WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 01:52 PM BST

PDB ID : 1A57
Title : THE THREE-DIMENSIONAL STRUCTURE OF A HELIX-LESS VARIANT OF INTESTINAL FATTY ACID BINDING PROTEIN, NMR, 20 STRUCTURES
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Deposited on : 1998-02-20

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	Percentile Ranks	Value
Clashscore		31
Ramachandran outliers		16.7%
Sidechain outliers		34.6%

Worse   *Better*

▌ Percentile relative to all structures

☐ Percentile relative to all NMR structures
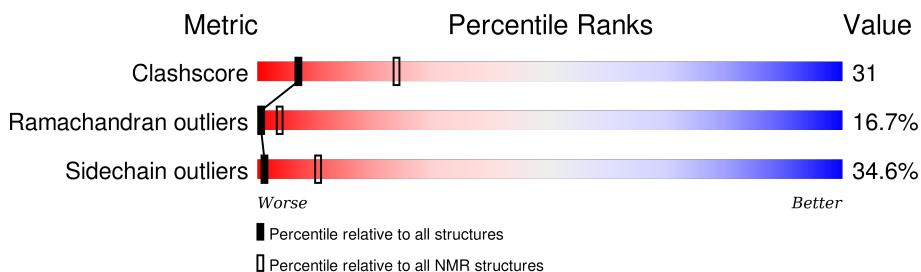
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	116	10% 50% 21% 8% 11%
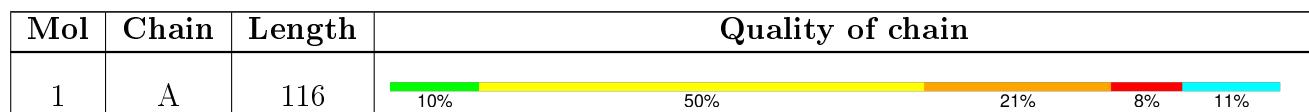
2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 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:2-A:8, A:21-A:116 (103)	0.64	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1838 atoms, of which 909 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INTESTINAL FATTY ACID-BINDING PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	116	1838	586	909	157	185	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	DELETION	UNP P02693
A	?	-	LYS	DELETION	UNP P02693
A	?	-	PHE	DELETION	UNP P02693
A	?	-	MET	DELETION	UNP P02693
A	?	-	GLU	DELETION	UNP P02693
A	?	-	LYS	DELETION	UNP P02693
A	?	-	MET	DELETION	UNP P02693
A	?	-	GLY	DELETION	UNP P02693
A	?	-	ILE	DELETION	UNP P02693
A	?	-	ASN	DELETION	UNP P02693
A	?	-	VAL	DELETION	UNP P02693
A	?	-	VAL	DELETION	UNP P02693
A	?	-	LYS	DELETION	UNP P02693
A	?	-	ARG	DELETION	UNP P02693
A	?	-	LYS	DELETION	UNP P02693
A	15	SER	LEU	ENGINEERED	UNP P02693

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: INTESTINAL FATTY ACID-BINDING PROTEIN
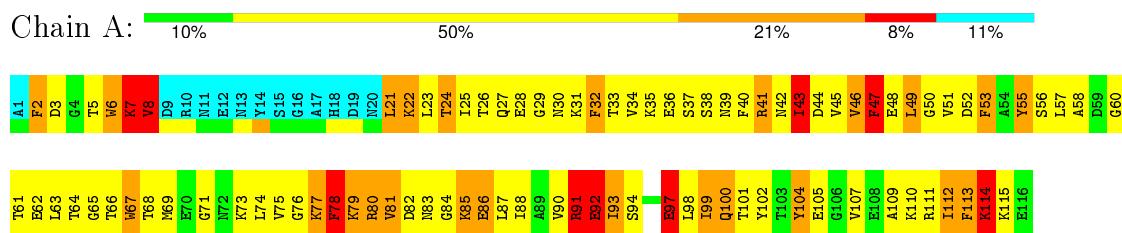
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN
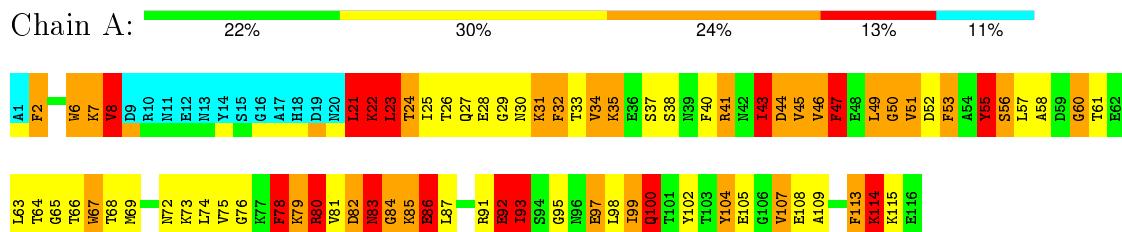
4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN
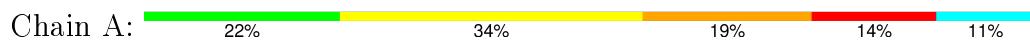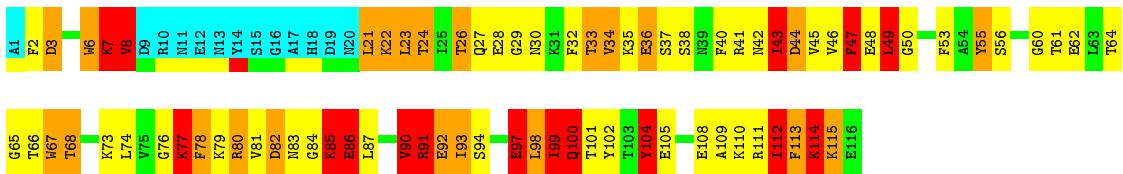
4.2.3 Score per residue for model 3

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN
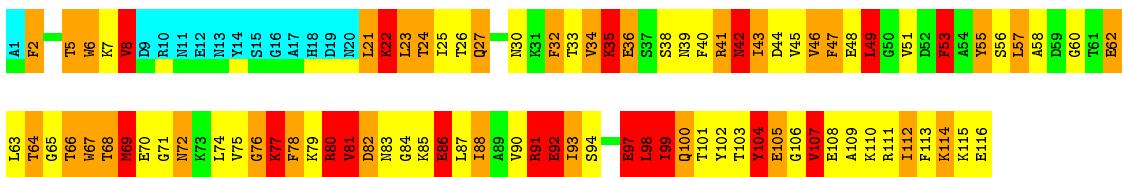
4.2.4 Score per residue for model 4

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN
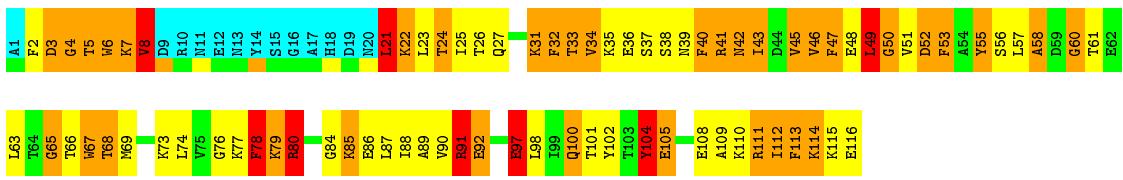
### 4.2.5 Score per residue for model 5

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN
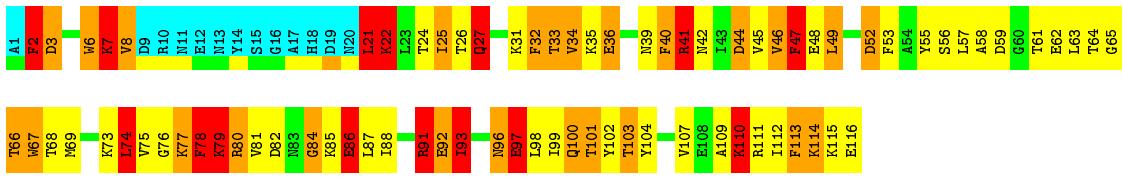
4.2.6 Score per residue for model 6

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

Chain A: 24% 31% 22% 12% 11%

A1 F2 D3 W6 K7 V8 D9 R10 N11 E12 N13 Y14 S15 G16 A17 H18 D19 N20 L21 K22 L23 T24 I25 T26 Q27 E28 G29 F32 T33 V34 K35 S38 N39 F40 R41 M42 I43 D44 V45 V46 F47 E48 L49 G50 V51 D52 F53 A54 Y55 S56 L57 A58 D59 G60 T61 E62 L63

T64 G65 T66 W67 T68 M69 E70 G71 N72 K73 L74 V75 G76 K77 F78 K79 R80 V81 D82 N83 G84 K85 E86 L87 I88 A89 V90 R91 E92 I93 S94 E97 L98 I99 Q100 T101 Y102 T103 Y104 E105 G106 V107 E108 A109 K110 R111 I112 F113 K114 K115 E116

4.2.7 Score per residue for model 7

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

Chain A: 20% 39% 20% 10% 11%

A1 F2 D3 G4 T5 W6 K7 V8 D9 R10 N11 E12 N13 Y14 S15 G16 A17 H18 D19 N20 L21 K22 L23 T24 I25 K31 F32 T33 V34 K35 E36 S37 S38 N39 F40 R41 M42 I43 D44 V45 V46 F47 E48 L49 G50 V51 D52 F53 A54 Y55 S56 L57 A58 D59 G60 T61 E62 L63 T64

G65 T66 W67 T68 M69 E70 L74 V75 G76 K77 F78 K79 R80 V81 D82 N83 G84 K85 E86 L87 I88 A89 V90 R91 E92 I93 S94 G95 N96 E97 L98 I99 Q100 T101 Y102 T103 Y104 E105 A109 K110 R111 I112 F113 K114 K115 E116

4.2.8 Score per residue for model 8

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

Chain A: 22% 34% 22% 12% 11%

A1 F2 D3 G4 T5 W6 K7 V8 D9 R10 N11 E12 N13 Y14 S15 G16 A17 H18 D19 N20 L21 K22 L23 T24 I25 T26 Q27 E28 G29 F32 T33 V34 K35 S38 N39 F40 R41 M42 I43 D44 V45 V46 F47 E48 L49 G50 V51 D52 F53 A54 Y55 S56 L57 A58 D59 L63 T64

G65 T66 W67 T68 M69 L74 V75 G76 K77 F78 K79 R80 V81 D82 N83 G84 K85 E86 L87 I88 A89 V90 R91 E92 I93 S94 E97 L98 I99 Q100 T101 Y102 T103 Y104 A109 K110 R111 I112 F113 K114 K115 E116
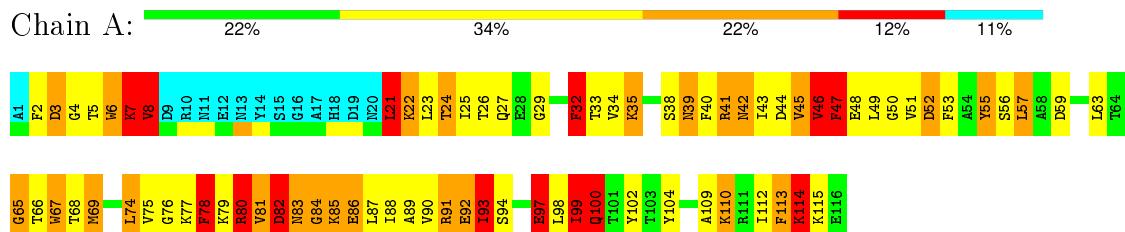
4.2.9 Score per residue for model 9

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

Chain A: 20% 34% 22% 13% 11%

A1 F2 D3 W6 K7 V8 D9 R10 N11 E12 N13 Y14 S15 G16 A17 H18 D19 N20 L21 K22 L23 T24 I25 T26 Q27 E28 G29 F32 T33 V34 K35 N39 F40 R41 M42 I43 D44 V45 V46 F47 E48 L49 G50 V51 D52 F53 A54 Y55 S56 L57 A58 D59 L63 T64 G65 T66

W67 T68 G71 N72 K73 L74 V75 G76 K77 F78 K79 R80 V81 D82 N83 G84 K85 E86 L87 I88 A89 V90 R91 E92 I93 E97 L98 I99 Q100 T101 Y102 T103 Y104 E105 G106 V107 E108 A109 K110 R111 I112 F113 K114 K115 E116

4.2.10 Score per residue for model 10

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

Chain A:
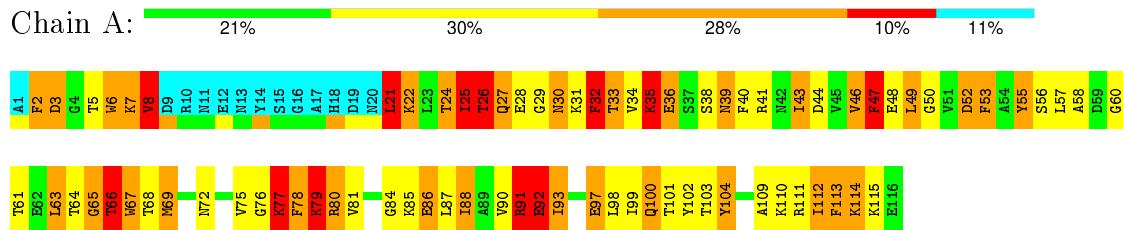
## 4.2.11 Score per residue for model 11

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

Chain A:
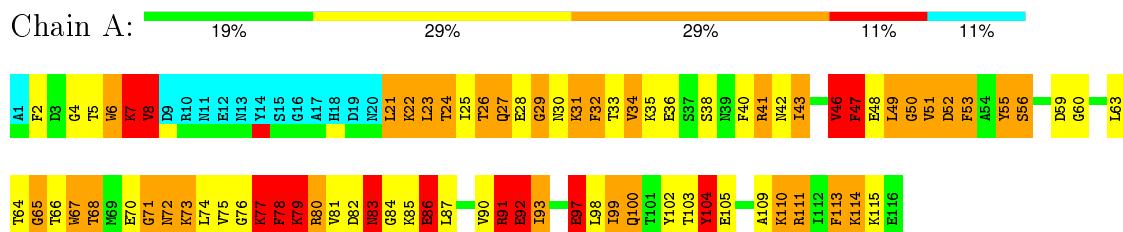
4.2.12 Score per residue for model 12

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

Chain A:
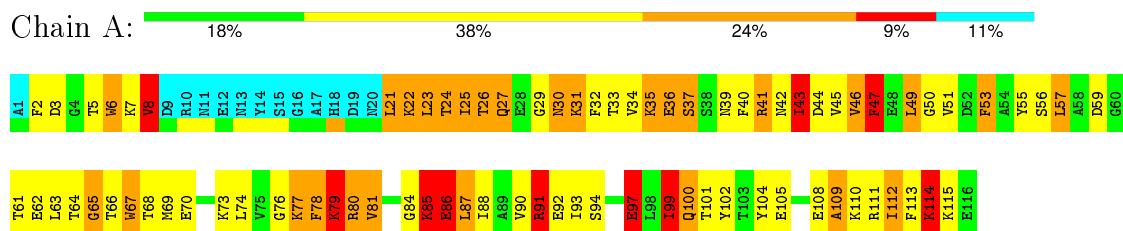
4.2.13 Score per residue for model 13

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

Chain A:
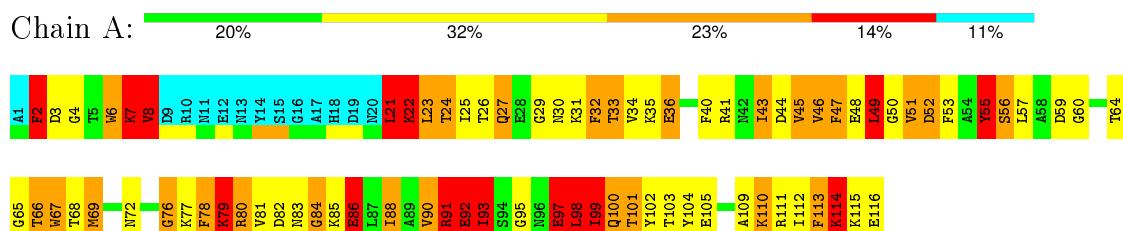
4.2.14 Score per residue for model 14

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN
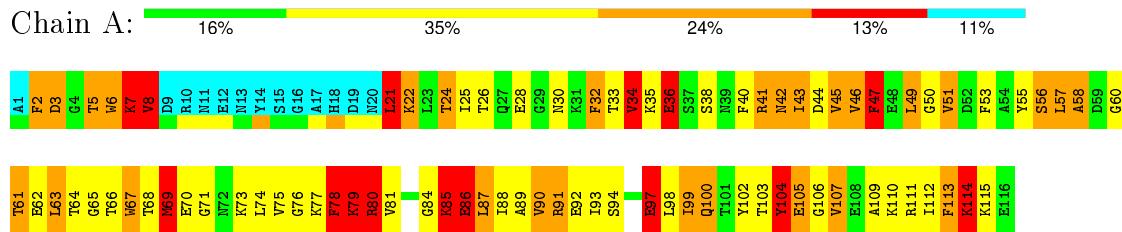
4.2.15 Score per residue for model 15

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN
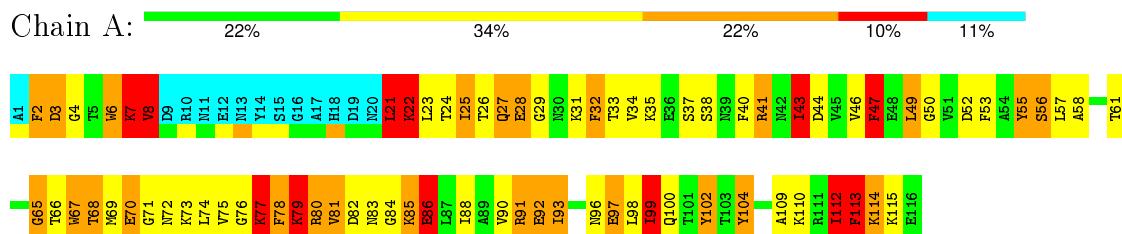
4.2.16 Score per residue for model 16

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN
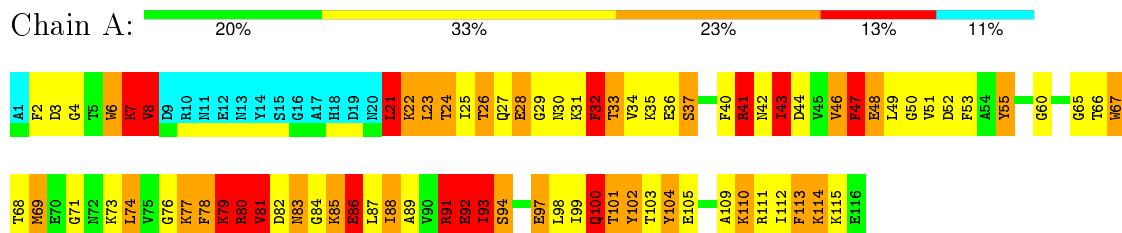
4.2.17 Score per residue for model 17

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN
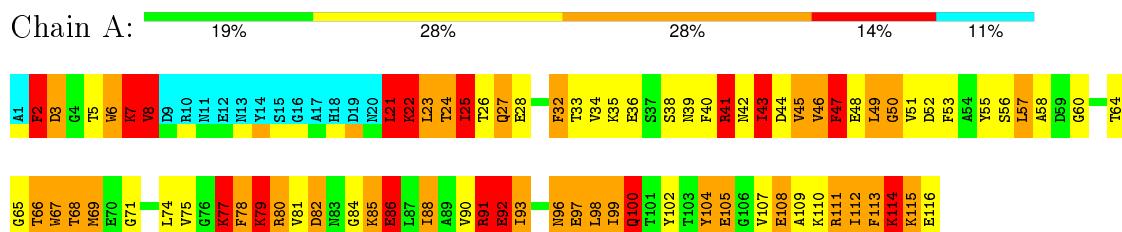
4.2.18 Score per residue for model 18

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN
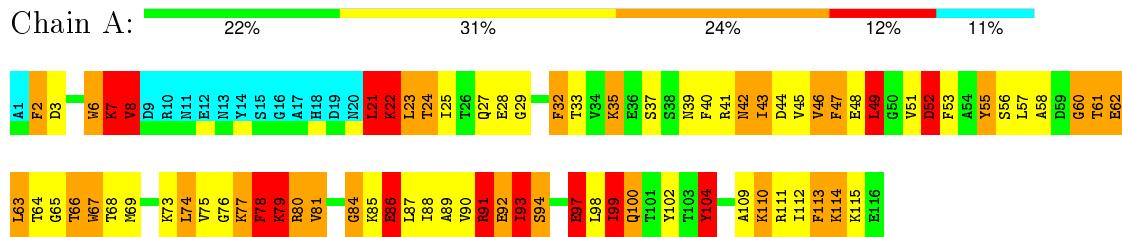

4.2.19 Score per residue for model 19

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN
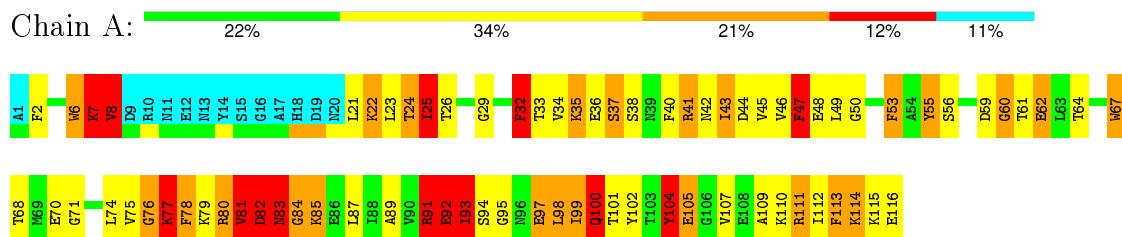
4.2.20 Score per residue for model 20

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN
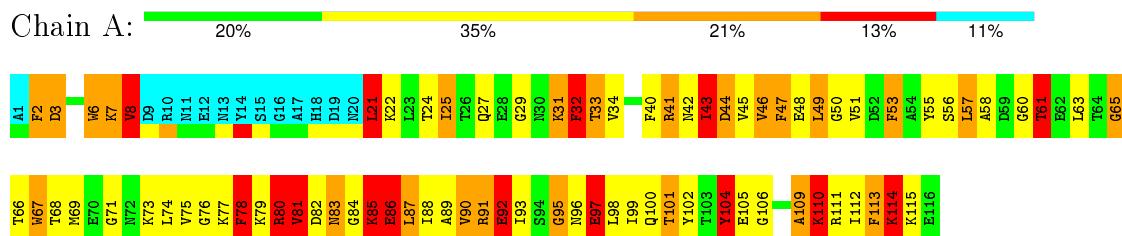
5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DISTANCE GEOMETRY WITH SIMU-LATED ANNEALING REFINEMENT*.

Of the 23 calculated structures, 20 were deposited, based on the following criterion: *FINAL PENALTY FUNCTION VALUES GREATER THAN 10.0 OR GREATER THAN TWO STAN-DARD DEVIATIONS FROM THE MEAN WERE OMITTED*.

