



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 05:19 PM BST

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

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

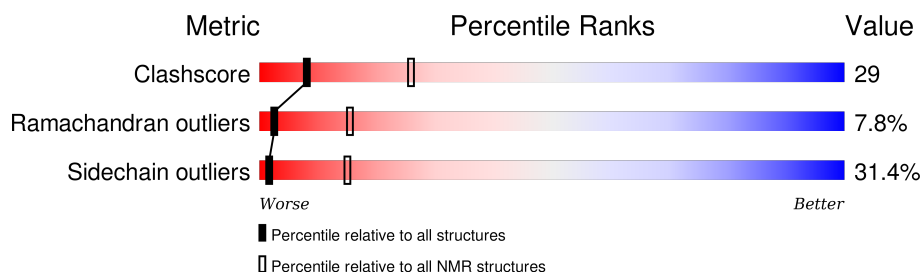
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	131	

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)	0.50	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

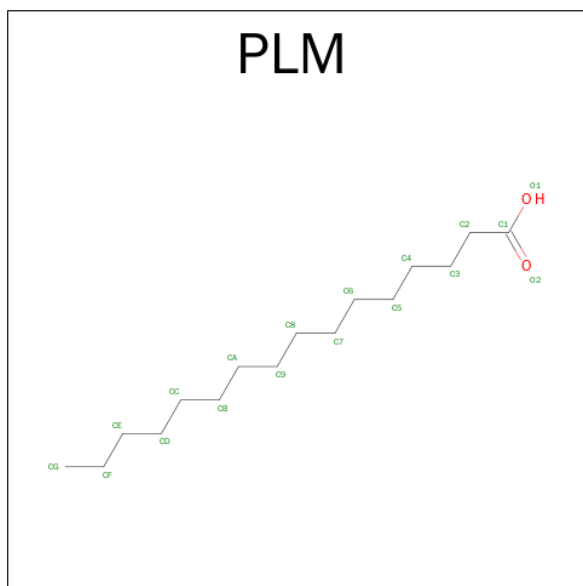
3 Entry composition [i](#)

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 (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



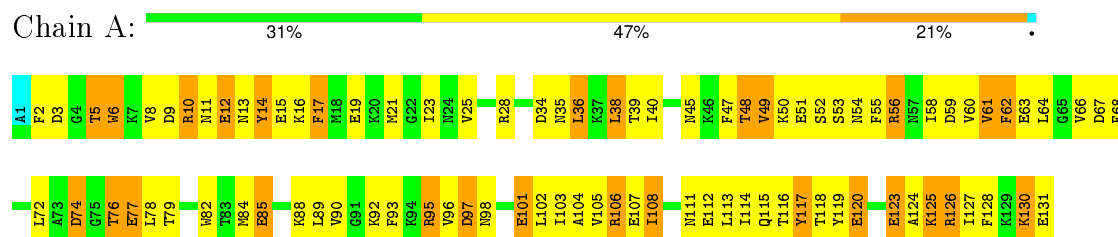
Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	O
			49	16	31	2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

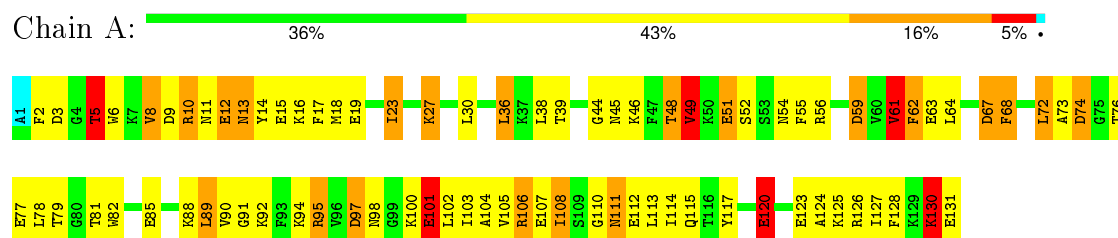


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

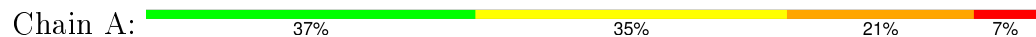
4.2.1 Score per residue for model 1

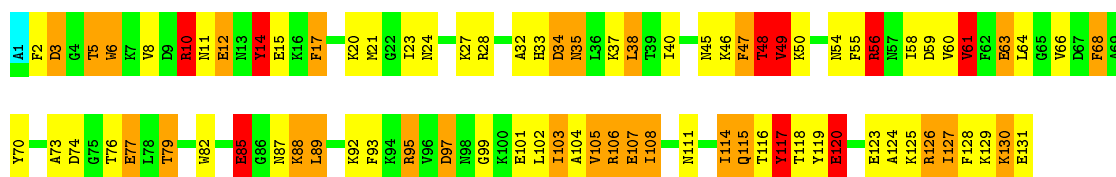
- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



4.2.2 Score per residue for model 2

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

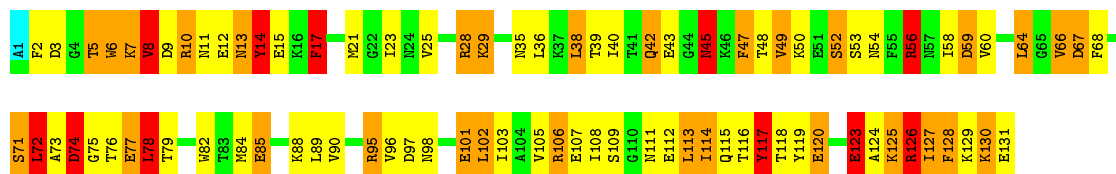




4.2.3 Score per residue for model 3

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

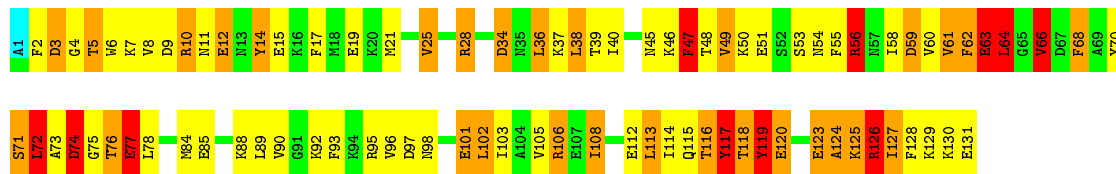
Chain A: 32% 36% 23% 8%



4.2.4 Score per residue for model 4

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

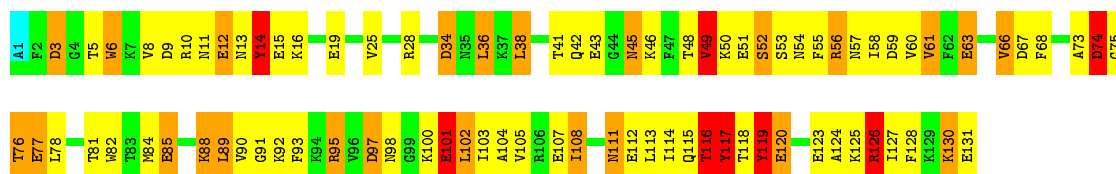
Chain A: 32% 37% 22% 8%



4.2.5 Score per residue for model 5

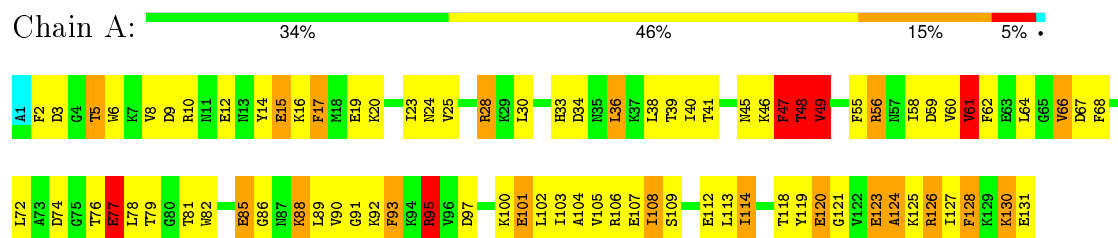
- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN

Chain A: 34% 41% 18% 6%



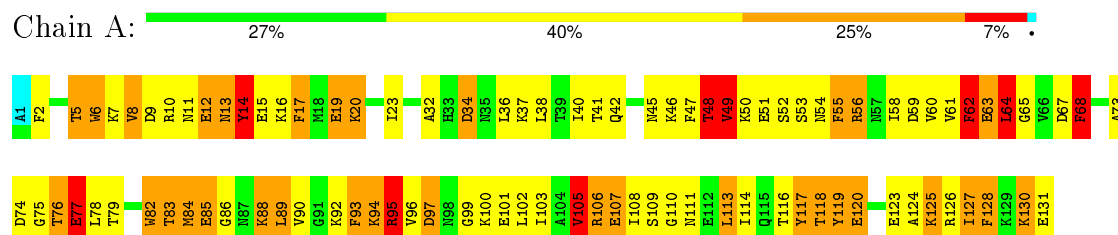
4.2.6 Score per residue for model 6

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



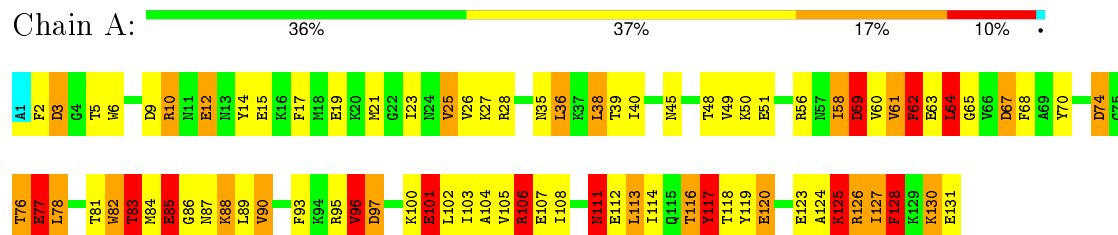
4.2.7 Score per residue for model 7

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



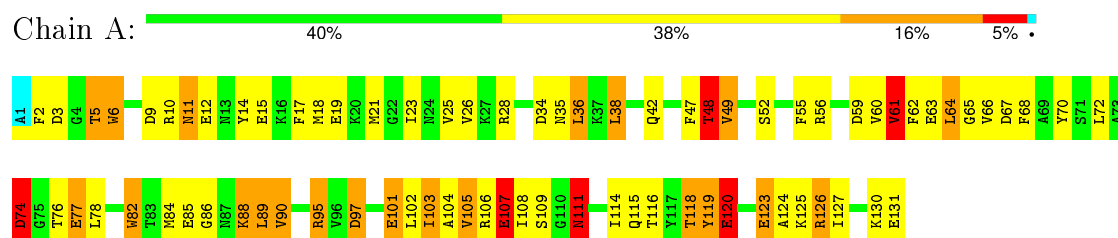
4.2.8 Score per residue for model 8

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



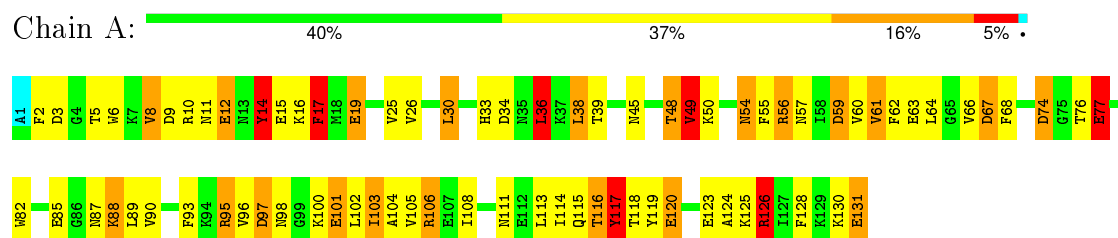
4.2.9 Score per residue for model 9

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



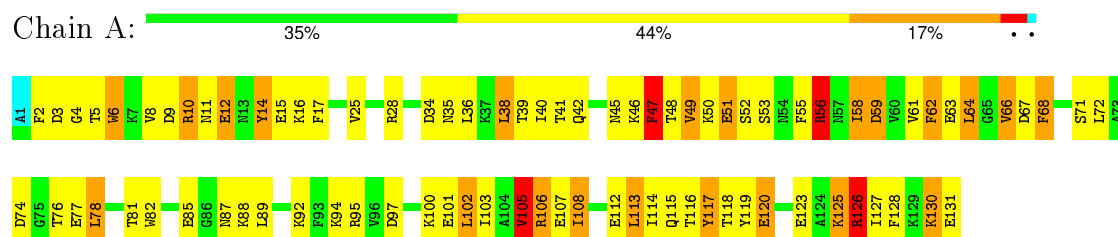
4.2.10 Score per residue for model 10

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



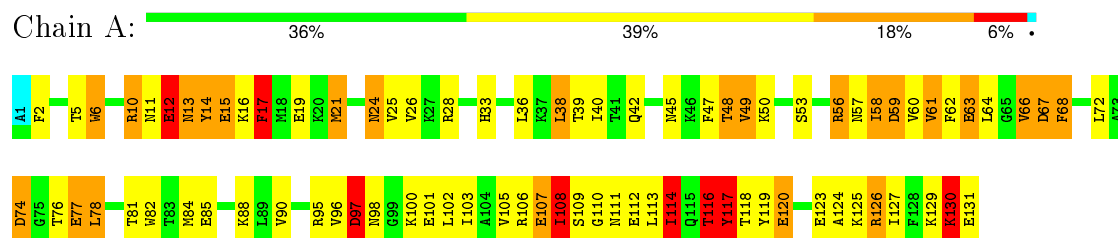
4.2.11 Score per residue for model 11

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



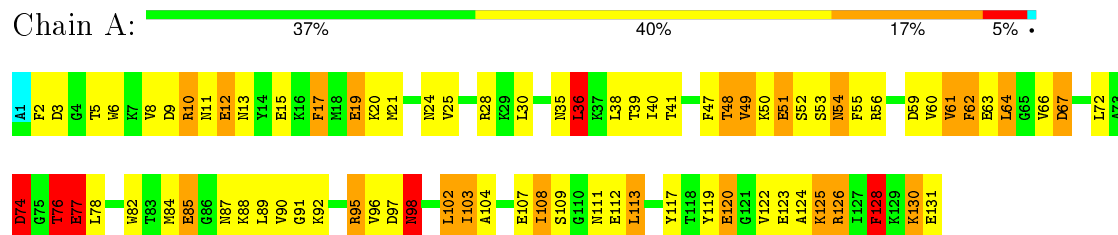
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



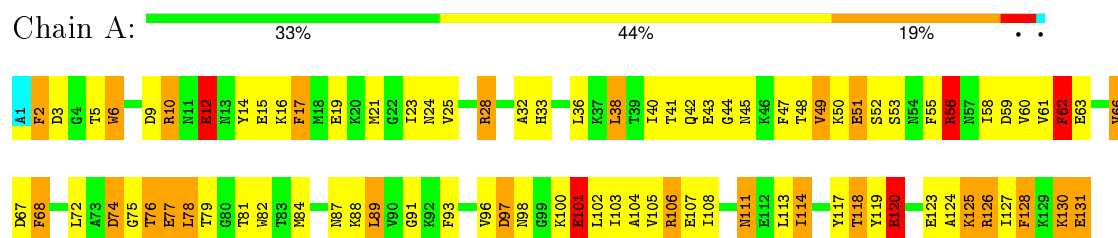
4.2.13 Score per residue for model 13

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



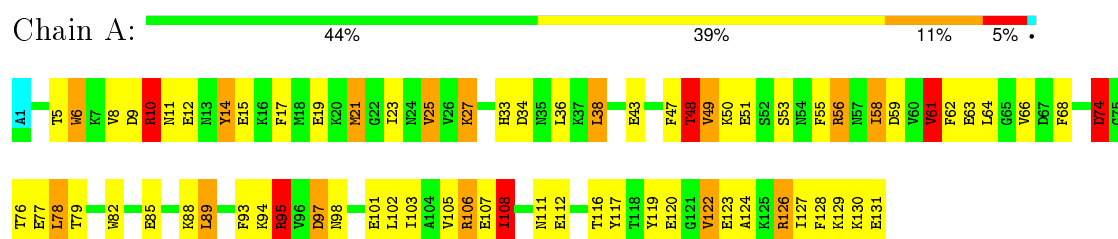
4.2.14 Score per residue for model 14

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



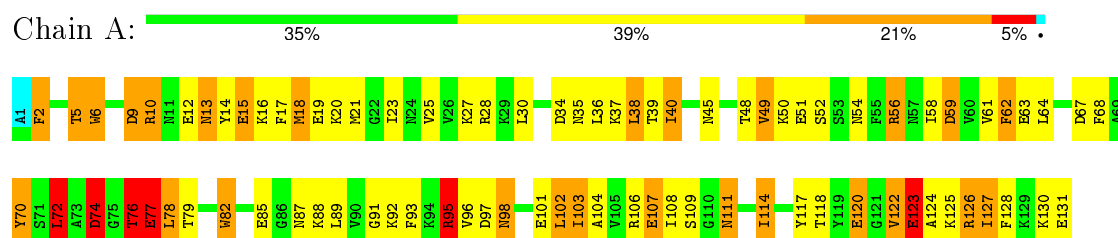
4.2.15 Score per residue for model 15

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



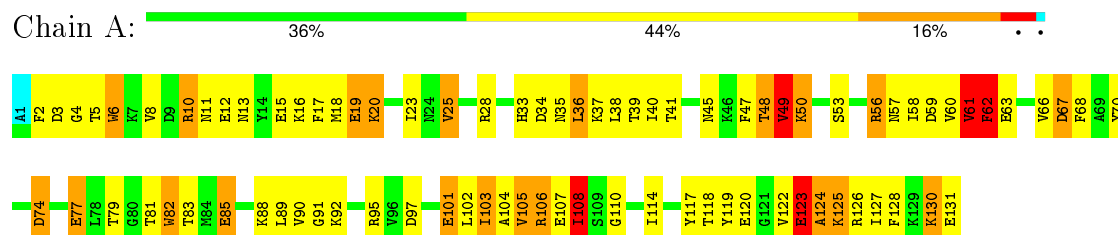
4.2.16 Score per residue for model 16

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



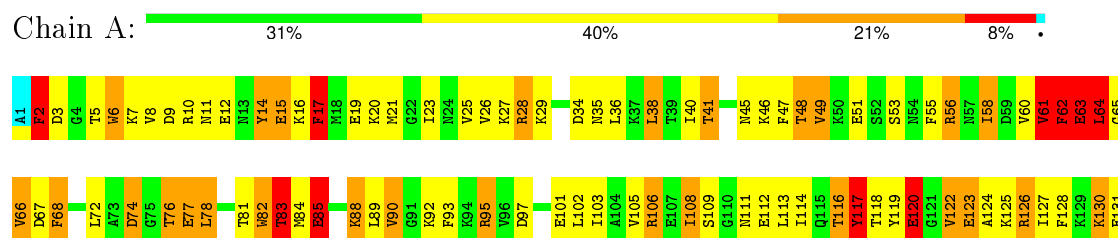
4.2.17 Score per residue for model 17

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



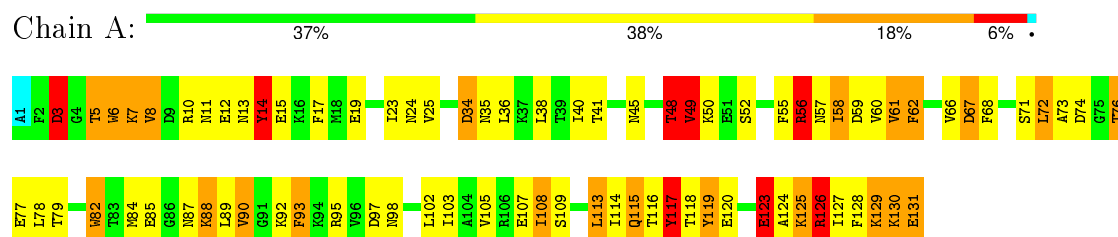
4.2.18 Score per residue for model 18

- Molecule 1: INTESTINAL FATTY ACID-BINDING PROTEIN



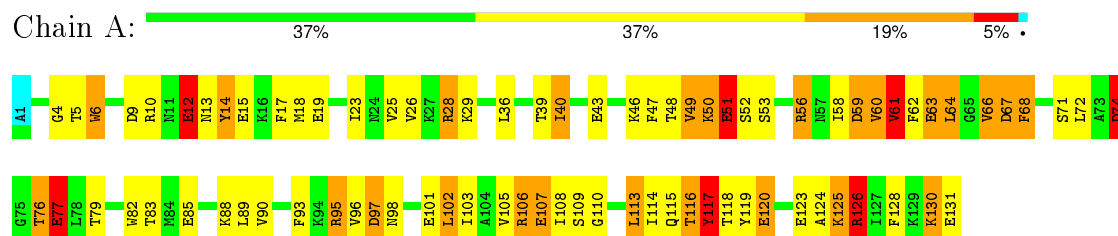
4.2.19 Score per residue for model 19

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

6 Model quality i

6.1 Standard geometry i

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	1.08±0.02	11±1/1068 (1.0±0.1%)	2.10±0.07	34±4/1429 (2.4±0.3%)
All	All	1.08	215/21360 (1.0%)	2.10	677/28580 (2.4%)

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

Mol	Chain	Chirality	Planarity
1	A	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	123	GLU	CD-OE2	7.58	1.33	1.25	14	16
1	A	15	GLU	CD-OE2	7.33	1.33	1.25	8	10
1	A	15	GLU	CD-OE1	7.31	1.33	1.25	14	10
1	A	131	GLU	CD-OE1	7.26	1.33	1.25	15	11
1	A	77	GLU	CD-OE2	7.20	1.33	1.25	5	14
1	A	77	GLU	CD-OE1	7.19	1.33	1.25	15	6
1	A	12	GLU	CD-OE2	7.18	1.33	1.25	2	7
1	A	12	GLU	CD-OE1	7.17	1.33	1.25	6	12
1	A	131	GLU	CD-OE2	7.04	1.33	1.25	3	9
1	A	19	GLU	CD-OE2	6.94	1.33	1.25	10	12
1	A	101	GLU	CD-OE2	6.83	1.33	1.25	3	8
1	A	120	GLU	CD-OE1	6.80	1.33	1.25	17	8
1	A	120	GLU	CD-OE2	6.80	1.33	1.25	10	10
1	A	85	GLU	CD-OE2	6.68	1.32	1.25	4	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	63	GLU	CD-OE1	6.67	1.32	1.25	15	6
1	A	123	GLU	CD-OE1	6.58	1.32	1.25	8	4
1	A	107	GLU	CD-OE1	6.53	1.32	1.25	2	5
1	A	107	GLU	CD-OE2	6.51	1.32	1.25	19	11
1	A	101	GLU	CD-OE1	6.38	1.32	1.25	20	5
1	A	85	GLU	CD-OE1	6.37	1.32	1.25	17	4
1	A	63	GLU	CD-OE2	6.33	1.32	1.25	2	9
1	A	19	GLU	CD-OE1	6.18	1.32	1.25	13	5
1	A	112	GLU	CD-OE2	6.12	1.32	1.25	4	4
1	A	112	GLU	CD-OE1	5.99	1.32	1.25	15	3
1	A	51	GLU	CD-OE2	5.73	1.31	1.25	13	6
1	A	43	GLU	CD-OE1	5.64	1.31	1.25	5	3
1	A	51	GLU	CD-OE1	5.58	1.31	1.25	15	3
1	A	43	GLU	CD-OE2	5.05	1.31	1.25	15	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	18.85	129.72	120.30	3	19
1	A	126	ARG	NE-CZ-NH1	18.74	129.67	120.30	8	18
1	A	10	ARG	NE-CZ-NH2	-16.46	112.07	120.30	16	17
1	A	56	ARG	NE-CZ-NH1	15.07	127.84	120.30	6	12
1	A	10	ARG	NE-CZ-NH1	14.62	127.61	120.30	3	14
1	A	28	ARG	NE-CZ-NH1	14.57	127.59	120.30	14	7
1	A	56	ARG	NE-CZ-NH2	-12.73	113.93	120.30	6	16
1	A	74	ASP	CB-CG-OD1	12.19	129.27	118.30	8	18
1	A	74	ASP	CB-CG-OD2	-11.64	107.82	118.30	3	18
1	A	97	ASP	CB-CG-OD1	11.53	128.68	118.30	4	16
1	A	95	ARG	NE-CZ-NH2	-10.91	114.85	120.30	5	15
1	A	59	ASP	CB-CG-OD2	-10.22	109.11	118.30	17	16
1	A	119	TYR	CB-CG-CD1	9.95	126.97	121.00	5	2
1	A	17	PHE	CB-CG-CD1	9.92	127.74	120.80	10	3
1	A	9	ASP	CB-CG-OD2	9.67	127.00	118.30	9	14
1	A	34	ASP	CB-CG-OD1	9.56	126.90	118.30	11	8
1	A	117	TYR	CB-CG-CD1	-9.27	115.44	121.00	2	3
1	A	59	ASP	CB-CG-OD1	-9.25	109.97	118.30	10	14
1	A	95	ARG	NE-CZ-NH1	-9.16	115.72	120.30	3	13
1	A	106	ARG	NE-CZ-NH1	9.13	124.86	120.30	20	12
1	A	56	ARG	CD-NE-CZ	8.86	136.01	123.60	16	19
1	A	97	ASP	CB-CG-OD2	8.85	126.27	118.30	10	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	117	TYR	CB-CG-CD2	-8.75	115.75	121.00	18	4
1	A	131	GLU	N-CA-CB	8.72	126.30	110.60	18	20
1	A	70	TYR	CB-CG-CD1	-8.69	115.78	121.00	16	2
1	A	3	ASP	CB-CG-OD2	-8.69	110.48	118.30	10	6
1	A	62	PHE	CB-CG-CD1	8.67	126.87	120.80	8	6
1	A	14	TYR	CB-CG-CD1	-8.60	115.84	121.00	2	7
1	A	106	ARG	NE-CZ-NH2	8.39	124.49	120.30	18	1
1	A	82	TRP	CD1-NE1-CE2	8.29	116.46	109.00	7	3
1	A	9	ASP	CB-CG-OD1	-8.27	110.86	118.30	1	13
1	A	3	ASP	CB-CG-OD1	-8.16	110.96	118.30	18	6
1	A	82	TRP	CD1-CG-CD2	8.12	112.80	106.30	7	3
1	A	14	TYR	CB-CG-CD2	-8.09	116.14	121.00	15	5
1	A	28	ARG	NE-CZ-NH2	-7.88	116.36	120.30	2	8
1	A	68	PHE	CB-CG-CD1	-7.68	115.42	120.80	7	1
1	A	82	TRP	CG-CD1-NE1	-7.59	102.51	110.10	7	4
1	A	67	ASP	CB-CG-OD1	7.58	125.13	118.30	20	5
1	A	47	PHE	CB-CG-CD1	7.53	126.07	120.80	4	1
1	A	5	THR	CA-CB-CG2	7.50	122.90	112.40	10	8
1	A	28	ARG	CD-NE-CZ	7.26	133.76	123.60	14	1
1	A	88	LYS	CB-CA-C	-7.19	96.02	110.40	2	17
1	A	66	VAL	CA-CB-CG1	7.18	121.67	110.90	10	13
1	A	76	THR	O-C-N	7.01	133.92	122.70	4	3
1	A	49	VAL	CB-CA-C	6.95	124.60	111.40	18	7
1	A	55	PHE	CB-CG-CD1	-6.89	115.97	120.80	9	1
1	A	79	THR	CA-CB-CG2	6.82	121.95	112.40	14	4
1	A	2	PHE	CB-CG-CD1	-6.78	116.05	120.80	18	1
1	A	58	ILE	CA-CB-CG2	6.77	124.45	110.90	15	6
1	A	6	TRP	CG-CD2-CE3	-6.71	127.86	133.90	20	8
1	A	6	TRP	CD1-CG-CD2	-6.67	100.96	106.30	17	9
1	A	5	THR	N-CA-CB	6.66	122.95	110.30	6	8
1	A	85	GLU	N-CA-CB	6.56	122.41	110.60	3	9
1	A	82	TRP	CE2-CD2-CG	-6.51	102.09	107.30	9	4
1	A	82	TRP	CB-CG-CD1	-6.45	118.61	127.00	8	3
1	A	17	PHE	CB-CG-CD2	-6.44	116.29	120.80	10	3
1	A	125	LYS	CB-CA-C	-6.44	97.52	110.40	3	9
1	A	67	ASP	CB-CG-OD2	-6.40	112.54	118.30	8	6
1	A	48	THR	N-CA-CB	6.40	122.45	110.30	7	12
1	A	62	PHE	CB-CG-CD2	-6.39	116.33	120.80	7	4
1	A	93	PHE	CB-CG-CD1	-6.36	116.35	120.80	19	3
1	A	85	GLU	CB-CA-C	6.28	122.95	110.40	18	10
1	A	77	GLU	OE1-CD-OE2	6.21	130.75	123.30	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	14	TYR	CG-CD2-CE2	-6.21	116.33	121.30	2	1
1	A	52	SER	N-CA-CB	-6.11	101.34	110.50	1	4
1	A	128	PHE	CB-CG-CD1	-6.09	116.54	120.80	13	2
1	A	6	TRP	CE2-CD2-CG	6.07	112.16	107.30	17	5
1	A	56	ARG	CB-CG-CD	6.04	127.31	111.60	13	7
1	A	47	PHE	CB-CG-CD2	-6.04	116.57	120.80	6	4
1	A	111	ASN	N-CA-CB	6.04	121.47	110.60	9	10
1	A	14	TYR	CD1-CG-CD2	6.01	124.52	117.90	2	1
1	A	95	ARG	N-CA-CB	-6.01	99.78	110.60	1	8
1	A	106	ARG	CD-NE-CZ	6.01	132.01	123.60	14	3
1	A	61	VAL	CA-CB-CG1	5.99	119.89	110.90	17	2
1	A	79	THR	CA-CB-OG1	5.99	121.58	109.00	16	4
1	A	95	ARG	CB-CG-CD	-5.94	96.16	111.60	6	3
1	A	119	TYR	CG-CD1-CE1	5.93	126.05	121.30	4	1
1	A	19	GLU	CG-CD-OE1	-5.92	106.46	118.30	13	1
1	A	126	ARG	O-C-N	5.90	132.14	122.70	8	4
1	A	126	ARG	NH1-CZ-NH2	-5.86	112.95	119.40	11	3
1	A	131	GLU	OE1-CD-OE2	5.80	130.26	123.30	9	3
1	A	101	GLU	C-N-CA	5.80	136.19	121.70	17	2
1	A	116	THR	O-C-N	5.75	131.89	122.70	12	2
1	A	26	VAL	N-CA-CB	5.68	123.99	111.50	10	2
1	A	76	THR	N-CA-CB	5.68	121.09	110.30	16	1
1	A	114	ILE	CB-CA-C	-5.61	100.38	111.60	14	6
1	A	117	TYR	N-CA-CB	5.61	120.69	110.60	18	8
1	A	62	PHE	CG-CD1-CE1	5.56	126.91	120.80	19	1
1	A	49	VAL	CA-CB-CG1	5.55	119.22	110.90	19	4
1	A	122	VAL	CG1-CB-CG2	-5.54	102.04	110.90	16	2
1	A	101	GLU	O-C-N	5.53	131.55	122.70	16	1
1	A	34	ASP	CB-CG-OD2	5.51	123.26	118.30	17	3
1	A	119	TYR	CZ-CE2-CD2	5.48	124.73	119.80	4	1
1	A	112	GLU	OE1-CD-OE2	5.47	129.87	123.30	5	1
1	A	6	TRP	CG-CD1-NE1	5.46	115.56	110.10	3	1
1	A	93	PHE	CB-CG-CD2	-5.45	116.99	120.80	6	1
1	A	5	THR	OG1-CB-CG2	5.41	122.44	110.00	16	3
1	A	119	TYR	CB-CG-CD2	5.39	124.24	121.00	9	2
1	A	67	ASP	CB-CA-C	-5.38	99.65	110.40	17	3
1	A	6	TRP	CB-CG-CD1	5.37	133.98	127.00	16	2
1	A	117	TYR	O-C-N	5.37	131.29	122.70	1	1
1	A	128	PHE	N-CA-CB	5.36	120.25	110.60	3	3
1	A	15	GLU	CG-CD-OE1	5.36	129.02	118.30	5	1
1	A	35	ASN	N-CA-CB	5.35	120.24	110.60	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	112	GLU	CG-CD-OE2	-5.31	107.67	118.30	13	2
1	A	47	PHE	CB-CA-C	-5.29	99.82	110.40	2	2
1	A	68	PHE	CB-CG-CD2	-5.28	117.11	120.80	3	2
1	A	78	LEU	N-CA-CB	-5.28	99.85	110.40	4	2
1	A	6	TRP	NE1-CE2-CD2	-5.25	102.05	107.30	11	1
1	A	66	VAL	CB-CA-C	5.24	121.36	111.40	19	3
1	A	123	GLU	OE1-CD-OE2	5.22	129.57	123.30	10	1
1	A	123	GLU	CG-CD-OE2	-5.22	107.86	118.30	5	1
1	A	61	VAL	N-CA-CB	5.22	122.98	111.50	20	1
1	A	105	VAL	CG1-CB-CG2	-5.11	102.72	110.90	11	2
1	A	11	ASN	CB-CA-C	-5.09	100.21	110.40	13	1
1	A	15	GLU	CG-CD-OE2	5.08	128.45	118.30	3	1
1	A	19	GLU	CG-CD-OE2	-5.06	108.17	118.30	1	1
1	A	115	GLN	O-C-N	5.05	130.78	122.70	2	1
1	A	129	LYS	N-CA-CB	-5.05	101.51	110.60	4	1
1	A	112	GLU	CG-CD-OE1	-5.03	108.23	118.30	5	1
1	A	45	ASN	N-CA-CB	5.03	119.64	110.60	3	1
1	A	117	TYR	CG-CD1-CE1	-5.00	117.30	121.30	20	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	62±18
2	A	18	31	31	2±2
All	All	21400	21620	21600	1234

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 29.

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:N	1:A:72:LEU:HD22	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:82:TRP:CG	1:A:83:THR:N	0.78	2.50	7	3
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: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: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:48:THR:HA	1:A:61:VAL:HA	0.74	1.57	4	7
1:A:36:LEU:HD11	1:A:38:LEU:CD1	0.74	2.12	6	5
1:A:114:ILE:HG12	1:A:127:ILE:HD13	0.74	1.60	7	2
1:A:72:LEU:N	1:A:72:LEU:HD13	0.74	1.97	3	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: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
1:A:56:ARG:HB2	1:A:58:ILE:HG22	0.70	1.61	18	6
1:A:89:LEU:HD23	1:A:106:ARG:HH11	0.70	1.45	1	1
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:CD2	1:A:72:LEU:N	0.69	2.54	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:7:LYS:O	1:A:8:VAL:HG12	0.67	1.90	3	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:11:ASN:HB3	1:A:14:TYR:CE1	0.67	2.25	2	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: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: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
1:A:62:PHE:CE1	1:A:82:TRP:CZ2	0.64	2.85	12	3
1:A:62:PHE:CE2	1:A:82:TRP:CD1	0.64	2.85	9	2
1:A:7:LYS:HB3	1:A:128:PHE:CZ	0.64	2.28	3	2
1:A:7:LYS:CB	1:A:128:PHE:CZ	0.64	2.80	19	1
1:A:7:LYS:N	1:A:128:PHE:CE2	0.64	2.65	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: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:114:ILE:HG23	1:A:127:ILE:HG12	0.63	1.70	9	2
1:A:62:PHE:CD1	1:A:68:PHE:CD1	0.63	2.87	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ASP:HB3	2:A:132:PLM:HG1	0.63	1.69	15	1
1:A:72:LEU:HD11	1:A:78:LEU:HD13	0.63	1.70	11	1
1:A:93:PHE:CB	1:A:102:LEU:HD23	0.63	2.22	2	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: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:HG3	1:A:28:ARG:HH11	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:68:PHE:N	1:A:68:PHE:CD1	0.61	2.69	7	2
1:A:90:VAL:HG12	1:A:105:VAL:HG23	0.61	1.73	17	2
1:A:82:TRP:CD1	1:A:82:TRP:C	0.61	2.72	18	2
1:A:48:THR:CG2	1:A:61:VAL:HG22	0.61	2.26	20	1
1:A:60:VAL:HG11	2:A:132:PLM:C2	0.61	2.25	13	2
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:90:VAL:HG12	1:A:105:VAL:HG22	0.61	1.73	6	1
1:A:62:PHE:CE2	1:A:68:PHE:CE2	0.61	2.89	10	2
1:A:106:ARG:HH11	1:A:106:ARG:HG2	0.60	1.55	3	2
1:A:38:LEU:HD22	1:A:128:PHE:CE2	0.60	2.31	17	4
1:A:6:TRP:CE3	1:A:113:LEU:HB3	0.60	2.32	19	2
1:A:62:PHE:CG	1:A:68:PHE:CE1	0.60	2.90	10	1
1:A:62:PHE:CZ	1:A:68:PHE:CD2	0.60	2.89	10	2
1:A:77:GLU:CB	1:A:96:VAL:HG22	0.60	2.27	13	3
1:A:76:THR:HG23	1:A:77:GLU:N	0.60	2.11	8	1
1:A:95:ARG:HE	1:A:100:LYS:N	0.60	1.94	7	1
1:A:36:LEU:HD11	1:A:38:LEU:HD13	0.60	1.73	6	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:82:TRP:CD1	0.59	2.71	8	1
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:60:VAL:CG1	1:A:62:PHE:CE2	0.58	2.86	4	3
1:A:6:TRP:HE1	1:A:40:ILE:HD12	0.58	1.59	6	2
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:89:LEU:HD13	1:A:106:ARG:HH11	0.58	1.58	9	1
1:A:114:ILE:HD12	1:A:127:ILE:HG12	0.58	1.76	6	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:48:THR:CB	1:A:61:VAL:HG12	0.57	2.29	5	5
1:A:36:LEU:O	1:A:36:LEU:HD23	0.57	2.00	8	2
1:A:113:LEU:HD23	1:A:113:LEU:C	0.57	2.19	3	1
1:A:2:PHE:CE1	1:A:108:ILE:HD12	0.57	2.34	4	1
1:A:62:PHE:CB	1:A:68:PHE:CZ	0.57	2.88	11	3
1:A:48:THR:HG22	1:A:61:VAL:HG11	0.57	1.76	6	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:65:GLY:N	1:A:82:TRP:CD1	0.57	2.73	18	3
1:A:14:TYR:CD2	1:A:126:ARG:CG	0.57	2.88	12	3
1:A:78:LEU:C	1:A:78:LEU:HD23	0.57	2.20	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:THR:HB	1:A:48:THR:HG23	0.57	1.77	11	2
1:A:105:VAL:HG12	1:A:116:THR:OG1	0.57	2.00	15	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: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:8:VAL:N	1:A:128:PHE:CD1	0.56	2.73	19	2
1:A:103:ILE:N	1:A:118:THR:O	0.56	2.39	5	12
1:A:82:TRP:CH2	1:A:84:MET:CB	0.56	2.88	18	2
1:A:49:VAL:HG11	2:A:132:PLM:O1	0.56	2.00	3	1
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: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
1:A:118:THR:HG23	1:A:119:TYR:N	0.56	2.16	5	2
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:77:GLU:HB2	1:A:96:VAL:HG22	0.56	1.77	13	2
1:A:46:LYS:CG	1:A:47:PHE:N	0.56	2.65	4	1
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: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:6:TRP:CZ3	1:A:113:LEU:CB	0.55	2.90	19	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:82:TRP:C	1:A:83:THR:HG22	0.55	2.23	8	2
1:A:72:LEU:H	1:A:72:LEU:HD22	0.55	1.58	16	1
1:A:21:MET:CE	1:A:119:TYR:CD1	0.55	2.89	12	1
1:A:14:TYR:CE1	1:A:17:PHE:CD2	0.55	2.95	12	2
1:A:49:VAL:CG1	1:A:62:PHE:CZ	0.55	2.89	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:TRP:CD1	1:A:40:ILE:HD12	0.55	2.36	2	3
1:A:95:ARG:C	1:A:95:ARG:HD2	0.54	2.21	7	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:38:LEU:HD12	1:A:128:PHE:CZ	0.54	2.38	5	1
1:A:14:TYR:CE2	1:A:126:ARG:HG2	0.54	2.37	4	4
1:A:13:ASN:ND2	1:A:17:PHE:CG	0.54	2.76	17	2
1:A:6:TRP:CZ3	1:A:113:LEU:HB2	0.54	2.38	19	3
1:A:105:VAL:HG13	1:A:107:GLU:HG2	0.53	1.79	12	1
1:A:38:LEU:HD23	1:A:49:VAL:CG2	0.53	2.33	5	1
1:A:14:TYR:CA	1:A:124:ALA:HA	0.53	2.32	2	1
1:A:47:PHE:HB3	1:A:62:PHE:CE1	0.53	2.38	12	1
1:A:105:VAL:HB	1:A:117:TYR:CE2	0.53	2.38	10	9
1:A:93:PHE:CZ	2:A:132:PLM:H41	0.53	2.39	18	1
1:A:64:LEU:HB2	1:A:82:TRP:CZ2	0.53	2.39	18	3
1:A:45:ASN:ND2	1:A:45:ASN:N	0.53	2.55	5	1
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: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:6:TRP:C	1:A:128:PHE:CE2	0.53	2.83	19	1
1:A:46:LYS:CB	1:A:63:GLU:CA	0.53	2.87	4	1
1:A:105:VAL:HG13	1:A:107:GLU:CG	0.53	2.33	12	1
1:A:62:PHE:HB2	1:A:68:PHE:CZ	0.53	2.38	1	1
1:A:78:LEU:HD12	1:A:102:LEU:HD23	0.53	1.81	16	1
1:A:6:TRP:CZ2	1:A:108:ILE:CD1	0.53	2.92	3	2
1:A:62:PHE:CE2	1:A:68:PHE:CD2	0.52	2.97	4	1
1:A:119:TYR:C	1:A:119:TYR:CD1	0.52	2.83	4	2
1:A:17:PHE:CD2	1:A:122:VAL:HA	0.52	2.40	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:LEU:HA	1:A:119:TYR:CA	0.52	2.33	4	1
1:A:102:LEU:CB	1:A:119:TYR:HA	0.52	2.35	4	7
1:A:62:PHE:CE2	2:A:132:PLM:H22	0.52	2.39	7	1
1:A:113:LEU:C	1:A:113:LEU:HD23	0.52	2.25	19	1
1:A:46:LYS:CB	1:A:62:PHE:C	0.52	2.78	4	1
1:A:95:ARG:CD	1:A:95:ARG:C	0.52	2.77	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:114:ILE:CG1	1:A:127:ILE:CD1	0.52	2.87	14	2
1:A:113:LEU:HD22	1:A:128:PHE:CE2	0.52	2.39	1	2
1:A:38:LEU:HD22	1:A:128:PHE:HE2	0.52	1.65	13	1
1:A:14:TYR:CE2	1:A:126:ARG:HD2	0.51	2.40	12	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:62:PHE:CE1	1:A:82:TRP:CE2	0.51	2.98	12	1
1:A:64:LEU:CB	1:A:82:TRP:CZ2	0.51	2.93	18	3
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:82:TRP:CZ3	1:A:84:MET:HB2	0.51	2.40	8	3
1:A:38:LEU:HD12	1:A:128:PHE:CE2	0.51	2.40	7	2
1:A:61:VAL:O	1:A:62:PHE:CD1	0.51	2.64	4	1
1:A:64:LEU:C	1:A:82:TRP:NE1	0.51	2.64	18	3
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:116:THR:O	1:A:117:TYR:CG	0.51	2.64	18	5
1:A:14:TYR:HE2	1:A:32:ALA:HB1	0.51	1.63	7	1
1:A:115:GLN:O	1:A:126:ARG:N	0.51	2.44	2	3
1:A:48:THR:HB	1:A:61:VAL:HB	0.51	1.82	4	2
1:A:72:LEU:H	1:A:72:LEU:HD13	0.51	1.66	3	1
1:A:8:VAL:HG11	1:A:36:LEU:HD23	0.51	1.82	19	1
1:A:38:LEU:HD23	1:A:49:VAL:HG21	0.51	1.81	5	1
1:A:14:TYR:CD2	1:A:126:ARG:HG2	0.51	2.41	5	3
1:A:30:LEU:HD22	1:A:33:HIS:CE1	0.51	2.40	10	1
1:A:127:ILE:HD13	1:A:127:ILE:N	0.51	2.20	16	1
1:A:72:LEU:HD23	2:A:132:PLM:HB2	0.51	1.83	6	1
2:A:132:PLM:C1	2:A:132:PLM:C5	0.51	2.89	7	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:104:ALA:HA	1:A:116:THR:O	0.51	2.06	2	1
1:A:14:TYR:CE2	1:A:32:ALA:CB	0.51	2.94	2	1
1:A:123:GLU:O	1:A:124:ALA:HB2	0.50	2.06	17	3
1:A:2:PHE:CZ	1:A:108:ILE:CG1	0.50	2.94	16	1
1:A:23:ILE:HD12	2:A:132:PLM:HG1	0.50	1.82	3	1
1:A:62:PHE:CE1	1:A:82:TRP:CH2	0.50	2.98	12	1
1:A:2:PHE:CZ	1:A:108:ILE:HG13	0.50	2.41	12	1
1:A:14:TYR:N	1:A:124:ALA:HA	0.50	2.20	2	1
1:A:113:LEU:HD21	1:A:115:GLN:CG	0.50	2.34	3	1
1:A:42:GLN:HG2	1:A:47:PHE:CE1	0.50	2.41	3	1
1:A:105:VAL:N	1:A:116:THR:O	0.50	2.44	4	6
1:A:8:VAL:CG1	1:A:36:LEU:HB3	0.50	2.37	3	2
1:A:48:THR:HB	1:A:61:VAL:CB	0.50	2.37	4	1
1:A:8:VAL:HB	1:A:128:PHE:CD1	0.50	2.42	10	6
1:A:115:GLN:HB2	1:A:126:ARG:HD2	0.50	1.83	11	1
1:A:2:PHE:CD1	1:A:2:PHE:N	0.50	2.80	6	2
1:A:17:PHE:CE2	1:A:118:THR:HA	0.50	2.41	10	1
1:A:92:LYS:C	1:A:93:PHE:CD1	0.50	2.85	19	2
1:A:102:LEU:CG	1:A:119:TYR:HA	0.50	2.37	11	3
1:A:11:ASN:CG	1:A:14:TYR:CE2	0.50	2.85	2	1
1:A:102:LEU:HD12	1:A:118:THR:O	0.50	2.06	2	1
1:A:55:PHE:CZ	2:A:132:PLM:HF2	0.50	2.42	14	2
1:A:49:VAL:HG11	2:A:132:PLM:H22	0.50	1.82	17	1
1:A:23:ILE:CG2	1:A:28:ARG:N	0.50	2.75	6	2
1:A:46:LYS:CB	1:A:63:GLU:N	0.50	2.75	4	1
1:A:38:LEU:HD11	2:A:132:PLM:O2	0.50	2.06	15	1
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:2:PHE:N	1:A:2:PHE:CD1	0.49	2.77	1	2
1:A:65:GLY:N	1:A:82:TRP:HE1	0.49	2.03	7	1
1:A:49:VAL:O	1:A:60:VAL:HG23	0.49	2.07	6	2
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:63:GLU:O	1:A:65:GLY:N	0.49	2.45	7	1
1:A:6:TRP:CA	1:A:128:PHE:CE2	0.49	2.95	19	2
1:A:36:LEU:HD13	1:A:51:GLU:OE2	0.49	2.08	1	1
1:A:113:LEU:HD23	1:A:128:PHE:CD1	0.49	2.42	20	1
1:A:105:VAL:HG21	1:A:117:TYR:CE2	0.49	2.43	19	1
1:A:75:GLY:C	1:A:76:THR:HG23	0.49	2.27	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:2:PHE:CZ	1:A:108:ILE:HG21	0.49	2.42	7	1
1:A:6:TRP:CH2	1:A:130:LYS:HG3	0.49	2.42	17	4
1:A:82:TRP:CE3	1:A:91:GLY:N	0.49	2.80	13	1
1:A:92:LYS:CG	1:A:103:ILE:CD1	0.49	2.90	11	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:68:PHE:CD1	1:A:68:PHE:N	0.49	2.81	15	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:HD23	1:A:78:LEU:O	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
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:46:LYS:HZ2	1:A:89:LEU:HD21	0.48	1.69	4	1
1:A:48:THR:HA	1:A:61:VAL:CA	0.48	2.36	4	1
1:A:42:GLN:NE2	1:A:47:PHE:CE2	0.48	2.81	14	2
1:A:76:THR:CG2	1:A:77:GLU:N	0.48	2.76	8	1
1:A:47:PHE:O	1:A:49:VAL:N	0.48	2.46	2	3
1:A:7:LYS:C	1:A:128:PHE:CE1	0.48	2.86	19	1
1:A:75:GLY:O	1:A:76:THR:HG22	0.48	2.06	7	2
1:A:114:ILE:HG23	1:A:127:ILE:HA	0.48	1.86	2	1
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:95:ARG:NE	1:A:100:LYS:N	0.48	2.61	7	1
1:A:77:GLU:HG2	1:A:96:VAL:HG21	0.48	1.85	7	2
1:A:115:GLN:HB2	1:A:126:ARG:CD	0.48	2.39	4	4
1:A:98:ASN:N	1:A:98:ASN:ND2	0.48	2.57	13	1
1:A:20:LYS:CE	1:A:120:GLU:CB	0.48	2.92	6	1
1:A:89:LEU:HD12	1:A:106:ARG:HD2	0.48	1.86	15	1
1:A:27:LYS:HD2	1:A:74:ASP:CB	0.48	2.39	16	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:115:GLN:O	1:A:116:THR:HG22	0.48	2.09	20	1
1:A:115:GLN:HB2	1:A:126:ARG:CG	0.48	2.39	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:HG23	1:A:27:LYS:HB3	0.48	1.85	16	1
1:A:49:VAL:HB	1:A:62:PHE:CE1	0.48	2.42	6	1
1:A:62:PHE:CG	1:A:68:PHE:CD1	0.48	3.02	10	2
1:A:96:VAL:CG2	1:A:97:ASP:N	0.48	2.77	12	1
1:A:75:GLY:HA3	1:A:78:LEU:CD1	0.48	2.38	3	1
1:A:56:ARG:CB	1:A:58:ILE:CG2	0.48	2.92	18	1
1:A:82:TRP:CD2	1:A:83:THR:CA	0.47	2.97	7	1
1:A:13:ASN:CG	1:A:17:PHE:CE2	0.47	2.88	17	1
1:A:16:LYS:HB3	1:A:17:PHE:CE2	0.47	2.44	17	1
1:A:115:GLN:C	1:A:116:THR:CG2	0.47	2.82	11	3
1:A:23:ILE:HD11	1:A:74:ASP:CB	0.47	2.38	20	1
1:A:6:TRP:HB3	1:A:128:PHE:CD2	0.47	2.44	18	2
1:A:36:LEU:HG	1:A:38:LEU:CD1	0.47	2.39	19	1
1:A:47:PHE:CZ	1:A:64:LEU:HD21	0.47	2.45	9	1
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: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:62:PHE:HB3	1:A:68:PHE:CZ	0.47	2.43	7	4
1:A:119:TYR:O	1:A:119:TYR:CG	0.47	2.68	2	3
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:51:GLU:O	1:A:53:SER:N	0.47	2.47	5	5
1:A:122:VAL:HG23	1:A:122:VAL:O	0.47	2.08	16	1
1:A:106:ARG:NH2	2:A:132:PLM:O1	0.47	2.47	3	4
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:56:ARG:HH21	1:A:58:ILE:HD12	0.47	1.69	11	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:95:ARG:CZ	1:A:99:GLY:CA	0.47	2.92	7	1
1:A:77:GLU:CB	1:A:96:VAL:HB	0.47	2.40	7	2
1:A:89:LEU:CD1	1:A:106:ARG:HH11	0.47	2.22	9	1
1:A:64:LEU:HA	1:A:82:TRP:CD1	0.47	2.45	8	2
1:A:17:PHE:HB3	1:A:122:VAL:CB	0.47	2.39	16	1
1:A:114:ILE:HG12	1:A:127:ILE:CD1	0.47	2.39	14	1
1:A:14:TYR:CE2	1:A:126:ARG:HD3	0.47	2.45	4	1
1:A:82:TRP:CZ3	1:A:106:ARG:NE	0.47	2.82	3	2
1:A:77:GLU:HG2	1:A:96:VAL:CG2	0.47	2.39	7	1
1:A:72:LEU:HD21	1:A:76:THR:C	0.47	2.30	16	1
1:A:84:MET:HA	1:A:89:LEU:HD23	0.47	1.86	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:CG	1:A:38:LEU:HD13	0.47	2.39	4	2
1:A:78:LEU:HD11	1:A:93:PHE:CG	0.47	2.44	15	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:90:VAL:CG1	1:A:105:VAL:HG23	0.47	2.40	4	1
1:A:40:ILE:CG1	1:A:49:VAL:CG2	0.47	2.93	12	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:117:TYR:N	1:A:123:GLU:O	0.47	2.46	16	1
1:A:42:GLN:CD	1:A:47:PHE:CZ	0.47	2.88	12	1
1:A:128:PHE:N	1:A:128:PHE:CD1	0.47	2.83	13	1
1:A:73:ALA:O	1:A:74:ASP:CB	0.47	2.63	4	2
1:A:78:LEU:HD13	1:A:95:ARG:HH21	0.47	1.70	6	1
1:A:40:ILE:CD1	1:A:49:VAL:HG23	0.47	2.40	19	1
1:A:55:PHE:CE1	2:A:132:PLM:HE2	0.47	2.44	15	2
1:A:74:ASP:CB	2:A:132:PLM:CG	0.46	2.92	1	2
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:46:LYS:HB3	1:A:63:GLU:N	0.46	2.25	4	1
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:41:THR:O	1:A:41:THR:HG22	0.46	2.10	5	1
1:A:49:VAL:HG12	1:A:62:PHE:CZ	0.46	2.45	17	1
1:A:39:THR:HB	1:A:50:LYS:HB3	0.46	1.86	11	2
1:A:93:PHE:O	1:A:102:LEU:N	0.46	2.49	7	1
1:A:106:ARG:CG	1:A:106:ARG:NH1	0.46	2.78	3	1
1:A:103:ILE:HG12	1:A:117:TYR:CD2	0.46	2.45	20	1
1:A:115:GLN:HE21	1:A:126:ARG:NE	0.46	2.08	19	1
1:A:113:LEU:CD1	1:A:128:PHE:CE2	0.46	2.98	4	1
1:A:107:GLU:O	1:A:109:SER:N	0.46	2.48	12	3
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:36:LEU:HD22	1:A:126:ARG:NH2	0.46	2.25	8	3
1:A:126:ARG:HH11	1:A:126:ARG:CG	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: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:92:LYS:HG3	1:A:103:ILE:CD1	0.46	2.41	11	1
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:96:VAL:HG23	1:A:97:ASP:N	0.46	2.25	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:PHE:HA	1:A:68:PHE:CE2	0.46	2.46	11	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:10:ARG:HB2	1:A:127:ILE:HB	0.46	1.88	8	1
1:A:72:LEU:CD1	1:A:78:LEU:HB2	0.46	2.41	16	1
1:A:17:PHE:N	1:A:17:PHE:CD1	0.46	2.84	16	1
1:A:36:LEU:CD2	1:A:126:ARG:NH2	0.46	2.79	16	1
1:A:102:LEU:CD1	1:A:102:LEU:C	0.46	2.84	20	1
1:A:10:ARG:HG3	1:A:127:ILE:HG21	0.46	1.88	2	1
1:A:101:GLU:CG	1:A:102:LEU:N	0.45	2.79	5	2
1:A:18:MET:O	1:A:23:ILE:HG12	0.45	2.11	17	1
1:A:20:LYS:HE3	1:A:120:GLU:CB	0.45	2.41	6	1
1:A:39:THR:HB	1:A:50:LYS:CB	0.45	2.41	17	9
1:A:55:PHE:CD2	1:A:73:ALA:CB	0.45	2.99	1	1
1:A:126:ARG:HH11	1:A:126:ARG:HG3	0.45	1.71	11	1
1:A:40:ILE:HG12	1:A:49:VAL:CG2	0.45	2.42	3	2
1:A:12:GLU:O	1:A:125:LYS:N	0.45	2.50	16	3
1:A:62:PHE:CE2	2:A:132:PLM:H32	0.45	2.46	8	1
1:A:6:TRP:HZ2	1:A:108:ILE:HD11	0.45	1.65	20	1
1:A:49:VAL:HG12	1:A:62:PHE:CE1	0.45	2.46	19	1
1:A:71:SER:C	1:A:72:LEU:CD1	0.45	2.85	4	1
1:A:60:VAL:HG13	1:A:60:VAL:O	0.45	2.11	12	1
1:A:55:PHE:CE2	1:A:73:ALA:CB	0.45	2.99	1	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: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:114:ILE:HG21	1:A:127:ILE:HD13	0.45	1.88	2	1
1:A:23:ILE:CG2	1:A:27:LYS:CB	0.45	2.94	2	1
1:A:90:VAL:HB	1:A:105:VAL:HG23	0.45	1.87	19	1
1:A:90:VAL:HB	1:A:105:VAL:CG2	0.45	2.42	19	1
1:A:6:TRP:CZ3	1:A:130:LYS:HG3	0.45	2.46	9	1
1:A:41:THR:HG22	1:A:41:THR:O	0.45	2.11	11	4
1:A:83:THR:CG2	1:A:90:VAL:CG2	0.45	2.89	20	2
1:A:16:LYS:HB3	1:A:17:PHE:CD2	0.45	2.47	17	1
1:A:48:THR:HB	1:A:61:VAL:HG13	0.45	1.85	2	1
1:A:68:PHE:C	1:A:68:PHE:CD1	0.45	2.89	2	1
1:A:71:SER:C	1:A:72:LEU:HD22	0.45	2.31	3	1
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:36:LEU:CD2	1:A:38:LEU:HD13	0.45	2.41	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:ILE:HG23	1:A:117:TYR:CD1	0.45	2.46	20	1
1:A:14:TYR:C	1:A:14:TYR:CD1	0.45	2.89	6	1
1:A:106:ARG:HB3	1:A:113:LEU:HD21	0.45	1.88	4	1
1:A:20:LYS:HE3	1:A:119:TYR:CG	0.45	2.47	13	1
1:A:116:THR:OG1	1:A:117:TYR:N	0.45	2.47	11	2
1:A:93:PHE:CE1	2:A:132:PLM:H41	0.45	2.47	6	1
1:A:36:LEU:HA	1:A:53:SER:CB	0.45	2.41	4	1
1:A:82:TRP:CH2	1:A:84:MET:HB2	0.45	2.47	7	2
1:A:49:VAL:HG22	1:A:60:VAL:HB	0.45	1.87	7	2
1:A:77:GLU:HB3	1:A:96:VAL:HG22	0.45	1.88	16	1
1:A:23:ILE:HG22	1:A:28:ARG:N	0.45	2.27	16	1
1:A:17:PHE:CD2	1:A:124:ALA:CB	0.45	2.99	19	2
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:113:LEU:HD23	1:A:128:PHE:CE2	0.44	2.47	13	1
1:A:116:THR:HB	1:A:125:LYS:CG	0.44	2.42	8	1
1:A:36:LEU:HD21	1:A:128:PHE:HE2	0.44	1.72	8	1
1:A:20:LYS:CE	1:A:122:VAL:HG12	0.44	2.42	16	1
1:A:55:PHE:C	1:A:56:ARG:HG2	0.44	2.32	14	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: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:60:VAL:HB	1:A:62:PHE:CZ	0.44	2.47	17	1
1:A:36:LEU:CD1	1:A:38:LEU:HD12	0.44	2.40	3	1
1:A:23:ILE:HG23	1:A:27:LYS:HG2	0.44	1.88	15	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:6:TRP:CZ3	1:A:130:LYS:CB	0.44	3.01	12	2
1:A:82:TRP:CE3	1:A:89:LEU:CD2	0.44	3.00	7	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:105:VAL:CG1	1:A:117:TYR:CZ	0.44	3.00	4	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:102:LEU:HD12	1:A:119:TYR:HA	0.44	1.89	17	1
1:A:72:LEU:HD22	2:A:132:PLM:H82	0.44	1.88	11	1
1:A:48:THR:OG1	1:A:61:VAL:HG13	0.44	2.13	20	1
1:A:38:LEU:CD2	1:A:49:VAL:HG22	0.44	2.42	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ILE:HG13	1:A:49:VAL:CG2	0.44	2.42	12	1
1:A:62:PHE:CZ	1:A:68:PHE:CE2	0.44	3.05	10	1
1:A:85:GLU:CG	1:A:90:VAL:HG21	0.44	2.42	7	1
1:A:105:VAL:O	1:A:107:GLU:N	0.44	2.51	7	2
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	3
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:116:THR:HB	1:A:125:LYS:CD	0.44	2.43	20	1
1:A:49:VAL:HG11	1:A:82:TRP:CH2	0.44	2.48	20	1
1:A:40:ILE:HG23	1:A:49:VAL:CG1	0.43	2.29	13	1
1:A:111:ASN:ND2	1:A:111:ASN:N	0.43	2.66	8	1
1:A:91:GLY:O	1:A:104:ALA:N	0.43	2.51	17	2
1:A:20:LYS:CE	1:A:122:VAL:CG1	0.43	2.96	16	1
1:A:66:VAL:O	1:A:68:PHE:CE2	0.43	2.71	11	1
1:A:127:ILE:O	1:A:127:ILE:HG22	0.43	2.12	3	1
1:A:46:LYS:HB2	1:A:64:LEU:N	0.43	2.28	4	1
1:A:38:LEU:HG	1:A:49:VAL:HG21	0.43	1.90	15	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:5:THR:C	1:A:6:TRP:CD1	0.43	2.92	3	1
1:A:21:MET:CE	1:A:95:ARG:HH12	0.43	2.27	15	1
1:A:17:PHE:CD1	1:A:17:PHE:O	0.43	2.72	12	2
1:A:111:ASN:N	1:A:111:ASN:HD22	0.43	2.11	8	1
1:A:70:TYR:HB3	1:A:78:LEU:HD23	0.43	1.90	16	1
1:A:114:ILE:HD13	1:A:127:ILE:HD12	0.43	1.89	11	1
1:A:6:TRP:CG	1:A:113:LEU:HD13	0.43	2.48	3	1
1:A:78:LEU:CD1	1:A:102:LEU:HD13	0.43	2.42	19	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:48:THR:CA	1:A:61:VAL:HA	0.43	2.39	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: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:82:TRP:CD2	1:A:91:GLY:HA2	0.43	2.49	1	1
1:A:23:ILE:HG21	1:A:28:ARG:HA	0.43	1.89	9	1
1:A:127:ILE:N	1:A:127:ILE:HD13	0.43	2.29	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:PHE:CE2	1:A:73:ALA:HB1	0.43	2.49	19	1
1:A:119:TYR:CE2	1:A:120:GLU:HG3	0.43	2.49	8	1
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:113:LEU:CD2	1:A:128:PHE:CD2	0.43	3.01	10	1
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:83:THR:O	1:A:90:VAL:N	0.43	2.51	8	2
1:A:20:LYS:HD3	1:A:122:VAL:CG1	0.43	2.43	16	1
1:A:33:HIS:C	1:A:33:HIS:CD2	0.43	2.91	2	1
1:A:38:LEU:HD21	1:A:106:ARG:HH12	0.43	1.73	3	1
1:A:60:VAL:O	1:A:60:VAL:HG13	0.43	2.13	3	1
1:A:20:LYS:CE	1:A:120:GLU:HB2	0.43	2.43	6	1
1:A:55:PHE:CE2	1:A:73:ALA:HA	0.43	2.49	4	1
1:A:17:PHE:HA	1:A:122:VAL:HG11	0.43	1.91	15	1
1:A:62:PHE:HB2	1:A:68:PHE:CE1	0.43	2.49	1	2
1:A:93:PHE:CE1	2:A:132:PLM:H42	0.43	2.49	8	2
1:A:113:LEU:CD2	1:A:128:PHE:CD1	0.43	3.02	20	1
1:A:6:TRP:CZ3	1:A:113:LEU:N	0.43	2.87	18	1
1:A:17:PHE:CD1	1:A:17:PHE:C	0.42	2.93	7	1
1:A:11:ASN:CG	1:A:14:TYR:CD2	0.42	2.92	7	1
1:A:64:LEU:HD12	1:A:64:LEU:H	0.42	1.74	16	1
1:A:105:VAL:HG11	1:A:117:TYR:CE2	0.42	2.48	4	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:75:GLY:O	1:A:76:THR:HG23	0.42	2.13	5	1
1:A:82:TRP:CD2	1:A:91:GLY:CA	0.42	3.03	13	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:49:VAL:HG22	1:A:60:VAL:CG1	0.42	2.44	5	1
1:A:92:LYS:HA	1:A:103:ILE:HD12	0.42	1.90	11	1
1:A:48:THR:OG1	1:A:61:VAL:CG1	0.42	2.67	20	1
1:A:40:ILE:HG12	1:A:49:VAL:HG23	0.42	1.89	3	1
1:A:36:LEU:CD2	1:A:128:PHE:CZ	0.42	3.02	6	1
1:A:78:LEU:CD1	1:A:93:PHE:HB3	0.42	2.44	19	1
1:A:6:TRP:CH2	1:A:113:LEU:HB2	0.42	2.49	18	1
1:A:10:ARG:O	1:A:127:ILE:N	0.42	2.53	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:TYR:CD2	1:A:126:ARG:HG3	0.42	2.49	20	1
1:A:116:THR:HG23	1:A:117:TYR:CE1	0.42	2.49	19	1
1:A:5:THR:HG23	1:A:39:THR:HG23	0.42	1.91	3	2
1:A:116:THR:HB	1:A:125:LYS:HG3	0.42	1.91	18	2
1:A:128:PHE:CD2	1:A:130:LYS:N	0.42	2.87	19	2
1:A:13:ASN:ND2	1:A:123:GLU:O	0.42	2.53	3	1
1:A:82:TRP:CZ3	1:A:91:GLY:HA3	0.42	2.50	1	1
1:A:93:PHE:HD2	1:A:102:LEU:HD22	0.42	1.75	8	2
1:A:93:PHE:N	1:A:102:LEU:O	0.42	2.53	16	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:103:ILE:HD12	1:A:104:ALA:H	0.42	1.75	10	1
1:A:17:PHE:C	1:A:17:PHE:CD1	0.42	2.93	10	1
1:A:55:PHE:CZ	2:A:132:PLM:HE2	0.42	2.50	4	1
1:A:23:ILE:HD11	1:A:74:ASP:HB3	0.42	1.92	15	1
1:A:6:TRP:CE2	1:A:113:LEU:HD13	0.42	2.50	18	1
1:A:63:GLU:O	1:A:64:LEU:C	0.42	2.58	18	1
1:A:98:ASN:ND2	1:A:100:LYS:HG2	0.42	2.29	12	1
1:A:108:ILE:HD13	1:A:112:GLU:O	0.42	2.15	1	1
1:A:62:PHE:O	1:A:63:GLU:C	0.42	2.58	7	1
1:A:62:PHE:CD1	1:A:62:PHE:N	0.42	2.88	9	1
1:A:82:TRP:CE3	1:A:90:VAL:C	0.42	2.93	6	2
1:A:23:ILE:HG23	1:A:27:LYS:CB	0.42	2.44	2	1
1:A:113:LEU:CD2	1:A:115:GLN:HG2	0.42	2.39	19	1
1:A:21:MET:HG3	1:A:119:TYR:CD2	0.42	2.50	4	1
1:A:62:PHE:CZ	1:A:82:TRP:CH2	0.42	3.08	12	1
1:A:62:PHE:CD2	1:A:82:TRP:NE1	0.42	2.87	1	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:101:GLU:HG2	1:A:102:LEU:N	0.42	2.30	8	1
1:A:56:ARG:HG3	1:A:58:ILE:CG2	0.42	2.44	16	1
1:A:102:LEU:CD1	1:A:119:TYR:HB2	0.42	2.45	6	1
1:A:92:LYS:O	1:A:93:PHE:CD1	0.42	2.72	18	1
1:A:5:THR:C	1:A:6:TRP:CG	0.42	2.93	2	3
1:A:106:ARG:HG3	1:A:106:ARG:NH1	0.42	2.30	17	1
1:A:106:ARG:NH1	1:A:106:ARG:CG	0.42	2.82	11	2
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:40:ILE:CG2	1:A:47:PHE:CD2	0.42	3.02	18	1
1:A:8:VAL:O	1:A:35:ASN:ND2	0.42	2.53	18	1
1:A:72:LEU:HD23	1:A:72:LEU:N	0.41	2.30	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:MET:O	1:A:23:ILE:CG1	0.41	2.68	16	1
1:A:119:TYR:CD2	1:A:120:GLU:HB2	0.41	2.50	4	2
1:A:113:LEU:C	1:A:113:LEU:CD2	0.41	2.89	3	1
1:A:28:ARG:HG3	1:A:29:LYS:N	0.41	2.29	3	1
1:A:8:VAL:HG13	1:A:36:LEU:HB3	0.41	1.90	19	1
1:A:83:THR:O	1:A:90:VAL:HG23	0.41	2.16	8	1
1:A:11:ASN:CG	1:A:14:TYR:CG	0.41	2.94	7	1
1:A:14:TYR:HA	1:A:124:ALA:HA	0.41	1.93	2	1
1:A:14:TYR:HB3	1:A:124:ALA:C	0.41	2.36	2	1
1:A:48:THR:O	1:A:50:LYS:N	0.41	2.53	2	1
1:A:7:LYS:C	1:A:8:VAL:HG12	0.41	2.36	3	1
1:A:62:PHE:CA	1:A:68:PHE:CZ	0.41	3.03	1	1
1:A:4:GLY:O	1:A:40:ILE:N	0.41	2.53	17	4
1:A:18:MET:CB	1:A:23:ILE:HG13	0.41	2.46	16	1
1:A:89:LEU:HD13	1:A:106:ARG:CD	0.41	2.46	2	1
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:51:GLU:HB2	1:A:60:VAL:CG2	0.41	2.46	8	1
1:A:113:LEU:O	1:A:128:PHE:N	0.41	2.52	3	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:113:LEU:CD2	1:A:128:PHE:CE2	0.41	3.04	10	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:98:ASN:ND2	1:A:119:TYR:OH	0.41	2.54	19	3
1:A:12:GLU:N	1:A:125:LYS:O	0.41	2.53	8	2
1:A:84:MET:CA	1:A:89:LEU:HD12	0.41	2.45	5	1
1:A:48:THR:HB	1:A:61:VAL:CG1	0.41	2.46	13	1
1:A:91:GLY:O	1:A:104:ALA:HB3	0.41	2.16	16	1
1:A:20:LYS:CD	1:A:122:VAL:CG1	0.41	2.99	16	1
1:A:47:PHE:CZ	1:A:89:LEU:HD21	0.41	2.51	11	1
1:A:63:GLU:OE1	1:A:66:VAL:HG11	0.41	2.16	12	1
1:A:102:LEU:CD1	1:A:119:TYR:CG	0.41	3.03	7	1
1:A:23:ILE:CD1	2:A:132:PLM:HG3	0.41	2.45	7	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:5:THR:O	1:A:131:GLU:N	0.41	2.54	19	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:23:ILE:HG22	1:A:24:ASN:N	0.41	2.31	14	1
1:A:10:ARG:HG3	1:A:127:ILE:CB	0.41	2.46	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:CD2	1:A:38:LEU:CD1	0.41	2.97	3	1
1:A:17:PHE:CE1	1:A:119:TYR:CB	0.41	3.04	3	1
1:A:5:THR:OG1	1:A:6:TRP:N	0.41	2.54	9	1
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: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:12:GLU:CB	1:A:125:LYS:HB2	0.41	2.46	20	2
1:A:105:VAL:HG12	1:A:105:VAL:O	0.41	2.15	2	1
1:A:55:PHE:CE2	2:A:132:PLM:HG2	0.41	2.51	2	1
1:A:115:GLN:HB2	1:A:126:ARG:HD3	0.41	1.93	3	1
1:A:8:VAL:HG21	1:A:126:ARG:HD2	0.41	1.92	6	1
1:A:61:VAL:C	1:A:62:PHE:CD1	0.41	2.95	6	1
1:A:41:THR:CG2	1:A:48:THR:HG23	0.41	2.46	19	1
1:A:3:ASP:N	1:A:3:ASP:OD1	0.41	2.54	19	1
1:A:55:PHE:CE1	2:A:132:PLM:CE	0.41	3.04	15	2
1:A:79:THR:O	1:A:94:LYS:N	0.41	2.53	15	1
1:A:21:MET:CE	1:A:72:LEU:HD13	0.41	2.46	9	1
1:A:74:ASP:HB2	2:A:132:PLM:CG	0.41	2.46	9	2
1:A:23:ILE:N	1:A:23:ILE:HD12	0.41	2.31	20	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:77:GLU:HB3	1:A:96:VAL:CG2	0.41	2.46	10	1
1:A:46:LYS:HD2	1:A:46:LYS:C	0.41	2.36	4	1
1:A:72:LEU:HD22	1:A:72:LEU:C	0.41	2.36	4	1
1:A:89:LEU:HD23	1:A:90:VAL:H	0.41	1.76	18	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: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:74:ASP:OD2	2:A:132:PLM:HG3	0.40	2.14	12	1
1:A:54:ASN:ND2	1:A:54:ASN:O	0.40	2.55	7	1
1:A:113:LEU:CD1	1:A:114:ILE:N	0.40	2.84	8	1
1:A:118:THR:O	1:A:118:THR:HG22	0.40	2.15	17	1
1:A:23:ILE:O	1:A:28:ARG:NH1	0.40	2.55	16	1
1:A:103:ILE:HG22	1:A:118:THR:HB	0.40	1.92	14	1
1:A:72:LEU:CD1	2:A:132:PLM:C8	0.40	3.00	20	1
1:A:54:ASN:OD1	1:A:55:PHE:N	0.40	2.54	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ASN:HB2	1:A:63:GLU:CG	0.40	2.45	4	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: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
1:A:108:ILE:HG13	1:A:113:LEU:HA	0.40	1.93	20	1
1:A:23:ILE:HD11	1:A:74:ASP:HB2	0.40	1.93	20	1
1:A:36:LEU:CD2	1:A:126:ARG:HH21	0.40	2.29	6	1
1:A:93:PHE:O	1:A:102:LEU:HD23	0.40	2.16	4	1
1:A:89:LEU:HD22	1:A:106:ARG:HH21	0.40	1.75	18	1
1:A:74:ASP:N	1:A:74:ASP:OD1	0.40	2.54	18	1
1:A:82:TRP:CE2	1:A:91:GLY:HA3	0.40	2.51	13	1
1:A:55:PHE:CD1	1:A:55:PHE:N	0.40	2.89	11	1
1:A:126:ARG:CD	1:A:126:ARG:N	0.40	2.84	20	1
1:A:75:GLY:HA3	1:A:78:LEU:HD12	0.40	1.92	3	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%)	2	15
All	All	2580/2620 (98%)	1828 (71%)	552 (21%)	200 (8%)	2	15

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	77	GLU	11
1	A	130	LYS	11
1	A	117	TYR	10
1	A	67	ASP	10
1	A	61	VAL	8

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Mol	Chain	Res	Type	Models (Total)
1	A	100	LYS	7
1	A	36	LEU	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
1	A	49	VAL	5
1	A	34	ASP	4
1	A	85	GLU	4
1	A	98	ASN	4
1	A	86	GLY	4
1	A	13	ASN	4
1	A	66	VAL	4
1	A	74	ASP	3
1	A	72	LEU	3
1	A	124	ALA	3
1	A	24	ASN	3
1	A	83	THR	3
1	A	8	VAL	3
1	A	123	GLU	3
1	A	10	ARG	2
1	A	45	ASN	2
1	A	44	GLY	2
1	A	2	PHE	2
1	A	35	ASN	2
1	A	7	LYS	2
1	A	12	GLU	2
1	A	76	THR	2
1	A	99	GLY	1
1	A	14	TYR	1
1	A	96	VAL	1
1	A	56	ARG	1
1	A	52	SER	1
1	A	75	GLY	1
1	A	63	GLU	1
1	A	48	THR	1
1	A	127	ILE	1
1	A	105	VAL	1
1	A	40	ILE	1
1	A	111	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	78	LEU	1
1	A	95	ARG	1
1	A	47	PHE	1
1	A	121	GLY	1
1	A	11	ASN	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%)	78±4 (69±4%)	35±4 (31±4%)	2	15
All	All	2260/2260 (100%)	1551 (69%)	709 (31%)	2	15

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	76	THR	19
1	A	49	VAL	16
1	A	64	LEU	15
1	A	89	LEU	15
1	A	61	VAL	15
1	A	45	ASN	14
1	A	38	LEU	13
1	A	95	ARG	13
1	A	120	GLU	13
1	A	88	LYS	12
1	A	113	LEU	12
1	A	125	LYS	12
1	A	56	ARG	11
1	A	59	ASP	11
1	A	17	PHE	11
1	A	97	ASP	11
1	A	11	ASN	11
1	A	10	ARG	10
1	A	108	ILE	10

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Mol	Chain	Res	Type	Models (Total)
1	A	78	LEU	10
1	A	16	LYS	10
1	A	111	ASN	10
1	A	74	ASP	10
1	A	126	ARG	10
1	A	68	PHE	10
1	A	14	TYR	10
1	A	90	VAL	9
1	A	46	LYS	8
1	A	62	PHE	8
1	A	13	ASN	8
1	A	102	LEU	8
1	A	5	THR	8
1	A	77	GLU	8
1	A	116	THR	8
1	A	21	MET	8
1	A	50	LYS	8
1	A	54	ASN	8
1	A	52	SER	8
1	A	92	LYS	8
1	A	87	ASN	8
1	A	101	GLU	8
1	A	98	ASN	7
1	A	12	GLU	7
1	A	58	ILE	7
1	A	85	GLU	7
1	A	130	LYS	7
1	A	128	PHE	7
1	A	84	MET	7
1	A	48	THR	7
1	A	105	VAL	7
1	A	72	LEU	6
1	A	2	PHE	6
1	A	109	SER	6
1	A	47	PHE	6
1	A	103	ILE	6
1	A	53	SER	6
1	A	36	LEU	6
1	A	127	ILE	6
1	A	28	ARG	6
1	A	25	VAL	5
1	A	33	HIS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	35	ASN	5
1	A	63	GLU	5
1	A	71	SER	5
1	A	118	THR	5
1	A	57	ASN	5
1	A	42	GLN	5
1	A	8	VAL	5
1	A	30	LEU	5
1	A	81	THR	5
1	A	15	GLU	4
1	A	18	MET	4
1	A	119	TYR	4
1	A	19	GLU	4
1	A	34	ASP	4
1	A	26	VAL	4
1	A	27	LYS	4
1	A	129	LYS	4
1	A	23	ILE	4
1	A	67	ASP	4
1	A	66	VAL	4
1	A	37	LYS	3
1	A	3	ASP	3
1	A	94	LYS	3
1	A	70	TYR	3
1	A	41	THR	3
1	A	20	LYS	3
1	A	123	GLU	3
1	A	107	GLU	3
1	A	55	PHE	3
1	A	24	ASN	3
1	A	7	LYS	3
1	A	29	LYS	3
1	A	40	ILE	2
1	A	122	VAL	2
1	A	106	ARG	2
1	A	131	GLU	2
1	A	115	GLN	2
1	A	117	TYR	2
1	A	83	THR	2
1	A	43	GLU	1
1	A	96	VAL	1
1	A	9	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	60	VAL	1
1	A	79	THR	1
1	A	51	GLU	1
1	A	112	GLU	1
1	A	114	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

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	-	14,17,17	0.52±0.03	0±0 (0±0%)

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	-	14,17,17	0.37±0.06	0±0 (0±0%)

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±0,13,15,15	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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