



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 10:31 AM UTC

PDB ID : 1A57 / pdb_00001a57
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

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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

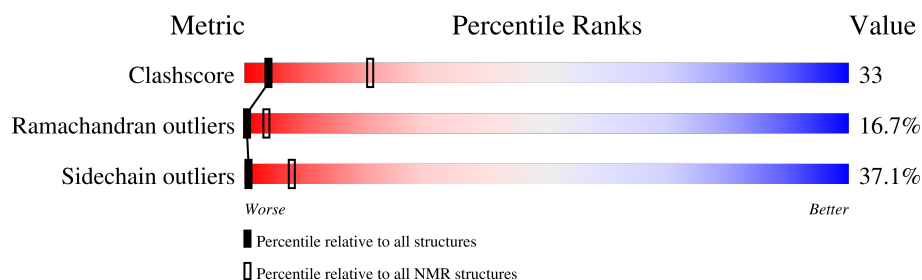
1 Overall quality at a glance

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	116	

2 Ensemble composition and analysis

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)	1.10	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

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
1	A	116	Total	C	H	N	O	S	0
			1838	586	909	157	185	1	

There are 16 discrepancies between the modelled and reference sequences:

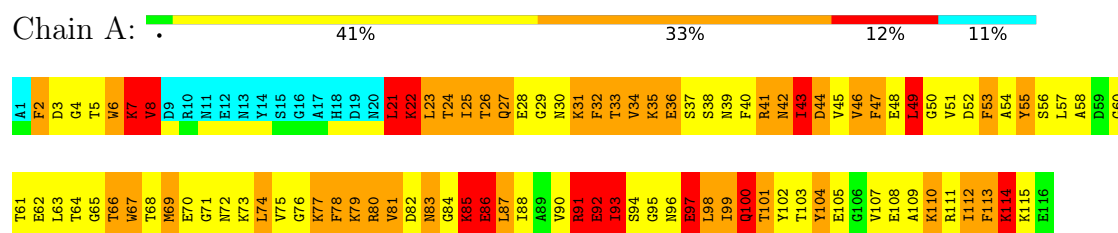
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P02693
A	?	-	LYS	deletion	UNP P02693
A	?	-	PHE	deletion	UNP P02693
A	?	-	MET	deletion	UNP P02693
A	?	-	GLU	deletion	UNP P02693
A	?	-	LYS	deletion	UNP P02693
A	?	-	MET	deletion	UNP P02693
A	?	-	GLY	deletion	UNP P02693
A	?	-	ILE	deletion	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 mutation	UNP P02693

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: INTESTINAL FATTY ACID-BINDING PROTEIN

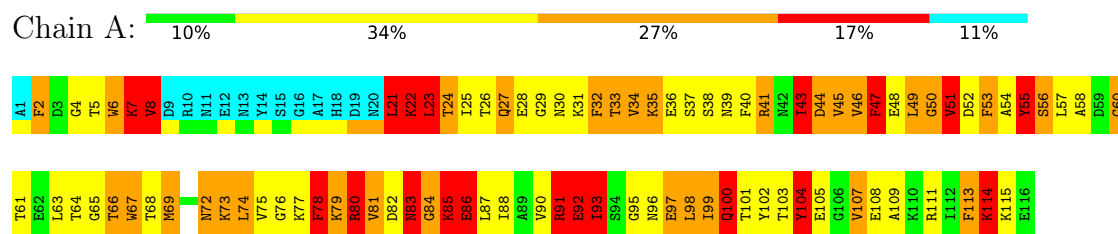


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

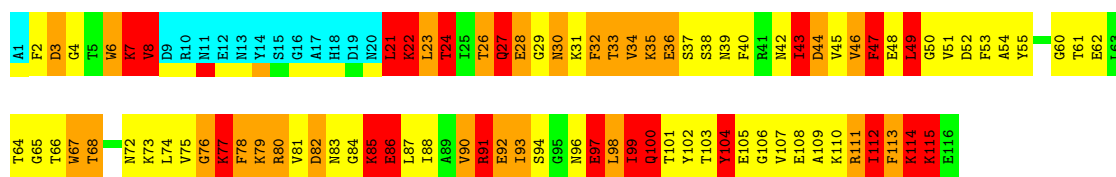
• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

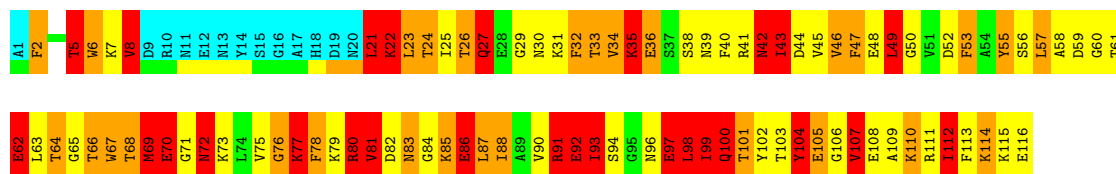




4.2.3 Score per residue for model 3

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

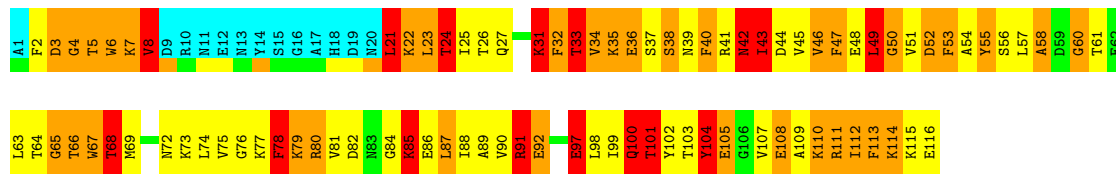
Chain A: 8% 34% 24% 23% 11%



4.2.4 Score per residue for model 4

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

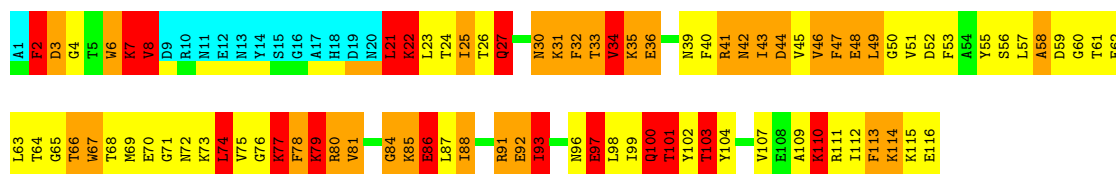
Chain A: 11% 34% 30% 14% 11%



4.2.5 Score per residue for model 5

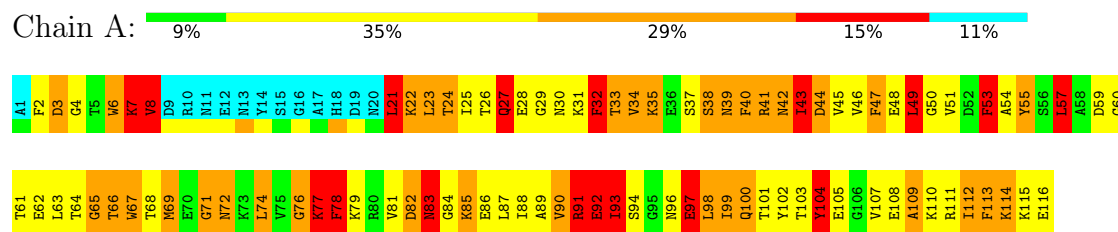
- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