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

Software name	Classification	Version
TINKER	refinement	
TINKER	structure solution	

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 (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	1.50±0.02	10±0/840 (1.2±0.1%)	2.69±0.06	71±6/1127 (6.3±0.5%)
All	All	1.50	207/16800 (1.2%)	2.69	1420/22540 (6.3%)

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	Models Total
1	A	104	TYR	CE1-CZ	-14.69	1.19	1.38	18	12
1	A	104	TYR	CE2-CZ	-14.64	1.19	1.38	17	8
1	A	55	TYR	CE1-CZ	-14.14	1.20	1.38	10	16
1	A	55	TYR	CE2-CZ	-14.08	1.20	1.38	7	4
1	A	102	TYR	CE1-CZ	-13.98	1.20	1.38	6	8
1	A	102	TYR	CE2-CZ	-13.85	1.20	1.38	3	12
1	A	113	PHE	CE1-CZ	-9.25	1.19	1.37	2	6
1	A	113	PHE	CE2-CZ	-9.24	1.19	1.37	3	14
1	A	78	PHE	CE2-CZ	-9.17	1.20	1.37	4	8
1	A	78	PHE	CE1-CZ	-9.13	1.20	1.37	14	12
1	A	40	PHE	CE2-CZ	-9.07	1.20	1.37	18	17
1	A	40	PHE	CE1-CZ	-8.95	1.20	1.37	19	3
1	A	32	PHE	CE1-CZ	-8.94	1.20	1.37	14	9
1	A	32	PHE	CE2-CZ	-8.88	1.20	1.37	2	11
1	A	53	PHE	CE2-CZ	-8.85	1.20	1.37	19	7
1	A	53	PHE	CE1-CZ	-8.83	1.20	1.37	2	13
1	A	2	PHE	CE2-CZ	-8.53	1.21	1.37	8	14
1	A	47	PHE	CE2-CZ	-8.35	1.21	1.37	14	6
1	A	2	PHE	CE1-CZ	-8.35	1.21	1.37	2	6
1	A	47	PHE	CE1-CZ	-8.29	1.21	1.37	9	14
1	A	67	TRP	CD1-NE1	-5.74	1.28	1.38	13	7

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	78	PHE	CB-CG-CD2	16.73	132.51	120.80	12	10
1	A	78	PHE	CB-CG-CD1	16.44	132.31	120.80	18	16
1	A	104	TYR	CB-CG-CD1	14.96	129.98	121.00	3	8
1	A	102	TYR	CB-CG-CD2	14.64	129.79	121.00	6	11
1	A	41	ARG	NE-CZ-NH1	13.61	127.11	120.30	14	11
1	A	67	TRP	CD1-NE1-CE2	12.96	120.66	109.00	18	20
1	A	111	ARG	NE-CZ-NH1	12.70	126.65	120.30	17	5
1	A	80	ARG	NE-CZ-NH1	12.59	126.59	120.30	1	8
1	A	47	PHE	CB-CG-CD2	12.49	129.54	120.80	14	13
1	A	80	ARG	NE-CZ-NH2	-12.46	114.07	120.30	3	12
1	A	104	TYR	CB-CG-CD2	12.14	128.28	121.00	2	12
1	A	102	TYR	CB-CG-CD1	12.11	128.26	121.00	15	13
1	A	6	TRP	CD1-NE1-CE2	12.09	119.88	109.00	9	18
1	A	91	ARG	NE-CZ-NH1	11.37	125.98	120.30	13	15
1	A	32	PHE	CB-CG-CD1	11.35	128.74	120.80	8	13
1	A	55	TYR	CB-CG-CD1	10.83	127.50	121.00	10	12
1	A	47	PHE	CB-CG-CD1	10.66	128.26	120.80	15	12
1	A	86	GLU	O-C-N	10.60	139.65	122.70	1	19
1	A	67	TRP	O-C-N	10.45	139.43	122.70	14	18
1	A	53	PHE	CB-CG-CD2	10.20	127.94	120.80	18	12
1	A	67	TRP	CG-CD1-NE1	-10.10	100.00	110.10	10	15
1	A	53	PHE	CB-CG-CD1	9.74	127.62	120.80	16	6
1	A	32	PHE	O-C-N	9.53	137.94	122.70	6	19
1	A	6	TRP	CE2-CD2-CG	9.49	114.89	107.30	13	13
1	A	88	ILE	O-C-N	9.41	137.75	122.70	17	14
1	A	109	ALA	O-C-N	9.40	137.74	122.70	20	16
1	A	6	TRP	NE1-CE2-CD2	-9.35	97.95	107.30	9	14
1	A	68	THR	O-C-N	9.34	137.64	122.70	16	18
1	A	6	TRP	CD1-CG-CD2	-9.27	98.88	106.30	13	16
1	A	113	PHE	CB-CG-CD2	9.20	127.24	120.80	6	5
1	A	41	ARG	NE-CZ-NH2	-8.85	115.88	120.30	4	10
1	A	7	LYS	O-C-N	8.68	136.59	122.70	7	19
1	A	111	ARG	NE-CZ-NH2	-8.64	115.98	120.30	7	8
1	A	6	TRP	NE1-CE2-CZ2	8.63	139.90	130.40	9	6
1	A	2	PHE	CB-CG-CD1	8.49	126.74	120.80	14	8
1	A	67	TRP	CE2-CD2-CG	-8.43	100.56	107.30	2	2
1	A	109	ALA	CB-CA-C	-8.42	97.47	110.10	18	19
1	A	112	ILE	O-C-N	8.41	136.16	122.70	15	14
1	A	67	TRP	NE1-CE2-CZ2	8.40	139.64	130.40	16	16
1	A	99	ILE	O-C-N	8.35	136.05	122.70	15	17
1	A	26	THR	O-C-N	8.19	135.80	122.70	10	11
1	A	3	ASP	CB-CG-OD1	8.19	125.67	118.30	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Models Total
1	A	32	PHE	CB-CG-CD2	8.16	126.51	120.80	13	6
1	A	67	TRP	CD1-CG-CD2	8.02	112.71	106.30	2	6
1	A	6	TRP	CB-CG-CD2	7.96	136.96	126.60	20	11
1	A	2	PHE	CB-CG-CD2	7.95	126.37	120.80	16	8
1	A	65	GLY	O-C-N	7.95	135.43	122.70	11	17
1	A	55	TYR	CB-CG-CD2	7.87	125.72	121.00	14	5
1	A	60	GLY	O-C-N	7.86	135.28	122.70	18	9
1	A	97	GLU	O-C-N	7.82	135.21	122.70	20	13
1	A	40	PHE	CB-CG-CD1	7.81	126.27	120.80	5	3
1	A	91	ARG	NE-CZ-NH2	-7.72	116.44	120.30	14	5
1	A	77	LYS	O-C-N	7.71	135.04	122.70	6	6
1	A	46	VAL	O-C-N	7.67	134.98	122.70	2	11
1	A	67	TRP	CA-CB-CG	-7.67	99.12	113.70	17	11
1	A	21	LEU	O-C-N	7.67	134.97	122.70	10	15
1	A	46	VAL	CG1-CB-CG2	-7.63	98.69	110.90	19	15
1	A	80	ARG	O-C-N	7.62	134.89	122.70	20	16
1	A	104	TYR	CZ-CE2-CD2	7.61	126.65	119.80	14	6
1	A	76	GLY	O-C-N	7.60	134.86	122.70	8	14
1	A	50	GLY	O-C-N	7.59	134.85	122.70	16	14
1	A	113	PHE	CB-CG-CD1	7.59	126.11	120.80	13	3
1	A	82	ASP	CB-CG-OD2	7.55	125.10	118.30	17	2
1	A	81	VAL	O-C-N	7.53	134.75	122.70	12	7
1	A	8	VAL	CA-C-O	7.53	135.91	120.10	12	13
1	A	92	GLU	O-C-N	7.52	134.73	122.70	19	18
1	A	98	LEU	O-C-N	7.50	134.70	122.70	3	6
1	A	55	TYR	O-C-N	7.50	134.69	122.70	11	2
1	A	22	LYS	O-C-N	7.42	134.57	122.70	19	18
1	A	84	GLY	O-C-N	7.41	134.56	122.70	6	16
1	A	34	VAL	CA-CB-CG1	7.31	121.86	110.90	16	8
1	A	29	GLY	O-C-N	7.30	134.38	122.70	6	10
1	A	44	ASP	CB-CG-OD2	7.27	124.84	118.30	2	1
1	A	75	VAL	CG1-CB-CG2	-7.14	99.48	110.90	3	14
1	A	79	LYS	N-CA-CB	-7.12	97.79	110.60	13	12
1	A	82	ASP	CB-CG-OD1	7.11	124.70	118.30	3	6
1	A	67	TRP	CH2-CZ2-CE2	7.09	124.49	117.40	12	12
1	A	100	GLN	O-C-N	7.09	134.04	122.70	13	12
1	A	104	TYR	CD1-CE1-CZ	7.06	126.16	119.80	4	3
1	A	43	ILE	CA-C-O	7.06	134.92	120.10	15	11
1	A	45	VAL	CG1-CB-CG2	-7.05	99.62	110.90	9	13
1	A	42	ASN	O-C-N	7.03	133.94	122.70	9	12
1	A	23	LEU	O-C-N	7.00	133.90	122.70	3	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models Worst	Total
1	A	66	THR	CA-CB-CG2	-6.95	102.67	112.40	5	1
1	A	6	TRP	O-C-N	6.95	133.81	122.70	17	6
1	A	90	VAL	CG1-CB-CG2	-6.95	99.79	110.90	12	12
1	A	48	GLU	O-C-N	6.91	133.75	122.70	16	11
1	A	40	PHE	O-C-N	6.80	133.57	122.70	5	4
1	A	32	PHE	CD1-CE1-CZ	6.78	128.23	120.10	14	4
1	A	55	TYR	CD1-CE1-CZ	6.75	125.87	119.80	8	6
1	A	93	ILE	O-C-N	6.71	133.43	122.70	19	4
1	A	78	PHE	CD1-CG-CD2	-6.67	109.62	118.30	14	8
1	A	34	VAL	N-CA-CB	-6.65	96.87	111.50	6	11
1	A	55	TYR	CG-CD2-CE2	-6.62	116.00	121.30	4	2
1	A	78	PHE	CD1-CE1-CZ	6.58	127.99	120.10	7	5
1	A	67	TRP	NE1-CE2-CD2	-6.55	100.75	107.30	16	7
1	A	35	LYS	CA-C-O	6.53	133.81	120.10	1	6
1	A	89	ALA	O-C-N	6.51	133.11	122.70	14	5
1	A	96	ASN	O-C-N	6.47	133.05	122.70	5	4
1	A	102	TYR	O-C-N	6.46	133.04	122.70	12	8
1	A	51	VAL	O-C-N	6.45	133.01	122.70	4	5
1	A	87	LEU	O-C-N	6.42	132.98	122.70	9	2
1	A	113	PHE	O-C-N	6.38	132.90	122.70	3	20
1	A	53	PHE	CD1-CE1-CZ	6.37	127.74	120.10	6	2
1	A	44	ASP	CB-CG-OD1	6.35	124.02	118.30	9	3
1	A	91	ARG	O-C-N	6.34	132.84	122.70	4	10
1	A	2	PHE	CD1-CE1-CZ	6.33	127.70	120.10	6	1
1	A	44	ASP	O-C-N	6.33	132.82	122.70	10	10
1	A	51	VAL	CG1-CB-CG2	-6.32	100.79	110.90	1	13
1	A	82	ASP	O-C-N	6.29	132.77	122.70	6	1
1	A	6	TRP	CB-CG-CD1	-6.26	118.86	127.00	19	1
1	A	55	TYR	CD1-CG-CD2	-6.22	111.05	117.90	3	3
1	A	22	LYS	CB-CA-C	-6.22	97.96	110.40	17	18
1	A	85	LYS	O-C-N	6.21	132.63	122.70	8	6
1	A	56	SER	O-C-N	6.16	132.56	122.70	15	7
1	A	34	VAL	CG1-CB-CG2	-6.14	101.08	110.90	2	5
1	A	81	VAL	CG1-CB-CG2	-6.13	101.09	110.90	17	8
1	A	113	PHE	CD1-CG-CD2	-6.11	110.35	118.30	17	1
1	A	95	GLY	O-C-N	6.10	132.47	122.70	1	2
1	A	52	ASP	O-C-N	6.06	132.39	122.70	8	4
1	A	39	ASN	O-C-N	6.03	132.34	122.70	7	2
1	A	7	LYS	CA-CB-CG	-6.02	100.16	113.40	15	14
1	A	32	PHE	CZ-CE2-CD2	6.01	127.32	120.10	17	3
1	A	4	GLY	O-C-N	5.98	132.27	122.70	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models Worst	Models Total
1	A	111	ARG	O-C-N	5.94	132.20	122.70	3	3
1	A	69	MET	O-C-N	5.87	132.09	122.70	14	2
1	A	64	THR	C-N-CA	-5.86	109.99	122.30	3	15
1	A	67	TRP	CB-CG-CD1	-5.86	119.38	127.00	12	2
1	A	8	VAL	CG1-CB-CG2	-5.85	101.54	110.90	4	9
1	A	113	PHE	CZ-CE2-CD2	5.85	127.12	120.10	16	4
1	A	8	VAL	N-CA-CB	-5.84	98.65	111.50	19	20
1	A	110	LYS	O-C-N	5.83	132.03	122.70	8	6
1	A	32	PHE	N-CA-C	-5.83	95.27	111.00	9	12
1	A	78	PHE	CA-C-N	-5.82	104.39	117.20	2	7
1	A	70	GLU	O-C-N	5.82	133.09	123.20	19	1
1	A	53	PHE	CZ-CE2-CD2	5.81	127.07	120.10	19	1
1	A	28	GLU	OE1-CD-OE2	5.81	130.27	123.30	16	2
1	A	6	TRP	CH2-CZ2-CE2	5.80	123.20	117.40	9	1
1	A	6	TRP	CB-CA-C	-5.79	98.81	110.40	3	8
1	A	27	GLN	O-C-N	5.76	131.92	122.70	5	3
1	A	51	VAL	CA-CB-CG1	5.73	119.50	110.90	12	2
1	A	26	THR	CA-C-N	-5.71	104.64	117.20	12	3
1	A	83	ASN	C-N-CA	-5.70	110.33	122.30	11	3
1	A	52	ASP	CB-CG-OD1	5.66	123.39	118.30	18	1
1	A	102	TYR	CD1-CG-CD2	-5.64	111.70	117.90	4	3
1	A	62	GLU	O-C-N	5.63	131.71	122.70	6	2
1	A	3	ASP	C-N-CA	-5.63	110.48	122.30	8	4
1	A	114	LYS	CA-C-O	5.61	131.87	120.10	8	3
1	A	78	PHE	CA-C-O	5.61	131.87	120.10	6	1
1	A	29	GLY	N-CA-C	-5.57	99.19	113.10	16	6
1	A	40	PHE	CZ-CE2-CD2	5.52	126.73	120.10	16	3
1	A	90	VAL	CA-CB-CG2	5.51	119.17	110.90	18	1
1	A	32	PHE	CA-C-N	-5.51	105.07	117.20	6	8
1	A	71	GLY	O-C-N	5.50	131.50	122.70	16	2
1	A	107	VAL	O-C-N	5.50	131.49	122.70	3	2
1	A	7	LYS	CA-C-N	-5.49	105.12	117.20	10	20
1	A	99	ILE	CA-C-O	-5.48	108.60	120.10	9	2
1	A	104	TYR	CD1-CG-CD2	-5.47	111.88	117.90	15	4
1	A	31	LYS	N-CA-C	-5.46	96.25	111.00	10	5
1	A	28	GLU	C-N-CA	-5.46	110.84	122.30	15	3
1	A	77	LYS	N-CA-CB	-5.46	100.78	110.60	16	5
1	A	30	ASN	O-C-N	5.43	131.39	122.70	1	1
1	A	100	GLN	CA-C-N	-5.42	105.28	117.20	13	2
1	A	75	VAL	CA-CB-CG1	5.41	119.01	110.90	17	1
1	A	74	LEU	O-C-N	5.38	131.32	122.70	5	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models Worst	Total
1	A	72	ASN	O-C-N	5.38	131.31	122.70	11	3
1	A	84	GLY	CA-C-N	-5.37	105.39	117.20	11	8
1	A	40	PHE	CB-CG-CD2	5.37	124.56	120.80	2	1
1	A	102	TYR	CG-CD2-CE2	5.35	125.58	121.30	16	1
1	A	34	VAL	CB-CA-C	5.32	121.50	111.40	16	4
1	A	23	LEU	N-CA-C	-5.30	96.69	111.00	13	4
1	A	48	GLU	OE1-CD-OE2	-5.28	116.96	123.30	9	3
1	A	22	LYS	CA-C-N	-5.27	105.61	117.20	13	4
1	A	98	LEU	CA-C-N	-5.25	105.65	117.20	9	2
1	A	88	ILE	CA-CB-CG2	5.25	121.39	110.90	20	1
1	A	38	SER	N-CA-CB	-5.24	102.64	110.50	11	1
1	A	55	TYR	CG-CD1-CE1	-5.24	117.11	121.30	7	1
1	A	76	GLY	N-CA-C	-5.24	100.01	113.10	8	1
1	A	2	PHE	O-C-N	5.20	131.03	122.70	17	3
1	A	6	TRP	CE2-CD2-CE3	-5.19	112.48	118.70	4	1
1	A	95	GLY	CA-C-N	-5.19	105.78	117.20	19	1
1	A	6	TRP	CZ3-CH2-CZ2	-5.17	115.39	121.60	15	2
1	A	91	ARG	CA-C-N	-5.17	105.83	117.20	13	1
1	A	76	GLY	C-N-CA	-5.16	108.81	121.70	13	1
1	A	109	ALA	N-CA-CB	-5.15	102.89	110.10	2	1
1	A	77	LYS	CA-C-N	-5.14	105.89	117.20	6	1
1	A	108	GLU	O-C-N	5.14	130.92	122.70	17	1
1	A	33	THR	N-CA-C	-5.11	97.21	111.00	20	4
1	A	34	VAL	CA-C-N	-5.08	106.03	117.20	1	1
1	A	84	GLY	N-CA-C	-5.07	100.44	113.10	5	2
1	A	43	ILE	N-CA-CB	-5.05	99.19	110.80	6	1
1	A	55	TYR	CZ-CE2-CD2	5.04	124.34	119.80	3	1
1	A	74	LEU	CA-C-N	-5.04	106.11	117.20	3	1
1	A	43	ILE	CG1-CB-CG2	-5.04	100.31	111.40	19	1
1	A	59	ASP	CB-CG-OD2	5.04	122.83	118.30	7	1
1	A	78	PHE	CB-CA-C	5.03	120.46	110.40	18	1
1	A	46	VAL	N-CA-CB	-5.02	100.45	111.50	14	1
1	A	2	PHE	CZ-CE2-CD2	5.02	126.12	120.10	15	1
1	A	45	VAL	O-C-N	5.01	130.72	122.70	8	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	827	827	827	52±11
All	All	16540	16540	16540	1031

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:101:THR:HG23	1:A:110:LYS:HG3	0.90	1.42	13	1
1:A:2:PHE:CE1	1:A:93:ILE:HD11	0.86	2.06	1	2
1:A:25:ILE:HG22	1:A:32:PHE:CD1	0.85	2.07	20	2
1:A:2:PHE:CZ	1:A:93:ILE:HD11	0.84	2.06	1	3
1:A:43:ILE:HD11	1:A:57:LEU:CD1	0.82	2.02	20	1
1:A:93:ILE:HD13	1:A:98:LEU:HD13	0.80	1.51	1	2
1:A:93:ILE:CD1	1:A:98:LEU:HD12	0.79	2.08	20	4
1:A:43:ILE:CG2	1:A:57:LEU:HD21	0.79	2.06	9	1
1:A:43:ILE:HD11	1:A:57:LEU:CG	0.78	2.08	20	1
1:A:91:ARG:CD	1:A:98:LEU:HD21	0.77	2.09	14	2
1:A:93:ILE:HD13	1:A:97:GLU:O	0.76	1.80	13	1
1:A:63:LEU:HD21	1:A:87:LEU:HD11	0.76	1.56	10	1
1:A:67:TRP:CE2	1:A:78:PHE:CE1	0.76	2.74	6	15
1:A:67:TRP:CZ2	1:A:78:PHE:CE2	0.75	2.74	10	7
1:A:25:ILE:HG21	1:A:32:PHE:CE1	0.75	2.17	3	3
1:A:67:TRP:CZ2	1:A:78:PHE:CZ	0.74	2.75	10	6
1:A:79:LYS:HG2	1:A:81:VAL:HG13	0.74	1.59	19	1
1:A:67:TRP:CZ2	1:A:78:PHE:CD1	0.73	2.77	14	7
1:A:62:GLU:O	1:A:63:LEU:HD12	0.72	1.84	14	2
1:A:67:TRP:CE2	1:A:78:PHE:CE2	0.72	2.78	16	3
1:A:79:LYS:CG	1:A:85:LYS:C	0.72	2.59	1	3
1:A:43:ILE:HD11	1:A:57:LEU:HG	0.70	1.62	20	1
1:A:91:ARG:HD2	1:A:98:LEU:HD21	0.70	1.63	14	2
1:A:93:ILE:HB	1:A:98:LEU:HD12	0.70	1.63	17	1
1:A:49:LEU:HD11	1:A:69:MET:CB	0.70	2.16	18	2
1:A:34:VAL:HG12	1:A:36:GLU:HG3	0.69	1.64	11	2
1:A:43:ILE:HG22	1:A:57:LEU:HD21	0.69	1.65	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:57:LEU:HD23	1:A:61:THR:HG21	0.69	1.65	20	1
1:A:97:GLU:CB	1:A:114:LYS:HA	0.69	2.17	7	19
1:A:6:TRP:CD2	1:A:115:LYS:HG3	0.68	2.23	2	19
1:A:2:PHE:CD1	1:A:25:ILE:HD13	0.68	2.24	5	1
1:A:67:TRP:CE2	1:A:78:PHE:CZ	0.68	2.81	17	8
1:A:67:TRP:CZ2	1:A:78:PHE:CE1	0.68	2.82	2	3
1:A:67:TRP:CZ2	1:A:78:PHE:CD2	0.67	2.83	17	4
1:A:25:ILE:HG21	1:A:32:PHE:CE2	0.67	2.24	7	2
1:A:66:THR:C	1:A:67:TRP:CD1	0.67	2.68	3	7
1:A:25:ILE:HG21	1:A:32:PHE:CZ	0.67	2.24	18	1
1:A:50:GLY:HA3	1:A:68:THR:HG22	0.66	1.67	11	1
1:A:93:ILE:HD12	1:A:98:LEU:HD12	0.65	1.68	18	4
1:A:25:ILE:HG23	1:A:33:THR:O	0.65	1.92	7	3
1:A:80:ARG:HG2	1:A:87:LEU:HD13	0.64	1.67	1	1
1:A:93:ILE:HA	1:A:98:LEU:HD12	0.64	1.69	9	2
1:A:99:ILE:HG22	1:A:100:GLN:N	0.64	2.06	14	11
1:A:49:LEU:HD21	1:A:69:MET:CB	0.64	2.23	13	3
1:A:21:LEU:HD13	1:A:21:LEU:N	0.63	2.08	13	1
1:A:7:LYS:HD3	1:A:113:PHE:HB3	0.63	1.68	17	9
1:A:21:LEU:HD23	1:A:21:LEU:N	0.63	2.09	4	2
1:A:99:ILE:HG23	1:A:110:LYS:HB2	0.62	1.71	11	1
1:A:8:VAL:HG11	1:A:21:LEU:HD22	0.62	1.68	20	1
1:A:8:VAL:HG11	1:A:21:LEU:O	0.62	1.94	1	3
1:A:91:ARG:HD3	1:A:98:LEU:HD21	0.62	1.72	20	2
1:A:23:LEU:HD22	1:A:25:ILE:HD11	0.62	1.71	3	2
1:A:67:TRP:CD1	1:A:78:PHE:CZ	0.62	2.87	8	5
1:A:67:TRP:NE1	1:A:78:PHE:CZ	0.62	2.68	8	10
1:A:32:PHE:CD1	1:A:49:LEU:HD23	0.62	2.29	17	1
1:A:67:TRP:CD1	1:A:67:TRP:N	0.61	2.68	7	5
1:A:83:ASN:N	1:A:83:ASN:ND2	0.61	2.47	11	1
1:A:49:LEU:HD22	1:A:69:MET:HB3	0.61	1.72	14	2
1:A:114:LYS:HD2	1:A:114:LYS:N	0.61	2.10	20	7
1:A:49:LEU:HD11	1:A:69:MET:HB3	0.61	1.73	18	1
1:A:77:LYS:O	1:A:78:PHE:CD1	0.61	2.54	16	2
1:A:114:LYS:CD	1:A:114:LYS:N	0.60	2.64	7	4
1:A:93:ILE:HD11	1:A:98:LEU:HD12	0.60	1.72	8	2
1:A:49:LEU:HD21	1:A:69:MET:HB3	0.60	1.71	6	3
1:A:67:TRP:CZ2	1:A:89:ALA:HB3	0.60	2.31	9	2
1:A:67:TRP:N	1:A:67:TRP:CD1	0.60	2.69	13	2
1:A:76:GLY:O	1:A:88:ILE:HG23	0.60	1.97	10	1
1:A:98:LEU:HD21	1:A:100:GLN:HB2	0.60	1.74	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:66:THR:C	1:A:67:TRP:CG	0.59	2.76	17	5
1:A:79:LYS:HG3	1:A:86:GLU:N	0.59	2.12	8	5
1:A:93:ILE:HD13	1:A:93:ILE:N	0.59	2.11	16	1
1:A:6:TRP:CE3	1:A:115:LYS:HG3	0.59	2.33	3	11
1:A:32:PHE:CE1	1:A:34:VAL:HG23	0.59	2.32	7	2
1:A:61:THR:HB	1:A:63:LEU:HD13	0.59	1.75	4	1
1:A:101:THR:HG23	1:A:110:LYS:CG	0.58	2.24	13	4
1:A:24:THR:N	1:A:35:LYS:HB3	0.58	2.13	2	12
1:A:80:ARG:NE	1:A:87:LEU:HD11	0.58	2.13	16	2
1:A:88:ILE:HG22	1:A:90:VAL:HG23	0.58	1.76	13	1
1:A:6:TRP:CE3	1:A:115:LYS:HB2	0.58	2.34	12	12
1:A:6:TRP:CZ3	1:A:93:ILE:HD11	0.58	2.34	7	2
1:A:25:ILE:HG21	1:A:32:PHE:HD2	0.57	1.60	14	1
1:A:2:PHE:CE1	1:A:25:ILE:HD13	0.57	2.34	5	1
1:A:21:LEU:HD12	1:A:21:LEU:N	0.57	2.14	6	1
1:A:79:LYS:HG2	1:A:85:LYS:C	0.57	2.19	1	4
1:A:86:GLU:C	1:A:87:LEU:HD12	0.57	2.20	1	1
1:A:63:LEU:HD21	1:A:87:LEU:HD23	0.57	1.74	5	1
1:A:24:THR:O	1:A:25:ILE:HD12	0.57	2.00	10	3
1:A:41:ARG:HG2	1:A:58:ALA:HB2	0.57	1.76	9	1
1:A:80:ARG:CG	1:A:87:LEU:HD13	0.56	2.30	20	2
1:A:91:ARG:NE	1:A:92:GLU:H	0.56	1.97	19	2
1:A:97:GLU:HB2	1:A:114:LYS:HA	0.56	1.77	12	8
1:A:67:TRP:CZ2	1:A:77:LYS:N	0.56	2.74	2	5
1:A:2:PHE:CZ	1:A:98:LEU:CD1	0.56	2.88	10	1
1:A:107:VAL:HG12	1:A:109:ALA:HB2	0.56	1.76	6	1
1:A:80:ARG:CD	1:A:87:LEU:HD11	0.56	2.30	19	2
1:A:6:TRP:CH2	1:A:93:ILE:CD1	0.56	2.88	7	2
1:A:25:ILE:CG2	1:A:32:PHE:CE1	0.56	2.88	3	1
1:A:91:ARG:C	1:A:92:GLU:CG	0.56	2.74	13	3
1:A:91:ARG:CD	1:A:98:LEU:CD2	0.56	2.83	6	1
1:A:99:ILE:HG12	1:A:112:ILE:HG22	0.56	1.75	3	1
1:A:67:TRP:NE1	1:A:78:PHE:CE1	0.56	2.73	13	9
1:A:6:TRP:CD2	1:A:115:LYS:CG	0.56	2.88	2	5
1:A:93:ILE:CD1	1:A:98:LEU:HD22	0.56	2.30	5	1
1:A:77:LYS:CG	1:A:78:PHE:N	0.56	2.68	16	4
1:A:6:TRP:CH2	1:A:93:ILE:HD11	0.55	2.36	7	1
1:A:90:VAL:O	1:A:101:THR:HG22	0.55	2.01	10	1
1:A:27:GLN:HB2	1:A:31:LYS:C	0.55	2.22	13	3
1:A:25:ILE:HG12	1:A:34:VAL:HG22	0.55	1.78	1	2
1:A:34:VAL:HG12	1:A:36:GLU:CG	0.55	2.32	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ILE:HG23	1:A:110:LYS:CB	0.55	2.30	11	1
1:A:25:ILE:HG22	1:A:32:PHE:HB2	0.55	1.79	11	1
1:A:85:LYS:CG	1:A:86:GLU:N	0.55	2.69	12	1
1:A:24:THR:HG22	1:A:25:ILE:N	0.55	2.15	15	1
1:A:93:ILE:N	1:A:93:ILE:HD13	0.55	2.17	14	1
1:A:114:LYS:N	1:A:114:LYS:CD	0.54	2.69	4	1
1:A:81:VAL:HG22	1:A:82:ASP:N	0.54	2.17	3	1
1:A:21:LEU:N	1:A:21:LEU:HD12	0.54	2.18	17	2
1:A:67:TRP:CH2	1:A:77:LYS:N	0.54	2.76	13	5
1:A:97:GLU:HB3	1:A:114:LYS:HA	0.54	1.78	13	7
1:A:8:VAL:HG21	1:A:21:LEU:O	0.54	2.02	8	3
1:A:91:ARG:CG	1:A:98:LEU:CD2	0.54	2.86	6	1
1:A:77:LYS:HG2	1:A:78:PHE:N	0.54	2.16	19	3
1:A:79:LYS:HG2	1:A:86:GLU:HA	0.54	1.80	5	7
1:A:32:PHE:CG	1:A:32:PHE:O	0.54	2.60	14	1
1:A:43:ILE:HG13	1:A:57:LEU:HD12	0.53	1.78	17	1
1:A:66:THR:O	1:A:66:THR:HG23	0.53	2.02	1	6
1:A:67:TRP:CE3	1:A:67:TRP:HA	0.53	2.36	18	8
1:A:78:PHE:N	1:A:78:PHE:CD1	0.53	2.76	15	4
1:A:67:TRP:NE1	1:A:78:PHE:CE2	0.53	2.77	2	3
1:A:32:PHE:CE1	1:A:34:VAL:CG2	0.53	2.92	8	1
1:A:114:LYS:N	1:A:114:LYS:HD2	0.53	2.19	13	5
1:A:88:ILE:HD12	1:A:103:THR:HG22	0.53	1.80	5	1
1:A:98:LEU:CD2	1:A:100:GLN:HB2	0.53	2.34	13	1
1:A:32:PHE:HZ	1:A:74:LEU:HD21	0.53	1.63	14	2
1:A:66:THR:N	1:A:78:PHE:CZ	0.53	2.77	5	4
1:A:66:THR:N	1:A:78:PHE:CE1	0.53	2.76	4	6
1:A:32:PHE:CZ	1:A:74:LEU:HD21	0.53	2.39	8	2
1:A:43:ILE:HG23	1:A:43:ILE:O	0.52	2.04	2	3
1:A:46:VAL:HG22	1:A:47:PHE:N	0.52	2.20	3	3
1:A:43:ILE:HD11	1:A:57:LEU:HD22	0.52	1.80	18	1
1:A:91:ARG:HG3	1:A:98:LEU:HD11	0.52	1.80	5	1
1:A:98:LEU:HD21	1:A:100:GLN:HG2	0.52	1.80	8	1
1:A:98:LEU:CD2	1:A:100:GLN:CG	0.52	2.87	14	3
1:A:49:LEU:HD21	1:A:69:MET:N	0.52	2.20	13	1
1:A:77:LYS:HG3	1:A:78:PHE:N	0.52	2.20	7	1
1:A:101:THR:HG23	1:A:110:LYS:HG2	0.52	1.82	16	3
1:A:67:TRP:CZ3	1:A:89:ALA:HB3	0.52	2.40	4	1
1:A:21:LEU:N	1:A:21:LEU:HD23	0.52	2.20	18	1
1:A:91:ARG:HD3	1:A:98:LEU:HD11	0.52	1.81	20	1
1:A:2:PHE:CE1	1:A:98:LEU:CD1	0.52	2.92	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ILE:HD11	1:A:97:GLU:N	0.52	2.20	10	1
1:A:46:VAL:C	1:A:47:PHE:CD1	0.51	2.83	4	5
1:A:83:ASN:N	1:A:83:ASN:HD22	0.51	2.00	11	1
1:A:24:THR:HB	1:A:35:LYS:HD2	0.51	1.82	4	8
1:A:79:LYS:CE	1:A:86:GLU:HB2	0.51	2.35	14	1
1:A:7:LYS:HD2	1:A:113:PHE:HB3	0.51	1.81	1	3
1:A:67:TRP:CH2	1:A:89:ALA:HB3	0.51	2.40	4	2
1:A:63:LEU:HD11	1:A:87:LEU:HD13	0.51	1.82	11	1
1:A:91:ARG:HG3	1:A:92:GLU:N	0.51	2.20	8	6
1:A:31:LYS:O	1:A:32:PHE:CG	0.51	2.64	20	3
1:A:98:LEU:HD23	1:A:100:GLN:HG2	0.51	1.80	2	1
1:A:32:PHE:N	1:A:32:PHE:CD1	0.51	2.78	6	2
1:A:80:ARG:NE	1:A:85:LYS:NZ	0.51	2.58	14	1
1:A:61:THR:HG22	1:A:63:LEU:HD13	0.51	1.82	14	2
1:A:49:LEU:HD21	1:A:69:MET:HB2	0.51	1.82	3	1
1:A:32:PHE:HB2	1:A:47:PHE:CE2	0.51	2.41	16	3
1:A:77:LYS:C	1:A:78:PHE:CD1	0.51	2.84	5	6
1:A:67:TRP:CE2	1:A:78:PHE:CD1	0.51	2.98	1	3
1:A:79:LYS:HD3	1:A:86:GLU:N	0.51	2.20	3	1
1:A:98:LEU:CD2	1:A:100:GLN:HG2	0.51	2.36	14	3
1:A:24:THR:HG22	1:A:24:THR:O	0.51	2.06	2	5
1:A:6:TRP:HB2	1:A:23:LEU:HB2	0.51	1.82	17	6
1:A:87:LEU:HG	1:A:87:LEU:O	0.51	2.06	14	1
1:A:45:VAL:HG22	1:A:57:LEU:HD11	0.51	1.83	14	1
1:A:79:LYS:CE	1:A:84:GLY:HA2	0.51	2.36	7	2
1:A:32:PHE:CE1	1:A:49:LEU:HD22	0.50	2.41	15	1
1:A:6:TRP:HB2	1:A:23:LEU:CB	0.50	2.36	6	10
1:A:80:ARG:HD3	1:A:87:LEU:HD11	0.50	1.83	16	1
1:A:47:PHE:CD2	1:A:67:TRP:HB2	0.50	2.41	15	1
1:A:104:TYR:C	1:A:104:TYR:CD1	0.50	2.85	14	3
1:A:53:PHE:N	1:A:53:PHE:CD1	0.50	2.79	7	4
1:A:6:TRP:CG	1:A:115:LYS:HG3	0.50	2.41	14	2
1:A:74:LEU:HD12	1:A:98:LEU:HD11	0.50	1.83	16	2
1:A:66:THR:HG23	1:A:66:THR:O	0.50	2.05	6	4
1:A:79:LYS:HG3	1:A:86:GLU:HA	0.50	1.84	1	1
1:A:24:THR:O	1:A:24:THR:HG22	0.50	2.05	11	1
1:A:93:ILE:N	1:A:98:LEU:HD12	0.50	2.21	2	1
1:A:99:ILE:CG2	1:A:110:LYS:HB2	0.50	2.36	15	1
1:A:27:GLN:CB	1:A:31:LYS:C	0.50	2.80	16	1
1:A:61:THR:CG2	1:A:63:LEU:CD1	0.50	2.90	10	1
1:A:34:VAL:HG12	1:A:36:GLU:HG2	0.50	1.84	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HD13	1:A:37:SER:O	0.50	2.06	4	1
1:A:98:LEU:O	1:A:98:LEU:HD23	0.50	2.07	13	1
1:A:80:ARG:HG3	1:A:87:LEU:HD13	0.50	1.83	20	1
1:A:32:PHE:CE1	1:A:34:VAL:HG22	0.50	2.42	8	1
1:A:33:THR:OG1	1:A:46:VAL:HG23	0.49	2.07	16	1
1:A:50:GLY:HA2	1:A:68:THR:HG22	0.49	1.85	4	1
1:A:47:PHE:CE1	1:A:67:TRP:HB2	0.49	2.43	18	1
1:A:79:LYS:HG2	1:A:86:GLU:N	0.49	2.22	11	3
1:A:93:ILE:CA	1:A:98:LEU:HD12	0.49	2.36	9	1
1:A:5:THR:HG22	1:A:24:THR:OG1	0.49	2.07	3	2
1:A:97:GLU:CB	1:A:114:LYS:CB	0.49	2.90	7	2
1:A:93:ILE:HD13	1:A:98:LEU:HD12	0.49	1.82	20	1
1:A:47:PHE:CD1	1:A:47:PHE:N	0.49	2.79	15	2
1:A:7:LYS:HD2	1:A:113:PHE:CB	0.49	2.36	13	6
1:A:81:VAL:HG12	1:A:82:ASP:N	0.49	2.22	8	1
1:A:6:TRP:CE3	1:A:115:LYS:CB	0.49	2.96	17	8
1:A:23:LEU:CD2	1:A:34:VAL:HG13	0.49	2.38	19	1
1:A:53:PHE:CD1	1:A:53:PHE:N	0.49	2.80	12	3
1:A:3:ASP:HA	1:A:26:THR:HB	0.49	1.85	10	1
1:A:47:PHE:CE2	1:A:67:TRP:CB	0.49	2.96	15	1
1:A:6:TRP:CH2	1:A:93:ILE:HD13	0.49	2.43	11	2
1:A:67:TRP:CH2	1:A:76:GLY:C	0.49	2.86	2	4
1:A:67:TRP:CZ3	1:A:76:GLY:C	0.49	2.86	19	3
1:A:97:GLU:HB3	1:A:114:LYS:HB2	0.49	1.84	12	5
1:A:86:GLU:OE2	1:A:103:THR:HG22	0.49	2.08	14	1
1:A:104:TYR:CD1	1:A:105:GLU:N	0.49	2.81	16	2
1:A:94:SER:CB	1:A:99:ILE:HD13	0.49	2.38	14	1
1:A:58:ALA:HB3	1:A:61:THR:OG1	0.49	2.08	14	2
1:A:74:LEU:CD1	1:A:98:LEU:HD11	0.49	2.37	18	1
1:A:74:LEU:N	1:A:91:ARG:O	0.48	2.46	15	17
1:A:61:THR:HG22	1:A:63:LEU:CD1	0.48	2.38	10	1
1:A:35:LYS:O	1:A:37:SER:N	0.48	2.46	7	7
1:A:104:TYR:CD1	1:A:104:TYR:C	0.48	2.86	11	5
1:A:89:ALA:HB1	1:A:100:GLN:NE2	0.48	2.23	16	1
1:A:2:PHE:CE2	1:A:98:LEU:HD12	0.48	2.43	3	1
1:A:97:GLU:CB	1:A:114:LYS:HB2	0.48	2.39	12	2
1:A:63:LEU:HD12	1:A:63:LEU:N	0.48	2.23	5	1
1:A:44:ASP:O	1:A:57:LEU:HD11	0.48	2.08	12	1
1:A:88:ILE:HD12	1:A:103:THR:O	0.48	2.08	3	1
1:A:91:ARG:CD	1:A:98:LEU:HD23	0.48	2.38	6	1
1:A:98:LEU:HD23	1:A:100:GLN:CG	0.48	2.37	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:TRP:CH2	1:A:77:LYS:CA	0.48	2.97	17	2
1:A:25:ILE:HG23	1:A:33:THR:H	0.48	1.69	13	1
1:A:85:LYS:HG3	1:A:86:GLU:N	0.48	2.23	17	8
1:A:47:PHE:N	1:A:47:PHE:CD1	0.48	2.81	16	4
1:A:27:GLN:CB	1:A:32:PHE:CD1	0.48	2.96	5	1
1:A:106:GLY:O	1:A:107:VAL:HG13	0.48	2.07	3	1
1:A:58:ALA:HB3	1:A:61:THR:CG2	0.48	2.39	1	1
1:A:7:LYS:CD	1:A:113:PHE:HB3	0.48	2.39	16	6
1:A:81:VAL:CG1	1:A:82:ASP:N	0.48	2.77	9	1
1:A:43:ILE:O	1:A:43:ILE:HG23	0.48	2.09	3	2
1:A:89:ALA:HB1	1:A:100:GLN:HE22	0.48	1.69	16	1
1:A:93:ILE:HG23	1:A:97:GLU:O	0.48	2.09	8	1
1:A:7:LYS:HB2	1:A:22:LYS:HA	0.48	1.86	17	1
1:A:79:LYS:HG2	1:A:86:GLU:CA	0.48	2.39	17	5
1:A:41:ARG:CD	1:A:41:ARG:N	0.48	2.76	16	2
1:A:49:LEU:HD22	1:A:69:MET:CB	0.47	2.39	7	1
1:A:46:VAL:C	1:A:47:PHE:CD2	0.47	2.87	18	6
1:A:2:PHE:CE1	1:A:98:LEU:HD13	0.47	2.43	10	1
1:A:99:ILE:CG2	1:A:110:LYS:CB	0.47	2.92	11	2
1:A:80:ARG:N	1:A:85:LYS:O	0.47	2.48	4	1
1:A:82:ASP:O	1:A:83:ASN:CB	0.47	2.61	6	3
1:A:98:LEU:HD23	1:A:100:GLN:HG3	0.47	1.85	18	2
1:A:83:ASN:ND2	1:A:84:GLY:N	0.47	2.62	19	1
1:A:53:PHE:CD1	1:A:55:TYR:HB2	0.47	2.44	1	1
1:A:58:ALA:HB3	1:A:61:THR:HG23	0.47	1.85	1	2
1:A:114:LYS:CD	1:A:114:LYS:O	0.47	2.62	8	2
1:A:79:LYS:HE2	1:A:86:GLU:CG	0.47	2.39	12	1
1:A:93:ILE:CD1	1:A:97:GLU:N	0.47	2.78	15	1
1:A:91:ARG:CG	1:A:92:GLU:N	0.47	2.77	17	8
1:A:24:THR:HB	1:A:35:LYS:CD	0.47	2.39	11	6
1:A:6:TRP:CZ3	1:A:115:LYS:HB2	0.47	2.44	17	1
1:A:99:ILE:CG2	1:A:100:GLN:N	0.47	2.78	13	3
1:A:97:GLU:CB	1:A:114:LYS:CA	0.47	2.91	7	2
1:A:93:ILE:HD11	1:A:97:GLU:H	0.47	1.69	10	1
1:A:67:TRP:CZ2	1:A:77:LYS:CA	0.47	2.98	2	1
1:A:2:PHE:CE2	1:A:98:LEU:CD1	0.47	2.98	3	1
1:A:32:PHE:CE2	1:A:69:MET:HG2	0.47	2.45	15	1
1:A:3:ASP:HA	1:A:26:THR:HA	0.47	1.86	10	1
1:A:79:LYS:HG3	1:A:85:LYS:C	0.47	2.29	1	1
1:A:41:ARG:CZ	1:A:43:ILE:HB	0.47	2.40	16	1
1:A:40:PHE:CD1	1:A:58:ALA:HB1	0.47	2.45	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:TRP:CE3	1:A:115:LYS:CG	0.47	2.98	3	2
1:A:99:ILE:CG2	1:A:110:LYS:HG2	0.47	2.39	13	1
1:A:97:GLU:HB3	1:A:114:LYS:CA	0.47	2.40	20	2
1:A:67:TRP:CD2	1:A:78:PHE:CE1	0.46	3.03	4	4
1:A:45:VAL:HG12	1:A:47:PHE:CE1	0.46	2.45	4	1
1:A:50:GLY:CA	1:A:68:THR:HG22	0.46	2.40	17	2
1:A:81:VAL:CG2	1:A:82:ASP:N	0.46	2.78	20	2
1:A:85:LYS:CG	1:A:85:LYS:O	0.46	2.63	1	1
1:A:80:ARG:HG2	1:A:87:LEU:CD1	0.46	2.41	19	1
1:A:73:LYS:HG3	1:A:92:GLU:HB3	0.46	1.86	9	1
1:A:67:TRP:CH2	1:A:77:LYS:HA	0.46	2.46	17	2
1:A:32:PHE:CZ	1:A:49:LEU:CD2	0.46	2.98	9	1
1:A:63:LEU:HG	1:A:87:LEU:HD21	0.46	1.88	10	1
1:A:97:GLU:HB3	1:A:114:LYS:CB	0.46	2.41	7	2
1:A:65:GLY:HA3	1:A:78:PHE:CD1	0.46	2.46	14	7
1:A:80:ARG:NE	1:A:85:LYS:HZ2	0.46	2.09	14	1
1:A:104:TYR:CE1	1:A:105:GLU:HG3	0.46	2.46	6	1
1:A:79:LYS:HD3	1:A:80:ARG:N	0.46	2.26	11	1
1:A:79:LYS:CG	1:A:86:GLU:N	0.46	2.79	9	3
1:A:79:LYS:HE2	1:A:84:GLY:CA	0.46	2.41	7	3
1:A:21:LEU:N	1:A:21:LEU:HD22	0.46	2.25	20	1
1:A:30:ASN:ND2	1:A:30:ASN:N	0.46	2.63	12	1
1:A:21:LEU:CD1	1:A:21:LEU:N	0.46	2.79	13	1
1:A:78:PHE:CD1	1:A:78:PHE:N	0.46	2.83	5	3
1:A:25:ILE:CG2	1:A:32:PHE:CZ	0.46	2.98	18	1
1:A:82:ASP:O	1:A:83:ASN:ND2	0.46	2.49	6	1
1:A:111:ARG:O	1:A:112:ILE:HG23	0.45	2.11	9	1
1:A:91:ARG:CG	1:A:92:GLU:H	0.45	2.24	10	1
1:A:39:ASN:O	1:A:41:ARG:N	0.45	2.49	10	1
1:A:53:PHE:CD1	1:A:53:PHE:C	0.45	2.90	1	1
1:A:27:GLN:HB3	1:A:32:PHE:CE1	0.45	2.47	9	1
1:A:49:LEU:CD2	1:A:50:GLY:N	0.45	2.79	1	1
1:A:67:TRP:HA	1:A:67:TRP:CE3	0.45	2.46	5	3
1:A:7:LYS:NZ	1:A:113:PHE:CD2	0.45	2.84	14	1
1:A:57:LEU:O	1:A:58:ALA:HB3	0.45	2.10	5	1
1:A:80:ARG:HG3	1:A:84:GLY:HA3	0.45	1.88	1	1
1:A:63:LEU:HD21	1:A:87:LEU:CD2	0.45	2.41	7	1
1:A:46:VAL:CG2	1:A:47:PHE:N	0.45	2.80	7	2
1:A:81:VAL:HG12	1:A:81:VAL:O	0.45	2.11	16	1
1:A:91:ARG:CG	1:A:98:LEU:HD21	0.45	2.42	6	1
1:A:93:ILE:HD12	1:A:98:LEU:HG	0.45	1.88	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:42:ASN:C	1:A:43:ILE:HG22	0.45	2.32	18	1
1:A:55:TYR:O	1:A:56:SER:C	0.45	2.55	11	1
1:A:7:LYS:HG3	1:A:114:LYS:O	0.45	2.12	9	4
1:A:91:ARG:HD3	1:A:100:GLN:HA	0.45	1.87	14	1
1:A:7:LYS:HA	1:A:114:LYS:HD3	0.45	1.88	11	1
1:A:32:PHE:CE1	1:A:49:LEU:CD2	0.45	3.00	5	2
1:A:6:TRP:CE2	1:A:115:LYS:HG3	0.45	2.47	14	2
1:A:27:GLN:HG3	1:A:32:PHE:N	0.45	2.26	20	3
1:A:65:GLY:HA3	1:A:78:PHE:CG	0.45	2.47	6	1
1:A:27:GLN:NE2	1:A:32:PHE:CE2	0.45	2.85	15	1
1:A:49:LEU:CD2	1:A:69:MET:N	0.45	2.79	13	1
1:A:65:GLY:C	1:A:78:PHE:CE2	0.45	2.90	15	1
1:A:46:VAL:C	1:A:47:PHE:CG	0.45	2.91	14	3
1:A:80:ARG:HG3	1:A:84:GLY:CA	0.45	2.42	1	1
1:A:27:GLN:CB	1:A:32:PHE:CE1	0.44	3.00	5	1
1:A:24:THR:HB	1:A:35:LYS:CB	0.44	2.42	13	3
1:A:43:ILE:HG13	1:A:57:LEU:HD13	0.44	1.88	12	1
1:A:90:VAL:O	1:A:90:VAL:HG12	0.44	2.11	17	3
1:A:61:THR:HB	1:A:63:LEU:CD1	0.44	2.43	7	1
1:A:58:ALA:HB3	1:A:61:THR:HB	0.44	1.89	10	1
1:A:114:LYS:HD2	1:A:114:LYS:O	0.44	2.13	2	1
1:A:6:TRP:CD1	1:A:25:ILE:HD12	0.44	2.48	10	1
1:A:42:ASN:H	1:A:42:ASN:ND2	0.44	2.11	3	1
1:A:6:TRP:CD1	1:A:115:LYS:HG3	0.44	2.48	14	1
1:A:104:TYR:O	1:A:106:GLY:N	0.44	2.51	14	2
1:A:91:ARG:HG3	1:A:98:LEU:CD1	0.44	2.43	5	1
1:A:91:ARG:HG2	1:A:98:LEU:CD2	0.44	2.42	6	1
1:A:27:GLN:HG3	1:A:32:PHE:CE1	0.44	2.48	5	1
1:A:53:PHE:CE1	1:A:65:GLY:C	0.44	2.90	10	1
1:A:97:GLU:O	1:A:98:LEU:HB2	0.44	2.12	13	1
1:A:88:ILE:CG2	1:A:90:VAL:HG23	0.44	2.40	13	1
1:A:79:LYS:HE2	1:A:84:GLY:HA2	0.44	1.88	13	1
1:A:47:PHE:CE2	1:A:67:TRP:HB2	0.44	2.48	15	1
1:A:105:GLU:O	1:A:107:VAL:HG23	0.44	2.12	14	1
1:A:21:LEU:N	1:A:21:LEU:CD2	0.44	2.80	4	1
1:A:80:ARG:CG	1:A:85:LYS:HG2	0.44	2.43	18	1
1:A:63:LEU:N	1:A:63:LEU:CD1	0.43	2.81	5	1
1:A:101:THR:HG21	1:A:108:GLU:OE2	0.43	2.13	12	1
1:A:109:ALA:C	1:A:110:LYS:CG	0.43	2.86	20	1
1:A:106:GLY:O	1:A:107:VAL:HG23	0.43	2.11	9	1
1:A:88:ILE:O	1:A:103:THR:N	0.43	2.52	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:45:VAL:HG12	1:A:47:PHE:HE1	0.43	1.71	4	1
1:A:26:THR:O	1:A:27:GLN:CG	0.43	2.66	12	1
1:A:80:ARG:HD3	1:A:84:GLY:HA3	0.43	1.90	1	1
1:A:80:ARG:O	1:A:82:ASP:N	0.43	2.51	20	2
1:A:21:LEU:H	1:A:21:LEU:HD12	0.43	1.71	17	1
1:A:48:GLU:HB3	1:A:51:VAL:HG21	0.43	1.90	16	1
1:A:91:ARG:HG2	1:A:92:GLU:N	0.43	2.27	20	1
1:A:27:GLN:HB2	1:A:31:LYS:O	0.43	2.13	16	1
1:A:25:ILE:CG2	1:A:32:PHE:CD1	0.43	2.93	16	2
1:A:49:LEU:O	1:A:51:VAL:N	0.43	2.51	1	1
1:A:93:ILE:HD12	1:A:98:LEU:HB2	0.43	1.91	11	1
1:A:29:GLY:O	1:A:30:ASN:ND2	0.43	2.52	11	1
1:A:7:LYS:CG	1:A:114:LYS:O	0.43	2.67	9	3
1:A:66:THR:O	1:A:67:TRP:CE3	0.43	2.72	14	1
1:A:114:LYS:HD3	1:A:114:LYS:C	0.43	2.33	13	1
1:A:43:ILE:CD1	1:A:57:LEU:CD1	0.43	2.88	20	1
1:A:4:GLY:N	1:A:26:THR:OG1	0.43	2.52	11	3
1:A:79:LYS:HG3	1:A:80:ARG:N	0.43	2.29	14	1
1:A:79:LYS:C	1:A:79:LYS:HD3	0.43	2.34	7	1
1:A:88:ILE:O	1:A:102:TYR:HA	0.43	2.13	16	1
1:A:90:VAL:HG12	1:A:90:VAL:O	0.43	2.13	13	2
1:A:80:ARG:HG3	1:A:87:LEU:CD1	0.43	2.44	20	1
1:A:114:LYS:HD2	1:A:114:LYS:C	0.43	2.34	1	1
1:A:70:GLU:O	1:A:73:LYS:N	0.43	2.51	15	1
1:A:58:ALA:HB3	1:A:61:THR:CB	0.43	2.44	10	1
1:A:98:LEU:HD22	1:A:100:GLN:HG2	0.43	1.91	3	1
1:A:62:GLU:O	1:A:64:THR:N	0.43	2.51	3	1
1:A:23:LEU:HD23	1:A:35:LYS:C	0.43	2.35	15	1
1:A:80:ARG:CZ	1:A:85:LYS:NZ	0.43	2.81	14	1
1:A:49:LEU:CD2	1:A:69:MET:CB	0.43	2.97	4	1
1:A:39:ASN:HD21	1:A:57:LEU:HD23	0.43	1.74	8	1
1:A:67:TRP:CD2	1:A:76:GLY:HA3	0.43	2.49	3	1
1:A:80:ARG:HB3	1:A:85:LYS:CB	0.43	2.44	13	3
1:A:53:PHE:CZ	1:A:78:PHE:CE1	0.43	3.06	19	1
1:A:7:LYS:HA	1:A:114:LYS:O	0.43	2.14	2	1
1:A:8:VAL:HG12	1:A:22:LYS:HG3	0.43	1.91	13	1
1:A:80:ARG:CD	1:A:87:LEU:CD1	0.43	2.97	3	1
1:A:32:PHE:CE2	1:A:69:MET:HB2	0.43	2.49	1	1
1:A:25:ILE:CG2	1:A:32:PHE:HB2	0.42	2.44	11	1
1:A:5:THR:C	1:A:6:TRP:CD1	0.42	2.92	3	2
1:A:97:GLU:CD	1:A:114:LYS:HB2	0.42	2.35	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:2:PHE:CZ	1:A:93:ILE:CD1	0.42	2.93	1	1
1:A:32:PHE:CE2	1:A:47:PHE:CE1	0.42	3.07	19	1
1:A:77:LYS:HD3	1:A:88:ILE:CD1	0.42	2.45	17	1
1:A:109:ALA:O	1:A:111:ARG:N	0.42	2.53	20	1
1:A:78:PHE:O	1:A:87:LEU:N	0.42	2.53	19	2
1:A:65:GLY:C	1:A:78:PHE:CZ	0.42	2.93	11	1
1:A:47:PHE:HB3	1:A:53:PHE:CZ	0.42	2.49	9	1
1:A:79:LYS:HE2	1:A:86:GLU:HB2	0.42	1.90	14	1
1:A:34:VAL:HG13	1:A:36:GLU:CB	0.42	2.44	14	1
1:A:101:THR:HG23	1:A:110:LYS:HB3	0.42	1.90	5	1
1:A:27:GLN:CA	1:A:32:PHE:HB3	0.42	2.44	6	1
1:A:95:GLY:N	1:A:97:GLU:OE2	0.42	2.52	20	1
1:A:65:GLY:CA	1:A:77:LYS:O	0.42	2.67	12	2
1:A:91:ARG:CD	1:A:92:GLU:H	0.42	2.28	13	1
1:A:80:ARG:O	1:A:84:GLY:N	0.42	2.52	8	1
1:A:91:ARG:HD3	1:A:92:GLU:N	0.42	2.30	3	1
1:A:106:GLY:C	1:A:107:VAL:HG23	0.42	2.34	14	1
1:A:21:LEU:HG	1:A:38:SER:CB	0.42	2.45	6	1
1:A:114:LYS:O	1:A:114:LYS:CD	0.42	2.67	14	1
1:A:55:TYR:O	1:A:57:LEU:N	0.42	2.53	6	2
1:A:32:PHE:O	1:A:47:PHE:CZ	0.42	2.73	18	1
1:A:102:TYR:O	1:A:104:TYR:N	0.42	2.53	15	1
1:A:8:VAL:HG12	1:A:8:VAL:O	0.42	2.15	19	1
1:A:34:VAL:CG1	1:A:36:GLU:HB2	0.42	2.45	5	1
1:A:98:LEU:C	1:A:98:LEU:HD23	0.42	2.34	13	2
1:A:31:LYS:HG3	1:A:32:PHE:N	0.42	2.28	4	1
1:A:79:LYS:HD3	1:A:79:LYS:C	0.42	2.35	13	1
1:A:41:ARG:HD3	1:A:43:ILE:HD12	0.42	1.92	15	1
1:A:114:LYS:CD	1:A:114:LYS:C	0.42	2.88	10	1
1:A:85:LYS:O	1:A:86:GLU:CG	0.42	2.68	1	1
1:A:23:LEU:HD11	1:A:100:GLN:OE1	0.41	2.14	17	1
1:A:49:LEU:HD12	1:A:50:GLY:N	0.41	2.30	7	1
1:A:111:ARG:HB3	1:A:113:PHE:CZ	0.41	2.50	4	1
1:A:43:ILE:CD1	1:A:57:LEU:HD22	0.41	2.45	18	1
1:A:27:GLN:CD	1:A:32:PHE:CE2	0.41	2.93	15	1
1:A:79:LYS:CD	1:A:80:ARG:N	0.41	2.83	11	1
1:A:24:THR:N	1:A:35:LYS:CB	0.41	2.83	14	1
1:A:34:VAL:CG1	1:A:36:GLU:CB	0.41	2.98	14	1
1:A:79:LYS:CE	1:A:85:LYS:N	0.41	2.83	5	1
1:A:85:LYS:O	1:A:86:GLU:HB2	0.41	2.16	5	1
1:A:52:ASP:N	1:A:66:THR:OG1	0.41	2.53	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LYS:CD	1:A:31:LYS:C	0.41	2.89	12	1
1:A:2:PHE:HZ	1:A:98:LEU:HD12	0.41	1.75	13	1
1:A:8:VAL:HG13	1:A:8:VAL:O	0.41	2.14	8	1
1:A:2:PHE:O	1:A:27:GLN:NE2	0.41	2.53	3	1
1:A:2:PHE:CZ	1:A:98:LEU:HD12	0.41	2.50	13	1
1:A:21:LEU:HD22	1:A:21:LEU:H	0.41	1.75	13	1
1:A:8:VAL:CG1	1:A:22:LYS:HG3	0.41	2.45	13	1
1:A:79:LYS:HE2	1:A:85:LYS:N	0.41	2.31	13	1
1:A:80:ARG:HD3	1:A:87:LEU:CD1	0.41	2.45	3	1
1:A:43:ILE:HD11	1:A:58:ALA:CA	0.41	2.46	15	1
1:A:66:THR:O	1:A:67:TRP:CD2	0.41	2.74	17	1
1:A:49:LEU:CD1	1:A:68:THR:HA	0.41	2.46	2	1
1:A:57:LEU:HB3	1:A:61:THR:HG21	0.41	1.92	20	1
1:A:6:TRP:CZ3	1:A:93:ILE:CD1	0.41	3.04	11	1
1:A:111:ARG:HB2	1:A:113:PHE:CE1	0.41	2.51	11	1
1:A:36:GLU:N	1:A:36:GLU:OE1	0.41	2.53	3	1
1:A:34:VAL:CG1	1:A:36:GLU:HB3	0.41	2.45	14	1
1:A:97:GLU:N	1:A:97:GLU:OE2	0.41	2.54	10	1
1:A:5:THR:HA	1:A:24:THR:HA	0.41	1.91	7	3
1:A:79:LYS:HE2	1:A:86:GLU:CB	0.41	2.46	14	1
1:A:27:GLN:HB2	1:A:32:PHE:CD1	0.41	2.51	5	1
1:A:62:GLU:HB2	1:A:81:VAL:HG12	0.41	1.92	5	1
1:A:97:GLU:CD	1:A:114:LYS:CB	0.41	2.89	4	1
1:A:80:ARG:CB	1:A:85:LYS:HB3	0.41	2.45	4	1
1:A:101:THR:O	1:A:101:THR:HG22	0.41	2.15	4	1
1:A:57:LEU:N	1:A:61:THR:O	0.41	2.54	10	1
1:A:6:TRP:CZ3	1:A:98:LEU:HB2	0.41	2.51	6	1
1:A:24:THR:C	1:A:25:ILE:HD12	0.41	2.36	20	1
1:A:58:ALA:N	1:A:61:THR:OG1	0.41	2.53	20	1
1:A:70:GLU:O	1:A:72:ASN:N	0.41	2.54	3	1
1:A:104:TYR:O	1:A:107:VAL:HG12	0.41	2.16	1	1
1:A:80:ARG:HG3	1:A:85:LYS:CB	0.41	2.46	12	1
1:A:25:ILE:HG22	1:A:32:PHE:HD1	0.41	1.74	13	1
1:A:41:ARG:HG2	1:A:42:ASN:N	0.40	2.31	17	1
1:A:25:ILE:HG13	1:A:34:VAL:HA	0.40	1.92	6	1
1:A:2:PHE:O	1:A:4:GLY:N	0.40	2.55	15	1
1:A:6:TRP:HB2	1:A:23:LEU:CA	0.40	2.46	17	1
1:A:93:ILE:CD1	1:A:98:LEU:HD13	0.40	2.40	5	1
1:A:67:TRP:CZ3	1:A:77:LYS:N	0.40	2.90	16	1
1:A:73:LYS:CD	1:A:73:LYS:N	0.40	2.84	11	1
1:A:41:ARG:HG2	1:A:58:ALA:CB	0.40	2.46	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:7:LYS:HE3	1:A:21:LEU:HD12	0.40	1.93	2	1
1:A:98:LEU:CD2	1:A:100:GLN:CB	0.40	2.99	13	1
1:A:21:LEU:C	1:A:22:LYS:HG2	0.40	2.36	1	1
1:A:93:ILE:CD1	1:A:93:ILE:N	0.40	2.79	16	1
1:A:104:TYR:CD1	1:A:105:GLU:HB2	0.40	2.52	4	1
1:A:101:THR:O	1:A:103:THR:N	0.40	2.54	10	1
1:A:80:ARG:CG	1:A:84:GLY:HA3	0.40	2.46	19	1
1:A:6:TRP:N	1:A:23:LEU:O	0.40	2.53	9	1
1:A:43:ILE:HG13	1:A:57:LEU:HD22	0.40	1.93	7	1
1:A:80:ARG:HB2	1:A:85:LYS:CB	0.40	2.47	10	1
1:A:101:THR:CG2	1:A:108:GLU:HG2	0.40	2.47	2	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	102/116 (88%)	55±5 (54±5%)	30±5 (30±4%)	17±3 (17±3%)	0	4
All	All	2040/2320 (88%)	1093 (54%)	607 (30%)	340 (17%)	0	4

All 60 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	8	VAL	19
1	A	24	THR	18
1	A	49	LEU	16
1	A	3	ASP	15
1	A	43	ILE	15
1	A	100	GLN	14
1	A	7	LYS	13
1	A	93	ILE	12
1	A	99	ILE	10
1	A	105	GLU	10
1	A	81	VAL	10

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Mol	Chain	Res	Type	Models (Total)
1	A	71	GLY	9
1	A	83	ASN	9
1	A	36	GLU	9
1	A	69	MET	8
1	A	86	GLU	8
1	A	60	GLY	8
1	A	22	LYS	8
1	A	114	LYS	8
1	A	57	LEU	7
1	A	25	ILE	7
1	A	85	LYS	6
1	A	63	LEU	6
1	A	112	ILE	6
1	A	58	ALA	5
1	A	61	THR	5
1	A	94	SER	5
1	A	47	PHE	5
1	A	77	LYS	5
1	A	66	THR	5
1	A	39	ASN	4
1	A	26	THR	4
1	A	97	GLU	4
1	A	52	ASP	4
1	A	27	GLN	4
1	A	41	ARG	3
1	A	79	LYS	3
1	A	82	ASP	3
1	A	4	GLY	2
1	A	30	ASN	2
1	A	2	PHE	2
1	A	80	ARG	2
1	A	115	LYS	2
1	A	92	GLU	2
1	A	107	VAL	2
1	A	95	GLY	2
1	A	74	LEU	1
1	A	38	SER	1
1	A	56	SER	1
1	A	59	ASP	1
1	A	50	GLY	1
1	A	28	GLU	1
1	A	21	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	44	ASP	1
1	A	110	LYS	1
1	A	98	LEU	1
1	A	62	GLU	1
1	A	5	THR	1
1	A	109	ALA	1
1	A	113	PHE	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	89/99 (90%)	58±4 (65±4%)	31±4 (35±4%)	1	10
All	All	1780/1980 (90%)	1165 (65%)	615 (35%)	1	10

All 80 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	33	THR	20
1	A	97	GLU	20
1	A	114	LYS	20
1	A	21	LEU	19
1	A	41	ARG	18
1	A	92	GLU	17
1	A	22	LYS	16
1	A	8	VAL	15
1	A	49	LEU	14
1	A	91	ARG	14
1	A	85	LYS	12
1	A	56	SER	12
1	A	27	GLN	12
1	A	77	LYS	12
1	A	110	LYS	11
1	A	38	SER	11
1	A	43	ILE	11
1	A	55	TYR	11

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Mol	Chain	Res	Type	Models (Total)
1	A	52	ASP	11
1	A	104	TYR	11
1	A	79	LYS	11
1	A	44	ASP	11
1	A	73	LYS	11
1	A	47	PHE	11
1	A	78	PHE	10
1	A	93	ILE	9
1	A	69	MET	9
1	A	83	ASN	9
1	A	87	LEU	9
1	A	42	ASN	9
1	A	80	ARG	8
1	A	59	ASP	8
1	A	112	ILE	8
1	A	32	PHE	8
1	A	30	ASN	6
1	A	116	GLU	6
1	A	3	ASP	6
1	A	28	GLU	6
1	A	100	GLN	6
1	A	35	LYS	6
1	A	36	GLU	6
1	A	111	ARG	6
1	A	98	LEU	5
1	A	86	GLU	5
1	A	70	GLU	5
1	A	57	LEU	5
1	A	94	SER	5
1	A	45	VAL	5
1	A	2	PHE	5
1	A	72	ASN	5
1	A	5	THR	5
1	A	31	LYS	5
1	A	46	VAL	5
1	A	105	GLU	5
1	A	62	GLU	5
1	A	37	SER	5
1	A	108	GLU	5
1	A	39	ASN	4
1	A	81	VAL	4
1	A	66	THR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	82	ASP	4
1	A	34	VAL	4
1	A	99	ILE	4
1	A	61	THR	4
1	A	48	GLU	4
1	A	68	THR	4
1	A	101	THR	4
1	A	51	VAL	4
1	A	25	ILE	4
1	A	96	ASN	3
1	A	53	PHE	3
1	A	90	VAL	3
1	A	107	VAL	3
1	A	63	LEU	3
1	A	40	PHE	3
1	A	74	LEU	2
1	A	103	THR	2
1	A	7	LYS	2
1	A	23	LEU	1
1	A	26	THR	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no carbohydrates 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 (i)

No chemical shift data were provided