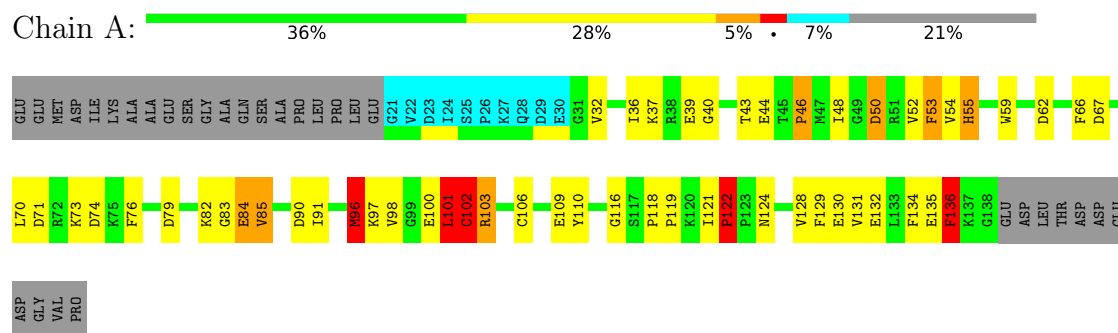
4.2.1 Score per residue for model 1

• Molecule 1: FKBP59-I



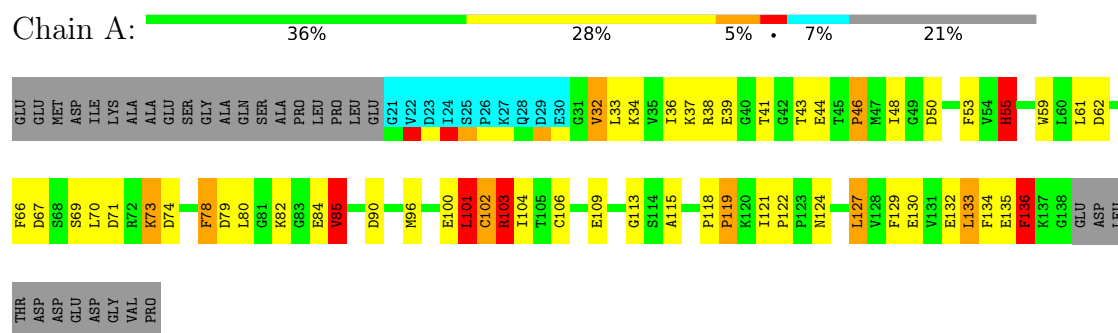
4.2.2 Score per residue for model 2

• Molecule 1: FKBP59-I



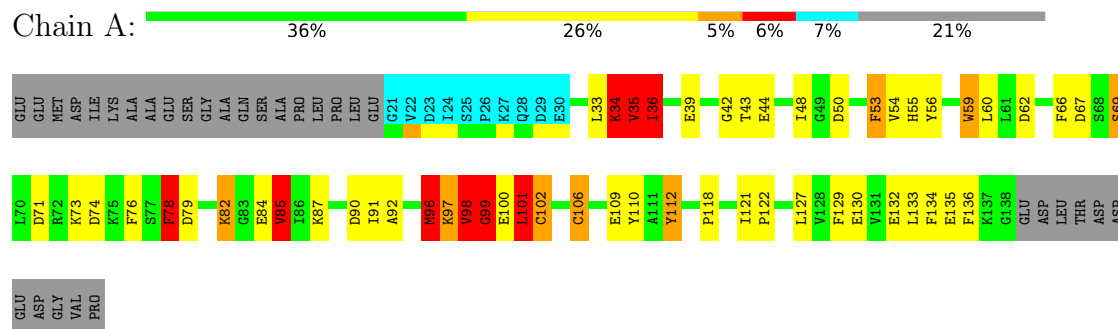
4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: FKBP59-I



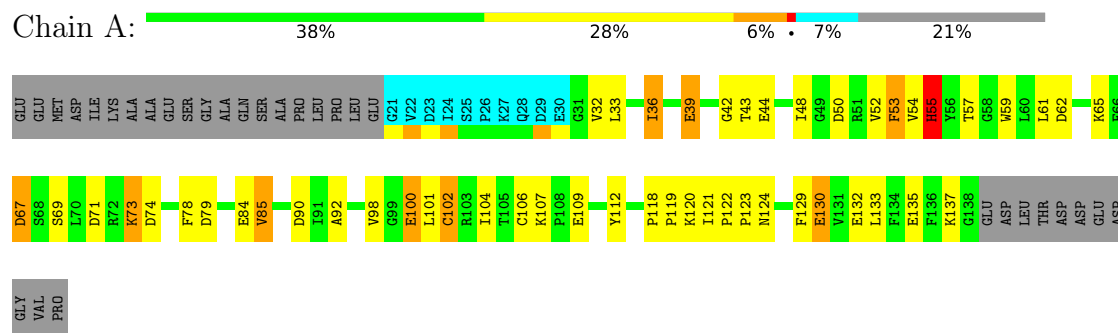
4.2.4 Score per residue for model 4

• Molecule 1: FKBP59-I



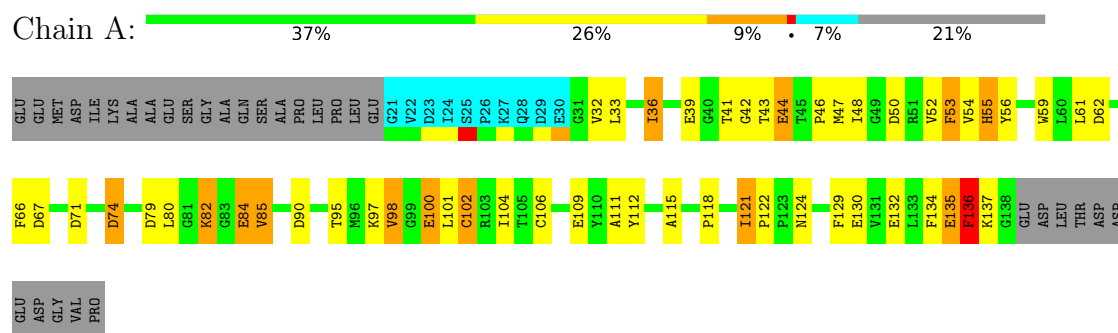
4.2.5 Score per residue for model 5

• Molecule 1: FKBP59-I



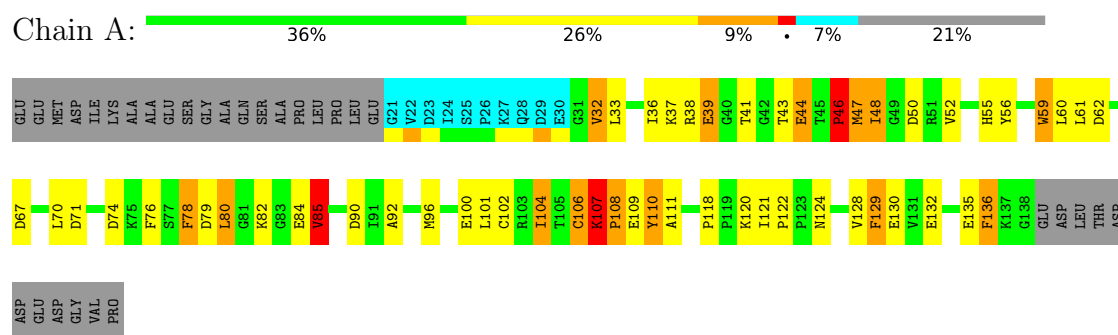
4.2.6 Score per residue for model 6

- Molecule 1: FKBP59-I



4.2.7 Score per residue for model 7

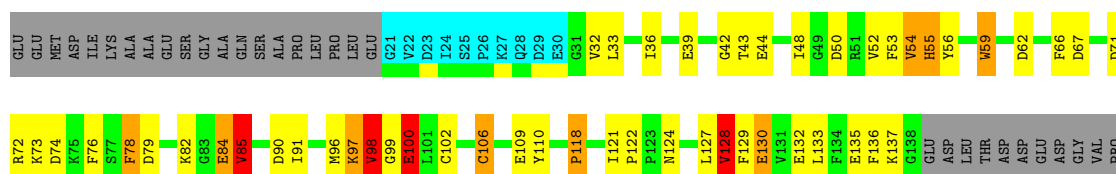
- Molecule 1: FKBP59-I



4.2.8 Score per residue for model 8

- Molecule 1: FKBP59-I

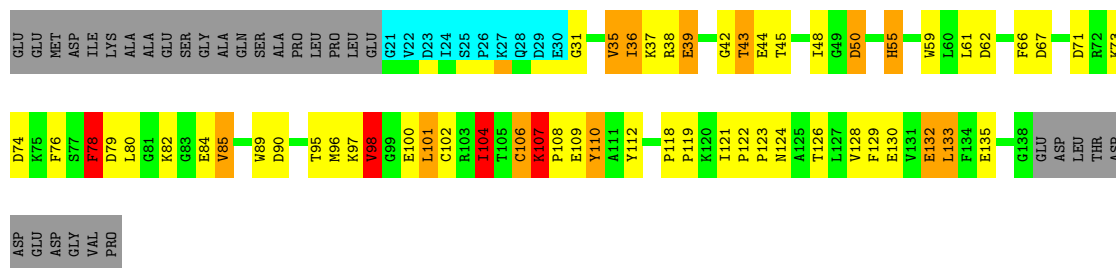




4.2.9 Score per residue for model 9

- Molecule 1: FKBP59-I

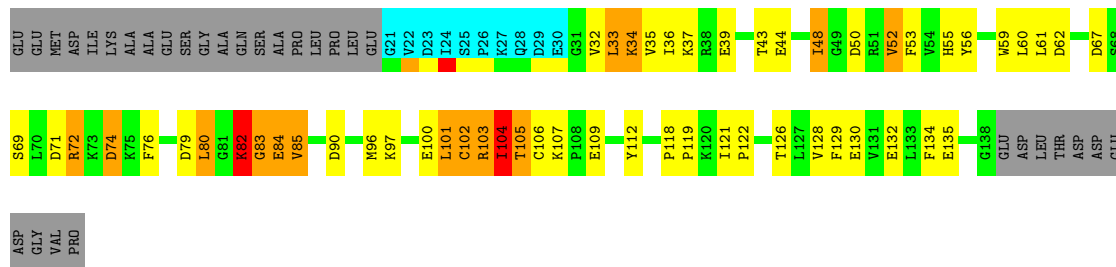
Chain A: 34% 28% 8% 7% 21%



4.2.10 Score per residue for model 10

- Molecule 1: FKBP59-I

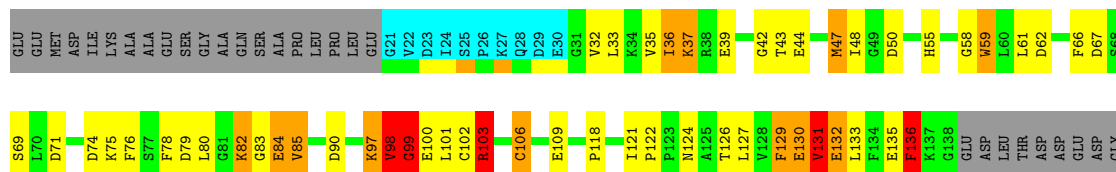
Chain A: 36% 26% 9% 7% 21%



4.2.11 Score per residue for model 11

- Molecule 1: FKBP59-I

Chain A: 36% 25% 8% 7% 21%

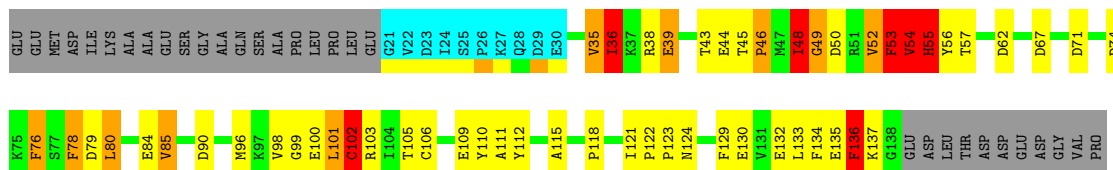


VAL
PRO

4.2.12 Score per residue for model 12

- Molecule 1: FKBP59-I

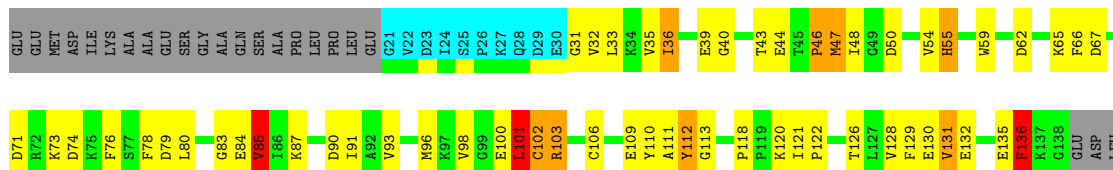
Chain A: 36% 26% 7% 5% 7% 21%



4.2.13 Score per residue for model 13

- Molecule 1: FKBP59-I

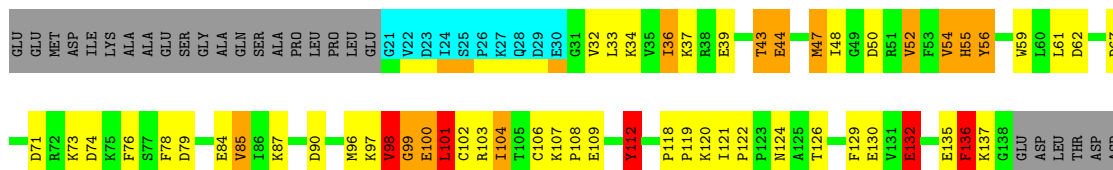
Chain A: 34% 32% 5% 7% 21%

THR
ASP
ASP
GLU
ASP
GLY
VAL
PRO

4.2.14 Score per residue for model 14

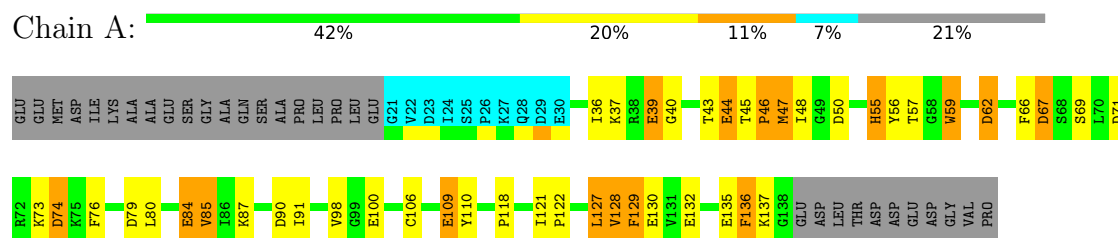
- Molecule 1: FKBP59-I

Chain A: 35% 26% 8% 7% 21%

GLU
ASP
GLY
VAL
PRO

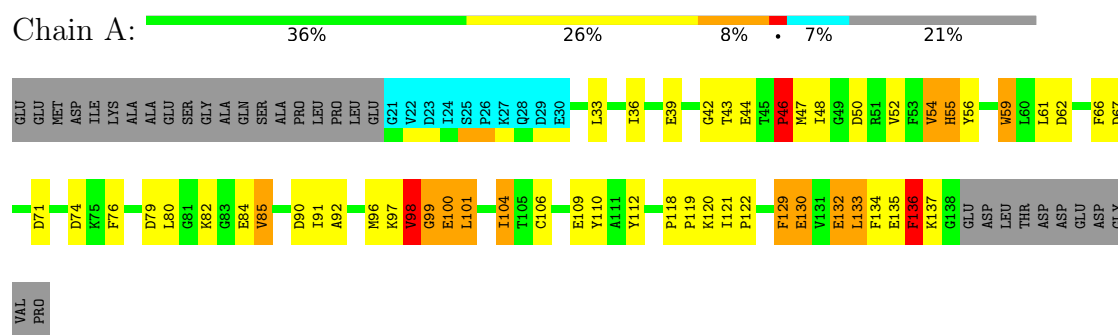
4.2.15 Score per residue for model 15

- Molecule 1: FKBP59-I



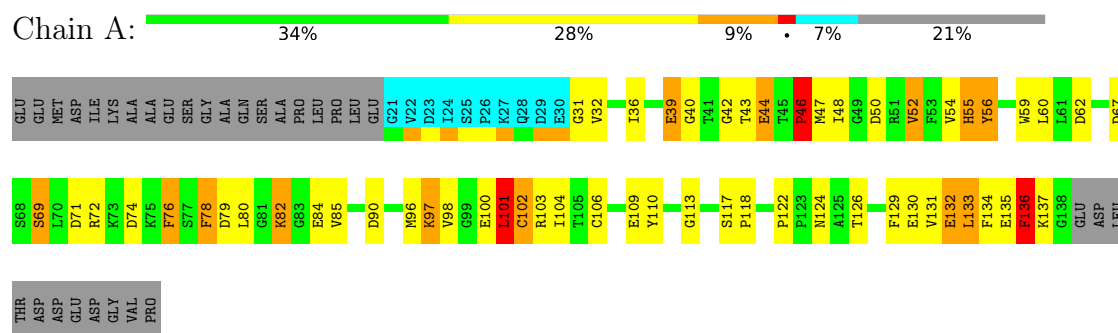
4.2.16 Score per residue for model 16

- Molecule 1: FKBP59-I



4.2.17 Score per residue for model 17

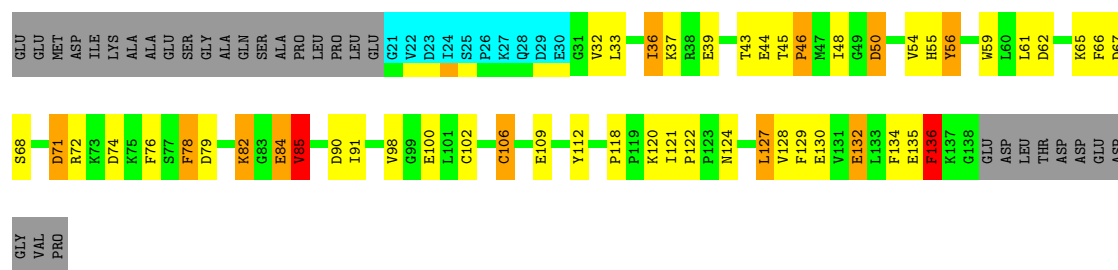
- Molecule 1: FKBP59-I



4.2.18 Score per residue for model 18

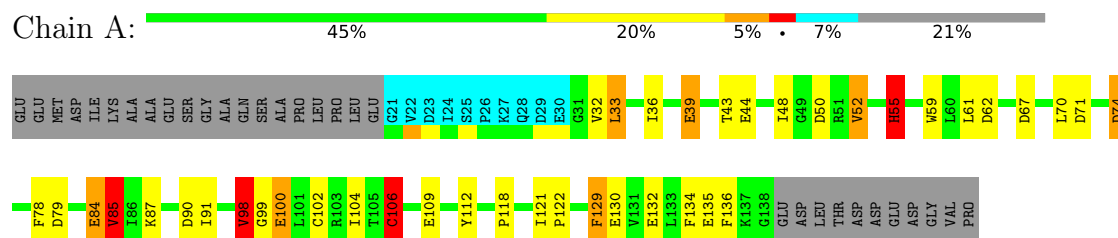
- Molecule 1: FKBP59-I





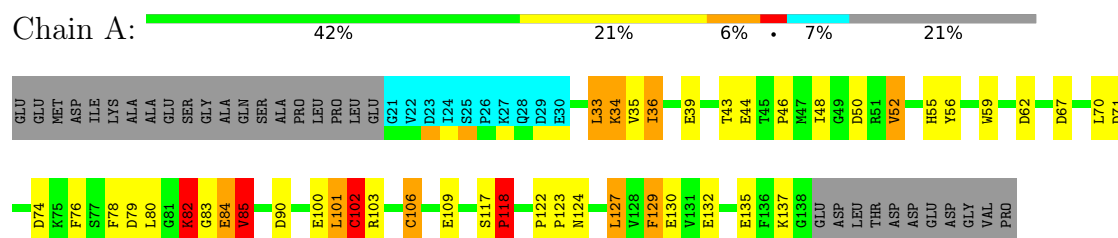
4.2.19 Score per residue for model 19

- Molecule 1: FKBP59-I



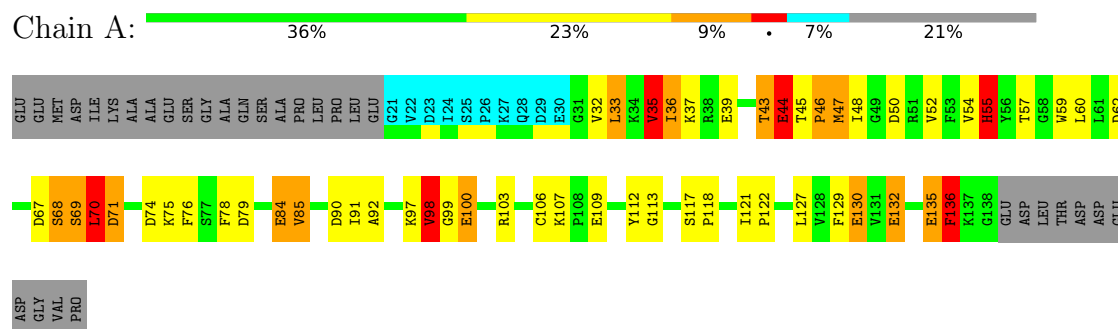
4.2.20 Score per residue for model 20

- Molecule 1: FKBP59-I



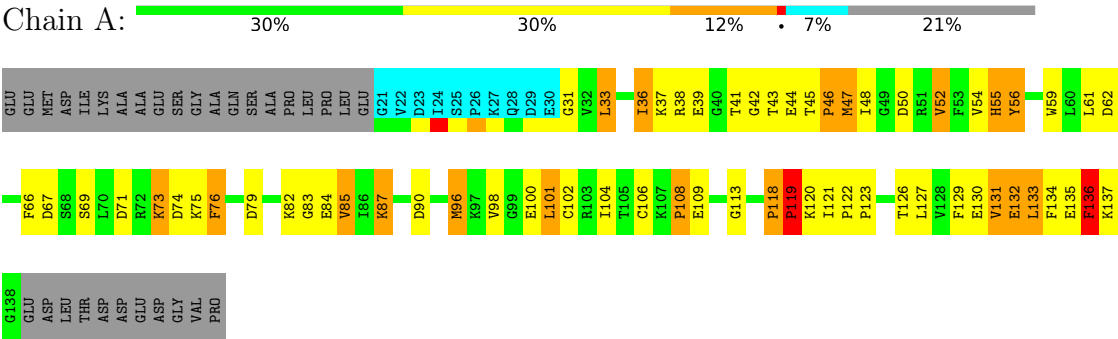
4.2.21 Score per residue for model 21

- Molecule 1: FKBP59-I



4.2.22 Score per residue for model 22

● Molecule 1: FKBP59-I



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: ?.

Of the ? calculated structures, 22 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
Discover	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	2.12±0.03	27±3/859 (3.1± 0.4%)	2.20±0.10	37±6/1159 (3.2± 0.5%)
All	All	2.12	591/18898 (3.1%)	2.20	813/25498 (3.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.6±0.7	2.5±1.3
All	All	14	55

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	137	LYS	CA-C	12.72	1.59	1.52	6	6
1	A	111	ALA	CA-C	11.44	1.57	1.52	13	3
1	A	100	GLU	CA-C	8.79	1.60	1.53	4	3
1	A	121	ILE	CA-C	8.69	1.60	1.53	16	20
1	A	122	PRO	CA-C	8.37	1.59	1.52	5	22
1	A	82	LYS	CA-C	8.30	1.57	1.52	10	2
1	A	107	LYS	CA-C	7.72	1.62	1.52	9	3
1	A	118	PRO	CA-C	7.59	1.59	1.52	20	22
1	A	132	GLU	CA-CB	7.33	1.63	1.53	9	2
1	A	45	THR	CA-C	7.18	1.59	1.52	18	3
1	A	98	VAL	N-CA	7.09	1.55	1.46	4	7
1	A	98	VAL	CA-C	6.67	1.60	1.52	18	11
1	A	102	CYS	CA-C	6.55	1.59	1.53	14	1
1	A	101	LEU	CA-C	6.48	1.60	1.52	9	6
1	A	55	HIS	CE1-NE2	6.47	1.39	1.32	1	7
1	A	101	LEU	C-N	6.43	1.39	1.33	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	45	THR	N-CA	6.34	1.50	1.46	18	2
1	A	71	ASP	CG-OD2	6.22	1.37	1.25	12	22
1	A	124	ASN	CA-C	6.21	1.59	1.53	6	8
1	A	33	LEU	CA-C	6.21	1.60	1.52	8	8
1	A	79	ASP	CG-OD2	6.18	1.37	1.25	15	22
1	A	109	GLU	CD-OE2	6.15	1.37	1.25	22	22
1	A	130	GLU	CD-OE2	6.14	1.37	1.25	10	22
1	A	67	ASP	CG-OD2	6.12	1.36	1.25	15	22
1	A	84	GLU	CD-OE2	6.11	1.36	1.25	19	22
1	A	100	GLU	CD-OE2	6.10	1.36	1.25	21	22
1	A	119	PRO	CA-C	6.10	1.59	1.53	16	3
1	A	62	ASP	CG-OD2	6.09	1.36	1.25	10	22
1	A	44	GLU	CD-OE2	6.07	1.36	1.25	22	22
1	A	74	ASP	CG-OD2	6.03	1.36	1.25	22	22
1	A	135	GLU	CD-OE2	6.03	1.36	1.25	15	22
1	A	50	ASP	CG-OD2	6.00	1.36	1.25	12	22
1	A	39	GLU	CD-OE2	5.97	1.36	1.25	10	22
1	A	32	VAL	N-CA	5.96	1.52	1.46	8	4
1	A	44	GLU	CA-C	5.96	1.58	1.53	12	1
1	A	132	GLU	CD-OE2	5.94	1.36	1.25	5	22
1	A	37	LYS	CA-C	5.94	1.57	1.52	7	11
1	A	106	CYS	CA-C	5.92	1.59	1.52	9	2
1	A	90	ASP	CG-OD2	5.90	1.36	1.25	21	22
1	A	56	TYR	CA-C	5.89	1.59	1.52	14	4
1	A	134	PHE	CA-C	5.89	1.57	1.52	12	4
1	A	104	ILE	CA-C	5.88	1.59	1.52	9	3
1	A	128	VAL	CA-C	5.86	1.60	1.52	10	1
1	A	135	GLU	CA-C	5.82	1.59	1.52	1	4
1	A	126	THR	CA-C	5.81	1.59	1.52	22	7
1	A	32	VAL	CA-C	5.80	1.59	1.52	17	3
1	A	47	MET	N-CA	5.74	1.53	1.46	7	1
1	A	62	ASP	CA-C	5.71	1.60	1.52	7	7
1	A	38	ARG	CA-C	5.71	1.58	1.52	12	4
1	A	48	ILE	CA-C	5.70	1.59	1.52	7	2
1	A	36	ILE	CA-C	5.69	1.59	1.52	4	1
1	A	55	HIS	ND1-CE1	5.67	1.38	1.32	14	9
1	A	76	PHE	CA-C	5.67	1.59	1.52	8	3
1	A	70	LEU	CA-C	5.58	1.60	1.52	21	1
1	A	39	GLU	N-CA	5.54	1.53	1.46	19	2
1	A	46	PRO	CA-C	5.52	1.58	1.52	20	1
1	A	120	LYS	CA-C	5.52	1.58	1.52	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	32	VAL	CA-CB	5.50	1.61	1.54	5	1
1	A	104	ILE	CA-CB	5.45	1.61	1.54	10	4
1	A	100	GLU	N-CA	5.42	1.53	1.46	5	2
1	A	36	ILE	N-CA	5.42	1.53	1.46	10	5
1	A	71	ASP	N-CA	5.41	1.53	1.46	18	1
1	A	112	TYR	CA-C	5.38	1.59	1.52	13	3
1	A	110	TYR	CA-C	5.37	1.60	1.52	7	1
1	A	53	PHE	CB-CG	5.35	1.62	1.50	12	1
1	A	117	SER	CA-C	5.30	1.58	1.52	1	3
1	A	112	TYR	N-CA	5.29	1.53	1.46	4	3
1	A	34	LYS	CA-C	5.29	1.58	1.52	4	1
1	A	78	PHE	CA-C	5.28	1.59	1.52	11	1
1	A	56	TYR	N-CA	5.22	1.52	1.46	18	1
1	A	39	GLU	CA-C	5.20	1.60	1.53	13	2
1	A	31	GLY	N-CA	5.20	1.52	1.45	9	1
1	A	89	TRP	CG-CD2	-5.18	1.34	1.43	9	1
1	A	96	MET	CA-C	5.16	1.58	1.52	4	1
1	A	35	VAL	CA-C	5.13	1.59	1.52	21	2
1	A	129	PHE	N-CA	5.12	1.52	1.45	6	1
1	A	65	LYS	CA-C	5.12	1.59	1.52	13	3
1	A	123	PRO	CA-C	5.12	1.57	1.52	9	1
1	A	106	CYS	CA-CB	5.11	1.60	1.54	17	1
1	A	58	GLY	CA-C	5.08	1.56	1.51	11	1
1	A	99	GLY	N-CA	5.06	1.52	1.45	14	1
1	A	95	THR	CA-C	5.05	1.59	1.52	9	2
1	A	43	THR	CA-C	5.01	1.56	1.52	10	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	69	SER	O-C-N	-35.20	75.77	122.59	21	1
1	A	55	HIS	CA-CB-CG	19.23	133.03	113.80	22	10
1	A	107	LYS	N-CA-C	17.13	147.67	109.81	7	2
1	A	69	SER	CA-C-O	-16.42	97.03	120.51	21	1
1	A	102	CYS	CB-CA-C	-15.17	91.97	114.87	14	1
1	A	122	PRO	CB-CA-C	14.43	128.52	110.92	2	1
1	A	107	LYS	N-CA-CB	-13.67	86.03	110.37	9	2
1	A	50	ASP	CA-CB-CG	12.41	125.02	112.60	11	20
1	A	46	PRO	CB-CA-C	12.41	125.16	109.89	13	4
1	A	52	VAL	N-CA-CB	-12.40	96.70	111.21	20	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	MET	N-CA-C	12.26	127.54	108.79	7	4
1	A	67	ASP	CA-CB-CG	12.15	124.75	112.60	9	4
1	A	55	HIS	ND1-CE1-NE2	12.14	120.54	108.40	8	22
1	A	98	VAL	O-C-N	-12.13	107.41	122.57	16	1
1	A	118	PRO	N-CA-C	11.62	124.88	110.70	8	21
1	A	129	PHE	CA-CB-CG	11.60	125.40	113.80	15	22
1	A	102	CYS	N-CA-CB	11.29	129.57	110.49	2	7
1	A	136	PHE	CA-CB-CG	11.24	125.04	113.80	21	16
1	A	53	PHE	CA-CB-CG	11.11	124.91	113.80	6	7
1	A	105	THR	CA-CB-CG2	10.76	128.79	110.50	10	1
1	A	36	ILE	N-CA-C	10.58	131.35	109.34	4	6
1	A	122	PRO	N-CA-C	10.55	123.57	110.70	2	2
1	A	82	LYS	N-CA-CB	-10.54	94.40	110.73	8	10
1	A	33	LEU	N-CA-CB	10.26	119.97	109.51	22	10
1	A	40	GLY	N-CA-C	10.21	123.56	112.33	13	5
1	A	71	ASP	CA-CB-CG	10.13	122.73	112.60	20	4
1	A	55	HIS	CE1-NE2-CD2	-10.00	99.00	109.00	22	22
1	A	43	THR	CA-CB-OG1	9.98	124.58	109.60	16	22
1	A	106	CYS	CB-CA-C	-9.98	93.34	113.80	17	1
1	A	53	PHE	N-CA-CB	-9.95	93.67	110.49	12	1
1	A	118	PRO	CB-CA-C	9.84	122.92	110.92	20	1
1	A	90	ASP	CA-CB-CG	9.77	122.36	112.60	6	11
1	A	46	PRO	N-CA-CB	-9.71	93.06	103.25	15	6
1	A	100	GLU	N-CA-C	9.65	131.35	110.80	5	5
1	A	101	LEU	N-CA-C	9.61	123.96	109.25	5	6
1	A	101	LEU	N-CA-CB	9.51	119.21	109.51	12	5
1	A	108	PRO	CB-CA-C	9.45	127.16	111.56	7	1
1	A	105	THR	N-CA-C	9.28	120.90	108.38	10	1
1	A	34	LYS	N-CA-C	9.26	122.12	108.60	4	2
1	A	132	GLU	N-CA-CB	-9.05	95.19	110.49	17	5
1	A	131	VAL	CA-CB-CG1	8.95	125.61	110.40	11	3
1	A	59	TRP	CA-CB-CG	8.88	130.47	113.60	11	3
1	A	35	VAL	N-CA-C	8.87	127.78	109.34	4	2
1	A	106	CYS	N-CA-CB	-8.78	95.23	111.13	9	2
1	A	98	VAL	N-CA-C	8.66	127.35	109.34	9	3
1	A	102	CYS	N-CA-C	8.46	118.22	108.49	12	4
1	A	33	LEU	CB-CA-C	8.43	127.19	110.42	1	2
1	A	121	ILE	N-CA-C	8.36	115.82	108.63	13	3
1	A	137	LYS	CB-CA-C	8.29	126.92	110.42	16	6
1	A	133	LEU	N-CA-C	8.28	123.21	109.46	17	3
1	A	68	SER	N-CA-C	8.17	128.21	110.80	18	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	84	GLU	CA-C-O	8.17	130.47	121.56	16	10
1	A	32	VAL	N-CA-C	8.16	119.12	108.35	6	9
1	A	137	LYS	N-CA-CB	-8.10	104.06	111.59	12	2
1	A	74	ASP	CA-CB-CG	8.08	120.68	112.60	14	11
1	A	100	GLU	CB-CA-C	8.05	125.79	116.54	14	5
1	A	55	HIS	CB-CG-CD2	-8.00	120.80	131.20	3	21
1	A	101	LEU	CB-CA-C	7.98	126.29	110.42	4	3
1	A	129	PHE	N-CA-CB	7.89	123.22	110.90	11	17
1	A	132	GLU	CB-CA-C	-7.81	94.88	110.42	17	2
1	A	74	ASP	N-CA-C	7.71	127.23	110.80	15	2
1	A	105	THR	OG1-CB-CG2	-7.71	93.89	109.30	10	1
1	A	103	ARG	CA-CB-CG	7.64	129.37	114.10	11	3
1	A	31	GLY	N-CA-C	7.54	125.54	115.59	13	4
1	A	134	PHE	CA-CB-CG	7.53	121.33	113.80	18	8
1	A	66	PHE	CA-CB-CG	7.43	121.23	113.80	11	13
1	A	56	TYR	N-CA-C	7.42	121.62	109.24	18	4
1	A	84	GLU	N-CA-CB	-7.41	97.97	110.49	8	5
1	A	113	GLY	N-CA-C	7.39	123.11	113.27	13	5
1	A	106	CYS	N-CA-C	7.38	120.09	108.79	7	18
1	A	105	THR	CA-CB-OG1	7.36	120.63	109.60	10	1
1	A	57	THR	N-CA-CB	7.30	121.87	110.71	12	4
1	A	39	GLU	N-CA-C	7.26	119.88	111.02	3	5
1	A	85	VAL	CB-CA-C	7.21	123.12	111.29	11	16
1	A	34	LYS	N-CA-CB	-7.18	99.50	110.77	20	1
1	A	76	PHE	CB-CA-C	7.17	123.46	109.33	10	14
1	A	76	PHE	CA-CB-CG	-7.17	106.64	113.80	4	12
1	A	130	GLU	CB-CG-CD	7.14	124.74	112.60	21	3
1	A	82	LYS	CA-CB-CG	7.12	128.34	114.10	10	1
1	A	99	GLY	N-CA-C	7.03	129.84	113.18	4	4
1	A	69	SER	N-CA-C	7.01	120.72	111.75	4	4
1	A	98	VAL	CA-CB-CG1	6.94	122.20	110.40	9	2
1	A	107	LYS	O-C-N	-6.94	113.34	121.32	9	1
1	A	97	LYS	CA-C-O	-6.92	113.51	121.47	4	2
1	A	36	ILE	N-CA-CB	6.90	118.79	110.31	12	4
1	A	124	ASN	CA-CB-CG	6.86	119.46	112.60	7	2
1	A	72	ARG	N-CA-C	6.85	119.17	110.61	10	2
1	A	79	ASP	CB-CA-C	6.84	121.08	110.14	13	11
1	A	62	ASP	N-CA-CB	-6.80	98.45	110.42	15	1
1	A	59	TRP	CB-CG-CD2	6.76	136.27	126.80	10	13
1	A	55	HIS	N-CA-CB	6.73	121.15	110.65	20	4
1	A	132	GLU	N-CA-C	6.66	116.78	108.19	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	53	PHE	CB-CA-C	6.64	121.09	110.19	2	4
1	A	128	VAL	CA-CB-CG1	6.64	121.69	110.40	8	1
1	A	84	GLU	N-CA-C	6.63	119.50	110.55	22	6
1	A	44	GLU	N-CA-C	6.63	120.67	110.20	11	9
1	A	84	GLU	CB-CA-C	6.62	123.59	110.42	21	11
1	A	54	VAL	N-CA-CB	-6.60	104.54	112.07	8	3
1	A	85	VAL	N-CA-CB	-6.59	100.36	111.23	16	8
1	A	46	PRO	N-CA-C	6.45	125.75	112.47	7	1
1	A	96	MET	N-CA-CB	-6.40	99.95	110.52	2	1
1	A	35	VAL	CB-CA-C	6.37	121.73	111.29	4	3
1	A	98	VAL	CB-CA-C	-6.36	100.86	111.29	2	3
1	A	54	VAL	CG1-CB-CG2	-6.35	96.82	110.80	16	4
1	A	91	ILE	CB-CA-C	6.35	120.06	111.87	21	6
1	A	62	ASP	CA-CB-CG	6.32	118.92	112.60	15	1
1	A	120	LYS	N-CA-C	6.32	120.33	112.24	16	2
1	A	71	ASP	N-CA-C	6.30	118.15	111.28	10	2
1	A	121	ILE	CA-C-N	6.28	126.84	120.38	2	1
1	A	121	ILE	C-N-CA	6.28	126.84	120.38	2	1
1	A	78	PHE	CA-CB-CG	6.17	119.97	113.80	14	12
1	A	85	VAL	CA-CB-CG2	6.15	120.86	110.40	14	9
1	A	119	PRO	N-CA-C	6.13	125.11	112.47	22	2
1	A	82	LYS	CB-CA-C	6.13	122.63	110.42	16	3
1	A	137	LYS	O-C-N	-6.11	117.57	122.03	12	1
1	A	47	MET	CB-CA-C	6.10	122.55	110.42	13	6
1	A	131	VAL	CB-CA-C	6.09	120.44	110.69	11	1
1	A	55	HIS	ND1-CG-CD2	6.08	112.18	106.10	1	2
1	A	82	LYS	CA-C-O	6.03	123.96	119.68	10	1
1	A	33	LEU	N-CA-C	6.03	116.56	108.23	20	1
1	A	55	HIS	CG-ND1-CE1	-6.02	99.07	109.30	8	21
1	A	56	TYR	N-CA-CB	6.00	121.27	110.83	22	3
1	A	32	VAL	CA-CB-CG2	5.97	120.55	110.40	10	4
1	A	128	VAL	CA-CB-CG2	5.94	120.50	110.40	10	2
1	A	103	ARG	N-CA-C	5.92	119.13	109.06	2	2
1	A	132	GLU	CB-CG-CD	5.91	122.65	112.60	17	1
1	A	45	THR	CB-CA-C	-5.91	100.66	108.76	21	2
1	A	69	SER	CA-C-N	5.90	128.19	120.28	11	4
1	A	69	SER	C-N-CA	5.90	128.19	120.28	11	4
1	A	54	VAL	CA-CB-CG2	5.88	120.40	110.40	14	4
1	A	133	LEU	N-CA-CB	-5.81	101.06	110.81	9	2
1	A	102	CYS	CA-C-O	5.79	124.36	120.19	3	1
1	A	137	LYS	CA-C-O	-5.79	116.02	119.55	22	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	74	ASP	N-CA-CB	-5.73	101.69	109.94	2	2
1	A	101	LEU	CD1-CG-CD2	5.72	123.39	110.80	17	1
1	A	124	ASN	OD1-CG-ND2	-5.72	116.88	122.60	6	4
1	A	53	PHE	CA-C-N	5.72	128.39	122.27	8	1
1	A	53	PHE	C-N-CA	5.72	128.39	122.27	8	1
1	A	107	LYS	CB-CG-CD	5.71	124.42	111.30	9	1
1	A	84	GLU	CA-C-N	5.70	132.23	121.97	16	2
1	A	84	GLU	C-N-CA	5.70	132.23	121.97	16	2
1	A	35	VAL	CA-C-N	5.69	132.22	121.97	4	1
1	A	35	VAL	C-N-CA	5.69	132.22	121.97	4	1
1	A	83	GLY	N-CA-C	-5.69	99.69	113.18	22	2
1	A	123	PRO	N-CA-C	5.67	121.21	113.84	22	3
1	A	134	PHE	CB-CA-C	5.66	120.20	110.86	4	2
1	A	127	LEU	N-CA-CB	-5.65	101.72	111.55	1	1
1	A	59	TRP	CB-CG-CD1	-5.63	118.45	126.90	10	1
1	A	137	LYS	N-CA-C	5.63	118.61	111.69	8	2
1	A	92	ALA	N-CA-C	5.62	117.48	111.36	7	4
1	A	106	CYS	CA-C-O	5.60	127.43	120.54	9	1
1	A	97	LYS	N-CA-C	5.59	118.84	109.95	17	5
1	A	34	LYS	CA-CB-CG	5.57	125.25	114.10	4	1
1	A	50	ASP	CB-CA-C	5.57	119.03	109.51	1	3
1	A	32	VAL	CB-CA-C	5.53	117.65	110.12	17	1
1	A	107	LYS	CB-CA-C	-5.53	99.28	110.17	7	1
1	A	100	GLU	N-CA-CB	5.47	119.73	110.49	5	1
1	A	131	VAL	CA-CB-CG2	5.44	119.64	110.40	17	1
1	A	70	LEU	N-CA-C	5.42	117.89	111.33	19	4
1	A	133	LEU	CB-CA-C	5.40	118.67	109.75	8	1
1	A	103	ARG	N-CA-CB	5.36	119.17	110.17	13	1
1	A	71	ASP	N-CA-CB	-5.35	102.03	110.06	17	1
1	A	115	ALA	N-CA-C	5.35	120.08	113.50	6	1
1	A	82	LYS	N-CA-C	5.30	120.40	113.30	9	1
1	A	44	GLU	CB-CG-CD	5.29	121.60	112.60	21	1
1	A	52	VAL	CA-CB-CG1	5.29	119.39	110.40	22	2
1	A	105	THR	N-CA-CB	5.29	119.59	111.24	10	1
1	A	124	ASN	N-CA-C	5.27	117.08	110.91	6	1
1	A	83	GLY	CA-C-N	5.27	131.60	121.54	10	1
1	A	83	GLY	C-N-CA	5.27	131.60	121.54	10	1
1	A	35	VAL	CA-CB-CG1	5.27	119.35	110.40	9	1
1	A	116	GLY	N-CA-C	5.26	119.49	112.65	2	1
1	A	43	THR	N-CA-C	5.25	119.17	112.87	13	1
1	A	44	GLU	CB-CA-C	5.24	120.85	110.42	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	117	SER	CA-C-N	5.23	125.77	120.38	20	1
1	A	117	SER	C-N-CA	5.23	125.77	120.38	20	1
1	A	68	SER	CA-C-N	5.22	131.51	121.54	21	1
1	A	68	SER	C-N-CA	5.22	131.51	121.54	21	1
1	A	130	GLU	N-CA-CB	5.22	118.29	109.94	3	1
1	A	128	VAL	N-CA-CB	-5.20	105.58	112.34	2	2
1	A	121	ILE	N-CA-CB	-5.19	103.94	111.21	18	1
1	A	36	ILE	CA-CB-CG2	5.18	119.31	110.50	3	1
1	A	99	GLY	CA-C-O	-5.18	115.05	119.56	12	1
1	A	122	PRO	N-CA-CB	-5.18	98.06	103.08	8	2
1	A	105	THR	CB-CA-C	5.16	119.11	111.17	12	1
1	A	126	THR	CA-CB-CG2	5.10	119.17	110.50	13	1
1	A	73	LYS	N-CA-CB	5.10	119.11	110.49	5	1
1	A	107	LYS	CA-C-N	5.09	126.21	119.84	7	1
1	A	107	LYS	C-N-CA	5.09	126.21	119.84	7	1
1	A	67	ASP	N-CA-C	5.08	115.24	108.38	15	1
1	A	41	THR	CA-CB-CG2	5.07	119.11	110.50	6	2
1	A	111	ALA	N-CA-CB	-5.05	101.95	110.49	6	1
1	A	112	TYR	CA-CB-CG	5.05	122.99	113.90	14	1
1	A	61	LEU	N-CA-C	5.04	117.51	111.71	1	1
1	A	87	LYS	CB-CA-C	5.04	120.84	110.31	22	1
1	A	124	ASN	O-C-N	-5.01	118.89	123.50	12	1
1	A	136	PHE	CB-CA-C	5.01	120.39	110.42	19	1
1	A	134	PHE	N-CA-C	5.00	117.84	111.69	19	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	132	GLU	CA	3
1	A	33	LEU	CA	2
1	A	101	LEU	CA	2
1	A	35	VAL	CA	1
1	A	107	LYS	CA	1
1	A	84	GLU	CA	1
1	A	105	THR	CA	1
1	A	103	ARG	CA	1
1	A	102	CYS	CA	1
1	A	106	CYS	CA	1

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	136	PHE	Sidechain	13
1	A	110	TYR	Sidechain	10
1	A	55	HIS	Sidechain	6
1	A	53	PHE	Sidechain	5
1	A	98	VAL	Peptide,Mainchain	5
1	A	78	PHE	Sidechain	4
1	A	112	TYR	Sidechain	4
1	A	56	TYR	Sidechain	4
1	A	104	ILE	Peptide	1
1	A	69	SER	Mainchain	1
1	A	76	PHE	Sidechain	1
1	A	134	PHE	Sidechain	1

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	839	846	846	5±3
All	All	18458	18612	18612	114

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:MET:SD	1:A:102:CYS:SG	0.79	2.80	7	3
1:A:54:VAL:HG23	1:A:76:PHE:HB3	0.71	1.60	12	2
1:A:104:ILE:HG22	1:A:106:CYS:SG	0.66	2.30	7	3
1:A:96:MET:HE3	1:A:101:LEU:HD22	0.66	1.67	17	1
1:A:103:ARG:HA	1:A:130:GLU:HA	0.62	1.71	11	1
1:A:35:VAL:O	1:A:102:CYS:SG	0.61	2.58	4	2
1:A:102:CYS:SG	1:A:103:ARG:N	0.60	2.75	20	5
1:A:106:CYS:SG	1:A:127:LEU:CD1	0.58	2.91	20	4
1:A:101:LEU:HD13	1:A:102:CYS:H	0.56	1.61	4	2
1:A:107:LYS:HG2	1:A:110:TYR:HB2	0.55	1.77	9	1
1:A:106:CYS:SG	1:A:127:LEU:CD2	0.55	2.95	18	1
1:A:103:ARG:HB2	1:A:131:VAL:H	0.55	1.62	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:LEU:HA	1:A:132:GLU:CB	0.52	2.35	14	2
1:A:96:MET:HE1	1:A:132:GLU:CD	0.52	2.30	17	1
1:A:36:ILE:HA	1:A:102:CYS:HB2	0.52	1.79	4	2
1:A:36:ILE:HD13	1:A:102:CYS:SG	0.51	2.46	18	4
1:A:106:CYS:SG	1:A:127:LEU:HB3	0.51	2.46	1	1
1:A:96:MET:SD	1:A:132:GLU:HB3	0.50	2.46	22	1
1:A:101:LEU:HD13	1:A:132:GLU:HG3	0.50	1.82	11	1
1:A:35:VAL:O	1:A:102:CYS:HB2	0.49	2.07	12	4
1:A:78:PHE:CG	1:A:85:VAL:HG11	0.49	2.43	18	11
1:A:101:LEU:HA	1:A:132:GLU:HB3	0.49	1.85	16	2
1:A:34:LYS:HB2	1:A:102:CYS:SG	0.49	2.47	10	1
1:A:34:LYS:HG2	1:A:102:CYS:SG	0.48	2.48	20	1
1:A:102:CYS:SG	1:A:103:ARG:NE	0.47	2.87	11	1
1:A:101:LEU:HD23	1:A:102:CYS:SG	0.47	2.49	17	1
1:A:101:LEU:HA	1:A:132:GLU:HA	0.47	1.86	22	1
1:A:36:ILE:HA	1:A:102:CYS:CB	0.47	2.40	4	2
1:A:36:ILE:CD1	1:A:102:CYS:SG	0.47	3.03	9	5
1:A:59:TRP:CE3	1:A:128:VAL:HG12	0.47	2.45	8	1
1:A:107:LYS:CG	1:A:110:TYR:HB2	0.47	2.40	9	1
1:A:35:VAL:C	1:A:102:CYS:HB3	0.47	2.35	4	1
1:A:96:MET:SD	1:A:133:LEU:HB2	0.46	2.49	22	2
1:A:32:VAL:HG13	1:A:106:CYS:HB3	0.46	1.87	7	1
1:A:82:LYS:HG3	1:A:83:GLY:H	0.46	1.70	10	4
1:A:106:CYS:SG	1:A:127:LEU:HD12	0.46	2.51	20	3
1:A:53:PHE:CE2	1:A:133:LEU:HG	0.46	2.46	12	1
1:A:106:CYS:HB2	1:A:107:LYS:HD2	0.45	1.88	7	1
1:A:100:GLU:O	1:A:132:GLU:HB3	0.45	2.11	16	1
1:A:106:CYS:SG	1:A:127:LEU:HB2	0.45	2.52	4	3
1:A:78:PHE:CD1	1:A:85:VAL:HG11	0.45	2.47	8	1
1:A:92:ALA:HB3	1:A:104:ILE:HD13	0.44	1.90	16	1
1:A:99:GLY:HA3	1:A:133:LEU:O	0.44	2.12	11	2
1:A:96:MET:SD	1:A:101:LEU:HD22	0.44	2.53	2	1
1:A:34:LYS:HB3	1:A:35:VAL:HG13	0.43	1.91	4	1
1:A:93:VAL:HG22	1:A:96:MET:CE	0.43	2.43	13	1
1:A:100:GLU:OE1	1:A:102:CYS:SG	0.43	2.77	19	1
1:A:96:MET:SD	1:A:132:GLU:OE2	0.43	2.77	14	1
1:A:96:MET:SD	1:A:101:LEU:HG	0.43	2.54	4	1
1:A:101:LEU:HD22	1:A:102:CYS:SG	0.43	2.54	13	1
1:A:97:LYS:O	1:A:98:VAL:C	0.42	2.62	14	5
1:A:102:CYS:SG	1:A:103:ARG:HG2	0.42	2.54	2	1
1:A:96:MET:CG	1:A:101:LEU:HD13	0.42	2.44	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:CYS:SG	1:A:107:LYS:HE3	0.42	2.55	9	1
1:A:36:ILE:HA	1:A:102:CYS:SG	0.42	2.54	13	1
1:A:106:CYS:SG	1:A:127:LEU:CB	0.42	3.08	22	1
1:A:55:HIS:CD2	1:A:70:LEU:HD12	0.41	2.50	2	1
1:A:59:TRP:HE3	1:A:128:VAL:HG13	0.41	1.76	15	1
1:A:98:VAL:O	1:A:98:VAL:HG12	0.41	2.16	19	1
1:A:48:ILE:HG23	1:A:49:GLY:H	0.41	1.76	12	1
1:A:48:ILE:O	1:A:80:LEU:HB3	0.40	2.16	12	1
1:A:70:LEU:HD22	1:A:75:LYS:HA	0.40	1.93	21	1
1:A:96:MET:HE2	1:A:133:LEU:HB2	0.40	1.92	9	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	107/149 (72%)	81±4 (76±4%)	19±3 (17±3%)	7±2 (6±2%)	2	18
All	All	2354/3278 (72%)	1792 (76%)	410 (17%)	152 (6%)	2	18

All 39 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	85	VAL	21
1	A	46	PRO	10
1	A	73	LYS	10
1	A	84	GLU	9
1	A	42	GLY	9
1	A	98	VAL	9
1	A	99	GLY	7
1	A	101	LEU	6
1	A	44	GLU	6
1	A	47	MET	6
1	A	120	LYS	5
1	A	119	PRO	4

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Mol	Chain	Res	Type	Models (Total)
1	A	32	VAL	3
1	A	115	ALA	3
1	A	100	GLU	3
1	A	74	ASP	3
1	A	39	GLU	3
1	A	118	PRO	3
1	A	102	CYS	2
1	A	41	THR	2
1	A	35	VAL	2
1	A	36	ILE	2
1	A	80	LEU	2
1	A	107	LYS	2
1	A	108	PRO	2
1	A	43	THR	2
1	A	69	SER	2
1	A	72	ARG	2
1	A	71	ASP	2
1	A	33	LEU	1
1	A	122	PRO	1
1	A	48	ILE	1
1	A	49	GLY	1
1	A	54	VAL	1
1	A	136	PHE	1
1	A	123	PRO	1
1	A	68	SER	1
1	A	70	LEU	1
1	A	75	LYS	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	90/124 (73%)	76±2 (85±3%)	14±2 (15±3%)	5	42
All	All	1980/2728 (73%)	1683 (85%)	297 (15%)	5	42

All 63 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	48	ILE	22
1	A	36	ILE	16
1	A	52	VAL	14
1	A	61	LEU	13
1	A	136	PHE	13
1	A	55	HIS	13
1	A	54	VAL	12
1	A	80	LEU	12
1	A	101	LEU	11
1	A	59	TRP	11
1	A	104	ILE	9
1	A	82	LYS	8
1	A	46	PRO	6
1	A	96	MET	6
1	A	103	ARG	6
1	A	87	LYS	6
1	A	129	PHE	6
1	A	39	GLU	5
1	A	127	LEU	5
1	A	60	LEU	5
1	A	112	TYR	5
1	A	33	LEU	5
1	A	34	LYS	4
1	A	50	ASP	4
1	A	131	VAL	4
1	A	133	LEU	4
1	A	91	ILE	4
1	A	102	CYS	4
1	A	107	LYS	4
1	A	130	GLU	4
1	A	128	VAL	4
1	A	98	VAL	3
1	A	100	GLU	3
1	A	97	LYS	3
1	A	35	VAL	3
1	A	108	PRO	3
1	A	132	GLU	3
1	A	56	TYR	3
1	A	73	LYS	2
1	A	119	PRO	2
1	A	67	ASP	2
1	A	84	GLU	2
1	A	135	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	37	LYS	2
1	A	122	PRO	1
1	A	70	LEU	1
1	A	69	SER	1
1	A	121	ILE	1
1	A	47	MET	1
1	A	72	ARG	1
1	A	74	ASP	1
1	A	105	THR	1
1	A	75	LYS	1
1	A	43	THR	1
1	A	45	THR	1
1	A	62	ASP	1
1	A	109	GLU	1
1	A	106	CYS	1
1	A	118	PRO	1
1	A	137	LYS	1
1	A	44	GLU	1
1	A	38	ARG	1
1	A	76	PHE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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