Chain A: 13% 35% 26% 15% 11%



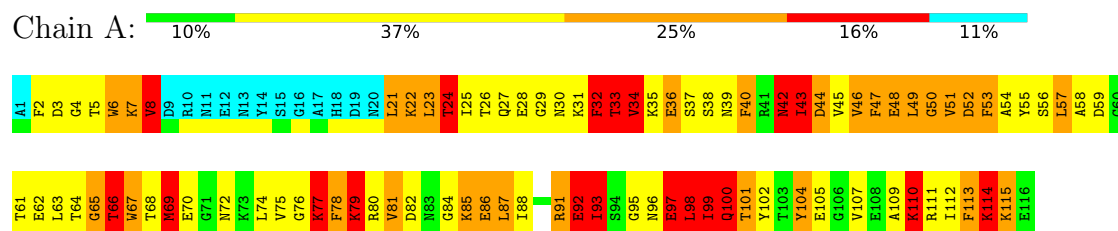
4.2.6 Score per residue for model 6

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



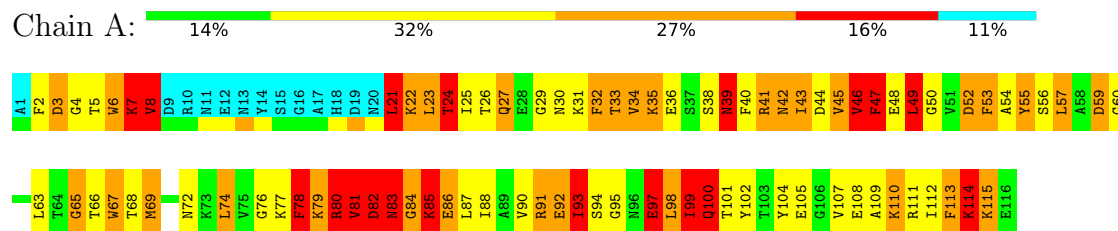
4.2.7 Score per residue for model 7

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



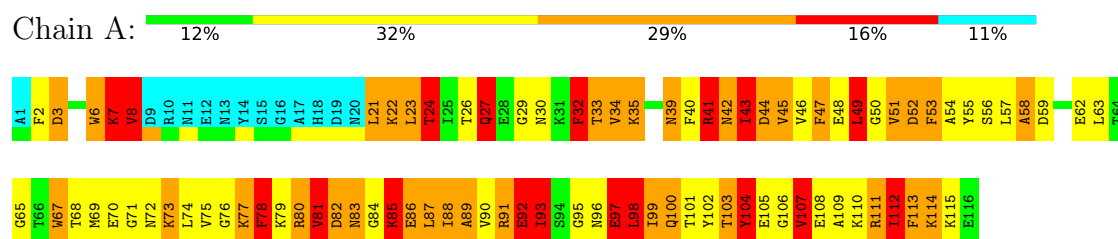
4.2.8 Score per residue for model 8

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



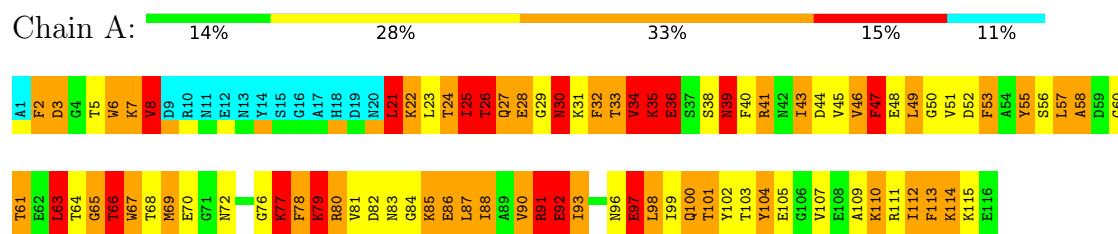
4.2.9 Score per residue for model 9

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



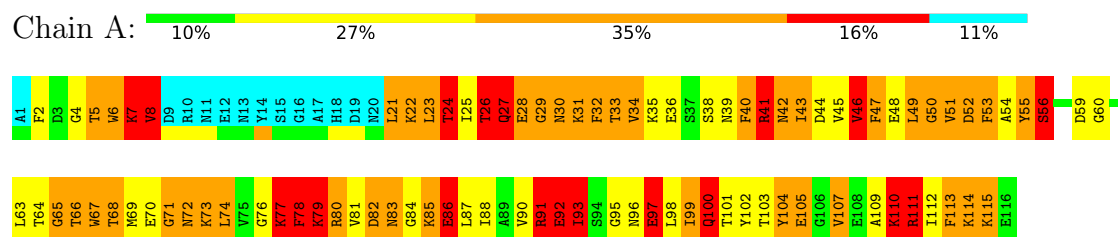
4.2.10 Score per residue for model 10

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



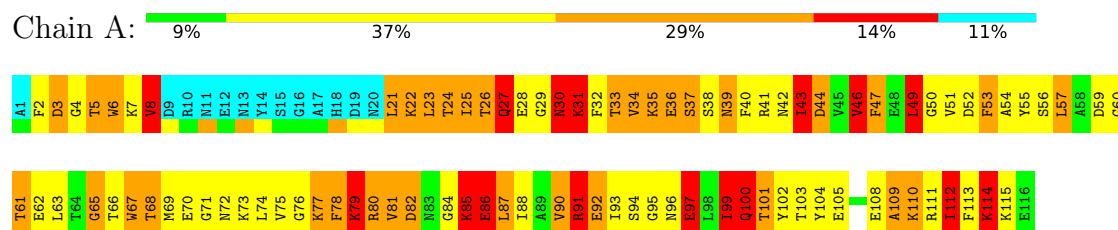
4.2.11 Score per residue for model 11

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



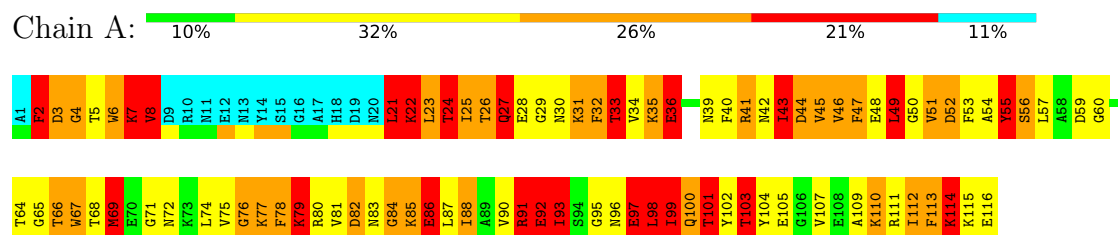
4.2.12 Score per residue for model 12

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



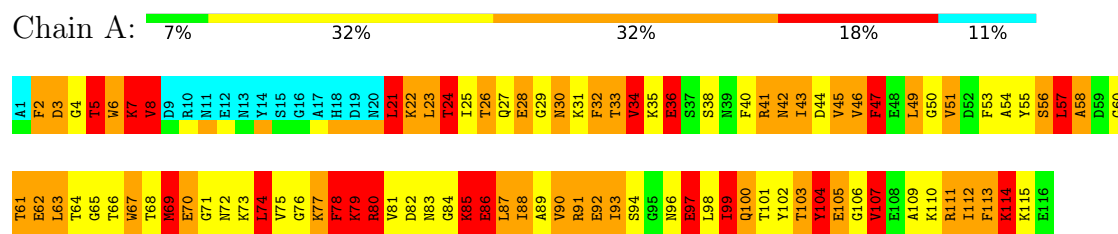
4.2.13 Score per residue for model 13

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



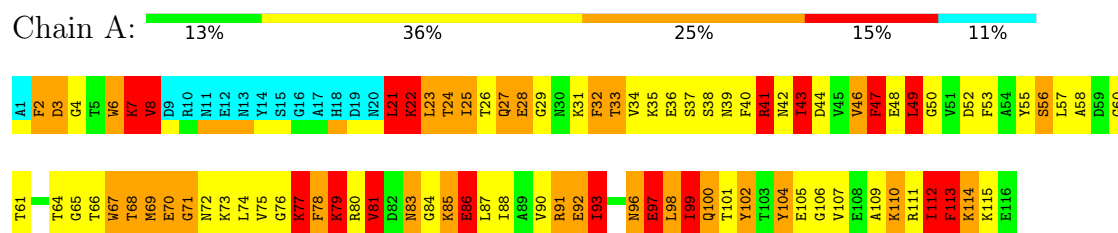
4.2.14 Score per residue for model 14

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



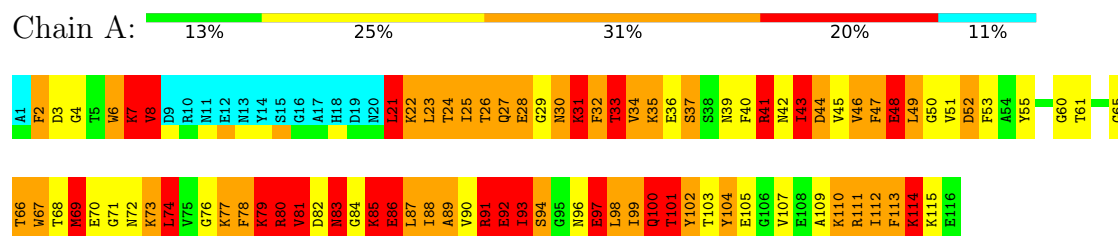
4.2.15 Score per residue for model 15

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



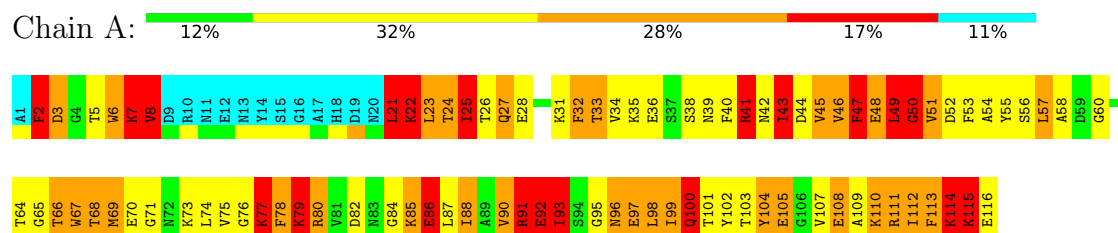
4.2.16 Score per residue for model 16

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



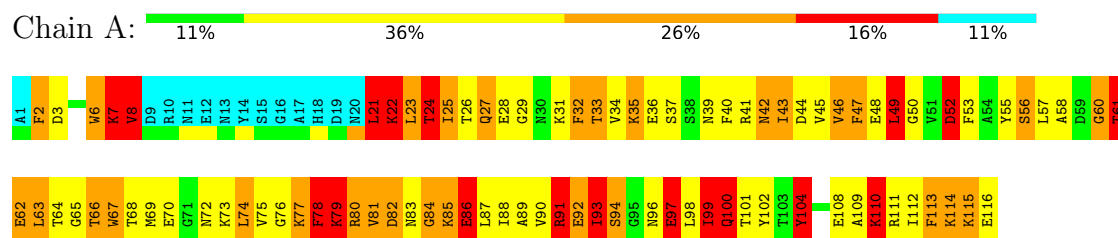
4.2.17 Score per residue for model 17

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



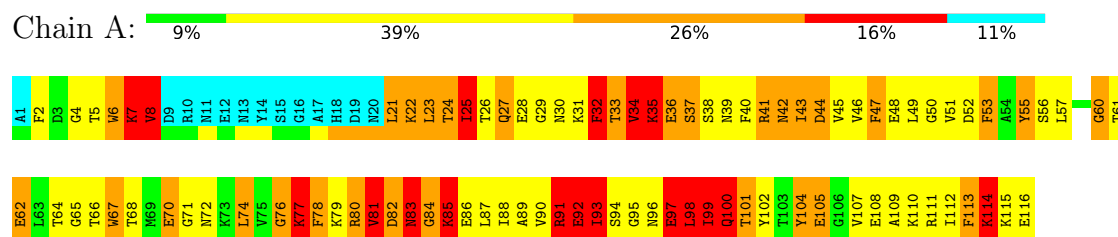
4.2.18 Score per residue for model 18

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



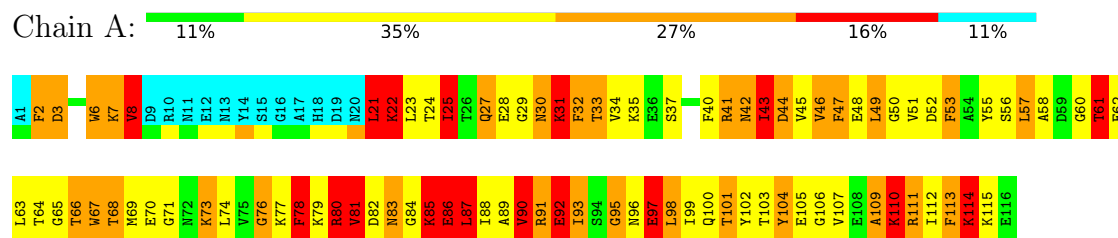
4.2.19 Score per residue for model 19

- 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

The models were refined using the following method: *DISTANCE GEOMETRY WITH SIMULATED 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 STANDARD 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.

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	1.46±0.02	10±0/840 (1.2± 0.1%)	3.07±0.05	116±9/1127 (10.3± 0.8%)
All	All	1.46	202/16800 (1.2%)	3.07	2327/22540 (10.3%)

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	Total
1	A	104	TYR	CE1-CZ	-7.83	1.19	1.38	18	12
1	A	104	TYR	CE2-CZ	-7.80	1.19	1.38	17	8
1	A	55	TYR	CE1-CZ	-7.53	1.20	1.38	10	16
1	A	55	TYR	CE2-CZ	-7.50	1.20	1.38	7	4
1	A	102	TYR	CE1-CZ	-7.45	1.20	1.38	6	8
1	A	102	TYR	CE2-CZ	-7.38	1.20	1.38	3	12
1	A	115	LYS	CA-C	-7.05	1.49	1.53	11	1
1	A	113	PHE	CE2-CZ	-6.29	1.19	1.38	3	14
1	A	113	PHE	CE1-CZ	-6.29	1.19	1.38	2	6
1	A	78	PHE	CE2-CZ	-6.24	1.20	1.38	4	8
1	A	78	PHE	CE1-CZ	-6.21	1.20	1.38	14	12
1	A	40	PHE	CE2-CZ	-6.18	1.20	1.38	18	17
1	A	40	PHE	CE1-CZ	-6.10	1.20	1.38	19	3
1	A	32	PHE	CE1-CZ	-6.10	1.20	1.38	14	9
1	A	32	PHE	CE2-CZ	-6.06	1.20	1.38	2	11
1	A	53	PHE	CE2-CZ	-6.04	1.20	1.38	19	7
1	A	53	PHE	CE1-CZ	-6.02	1.20	1.38	2	13
1	A	2	PHE	CE2-CZ	-5.83	1.21	1.38	8	14
1	A	47	PHE	CE2-CZ	-5.72	1.21	1.38	14	6
1	A	2	PHE	CE1-CZ	-5.72	1.21	1.38	2	6
1	A	47	PHE	CE1-CZ	-5.68	1.21	1.38	9	13
1	A	8	VAL	C-N	5.58	1.37	1.33	2	1
1	A	76	GLY	C-O	-5.17	1.20	1.23	16	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	88	ILE	O-C-N	14.19	137.75	122.57	17	15
1	A	29	GLY	N-CA-C	-13.45	99.19	113.58	16	10
1	A	32	PHE	O-C-N	13.34	136.66	123.46	13	20
1	A	43	ILE	CA-C-O	13.08	131.86	120.22	19	16
1	A	86	GLU	O-C-N	12.83	139.65	122.59	1	20
1	A	50	GLY	O-C-N	12.20	133.67	122.57	20	20
1	A	8	VAL	CA-C-O	12.10	135.91	120.78	12	20
1	A	55	TYR	O-C-N	12.03	134.69	122.30	11	5
1	A	68	THR	O-C-N	11.56	136.57	122.35	10	18
1	A	99	ILE	O-C-N	11.29	135.40	123.20	9	19
1	A	112	ILE	O-C-N	11.20	135.94	122.72	8	19
1	A	99	ILE	CA-C-O	-11.10	108.60	120.36	9	18
1	A	34	VAL	N-CA-CB	-11.02	98.43	111.00	13	19
1	A	64	THR	CA-C-N	-11.00	109.99	122.42	3	16
1	A	64	THR	C-N-CA	-11.00	109.99	122.42	3	16
1	A	67	TRP	O-C-N	10.93	136.06	123.27	15	20
1	A	92	GLU	O-C-N	10.89	134.73	123.62	19	20
1	A	109	ALA	O-C-N	10.83	137.74	122.36	20	20
1	A	76	GLY	CA-C-O	-10.76	113.48	120.91	15	8
1	A	97	GLU	O-C-N	10.62	135.21	123.52	20	19
1	A	46	VAL	O-C-N	10.58	134.98	123.02	2	17
1	A	7	LYS	O-C-N	10.53	136.59	122.59	7	20
1	A	42	ASN	O-C-N	10.35	133.94	122.15	9	17
1	A	76	GLY	O-C-N	10.31	133.82	123.92	4	14
1	A	32	PHE	N-CA-C	-10.26	95.27	110.46	9	19
1	A	23	LEU	CA-C-O	-10.25	109.90	121.89	18	20
1	A	84	GLY	O-C-N	10.23	132.01	122.19	19	19
1	A	81	VAL	O-C-N	10.21	132.22	121.90	10	18
1	A	80	ARG	O-C-N	10.20	134.89	122.35	20	17
1	A	91	ARG	O-C-N	10.19	132.58	123.41	2	20
1	A	35	LYS	CA-C-O	9.95	133.81	122.37	1	8
1	A	26	THR	O-C-N	9.94	135.80	122.59	10	14
1	A	22	LYS	O-C-N	9.90	134.57	123.48	19	20
1	A	46	VAL	N-CA-CB	-9.86	100.83	112.07	5	9
1	A	65	GLY	O-C-N	9.83	134.86	123.66	18	16
1	A	6	TRP	O-C-N	9.80	133.56	123.26	8	9
1	A	98	LEU	O-C-N	9.79	134.70	123.05	3	12
1	A	96	ASN	OD1-CG-ND2	9.69	132.29	122.60	3	14
1	A	60	GLY	O-C-N	9.68	135.28	122.70	18	14
1	A	51	VAL	O-C-N	9.67	129.43	121.98	17	15
1	A	45	VAL	CA-C-N	-9.61	111.62	122.48	20	15
1	A	45	VAL	C-N-CA	-9.61	111.62	122.48	20	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	115	LYS	N-CA-CB	-9.60	102.66	111.59	18	2
1	A	30	ASN	CA-C-O	-9.58	112.76	121.67	11	7
1	A	21	LEU	O-C-N	9.58	134.97	122.23	10	20
1	A	88	ILE	CA-C-O	-9.49	112.09	121.58	6	10
1	A	27	GLN	OE1-CD-NE2	9.45	132.05	122.60	12	16
1	A	77	LYS	O-C-N	9.36	135.04	122.59	6	9
1	A	87	LEU	O-C-N	9.33	131.42	122.18	12	12
1	A	6	TRP	CA-C-O	-9.28	111.12	121.51	17	15
1	A	42	ASN	N-CA-C	-9.18	101.36	111.36	9	6
1	A	43	ILE	N-CA-CB	-9.08	100.53	112.34	19	11
1	A	3	ASP	CA-C-N	-9.04	111.07	121.83	2	7
1	A	3	ASP	C-N-CA	-9.04	111.07	121.83	2	7
1	A	29	GLY	O-C-N	8.98	134.38	122.70	6	13
1	A	115	LYS	N-CA-C	8.92	117.31	108.75	11	1
1	A	78	PHE	CA-C-O	8.91	131.87	121.44	6	14
1	A	23	LEU	N-CA-C	-8.86	96.69	110.42	13	20
1	A	84	GLY	N-CA-C	-8.81	101.83	112.49	19	10
1	A	48	GLU	O-C-N	8.71	132.79	121.99	20	14
1	A	102	TYR	O-C-N	8.71	133.04	122.58	12	12
1	A	39	ASN	O-C-N	8.71	131.35	122.12	17	6
1	A	93	ILE	O-C-N	8.69	133.43	122.57	19	12
1	A	31	LYS	N-CA-C	-8.61	98.92	110.55	8	16
1	A	100	GLN	O-C-N	8.61	134.04	122.59	13	17
1	A	62	GLU	O-C-N	8.56	130.66	122.18	9	4
1	A	44	ASP	CA-C-N	-8.54	114.85	122.96	16	9
1	A	44	ASP	C-N-CA	-8.54	114.85	122.96	16	9
1	A	58	ALA	CB-CA-C	-8.53	105.64	115.79	10	1
1	A	85	LYS	O-C-N	8.49	131.95	122.11	14	15
1	A	28	GLU	CA-C-N	-8.48	110.84	120.42	15	5
1	A	28	GLU	C-N-CA	-8.48	110.84	120.42	15	5
1	A	115	LYS	CA-C-O	8.46	123.66	118.33	11	3
1	A	23	LEU	O-C-N	8.41	132.52	122.68	18	14
1	A	78	PHE	CA-CB-CG	8.41	122.21	113.80	2	12
1	A	85	LYS	CA-C-O	-8.39	111.99	120.80	14	13
1	A	52	ASP	O-C-N	8.35	132.39	122.96	8	12
1	A	33	THR	CA-C-N	-8.34	109.64	120.98	9	16
1	A	33	THR	C-N-CA	-8.34	109.64	120.98	9	16
1	A	89	ALA	O-C-N	8.32	133.11	122.71	14	4
1	A	101	THR	CA-C-N	-8.31	109.31	120.95	16	12
1	A	101	THR	C-N-CA	-8.31	109.31	120.95	16	12
1	A	40	PHE	O-C-N	8.29	131.89	122.11	14	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	LYS	CA-C-O	-8.25	111.21	120.54	17	16
1	A	34	VAL	N-CA-C	-8.25	98.98	109.30	9	9
1	A	85	LYS	N-CA-C	8.20	120.13	111.03	7	4
1	A	96	ASN	O-C-N	8.10	133.05	122.19	5	10
1	A	70	GLU	O-C-N	8.06	133.09	123.33	19	6
1	A	76	GLY	N-CA-C	-8.03	100.01	110.29	8	9
1	A	56	SER	O-C-N	8.00	132.39	122.63	10	11
1	A	35	LYS	N-CA-C	7.98	121.87	112.93	4	9
1	A	34	VAL	CB-CA-C	7.96	121.50	111.15	16	9
1	A	114	LYS	CA-C-O	7.95	131.87	120.51	8	6
1	A	28	GLU	N-CA-C	-7.92	103.64	113.38	2	5
1	A	110	LYS	O-C-N	7.88	131.97	122.20	13	15
1	A	75	VAL	CA-C-O	7.87	129.47	122.63	7	6
1	A	67	TRP	CG-CD1-NE1	-7.84	100.00	110.20	10	10
1	A	72	ASN	CA-CB-CG	-7.81	104.79	112.60	19	11
1	A	32	PHE	CA-C-N	-7.75	111.85	122.86	2	15
1	A	32	PHE	C-N-CA	-7.75	111.85	122.86	2	15
1	A	113	PHE	O-C-N	7.75	132.90	122.59	3	20
1	A	109	ALA	CB-CA-C	-7.71	98.72	111.68	7	15
1	A	111	ARG	O-C-N	7.65	132.20	123.48	3	9
1	A	8	VAL	N-CA-CB	-7.62	98.65	111.23	19	20
1	A	67	TRP	CA-CB-CG	-7.62	99.12	113.60	17	11
1	A	28	GLU	CA-C-O	-7.58	113.54	117.94	12	2
1	A	95	GLY	O-C-N	7.58	131.88	122.41	7	8
1	A	79	LYS	N-CA-CB	-7.51	97.79	110.49	13	13
1	A	44	ASP	O-C-N	7.51	132.25	123.02	14	17
1	A	107	VAL	O-C-N	7.47	130.87	123.03	17	13
1	A	28	GLU	O-C-N	7.41	127.03	121.47	12	6
1	A	33	THR	N-CA-C	-7.41	98.66	110.14	1	10
1	A	4	GLY	O-C-N	7.36	132.27	122.70	4	1
1	A	96	ASN	CA-CB-CG	-7.34	105.26	112.60	18	8
1	A	6	TRP	NE1-CE2-CD2	-7.27	97.95	107.40	9	9
1	A	6	TRP	CB-CG-CD2	7.25	136.96	126.80	20	9
1	A	86	GLU	CA-C-O	-7.15	112.77	120.92	20	6
1	A	69	MET	O-C-N	7.15	132.09	122.59	14	6
1	A	31	LYS	CA-C-N	-7.12	112.14	122.19	2	13
1	A	31	LYS	C-N-CA	-7.12	112.14	122.19	2	13
1	A	72	ASN	O-C-N	7.11	131.03	122.21	13	13
1	A	27	GLN	O-C-N	7.11	131.92	122.82	5	7
1	A	100	GLN	OE1-CD-NE2	7.10	129.70	122.60	16	4
1	A	90	VAL	CA-C-N	-7.10	109.47	121.75	20	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	90	VAL	C-N-CA	-7.10	109.47	121.75	20	13
1	A	75	VAL	O-C-N	7.08	127.90	121.96	3	2
1	A	103	THR	N-CA-C	-6.99	99.55	109.96	14	6
1	A	99	ILE	N-CA-CB	-6.99	103.72	111.41	4	2
1	A	95	GLY	N-CA-C	-6.97	105.61	115.30	7	2
1	A	7	LYS	CA-CB-CG	-6.97	100.16	114.10	15	19
1	A	75	VAL	N-CA-CB	-6.95	105.31	112.06	13	5
1	A	2	PHE	N-CA-C	-6.95	103.92	112.88	18	7
1	A	82	ASP	CA-C-O	-6.95	113.47	120.90	7	9
1	A	74	LEU	O-C-N	6.95	129.06	122.18	14	8
1	A	78	PHE	CB-CG-CD2	6.95	132.51	120.70	12	6
1	A	24	THR	CA-C-O	6.92	130.40	120.51	14	3
1	A	88	ILE	N-CA-C	-6.88	98.91	109.78	6	5
1	A	22	LYS	CB-CA-C	-6.87	98.93	109.99	16	18
1	A	109	ALA	CA-C-O	-6.84	114.30	122.03	2	3
1	A	25	ILE	N-CA-CB	-6.84	103.06	111.67	16	3
1	A	78	PHE	CB-CG-CD1	6.83	132.31	120.70	18	4
1	A	101	THR	N-CA-C	6.79	119.69	111.82	7	3
1	A	33	THR	CB-CA-C	6.77	120.84	110.62	2	11
1	A	71	GLY	O-C-N	6.77	131.50	122.70	16	7
1	A	111	ARG	CA-C-N	-6.76	112.33	121.66	7	11
1	A	111	ARG	C-N-CA	-6.76	112.33	121.66	7	11
1	A	77	LYS	N-CA-CB	-6.75	101.07	111.46	3	8
1	A	34	VAL	CA-CB-CG1	6.74	121.86	110.40	16	6
1	A	102	TYR	CA-C-O	-6.72	113.30	121.36	20	3
1	A	4	GLY	CA-C-O	-6.68	114.91	121.86	1	8
1	A	30	ASN	O-C-N	6.68	129.73	122.05	6	3
1	A	108	GLU	O-C-N	6.67	130.92	122.65	17	3
1	A	111	ARG	N-CA-C	-6.67	104.16	112.90	12	10
1	A	76	GLY	CA-C-N	-6.66	108.81	121.54	13	4
1	A	76	GLY	C-N-CA	-6.66	108.81	121.54	13	4
1	A	6	TRP	CB-CA-C	-6.66	100.52	110.24	13	7
1	A	21	LEU	N-CA-C	-6.66	101.56	110.55	9	1
1	A	78	PHE	N-CA-C	-6.65	99.83	110.14	13	6
1	A	75	VAL	N-CA-C	6.64	117.44	107.75	9	7
1	A	49	LEU	CA-C-O	6.64	130.00	120.51	9	4
1	A	39	ASN	CA-CB-CG	-6.60	106.00	112.60	6	5
1	A	47	PHE	CA-CB-CG	-6.60	107.20	113.80	1	17
1	A	21	LEU	CA-C-O	-6.54	114.42	121.36	4	9
1	A	45	VAL	O-C-N	6.54	129.05	122.71	1	7
1	A	67	TRP	CD1-NE1-CE2	6.53	120.66	108.90	18	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	6	TRP	NE1-CE2-CZ2	6.53	139.90	130.10	9	1
1	A	108	GLU	CA-C-N	-6.51	112.84	122.41	8	3
1	A	108	GLU	C-N-CA	-6.51	112.84	122.41	8	3
1	A	52	ASP	CA-C-N	-6.51	111.58	121.86	16	4
1	A	52	ASP	C-N-CA	-6.51	111.58	121.86	16	4
1	A	108	GLU	CA-C-O	-6.50	114.89	122.37	19	1
1	A	82	ASP	O-C-N	6.48	132.77	122.41	6	7
1	A	92	GLU	CA-C-O	-6.47	113.56	120.09	19	6
1	A	96	ASN	N-CA-C	-6.46	103.52	112.30	19	1
1	A	56	SER	CA-C-O	-6.46	114.63	121.99	1	9
1	A	113	PHE	CA-C-O	-6.45	114.03	120.80	4	9
1	A	5	THR	CA-C-O	-6.44	114.03	121.82	3	6
1	A	73	LYS	CA-C-O	-6.42	113.93	121.44	3	5
1	A	6	TRP	CE2-CD2-CG	6.41	114.89	107.20	13	9
1	A	30	ASN	CA-C-N	-6.41	111.20	121.58	19	6
1	A	30	ASN	C-N-CA	-6.41	111.20	121.58	19	6
1	A	88	ILE	CA-CB-CG2	6.41	121.39	110.50	20	11
1	A	55	TYR	CA-C-N	-6.39	112.60	122.05	20	6
1	A	55	TYR	C-N-CA	-6.39	112.60	122.05	20	6
1	A	59	ASP	O-C-N	6.38	128.57	121.87	8	1
1	A	57	LEU	CA-C-O	-6.37	114.78	121.98	10	3
1	A	67	TRP	NE1-CE2-CZ2	6.36	139.64	130.10	16	6
1	A	2	PHE	O-C-N	6.34	131.03	122.59	17	8
1	A	72	ASN	CA-C-O	-6.33	114.92	122.27	16	3
1	A	49	LEU	N-CA-CB	-6.33	102.84	112.28	17	1
1	A	36	GLU	CA-C-N	-6.33	112.45	121.50	8	4
1	A	36	GLU	C-N-CA	-6.33	112.45	121.50	8	4
1	A	6	TRP	CE2-CD2-CE3	-6.32	112.48	118.80	4	5
1	A	66	THR	N-CA-C	6.32	118.73	107.80	11	5
1	A	61	THR	O-C-N	6.30	129.56	122.32	3	3
1	A	102	TYR	N-CA-C	-6.28	103.56	110.91	15	2
1	A	90	VAL	N-CA-C	-6.26	100.92	109.37	14	1
1	A	54	ALA	CA-C-N	-6.25	112.10	121.72	13	5
1	A	54	ALA	C-N-CA	-6.25	112.10	121.72	13	5
1	A	54	ALA	O-C-N	6.20	130.19	122.63	14	3
1	A	97	GLU	CA-C-O	-6.18	114.62	121.23	4	2
1	A	105	GLU	N-CA-CB	-6.17	103.08	112.28	10	3
1	A	39	ASN	N-CA-C	-6.16	105.02	112.54	9	3
1	A	66	THR	O-C-N	-6.16	115.62	123.26	20	1
1	A	47	PHE	CA-C-O	-6.16	114.54	120.94	18	5
1	A	109	ALA	CA-C-N	-6.15	114.23	122.72	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	109	ALA	C-N-CA	-6.15	114.23	122.72	1	2
1	A	42	ASN	CB-CG-ND2	-6.14	107.19	116.40	8	6
1	A	50	GLY	CA-C-O	-6.13	112.67	120.03	20	1
1	A	104	TYR	CB-CG-CD1	6.12	129.98	120.80	3	1
1	A	90	VAL	CB-CA-C	-6.12	102.22	111.33	18	4
1	A	6	TRP	CD1-NE1-CE2	6.10	119.88	108.90	9	4
1	A	39	ASN	CA-C-N	-6.03	114.02	123.13	3	6
1	A	39	ASN	C-N-CA	-6.03	114.02	123.13	3	6
1	A	42	ASN	CA-C-N	-6.03	113.65	122.58	8	3
1	A	42	ASN	C-N-CA	-6.03	113.65	122.58	8	3
1	A	53	PHE	CA-CB-CG	-6.02	107.78	113.80	17	4
1	A	39	ASN	OD1-CG-ND2	6.02	128.62	122.60	8	2
1	A	41	ARG	CA-C-N	-6.00	111.78	120.29	13	7
1	A	41	ARG	C-N-CA	-6.00	111.78	120.29	13	7
1	A	102	TYR	CB-CG-CD2	5.99	129.79	120.80	6	2
1	A	78	PHE	CD1-CG-CD2	-5.99	109.62	118.60	14	7
1	A	83	ASN	CA-C-N	-5.97	110.84	121.00	13	4
1	A	83	ASN	C-N-CA	-5.97	110.84	121.00	13	4
1	A	54	ALA	N-CA-C	-5.96	100.85	110.32	4	6
1	A	89	ALA	CA-C-N	-5.96	111.57	121.63	9	4
1	A	89	ALA	C-N-CA	-5.96	111.57	121.63	9	4
1	A	24	THR	CA-C-N	-5.95	115.28	122.90	11	7
1	A	24	THR	C-N-CA	-5.95	115.28	122.90	11	7
1	A	66	THR	N-CA-CB	-5.95	101.57	111.57	19	4
1	A	100	GLN	N-CA-C	-5.95	98.13	110.80	15	3
1	A	67	TRP	N-CA-C	-5.94	100.50	109.95	16	1
1	A	46	VAL	CA-C-O	-5.93	115.76	121.63	2	2
1	A	51	VAL	N-CA-C	5.92	114.88	106.53	20	2
1	A	68	THR	CA-C-O	-5.90	114.37	121.34	7	3
1	A	83	ASN	CA-CB-CG	-5.89	106.71	112.60	3	4
1	A	53	PHE	N-CA-C	5.89	117.48	108.52	11	4
1	A	4	GLY	CA-C-N	-5.89	112.49	122.67	6	5
1	A	4	GLY	C-N-CA	-5.89	112.49	122.67	6	5
1	A	107	VAL	N-CA-CB	-5.87	103.61	112.35	16	2
1	A	67	TRP	CA-C-O	-5.86	113.19	120.57	14	2
1	A	70	GLU	N-CA-C	-5.83	104.83	111.07	14	1
1	A	91	ARG	N-CA-C	5.83	115.93	108.24	10	2
1	A	56	SER	N-CA-C	-5.82	102.84	110.53	9	1
1	A	37	SER	O-C-N	5.81	130.01	123.27	6	1
1	A	8	VAL	N-CA-C	5.80	121.41	109.34	11	11
1	A	3	ASP	N-CA-C	5.78	117.38	110.44	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	26	THR	CA-CB-OG1	5.77	118.26	109.60	9	5
1	A	54	ALA	CA-C-O	-5.75	114.61	120.71	13	7
1	A	41	ARG	N-CA-C	5.74	117.78	110.61	9	1
1	A	101	THR	O-C-N	5.74	129.93	122.87	3	6
1	A	79	LYS	N-CA-C	5.72	117.22	108.52	12	4
1	A	31	LYS	O-C-N	5.72	130.35	123.26	19	4
1	A	47	PHE	CA-C-N	-5.71	115.33	123.20	15	2
1	A	47	PHE	C-N-CA	-5.71	115.33	123.20	15	2
1	A	80	ARG	NE-CZ-NH2	-5.70	114.07	119.20	3	5
1	A	27	GLN	CG-CD-NE2	-5.70	107.86	116.40	14	5
1	A	46	VAL	CA-C-N	-5.68	112.55	122.84	18	2
1	A	46	VAL	C-N-CA	-5.68	112.55	122.84	18	2
1	A	26	THR	CA-C-N	-5.67	112.19	120.75	15	7
1	A	26	THR	C-N-CA	-5.67	112.19	120.75	15	7
1	A	80	ARG	CA-C-O	-5.65	115.04	120.92	2	4
1	A	101	THR	CA-C-O	5.64	126.94	120.84	4	1
1	A	83	ASN	CA-C-O	-5.62	113.66	119.51	15	2
1	A	41	ARG	NE-CZ-NH1	5.61	127.11	121.50	14	1
1	A	48	GLU	N-CA-CB	-5.60	101.84	110.25	13	4
1	A	34	VAL	CA-C-O	5.59	126.93	120.67	1	1
1	A	104	TYR	N-CA-C	5.59	117.52	108.41	18	2
1	A	105	GLU	CA-C-N	-5.57	113.76	122.51	8	1
1	A	105	GLU	C-N-CA	-5.57	113.76	122.51	8	1
1	A	82	ASP	CA-C-N	-5.57	113.40	122.26	13	1
1	A	82	ASP	C-N-CA	-5.57	113.40	122.26	13	1
1	A	103	THR	CA-C-O	5.56	127.62	121.39	6	1
1	A	46	VAL	CB-CA-C	-5.55	104.15	111.70	20	1
1	A	23	LEU	N-CA-CB	5.55	119.25	110.87	12	3
1	A	67	TRP	CE2-CD2-CG	-5.53	100.56	107.20	2	1
1	A	46	VAL	CG1-CB-CG2	-5.50	98.69	110.80	19	2
1	A	113	PHE	CD1-CG-CD2	-5.50	110.35	118.60	17	1
1	A	23	LEU	CB-CA-C	5.50	118.87	109.80	4	1
1	A	37	SER	CA-C-N	-5.47	114.13	122.23	20	1
1	A	37	SER	C-N-CA	-5.47	114.13	122.23	20	1
1	A	49	LEU	CD1-CG-CD2	-5.45	98.80	110.80	15	3
1	A	96	ASN	CB-CG-ND2	-5.45	108.23	116.40	6	5
1	A	109	ALA	N-CA-CB	-5.44	102.89	110.29	2	1
1	A	24	THR	CA-CB-OG1	5.44	117.76	109.60	13	2
1	A	90	VAL	CA-C-O	-5.43	114.83	121.13	14	1
1	A	107	VAL	N-CA-C	5.43	115.37	107.88	9	2
1	A	98	LEU	N-CA-CB	-5.42	102.04	110.55	16	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	61	THR	CA-C-N	-5.41	115.57	122.77	10	1
1	A	61	THR	C-N-CA	-5.41	115.57	122.77	10	1
1	A	33	THR	O-C-N	5.40	129.51	123.19	7	2
1	A	85	LYS	N-CA-CB	-5.39	102.44	110.10	10	3
1	A	28	GLU	N-CA-CB	-5.39	103.86	110.98	13	2
1	A	81	VAL	CA-C-O	-5.39	114.05	120.78	12	1
1	A	41	ARG	CB-CA-C	-5.39	102.74	114.10	10	1
1	A	67	TRP	CH2-CZ2-CE2	5.38	124.49	117.50	12	3
1	A	6	TRP	CB-CG-CD1	-5.36	118.86	126.90	19	1
1	A	58	ALA	N-CA-CB	-5.36	104.58	112.78	5	1
1	A	100	GLN	CG-CD-NE2	-5.35	108.37	116.40	5	1
1	A	51	VAL	CA-CB-CG1	5.35	119.50	110.40	12	1
1	A	43	ILE	CB-CA-C	5.35	116.51	110.41	19	1
1	A	63	LEU	O-C-N	5.35	129.23	122.28	10	1
1	A	85	LYS	CA-CB-CG	-5.35	103.41	114.10	20	2
1	A	58	ALA	O-C-N	5.34	129.53	122.43	9	1
1	A	68	THR	CA-CB-OG1	5.33	117.60	109.60	20	2
1	A	4	GLY	N-CA-C	-5.33	104.49	111.37	19	1
1	A	45	VAL	CB-CA-C	5.33	117.92	110.99	10	1
1	A	90	VAL	O-C-N	5.33	128.48	122.67	18	3
1	A	103	THR	O-C-N	5.32	129.72	122.48	13	2
1	A	47	PHE	O-C-N	5.32	128.57	123.04	6	1
1	A	30	ASN	CB-CA-C	-5.29	103.19	111.39	9	1
1	A	40	PHE	N-CA-C	-5.29	105.16	111.03	16	1
1	A	27	GLN	CA-C-N	-5.28	115.27	122.87	5	1
1	A	27	GLN	C-N-CA	-5.28	115.27	122.87	5	1
1	A	36	GLU	CB-CG-CD	-5.27	103.64	112.60	4	2
1	A	51	VAL	N-CA-CB	5.27	115.97	111.64	17	1
1	A	38	SER	O-C-N	5.25	129.57	122.59	4	1
1	A	51	VAL	CA-C-N	-5.25	112.68	121.39	6	1
1	A	51	VAL	C-N-CA	-5.25	112.68	121.39	6	1
1	A	51	VAL	CB-CA-C	-5.24	106.45	111.06	13	1
1	A	111	ARG	NE-CZ-NH2	5.22	123.90	119.20	18	2
1	A	8	VAL	O-C-N	-5.22	116.05	122.57	15	1
1	A	50	GLY	N-CA-C	-5.22	104.37	113.76	20	1
1	A	93	ILE	CA-C-O	-5.21	114.27	120.78	1	1
1	A	78	PHE	CB-CA-C	5.21	120.46	109.79	18	2
1	A	86	GLU	N-CA-C	5.20	117.42	110.35	2	1
1	A	47	PHE	CB-CG-CD2	5.20	129.54	120.70	14	2
1	A	48	GLU	CA-C-O	-5.18	115.48	121.49	19	1
1	A	84	GLY	CA-C-O	5.18	126.04	119.72	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	90	VAL	CA-CB-CG2	5.16	119.17	110.40	18	1
1	A	106	GLY	CA-C-O	5.15	124.77	119.00	15	1
1	A	111	ARG	NE-CZ-NH1	5.15	126.65	121.50	17	1
1	A	75	VAL	CG1-CB-CG2	-5.15	99.48	110.80	3	2
1	A	41	ARG	CA-C-O	-5.14	115.41	120.80	16	1
1	A	38	SER	N-CA-CB	-5.13	102.64	110.49	11	1
1	A	40	PHE	CA-C-O	-5.13	116.01	122.63	13	1
1	A	41	ARG	O-C-N	5.13	129.41	122.59	20	1
1	A	30	ASN	CA-CB-CG	5.12	117.72	112.60	2	1
1	A	67	TRP	NE1-CE2-CD2	-5.12	100.75	107.40	16	1
1	A	27	GLN	CA-C-O	-5.11	115.92	121.44	1	1
1	A	79	LYS	O-C-N	5.10	129.37	122.59	10	2
1	A	64	THR	O-C-N	5.10	129.37	122.59	13	1
1	A	80	ARG	NE-CZ-NH1	5.09	126.59	121.50	1	1
1	A	106	GLY	CA-C-N	-5.09	117.93	123.08	2	1
1	A	106	GLY	C-N-CA	-5.09	117.93	123.08	2	1
1	A	85	LYS	CA-C-N	-5.09	113.64	120.82	3	1
1	A	85	LYS	C-N-CA	-5.09	113.64	120.82	3	1
1	A	45	VAL	CG1-CB-CG2	-5.08	99.62	110.80	9	1
1	A	46	VAL	N-CA-C	5.07	115.94	110.21	19	1
1	A	75	VAL	CA-CB-CG1	5.07	119.01	110.40	17	1
1	A	32	PHE	CB-CA-C	5.06	118.25	110.62	10	1
1	A	62	GLU	CB-CG-CD	-5.04	104.03	112.60	3	1
1	A	5	THR	O-C-N	5.03	128.67	122.84	12	1
1	A	93	ILE	CA-C-N	-5.02	115.71	123.14	17	1
1	A	93	ILE	C-N-CA	-5.02	115.71	123.14	17	1
1	A	67	TRP	CB-CG-CD1	-5.01	119.38	126.90	12	1
1	A	37	SER	CA-C-O	-5.00	114.94	120.30	6	1
1	A	90	VAL	CG1-CB-CG2	-5.00	99.79	110.80	12	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	827	827	827	55±10
All	All	16540	16540	16540	1108

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	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:79:LYS:CG	1:A:85:LYS:C	0.76	2.59	1	4
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:66:THR:C	1:A:67:TRP:CD1	0.72	2.68	3	7
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ILE:HG21	1:A:32:PHE:CE2	0.67	2.24	7	2
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: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:66:THR:C	1:A:67:TRP:CG	0.64	2.76	17	7
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	3
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:NE1	1:A:78:PHE:CZ	0.62	2.68	8	10
1:A:67:TRP:CD1	1:A:78:PHE:CZ	0.62	2.87	8	5
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	7
1:A:79:LYS:HG2	1:A:85:LYS:C	0.61	2.19	1	6
1:A:83:ASN:ND2	1:A:83:ASN:N	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:N	1:A:114:LYS:HD2	0.61	2.10	20	12
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:86:GLU:C	1:A:87:LEU:HD12	0.61	2.20	1	1
1:A:91:ARG:C	1:A:92:GLU:CG	0.61	2.74	13	7
1:A:114:LYS:CD	1:A:114:LYS:N	0.60	2.64	7	2
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:27:GLN:HB2	1:A:31:LYS:C	0.60	2.22	13	3
1:A:67:TRP:CZ2	1:A:89:ALA:HB3	0.60	2.31	9	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
1:A:79:LYS:HG3	1:A:86:GLU:N	0.59	2.12	8	5
1:A:93:ILE:N	1:A:93:ILE:HD13	0.59	2.11	16	2
1:A:6:TRP:CE3	1:A:115:LYS:HG3	0.59	2.33	3	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:21:LEU:N	1:A:21:LEU:HD12	0.57	2.14	6	3
1:A:2:PHE:CE1	1:A:25:ILE:HD13	0.57	2.34	5	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:67:TRP:CZ2	1:A:77:LYS:N	0.56	2.74	2	5
1:A:97:GLU:HB2	1:A:114:LYS:HA	0.56	1.77	12	8
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:25:ILE:CG2	1:A:32:PHE:CE1	0.56	2.88	3	1
1:A:46:VAL:C	1:A:47:PHE:CD1	0.56	2.83	4	5
1:A:6:TRP:CH2	1:A:93:ILE:CD1	0.56	2.88	7	2
1:A:80:ARG:CD	1:A:87:LEU:HD11	0.56	2.30	19	2
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:6:TRP:CD2	1:A:115:LYS:CG	0.56	2.88	2	5
1:A:67:TRP:NE1	1:A:78:PHE:CE1	0.56	2.73	13	9
1:A:77:LYS:C	1:A:78:PHE:CD1	0.56	2.84	5	6
1:A:77:LYS:CG	1:A:78:PHE:N	0.56	2.68	16	4
1:A:93:ILE:CD1	1:A:98:LEU:HD22	0.56	2.30	5	1
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:25:ILE:HG12	1:A:34:VAL:HG22	0.55	1.78	1	2
1:A:104:TYR:C	1:A:104:TYR:CD1	0.55	2.85	14	9
1:A:25:ILE:HG22	1:A:32:PHE:HB2	0.55	1.79	11	1
1:A:34:VAL:HG12	1:A:36:GLU:CG	0.55	2.32	11	1
1:A:99:ILE:HG23	1:A:110:LYS:CB	0.55	2.30	11	1
1:A:24:THR:HG22	1:A:25:ILE:N	0.55	2.15	15	1
1:A:27:GLN:CB	1:A:31:LYS:C	0.55	2.80	16	3
1:A:85:LYS:CG	1:A:86:GLU:N	0.55	2.69	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:VAL:HG22	1:A:82:ASP:N	0.54	2.17	3	1
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:80:ARG:NE	1:A:85:LYS:HZ2	0.54	2.01	14	1
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:67:TRP:CH2	1:A:76:GLY:C	0.54	2.86	2	4
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:67:TRP:CZ3	1:A:76:GLY:C	0.53	2.86	19	6
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	10
1:A:67:TRP:CE3	1:A:67:TRP:HA	0.53	2.36	18	11
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:78:PHE:N	1:A:78:PHE:CD1	0.53	2.76	15	1
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:CE1	0.53	2.76	4	6
1:A:66:THR:N	1:A:78:PHE:CZ	0.53	2.77	5	4
1:A:32:PHE:CZ	1:A:74:LEU:HD21	0.53	2.39	8	2
1:A:43:ILE:O	1:A:43:ILE:HG23	0.52	2.04	2	5
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:46:VAL:C	1:A:47:PHE:CD2	0.52	2.88	1	6
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: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:77:LYS:HG3	1:A:78:PHE:N	0.52	2.20	7	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
1:A:93:ILE:HD11	1:A:97:GLU:N	0.52	2.20	10	1
1:A:7:LYS:HD2	1:A:113:PHE:HB3	0.51	1.81	1	3
1:A:24:THR:HB	1:A:35:LYS:HD2	0.51	1.82	4	8
1:A:67:TRP:CH2	1:A:89:ALA:HB3	0.51	2.40	4	2
1:A:83:ASN:N	1:A:83:ASN:HD22	0.51	2.00	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:LYS:CE	1:A:86:GLU:HB2	0.51	2.35	14	1
1:A:91:ARG:HG3	1:A:92:GLU:N	0.51	2.20	8	6
1:A:63:LEU:HD11	1:A:87:LEU:HD13	0.51	1.82	11	1
1:A:79:LYS:HG3	1:A:85:LYS:C	0.51	2.29	1	1
1:A:98:LEU:HD23	1:A:100:GLN:HG2	0.51	1.80	2	1
1:A:31:LYS:O	1:A:32:PHE:CG	0.51	2.64	20	3
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:49:LEU:HD21	1:A:69:MET:HB2	0.51	1.82	3	1
1:A:61:THR:HG22	1:A:63:LEU:HD13	0.51	1.82	14	2
1:A:32:PHE:HB2	1:A:47:PHE:CE2	0.51	2.41	16	3
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:6:TRP:HB2	1:A:23:LEU:HB2	0.51	1.82	17	6
1:A:24:THR:O	1:A:24:THR:HG22	0.51	2.06	2	5
1:A:79:LYS:CE	1:A:84:GLY:HA2	0.51	2.36	7	2
1:A:45:VAL:HG22	1:A:57:LEU:HD11	0.51	1.83	14	1
1:A:87:LEU:O	1:A:87:LEU:HG	0.51	2.06	14	1
1:A:6:TRP:HB2	1:A:23:LEU:CB	0.50	2.36	6	10
1:A:32:PHE:CE1	1:A:49:LEU:HD22	0.50	2.41	15	1
1:A:80:ARG:HD3	1:A:87:LEU:HD11	0.50	1.83	16	1
1:A:53:PHE:N	1:A:53:PHE:CD1	0.50	2.79	7	7
1:A:47:PHE:CD2	1:A:67:TRP:HB2	0.50	2.41	15	1
1:A:6:TRP:CG	1:A:115:LYS:HG3	0.50	2.41	14	2
1:A:53:PHE:CD1	1:A:53:PHE:C	0.50	2.90	1	2
1:A:74:LEU:HD12	1:A:98:LEU:HD11	0.50	1.83	16	2
1:A:79:LYS:HG3	1:A:86:GLU:HA	0.50	1.84	1	1
1:A:93:ILE:N	1:A:98:LEU:HD12	0.50	2.21	2	1
1:A:42:ASN:C	1:A:43:ILE:HG22	0.50	2.32	18	1
1:A:34:VAL:HG12	1:A:36:GLU:HG2	0.50	1.84	10	1
1:A:61:THR:CG2	1:A:63:LEU:CD1	0.50	2.90	10	1
1:A:55:TYR:O	1:A:56:SER:C	0.50	2.55	11	1
1:A:65:GLY:C	1:A:78:PHE:CE2	0.50	2.90	15	1
1:A:99:ILE:CG2	1:A:110:LYS:HB2	0.50	2.36	15	1
1:A:21:LEU:HD13	1:A:37:SER:O	0.50	2.06	4	1
1:A:32:PHE:CE1	1:A:34:VAL:HG22	0.50	2.42	8	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:5:THR:HG22	1:A:24:THR:OG1	0.49	2.07	3	2
1:A:93:ILE:CA	1:A:98:LEU:HD12	0.49	2.36	9	1
1:A:46:VAL:C	1:A:47:PHE:CG	0.49	2.91	14	5
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:7:LYS:HD2	1:A:113:PHE:CB	0.49	2.36	13	6
1:A:47:PHE:CD1	1:A:47:PHE:N	0.49	2.79	15	6
1:A:81:VAL:HG12	1:A:82:ASP:N	0.49	2.22	8	1
1:A:3:ASP:HA	1:A:26:THR:HB	0.49	1.85	10	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:6:TRP:CH2	1:A:93:ILE:HD13	0.49	2.43	11	2
1:A:47:PHE:CE2	1:A:67:TRP:CB	0.49	2.96	15	1
1:A:97:GLU:HB3	1:A:114:LYS:HB2	0.49	1.84	12	5
1:A:104:TYR:CD1	1:A:105:GLU:N	0.49	2.81	16	2
1:A:86:GLU:OE2	1:A:103:THR:HG22	0.49	2.08	14	1
1:A:58:ALA:HB3	1:A:61:THR:OG1	0.49	2.08	14	2
1:A:94:SER:CB	1:A:99:ILE:HD13	0.49	2.38	14	1
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:2:PHE:CE2	1:A:98:LEU:HD12	0.48	2.43	3	1
1:A:53:PHE:CE1	1:A:65:GLY:C	0.48	2.90	10	1
1:A:89:ALA:HB1	1:A:100:GLN:NE2	0.48	2.23	16	1
1:A:109:ALA:C	1:A:110:LYS:CG	0.48	2.86	20	1
1:A:88:ILE:HD12	1:A:103:THR:O	0.48	2.08	3	1
1:A:63:LEU:HD12	1:A:63:LEU:N	0.48	2.23	5	1
1:A:97:GLU:CB	1:A:114:LYS:HB2	0.48	2.39	12	2
1:A:44:ASP:O	1:A:57:LEU:HD11	0.48	2.08	12	1
1:A:91:ARG:CD	1:A:98:LEU:HD23	0.48	2.38	6	1
1:A:67:TRP:CH2	1:A:77:LYS:CA	0.48	2.97	17	2
1:A:98:LEU:HD23	1:A:100:GLN:CG	0.48	2.37	17	1
1:A:25:ILE:HG23	1:A:33:THR:H	0.48	1.69	13	1
1:A:58:ALA:HB3	1:A:61:THR:CG2	0.48	2.39	1	1
1:A:106:GLY:O	1:A:107:VAL:HG13	0.48	2.07	3	1
1:A:27:GLN:CB	1:A:32:PHE:CD1	0.48	2.96	5	1
1:A:85:LYS:HG3	1:A:86:GLU:N	0.48	2.23	17	8
1:A:114:LYS:C	1:A:114:LYS:HD3	0.48	2.33	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LYS:CD	1:A:113:PHE:HB3	0.48	2.39	16	6
1:A:93:ILE:HG23	1:A:97:GLU:O	0.48	2.09	8	1
1:A:81:VAL:CG1	1:A:82:ASP:N	0.48	2.77	9	1
1:A:89:ALA:HB1	1:A:100:GLN:HE22	0.48	1.69	16	1
1:A:79:LYS:HG2	1:A:86:GLU:CA	0.48	2.39	17	5
1:A:79:LYS:C	1:A:79:LYS:HD3	0.48	2.34	7	3
1:A:41:ARG:CD	1:A:41:ARG:N	0.48	2.76	16	2
1:A:82:ASP:C	1:A:83:ASN:CG	0.48	2.82	11	1
1:A:7:LYS:HB2	1:A:22:LYS:HA	0.48	1.86	17	1
1:A:114:LYS:HD2	1:A:114:LYS:C	0.47	2.34	1	2
1:A:49:LEU:HD22	1:A:69:MET:CB	0.47	2.39	7	1
1:A:2:PHE:CE1	1:A:98:LEU:HD13	0.47	2.43	10	1
1:A:106:GLY:C	1:A:107:VAL:HG23	0.47	2.34	14	1
1:A:80:ARG:N	1:A:85:LYS:O	0.47	2.48	4	1
1:A:99:ILE:CG2	1:A:110:LYS:CB	0.47	2.92	11	2
1:A:23:LEU:HD23	1:A:35:LYS:C	0.47	2.35	15	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:97:GLU:CD	1:A:114:LYS:HB2	0.47	2.35	4	2
1:A:53:PHE:CD1	1:A:55:TYR:HB2	0.47	2.44	1	1
1:A:83:ASN:ND2	1:A:84:GLY:N	0.47	2.62	19	1
1:A:58:ALA:HB3	1:A:61:THR:HG23	0.47	1.85	1	2
1:A:114:LYS:O	1:A:114:LYS:CD	0.47	2.62	8	3
1:A:79:LYS:HE2	1:A:86:GLU:CG	0.47	2.39	12	1
1:A:24:THR:HB	1:A:35:LYS:CD	0.47	2.39	11	6
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:5:THR:C	1:A:6:TRP:CD1	0.47	2.92	3	2
1:A:91:ARG:CG	1:A:92:GLU:N	0.47	2.77	17	8
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:65:GLY:C	1:A:78:PHE:CZ	0.47	2.93	11	1
1:A:98:LEU:HD23	1:A:98:LEU:C	0.47	2.34	13	1
1:A:99:ILE:CG2	1:A:100:GLN:N	0.47	2.78	13	3
1:A:93:ILE:CD1	1:A:97:GLU:N	0.47	2.78	15	1
1:A:6:TRP:CZ3	1:A:115:LYS:HB2	0.47	2.44	17	1
1:A:78:PHE:CD1	1:A:78:PHE:N	0.47	2.82	9	6
1:A:3:ASP:HA	1:A:26:THR:HA	0.47	1.86	10	1
1:A:114:LYS:N	1:A:114:LYS:CD	0.47	2.78	20	3
1:A:32:PHE:CE2	1:A:69:MET:HG2	0.47	2.45	15	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:114:LYS:CD	1:A:114:LYS:C	0.47	2.88	10	1
1:A:41:ARG:CZ	1:A:43:ILE:HB	0.47	2.40	16	1
1:A:6:TRP:CE3	1:A:115:LYS:CG	0.47	2.98	3	2
1:A:97:GLU:HB3	1:A:114:LYS:CA	0.47	2.40	20	2
1:A:99:ILE:CG2	1:A:110:LYS:HG2	0.47	2.39	13	1
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:85:LYS:O	1:A:85:LYS:CG	0.46	2.63	1	1
1:A:81:VAL:CG2	1:A:82:ASP:N	0.46	2.78	20	2
1:A:50:GLY:CA	1:A:68:THR:HG22	0.46	2.40	17	2
1:A:67:TRP:CH2	1:A:77:LYS:HA	0.46	2.46	17	2
1:A:73:LYS:HG3	1:A:92:GLU:HB3	0.46	1.86	9	1
1:A:31:LYS:CD	1:A:31:LYS:C	0.46	2.89	12	1
1:A:27:GLN:CD	1:A:32:PHE:CE2	0.46	2.93	15	1
1:A:80:ARG:HG2	1:A:87:LEU:CD1	0.46	2.41	19	1
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:98:LEU:C	1:A:98:LEU:HD23	0.46	2.36	16	1
1:A:65:GLY:HA3	1:A:78:PHE:CD1	0.46	2.46	14	7
1:A:104:TYR:CE1	1:A:105:GLU:HG3	0.46	2.46	6	1
1:A:97:GLU:HB3	1:A:114:LYS:CB	0.46	2.41	7	2
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:79:LYS:HD3	1:A:80:ARG:N	0.46	2.26	11	1
1:A:21:LEU:HD22	1:A:21:LEU:N	0.46	2.25	20	1
1:A:32:PHE:CE2	1:A:69:MET:HE2	0.46	2.45	9	1
1:A:21:LEU:N	1:A:21:LEU:CD1	0.46	2.79	13	1
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:39:ASN:O	1:A:41:ARG:N	0.45	2.49	10	1
1:A:91:ARG:CG	1:A:92:GLU:H	0.45	2.24	10	1
1:A:49:LEU:CD2	1:A:50:GLY:N	0.45	2.79	1	1
1:A:97:GLU:CD	1:A:114:LYS:CB	0.45	2.89	4	1
1:A:27:GLN:HB3	1:A:32:PHE:CE1	0.45	2.47	9	1
1:A:32:PHE:HE2	1:A:69:MET:HE2	0.45	1.72	9	1
1:A:7:LYS:NZ	1:A:113:PHE:CD2	0.45	2.84	14	1
1:A:24:THR:C	1:A:25:ILE:HD12	0.45	2.36	20	2
1:A:80:ARG:HG3	1:A:84:GLY:HA3	0.45	1.88	1	1
1:A:57:LEU:O	1:A:58:ALA:HB3	0.45	2.10	5	1
1:A:30:ASN:N	1:A:30:ASN:ND2	0.45	2.63	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:C	1:A:22:LYS:HG2	0.45	2.36	1	3
1:A:46:VAL:CG2	1:A:47:PHE:N	0.45	2.80	7	2
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
1:A:63:LEU:HD21	1:A:87:LEU:CD2	0.45	2.41	7	1
1:A:81:VAL:HG12	1:A:81:VAL:O	0.45	2.11	16	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:6:TRP:CE2	1:A:115:LYS:HG3	0.45	2.47	14	2
1:A:32:PHE:CE1	1:A:49:LEU:CD2	0.45	3.00	5	2
1:A:7:LYS:HA	1:A:114:LYS:HD3	0.45	1.88	11	1
1:A:65:GLY:HA3	1:A:78:PHE:CG	0.45	2.47	6	1
1:A:27:GLN:HG3	1:A:32:PHE:N	0.45	2.26	20	3
1:A:49:LEU:CD2	1:A:69:MET:N	0.45	2.79	13	1
1:A:27:GLN:NE2	1:A:32:PHE:CE2	0.45	2.85	15	1
1:A:79:LYS:C	1:A:80:ARG:HG2	0.45	2.36	16	1
1:A:80:ARG:HG3	1:A:84:GLY:CA	0.45	2.42	1	1
1:A:93:ILE:HD12	1:A:97:GLU:C	0.45	2.37	2	1
1:A:42:ASN:O	1:A:43:ILE:C	0.44	2.59	3	4
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:2:PHE:CD2	1:A:69:MET:HE3	0.44	2.46	16	1
1:A:114:LYS:HD2	1:A:114:LYS:O	0.44	2.13	2	1
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:90:VAL:HG12	1:A:90:VAL:O	0.44	2.11	17	1
1:A:42:ASN:ND2	1:A:42:ASN:H	0.44	2.11	3	1
1:A:6:TRP:CD1	1:A:25:ILE:HD12	0.44	2.48	10	1
1:A:111:ARG:C	1:A:112:ILE:CG1	0.44	2.91	15	1
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: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:27:GLN:HG3	1:A:32:PHE:CE1	0.44	2.48	5	1
1:A:79:LYS:HE2	1:A:84:GLY:HA2	0.44	1.88	13	1
1:A:88:ILE:CG2	1:A:90:VAL:HG23	0.44	2.40	13	1
1:A:97:GLU:O	1:A:98:LEU:HB2	0.44	2.12	13	1
1:A:47:PHE:CE2	1:A:67:TRP:HB2	0.44	2.48	15	1
1:A:21:LEU:N	1:A:21:LEU:CD2	0.44	2.80	4	1
1:A:105:GLU:O	1:A:107:VAL:HG23	0.44	2.12	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:ARG:CG	1:A:85:LYS:HG2	0.44	2.43	18	1
1:A:47:PHE:C	1:A:47:PHE:CD1	0.43	2.96	19	3
1:A:36:GLU:CD	1:A:36:GLU:C	0.43	2.86	3	2
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:80:ARG:HD3	1:A:84:GLY:HA3	0.43	1.90	1	1
1:A:45:VAL:HG12	1:A:47:PHE:HE1	0.43	1.71	4	1
1:A:88:ILE:O	1:A:103:THR:N	0.43	2.52	16	5
1:A:106:GLY:O	1:A:107:VAL:HG23	0.43	2.11	9	1
1:A:26:THR:O	1:A:27:GLN:CG	0.43	2.66	12	1
1:A:27:GLN:CD	1:A:32:PHE:CZ	0.43	2.96	2	1
1:A:48:GLU:HB3	1:A:51:VAL:HG21	0.43	1.90	16	1
1:A:21:LEU:HD12	1:A:21:LEU:H	0.43	1.71	17	1
1:A:80:ARG:O	1:A:82:ASP:N	0.43	2.51	20	2
1:A:91:ARG:HG2	1:A:92:GLU:N	0.43	2.27	20	1
1:A:49:LEU:O	1:A:51:VAL:N	0.43	2.51	1	1
1:A:83:ASN:ND2	1:A:83:ASN:C	0.43	2.75	6	1
1:A:25:ILE:CG2	1:A:32:PHE:CD1	0.43	2.93	16	2
1:A:27:GLN:HB2	1:A:31:LYS:O	0.43	2.13	16	1
1:A:80:ARG:C	1:A:82:ASP:N	0.43	2.76	18	2
1:A:7:LYS:CG	1:A:114:LYS:O	0.43	2.67	9	3
1:A:29:GLY:O	1:A:30:ASN:ND2	0.43	2.52	11	1
1:A:93:ILE:HD12	1:A:98:LEU:HB2	0.43	1.91	11	1
1:A:66:THR:O	1:A:67:TRP:CE3	0.43	2.72	14	1
1:A:43:ILE:CD1	1:A:57:LEU:CD1	0.43	2.88	20	1
1:A:49:LEU:C	1:A:49:LEU:HD12	0.43	2.39	2	1
1:A:90:VAL:O	1:A:90:VAL:HG12	0.43	2.13	13	4
1:A:114:LYS:C	1:A:114:LYS:HD2	0.43	2.38	10	2
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:88:ILE:O	1:A:102:TYR:HA	0.43	2.13	16	1
1:A:80:ARG:HG3	1:A:87:LEU:CD1	0.43	2.44	20	1
1:A:62:GLU:O	1:A:64:THR:N	0.43	2.51	3	1
1:A:98:LEU:HD22	1:A:100:GLN:HG2	0.43	1.91	3	1
1:A:58:ALA:HB3	1:A:61:THR:CB	0.43	2.44	10	1
1:A:70:GLU:O	1:A:73:LYS:N	0.43	2.51	15	1
1:A:67:TRP:CD2	1:A:76:GLY:HA3	0.43	2.49	3	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:80:ARG:CZ	1:A:85:LYS:NZ	0.43	2.81	14	1
1:A:32:PHE:CE2	1:A:69:MET:HB2	0.43	2.49	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LYS:HA	1:A:114:LYS:O	0.43	2.14	2	1
1:A:80:ARG:CD	1:A:87:LEU:CD1	0.43	2.97	3	1
1:A:80:ARG:HB3	1:A:85:LYS:CB	0.43	2.44	13	3
1:A:8:VAL:HG12	1:A:22:LYS:HG3	0.43	1.91	13	1
1:A:53:PHE:CZ	1:A:78:PHE:CE1	0.43	3.06	19	1
1:A:2:PHE:CZ	1:A:93:ILE:CD1	0.42	2.93	1	1
1:A:23:LEU:C	1:A:35:LYS:HB3	0.42	2.39	16	3
1:A:25:ILE:CG2	1:A:32:PHE:HB2	0.42	2.44	11	1
1:A:70:GLU:CD	1:A:70:GLU:C	0.42	2.87	15	1
1:A:77:LYS:HD3	1:A:88:ILE:CD1	0.42	2.45	17	1
1:A:32:PHE:CE2	1:A:47:PHE:CE1	0.42	3.07	19	1
1:A:109:ALA:O	1:A:111:ARG:N	0.42	2.53	20	1
1:A:49:LEU:C	1:A:49:LEU:CD1	0.42	2.92	2	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:78:PHE:O	1:A:87:LEU:N	0.42	2.53	19	2
1:A:47:PHE:HB3	1:A:53:PHE:CZ	0.42	2.49	9	1
1:A:34:VAL:HG13	1:A:36:GLU:CB	0.42	2.44	14	1
1:A:79:LYS:HE2	1:A:86:GLU:HB2	0.42	1.90	14	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:91:ARG:HD3	1:A:92:GLU:N	0.42	2.30	3	1
1:A:80:ARG:O	1:A:84:GLY:N	0.42	2.52	8	1
1:A:113:PHE:C	1:A:114:LYS:CG	0.42	2.91	17	1
1:A:21:LEU:HG	1:A:38:SER:CB	0.42	2.45	6	1
1:A:97:GLU:N	1:A:97:GLU:CD	0.42	2.77	16	3
1:A:70:GLU:CD	1:A:70:GLU:N	0.42	2.78	16	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:34:VAL:CG1	1:A:36:GLU:HB2	0.42	2.45	5	1
1:A:35:LYS:O	1:A:36:GLU:C	0.42	2.62	13	1
1:A:102:TYR:O	1:A:104:TYR:N	0.42	2.53	15	1
1:A:42:ASN:C	1:A:43:ILE:CG2	0.42	2.92	18	1
1:A:8:VAL:O	1:A:8:VAL:HG12	0.42	2.15	19	1
1:A:31:LYS:HG3	1:A:32:PHE:N	0.42	2.28	4	1
1:A:24:THR:C	1:A:25:ILE:CG1	0.42	2.93	10	1
1:A:66:THR:C	1:A:78:PHE:CZ	0.42	2.98	15	1
1:A:85:LYS:O	1:A:86:GLU:CG	0.42	2.68	1	1
1:A:41:ARG:HD3	1:A:43:ILE:HD12	0.42	1.92	15	1
1:A:111:ARG:HB3	1:A:113:PHE:CZ	0.41	2.50	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:C	1:A:22:LYS:CG	0.41	2.93	5	1
1:A:49:LEU:HD12	1:A:50:GLY:N	0.41	2.30	7	1
1:A:23:LEU:HD11	1:A:100:GLN:OE1	0.41	2.14	17	1
1:A:113:PHE:C	1:A:114:LYS:HG3	0.41	2.40	17	1
1:A:43:ILE:CD1	1:A:57:LEU:HD22	0.41	2.45	18	1
1:A:21:LEU:C	1:A:22:LYS:HG3	0.41	2.40	20	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:79:LYS:CD	1:A:80:ARG:N	0.41	2.83	11	1
1:A:2:PHE:HZ	1:A:98:LEU:HD12	0.41	1.75	13	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:52:ASP:N	1:A:66:THR:OG1	0.41	2.53	18	1
1:A:110:LYS:C	1:A:111:ARG:CG	0.41	2.93	20	1
1:A:2:PHE:O	1:A:27:GLN:NE2	0.41	2.53	3	1
1:A:8:VAL:HG13	1:A:8:VAL:O	0.41	2.14	8	1
1:A:27:GLN:CD	1:A:27:GLN:N	0.41	2.79	19	1
1:A:2:PHE:CZ	1:A:98:LEU:HD12	0.41	2.50	13	1
1:A:8:VAL:CG1	1:A:22:LYS:HG3	0.41	2.45	13	1
1:A:21:LEU:H	1:A:21:LEU:HD22	0.41	1.75	13	1
1:A:104:TYR:CD1	1:A:104:TYR:C	0.41	2.99	16	1
1:A:80:ARG:HD3	1:A:87:LEU:CD1	0.41	2.45	3	1
1:A:38:SER:C	1:A:40:PHE:N	0.41	2.77	6	1
1:A:79:LYS:HE2	1:A:85:LYS:N	0.41	2.31	13	1
1:A:49:LEU:CD1	1:A:68:THR:HA	0.41	2.46	2	1
1:A:79:LYS:CD	1:A:79:LYS:C	0.41	2.93	11	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:57:LEU:HB3	1:A:61:THR:HG21	0.41	1.92	20	1
1:A:36:GLU:N	1:A:36:GLU:OE1	0.41	2.53	3	1
1:A:65:GLY:C	1:A:66:THR:HG22	0.41	2.41	7	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:93:ILE:C	1:A:93:ILE:HD12	0.41	2.41	13	1
1:A:111:ARG:C	1:A:112:ILE:HD12	0.41	2.41	14	1
1:A:97:GLU:N	1:A:97:GLU:OE2	0.41	2.54	10	1
1:A:114:LYS:C	1:A:114:LYS:CD	0.41	2.94	12	1
1:A:34:VAL:CG1	1:A:36:GLU:HB3	0.41	2.45	14	1
1:A:104:TYR:O	1:A:107:VAL:HG12	0.41	2.16	1	1
1:A:70:GLU:O	1:A:72:ASN:N	0.41	2.54	3	1
1:A:80:ARG:CB	1:A:85:LYS:HB3	0.41	2.45	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:THR:O	1:A:101:THR:HG22	0.41	2.15	4	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:6:TRP:CZ3	1:A:98:LEU:HB2	0.41	2.51	6	1
1:A:5:THR:HA	1:A:24:THR:HA	0.41	1.91	7	3
1:A:57:LEU:N	1:A:61:THR:O	0.41	2.54	10	1
1:A:40:PHE:C	1:A:41:ARG:HD2	0.41	2.41	11	1
1:A:79:LYS:HE2	1:A:86:GLU:CB	0.41	2.46	14	1
1:A:58:ALA:N	1:A:61:THR:OG1	0.41	2.53	20	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:25:ILE:HG13	1:A:34:VAL:HA	0.40	1.92	6	1
1:A:41:ARG:HG2	1:A:42:ASN:N	0.40	2.31	17	1
1:A:93:ILE:CD1	1:A:98:LEU:HD13	0.40	2.40	5	1
1:A:2:PHE:O	1:A:4:GLY:N	0.40	2.55	15	1
1:A:67:TRP:CZ3	1:A:77:LYS:N	0.40	2.90	16	1
1:A:6:TRP:HB2	1:A:23:LEU:CA	0.40	2.46	17	1
1:A:7:LYS:HE3	1:A:21:LEU:HD12	0.40	1.93	2	1
1:A:24:THR:HG22	1:A:24:THR:O	0.40	2.15	8	1
1:A:41:ARG:HG2	1:A:58:ALA:CB	0.40	2.46	9	1
1:A:114:LYS:HD3	1:A:114:LYS:C	0.40	2.42	9	1
1:A:73:LYS:N	1:A:73:LYS:CD	0.40	2.84	11	1
1:A:98:LEU:CD2	1:A:100:GLN:CB	0.40	2.99	13	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:93:ILE:N	1:A:93:ILE:CD1	0.40	2.79	16	1
1:A:101:THR:CG2	1:A:108:GLU:HG2	0.40	2.47	2	1
1:A:43:ILE:HG13	1:A:57:LEU:HD22	0.40	1.93	7	1
1:A:49:LEU:HD12	1:A:49:LEU:C	0.40	2.42	7	1
1:A:6:TRP:N	1:A:23:LEU:O	0.40	2.53	9	1
1:A:80:ARG:HB2	1:A:85:LYS:CB	0.40	2.47	10	1
1:A:80:ARG:CG	1:A:84:GLY:HA3	0.40	2.46	19	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	3
All	All	2040/2320 (88%)	1093 (54%)	607 (30%)	340 (17%)	0	3

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	43	ILE	15
1	A	3	ASP	15
1	A	100	GLN	14
1	A	7	LYS	13
1	A	93	ILE	12
1	A	81	VAL	10
1	A	105	GLU	10
1	A	99	ILE	10
1	A	83	ASN	9
1	A	36	GLU	9
1	A	71	GLY	9
1	A	22	LYS	8
1	A	60	GLY	8
1	A	86	GLU	8
1	A	114	LYS	8
1	A	69	MET	8
1	A	57	LEU	7
1	A	25	ILE	7
1	A	63	LEU	6
1	A	85	LYS	6
1	A	112	ILE	6
1	A	47	PHE	5
1	A	58	ALA	5
1	A	66	THR	5
1	A	94	SER	5
1	A	77	LYS	5
1	A	61	THR	5
1	A	26	THR	4
1	A	97	GLU	4
1	A	39	ASN	4
1	A	52	ASP	4
1	A	27	GLN	4
1	A	82	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	41	ARG	3
1	A	79	LYS	3
1	A	30	ASN	2
1	A	115	LYS	2
1	A	92	GLU	2
1	A	4	GLY	2
1	A	2	PHE	2
1	A	95	GLY	2
1	A	107	VAL	2
1	A	80	ARG	2
1	A	5	THR	1
1	A	21	LEU	1
1	A	74	LEU	1
1	A	38	SER	1
1	A	44	ASP	1
1	A	59	ASP	1
1	A	28	GLU	1
1	A	56	SER	1
1	A	109	ALA	1
1	A	98	LEU	1
1	A	113	PHE	1
1	A	50	GLY	1
1	A	62	GLU	1
1	A	110	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	89/99 (90%)	56±4 (63±4%)	33±4 (37±4%)	1	8
All	All	1780/1980 (90%)	1119 (63%)	661 (37%)	1	8

All 82 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	21	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	33	THR	20
1	A	97	GLU	20
1	A	114	LYS	20
1	A	8	VAL	19
1	A	22	LYS	17
1	A	41	ARG	17
1	A	92	GLU	17
1	A	49	LEU	15
1	A	91	ARG	13
1	A	27	GLN	12
1	A	38	SER	12
1	A	43	ILE	12
1	A	85	LYS	12
1	A	77	LYS	12
1	A	110	LYS	12
1	A	44	ASP	11
1	A	73	LYS	11
1	A	93	ILE	11
1	A	79	LYS	11
1	A	56	SER	10
1	A	34	VAL	10
1	A	42	ASN	10
1	A	69	MET	10
1	A	70	GLU	10
1	A	78	PHE	9
1	A	83	ASN	9
1	A	104	TYR	9
1	A	112	ILE	9
1	A	52	ASP	9
1	A	59	ASP	8
1	A	81	VAL	8
1	A	116	GLU	8
1	A	51	VAL	7
1	A	55	TYR	7
1	A	80	ARG	7
1	A	28	GLU	7
1	A	30	ASN	7
1	A	35	LYS	7
1	A	36	GLU	7
1	A	99	ILE	7
1	A	87	LEU	7
1	A	48	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	7	LYS	6
1	A	45	VAL	6
1	A	57	LEU	6
1	A	86	GLU	6
1	A	103	THR	6
1	A	107	VAL	6
1	A	108	GLU	6
1	A	62	GLU	6
1	A	90	VAL	6
1	A	111	ARG	6
1	A	98	LEU	6
1	A	100	GLN	6
1	A	3	ASP	6
1	A	37	SER	5
1	A	72	ASN	5
1	A	74	LEU	5
1	A	47	PHE	5
1	A	61	THR	5
1	A	94	SER	5
1	A	5	THR	5
1	A	68	THR	5
1	A	31	LYS	5
1	A	101	THR	5
1	A	105	GLU	5
1	A	46	VAL	5
1	A	25	ILE	5
1	A	82	ASP	4
1	A	2	PHE	4
1	A	32	PHE	4
1	A	39	ASN	4
1	A	66	THR	4
1	A	24	THR	3
1	A	63	LEU	3
1	A	26	THR	2
1	A	53	PHE	2
1	A	96	ASN	2
1	A	23	LEU	1
1	A	115	LYS	1
1	A	40	PHE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided