



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 03:08 PM UTC

PDB ID : 1URE / pdb_00001ure
Title : NMR STRUCTURE OF INTESTINAL FATTY ACID-BINDING PROTEIN
COMPLEXED WITH PALMITATE, 20 STRUCTURES
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Deposited on : 1996-06-17

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

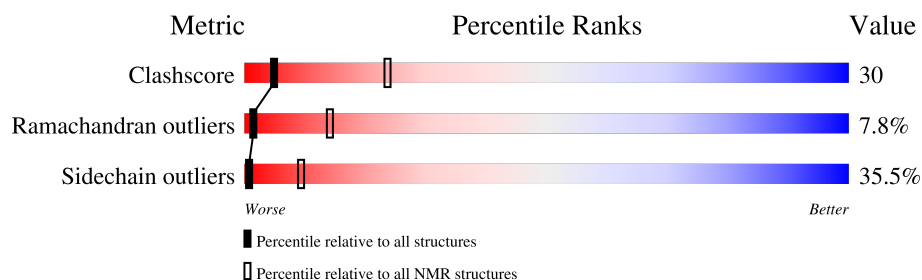
1 Overall quality at a glance

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	131	24% 51% 22% ..

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 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:131 (130)	0.86	12

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

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

The models can be grouped into 3 clusters and 7 single-model clusters were found.

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

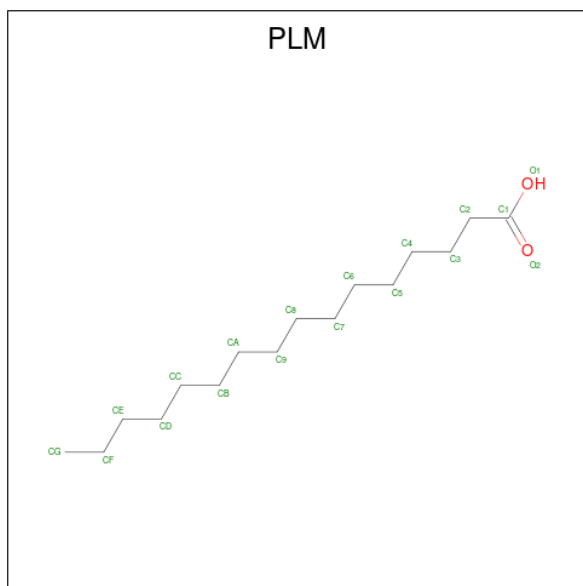
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2163 atoms, of which 1088 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	131	Total	C	H	N	O	S	0
			2114	670	1057	180	204	3	

- Molecule 2 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	O
			49	16	31	2

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

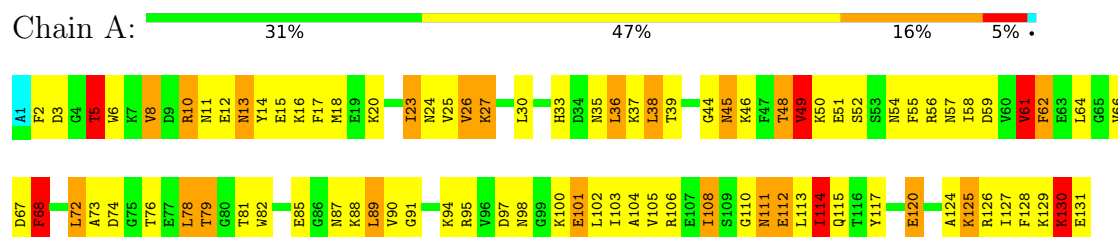


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

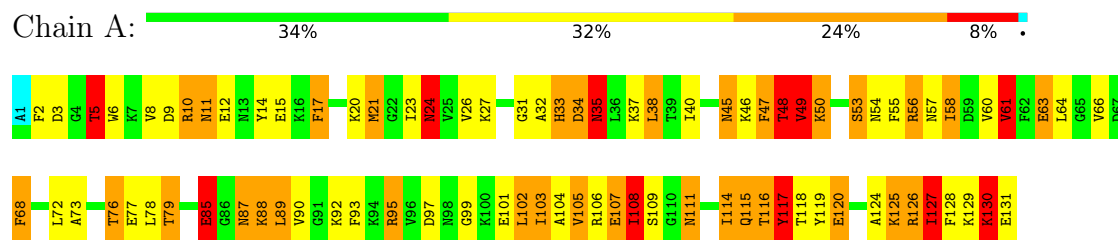
4.2.1 Score per residue for model 1

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



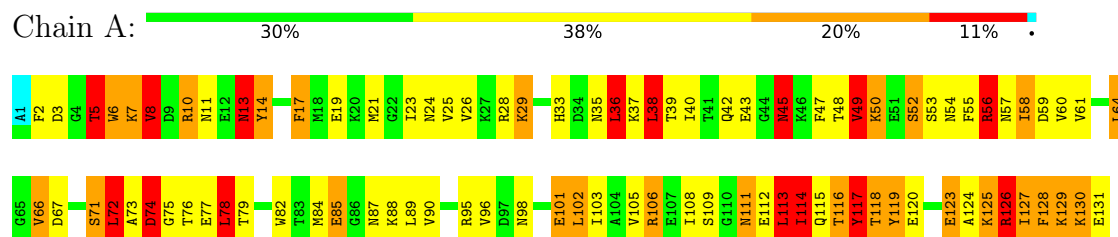
4.2.2 Score per residue for model 2

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



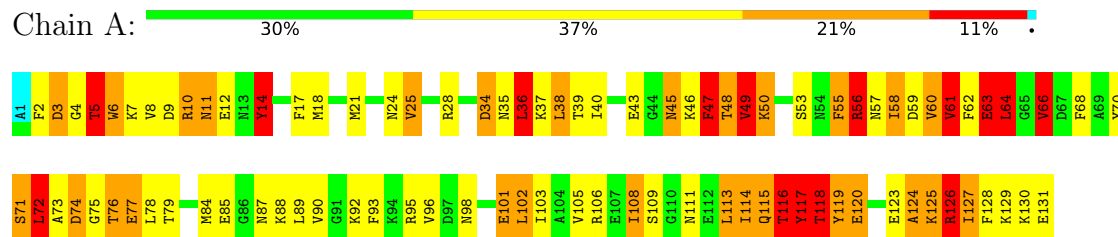
4.2.3 Score per residue for model 3

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



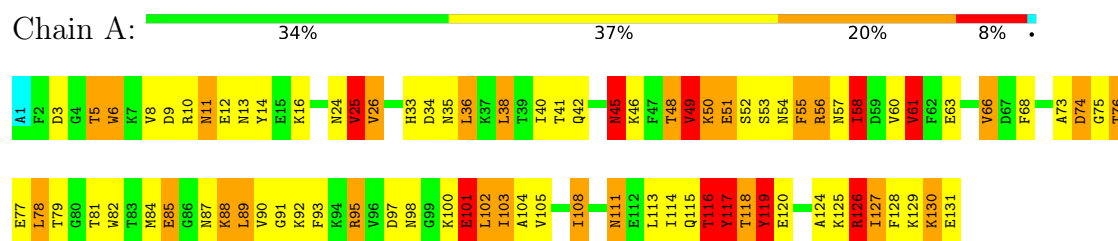
4.2.4 Score per residue for model 4

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



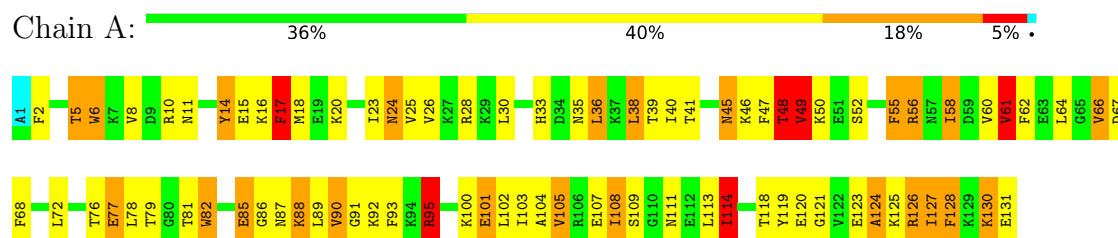
4.2.5 Score per residue for model 5

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



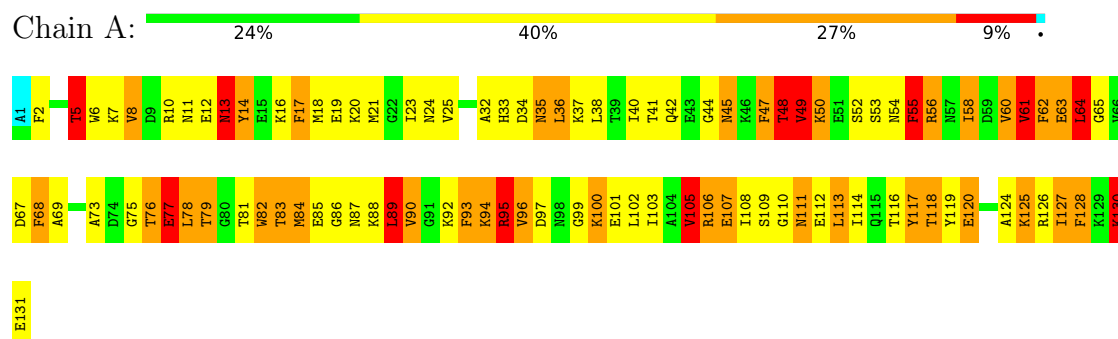
4.2.6 Score per residue for model 6

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



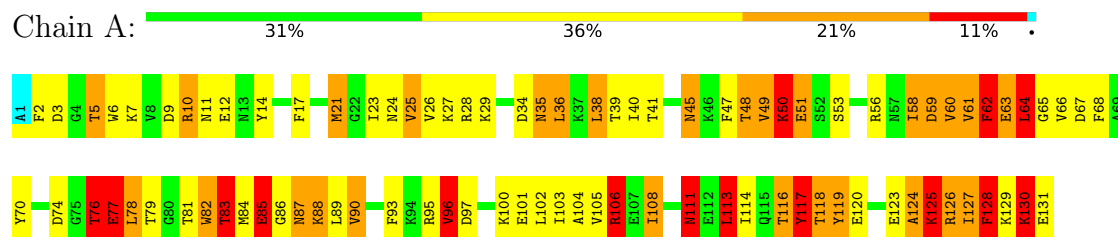
4.2.7 Score per residue for model 7

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



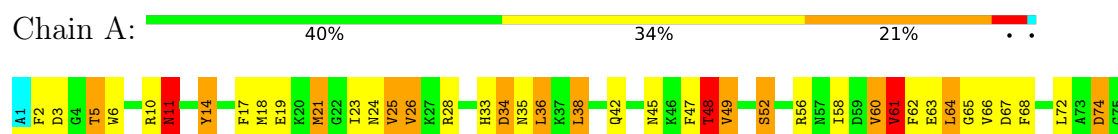
4.2.8 Score per residue for model 8

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



4.2.9 Score per residue for model 9

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

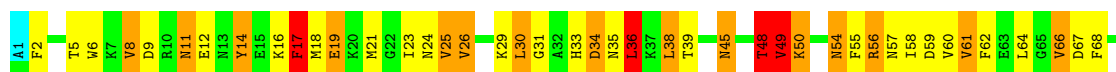




4.2.10 Score per residue for model 10

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

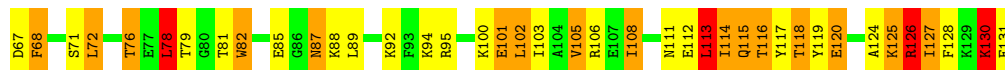
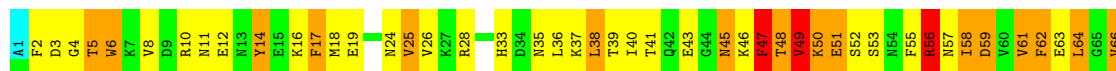
Chain A: 36% 35% 24% 5%



4.2.11 Score per residue for model 11

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

Chain A: 34% 36% 24% 5%



4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

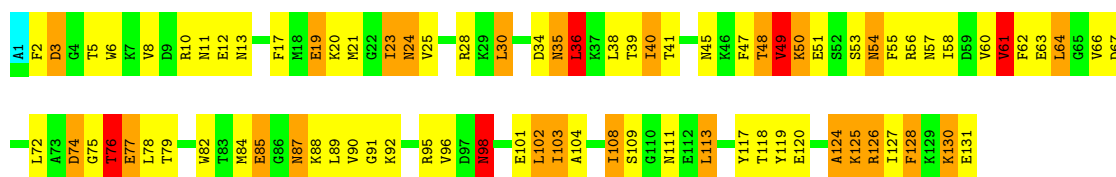
Chain A: 31% 37% 24% 8%



4.2.13 Score per residue for model 13

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

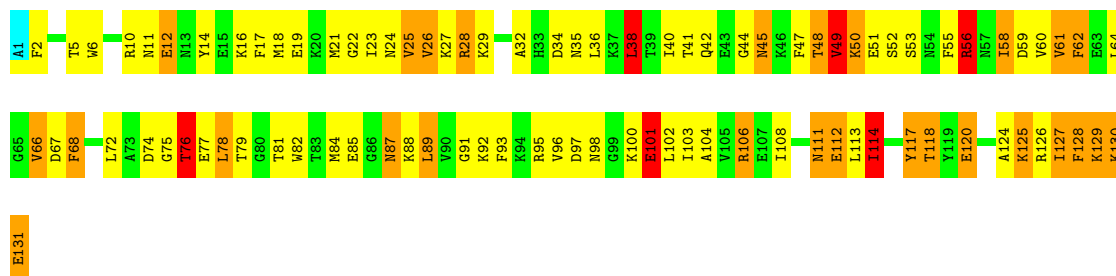
Chain A: 37% 40% 18%



4.2.14 Score per residue for model 14

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

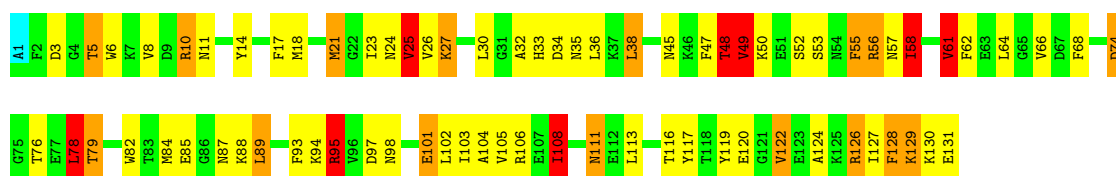
Chain A: 30% 44% 21% 5% •



4.2.15 Score per residue for model 15

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

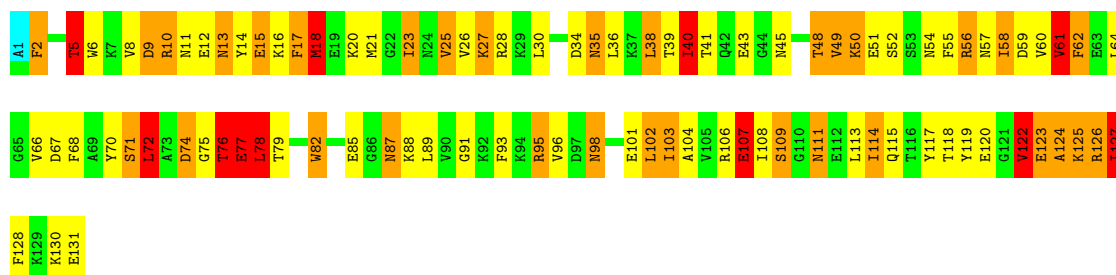
Chain A: 43% 38% 12% 6% •



4.2.16 Score per residue for model 16

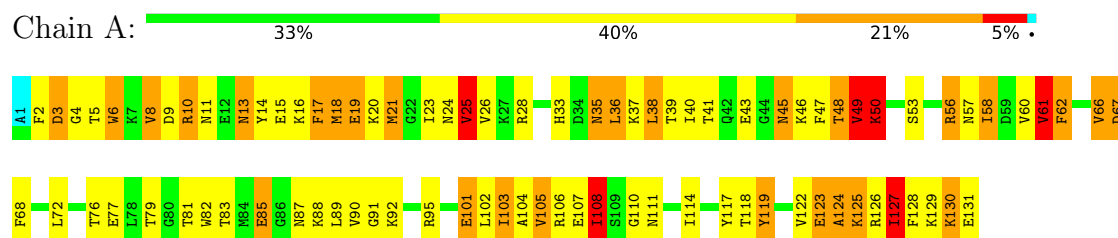
- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

Chain A: 28% 38% 24% 8% •



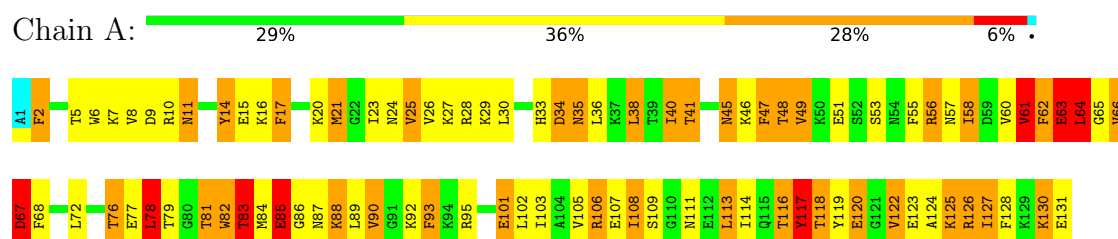
4.2.17 Score per residue for model 17

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



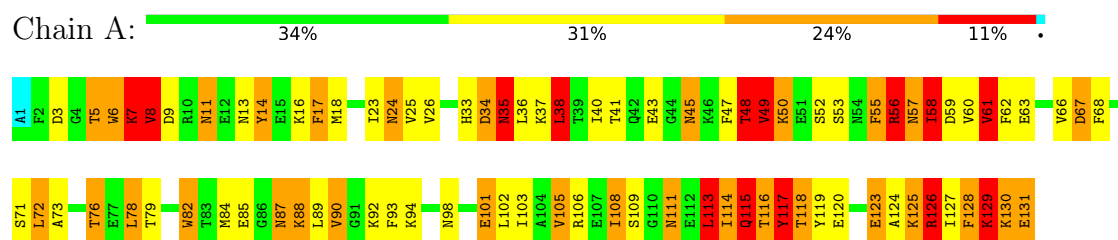
4.2.18 Score per residue for model 18

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



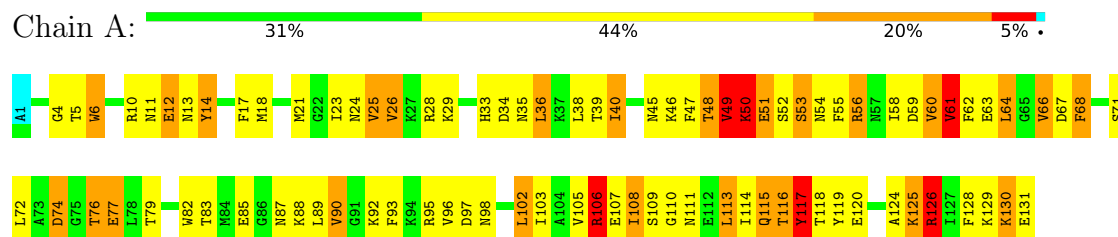
4.2.19 Score per residue for model 19

- 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 26 calculated structures, 20 were deposited, based on the following criterion: *FINAL PENALTY FUNCTION VALUES LESS THAN 10.0*.

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

Bond lengths and bond angles in the following residue types are not validated in this section: PLM

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	1.13±0.02	0±0/1068 (0.0± 0.0%)	2.32±0.06	54±8/1429 (3.8± 0.6%)
All	All	1.13	3/21360 (0.0%)	2.32	1084/28580 (3.8%)

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

Mol	Chain	Chirality	Planarity
1	A	1.0±0.0	0.0±0.0
All	All	20	0

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	117	TYR	CA-C	-6.09	1.48	1.53	15	2
1	A	103	ILE	CA-CB	-5.13	1.50	1.55	17	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	126	ARG	NE-CZ-NH2	11.69	129.72	119.20	3	16
1	A	49	VAL	CB-CA-C	10.49	124.01	111.32	17	13
1	A	11	ASN	CA-CB-CG	10.17	122.77	112.60	13	13
1	A	25	VAL	N-CA-CB	9.97	122.21	110.55	14	6
1	A	35	ASN	CA-CB-CG	9.36	121.96	112.60	8	15
1	A	131	GLU	N-CA-CB	9.29	126.30	110.50	18	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	49	VAL	N-CA-CB	9.18	121.44	111.89	9	11
1	A	101	GLU	CA-C-N	9.14	135.34	122.72	12	14
1	A	101	GLU	C-N-CA	9.14	135.34	122.72	12	14
1	A	26	VAL	N-CA-CB	8.94	123.99	110.58	10	9
1	A	87	ASN	CA-CB-CG	8.63	121.23	112.60	10	15
1	A	58	ILE	N-CA-C	8.55	119.00	106.85	19	14
1	A	66	VAL	N-CA-CB	8.55	121.86	111.60	1	7
1	A	85	GLU	N-CA-CB	8.55	120.96	110.53	6	13
1	A	88	LYS	CB-CA-C	-8.51	97.82	110.24	4	16
1	A	24	ASN	CA-CB-CG	8.49	121.09	112.60	18	18
1	A	116	THR	O-C-N	8.36	129.38	123.11	11	6
1	A	56	ARG	CD-NE-CZ	8.29	136.01	124.40	16	17
1	A	50	LYS	N-CA-C	-8.27	99.10	110.35	5	15
1	A	58	ILE	CA-CB-CG2	8.20	124.45	110.50	15	13
1	A	26	VAL	N-CA-C	8.17	118.97	110.72	2	6
1	A	126	ARG	NE-CZ-NH1	8.17	129.67	121.50	8	18
1	A	124	ALA	CA-C-O	-8.17	112.57	121.31	8	4
1	A	48	THR	N-CA-CB	8.02	122.28	110.49	19	19
1	A	79	THR	CA-CB-OG1	7.98	121.58	109.60	16	16
1	A	5	THR	N-CA-CB	7.93	121.69	110.04	14	14
1	A	10	ARG	NE-CZ-NH2	-7.92	112.07	119.20	16	9
1	A	17	PHE	CA-CB-CG	-7.82	105.98	113.80	17	3
1	A	33	HIS	CA-CB-CG	-7.72	106.08	113.80	19	11
1	A	111	ASN	CA-CB-CG	7.66	120.26	112.60	18	9
1	A	63	GLU	N-CA-C	-7.66	98.81	110.30	7	4
1	A	23	ILE	CA-C-O	-7.61	116.01	122.63	16	2
1	A	57	ASN	CA-C-N	7.59	132.69	120.55	15	7
1	A	57	ASN	C-N-CA	7.59	132.69	120.55	15	7
1	A	49	VAL	N-CA-C	7.55	118.09	107.37	14	6
1	A	56	ARG	NE-CZ-NH2	7.55	125.99	119.20	1	9
1	A	60	VAL	N-CA-C	7.52	114.26	106.21	4	1
1	A	66	VAL	CB-CA-C	7.49	121.36	111.85	19	12
1	A	36	LEU	CA-C-O	-7.42	112.64	120.58	3	1
1	A	35	ASN	OD1-CG-ND2	7.32	129.92	122.60	11	20
1	A	47	PHE	CB-CA-C	-7.32	100.65	111.77	17	10
1	A	5	THR	CA-CB-CG2	7.29	122.90	110.50	10	8
1	A	127	ILE	CB-CA-C	-7.27	103.43	111.35	16	4
1	A	85	GLU	CB-CA-C	7.27	122.95	111.91	18	13
1	A	111	ASN	N-CA-CB	7.27	121.24	110.49	13	13
1	A	115	GLN	N-CA-C	-7.24	101.50	110.41	4	5
1	A	67	ASP	CB-CA-C	-7.24	99.65	109.71	17	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	52	SER	N-CA-CB	-7.23	101.34	110.45	1	5
1	A	61	VAL	N-CA-CB	7.21	120.14	110.26	19	10
1	A	114	ILE	CB-CA-C	-7.17	100.38	111.71	14	11
1	A	14	TYR	N-CA-C	7.16	119.08	111.28	6	5
1	A	101	GLU	O-C-N	7.14	131.55	123.27	16	6
1	A	118	THR	N-CA-C	7.11	117.66	108.34	4	9
1	A	34	ASP	N-CA-C	6.98	120.68	111.75	15	4
1	A	56	ARG	CB-CG-CD	6.96	127.31	111.30	13	10
1	A	119	TYR	N-CA-C	-6.91	103.83	111.36	16	5
1	A	19	GLU	CA-C-O	6.90	127.90	119.97	17	6
1	A	115	GLN	O-C-N	6.90	130.78	123.06	2	2
1	A	45	ASN	OD1-CG-ND2	6.88	129.48	122.60	15	20
1	A	57	ASN	N-CA-C	-6.86	100.14	109.54	18	8
1	A	117	TYR	CB-CA-C	-6.86	102.44	111.42	14	2
1	A	34	ASP	CA-CB-CG	6.84	119.44	112.60	9	9
1	A	6	TRP	CA-C-O	-6.80	113.98	121.33	4	5
1	A	76	THR	O-C-N	6.77	133.92	122.21	4	11
1	A	125	LYS	CB-CA-C	-6.77	98.09	109.53	19	9
1	A	95	ARG	N-CA-CB	-6.77	100.17	110.45	11	11
1	A	79	THR	N-CA-C	-6.76	101.80	110.53	11	2
1	A	9	ASP	CA-C-O	6.76	126.20	118.97	17	2
1	A	128	PHE	N-CA-CB	6.75	120.25	110.06	3	5
1	A	78	LEU	CB-CA-C	-6.75	103.06	111.43	7	2
1	A	79	THR	CA-CB-CG2	6.73	121.95	110.50	14	5
1	A	24	ASN	CA-C-O	-6.73	113.87	121.81	5	5
1	A	78	LEU	N-CA-CB	-6.70	99.85	110.77	4	11
1	A	3	ASP	CA-CB-CG	-6.69	105.91	112.60	11	4
1	A	28	ARG	CD-NE-CZ	6.68	133.76	124.40	14	1
1	A	119	TYR	O-C-N	6.67	129.75	122.15	16	1
1	A	9	ASP	N-CA-C	-6.65	105.29	113.41	10	1
1	A	66	VAL	CA-CB-CG1	6.63	121.67	110.40	10	8
1	A	122	VAL	O-C-N	6.63	129.01	122.05	16	1
1	A	95	ARG	CB-CG-CD	-6.58	96.16	111.30	6	10
1	A	5	THR	OG1-CB-CG2	6.57	122.44	109.30	16	11
1	A	117	TYR	O-C-N	6.54	131.29	122.59	1	4
1	A	51	GLU	N-CA-C	-6.51	102.45	110.65	12	2
1	A	96	VAL	N-CA-C	-6.50	106.49	111.62	7	1
1	A	56	ARG	CA-C-N	6.46	131.03	122.06	3	8
1	A	56	ARG	C-N-CA	6.46	131.03	122.06	3	8
1	A	13	ASN	CA-CB-CG	6.44	119.04	112.60	17	2
1	A	55	PHE	CA-C-O	-6.41	114.30	120.90	6	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	21	MET	N-CA-C	-6.40	103.59	111.40	7	3
1	A	82	TRP	N-CA-C	-6.40	99.81	109.79	18	9
1	A	129	LYS	N-CA-CB	-6.39	101.98	111.43	14	10
1	A	48	THR	CB-CA-C	6.36	120.52	109.65	20	1
1	A	57	ASN	O-C-N	6.34	130.01	122.46	13	2
1	A	56	ARG	NE-CZ-NH1	6.34	127.84	121.50	6	6
1	A	40	ILE	O-C-N	6.28	129.87	122.83	18	2
1	A	53	SER	CA-C-O	-6.28	114.72	121.56	2	4
1	A	76	THR	N-CA-CB	6.27	121.09	110.49	16	3
1	A	5	THR	CA-CB-OG1	6.26	119.00	109.60	15	4
1	A	37	LYS	N-CA-C	-6.26	100.14	109.15	19	2
1	A	113	LEU	N-CA-C	-6.24	100.12	110.17	19	8
1	A	9	ASP	CA-CB-CG	6.19	118.79	112.60	16	6
1	A	31	GLY	CA-C-N	6.19	128.57	120.28	2	1
1	A	31	GLY	C-N-CA	6.19	128.57	120.28	2	1
1	A	128	PHE	CA-CB-CG	-6.18	107.62	113.80	19	3
1	A	87	ASN	OD1-CG-ND2	6.18	128.78	122.60	3	20
1	A	127	ILE	N-CA-C	6.17	117.31	107.98	6	5
1	A	66	VAL	CA-C-O	-6.14	117.28	122.63	10	1
1	A	10	ARG	NE-CZ-NH1	6.11	127.61	121.50	3	8
1	A	48	THR	CA-CB-OG1	6.11	118.76	109.60	20	8
1	A	114	ILE	O-C-N	6.09	129.62	123.10	3	2
1	A	28	ARG	NE-CZ-NH1	6.09	127.59	121.50	14	1
1	A	6	TRP	CG-CD2-CE3	-6.04	127.86	133.90	20	4
1	A	124	ALA	O-C-N	6.04	129.45	122.99	8	2
1	A	117	TYR	N-CA-CB	6.04	120.69	110.49	18	8
1	A	17	PHE	O-C-N	-5.98	114.92	122.27	3	3
1	A	108	ILE	N-CA-CB	5.95	117.33	110.49	2	1
1	A	45	ASN	N-CA-CB	5.94	118.93	110.67	1	4
1	A	82	TRP	CG-CD1-NE1	-5.92	102.51	110.20	7	1
1	A	106	ARG	NE-CZ-NH2	5.88	124.49	119.20	18	1
1	A	106	ARG	CB-CA-C	-5.88	101.71	111.41	20	4
1	A	97	ASP	N-CA-C	5.87	118.46	111.71	10	1
1	A	38	LEU	N-CA-CB	-5.86	100.72	110.39	19	2
1	A	26	VAL	O-C-N	5.86	127.79	121.87	1	1
1	A	45	ASN	CA-CB-CG	5.84	118.44	112.60	17	4
1	A	3	ASP	CA-C-O	5.80	127.47	120.27	15	1
1	A	115	GLN	N-CA-CB	5.80	119.24	110.42	11	1
1	A	95	ARG	NE-CZ-NH1	-5.78	115.72	121.50	3	3
1	A	71	SER	O-C-N	5.76	130.35	122.29	16	1
1	A	116	THR	CA-CB-OG1	-5.76	100.96	109.60	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	126	ARG	O-C-N	5.75	132.14	122.93	8	3
1	A	105	VAL	CA-C-O	5.75	126.08	120.27	12	2
1	A	125	LYS	O-C-N	5.75	129.66	122.65	4	1
1	A	95	ARG	NE-CZ-NH2	5.74	124.37	119.20	6	3
1	A	24	ASN	O-C-N	5.74	128.97	122.20	8	2
1	A	111	ASN	O-C-N	5.72	128.91	122.27	3	2
1	A	56	ARG	O-C-N	5.67	129.21	123.26	11	2
1	A	81	THR	CB-CA-C	-5.67	100.75	110.95	7	2
1	A	107	GLU	CA-C-N	-5.66	111.78	121.97	18	2
1	A	107	GLU	C-N-CA	-5.66	111.78	121.97	18	2
1	A	35	ASN	N-CA-CB	5.64	120.03	110.49	9	3
1	A	25	VAL	N-CA-C	5.64	121.07	109.34	16	5
1	A	87	ASN	N-CA-C	5.63	120.15	113.28	3	1
1	A	61	VAL	CA-C-N	-5.63	114.39	122.67	4	1
1	A	61	VAL	C-N-CA	-5.63	114.39	122.67	4	1
1	A	62	PHE	CA-CB-CG	5.62	119.42	113.80	8	1
1	A	104	ALA	CA-C-O	-5.59	114.12	120.32	15	1
1	A	5	THR	CB-CA-C	5.58	118.94	109.50	12	5
1	A	96	VAL	N-CA-CB	-5.58	102.02	111.23	10	1
1	A	57	ASN	CA-CB-CG	-5.58	107.02	112.60	4	1
1	A	60	VAL	N-CA-CB	-5.58	106.70	112.28	4	1
1	A	61	VAL	CA-CB-CG1	5.58	119.89	110.40	17	2
1	A	111	ASN	OD1-CG-ND2	5.58	128.18	122.60	9	20
1	A	6	TRP	O-C-N	5.56	129.59	123.25	4	2
1	A	11	ASN	N-CA-CB	-5.55	101.72	111.49	2	1
1	A	58	ILE	N-CA-CB	-5.55	105.44	112.15	17	5
1	A	72	LEU	O-C-N	5.54	128.67	121.79	11	1
1	A	109	SER	CA-C-N	5.54	132.27	121.41	2	3
1	A	109	SER	C-N-CA	5.54	132.27	121.41	2	3
1	A	33	HIS	ND1-CE1-NE2	5.54	113.94	108.40	20	1
1	A	82	TRP	CB-CG-CD1	-5.52	118.61	126.90	8	1
1	A	28	ARG	NE-CZ-NH2	5.50	124.15	119.20	11	2
1	A	93	PHE	CA-CB-CG	-5.49	108.31	113.80	20	2
1	A	78	LEU	N-CA-C	-5.48	101.93	110.42	9	1
1	A	113	LEU	CA-C-O	-5.46	114.64	120.92	12	3
1	A	18	MET	N-CA-C	-5.46	105.88	112.54	17	3
1	A	76	THR	OG1-CB-CG2	5.45	120.21	109.30	11	1
1	A	36	LEU	CB-CA-C	-5.45	101.81	110.81	3	1
1	A	47	PHE	CA-CB-CG	5.44	119.24	113.80	7	1
1	A	85	GLU	O-C-N	5.44	127.97	122.09	12	1
1	A	106	ARG	CD-NE-CZ	5.43	132.01	124.40	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	109	SER	CA-C-O	-5.43	115.85	122.64	12	1
1	A	16	LYS	CA-C-O	5.43	126.05	119.31	19	1
1	A	30	LEU	N-CA-C	-5.43	106.16	112.89	13	1
1	A	15	GLU	CA-C-N	5.42	127.54	120.28	17	2
1	A	15	GLU	C-N-CA	5.42	127.54	120.28	17	2
1	A	89	LEU	N-CA-C	-5.41	101.72	110.32	7	2
1	A	66	VAL	N-CA-C	-5.40	107.55	113.43	18	1
1	A	44	GLY	O-C-N	5.39	129.71	122.70	7	1
1	A	7	LYS	CA-C-O	-5.39	112.80	120.51	19	2
1	A	9	ASP	CA-C-N	-5.39	113.79	121.33	18	1
1	A	9	ASP	C-N-CA	-5.39	113.79	121.33	18	1
1	A	34	ASP	CA-C-O	-5.38	114.83	121.02	18	1
1	A	56	ARG	CA-CB-CG	-5.38	103.34	114.10	5	1
1	A	8	VAL	CB-CA-C	5.36	120.08	111.29	16	1
1	A	35	ASN	O-C-N	5.34	128.70	122.67	3	1
1	A	100	LYS	CA-C-N	5.34	131.38	121.62	7	2
1	A	100	LYS	C-N-CA	5.34	131.38	121.62	7	2
1	A	107	GLU	N-CA-C	5.31	117.77	108.52	2	3
1	A	17	PHE	CA-C-O	5.31	126.08	119.97	3	3
1	A	115	GLN	CB-CA-C	-5.31	103.00	111.17	16	1
1	A	50	LYS	CA-C-O	-5.31	115.35	121.19	2	1
1	A	115	GLN	CA-C-O	-5.29	115.70	121.89	11	2
1	A	129	LYS	N-CA-C	-5.28	105.69	113.61	15	1
1	A	61	VAL	N-CA-C	5.28	116.89	108.87	7	1
1	A	127	ILE	N-CA-CB	5.27	116.67	110.82	18	1
1	A	112	GLU	O-C-N	5.27	129.35	123.40	7	1
1	A	10	ARG	O-C-N	5.26	129.59	122.59	8	1
1	A	18	MET	CA-C-O	5.26	125.85	119.38	19	2
1	A	25	VAL	O-C-N	5.25	127.06	121.91	14	1
1	A	79	THR	OG1-CB-CG2	5.25	119.79	109.30	4	3
1	A	69	ALA	CA-C-O	-5.24	114.67	120.38	7	1
1	A	57	ASN	CA-C-O	-5.20	114.46	120.49	4	2
1	A	101	GLU	CA-C-O	-5.20	115.55	121.58	17	1
1	A	19	GLU	CG-CD-OE1	-5.19	106.46	118.40	13	1
1	A	49	VAL	CA-CB-CG1	5.19	119.22	110.40	19	3
1	A	32	ALA	O-C-N	5.18	128.96	122.23	15	1
1	A	117	TYR	CA-C-O	-5.17	113.12	120.51	10	2
1	A	38	LEU	CA-C-O	-5.16	115.38	121.16	14	1
1	A	68	PHE	CA-CB-CG	5.15	118.95	113.80	1	1
1	A	13	ASN	O-C-N	5.15	126.94	121.89	3	1
1	A	79	THR	CA-C-N	-5.15	113.81	120.91	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	79	THR	C-N-CA	-5.15	113.81	120.91	1	1
1	A	127	ILE	CA-CB-CG1	5.14	119.14	110.40	14	1
1	A	76	THR	CA-C-N	5.13	131.35	121.54	4	1
1	A	76	THR	C-N-CA	5.13	131.35	121.54	4	1
1	A	11	ASN	CB-CA-C	-5.13	100.21	110.42	13	2
1	A	59	ASP	N-CA-CB	5.13	117.54	109.69	11	1
1	A	30	LEU	O-C-N	5.12	128.57	122.27	18	1
1	A	33	HIS	CE1-NE2-CD2	-5.12	103.88	109.00	1	1
1	A	92	LYS	CA-CB-CG	-5.11	103.88	114.10	14	1
1	A	112	GLU	CA-C-O	-5.10	114.84	120.24	14	1
1	A	111	ASN	CA-C-O	-5.08	113.31	118.90	3	2
1	A	93	PHE	CA-C-N	5.08	130.16	123.00	7	1
1	A	93	PHE	C-N-CA	5.08	130.16	123.00	7	1
1	A	38	LEU	O-C-N	-5.07	117.29	123.27	3	1
1	A	109	SER	O-C-N	5.06	129.19	122.56	12	1
1	A	131	GLU	CB-CA-C	5.05	119.70	110.10	3	1
1	A	22	GLY	O-C-N	5.05	129.27	122.70	14	1
1	A	89	LEU	CB-CA-C	5.04	118.02	109.50	2	1
1	A	90	VAL	O-C-N	5.03	128.35	122.97	6	1
1	A	37	LYS	CA-C-N	-5.03	116.01	123.05	3	1
1	A	37	LYS	C-N-CA	-5.03	116.01	123.05	3	1
1	A	113	LEU	O-C-N	5.03	128.99	123.16	15	1
1	A	33	HIS	CG-CD2-NE2	-5.02	102.18	107.20	12	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	79	THR	CB	20

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	1052	1050	1049	64±18

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
2	A	18	31	31	2±2
All	All	21400	21620	21600	1276

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 30.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ILE:HD12	1:A:127:ILE:HD12	0.97	1.31	16	1
1:A:40:ILE:HG23	1:A:49:VAL:HG12	0.94	1.39	13	1
1:A:6:TRP:CZ2	1:A:108:ILE:HD11	0.92	2.00	20	8
1:A:72:LEU:HD22	1:A:72:LEU:N	0.88	1.83	16	1
1:A:48:THR:HA	1:A:61:VAL:HG13	0.87	1.46	9	6
1:A:83:THR:HG22	1:A:90:VAL:HG22	0.82	1.51	20	1
1:A:48:THR:HB	1:A:61:VAL:HG12	0.82	1.52	17	11
1:A:36:LEU:HD21	1:A:38:LEU:HD13	0.80	1.53	13	6
1:A:49:VAL:HG11	1:A:62:PHE:CZ	0.79	2.12	1	1
1:A:114:ILE:HG23	1:A:127:ILE:CD1	0.79	2.07	16	1
1:A:72:LEU:HD21	1:A:78:LEU:HD13	0.79	1.53	18	2
1:A:48:THR:HG22	1:A:61:VAL:CG1	0.78	2.09	6	4
1:A:48:THR:HG23	1:A:61:VAL:HG22	0.78	1.55	20	1
1:A:114:ILE:HG12	1:A:127:ILE:HG23	0.77	1.56	2	4
1:A:17:PHE:CZ	1:A:21:MET:HE2	0.77	2.14	18	2
1:A:114:ILE:HD12	1:A:127:ILE:CD1	0.75	2.11	16	1
1:A:6:TRP:CH2	1:A:108:ILE:HD11	0.75	2.16	20	13
1:A:21:MET:HE1	1:A:72:LEU:HD13	0.75	1.59	9	1
1:A:47:PHE:CE2	1:A:89:LEU:HD21	0.74	2.17	11	1
1:A:114:ILE:HG22	1:A:116:THR:CG2	0.74	2.12	2	3
1:A:36:LEU:HD11	1:A:38:LEU:CD1	0.74	2.12	6	5
1:A:48:THR:HA	1:A:61:VAL:HA	0.74	1.57	4	7
1:A:72:LEU:N	1:A:72:LEU:HD13	0.74	1.97	3	2
1:A:114:ILE:HG12	1:A:127:ILE:HD13	0.74	1.60	7	2
1:A:113:LEU:HD21	1:A:115:GLN:HG2	0.73	1.60	3	2
1:A:49:VAL:HG13	1:A:60:VAL:HB	0.73	1.60	2	3
1:A:90:VAL:HG12	1:A:105:VAL:CG2	0.73	2.14	6	3
1:A:82:TRP:CG	1:A:83:THR:N	0.73	2.50	7	3
1:A:48:THR:OG1	1:A:61:VAL:HG12	0.73	1.84	5	3
1:A:83:THR:HG23	1:A:90:VAL:HG23	0.72	1.61	18	2
1:A:117:TYR:HB2	1:A:124:ALA:HB3	0.72	1.60	14	3
1:A:103:ILE:HG23	1:A:117:TYR:HB3	0.71	1.62	3	6
1:A:70:TYR:HB3	1:A:78:LEU:HD22	0.71	1.62	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:LEU:HD23	1:A:106:ARG:HH11	0.70	1.45	1	1
1:A:56:ARG:HB2	1:A:58:ILE:HG22	0.70	1.61	18	6
1:A:14:TYR:HA	1:A:124:ALA:HB1	0.70	1.62	4	7
1:A:38:LEU:CD2	1:A:49:VAL:HG21	0.69	2.17	5	1
1:A:20:LYS:HD3	1:A:122:VAL:HG11	0.69	1.62	17	1
1:A:114:ILE:HG22	1:A:116:THR:HG22	0.69	1.64	10	2
1:A:17:PHE:CB	1:A:124:ALA:HB2	0.69	2.18	7	11
1:A:82:TRP:CD2	1:A:83:THR:N	0.69	2.60	7	3
1:A:70:TYR:O	1:A:72:LEU:HD13	0.69	1.88	16	1
1:A:72:LEU:N	1:A:72:LEU:CD2	0.69	2.54	16	1
1:A:65:GLY:N	1:A:82:TRP:NE1	0.69	2.41	7	3
1:A:83:THR:HG22	1:A:90:VAL:CG2	0.68	2.17	20	1
1:A:114:ILE:HG23	1:A:127:ILE:HD12	0.68	1.66	16	2
1:A:49:VAL:HG12	1:A:60:VAL:CG1	0.68	2.19	3	1
1:A:56:ARG:HB3	1:A:58:ILE:HG22	0.68	1.65	19	2
1:A:64:LEU:HB3	1:A:82:TRP:CD2	0.67	2.24	7	3
1:A:74:ASP:N	2:A:132:PLM:HG3	0.67	2.04	4	1
1:A:83:THR:CG2	1:A:90:VAL:HG22	0.67	2.20	20	1
1:A:7:LYS:O	1:A:8:VAL:HG12	0.67	1.90	3	1
1:A:114:ILE:CG2	1:A:127:ILE:HD13	0.67	2.19	18	3
1:A:103:ILE:HD13	1:A:104:ALA:N	0.67	2.05	13	2
1:A:11:ASN:HB3	1:A:14:TYR:CE1	0.67	2.25	2	1
1:A:48:THR:CA	1:A:61:VAL:HG13	0.67	2.19	9	4
1:A:108:ILE:CG1	1:A:113:LEU:HD12	0.67	2.20	13	1
1:A:36:LEU:HD22	1:A:128:PHE:CE1	0.67	2.25	11	1
1:A:49:VAL:HG13	1:A:60:VAL:CG1	0.66	2.20	2	1
1:A:64:LEU:CB	1:A:82:TRP:CE2	0.66	2.79	8	3
1:A:49:VAL:HG13	1:A:60:VAL:CB	0.66	2.20	2	1
1:A:108:ILE:HD13	1:A:113:LEU:HD12	0.66	1.66	7	1
1:A:48:THR:CB	1:A:61:VAL:HG13	0.66	2.21	2	2
1:A:60:VAL:HG11	2:A:132:PLM:H21	0.66	1.68	13	2
1:A:62:PHE:CE1	1:A:68:PHE:CB	0.66	2.79	4	1
1:A:6:TRP:NE1	1:A:40:ILE:HD12	0.65	2.06	6	3
1:A:82:TRP:CD1	1:A:82:TRP:C	0.65	2.72	18	2
1:A:49:VAL:HG12	1:A:60:VAL:HG12	0.65	1.67	3	1
1:A:64:LEU:HB3	1:A:82:TRP:CE2	0.65	2.26	7	3
1:A:46:LYS:HG3	1:A:47:PHE:N	0.65	2.05	4	1
1:A:17:PHE:CE1	1:A:21:MET:HE2	0.65	2.27	18	1
1:A:14:TYR:CE2	1:A:32:ALA:HB1	0.65	2.27	7	2
1:A:11:ASN:CB	1:A:14:TYR:CZ	0.65	2.80	2	1
1:A:114:ILE:HG13	1:A:127:ILE:HD13	0.64	1.69	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:PHE:CE1	1:A:82:TRP:CZ2	0.64	2.85	12	3
1:A:7:LYS:HB3	1:A:128:PHE:CZ	0.64	2.28	3	2
1:A:62:PHE:CE2	1:A:82:TRP:CD1	0.64	2.85	9	2
1:A:82:TRP:C	1:A:82:TRP:CD1	0.64	2.71	8	1
1:A:7:LYS:N	1:A:128:PHE:CE2	0.64	2.65	19	1
1:A:7:LYS:CB	1:A:128:PHE:CZ	0.64	2.80	19	1
1:A:105:VAL:HG12	1:A:116:THR:O	0.63	1.94	18	1
1:A:89:LEU:HD23	1:A:106:ARG:HD2	0.63	1.70	4	2
1:A:21:MET:HE1	1:A:72:LEU:HG	0.63	1.70	17	1
1:A:84:MET:HE3	1:A:86:GLY:O	0.63	1.91	18	1
1:A:8:VAL:CG1	1:A:36:LEU:HD23	0.63	2.22	19	1
1:A:114:ILE:HG23	1:A:127:ILE:HD13	0.63	1.70	12	5
1:A:72:LEU:HD11	1:A:78:LEU:HD12	0.63	1.70	9	1
1:A:62:PHE:CD1	1:A:68:PHE:CD1	0.63	2.87	20	3
1:A:114:ILE:HG23	1:A:127:ILE:HG12	0.63	1.70	9	2
1:A:74:ASP:HB3	2:A:132:PLM:HG1	0.63	1.69	15	1
1:A:93:PHE:CB	1:A:102:LEU:HD23	0.63	2.22	2	1
1:A:72:LEU:HD11	1:A:78:LEU:HD13	0.63	1.70	11	1
1:A:48:THR:HG22	1:A:61:VAL:HG13	0.63	1.70	1	4
1:A:11:ASN:ND2	1:A:14:TYR:CE2	0.63	2.67	2	1
1:A:93:PHE:HB2	1:A:102:LEU:HD23	0.63	1.70	2	1
1:A:56:ARG:CB	1:A:58:ILE:HG22	0.63	2.24	18	3
1:A:11:ASN:HB3	1:A:14:TYR:CD1	0.63	2.29	2	2
1:A:62:PHE:CZ	1:A:82:TRP:CZ2	0.63	2.87	11	2
1:A:47:PHE:CE1	1:A:64:LEU:HD21	0.62	2.29	13	3
1:A:105:VAL:CG1	1:A:116:THR:HG23	0.62	2.24	4	1
1:A:116:THR:OG1	1:A:117:TYR:CE2	0.62	2.52	2	1
1:A:6:TRP:HA	1:A:128:PHE:CE2	0.62	2.28	19	2
1:A:36:LEU:HD11	1:A:38:LEU:HD12	0.62	1.71	3	4
1:A:113:LEU:C	1:A:113:LEU:HD23	0.62	2.19	3	2
1:A:78:LEU:C	1:A:78:LEU:HD23	0.62	2.20	8	1
1:A:95:ARG:HD2	1:A:95:ARG:N	0.62	2.10	7	2
1:A:20:LYS:HG2	1:A:122:VAL:HG21	0.62	1.71	17	1
1:A:28:ARG:HH11	1:A:28:ARG:HG3	0.62	1.53	20	1
1:A:20:LYS:HB2	1:A:122:VAL:HG21	0.62	1.71	18	1
1:A:46:LYS:HB2	1:A:63:GLU:CA	0.61	2.25	4	1
1:A:6:TRP:CE3	1:A:113:LEU:CB	0.61	2.83	3	2
1:A:103:ILE:HG23	1:A:117:TYR:CB	0.61	2.25	3	3
1:A:90:VAL:HG12	1:A:105:VAL:HG23	0.61	1.73	17	2
1:A:68:PHE:N	1:A:68:PHE:CD1	0.61	2.69	7	3
1:A:48:THR:CG2	1:A:61:VAL:HG22	0.61	2.26	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:VAL:HG11	2:A:132:PLM:C2	0.61	2.25	13	2
1:A:62:PHE:CE2	1:A:68:PHE:CE2	0.61	2.89	10	2
1:A:90:VAL:HG12	1:A:105:VAL:HG22	0.61	1.73	6	1
1:A:89:LEU:HD22	1:A:106:ARG:HD2	0.61	1.70	8	1
1:A:62:PHE:CD2	1:A:68:PHE:CZ	0.61	2.89	10	2
1:A:106:ARG:HG2	1:A:106:ARG:HH11	0.60	1.55	3	2
1:A:6:TRP:CE3	1:A:113:LEU:HB3	0.60	2.32	19	2
1:A:38:LEU:HD22	1:A:128:PHE:CE2	0.60	2.31	17	4
1:A:62:PHE:CZ	1:A:68:PHE:CD2	0.60	2.89	10	2
1:A:62:PHE:CG	1:A:68:PHE:CE1	0.60	2.90	10	1
1:A:76:THR:HG23	1:A:77:GLU:N	0.60	2.11	8	1
1:A:77:GLU:CB	1:A:96:VAL:HG22	0.60	2.27	13	3
1:A:36:LEU:HD11	1:A:38:LEU:HD13	0.60	1.73	6	4
1:A:95:ARG:HE	1:A:100:LYS:N	0.60	1.94	7	1
1:A:114:ILE:CD1	1:A:127:ILE:HD12	0.60	2.18	16	2
1:A:114:ILE:HD13	1:A:127:ILE:HG23	0.60	1.72	6	1
1:A:105:VAL:HG12	1:A:116:THR:HG23	0.60	1.74	4	3
1:A:108:ILE:HG12	1:A:113:LEU:HD12	0.60	1.73	13	1
1:A:11:ASN:CB	1:A:14:TYR:CE1	0.60	2.85	2	1
1:A:62:PHE:CE1	1:A:68:PHE:CG	0.60	2.90	10	2
1:A:105:VAL:HG11	1:A:117:TYR:CZ	0.60	2.31	4	2
1:A:102:LEU:HD12	1:A:119:TYR:CD1	0.60	2.32	9	1
1:A:72:LEU:HD12	1:A:76:THR:O	0.59	1.97	19	2
1:A:72:LEU:HD21	1:A:77:GLU:N	0.59	2.11	16	1
1:A:82:TRP:C	1:A:83:THR:HG22	0.59	2.23	8	2
1:A:14:TYR:CD1	1:A:124:ALA:HB1	0.59	2.31	3	3
1:A:113:LEU:HD22	1:A:128:PHE:CD2	0.59	2.32	1	2
1:A:95:ARG:CZ	1:A:99:GLY:HA2	0.59	2.27	7	1
1:A:5:THR:HG22	1:A:39:THR:HG23	0.59	1.74	1	2
1:A:6:TRP:HA	1:A:128:PHE:CD2	0.59	2.33	3	2
1:A:40:ILE:CG2	1:A:47:PHE:CE1	0.59	2.86	4	1
1:A:113:LEU:HD13	1:A:128:PHE:CE2	0.59	2.33	4	1
1:A:82:TRP:CH2	1:A:106:ARG:CZ	0.59	2.85	12	2
1:A:6:TRP:HE1	1:A:40:ILE:HD12	0.58	1.59	6	2
1:A:60:VAL:CG1	1:A:62:PHE:CE2	0.58	2.86	4	3
1:A:114:ILE:CG1	1:A:127:ILE:HD13	0.58	2.29	1	3
1:A:36:LEU:HD21	1:A:38:LEU:CD1	0.58	2.28	3	1
1:A:102:LEU:HD13	1:A:119:TYR:HB2	0.58	1.74	4	1
1:A:62:PHE:CD2	1:A:82:TRP:CD1	0.58	2.91	20	3
1:A:6:TRP:CH2	1:A:108:ILE:CD1	0.58	2.86	2	4
1:A:114:ILE:HD12	1:A:127:ILE:HG12	0.58	1.76	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:LEU:HD13	1:A:106:ARG:HH11	0.58	1.58	9	1
1:A:17:PHE:CE2	1:A:18:MET:HE2	0.58	2.32	6	1
1:A:95:ARG:HD2	1:A:95:ARG:C	0.58	2.21	7	1
1:A:62:PHE:CD1	1:A:68:PHE:CG	0.58	2.90	10	1
1:A:102:LEU:HA	1:A:119:TYR:HA	0.58	1.76	4	12
1:A:6:TRP:C	1:A:128:PHE:CE2	0.57	2.83	19	2
1:A:48:THR:CB	1:A:61:VAL:HG12	0.57	2.29	5	5
1:A:36:LEU:HD23	1:A:36:LEU:O	0.57	2.00	8	2
1:A:2:PHE:CE1	1:A:108:ILE:HD12	0.57	2.34	4	1
1:A:17:PHE:CZ	1:A:21:MET:HE3	0.57	2.34	20	1
1:A:48:THR:HG22	1:A:61:VAL:HG11	0.57	1.76	6	2
1:A:62:PHE:CB	1:A:68:PHE:CZ	0.57	2.88	11	3
1:A:119:TYR:C	1:A:119:TYR:CD1	0.57	2.83	4	2
1:A:48:THR:HA	1:A:61:VAL:CG1	0.57	2.26	9	1
1:A:6:TRP:HH2	1:A:108:ILE:HD11	0.57	1.58	1	2
1:A:117:TYR:O	1:A:124:ALA:N	0.57	2.38	2	2
1:A:114:ILE:CG2	1:A:127:ILE:HD12	0.57	2.29	4	1
1:A:46:LYS:CB	1:A:62:PHE:C	0.57	2.78	4	1
1:A:65:GLY:N	1:A:82:TRP:CD1	0.57	2.73	18	3
1:A:41:THR:HB	1:A:48:THR:HG23	0.57	1.77	11	2
1:A:14:TYR:CD2	1:A:126:ARG:CG	0.57	2.88	12	3
1:A:105:VAL:HG12	1:A:116:THR:OG1	0.57	2.00	15	1
1:A:95:ARG:C	1:A:95:ARG:CD	0.56	2.77	7	1
1:A:62:PHE:CE1	1:A:68:PHE:CD2	0.56	2.92	10	1
1:A:6:TRP:CE3	1:A:130:LYS:HA	0.56	2.35	15	9
1:A:8:VAL:N	1:A:128:PHE:CD1	0.56	2.73	19	2
1:A:36:LEU:HD13	1:A:53:SER:OG	0.56	1.99	5	1
1:A:36:LEU:HD22	1:A:126:ARG:HH21	0.56	1.59	8	1
1:A:13:ASN:ND2	1:A:17:PHE:CD1	0.56	2.73	16	1
1:A:103:ILE:N	1:A:118:THR:O	0.56	2.39	5	12
1:A:49:VAL:HG11	2:A:132:PLM:O1	0.56	2.00	3	1
1:A:82:TRP:CH2	1:A:84:MET:CB	0.56	2.88	18	2
1:A:105:VAL:CG2	1:A:117:TYR:CE2	0.56	2.88	19	1
1:A:56:ARG:HB2	1:A:58:ILE:CG2	0.56	2.31	18	1
1:A:103:ILE:CG2	1:A:118:THR:HB	0.56	2.30	7	3
1:A:64:LEU:C	1:A:82:TRP:NE1	0.56	2.64	18	3
1:A:105:VAL:HB	1:A:117:TYR:CD2	0.56	2.34	11	1
1:A:90:VAL:HG12	1:A:104:ALA:O	0.56	1.99	8	1
1:A:36:LEU:HD22	1:A:128:PHE:HE1	0.56	1.58	11	1
1:A:79:THR:HG22	1:A:94:LYS:O	0.56	1.99	7	1
1:A:72:LEU:HG	1:A:76:THR:N	0.56	2.16	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:TRP:CA	1:A:128:PHE:CD2	0.56	2.89	3	2
1:A:62:PHE:CZ	1:A:68:PHE:CG	0.56	2.93	4	1
1:A:118:THR:HG23	1:A:119:TYR:N	0.56	2.16	5	2
1:A:46:LYS:CG	1:A:47:PHE:N	0.56	2.65	4	1
1:A:77:GLU:HB2	1:A:96:VAL:HG22	0.56	1.77	13	2
1:A:14:TYR:CE2	1:A:126:ARG:CD	0.55	2.89	12	2
1:A:103:ILE:HG23	1:A:117:TYR:CG	0.55	2.37	20	1
1:A:102:LEU:HD22	1:A:119:TYR:HD1	0.55	1.60	4	1
1:A:14:TYR:HA	1:A:124:ALA:CB	0.55	2.30	2	4
1:A:17:PHE:HB2	1:A:124:ALA:HB2	0.55	1.78	9	4
1:A:67:ASP:HA	1:A:81:THR:HG22	0.55	1.77	1	2
1:A:55:PHE:CE1	1:A:73:ALA:HB1	0.55	2.37	7	2
1:A:6:TRP:CZ3	1:A:113:LEU:CB	0.55	2.90	19	2
1:A:20:LYS:CE	1:A:119:TYR:HB3	0.55	2.32	7	1
1:A:60:VAL:HG12	1:A:61:VAL:N	0.55	2.17	9	2
1:A:82:TRP:CE3	1:A:91:GLY:CA	0.55	2.89	1	3
1:A:8:VAL:HG12	1:A:36:LEU:HB3	0.55	1.78	11	2
1:A:72:LEU:HD22	1:A:72:LEU:H	0.55	1.58	16	1
1:A:49:VAL:CG1	1:A:62:PHE:CZ	0.55	2.89	1	2
1:A:6:TRP:CD1	1:A:40:ILE:HD12	0.55	2.36	2	3
1:A:11:ASN:CG	1:A:14:TYR:CE2	0.55	2.85	2	1
1:A:92:LYS:C	1:A:93:PHE:CD1	0.55	2.85	19	2
1:A:14:TYR:CE1	1:A:17:PHE:CD2	0.55	2.95	12	2
1:A:21:MET:CE	1:A:119:TYR:CD1	0.55	2.89	12	1
1:A:113:LEU:HD23	1:A:114:ILE:N	0.54	2.17	19	3
1:A:62:PHE:CE1	1:A:68:PHE:HB3	0.54	2.37	4	1
1:A:40:ILE:HD13	1:A:49:VAL:HG23	0.54	1.79	17	2
1:A:38:LEU:HD13	1:A:128:PHE:CZ	0.54	2.37	16	1
1:A:82:TRP:CZ2	1:A:106:ARG:CZ	0.54	2.90	16	1
1:A:6:TRP:CZ3	1:A:130:LYS:CG	0.54	2.91	17	2
1:A:62:PHE:HB3	1:A:68:PHE:CE1	0.54	2.37	16	1
1:A:105:VAL:CG1	1:A:117:TYR:CE2	0.54	2.89	4	3
1:A:82:TRP:CZ3	1:A:84:MET:N	0.54	2.75	7	1
1:A:102:LEU:HG	1:A:119:TYR:HA	0.54	1.80	8	8
1:A:60:VAL:HG12	1:A:62:PHE:CE2	0.54	2.36	14	1
1:A:14:TYR:CE2	1:A:126:ARG:HG2	0.54	2.37	4	4
1:A:38:LEU:HD12	1:A:128:PHE:CZ	0.54	2.38	5	1
1:A:75:GLY:C	1:A:76:THR:HG23	0.54	2.27	5	2
1:A:6:TRP:CZ3	1:A:113:LEU:HB2	0.54	2.38	19	3
1:A:13:ASN:ND2	1:A:17:PHE:CG	0.54	2.76	17	2
1:A:14:TYR:CA	1:A:124:ALA:HA	0.53	2.32	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LEU:HD23	1:A:49:VAL:CG2	0.53	2.33	5	1
1:A:105:VAL:HG13	1:A:107:GLU:HG2	0.53	1.79	12	1
1:A:105:VAL:HB	1:A:117:TYR:CE2	0.53	2.38	10	9
1:A:47:PHE:HB3	1:A:62:PHE:CE1	0.53	2.38	12	1
1:A:93:PHE:CZ	2:A:132:PLM:H41	0.53	2.39	18	1
1:A:45:ASN:ND2	1:A:45:ASN:N	0.53	2.55	5	1
1:A:64:LEU:HB2	1:A:82:TRP:CZ2	0.53	2.39	18	3
1:A:13:ASN:ND2	1:A:17:PHE:CD2	0.53	2.77	17	1
1:A:78:LEU:HG	1:A:93:PHE:HB3	0.53	1.80	19	2
1:A:85:GLU:HG2	1:A:90:VAL:HG21	0.53	1.81	7	1
1:A:38:LEU:HD21	1:A:49:VAL:HG21	0.53	1.79	5	1
1:A:14:TYR:OH	1:A:18:MET:HE3	0.53	2.03	6	1
1:A:17:PHE:CE2	1:A:117:TYR:CD2	0.53	2.97	14	1
1:A:62:PHE:CE2	1:A:82:TRP:NE1	0.53	2.77	1	1
1:A:7:LYS:CG	1:A:36:LEU:O	0.53	2.57	3	1
1:A:46:LYS:CB	1:A:63:GLU:CA	0.53	2.87	4	1
1:A:62:PHE:HB2	1:A:68:PHE:CZ	0.53	2.38	1	1
1:A:105:VAL:HG13	1:A:107:GLU:CG	0.53	2.33	12	1
1:A:7:LYS:C	1:A:128:PHE:CE1	0.53	2.86	19	1
1:A:6:TRP:CZ2	1:A:108:ILE:CD1	0.53	2.92	3	2
1:A:78:LEU:HD12	1:A:102:LEU:HD23	0.53	1.81	16	1
1:A:62:PHE:CE2	1:A:68:PHE:CD2	0.52	2.97	4	1
1:A:21:MET:HE2	1:A:95:ARG:HH12	0.52	1.63	15	1
1:A:102:LEU:HA	1:A:119:TYR:CA	0.52	2.33	4	1
1:A:17:PHE:CD2	1:A:122:VAL:HA	0.52	2.40	16	1
1:A:13:ASN:CG	1:A:17:PHE:CE2	0.52	2.88	17	1
1:A:102:LEU:CB	1:A:119:TYR:HA	0.52	2.35	4	7
1:A:115:GLN:C	1:A:116:THR:CG2	0.52	2.82	11	4
1:A:62:PHE:CE2	2:A:132:PLM:H22	0.52	2.39	7	1
1:A:114:ILE:HG22	1:A:116:THR:HG23	0.52	1.78	2	1
1:A:82:TRP:CZ2	1:A:106:ARG:NH2	0.52	2.78	11	1
1:A:113:LEU:HD22	1:A:128:PHE:CE2	0.52	2.39	1	2
1:A:114:ILE:CG1	1:A:127:ILE:CD1	0.52	2.87	14	2
1:A:38:LEU:HD22	1:A:128:PHE:HE2	0.52	1.65	13	1
1:A:72:LEU:HD21	1:A:76:THR:C	0.52	2.30	16	1
1:A:114:ILE:HG13	1:A:127:ILE:CD1	0.51	2.33	3	2
1:A:74:ASP:HB2	2:A:132:PLM:HG1	0.51	1.81	5	1
1:A:14:TYR:CE2	1:A:126:ARG:HD2	0.51	2.40	12	1
1:A:64:LEU:CB	1:A:82:TRP:CZ2	0.51	2.93	18	3
1:A:18:MET:HE1	1:A:31:GLY:HA3	0.51	1.83	10	1
1:A:62:PHE:CE1	1:A:82:TRP:CE2	0.51	2.98	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ASN:ND2	1:A:55:PHE:N	0.51	2.58	13	1
1:A:6:TRP:CZ3	1:A:130:LYS:HB2	0.51	2.40	2	12
1:A:77:GLU:CG	1:A:96:VAL:CG2	0.51	2.88	7	1
1:A:60:VAL:HG12	1:A:62:PHE:CD2	0.51	2.40	13	2
1:A:17:PHE:HB3	1:A:122:VAL:HB	0.51	1.81	16	1
1:A:61:VAL:O	1:A:62:PHE:CD1	0.51	2.64	4	1
1:A:38:LEU:HD12	1:A:128:PHE:CE2	0.51	2.40	7	2
1:A:82:TRP:CZ3	1:A:84:MET:HB2	0.51	2.40	8	3
1:A:42:GLN:CD	1:A:47:PHE:CZ	0.51	2.88	12	1
1:A:11:ASN:ND2	1:A:14:TYR:CD2	0.51	2.78	2	2
1:A:128:PHE:CG	1:A:129:LYS:N	0.51	2.79	19	2
1:A:115:GLN:O	1:A:126:ARG:N	0.51	2.44	2	3
1:A:72:LEU:HD13	1:A:72:LEU:H	0.51	1.66	3	1
1:A:48:THR:HB	1:A:61:VAL:HB	0.51	1.82	4	2
1:A:14:TYR:HE2	1:A:32:ALA:HB1	0.51	1.63	7	1
1:A:116:THR:O	1:A:117:TYR:CG	0.51	2.64	18	5
1:A:8:VAL:HG11	1:A:36:LEU:HD23	0.51	1.82	19	1
1:A:14:TYR:CD2	1:A:126:ARG:HG2	0.51	2.41	5	3
1:A:38:LEU:HD23	1:A:49:VAL:HG21	0.51	1.81	5	1
1:A:30:LEU:HD22	1:A:33:HIS:CE1	0.51	2.40	10	1
1:A:72:LEU:HD23	2:A:132:PLM:HB2	0.51	1.83	6	1
1:A:127:ILE:N	1:A:127:ILE:HD13	0.51	2.20	16	2
1:A:14:TYR:CE2	1:A:32:ALA:CB	0.51	2.94	2	1
1:A:104:ALA:HA	1:A:116:THR:O	0.51	2.06	2	1
1:A:17:PHE:HB3	1:A:124:ALA:HB2	0.51	1.82	7	4
1:A:82:TRP:CZ3	1:A:91:GLY:N	0.51	2.79	5	2
2:A:132:PLM:C1	2:A:132:PLM:C5	0.51	2.89	7	2
1:A:70:TYR:CB	1:A:78:LEU:HD22	0.51	2.36	8	1
1:A:62:PHE:CB	1:A:68:PHE:CE1	0.51	2.93	16	1
1:A:23:ILE:HD12	2:A:132:PLM:HG1	0.50	1.82	3	1
1:A:123:GLU:O	1:A:124:ALA:HB2	0.50	2.06	17	2
1:A:2:PHE:CZ	1:A:108:ILE:CG1	0.50	2.94	16	1
1:A:14:TYR:N	1:A:124:ALA:HA	0.50	2.20	2	1
1:A:42:GLN:HG2	1:A:47:PHE:CE1	0.50	2.41	3	1
1:A:113:LEU:HD21	1:A:115:GLN:CG	0.50	2.34	3	1
1:A:2:PHE:CZ	1:A:108:ILE:HG13	0.50	2.41	12	1
1:A:62:PHE:CE1	1:A:82:TRP:CH2	0.50	2.98	12	1
1:A:105:VAL:N	1:A:116:THR:O	0.50	2.44	4	6
1:A:46:LYS:HZ2	1:A:89:LEU:HD21	0.50	1.67	4	1
1:A:102:LEU:C	1:A:102:LEU:CD1	0.50	2.84	20	1
1:A:8:VAL:CG1	1:A:36:LEU:HB3	0.50	2.37	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:THR:HB	1:A:61:VAL:CB	0.50	2.37	4	1
1:A:2:PHE:N	1:A:2:PHE:CD1	0.50	2.80	6	3
1:A:8:VAL:HB	1:A:128:PHE:CD1	0.50	2.42	10	6
1:A:71:SER:C	1:A:72:LEU:CD1	0.50	2.85	4	1
1:A:17:PHE:CE2	1:A:118:THR:HA	0.50	2.41	10	1
1:A:115:GLN:HB2	1:A:126:ARG:HD2	0.50	1.83	11	1
1:A:102:LEU:HD12	1:A:118:THR:O	0.50	2.06	2	1
1:A:102:LEU:CG	1:A:119:TYR:HA	0.50	2.37	11	3
1:A:46:LYS:CB	1:A:63:GLU:N	0.50	2.75	4	1
1:A:23:ILE:CG2	1:A:28:ARG:N	0.50	2.75	6	2
1:A:55:PHE:CZ	2:A:132:PLM:HF2	0.50	2.42	14	2
1:A:38:LEU:HD11	2:A:132:PLM:O2	0.50	2.06	15	1
1:A:49:VAL:HG11	2:A:132:PLM:H22	0.50	1.82	17	1
1:A:68:PHE:CD1	1:A:68:PHE:C	0.50	2.89	2	1
1:A:71:SER:C	1:A:72:LEU:HD22	0.50	2.31	3	2
1:A:72:LEU:CD1	1:A:78:LEU:HD12	0.50	2.37	9	1
1:A:2:PHE:CE2	1:A:89:LEU:HD13	0.49	2.41	1	1
1:A:14:TYR:CD1	1:A:14:TYR:C	0.49	2.89	6	1
1:A:49:VAL:O	1:A:60:VAL:HG23	0.49	2.07	6	2
1:A:65:GLY:N	1:A:82:TRP:HE1	0.49	2.03	7	1
1:A:46:LYS:HG3	1:A:47:PHE:HB2	0.49	1.85	4	1
1:A:46:LYS:CB	1:A:63:GLU:HA	0.49	2.37	4	1
1:A:55:PHE:C	1:A:56:ARG:HG2	0.49	2.32	14	1
1:A:6:TRP:CA	1:A:128:PHE:CE2	0.49	2.95	19	2
1:A:63:GLU:O	1:A:65:GLY:N	0.49	2.45	7	1
1:A:36:LEU:HD13	1:A:51:GLU:OE2	0.49	2.08	1	1
1:A:105:VAL:HG21	1:A:117:TYR:CE2	0.49	2.43	19	1
1:A:113:LEU:HD23	1:A:128:PHE:CD1	0.49	2.42	20	1
1:A:14:TYR:CE1	1:A:32:ALA:HB1	0.49	2.43	14	1
1:A:23:ILE:CD1	1:A:74:ASP:HB3	0.49	2.37	15	1
1:A:6:TRP:CH2	1:A:130:LYS:HG3	0.49	2.42	17	4
1:A:2:PHE:CZ	1:A:108:ILE:HG21	0.49	2.42	7	1
1:A:92:LYS:CG	1:A:103:ILE:CD1	0.49	2.90	11	1
1:A:82:TRP:CE3	1:A:91:GLY:N	0.49	2.80	13	1
1:A:78:LEU:HD21	1:A:93:PHE:CD1	0.49	2.43	14	1
1:A:82:TRP:CH2	1:A:106:ARG:NE	0.49	2.81	12	2
1:A:74:ASP:HB3	2:A:132:PLM:CG	0.49	2.37	1	1
1:A:14:TYR:CA	1:A:124:ALA:HB1	0.49	2.37	5	3
1:A:78:LEU:O	1:A:78:LEU:HD23	0.49	2.07	18	1
1:A:62:PHE:CD2	1:A:68:PHE:CE1	0.49	3.01	17	1
1:A:62:PHE:CE2	1:A:82:TRP:CG	0.49	3.01	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:VAL:CB	1:A:117:TYR:CE2	0.49	2.96	19	1
1:A:48:THR:CG2	1:A:61:VAL:HG13	0.48	2.38	1	4
1:A:77:GLU:CG	1:A:96:VAL:HG21	0.48	2.39	7	1
1:A:2:PHE:CE1	1:A:108:ILE:CG1	0.48	2.96	16	1
1:A:116:THR:OG1	1:A:117:TYR:CD2	0.48	2.62	2	1
1:A:7:LYS:N	1:A:128:PHE:CD2	0.48	2.81	3	1
1:A:48:THR:HA	1:A:61:VAL:CA	0.48	2.36	4	1
1:A:47:PHE:O	1:A:49:VAL:N	0.48	2.46	2	3
1:A:76:THR:CG2	1:A:77:GLU:N	0.48	2.76	8	1
1:A:42:GLN:NE2	1:A:47:PHE:CE2	0.48	2.81	14	2
1:A:5:THR:C	1:A:6:TRP:CD1	0.48	2.92	3	3
1:A:114:ILE:HG23	1:A:127:ILE:HA	0.48	1.86	2	1
1:A:75:GLY:O	1:A:76:THR:HG22	0.48	2.06	7	2
1:A:82:TRP:CD2	1:A:83:THR:HA	0.48	2.44	7	1
1:A:47:PHE:CD1	1:A:64:LEU:HD21	0.48	2.44	18	1
1:A:115:GLN:HB2	1:A:126:ARG:CD	0.48	2.39	4	4
1:A:20:LYS:CE	1:A:120:GLU:CB	0.48	2.92	6	1
1:A:77:GLU:HG2	1:A:96:VAL:HG21	0.48	1.85	7	2
1:A:95:ARG:NE	1:A:100:LYS:N	0.48	2.61	7	1
1:A:98:ASN:N	1:A:98:ASN:ND2	0.48	2.57	13	1
1:A:89:LEU:HD12	1:A:106:ARG:HD2	0.48	1.86	15	1
1:A:115:GLN:HB2	1:A:126:ARG:CG	0.48	2.39	4	1
1:A:36:LEU:HD11	1:A:51:GLU:OE2	0.48	2.09	11	1
1:A:102:LEU:HD23	1:A:103:ILE:N	0.48	2.24	15	2
1:A:27:LYS:HD2	1:A:74:ASP:CB	0.48	2.39	16	1
1:A:115:GLN:O	1:A:116:THR:HG22	0.48	2.09	20	1
1:A:62:PHE:CG	1:A:68:PHE:CD1	0.48	3.02	10	2
1:A:49:VAL:HB	1:A:62:PHE:CE1	0.48	2.42	6	1
1:A:23:ILE:HG23	1:A:27:LYS:HB3	0.48	1.85	16	1
1:A:75:GLY:HA3	1:A:78:LEU:CD1	0.48	2.38	3	1
1:A:2:PHE:CD1	1:A:2:PHE:N	0.48	2.81	9	1
1:A:96:VAL:CG2	1:A:97:ASP:N	0.48	2.77	12	1
1:A:56:ARG:CB	1:A:58:ILE:CG2	0.48	2.92	18	1
1:A:6:TRP:HB3	1:A:128:PHE:CD2	0.47	2.44	18	2
1:A:82:TRP:CD2	1:A:83:THR:CA	0.47	2.97	7	1
1:A:16:LYS:HB3	1:A:17:PHE:CE2	0.47	2.44	17	1
1:A:36:LEU:HG	1:A:38:LEU:CD1	0.47	2.39	19	1
1:A:23:ILE:HD11	1:A:74:ASP:CB	0.47	2.38	20	1
1:A:11:ASN:HB3	1:A:14:TYR:CZ	0.47	2.41	2	1
1:A:7:LYS:HA	1:A:36:LEU:O	0.47	2.09	3	2
1:A:47:PHE:CZ	1:A:64:LEU:HD21	0.47	2.45	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:LEU:HD22	2:A:132:PLM:C9	0.47	2.38	11	1
1:A:102:LEU:HD13	1:A:103:ILE:N	0.47	2.23	20	1
1:A:119:TYR:O	1:A:119:TYR:CG	0.47	2.68	2	2
1:A:23:ILE:CD1	2:A:132:PLM:HG1	0.47	2.39	3	1
1:A:40:ILE:HD13	1:A:49:VAL:HG12	0.47	1.84	4	1
1:A:62:PHE:HB3	1:A:68:PHE:CZ	0.47	2.43	7	4
1:A:106:ARG:NH2	2:A:132:PLM:O1	0.47	2.47	3	4
1:A:51:GLU:O	1:A:53:SER:N	0.47	2.47	5	5
1:A:17:PHE:CD1	1:A:17:PHE:C	0.47	2.93	7	3
1:A:122:VAL:O	1:A:122:VAL:HG23	0.47	2.08	16	1
1:A:60:VAL:CG1	1:A:61:VAL:N	0.47	2.77	20	1
1:A:49:VAL:CG1	1:A:62:PHE:CE1	0.47	2.98	1	1
1:A:72:LEU:N	1:A:72:LEU:CD1	0.47	2.70	3	2
1:A:23:ILE:HG21	1:A:28:ARG:CA	0.47	2.39	6	1
1:A:11:ASN:CG	1:A:14:TYR:CD2	0.47	2.92	7	1
1:A:56:ARG:HH21	1:A:58:ILE:HD12	0.47	1.69	11	1
1:A:17:PHE:C	1:A:17:PHE:CD1	0.47	2.93	10	2
1:A:14:TYR:CE2	1:A:126:ARG:HD3	0.47	2.45	4	1
1:A:77:GLU:CB	1:A:96:VAL:HB	0.47	2.40	7	2
1:A:95:ARG:CZ	1:A:99:GLY:CA	0.47	2.92	7	1
1:A:64:LEU:HA	1:A:82:TRP:CD1	0.47	2.45	8	2
1:A:89:LEU:CD1	1:A:106:ARG:HH11	0.47	2.22	9	1
1:A:114:ILE:HG12	1:A:127:ILE:CD1	0.47	2.39	14	1
1:A:17:PHE:HB3	1:A:122:VAL:CB	0.47	2.39	16	1
1:A:82:TRP:CZ3	1:A:106:ARG:NE	0.47	2.82	3	2
1:A:36:LEU:CG	1:A:38:LEU:HD13	0.47	2.39	4	2
1:A:77:GLU:HG2	1:A:96:VAL:CG2	0.47	2.39	7	1
1:A:84:MET:HA	1:A:89:LEU:HD23	0.47	1.86	14	1
1:A:78:LEU:HD11	1:A:93:PHE:CG	0.47	2.44	15	1
1:A:90:VAL:CG1	1:A:105:VAL:HG23	0.47	2.40	4	1
1:A:68:PHE:CZ	1:A:81:THR:HA	0.47	2.44	18	2
1:A:78:LEU:HD12	1:A:102:LEU:HD13	0.47	1.85	11	1
1:A:14:TYR:CE1	1:A:18:MET:HE3	0.47	2.45	4	1
1:A:108:ILE:CD1	1:A:113:LEU:HD12	0.47	2.39	7	1
1:A:62:PHE:O	1:A:64:LEU:N	0.47	2.48	8	2
1:A:63:GLU:O	1:A:64:LEU:C	0.47	2.58	18	2
1:A:40:ILE:CG1	1:A:49:VAL:CG2	0.47	2.93	12	1
1:A:117:TYR:N	1:A:123:GLU:O	0.47	2.46	16	1
1:A:73:ALA:O	1:A:74:ASP:CB	0.47	2.63	4	2
1:A:55:PHE:CE1	2:A:132:PLM:HE2	0.47	2.44	15	2
1:A:62:PHE:O	1:A:63:GLU:C	0.47	2.58	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:HD13	1:A:95:ARG:HH21	0.47	1.70	6	1
1:A:82:TRP:CE3	1:A:90:VAL:C	0.47	2.93	6	2
1:A:128:PHE:CD1	1:A:128:PHE:N	0.47	2.83	13	1
1:A:40:ILE:CD1	1:A:49:VAL:HG23	0.47	2.40	19	1
1:A:74:ASP:CB	2:A:132:PLM:CG	0.46	2.92	1	2
1:A:46:LYS:HB3	1:A:63:GLU:N	0.46	2.25	4	1
1:A:2:PHE:CE1	1:A:108:ILE:HG12	0.46	2.44	16	1
1:A:14:TYR:CG	1:A:124:ALA:HB1	0.46	2.45	19	1
1:A:5:THR:C	1:A:6:TRP:CG	0.46	2.93	2	6
1:A:17:PHE:CE1	1:A:119:TYR:HB2	0.46	2.45	12	2
1:A:14:TYR:CD2	1:A:126:ARG:HD3	0.46	2.45	15	1
1:A:113:LEU:C	1:A:113:LEU:CD2	0.46	2.89	3	1
1:A:39:THR:HB	1:A:50:LYS:HB3	0.46	1.86	11	2
1:A:49:VAL:HG12	1:A:62:PHE:CZ	0.46	2.45	17	1
1:A:106:ARG:NH1	1:A:106:ARG:CG	0.46	2.78	3	3
1:A:93:PHE:O	1:A:102:LEU:N	0.46	2.49	7	1
1:A:14:TYR:HB3	1:A:124:ALA:C	0.46	2.36	2	1
1:A:7:LYS:C	1:A:8:VAL:HG12	0.46	2.36	3	1
1:A:113:LEU:CD1	1:A:128:PHE:CE2	0.46	2.98	4	1
1:A:11:ASN:CG	1:A:14:TYR:CG	0.46	2.94	7	1
1:A:115:GLN:HE21	1:A:126:ARG:NE	0.46	2.08	19	1
1:A:103:ILE:HG12	1:A:117:TYR:CD2	0.46	2.45	20	1
1:A:10:ARG:HG3	1:A:127:ILE:CG2	0.46	2.41	2	1
1:A:7:LYS:CA	1:A:36:LEU:O	0.46	2.63	3	1
1:A:107:GLU:O	1:A:109:SER:N	0.46	2.48	12	3
1:A:36:LEU:HD22	1:A:126:ARG:NH2	0.46	2.25	8	3
1:A:126:ARG:CG	1:A:126:ARG:HH11	0.46	2.24	11	1
1:A:103:ILE:CG1	1:A:104:ALA:N	0.46	2.78	6	3
1:A:6:TRP:CE3	1:A:113:LEU:HB2	0.46	2.45	3	1
1:A:39:THR:HG22	1:A:39:THR:O	0.46	2.10	6	1
1:A:92:LYS:HG3	1:A:103:ILE:CD1	0.46	2.41	11	1
1:A:6:TRP:CH2	1:A:130:LYS:HD2	0.46	2.46	13	2
1:A:114:ILE:HG12	1:A:127:ILE:HD12	0.46	1.87	17	1
1:A:6:TRP:CG	1:A:113:LEU:CD1	0.46	2.99	3	1
1:A:36:LEU:HD21	1:A:128:PHE:CZ	0.46	2.45	6	1
1:A:62:PHE:HA	1:A:68:PHE:CE2	0.46	2.46	11	1
1:A:10:ARG:HG3	1:A:127:ILE:HG21	0.46	1.88	2	1
1:A:10:ARG:HB2	1:A:127:ILE:HB	0.46	1.88	8	1
1:A:17:PHE:CD1	1:A:17:PHE:N	0.46	2.84	16	1
1:A:36:LEU:CD2	1:A:126:ARG:NH2	0.46	2.79	16	1
1:A:72:LEU:CD1	1:A:78:LEU:HB2	0.46	2.41	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LYS:HE3	1:A:120:GLU:CB	0.45	2.41	6	1
1:A:18:MET:O	1:A:23:ILE:HG12	0.45	2.11	17	1
1:A:55:PHE:CD2	1:A:73:ALA:CB	0.45	2.99	1	1
1:A:39:THR:HB	1:A:50:LYS:CB	0.45	2.41	17	9
1:A:40:ILE:HG12	1:A:49:VAL:CG2	0.45	2.42	3	2
1:A:126:ARG:HH11	1:A:126:ARG:HG3	0.45	1.71	11	1
1:A:46:LYS:HD2	1:A:46:LYS:C	0.45	2.36	4	1
1:A:62:PHE:CE2	2:A:132:PLM:H32	0.45	2.46	8	1
1:A:12:GLU:O	1:A:125:LYS:N	0.45	2.50	16	3
1:A:49:VAL:HG12	1:A:62:PHE:CE1	0.45	2.46	19	1
1:A:6:TRP:HZ2	1:A:108:ILE:HD11	0.45	1.65	20	1
1:A:55:PHE:CE2	1:A:73:ALA:CB	0.45	2.99	1	1
1:A:11:ASN:HB3	1:A:14:TYR:CG	0.45	2.45	2	1
1:A:116:THR:CB	1:A:125:LYS:HA	0.45	2.41	2	1
1:A:60:VAL:O	1:A:60:VAL:HG13	0.45	2.11	12	2
1:A:72:LEU:HD22	1:A:72:LEU:C	0.45	2.36	4	1
1:A:61:VAL:C	1:A:62:PHE:CD1	0.45	2.95	6	1
1:A:2:PHE:CE1	1:A:108:ILE:HG13	0.45	2.47	13	1
1:A:6:TRP:CD1	1:A:40:ILE:HG13	0.45	2.46	16	1
1:A:23:ILE:CG2	1:A:27:LYS:CB	0.45	2.94	2	1
1:A:114:ILE:HG21	1:A:127:ILE:HD13	0.45	1.88	2	1
1:A:90:VAL:HB	1:A:105:VAL:CG2	0.45	2.42	19	1
1:A:90:VAL:HB	1:A:105:VAL:HG23	0.45	1.87	19	1
1:A:48:THR:HB	1:A:61:VAL:HG13	0.45	1.85	2	1
1:A:41:THR:HG22	1:A:41:THR:O	0.45	2.11	11	2
1:A:6:TRP:CZ3	1:A:130:LYS:HG3	0.45	2.46	9	1
1:A:16:LYS:HB3	1:A:17:PHE:CD2	0.45	2.47	17	1
1:A:83:THR:CG2	1:A:90:VAL:CG2	0.45	2.89	20	2
1:A:89:LEU:HD23	1:A:90:VAL:N	0.45	2.27	18	1
1:A:68:PHE:O	1:A:79:THR:HB	0.45	2.11	1	1
1:A:106:ARG:HB3	1:A:113:LEU:HD21	0.45	1.88	4	1
1:A:36:LEU:CD2	1:A:38:LEU:HD13	0.45	2.41	9	1
1:A:103:ILE:HG23	1:A:117:TYR:CD1	0.45	2.46	20	1
1:A:36:LEU:HA	1:A:53:SER:CB	0.45	2.41	4	1
1:A:93:PHE:CE1	2:A:132:PLM:H41	0.45	2.47	6	1
1:A:20:LYS:HE3	1:A:119:TYR:CG	0.45	2.47	13	1
1:A:17:PHE:CD2	1:A:124:ALA:CB	0.45	2.99	19	2
1:A:49:VAL:HG22	1:A:60:VAL:HB	0.45	1.87	7	2
1:A:82:TRP:CH2	1:A:84:MET:HB2	0.45	2.47	7	2
1:A:41:THR:O	1:A:41:THR:HG22	0.45	2.11	13	3
1:A:23:ILE:HG22	1:A:28:ARG:N	0.45	2.27	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:GLU:HB3	1:A:96:VAL:HG22	0.45	1.88	16	1
1:A:105:VAL:O	1:A:105:VAL:HG13	0.45	2.12	5	1
1:A:82:TRP:CH2	1:A:84:MET:HB3	0.45	2.47	18	1
1:A:92:LYS:C	1:A:93:PHE:CG	0.45	2.95	18	1
1:A:17:PHE:CE1	1:A:21:MET:HG2	0.44	2.47	3	1
1:A:14:TYR:CE2	1:A:126:ARG:CG	0.44	2.99	4	1
1:A:36:LEU:HD21	1:A:128:PHE:HE2	0.44	1.72	8	1
1:A:70:TYR:CD1	1:A:70:TYR:C	0.44	2.96	8	1
1:A:116:THR:HB	1:A:125:LYS:CG	0.44	2.42	8	1
1:A:113:LEU:HD23	1:A:128:PHE:CE2	0.44	2.47	13	1
1:A:20:LYS:CE	1:A:122:VAL:HG12	0.44	2.42	16	1
1:A:36:LEU:CD1	1:A:38:LEU:HD12	0.44	2.40	3	1
1:A:36:LEU:HD12	1:A:37:LYS:N	0.44	2.26	17	2
1:A:49:VAL:CG1	1:A:60:VAL:HB	0.44	2.41	19	2
1:A:96:VAL:HG23	1:A:97:ASP:N	0.44	2.25	12	2
1:A:23:ILE:HG23	1:A:27:LYS:HG2	0.44	1.88	15	1
1:A:60:VAL:HB	1:A:62:PHE:CZ	0.44	2.47	17	1
1:A:82:TRP:O	1:A:83:THR:CB	0.44	2.65	8	2
1:A:83:THR:HG23	1:A:90:VAL:HG22	0.44	1.89	17	1
1:A:114:ILE:CG1	1:A:127:ILE:HD12	0.44	2.42	17	1
1:A:46:LYS:HB2	1:A:63:GLU:C	0.44	2.37	4	1
1:A:105:VAL:CG1	1:A:117:TYR:CZ	0.44	3.00	4	1
1:A:6:TRP:CZ3	1:A:130:LYS:CB	0.44	3.01	12	2
1:A:101:GLU:CG	1:A:102:LEU:N	0.44	2.79	5	2
1:A:82:TRP:CE3	1:A:89:LEU:CD2	0.44	3.00	7	1
1:A:102:LEU:C	1:A:103:ILE:CG2	0.44	2.90	9	1
1:A:20:LYS:HE3	1:A:119:TYR:CD1	0.44	2.47	13	1
1:A:77:GLU:HG2	1:A:96:VAL:HG11	0.44	1.88	16	1
1:A:93:PHE:CZ	2:A:132:PLM:C4	0.44	3.01	18	1
1:A:82:TRP:CE2	1:A:83:THR:HA	0.44	2.48	7	1
1:A:38:LEU:HG	1:A:49:VAL:CG2	0.44	2.43	9	2
1:A:72:LEU:HD22	2:A:132:PLM:H82	0.44	1.88	11	1
1:A:102:LEU:HD12	1:A:119:TYR:HA	0.44	1.89	17	1
1:A:115:GLN:C	1:A:116:THR:HG22	0.44	2.38	4	2
1:A:38:LEU:CD2	1:A:49:VAL:HG22	0.44	2.42	18	1
1:A:48:THR:OG1	1:A:61:VAL:HG13	0.44	2.13	20	1
1:A:62:PHE:CZ	1:A:68:PHE:CE2	0.44	3.05	10	1
1:A:40:ILE:HG13	1:A:49:VAL:CG2	0.44	2.42	12	1
1:A:42:GLN:CD	1:A:47:PHE:CE2	0.44	2.95	12	1
1:A:33:HIS:CD2	1:A:33:HIS:C	0.44	2.91	2	1
1:A:105:VAL:O	1:A:107:GLU:N	0.44	2.51	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:GLU:CG	1:A:90:VAL:HG21	0.44	2.42	7	1
1:A:82:TRP:CZ3	1:A:106:ARG:CD	0.44	3.01	16	1
1:A:103:ILE:HG13	1:A:104:ALA:N	0.44	2.28	9	2
1:A:89:LEU:O	1:A:105:VAL:HG23	0.44	2.13	8	1
1:A:70:TYR:CE2	2:A:132:PLM:C6	0.44	3.01	16	1
1:A:49:VAL:HG11	1:A:82:TRP:CH2	0.44	2.48	20	1
1:A:116:THR:HB	1:A:125:LYS:CD	0.44	2.43	20	1
1:A:127:ILE:HG22	1:A:127:ILE:O	0.43	2.12	3	1
1:A:46:LYS:HB2	1:A:64:LEU:N	0.43	2.28	4	1
1:A:68:PHE:CD1	1:A:68:PHE:N	0.43	2.86	6	1
1:A:91:GLY:O	1:A:104:ALA:N	0.43	2.51	17	2
1:A:111:ASN:N	1:A:111:ASN:ND2	0.43	2.66	8	1
1:A:66:VAL:O	1:A:68:PHE:CE2	0.43	2.71	11	1
1:A:40:ILE:HG23	1:A:49:VAL:CG1	0.43	2.29	13	1
1:A:38:LEU:HG	1:A:49:VAL:HG21	0.43	1.90	15	1
1:A:20:LYS:CE	1:A:122:VAL:CG1	0.43	2.96	16	1
1:A:82:TRP:CZ3	1:A:89:LEU:HD21	0.43	2.48	7	1
1:A:85:GLU:CG	1:A:90:VAL:CG2	0.43	2.96	18	3
1:A:6:TRP:CG	1:A:113:LEU:HD13	0.43	2.48	3	1
1:A:111:ASN:N	1:A:111:ASN:HD22	0.43	2.11	8	1
1:A:114:ILE:HD13	1:A:127:ILE:HD12	0.43	1.89	11	1
1:A:17:PHE:CD1	1:A:17:PHE:O	0.43	2.72	12	2
1:A:70:TYR:HB3	1:A:78:LEU:HD23	0.43	1.90	16	1
1:A:78:LEU:CD1	1:A:102:LEU:HD13	0.43	2.42	19	1
1:A:48:THR:CA	1:A:61:VAL:HA	0.43	2.39	4	1
1:A:20:LYS:HE3	1:A:119:TYR:HB3	0.43	1.90	7	1
2:A:132:PLM:C1	2:A:132:PLM:H51	0.43	2.43	7	1
1:A:62:PHE:N	1:A:62:PHE:CD1	0.43	2.86	15	2
1:A:6:TRP:O	1:A:38:LEU:N	0.43	2.51	2	4
1:A:118:THR:OG1	1:A:119:TYR:N	0.43	2.52	2	2
1:A:60:VAL:O	1:A:60:VAL:HG12	0.43	2.13	4	1
1:A:20:LYS:HE3	1:A:119:TYR:CB	0.43	2.44	7	1
1:A:106:ARG:NH1	2:A:132:PLM:O1	0.43	2.50	18	2
1:A:78:LEU:HD21	1:A:93:PHE:CE1	0.43	2.49	16	1
1:A:125:LYS:C	1:A:126:ARG:HD2	0.43	2.39	20	1
1:A:82:TRP:CD2	1:A:91:GLY:HA2	0.43	2.49	1	1
1:A:116:THR:OG1	1:A:117:TYR:N	0.43	2.47	11	2
1:A:65:GLY:H	1:A:82:TRP:CD1	0.43	2.32	7	1
1:A:23:ILE:HG21	1:A:28:ARG:HA	0.43	1.89	9	1
1:A:61:VAL:C	1:A:62:PHE:CG	0.43	2.96	17	1
1:A:55:PHE:CE2	1:A:73:ALA:HB1	0.43	2.49	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ILE:HG21	1:A:47:PHE:CE2	0.43	2.49	3	1
1:A:114:ILE:CD1	1:A:127:ILE:HG12	0.43	2.43	6	1
1:A:119:TYR:CE2	1:A:120:GLU:HG3	0.43	2.49	8	1
1:A:113:LEU:CD2	1:A:128:PHE:CD2	0.43	3.01	10	1
1:A:38:LEU:HD21	1:A:106:ARG:HH12	0.43	1.73	3	1
1:A:55:PHE:CE2	1:A:73:ALA:HA	0.43	2.49	4	1
1:A:20:LYS:CE	1:A:120:GLU:HB2	0.43	2.43	6	1
1:A:83:THR:O	1:A:90:VAL:N	0.43	2.51	8	2
1:A:6:TRP:CH2	1:A:130:LYS:CG	0.43	3.02	12	2
1:A:78:LEU:HD11	1:A:102:LEU:CD2	0.43	2.44	13	1
1:A:102:LEU:HD11	1:A:117:TYR:HD1	0.43	1.72	13	1
1:A:17:PHE:HA	1:A:122:VAL:HG11	0.43	1.91	15	1
1:A:20:LYS:HD3	1:A:122:VAL:CG1	0.43	2.43	16	1
1:A:116:THR:C	1:A:117:TYR:CD1	0.43	2.97	19	1
1:A:62:PHE:HB2	1:A:68:PHE:CE1	0.43	2.49	1	2
1:A:112:GLU:N	1:A:112:GLU:CD	0.43	2.76	3	1
1:A:93:PHE:CE1	2:A:132:PLM:H42	0.43	2.49	8	2
1:A:6:TRP:CZ3	1:A:113:LEU:N	0.43	2.87	18	1
1:A:113:LEU:CD2	1:A:128:PHE:CD1	0.43	3.02	20	1
1:A:105:VAL:HG11	1:A:117:TYR:CE2	0.42	2.48	4	1
1:A:64:LEU:H	1:A:64:LEU:HD12	0.42	1.74	16	1
1:A:20:LYS:CE	1:A:119:TYR:CB	0.42	2.97	7	1
1:A:77:GLU:CG	1:A:96:VAL:HG22	0.42	2.44	8	1
1:A:89:LEU:CD2	1:A:106:ARG:HH21	0.42	2.27	18	1
1:A:23:ILE:CG2	1:A:27:LYS:HB2	0.42	2.43	1	1
1:A:14:TYR:HA	1:A:124:ALA:CA	0.42	2.44	2	1
1:A:77:GLU:HB3	1:A:96:VAL:HB	0.42	1.89	3	1
1:A:119:TYR:CG	1:A:120:GLU:N	0.42	2.87	4	1
1:A:82:TRP:CD2	1:A:91:GLY:CA	0.42	3.03	13	1
1:A:40:ILE:HG12	1:A:49:VAL:HG23	0.42	1.89	3	1
1:A:49:VAL:HG22	1:A:60:VAL:CG1	0.42	2.44	5	1
1:A:75:GLY:C	1:A:76:THR:CG2	0.42	2.91	5	1
1:A:36:LEU:CD2	1:A:128:PHE:CZ	0.42	3.02	6	1
1:A:92:LYS:HA	1:A:103:ILE:HD12	0.42	1.90	11	1
1:A:6:TRP:CH2	1:A:113:LEU:HB2	0.42	2.49	18	1
1:A:78:LEU:CD1	1:A:93:PHE:HB3	0.42	2.44	19	1
1:A:48:THR:OG1	1:A:61:VAL:CG1	0.42	2.67	20	1
1:A:10:ARG:O	1:A:127:ILE:N	0.42	2.53	11	3
1:A:21:MET:HE3	1:A:119:TYR:CD1	0.42	2.50	12	1
1:A:116:THR:HG23	1:A:117:TYR:CE1	0.42	2.49	19	1
1:A:14:TYR:CD2	1:A:126:ARG:HG3	0.42	2.49	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:THR:HG23	1:A:39:THR:HG23	0.42	1.91	3	2
1:A:13:ASN:ND2	1:A:123:GLU:O	0.42	2.53	3	1
1:A:128:PHE:CD2	1:A:130:LYS:N	0.42	2.87	19	2
1:A:75:GLY:O	1:A:76:THR:HG23	0.42	2.13	5	1
1:A:116:THR:HB	1:A:125:LYS:HG3	0.42	1.91	18	2
1:A:82:TRP:CZ3	1:A:91:GLY:HA3	0.42	2.50	1	1
1:A:55:PHE:CZ	2:A:132:PLM:HE2	0.42	2.50	4	1
1:A:93:PHE:HD2	1:A:102:LEU:HD22	0.42	1.75	8	2
1:A:103:ILE:HD12	1:A:104:ALA:H	0.42	1.75	10	1
1:A:8:VAL:HB	1:A:128:PHE:CE1	0.42	2.50	11	1
1:A:8:VAL:HG21	1:A:11:ASN:OD1	0.42	2.15	11	1
1:A:119:TYR:CD1	1:A:119:TYR:C	0.42	2.98	13	1
1:A:23:ILE:HD11	1:A:74:ASP:HB3	0.42	1.92	15	1
1:A:93:PHE:N	1:A:102:LEU:O	0.42	2.53	16	1
1:A:6:TRP:CE2	1:A:113:LEU:HD13	0.42	2.50	18	1
1:A:108:ILE:HD13	1:A:112:GLU:O	0.42	2.15	1	1
1:A:23:ILE:HG23	1:A:27:LYS:CB	0.42	2.44	2	1
1:A:21:MET:HG3	1:A:119:TYR:CD2	0.42	2.50	4	1
1:A:62:PHE:CD1	1:A:62:PHE:N	0.42	2.88	9	1
1:A:98:ASN:ND2	1:A:100:LYS:HG2	0.42	2.29	12	1
1:A:36:LEU:HD12	1:A:36:LEU:C	0.42	2.39	17	1
1:A:113:LEU:CD2	1:A:115:GLN:HG2	0.42	2.39	19	1
1:A:62:PHE:CD2	1:A:82:TRP:NE1	0.42	2.87	1	1
1:A:102:LEU:CD1	1:A:119:TYR:HB2	0.42	2.45	6	1
1:A:101:GLU:HG2	1:A:102:LEU:N	0.42	2.30	8	1
1:A:65:GLY:N	1:A:82:TRP:O	0.42	2.53	9	1
1:A:74:ASP:HB3	2:A:132:PLM:HG3	0.42	1.91	9	1
1:A:62:PHE:CZ	1:A:82:TRP:CH2	0.42	3.08	12	1
1:A:21:MET:CE	1:A:95:ARG:HH12	0.42	2.27	15	1
1:A:56:ARG:HG3	1:A:58:ILE:CG2	0.42	2.44	16	1
1:A:92:LYS:O	1:A:93:PHE:CD1	0.42	2.72	18	1
1:A:7:LYS:HG2	1:A:8:VAL:N	0.42	2.30	3	1
1:A:49:VAL:HG11	1:A:82:TRP:CZ2	0.42	2.50	10	1
1:A:106:ARG:NH1	1:A:106:ARG:HG3	0.42	2.30	17	1
1:A:8:VAL:O	1:A:35:ASN:ND2	0.42	2.53	18	1
1:A:40:ILE:CG2	1:A:47:PHE:CD2	0.42	3.02	18	1
1:A:72:LEU:HD23	1:A:72:LEU:N	0.41	2.30	1	1
1:A:28:ARG:HG3	1:A:29:LYS:N	0.41	2.29	3	1
1:A:119:TYR:CD2	1:A:120:GLU:HB2	0.41	2.50	4	2
1:A:18:MET:O	1:A:23:ILE:CG1	0.41	2.68	16	1
1:A:8:VAL:HG13	1:A:36:LEU:HB3	0.41	1.90	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:THR:O	1:A:90:VAL:HG23	0.41	2.16	8	1
1:A:14:TYR:HA	1:A:124:ALA:HA	0.41	1.93	2	1
1:A:48:THR:O	1:A:50:LYS:N	0.41	2.53	2	1
1:A:62:PHE:CA	1:A:68:PHE:CZ	0.41	3.03	1	1
1:A:89:LEU:HD13	1:A:106:ARG:CD	0.41	2.46	2	1
1:A:4:GLY:O	1:A:40:ILE:N	0.41	2.53	17	4
1:A:6:TRP:CD1	1:A:40:ILE:CG1	0.41	3.04	4	1
1:A:17:PHE:CB	1:A:124:ALA:CB	0.41	2.98	4	1
1:A:18:MET:CB	1:A:23:ILE:HG13	0.41	2.46	16	1
1:A:113:LEU:O	1:A:128:PHE:N	0.41	2.52	3	1
1:A:63:GLU:O	1:A:66:VAL:N	0.41	2.52	4	1
1:A:102:LEU:CA	1:A:119:TYR:HA	0.41	2.44	4	1
1:A:23:ILE:CG2	1:A:28:ARG:CA	0.41	2.98	6	1
1:A:23:ILE:CG2	1:A:28:ARG:HB3	0.41	2.46	6	1
1:A:51:GLU:HB2	1:A:60:VAL:CG2	0.41	2.46	8	1
1:A:113:LEU:CD2	1:A:128:PHE:CE2	0.41	3.04	10	1
1:A:84:MET:CA	1:A:89:LEU:HD12	0.41	2.45	5	1
1:A:12:GLU:N	1:A:125:LYS:O	0.41	2.53	8	2
1:A:47:PHE:CZ	1:A:89:LEU:HD21	0.41	2.51	11	1
1:A:98:ASN:ND2	1:A:119:TYR:OH	0.41	2.54	19	3
1:A:48:THR:HB	1:A:61:VAL:CG1	0.41	2.46	13	1
1:A:13:ASN:CG	1:A:17:PHE:CE1	0.41	2.99	16	1
1:A:20:LYS:CD	1:A:122:VAL:CG1	0.41	2.99	16	1
1:A:91:GLY:O	1:A:104:ALA:HB3	0.41	2.16	16	1
1:A:11:ASN:ND2	1:A:126:ARG:HA	0.41	2.31	2	1
1:A:36:LEU:CG	1:A:38:LEU:HD12	0.41	2.46	3	1
1:A:23:ILE:CD1	2:A:132:PLM:HG3	0.41	2.45	7	1
1:A:102:LEU:CD1	1:A:119:TYR:CG	0.41	3.03	7	1
1:A:63:GLU:OE1	1:A:66:VAL:HG11	0.41	2.16	12	1
1:A:5:THR:O	1:A:131:GLU:N	0.41	2.54	19	1
1:A:10:ARG:HG3	1:A:127:ILE:CB	0.41	2.46	2	1
1:A:17:PHE:CE1	1:A:119:TYR:CB	0.41	3.04	3	1
1:A:36:LEU:CD2	1:A:38:LEU:CD1	0.41	2.97	3	1
1:A:78:LEU:C	1:A:78:LEU:CD2	0.41	2.91	8	1
1:A:23:ILE:HG22	1:A:24:ASN:N	0.41	2.31	14	1
1:A:70:TYR:HB3	1:A:78:LEU:CD2	0.41	2.46	16	1
1:A:82:TRP:CZ3	1:A:106:ARG:HD3	0.41	2.51	16	1
1:A:55:PHE:CE2	2:A:132:PLM:HG2	0.41	2.51	2	1
1:A:105:VAL:O	1:A:105:VAL:HG12	0.41	2.15	2	1
1:A:115:GLN:HB2	1:A:126:ARG:HD3	0.41	1.93	3	1
1:A:55:PHE:CE1	2:A:132:PLM:CE	0.41	3.04	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:VAL:HG21	1:A:126:ARG:HD2	0.41	1.92	6	1
1:A:5:THR:OG1	1:A:6:TRP:N	0.41	2.54	9	1
1:A:12:GLU:CB	1:A:125:LYS:HB2	0.41	2.46	20	2
1:A:62:PHE:CE1	1:A:82:TRP:CD1	0.41	3.09	13	1
1:A:77:GLU:CB	1:A:96:VAL:CG2	0.41	2.98	13	1
1:A:79:THR:O	1:A:94:LYS:N	0.41	2.53	15	1
1:A:72:LEU:HG	1:A:75:GLY:C	0.41	2.41	16	1
1:A:18:MET:HB3	1:A:23:ILE:CG1	0.41	2.45	17	1
1:A:106:ARG:HG3	1:A:106:ARG:HH11	0.41	1.75	17	1
1:A:67:ASP:C	1:A:68:PHE:CD1	0.41	2.99	18	1
1:A:41:THR:CG2	1:A:48:THR:HG23	0.41	2.46	19	1
1:A:114:ILE:CG2	1:A:116:THR:CG2	0.41	2.91	2	1
1:A:117:TYR:O	1:A:123:GLU:HA	0.41	2.15	4	2
1:A:74:ASP:HB2	2:A:132:PLM:CG	0.41	2.46	9	2
1:A:77:GLU:HB3	1:A:96:VAL:CG2	0.41	2.46	10	1
1:A:89:LEU:HD23	1:A:90:VAL:H	0.41	1.76	18	1
1:A:23:ILE:N	1:A:23:ILE:HD12	0.41	2.31	20	1
1:A:6:TRP:CZ2	1:A:130:LYS:HG3	0.40	2.51	2	1
1:A:55:PHE:CD1	1:A:73:ALA:CB	0.40	3.04	2	1
1:A:63:GLU:OE1	1:A:66:VAL:HG21	0.40	2.15	2	1
1:A:89:LEU:O	1:A:106:ARG:N	0.40	2.54	7	1
1:A:59:ASP:OD1	1:A:59:ASP:N	0.40	2.54	8	1
1:A:123:GLU:O	1:A:124:ALA:HB3	0.40	2.16	16	1
1:A:116:THR:O	1:A:116:THR:OG1	0.40	2.37	20	1
1:A:53:SER:C	1:A:55:PHE:N	0.40	2.79	2	1
1:A:45:ASN:HB2	1:A:63:GLU:CG	0.40	2.45	4	1
1:A:54:ASN:O	1:A:54:ASN:ND2	0.40	2.55	7	1
1:A:113:LEU:CD1	1:A:114:ILE:N	0.40	2.84	8	1
1:A:54:ASN:OD1	1:A:55:PHE:N	0.40	2.54	10	1
1:A:74:ASP:OD2	2:A:132:PLM:HG3	0.40	2.14	12	1
1:A:103:ILE:HG22	1:A:118:THR:HB	0.40	1.92	14	1
1:A:23:ILE:O	1:A:28:ARG:NH1	0.40	2.55	16	1
1:A:118:THR:HG22	1:A:118:THR:O	0.40	2.15	17	1
1:A:72:LEU:CD1	2:A:132:PLM:C8	0.40	3.00	20	1
1:A:72:LEU:HD21	1:A:78:LEU:CD1	0.40	2.46	9	1
1:A:78:LEU:HG	1:A:93:PHE:CD1	0.40	2.51	16	1
1:A:106:ARG:NE	1:A:115:GLN:OE1	0.40	2.54	1	1
1:A:93:PHE:O	1:A:102:LEU:HD23	0.40	2.16	4	1
1:A:36:LEU:CD2	1:A:126:ARG:HH21	0.40	2.29	6	1
1:A:20:LYS:NZ	1:A:119:TYR:CB	0.40	2.84	7	1
1:A:36:LEU:CD2	1:A:128:PHE:CE2	0.40	3.05	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:LEU:HD22	1:A:106:ARG:HH21	0.40	1.75	18	1
1:A:23:ILE:HD11	1:A:74:ASP:HB2	0.40	1.93	20	1
1:A:23:ILE:CD1	1:A:74:ASP:CG	0.40	2.94	20	1
1:A:108:ILE:HG13	1:A:113:LEU:HA	0.40	1.93	20	1
1:A:75:GLY:HA3	1:A:78:LEU:HD12	0.40	1.92	3	1
1:A:55:PHE:CD1	1:A:55:PHE:N	0.40	2.89	11	1
1:A:82:TRP:CE2	1:A:91:GLY:HA3	0.40	2.51	13	1
1:A:126:ARG:CD	1:A:126:ARG:N	0.40	2.84	20	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	129/131 (98%)	91±5 (71±4%)	28±4 (21±3%)	10±3 (8±2%)	1	14
All	All	2580/2620 (98%)	1828 (71%)	552 (21%)	200 (8%)	1	14

All 54 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	25	VAL	16
1	A	130	LYS	11
1	A	77	GLU	11
1	A	117	TYR	10
1	A	67	ASP	10
1	A	61	VAL	8
1	A	36	LEU	7
1	A	100	LYS	7
1	A	120	GLU	7
1	A	108	ILE	7
1	A	101	GLU	6
1	A	64	LEU	6
1	A	3	ASP	5
1	A	110	GLY	5

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Mol	Chain	Res	Type	Models (Total)
1	A	49	VAL	5
1	A	13	ASN	4
1	A	98	ASN	4
1	A	85	GLU	4
1	A	34	ASP	4
1	A	66	VAL	4
1	A	86	GLY	4
1	A	8	VAL	3
1	A	24	ASN	3
1	A	72	LEU	3
1	A	74	ASP	3
1	A	123	GLU	3
1	A	124	ALA	3
1	A	83	THR	3
1	A	12	GLU	2
1	A	44	GLY	2
1	A	35	ASN	2
1	A	7	LYS	2
1	A	45	ASN	2
1	A	10	ARG	2
1	A	2	PHE	2
1	A	76	THR	2
1	A	99	GLY	1
1	A	127	ILE	1
1	A	47	PHE	1
1	A	56	ARG	1
1	A	63	GLU	1
1	A	75	GLY	1
1	A	52	SER	1
1	A	48	THR	1
1	A	121	GLY	1
1	A	14	TYR	1
1	A	95	ARG	1
1	A	105	VAL	1
1	A	78	LEU	1
1	A	96	VAL	1
1	A	11	ASN	1
1	A	111	ASN	1
1	A	40	ILE	1
1	A	109	SER	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	113/113 (100%)	73±4 (65±4%)	40±4 (35±4%)	1	9
All	All	2260/2260 (100%)	1458 (65%)	802 (35%)	1	9

All 108 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	61	VAL	20
1	A	76	THR	19
1	A	38	LEU	18
1	A	49	VAL	17
1	A	64	LEU	16
1	A	120	GLU	16
1	A	125	LYS	16
1	A	89	LEU	15
1	A	45	ASN	13
1	A	26	VAL	12
1	A	90	VAL	12
1	A	108	ILE	12
1	A	88	LYS	12
1	A	113	LEU	12
1	A	59	ASP	11
1	A	111	ASN	11
1	A	130	LYS	11
1	A	56	ARG	11
1	A	5	THR	10
1	A	10	ARG	10
1	A	11	ASN	10
1	A	16	LYS	10
1	A	78	LEU	10
1	A	21	MET	10
1	A	127	ILE	10
1	A	36	LEU	10
1	A	50	LYS	10
1	A	58	ILE	10
1	A	68	PHE	9

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Mol	Chain	Res	Type	Models (Total)
1	A	97	ASP	9
1	A	102	LEU	9
1	A	105	VAL	9
1	A	74	ASP	9
1	A	126	ARG	9
1	A	63	GLU	9
1	A	77	GLU	9
1	A	8	VAL	8
1	A	13	ASN	8
1	A	46	LYS	8
1	A	54	ASN	8
1	A	62	PHE	8
1	A	72	LEU	8
1	A	101	GLU	8
1	A	87	ASN	8
1	A	92	LYS	8
1	A	95	ARG	8
1	A	14	TYR	8
1	A	52	SER	8
1	A	84	MET	8
1	A	25	VAL	8
1	A	116	THR	8
1	A	23	ILE	7
1	A	30	LEU	7
1	A	12	GLU	7
1	A	35	ASN	7
1	A	48	THR	7
1	A	85	GLU	7
1	A	103	ILE	7
1	A	128	PHE	7
1	A	98	ASN	7
1	A	15	GLU	6
1	A	18	MET	6
1	A	27	LYS	6
1	A	129	LYS	6
1	A	29	LYS	6
1	A	43	GLU	6
1	A	53	SER	6
1	A	66	VAL	6
1	A	67	ASP	6
1	A	109	SER	6
1	A	28	ARG	6

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Mol	Chain	Res	Type	Models (Total)
1	A	118	THR	6
1	A	114	ILE	5
1	A	17	PHE	5
1	A	2	PHE	5
1	A	71	SER	5
1	A	81	THR	5
1	A	41	THR	5
1	A	107	GLU	5
1	A	60	VAL	5
1	A	37	LYS	4
1	A	94	LYS	4
1	A	3	ASP	4
1	A	24	ASN	4
1	A	34	ASP	4
1	A	106	ARG	4
1	A	40	ILE	4
1	A	19	GLU	4
1	A	51	GLU	4
1	A	123	GLU	4
1	A	57	ASN	4
1	A	112	GLU	3
1	A	7	LYS	3
1	A	47	PHE	3
1	A	42	GLN	3
1	A	33	HIS	3
1	A	55	PHE	3
1	A	122	VAL	3
1	A	20	LYS	2
1	A	119	TYR	2
1	A	117	TYR	2
1	A	83	THR	2
1	A	115	GLN	2
1	A	131	GLU	2
1	A	79	THR	1
1	A	70	TYR	1
1	A	96	VAL	1
1	A	9	ASP	1

6.3.3 RNA ⓘ

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	PLM	A	132	-	17,17,17	0.78±0.05	0±0 (0±1%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	PLM	A	132	-	17,17,17	0.61±0.18	0±1 (2±3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLM	A	132	-	-	0±0,15,15,15	-

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	132	PLM	C2-C1	2.09	1.55	1.50	9	2

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

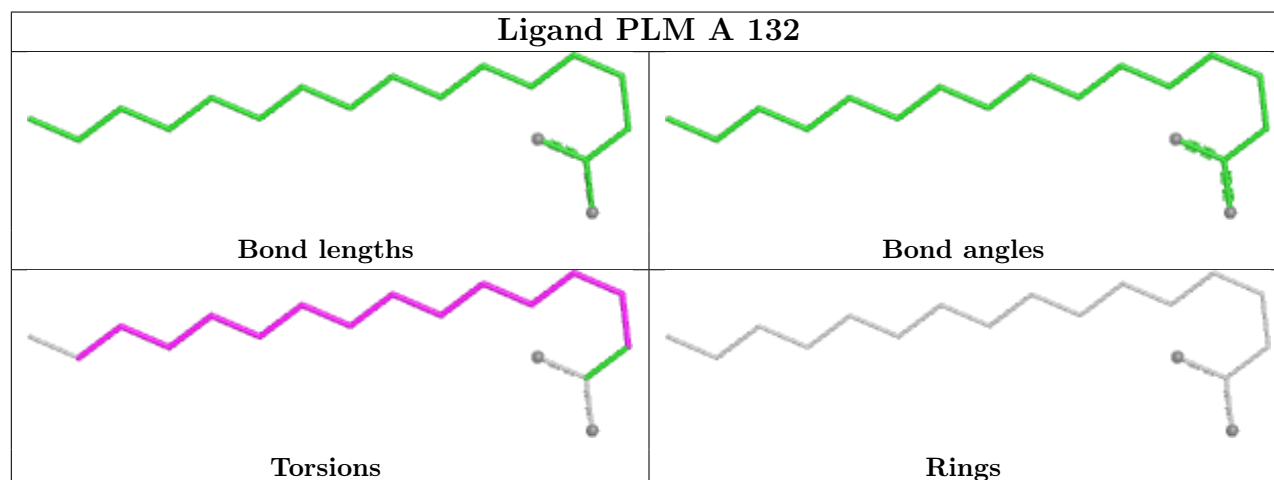
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	132	PLM	O2-C1-C2	2.52	115.09	123.09	5	5
2	A	132	PLM	O1-C1-C2	2.18	120.89	114.00	5	1
2	A	132	PLM	O1-C1-O2	2.02	128.53	123.33	20	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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