Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 04:41 PM BST

PDB ID	:	1ROU
Title	:	STRUCTURE OF FKBP59-I, THE N-TERMINAL DOMAIN OF A 59 KDA FK506-BINDING PROTEIN, NMR, 22 STRUCTURES
Authors	:	Craescu, C.T.; Rouviere, N.; Popescu, A.; Cerpolini, E.; Lebeau, M.-C.; Baulieu, E.-E.; Mispelter, J.
Deposited on	:	1996-06-14

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

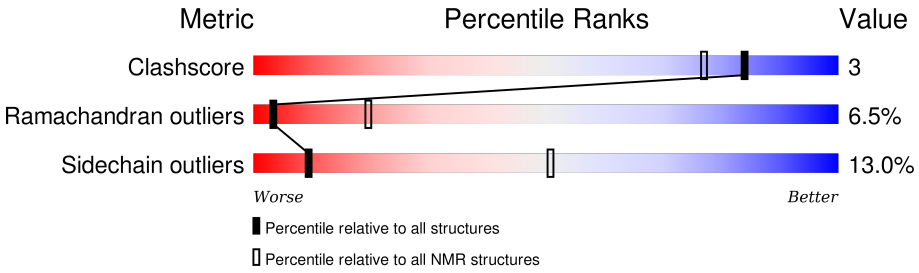
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	149	40% 30% • 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)	0.69	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
			Total	C	H	N	O	S	
1	A	118	1832	589	918	148	173	4	0

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

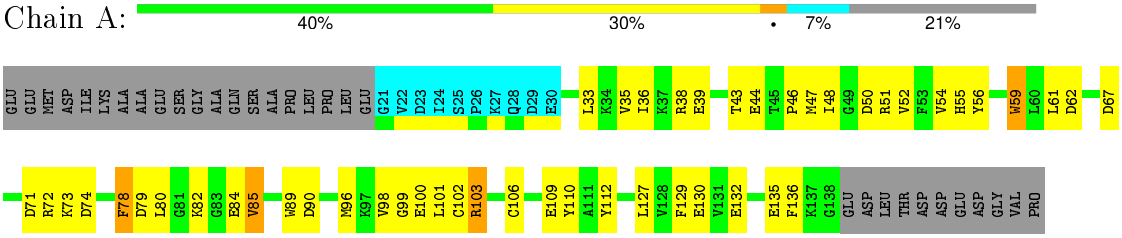
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

Chain A:



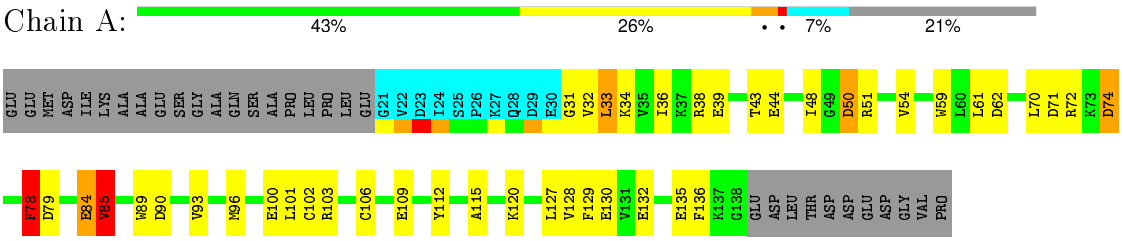
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: FKBP59-I

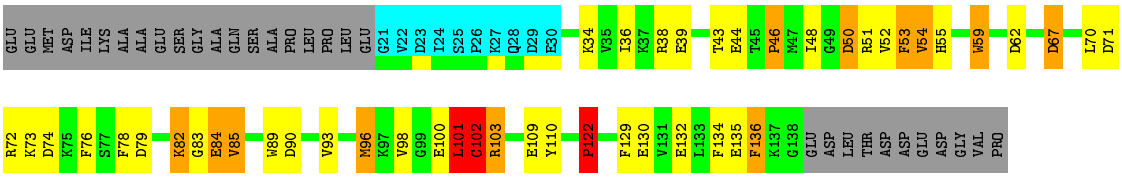
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: FKBP59-I

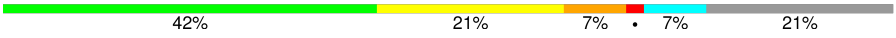
Chain A:

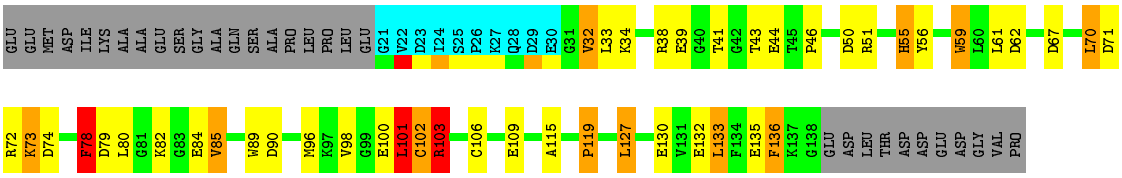


4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: FKBP59-I

Chain A:

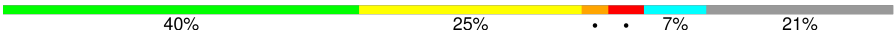


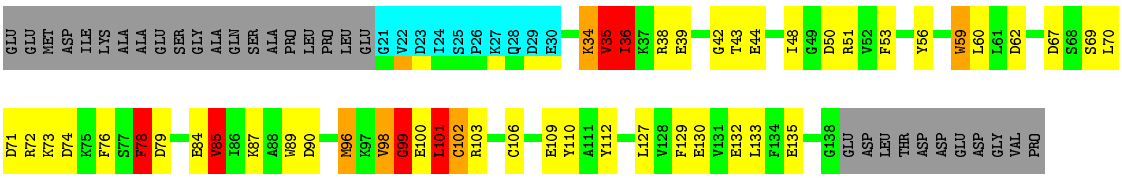


4.2.4 Score per residue for model 4

- Molecule 1: FKBP59-I

Chain A:

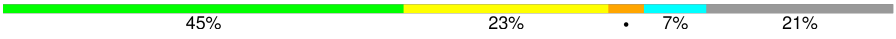


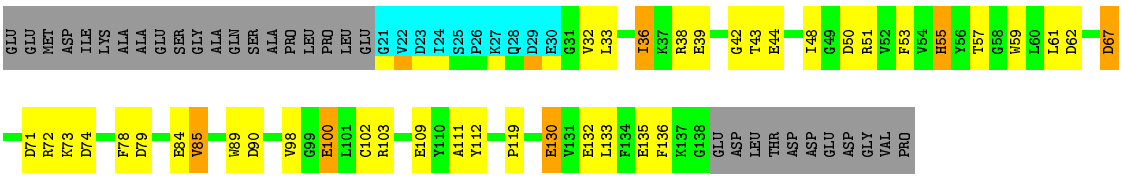


4.2.5 Score per residue for model 5

- Molecule 1: FKBP59-I

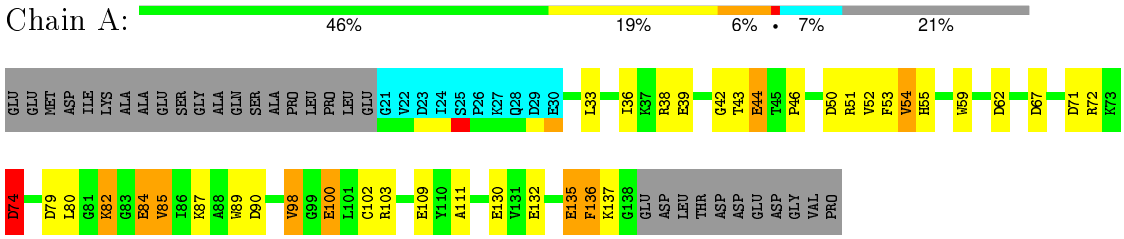
Chain A:





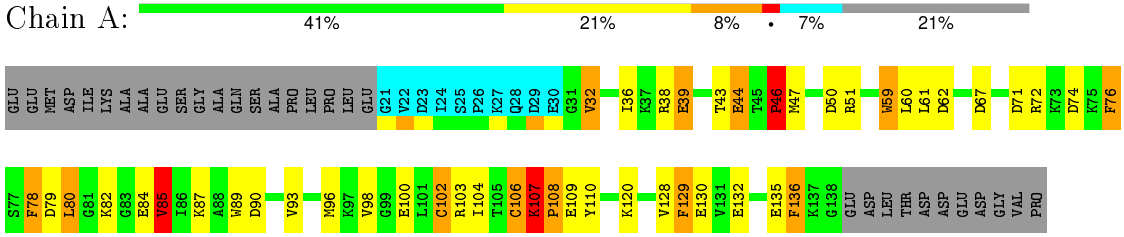
4.2.6 Score per residue for model 6

- Molecule 1: FKBP59-I



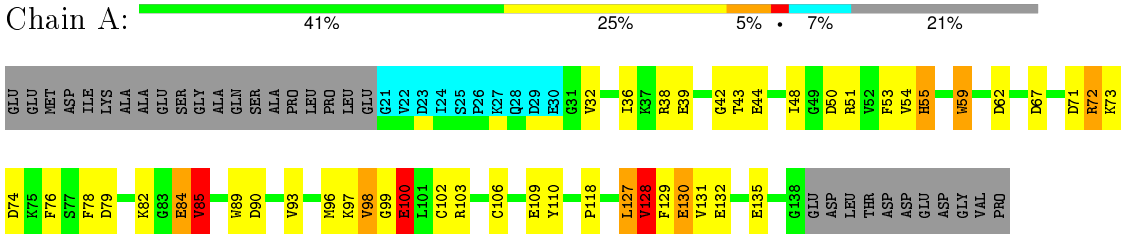
4.2.7 Score per residue for model 7

- Molecule 1: FKBP59-I



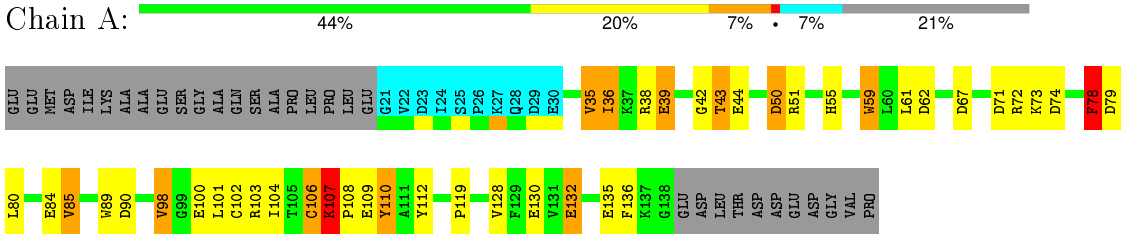
4.2.8 Score per residue for model 8

- Molecule 1: FKBP59-I



4.2.9 Score per residue for model 9

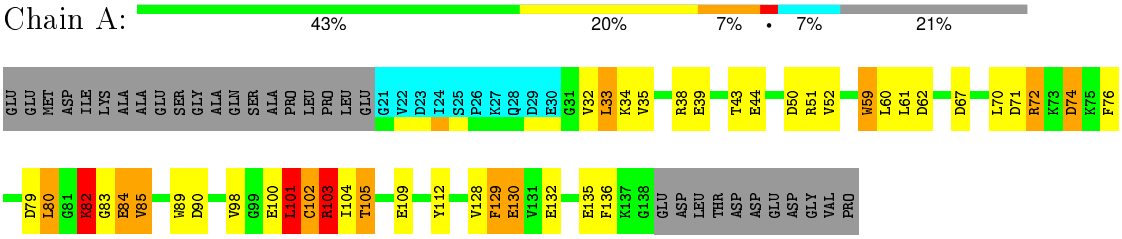
- Molecule 1: FKBP59-I



4.2.10 Score per residue for model 10

- Molecule 1: FKBP59-I

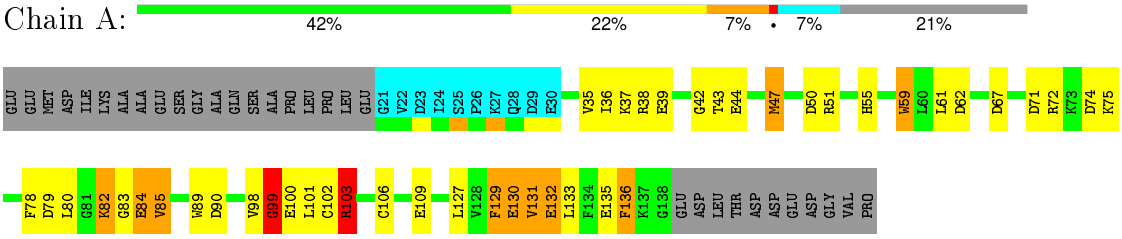
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: FKBP59-I

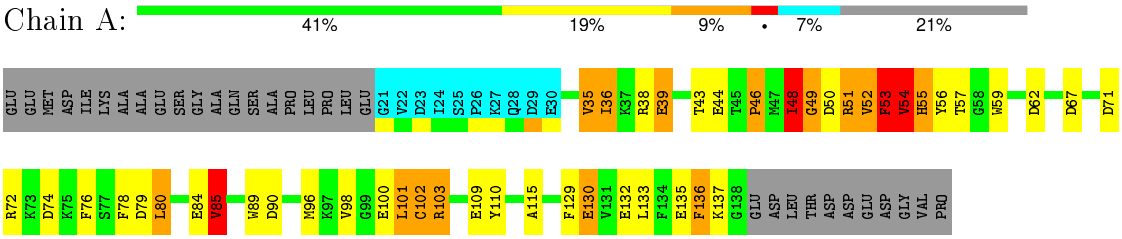
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: FKBP59-I

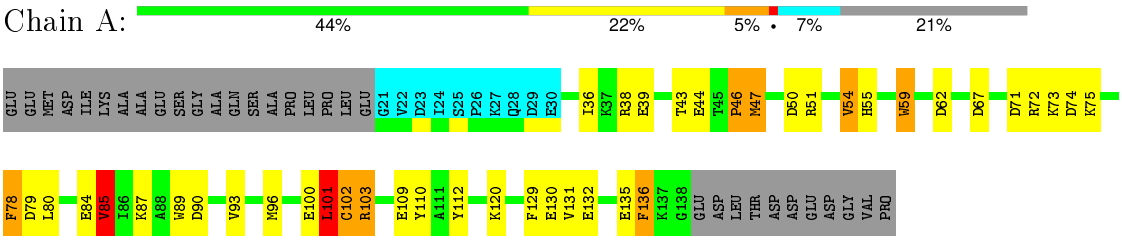
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: FKBP59-I

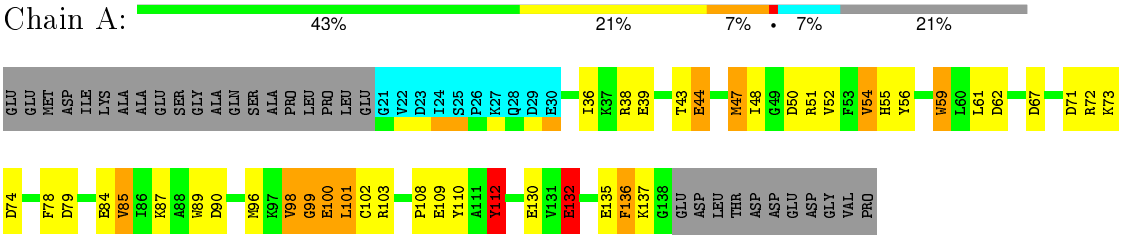
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: FKBP59-I

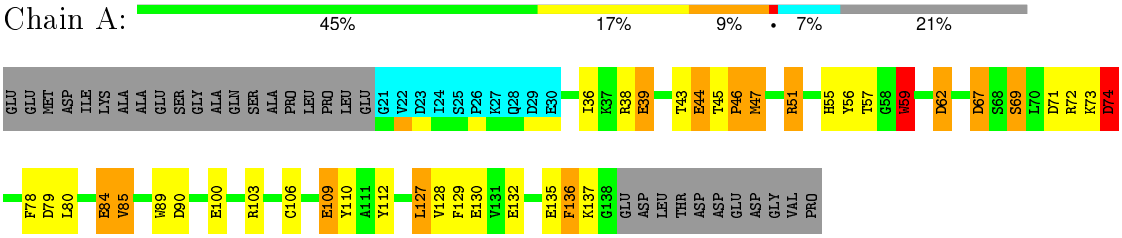
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: FKBP59-I

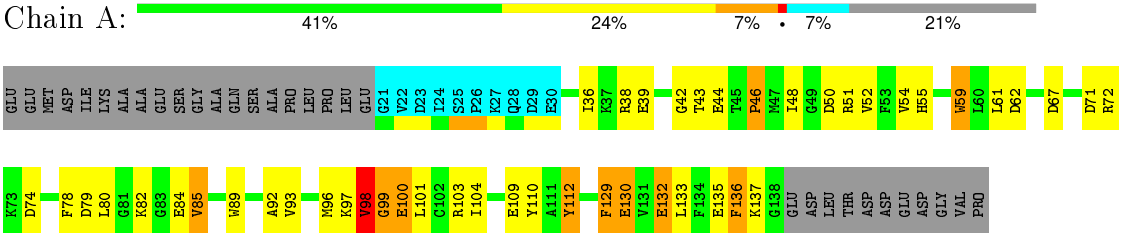
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: FKBP59-I

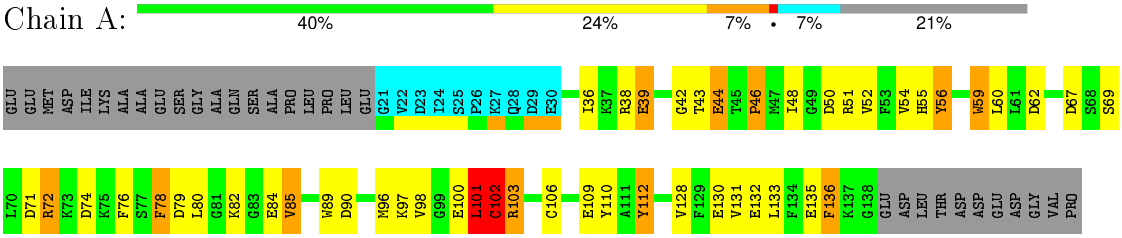
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: FKBP59-I

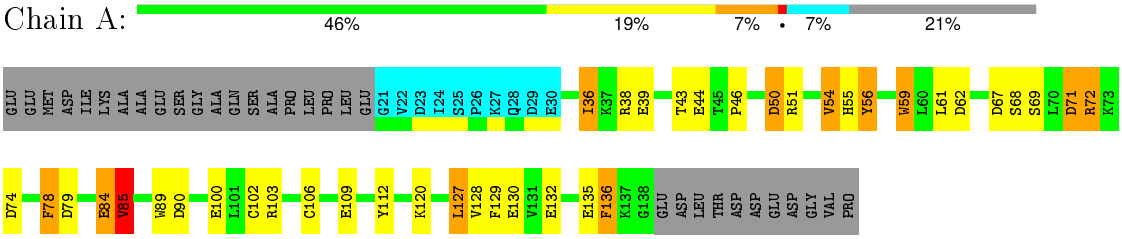
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: FKBP59-I

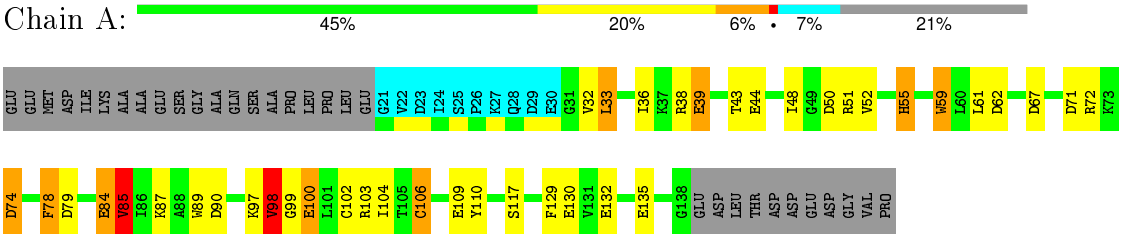
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: FKBP59-I

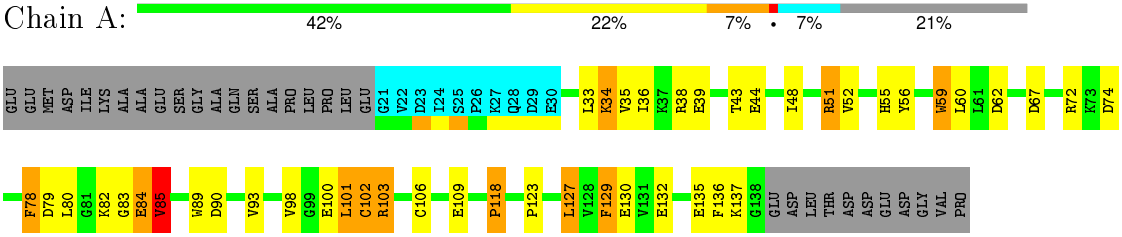
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: FKBP59-I

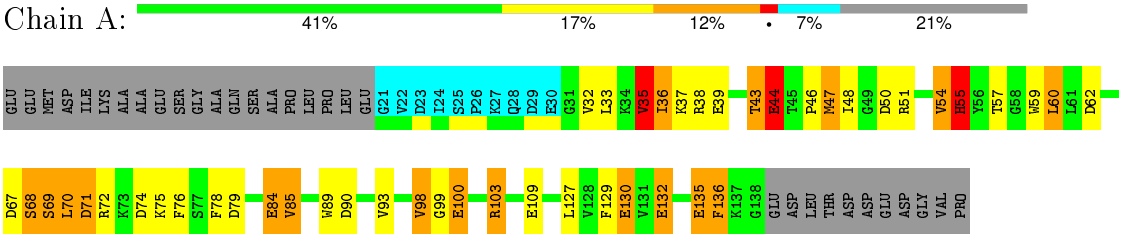
Chain A:



4.2.21 Score per residue for model 21

- Molecule 1: FKBP59-I

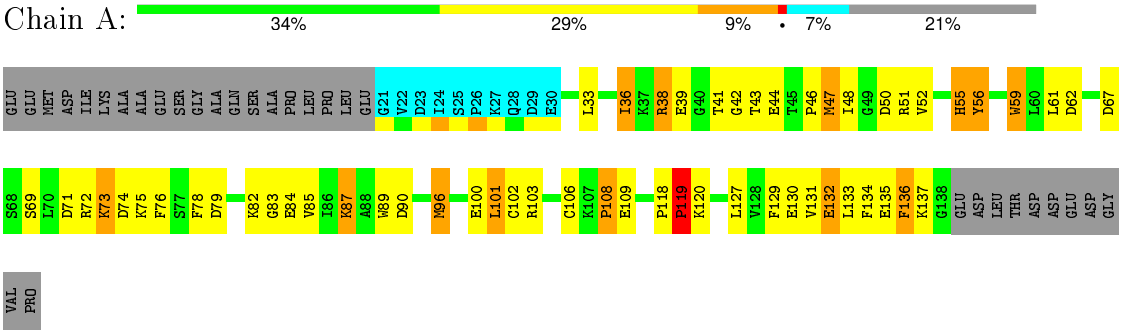
Chain A:



4.2.22 Score per residue for model 22

- Molecule 1: FKBP59-I

Chain A:



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. No validations of the models with respect to experimental NMR restraints is performed at this time.

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	1.65±0.01	9±1/859 (1.0±0.1%)	1.98±0.10	39±4/1159 (3.4±0.4%)
All	All	1.65	188/18898 (1.0%)	1.99	867/25498 (3.4%)

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	109	GLU	CD-OE2	10.36	1.37	1.25	22	22
1	A	130	GLU	CD-OE2	10.33	1.37	1.25	10	22
1	A	84	GLU	CD-OE2	10.28	1.36	1.25	19	22
1	A	100	GLU	CD-OE2	10.27	1.36	1.25	21	22
1	A	44	GLU	CD-OE2	10.22	1.36	1.25	22	22
1	A	135	GLU	CD-OE2	10.14	1.36	1.25	15	22
1	A	39	GLU	CD-OE2	10.04	1.36	1.25	10	22
1	A	132	GLU	CD-OE2	9.99	1.36	1.25	5	22
1	A	53	PHE	CB-CG	6.82	1.62	1.51	12	1
1	A	89	TRP	CG-CD2	-5.43	1.34	1.43	9	2
1	A	71	ASP	CG-OD2	5.14	1.37	1.25	12	3
1	A	79	ASP	CG-OD2	5.10	1.37	1.25	15	1
1	A	67	ASP	CG-OD2	5.06	1.36	1.25	15	2
1	A	62	ASP	CG-OD2	5.03	1.36	1.25	10	3

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	69	SER	O-C-N	-29.33	75.77	122.70	21	1
1	A	69	SER	CA-C-N	25.27	172.79	117.20	21	1
1	A	107	LYS	N-CA-CB	-13.65	86.03	110.60	9	2
1	A	107	LYS	N-CA-C	13.58	147.67	111.00	7	2
1	A	53	PHE	CB-CG-CD2	-11.76	112.57	120.80	12	1
1	A	105	THR	CA-CB-CG2	11.71	128.79	112.40	10	1
1	A	55	HIS	CA-CB-CG	11.43	133.03	113.60	22	2
1	A	69	SER	CA-C-O	-10.99	97.03	120.10	21	1
1	A	102	CYS	N-CA-CB	10.54	129.57	110.60	2	3
1	A	131	VAL	CA-CB-CG1	9.81	125.61	110.90	11	3
1	A	53	PHE	N-CA-CB	-9.40	93.67	110.60	12	1
1	A	98	VAL	O-C-N	-9.29	107.41	123.20	16	1
1	A	102	CYS	CB-CA-C	-9.22	91.97	110.40	14	1
1	A	103	ARG	NE-CZ-NH1	9.14	124.87	120.30	11	22
1	A	72	ARG	NE-CZ-NH1	9.10	124.85	120.30	8	22
1	A	82	LYS	N-CA-CB	-9.00	94.40	110.60	8	6
1	A	38	ARG	NE-CZ-NH1	8.99	124.80	120.30	8	22
1	A	33	LEU	CB-CA-C	8.94	127.19	110.20	1	7
1	A	51	ARG	NE-CZ-NH1	8.93	124.77	120.30	12	22
1	A	59	TRP	CA-CB-CG	8.82	130.47	113.70	11	3
1	A	54	VAL	CG1-CB-CG2	-8.80	96.82	110.90	16	9
1	A	132	GLU	N-CA-CB	8.63	126.13	110.60	9	5
1	A	50	ASP	CB-CG-OD1	8.55	126.00	118.30	16	10
1	A	106	CYS	N-CA-CB	-8.54	95.23	110.60	9	2
1	A	46	PRO	N-CA-CB	-8.53	93.06	103.30	15	3
1	A	106	CYS	CB-CA-C	-8.53	93.34	110.40	17	1
1	A	101	LEU	CB-CA-C	8.47	126.29	110.20	4	4
1	A	137	LYS	CB-CA-C	8.26	126.92	110.40	16	6
1	A	50	ASP	CB-CG-OD2	-8.20	110.92	118.30	16	18
1	A	90	ASP	CB-CG-OD2	-8.18	110.94	118.30	21	21
1	A	78	PHE	CB-CG-CD2	-8.06	115.16	120.80	21	9
1	A	132	GLU	CB-CA-C	-7.76	94.88	110.40	17	3
1	A	100	GLU	CB-CA-C	7.70	125.79	110.40	14	5
1	A	90	ASP	CB-CG-OD1	7.61	125.15	118.30	21	19
1	A	71	ASP	CB-CG-OD1	7.54	125.09	118.30	5	20
1	A	36	ILE	N-CA-C	7.54	131.35	111.00	4	2
1	A	100	GLU	N-CA-C	7.54	131.35	111.00	5	1
1	A	98	VAL	CA-CB-CG1	7.54	122.20	110.90	9	2
1	A	71	ASP	CB-CG-OD2	-7.53	111.52	118.30	5	21
1	A	67	ASP	CB-CG-OD2	-7.48	111.57	118.30	15	20
1	A	56	TYR	CB-CG-CD2	-7.48	116.51	121.00	18	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	59	TRP	CB-CG-CD2	7.44	136.27	126.60	10	16
1	A	43	THR	CA-CB-OG1	7.42	124.58	109.00	16	22
1	A	84	GLU	CA-C-N	-7.37	100.99	117.20	16	10
1	A	67	ASP	CB-CG-OD1	7.33	124.90	118.30	17	20
1	A	74	ASP	CB-CG-OD1	7.29	124.86	118.30	12	22
1	A	74	ASP	CB-CG-OD2	-7.28	111.75	118.30	2	22
1	A	103	ARG	CA-CB-CG	7.26	129.37	113.40	11	3
1	A	70	LEU	CB-CG-CD2	7.25	123.32	111.00	10	4
1	A	128	VAL	CA-CB-CG1	7.20	121.69	110.90	8	2
1	A	84	GLU	N-CA-CB	-7.02	97.97	110.60	8	4
1	A	103	ARG	NE-CZ-NH2	-7.02	116.79	120.30	4	22
1	A	89	TRP	CD1-NE1-CE2	-7.02	102.69	109.00	22	22
1	A	129	PHE	N-CA-CB	7.01	123.22	110.60	11	13
1	A	105	THR	OG1-CB-CG2	-7.01	93.89	110.00	10	1
1	A	82	LYS	CA-CB-CG	6.79	128.34	113.40	10	1
1	A	79	ASP	CB-CG-OD2	-6.76	112.22	118.30	7	22
1	A	62	ASP	N-CA-CB	-6.75	98.45	110.60	15	1
1	A	52	VAL	N-CA-CB	-6.72	96.70	111.50	20	8
1	A	99	GLY	N-CA-C	6.70	129.84	113.10	4	4
1	A	62	ASP	CB-CG-OD2	-6.69	112.28	118.30	21	22
1	A	85	VAL	CA-CB-CG2	6.64	120.86	110.90	14	15
1	A	59	TRP	CD1-NE1-CE2	-6.63	103.03	109.00	16	22
1	A	122	PRO	CB-CA-C	6.61	128.52	112.00	2	1
1	A	98	VAL	CG1-CB-CG2	-6.60	100.34	110.90	19	11
1	A	84	GLU	CB-CA-C	6.59	123.59	110.40	21	8
1	A	59	TRP	CB-CG-CD1	-6.58	118.45	127.00	10	10
1	A	101	LEU	CB-CG-CD2	6.56	122.15	111.00	12	3
1	A	76	PHE	CB-CA-C	6.53	123.46	110.40	10	5
1	A	38	ARG	NE-CZ-NH2	-6.49	117.06	120.30	1	21
1	A	32	VAL	CA-CB-CG2	6.43	120.55	110.90	10	4
1	A	128	VAL	CA-CB-CG2	6.40	120.50	110.90	10	3
1	A	68	SER	N-CA-C	6.37	128.21	111.00	18	2
1	A	54	VAL	CA-CB-CG2	6.33	120.40	110.90	14	4
1	A	33	LEU	N-CA-CB	6.31	123.03	110.40	20	6
1	A	79	ASP	CB-CG-OD1	6.28	123.95	118.30	7	21
1	A	51	ARG	NE-CZ-NH2	-6.25	117.17	120.30	11	20
1	A	78	PHE	CB-CG-CD1	-6.25	116.43	120.80	11	10
1	A	72	ARG	NE-CZ-NH2	-6.22	117.19	120.30	22	20
1	A	35	VAL	N-CA-C	6.22	127.78	111.00	4	2
1	A	62	ASP	CB-CG-OD1	6.21	123.89	118.30	21	17
1	A	93	VAL	CG1-CB-CG2	-6.20	100.97	110.90	16	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	56	TYR	CB-CG-CD1	6.20	124.72	121.00	18	2
1	A	85	VAL	CB-CA-C	6.17	123.12	111.40	11	12
1	A	34	LYS	N-CA-CB	-6.16	99.50	110.60	20	1
1	A	47	MET	N-CA-C	6.13	127.54	111.00	7	1
1	A	82	LYS	CB-CA-C	6.11	122.63	110.40	16	2
1	A	57	THR	N-CA-CB	6.09	121.87	110.30	12	4
1	A	47	MET	CB-CA-C	6.08	122.55	110.40	13	6
1	A	108	PRO	CB-CA-C	6.06	127.16	112.00	7	1
1	A	98	VAL	N-CA-C	6.06	127.35	111.00	9	2
1	A	136	PHE	CB-CG-CD1	-6.04	116.58	120.80	7	4
1	A	74	ASP	N-CA-C	6.01	127.23	111.00	15	1
1	A	79	ASP	CB-CA-C	5.93	122.27	110.40	8	6
1	A	56	TYR	N-CA-CB	5.93	121.27	110.60	22	2
1	A	96	MET	N-CA-CB	-5.91	99.95	110.60	2	1
1	A	60	LEU	CA-CB-CG	5.88	128.82	115.30	21	2
1	A	55	HIS	N-CA-CB	5.86	121.15	110.60	20	2
1	A	131	VAL	CA-CB-CG2	5.83	119.64	110.90	17	1
1	A	111	ALA	N-CA-CB	-5.82	101.95	110.10	6	2
1	A	101	LEU	N-CA-CB	5.76	121.93	110.40	17	3
1	A	136	PHE	CB-CG-CD2	-5.74	116.78	120.80	9	3
1	A	52	VAL	CA-CB-CG1	5.66	119.39	110.90	22	2
1	A	112	TYR	CB-CG-CD1	-5.65	117.61	121.00	17	4
1	A	35	VAL	CA-CB-CG1	5.64	119.35	110.90	9	1
1	A	31	GLY	N-CA-C	5.63	127.17	113.10	1	1
1	A	69	SER	N-CA-CB	5.59	118.89	110.50	15	2
1	A	134	PHE	CB-CG-CD1	5.58	124.70	120.80	2	1
1	A	107	LYS	CB-CA-C	-5.56	99.28	110.40	7	1
1	A	98	VAL	CB-CA-C	-5.55	100.86	111.40	2	1
1	A	105	THR	CA-CB-OG1	5.54	120.63	109.00	10	1
1	A	35	VAL	CB-CA-C	5.44	121.73	111.40	4	2
1	A	110	TYR	CB-CG-CD2	-5.41	117.76	121.00	19	2
1	A	89	TRP	CG-CD2-CE3	-5.40	129.04	133.90	9	4
1	A	34	LYS	CA-CB-CG	5.39	125.25	113.40	4	1
1	A	69	SER	CB-CA-C	5.37	120.30	110.10	18	1
1	A	83	GLY	N-CA-C	-5.37	99.69	113.10	22	1
1	A	53	PHE	CB-CA-C	5.34	121.09	110.40	2	2
1	A	131	VAL	CG1-CB-CG2	-5.33	102.37	110.90	17	2
1	A	98	VAL	CA-CB-CG2	5.29	118.83	110.90	5	1
1	A	50	ASP	CA-CB-CG	5.28	125.02	113.40	11	1
1	A	46	PRO	CB-CA-C	5.26	125.16	112.00	13	1
1	A	46	PRO	N-CA-C	5.25	125.75	112.10	7	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	44	GLU	CB-CA-C	5.23	120.85	110.40	15	1
1	A	87	LYS	CB-CA-C	5.22	120.84	110.40	22	1
1	A	32	VAL	CG1-CB-CG2	-5.20	102.58	110.90	8	2
1	A	67	ASP	CA-CB-CG	5.16	124.75	113.40	9	1
1	A	55	HIS	CG-ND1-CE1	-5.10	99.07	105.70	8	1
1	A	52	VAL	CA-CB-CG2	5.09	118.53	110.90	2	2
1	A	137	LYS	CA-C-N	5.08	126.37	116.20	16	1
1	A	74	ASP	N-CA-CB	-5.08	101.46	110.60	4	1
1	A	100	GLU	N-CA-CB	5.08	119.73	110.60	5	1
1	A	85	VAL	N-CA-CB	-5.07	100.36	111.50	16	1
1	A	112	TYR	CA-CB-CG	5.05	122.99	113.40	14	1
1	A	137	LYS	N-CA-CB	-5.04	101.53	110.60	15	1
1	A	119	PRO	N-CA-C	5.00	125.11	112.10	22	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	112	TYR	Sidechain	4
1	A	56	TYR	Sidechain	4
1	A	78	PHE	Sidechain	4
1	A	76	PHE	Sidechain	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	104	ILE	Peptide	1
1	A	134	PHE	Sidechain	1
1	A	69	SER	Mainchain	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	107

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: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
1:A:101:LEU:HA	1:A:132:GLU:CB	0.52	2.35	14	2
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:96:MET:CE	1:A:101:LEU:HD22	0.45	2.41	17	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: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
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:35:VAL:C	1:A:102:CYS:HB3	0.42	2.35	4	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

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	107/149 (72%)	81±4 (76±4%)	19±3 (17±3%)	7±2 (6±2%)	3	19
All	All	2354/3278 (72%)	1792 (76%)	410 (17%)	152 (6%)	3	19

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	73	LYS	10
1	A	46	PRO	10
1	A	84	GLU	9
1	A	42	GLY	9
1	A	98	VAL	9
1	A	99	GLY	7
1	A	47	MET	6
1	A	101	LEU	6
1	A	44	GLU	6
1	A	120	LYS	5
1	A	119	PRO	4
1	A	32	VAL	3
1	A	74	ASP	3
1	A	115	ALA	3
1	A	100	GLU	3
1	A	39	GLU	3
1	A	118	PRO	3
1	A	43	THR	2
1	A	41	THR	2
1	A	36	ILE	2
1	A	80	LEU	2
1	A	107	LYS	2
1	A	72	ARG	2
1	A	102	CYS	2
1	A	69	SER	2
1	A	108	PRO	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	71	ASP	2
1	A	35	VAL	2
1	A	49	GLY	1
1	A	68	SER	1
1	A	54	VAL	1
1	A	75	LYS	1
1	A	70	LEU	1
1	A	48	ILE	1
1	A	33	LEU	1
1	A	123	PRO	1
1	A	136	PHE	1
1	A	122	PRO	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	90/124 (73%)	78±2 (87±3%)	12±2 (13±3%)	9 51
All	All	1980/2728 (73%)	1722 (87%)	258 (13%)	9 51

All 58 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	36	ILE	16
1	A	59	TRP	16
1	A	55	HIS	14
1	A	48	ILE	13
1	A	136	PHE	13
1	A	80	LEU	12
1	A	61	LEU	12
1	A	101	LEU	11
1	A	129	PHE	8
1	A	54	VAL	7
1	A	87	LYS	7
1	A	130	GLU	6
1	A	127	LEU	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	46	PRO	6
1	A	112	TYR	6
1	A	102	CYS	6
1	A	82	LYS	6
1	A	103	ARG	5
1	A	60	LEU	5
1	A	50	ASP	4
1	A	74	ASP	4
1	A	97	LYS	4
1	A	96	MET	4
1	A	133	LEU	4
1	A	34	LYS	3
1	A	100	GLU	3
1	A	39	GLU	3
1	A	128	VAL	3
1	A	108	PRO	3
1	A	56	TYR	3
1	A	35	VAL	3
1	A	67	ASP	3
1	A	51	ARG	3
1	A	84	GLU	2
1	A	73	LYS	2
1	A	75	LYS	2
1	A	135	GLU	2
1	A	119	PRO	2
1	A	107	LYS	2
1	A	72	ARG	2
1	A	76	PHE	2
1	A	33	LEU	2
1	A	37	LYS	2
1	A	132	GLU	2
1	A	62	ASP	1
1	A	45	THR	1
1	A	117	SER	1
1	A	70	LEU	1
1	A	38	ARG	1
1	A	52	VAL	1
1	A	105	THR	1
1	A	44	GLU	1
1	A	69	SER	1
1	A	122	PRO	1
1	A	106	CYS	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	137	LYS	1
1	A	109	GLU	1
1	A	118	PRO	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 carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided