



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:22 PM UTC

PDB ID : 2JMH / pdb_00002jmh
Title : NMR solution structure of Blo t 5, a major mite allergen from Blomia tropicalis
Authors : Naik, M.T.; Chang, C.; Kuo, I.; Chua, K.; Huang, T.
Deposited on : 2006-11-12

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

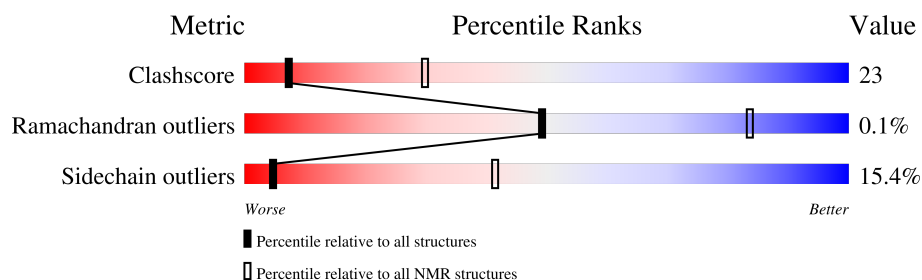
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	119	

2 Ensemble composition and analysis

This entry contains 21 models. Model 21 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:18-A:78, A:83-A:117 (96)	0.35	21

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 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 5, 7, 10, 14, 16, 17, 20, 21
2	3, 6, 8, 12, 13, 18
3	9, 15
Single-model clusters	11; 19

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1954 atoms, of which 978 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mite allergen Blo t 5.

Mol	Chain	Residues	Atoms						Trace
1	A	117	Total	C	H	N	O	S	0
			1954	608	978	172	194	2	

There are 2 discrepancies between the modelled and reference sequences:

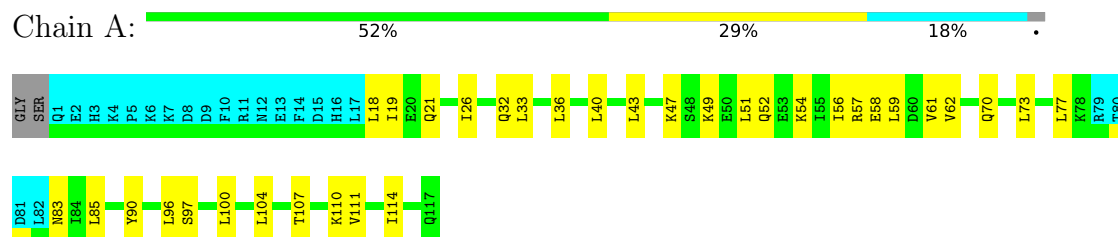
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O96870
A	0	SER	-	expression tag	UNP O96870

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: Mite allergen Blo t 5

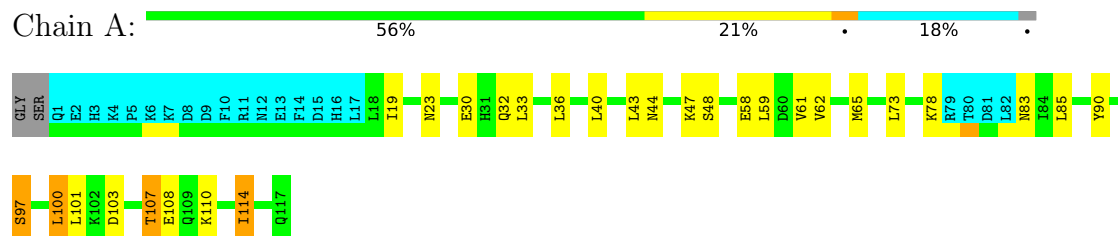


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

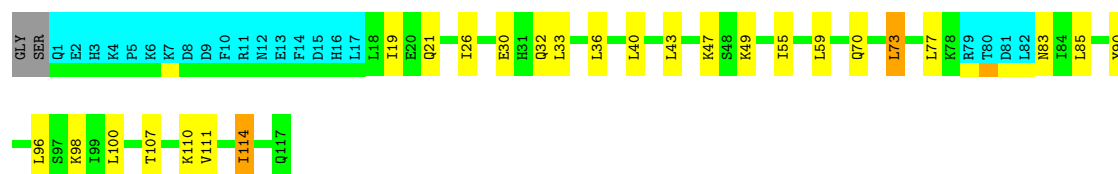
- Molecule 1: Mite allergen Blo t 5



4.2.2 Score per residue for model 2

- Molecule 1: Mite allergen Blo t 5

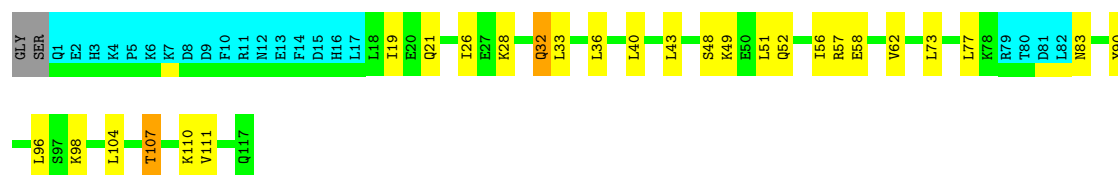




4.2.3 Score per residue for model 3

- Molecule 1: Mite allergen Blo t 5

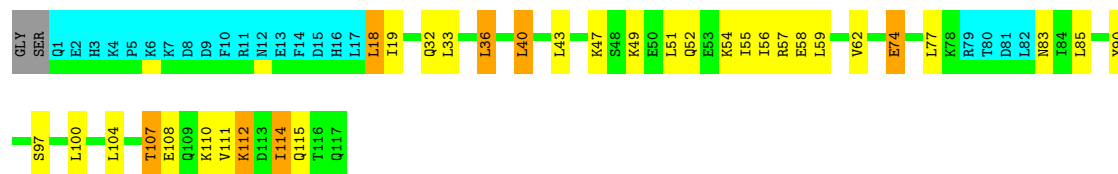
Chain A: 58% 21% 18%



4.2.4 Score per residue for model 4

- Molecule 1: Mite allergen Blo t 5

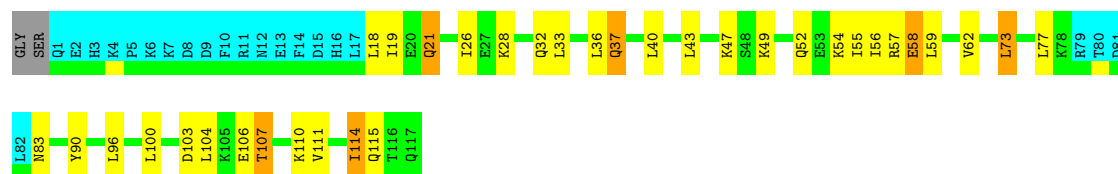
Chain A: 53% 22% 6% 18%



4.2.5 Score per residue for model 5

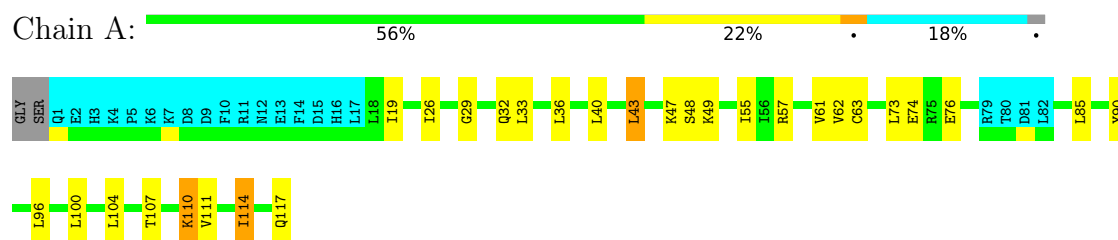
- Molecule 1: Mite allergen Blo t 5

Chain A: 51% 24% 5% 18%



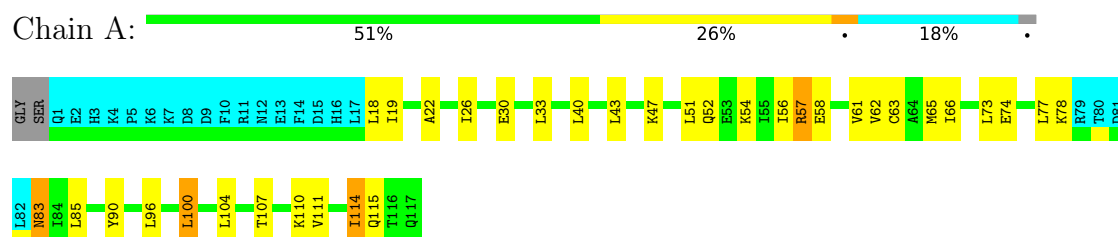
4.2.6 Score per residue for model 6

- Molecule 1: Mite allergen Blo t 5



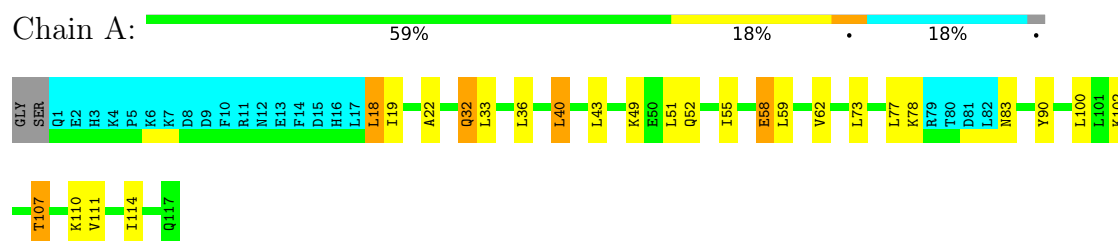
4.2.7 Score per residue for model 7

- Molecule 1: Mite allergen Blo t 5



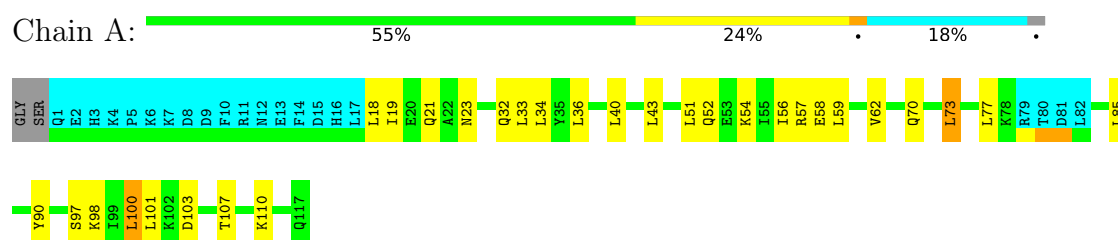
4.2.8 Score per residue for model 8

- Molecule 1: Mite allergen Blo t 5



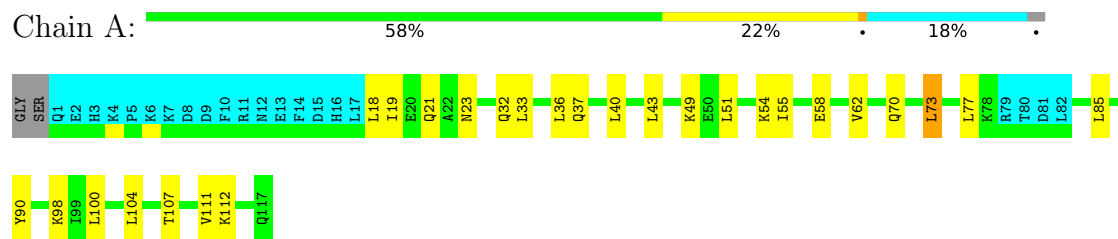
4.2.9 Score per residue for model 9

- Molecule 1: Mite allergen Blo t 5



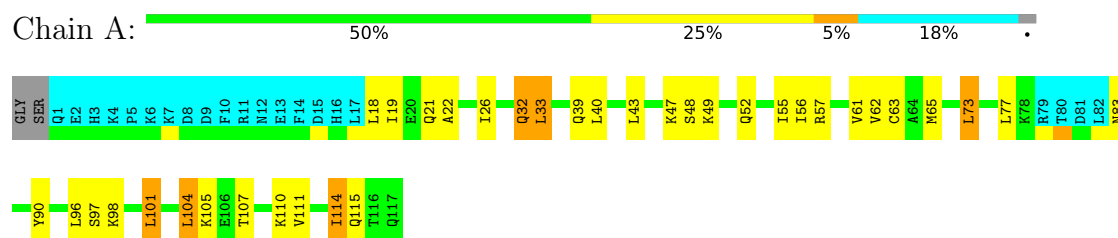
4.2.10 Score per residue for model 10

- Molecule 1: Mite allergen Blo t 5



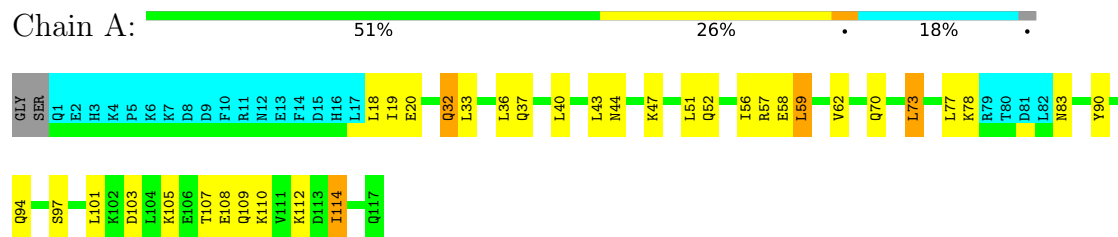
4.2.11 Score per residue for model 11

- Molecule 1: Mite allergen Blo t 5



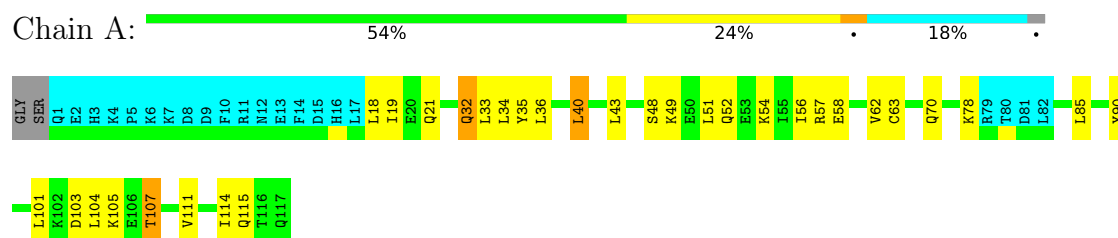
4.2.12 Score per residue for model 12

- Molecule 1: Mite allergen Blo t 5



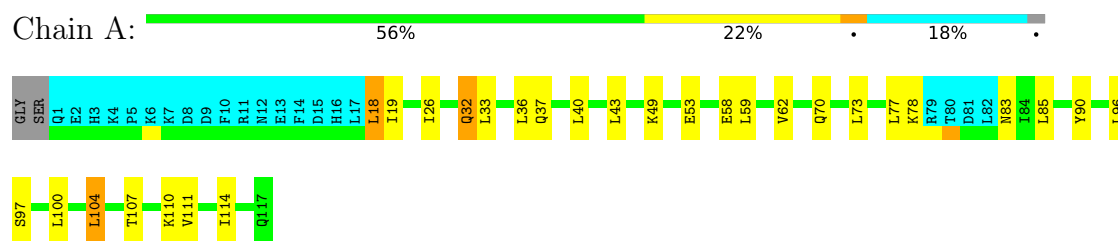
4.2.13 Score per residue for model 13

- Molecule 1: Mite allergen Blo t 5



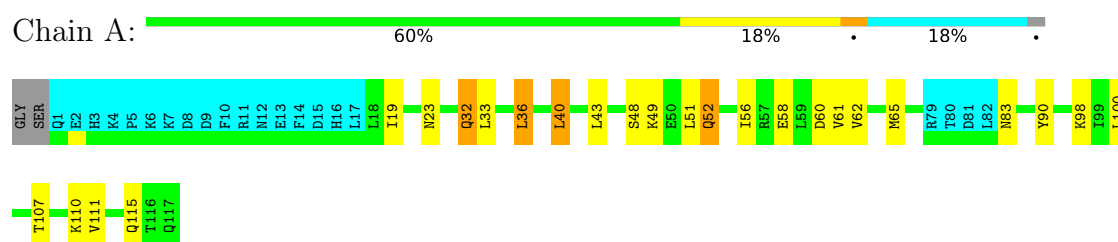
4.2.14 Score per residue for model 14

- Molecule 1: Mite allergen Blo t 5



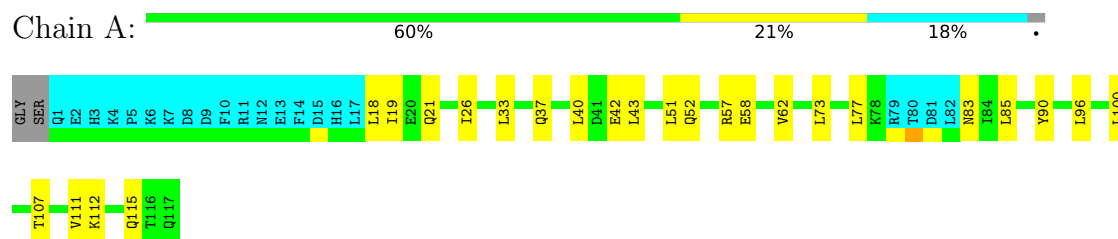
4.2.15 Score per residue for model 15

- Molecule 1: Mite allergen Blo t 5



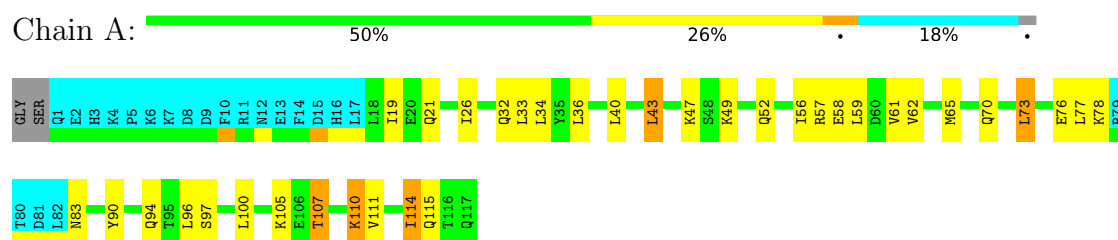
4.2.16 Score per residue for model 16

- Molecule 1: Mite allergen Blo t 5



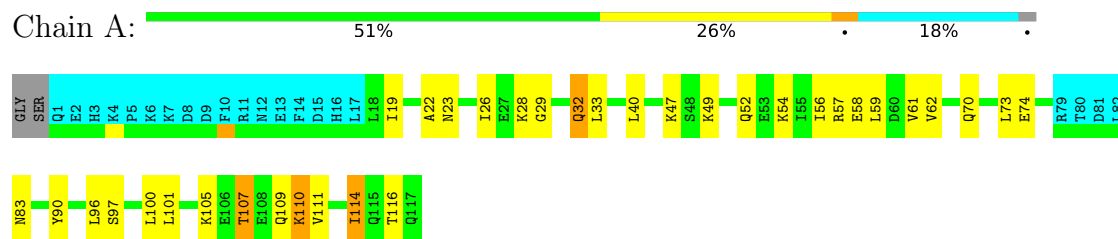
4.2.17 Score per residue for model 17

- Molecule 1: Mite allergen Blo t 5



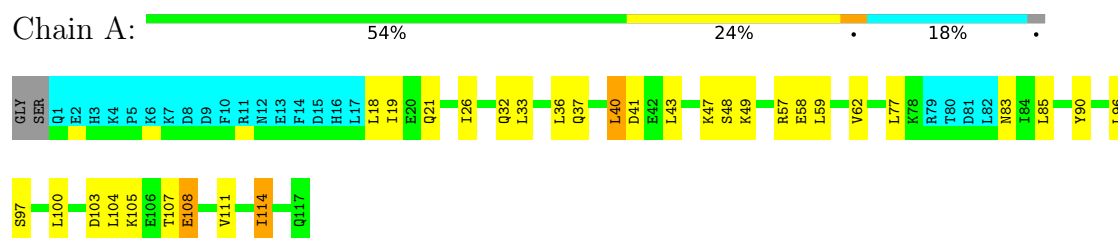
4.2.18 Score per residue for model 18

- Molecule 1: Mite allergen Blo t 5



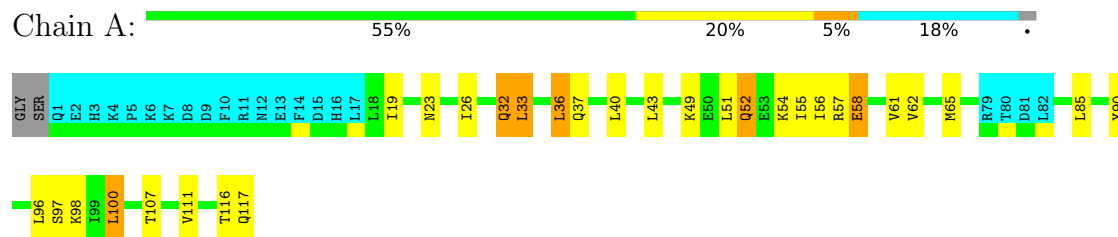
4.2.19 Score per residue for model 19

- Molecule 1: Mite allergen Blo t 5



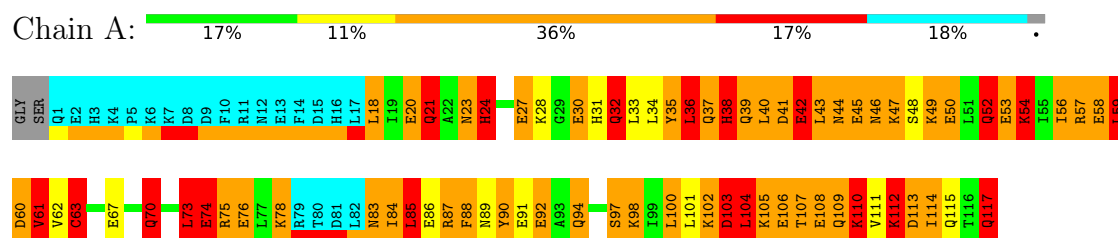
4.2.20 Score per residue for model 20

- Molecule 1: Mite allergen Blo t 5



4.2.21 Score per residue for model 21 (medoid)

- Molecule 1: Mite allergen Blo t 5



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 21 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	refinement	2.1
CYANA	structure solution	2.1
Sparky	structure solution	3.112

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.96±3.24	11±49/793 (1.4± 6.2%)	1.08±2.29	12±52/1061 (1.1± 4.9%)
All	All	3.38	231/16653 (1.4%)	2.53	242/22281 (1.1%)

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	87	ARG	CZ-NH1	-79.57	0.21	1.32	21	1
1	A	38	HIS	CE1-NE2	-72.70	0.59	1.32	21	1
1	A	57	ARG	CZ-NH1	-58.83	0.50	1.32	21	1
1	A	76	GLU	CD-OE1	-56.55	0.17	1.25	21	1
1	A	75	ARG	CZ-NH1	-55.41	0.55	1.32	21	1
1	A	67	GLU	CD-OE1	-52.69	0.25	1.25	21	1
1	A	24	HIS	CE1-NE2	-52.32	0.80	1.32	21	1
1	A	52	GLN	CD-OE1	-51.80	0.25	1.23	21	1
1	A	38	HIS	CG-ND1	-51.33	0.81	1.38	21	1
1	A	30	GLU	CD-OE1	-50.78	0.28	1.25	21	1
1	A	87	ARG	CZ-NH2	-50.60	0.67	1.33	21	1
1	A	108	GLU	CD-OE2	-49.84	0.30	1.25	21	1
1	A	75	ARG	CZ-NH2	-49.53	0.69	1.33	21	1
1	A	87	ARG	CD-NE	-48.62	0.78	1.46	21	1
1	A	75	ARG	CD-NE	-47.93	0.79	1.46	21	1
1	A	92	GLU	CD-OE2	-47.46	0.35	1.25	21	1
1	A	91	GLU	CD-OE2	-46.95	0.36	1.25	21	1
1	A	21	GLN	CD-OE1	-46.07	0.36	1.23	21	1
1	A	106	GLU	CD-OE2	-45.68	0.38	1.25	21	1
1	A	27	GLU	CD-OE2	-45.23	0.39	1.25	21	1
1	A	86	GLU	CD-OE2	-45.05	0.39	1.25	21	1
1	A	87	ARG	NE-CZ	-44.55	0.84	1.33	21	1
1	A	20	GLU	CD-OE2	-44.39	0.41	1.25	21	1
1	A	117	GLN	CD-OE1	-44.11	0.39	1.23	21	1
1	A	103	ASP	CG-OD2	-43.89	0.41	1.25	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	45	GLU	CD-OE1	-43.78	0.42	1.25	21	1
1	A	50	GLU	CD-OE2	-43.26	0.43	1.25	21	1
1	A	20	GLU	CD-OE1	-43.05	0.43	1.25	21	1
1	A	94	GLN	CD-OE1	-42.83	0.42	1.23	21	1
1	A	27	GLU	CD-OE1	-42.70	0.44	1.25	21	1
1	A	106	GLU	CD-OE1	-42.48	0.44	1.25	21	1
1	A	113	ASP	CG-OD2	-41.45	0.46	1.25	21	1
1	A	42	GLU	CD-OE2	-40.91	0.47	1.25	21	1
1	A	74	GLU	CD-OE2	-40.23	0.48	1.25	21	1
1	A	70	GLN	CD-OE1	-40.13	0.47	1.23	21	1
1	A	41	ASP	CG-OD2	-39.50	0.50	1.25	21	1
1	A	45	GLU	CD-OE2	-39.15	0.51	1.25	21	1
1	A	24	HIS	CG-CD2	-39.07	0.92	1.35	21	1
1	A	44	ASN	CG-OD1	-38.79	0.49	1.23	21	1
1	A	91	GLU	CD-OE1	-38.44	0.52	1.25	21	1
1	A	86	GLU	CD-OE1	-38.25	0.52	1.25	21	1
1	A	38	HIS	CG-CD2	-38.24	0.93	1.35	21	1
1	A	50	GLU	CD-OE1	-38.12	0.53	1.25	21	1
1	A	24	HIS	CG-ND1	-37.25	0.97	1.38	21	1
1	A	37	GLN	CD-OE1	-37.09	0.53	1.23	21	1
1	A	42	GLU	CD-OE1	-37.08	0.54	1.25	21	1
1	A	53	GLU	CD-OE1	-36.77	0.55	1.25	21	1
1	A	74	GLU	CD-OE1	-35.88	0.57	1.25	21	1
1	A	113	ASP	CG-OD1	-35.77	0.57	1.25	21	1
1	A	108	GLU	CD-OE1	-35.75	0.57	1.25	21	1
1	A	75	ARG	NE-CZ	-35.62	0.93	1.33	21	1
1	A	41	ASP	CG-OD1	-35.54	0.57	1.25	21	1
1	A	53	GLU	CD-OE2	-35.51	0.57	1.25	21	1
1	A	60	ASP	CG-OD1	-35.17	0.58	1.25	21	1
1	A	92	GLU	CD-OE1	-34.72	0.59	1.25	21	1
1	A	94	GLN	CD-NE2	-34.31	0.61	1.33	21	1
1	A	32	GLN	CD-OE1	-34.15	0.58	1.23	21	1
1	A	85	LEU	CG-CD2	-34.13	0.40	1.52	21	1
1	A	76	GLU	CD-OE2	-34.05	0.60	1.25	21	1
1	A	35	TYR	CG-CD2	-33.43	0.69	1.39	21	1
1	A	40	LEU	CG-CD2	-33.17	0.43	1.52	21	1
1	A	88	PHE	CG-CD2	-32.68	0.70	1.38	21	1
1	A	60	ASP	CG-OD2	-32.66	0.63	1.25	21	1
1	A	58	GLU	CD-OE2	-31.44	0.65	1.25	21	1
1	A	30	GLU	CD-OE2	-31.31	0.65	1.25	21	1
1	A	88	PHE	CG-CD1	-31.04	0.73	1.38	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	117	GLN	CD-NE2	-30.64	0.69	1.33	21	1
1	A	58	GLU	CD-OE1	-30.26	0.67	1.25	21	1
1	A	35	TYR	CG-CD1	-30.23	0.75	1.39	21	1
1	A	21	GLN	CG-CD	-30.10	0.76	1.52	21	1
1	A	28	LYS	CE-NZ	-30.07	0.59	1.49	21	1
1	A	35	TYR	CE1-CZ	-29.94	0.66	1.38	21	1
1	A	31	HIS	CD2-NE2	-29.76	1.05	1.37	21	1
1	A	103	ASP	CG-OD1	-29.63	0.69	1.25	21	1
1	A	43	LEU	CG-CD2	-29.24	0.56	1.52	21	1
1	A	97	SER	CB-OG	-29.14	0.83	1.42	21	1
1	A	90	TYR	CG-CD2	-28.93	0.78	1.39	21	1
1	A	117	GLN	CG-CD	-28.80	0.80	1.52	21	1
1	A	115	GLN	CD-OE1	-28.69	0.69	1.23	21	1
1	A	110	LYS	CE-NZ	-28.43	0.64	1.49	21	1
1	A	57	ARG	NE-CZ	-28.35	1.01	1.33	21	1
1	A	78	LYS	CE-NZ	-27.86	0.65	1.49	21	1
1	A	39	GLN	CD-NE2	-27.75	0.74	1.33	21	1
1	A	98	LYS	CE-NZ	-27.73	0.66	1.49	21	1
1	A	90	TYR	CG-CD1	-27.36	0.81	1.39	21	1
1	A	117	GLN	C-O	-27.18	0.69	1.23	21	1
1	A	56	ILE	CB-CG1	-27.18	0.99	1.53	21	1
1	A	35	TYR	CE2-CZ	-27.16	0.73	1.38	21	1
1	A	52	GLN	CD-NE2	-26.85	0.76	1.33	21	1
1	A	36	LEU	CG-CD1	-26.44	0.65	1.52	21	1
1	A	74	GLU	CG-CD	-26.27	0.86	1.52	21	1
1	A	36	LEU	CG-CD2	-26.17	0.66	1.52	21	1
1	A	24	HIS	ND1-CE1	-26.08	1.06	1.32	21	1
1	A	31	HIS	CG-ND1	-26.00	1.09	1.38	21	1
1	A	39	GLN	CD-OE1	-25.85	0.74	1.23	21	1
1	A	90	TYR	CE1-CZ	-25.84	0.76	1.38	21	1
1	A	100	LEU	CG-CD2	-25.18	0.69	1.52	21	1
1	A	105	LYS	CE-NZ	-25.10	0.74	1.49	21	1
1	A	67	GLU	CD-OE2	-25.07	0.77	1.25	21	1
1	A	109	GLN	CD-OE1	-24.96	0.76	1.23	21	1
1	A	40	LEU	CG-CD1	-24.91	0.70	1.52	21	1
1	A	61	VAL	CB-CG1	-24.87	0.70	1.52	21	1
1	A	61	VAL	CB-CG2	-24.81	0.70	1.52	21	1
1	A	90	TYR	CE2-CZ	-24.50	0.79	1.38	21	1
1	A	76	GLU	CG-CD	-24.25	0.91	1.52	21	1
1	A	94	GLN	CB-CG	-24.23	0.79	1.52	21	1
1	A	44	ASN	CG-ND2	-24.20	0.82	1.33	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	54	LYS	CD-CE	-24.01	0.80	1.52	21	1
1	A	45	GLU	CG-CD	-23.95	0.92	1.52	21	1
1	A	24	HIS	CD2-NE2	-23.95	1.11	1.37	21	1
1	A	85	LEU	CG-CD1	-23.71	0.74	1.52	21	1
1	A	109	GLN	CD-NE2	-23.67	0.83	1.33	21	1
1	A	88	PHE	CE1-CZ	-23.26	0.68	1.38	21	1
1	A	43	LEU	CG-CD1	-23.20	0.76	1.52	21	1
1	A	57	ARG	CZ-NH2	-23.16	1.03	1.33	21	1
1	A	109	GLN	CG-CD	-23.13	0.94	1.52	21	1
1	A	18	LEU	CG-CD1	-22.89	0.77	1.52	21	1
1	A	37	GLN	CG-CD	-22.67	0.95	1.52	21	1
1	A	112	LYS	CB-CG	-22.62	0.84	1.52	21	1
1	A	31	HIS	ND1-CE1	-22.51	1.10	1.32	21	1
1	A	108	GLU	CB-CG	-22.31	0.85	1.52	21	1
1	A	38	HIS	CD2-NE2	-22.31	1.13	1.37	21	1
1	A	88	PHE	CE2-CZ	-22.11	0.72	1.38	21	1
1	A	73	LEU	CG-CD1	-21.91	0.80	1.52	21	1
1	A	98	LYS	CD-CE	-21.88	0.86	1.52	21	1
1	A	110	LYS	CG-CD	-21.88	0.86	1.52	21	1
1	A	54	LYS	CE-NZ	-21.82	0.83	1.49	21	1
1	A	31	HIS	CB-CG	-21.65	1.19	1.50	21	1
1	A	48	SER	CB-OG	-21.56	0.99	1.42	21	1
1	A	27	GLU	CG-CD	-21.35	0.98	1.52	21	1
1	A	57	ARG	CD-NE	-21.29	1.16	1.46	21	1
1	A	63	CYS	CB-SG	-21.18	1.11	1.81	21	1
1	A	20	GLU	CG-CD	-21.18	0.99	1.52	21	1
1	A	89	ASN	CG-OD1	-21.07	0.83	1.23	21	1
1	A	106	GLU	CG-CD	-20.90	0.99	1.52	21	1
1	A	59	LEU	CG-CD1	-20.80	0.83	1.52	21	1
1	A	115	GLN	CD-NE2	-20.76	0.89	1.33	21	1
1	A	89	ASN	CG-ND2	-20.32	0.90	1.33	21	1
1	A	91	GLU	CG-CD	-20.31	1.01	1.52	21	1
1	A	73	LEU	CG-CD2	-20.29	0.85	1.52	21	1
1	A	50	GLU	CB-CG	-20.25	0.91	1.52	21	1
1	A	59	LEU	CG-CD2	-20.09	0.86	1.52	21	1
1	A	104	LEU	CG-CD1	-20.04	0.86	1.52	21	1
1	A	47	LYS	CE-NZ	-19.91	0.89	1.49	21	1
1	A	70	GLN	CB-CG	-19.71	0.93	1.52	21	1
1	A	105	LYS	CG-CD	-19.55	0.93	1.52	21	1
1	A	18	LEU	CG-CD2	-19.54	0.88	1.52	21	1
1	A	36	LEU	CB-CG	-19.31	1.14	1.53	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	100	LEU	CB-CG	-19.29	1.14	1.53	21	1
1	A	24	HIS	CB-CG	-18.87	1.23	1.50	21	1
1	A	70	GLN	CD-NE2	-18.40	0.94	1.33	21	1
1	A	117	GLN	CB-CG	-18.23	0.97	1.52	21	1
1	A	108	GLU	CG-CD	-18.04	1.06	1.52	21	1
1	A	73	LEU	CB-CG	-17.98	1.17	1.53	21	1
1	A	112	LYS	CE-NZ	-17.94	0.95	1.49	21	1
1	A	83	ASN	CG-OD1	-17.66	0.90	1.23	21	1
1	A	28	LYS	CD-CE	-17.55	0.99	1.52	21	1
1	A	105	LYS	CD-CE	-17.29	1.00	1.52	21	1
1	A	86	GLU	CG-CD	-16.96	1.09	1.52	21	1
1	A	104	LEU	CG-CD2	-16.81	0.97	1.52	21	1
1	A	21	GLN	CD-NE2	-16.61	0.98	1.33	21	1
1	A	100	LEU	CG-CD1	-16.53	0.97	1.52	21	1
1	A	101	LEU	CG-CD1	-16.46	0.98	1.52	21	1
1	A	52	GLN	CG-CD	-16.45	1.10	1.52	21	1
1	A	20	GLU	CB-CG	-16.43	1.03	1.52	21	1
1	A	38	HIS	ND1-CE1	-16.26	1.16	1.32	21	1
1	A	107	THR	CB-OG1	-16.22	1.17	1.43	21	1
1	A	56	ILE	CB-CG2	-16.04	0.99	1.52	21	1
1	A	31	HIS	CE1-NE2	-15.99	1.16	1.32	21	1
1	A	45	GLU	CB-CG	-15.92	1.04	1.52	21	1
1	A	30	GLU	CG-CD	-15.82	1.12	1.52	21	1
1	A	67	GLU	CG-CD	-15.55	1.13	1.52	21	1
1	A	117	GLN	CA-CB	-15.46	1.22	1.53	21	1
1	A	92	GLU	CG-CD	-15.42	1.13	1.52	21	1
1	A	46	ASN	CG-OD1	-15.35	0.94	1.23	21	1
1	A	34	LEU	CB-CG	-15.16	1.23	1.53	21	1
1	A	84	ILE	CG1-CD1	-14.87	0.93	1.51	21	1
1	A	87	ARG	CG-CD	-14.77	1.08	1.52	21	1
1	A	117	GLN	CA-C	-14.70	1.22	1.52	21	1
1	A	46	ASN	CB-CG	-14.60	1.15	1.52	21	1
1	A	102	LYS	CB-CG	-14.60	1.08	1.52	21	1
1	A	50	GLU	CG-CD	-14.26	1.16	1.52	21	1
1	A	115	GLN	CG-CD	-14.02	1.17	1.52	21	1
1	A	42	GLU	CB-CG	-13.77	1.11	1.52	21	1
1	A	49	LYS	CE-NZ	-13.63	1.08	1.49	21	1
1	A	32	GLN	CG-CD	-13.49	1.18	1.52	21	1
1	A	42	GLU	CG-CD	-13.43	1.18	1.52	21	1
1	A	98	LYS	CG-CD	-12.88	1.13	1.52	21	1
1	A	18	LEU	CB-CG	-12.78	1.27	1.53	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	31	HIS	CG-CD2	-12.74	1.21	1.35	21	1
1	A	75	ARG	CB-CG	-12.28	1.15	1.52	21	1
1	A	94	GLN	CG-CD	-12.21	1.21	1.52	21	1
1	A	101	LEU	CG-CD2	-12.05	1.12	1.52	21	1
1	A	38	HIS	CB-CG	-11.81	1.33	1.50	21	1
1	A	102	LYS	CE-NZ	-11.71	1.14	1.49	21	1
1	A	104	LEU	CB-CG	-11.54	1.30	1.53	21	1
1	A	75	ARG	CG-CD	-11.31	1.18	1.52	21	1
1	A	32	GLN	CB-CG	-11.23	1.18	1.52	21	1
1	A	27	GLU	CB-CG	-11.10	1.19	1.52	21	1
1	A	70	GLN	CG-CD	-11.04	1.24	1.52	21	1
1	A	28	LYS	CG-CD	-11.00	1.19	1.52	21	1
1	A	56	ILE	CG1-CD1	-10.72	1.09	1.51	21	1
1	A	21	GLN	CB-CG	-10.57	1.20	1.52	21	1
1	A	32	GLN	CD-NE2	-10.03	1.12	1.33	21	1
1	A	102	LYS	CD-CE	-9.84	1.23	1.52	21	1
1	A	87	ARG	CB-CG	-9.69	1.23	1.52	21	1
1	A	113	ASP	CB-CG	-9.49	1.28	1.52	21	1
1	A	76	GLU	CB-CG	-8.63	1.26	1.52	21	1
1	A	53	GLU	CG-CD	-8.57	1.30	1.52	21	1
1	A	23	ASN	CG-OD1	-8.47	1.07	1.23	21	1
1	A	111	VAL	CB-CG2	-8.43	1.24	1.52	21	1
1	A	34	LEU	CG-CD2	-8.30	1.25	1.52	21	1
1	A	107	THR	CB-CG2	-8.23	1.25	1.52	21	1
1	A	109	GLN	CB-CG	-8.01	1.28	1.52	21	1
1	A	111	VAL	CB-CG1	-7.96	1.26	1.52	21	1
1	A	78	LYS	CD-CE	-7.79	1.29	1.52	21	1
1	A	74	GLU	CB-CG	-7.76	1.29	1.52	21	1
1	A	83	ASN	CG-ND2	-7.61	1.17	1.33	21	1
1	A	91	GLU	CB-CG	-7.52	1.29	1.52	21	1
1	A	52	GLN	CB-CG	-7.35	1.30	1.52	21	1
1	A	58	GLU	CG-CD	-7.28	1.33	1.52	21	1
1	A	110	LYS	CD-CE	-7.25	1.30	1.52	21	1
1	A	37	GLN	CD-NE2	-6.88	1.18	1.33	21	1
1	A	30	GLU	CB-CG	-6.74	1.32	1.52	21	1
1	A	41	ASP	CB-CG	-6.70	1.35	1.52	21	1
1	A	112	LYS	CD-CE	-6.67	1.32	1.52	21	1
1	A	105	LYS	CB-CG	-6.26	1.33	1.52	21	1
1	A	34	LEU	CG-CD1	-5.80	1.33	1.52	21	1
1	A	103	ASP	CB-CG	-5.71	1.37	1.52	21	1
1	A	110	LYS	CB-CG	-5.62	1.35	1.52	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	47	LYS	CB-CG	-5.06	1.37	1.52	21	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	94	GLN	OE1-CD-NE2	-92.21	30.39	122.60	21	1
1	A	44	ASN	OD1-CG-ND2	-67.95	54.65	122.60	21	1
1	A	52	GLN	OE1-CD-NE2	-67.39	55.21	122.60	21	1
1	A	88	PHE	CD1-CG-CD2	-66.08	19.48	118.60	21	1
1	A	35	TYR	CD1-CG-CD2	-65.65	19.63	118.10	21	1
1	A	87	ARG	NH1-CZ-NH2	-59.05	42.54	119.30	21	1
1	A	87	ARG	NE-CZ-NH2	56.80	170.32	119.20	21	1
1	A	88	PHE	CE1-CZ-CE2	-55.63	19.86	120.00	21	1
1	A	35	TYR	CE1-CZ-CE2	-49.86	20.58	120.30	21	1
1	A	90	TYR	CD1-CG-CD2	-43.21	53.28	118.10	21	1
1	A	41	ASP	OD1-CG-OD2	-42.78	20.23	122.90	21	1
1	A	39	GLN	OE1-CD-NE2	-41.26	81.34	122.60	21	1
1	A	103	ASP	OD1-CG-OD2	-40.38	25.99	122.90	21	1
1	A	85	LEU	CD1-CG-CD2	-39.89	23.05	110.80	21	1
1	A	40	LEU	CD1-CG-CD2	-39.84	23.15	110.80	21	1
1	A	113	ASP	OD1-CG-OD2	-39.73	27.55	122.90	21	1
1	A	38	HIS	ND1-CG-CD2	-38.55	67.55	106.10	21	1
1	A	21	GLN	CG-CD-OE1	-37.32	46.17	120.80	21	1
1	A	50	GLU	OE1-CD-OE2	-36.47	35.38	122.90	21	1
1	A	108	GLU	OE1-CD-OE2	-36.33	35.70	122.90	21	1
1	A	57	ARG	NE-CZ-NH2	36.02	151.62	119.20	21	1
1	A	60	ASP	OD1-CG-OD2	-35.96	36.60	122.90	21	1
1	A	106	GLU	OE1-CD-OE2	-35.14	38.57	122.90	21	1
1	A	76	GLU	CB-CG-CD	34.56	171.36	112.60	21	1
1	A	92	GLU	OE1-CD-OE2	-34.56	39.95	122.90	21	1
1	A	86	GLU	OE1-CD-OE2	-33.62	42.22	122.90	21	1
1	A	94	GLN	CG-CD-NE2	33.56	166.75	116.40	21	1
1	A	87	ARG	CD-NE-CZ	33.39	171.15	124.40	21	1
1	A	27	GLU	OE1-CD-OE2	-33.24	43.12	122.90	21	1
1	A	35	TYR	CB-CG-CD1	33.17	170.55	120.80	21	1
1	A	52	GLN	CG-CD-NE2	33.16	166.14	116.40	21	1
1	A	35	TYR	CG-CD1-CE1	32.94	170.61	121.20	21	1
1	A	35	TYR	CB-CG-CD2	32.68	169.82	120.80	21	1
1	A	30	GLU	OE1-CD-OE2	-32.60	44.67	122.90	21	1
1	A	90	TYR	CE1-CZ-CE2	-32.45	55.40	120.30	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	20	GLU	OE1-CD-OE2	-32.43	45.07	122.90	21	1
1	A	35	TYR	CG-CD2-CE2	32.42	169.84	121.20	21	1
1	A	36	LEU	CD1-CG-CD2	-31.67	41.12	110.80	21	1
1	A	38	HIS	CG-CD2-NE2	31.58	138.78	107.20	21	1
1	A	89	ASN	OD1-CG-ND2	-31.47	91.13	122.60	21	1
1	A	21	GLN	CG-CD-NE2	30.98	162.87	116.40	21	1
1	A	70	GLN	OE1-CD-NE2	-30.96	91.64	122.60	21	1
1	A	42	GLU	OE1-CD-OE2	-30.67	49.28	122.90	21	1
1	A	53	GLU	OE1-CD-OE2	-30.26	50.27	122.90	21	1
1	A	88	PHE	CG-CD1-CE1	29.31	170.53	120.70	21	1
1	A	91	GLU	OE1-CD-OE2	-29.31	52.56	122.90	21	1
1	A	88	PHE	CB-CG-CD1	29.30	170.52	120.70	21	1
1	A	88	PHE	CB-CG-CD2	29.00	170.00	120.70	21	1
1	A	88	PHE	CG-CD2-CE2	28.99	169.99	120.70	21	1
1	A	75	ARG	NH1-CZ-NH2	-28.84	81.81	119.30	21	1
1	A	21	GLN	OE1-CD-NE2	28.37	150.97	122.60	21	1
1	A	75	ARG	NE-CZ-NH2	28.13	144.52	119.20	21	1
1	A	35	TYR	CZ-CE2-CD2	28.08	170.14	119.60	21	1
1	A	44	ASN	CB-CG-ND2	28.00	158.40	116.40	21	1
1	A	88	PHE	CZ-CE2-CD2	27.96	170.33	120.00	21	1
1	A	88	PHE	CD1-CE1-CZ	27.67	169.81	120.00	21	1
1	A	35	TYR	CD1-CE1-CZ	27.56	169.21	119.60	21	1
1	A	76	GLU	OE1-CD-OE2	-27.24	57.52	122.90	21	1
1	A	37	GLN	CG-CD-OE1	-27.04	66.72	120.80	21	1
1	A	27	GLU	CB-CG-CD	26.68	157.95	112.60	21	1
1	A	87	ARG	NE-CZ-NH1	25.64	147.14	121.50	21	1
1	A	110	LYS	CB-CG-CD	25.36	169.62	111.30	21	1
1	A	109	GLN	CB-CG-CD	24.96	155.03	112.60	21	1
1	A	21	GLN	CB-CG-CD	24.81	154.78	112.60	21	1
1	A	37	GLN	CG-CD-NE2	24.16	152.64	116.40	21	1
1	A	108	GLU	CB-CG-CD	23.74	152.95	112.60	21	1
1	A	110	LYS	CG-CD-CE	23.27	164.81	111.30	21	1
1	A	45	GLU	CB-CG-CD	22.97	151.65	112.60	21	1
1	A	41	ASP	CB-CG-OD1	22.71	170.62	118.40	21	1
1	A	70	GLN	CG-CD-NE2	22.66	150.39	116.40	21	1
1	A	54	LYS	CG-CD-CE	22.56	163.19	111.30	21	1
1	A	103	ASP	CB-CG-OD1	22.52	170.20	118.40	21	1
1	A	90	TYR	CB-CG-CD1	22.12	153.98	120.80	21	1
1	A	41	ASP	CB-CG-OD2	22.06	169.15	118.40	21	1
1	A	73	LEU	CD1-CG-CD2	-22.05	62.30	110.80	21	1
1	A	90	TYR	CG-CD1-CE1	21.90	154.04	121.20	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	87	ARG	CG-CD-NE	21.82	160.00	112.00	21	1
1	A	76	GLU	CG-CD-OE2	21.56	167.99	118.40	21	1
1	A	108	GLU	CG-CD-OE1	21.47	167.78	118.40	21	1
1	A	113	ASP	CB-CG-OD1	21.42	167.68	118.40	21	1
1	A	90	TYR	CB-CG-CD2	21.30	152.74	120.80	21	1
1	A	67	GLU	OE1-CD-OE2	-21.27	71.85	122.90	21	1
1	A	94	GLN	CB-CG-CD	21.24	148.71	112.60	21	1
1	A	90	TYR	CG-CD2-CE2	21.09	152.84	121.20	21	1
1	A	30	GLU	CG-CD-OE2	21.08	166.89	118.40	21	1
1	A	94	GLN	CG-CD-OE1	21.03	162.87	120.80	21	1
1	A	57	ARG	CD-NE-CZ	20.78	153.49	124.40	21	1
1	A	92	GLU	CG-CD-OE1	20.39	165.31	118.40	21	1
1	A	113	ASP	CB-CG-OD2	20.16	164.77	118.40	21	1
1	A	67	GLU	CG-CD-OE2	20.02	164.45	118.40	21	1
1	A	50	GLU	CG-CD-OE1	19.88	164.11	118.40	21	1
1	A	61	VAL	CG1-CB-CG2	-19.87	67.09	110.80	21	1
1	A	85	LEU	CB-CG-CD1	19.81	170.13	110.70	21	1
1	A	38	HIS	CE1-NE2-CD2	-19.77	89.23	109.00	21	1
1	A	40	LEU	CB-CG-CD1	19.76	169.97	110.70	21	1
1	A	103	ASP	CB-CG-OD2	19.74	163.81	118.40	21	1
1	A	58	GLU	OE1-CD-OE2	-19.56	75.97	122.90	21	1
1	A	43	LEU	CD1-CG-CD2	-19.37	68.19	110.80	21	1
1	A	60	ASP	CB-CG-OD2	19.18	162.52	118.40	21	1
1	A	106	GLU	CG-CD-OE1	19.07	162.27	118.40	21	1
1	A	86	GLU	CG-CD-OE1	19.00	162.11	118.40	21	1
1	A	75	ARG	CB-CG-CD	18.99	154.99	111.30	21	1
1	A	32	GLN	CG-CD-NE2	18.88	144.72	116.40	21	1
1	A	57	ARG	NE-CZ-NH1	-18.65	102.85	121.50	21	1
1	A	45	GLU	OE1-CD-OE2	-18.65	78.14	122.90	21	1
1	A	90	TYR	CZ-CE2-CD2	18.48	152.86	119.60	21	1
1	A	60	ASP	CB-CG-OD1	18.47	160.88	118.40	21	1
1	A	50	GLU	CG-CD-OE2	18.31	160.51	118.40	21	1
1	A	61	VAL	CA-CB-CG2	18.09	141.16	110.40	21	1
1	A	37	GLN	OE1-CD-NE2	18.03	140.63	122.60	21	1
1	A	27	GLU	CG-CD-OE1	18.01	159.82	118.40	21	1
1	A	61	VAL	CA-CB-CG1	18.00	141.00	110.40	21	1
1	A	90	TYR	CD1-CE1-CZ	17.77	151.58	119.60	21	1
1	A	85	LEU	CB-CG-CD2	17.74	163.92	110.70	21	1
1	A	40	LEU	CB-CG-CD2	17.72	163.87	110.70	21	1
1	A	106	GLU	CG-CD-OE2	17.72	159.16	118.40	21	1
1	A	91	GLU	CG-CD-OE1	17.67	159.04	118.40	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	24	HIS	ND1-CG-CD2	-17.60	88.50	106.10	21	1
1	A	52	GLN	CB-CG-CD	17.50	142.34	112.60	21	1
1	A	117	GLN	CG-CD-NE2	17.35	142.42	116.40	21	1
1	A	105	LYS	CB-CG-CD	17.27	151.03	111.30	21	1
1	A	20	GLU	CG-CD-OE1	17.27	158.12	118.40	21	1
1	A	36	LEU	CB-CG-CD2	16.90	161.39	110.70	21	1
1	A	42	GLU	CG-CD-OE1	16.89	157.26	118.40	21	1
1	A	27	GLU	CG-CD-OE2	16.81	157.05	118.40	21	1
1	A	35	TYR	OH-CZ-CE2	16.76	170.19	119.90	21	1
1	A	104	LEU	CD1-CG-CD2	-16.74	73.97	110.80	21	1
1	A	20	GLU	CG-CD-OE2	16.70	156.81	118.40	21	1
1	A	75	ARG	CD-NE-CZ	16.66	147.73	124.40	21	1
1	A	108	GLU	CG-CD-OE2	16.57	156.52	118.40	21	1
1	A	35	TYR	CE1-CZ-OH	16.44	169.23	119.90	21	1
1	A	37	GLN	CB-CG-CD	16.39	140.46	112.60	21	1
1	A	112	LYS	CB-CG-CD	16.33	148.86	111.30	21	1
1	A	115	GLN	OE1-CD-NE2	-16.25	106.34	122.60	21	1
1	A	86	GLU	CG-CD-OE2	16.21	155.68	118.40	21	1
1	A	91	GLU	CB-CG-CD	16.20	140.13	112.60	21	1
1	A	53	GLU	CG-CD-OE2	16.16	155.56	118.40	21	1
1	A	92	GLU	CG-CD-OE2	15.80	154.75	118.40	21	1
1	A	53	GLU	CG-CD-OE1	15.55	154.17	118.40	21	1
1	A	112	LYS	CA-CB-CG	15.46	145.02	114.10	21	1
1	A	38	HIS	CB-CG-CD2	15.35	151.16	131.20	21	1
1	A	42	GLU	CG-CD-OE2	15.24	153.46	118.40	21	1
1	A	70	GLN	CB-CG-CD	14.83	137.80	112.60	21	1
1	A	18	LEU	CD1-CG-CD2	-14.79	78.25	110.80	21	1
1	A	38	HIS	CG-ND1-CE1	14.78	134.42	109.30	21	1
1	A	87	ARG	CB-CG-CD	14.42	144.47	111.30	21	1
1	A	117	GLN	OE1-CD-NE2	-13.79	108.81	122.60	21	1
1	A	50	GLU	CB-CG-CD	13.71	135.90	112.60	21	1
1	A	94	GLN	CA-CB-CG	13.46	141.01	114.10	21	1
1	A	39	GLN	CG-CD-NE2	13.46	136.58	116.40	21	1
1	A	105	LYS	CD-CE-NZ	13.40	154.79	111.90	21	1
1	A	24	HIS	CG-CD2-NE2	13.15	120.35	107.20	21	1
1	A	44	ASN	CB-CG-OD1	13.08	146.96	120.80	21	1
1	A	30	GLU	CG-CD-OE1	13.06	148.44	118.40	21	1
1	A	91	GLU	CG-CD-OE2	13.04	148.40	118.40	21	1
1	A	108	GLU	CA-CB-CG	13.00	140.11	114.10	21	1
1	A	59	LEU	CD1-CG-CD2	-12.76	82.73	110.80	21	1
1	A	36	LEU	CB-CG-CD1	12.65	148.66	110.70	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	38	HIS	CB-CG-ND1	12.39	141.29	122.70	21	1
1	A	75	ARG	NE-CZ-NH1	12.18	133.68	121.50	21	1
1	A	43	LEU	CB-CG-CD1	12.15	147.16	110.70	21	1
1	A	75	ARG	CG-CD-NE	12.14	138.71	112.00	21	1
1	A	83	ASN	OD1-CG-ND2	-11.95	110.66	122.60	21	1
1	A	105	LYS	CG-CD-CE	11.94	138.77	111.30	21	1
1	A	45	GLU	CG-CD-OE2	11.75	145.42	118.40	21	1
1	A	117	GLN	CA-C-O	11.36	140.11	120.80	21	1
1	A	89	ASN	CB-CG-ND2	11.28	133.31	116.40	21	1
1	A	70	GLN	CA-CB-CG	11.10	136.30	114.10	21	1
1	A	110	LYS	CD-CE-NZ	11.09	147.38	111.90	21	1
1	A	90	TYR	OH-CZ-CE2	11.02	152.96	119.90	21	1
1	A	32	GLN	CG-CD-OE1	-11.00	98.80	120.80	21	1
1	A	20	GLU	CB-CG-CD	10.99	131.28	112.60	21	1
1	A	100	LEU	CB-CG-CD1	10.93	143.49	110.70	21	1
1	A	73	LEU	CB-CG-CD1	10.65	142.66	110.70	21	1
1	A	39	GLN	CG-CD-OE1	10.64	142.08	120.80	21	1
1	A	58	GLU	CG-CD-OE1	10.64	142.86	118.40	21	1
1	A	115	GLN	CG-CD-NE2	10.60	132.30	116.40	21	1
1	A	57	ARG	NH1-CZ-NH2	-10.59	105.54	119.30	21	1
1	A	90	TYR	CE1-CZ-OH	10.58	151.64	119.90	21	1
1	A	50	GLU	CA-CB-CG	10.16	134.42	114.10	21	1
1	A	18	LEU	CB-CG-CD2	10.04	140.81	110.70	21	1
1	A	56	ILE	CB-CG1-CD1	10.03	134.86	113.80	21	1
1	A	58	GLU	CG-CD-OE2	9.90	141.17	118.40	21	1
1	A	100	LEU	CD1-CG-CD2	-9.81	89.21	110.80	21	1
1	A	98	LYS	CG-CD-CE	9.72	133.65	111.30	21	1
1	A	30	GLU	CB-CG-CD	9.64	129.00	112.60	21	1
1	A	83	ASN	CB-CG-ND2	9.57	130.76	116.40	21	1
1	A	46	ASN	CB-CG-OD1	-9.41	101.97	120.80	21	1
1	A	117	GLN	CB-CG-CD	9.19	128.22	112.60	21	1
1	A	74	GLU	OE1-CD-OE2	-9.06	101.15	122.90	21	1
1	A	52	GLN	CG-CD-OE1	8.93	138.65	120.80	21	1
1	A	112	LYS	CD-CE-NZ	8.89	140.36	111.90	21	1
1	A	54	LYS	CD-CE-NZ	8.86	140.24	111.90	21	1
1	A	46	ASN	OD1-CG-ND2	8.80	131.40	122.60	21	1
1	A	56	ILE	CA-CB-CG2	8.51	124.97	110.50	21	1
1	A	31	HIS	ND1-CE1-NE2	8.47	116.87	108.40	21	1
1	A	73	LEU	CB-CG-CD2	8.43	135.99	110.70	21	1
1	A	97	SER	CA-CB-OG	8.40	127.91	111.10	21	1
1	A	63	CYS	CA-CB-SG	8.35	133.61	114.40	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	LYS	CD-CE-NZ	8.27	138.37	111.90	21	1
1	A	24	HIS	CG-ND1-CE1	8.26	123.35	109.30	21	1
1	A	86	GLU	CB-CG-CD	8.25	126.62	112.60	21	1
1	A	104	LEU	CB-CG-CD2	8.09	134.98	110.70	21	1
1	A	56	ILE	CA-CB-CG1	8.07	124.12	110.40	21	1
1	A	84	ILE	CB-CG1-CD1	8.05	130.70	113.80	21	1
1	A	102	LYS	CG-CD-CE	7.87	129.41	111.30	21	1
1	A	45	GLU	CG-CD-OE1	7.84	136.44	118.40	21	1
1	A	104	LEU	CB-CG-CD1	7.80	134.10	110.70	21	1
1	A	43	LEU	CB-CG-CD2	7.64	133.62	110.70	21	1
1	A	78	LYS	CD-CE-NZ	7.61	136.24	111.90	21	1
1	A	46	ASN	CA-CB-CG	7.60	120.20	112.60	21	1
1	A	89	ASN	CB-CG-OD1	7.38	135.56	120.80	21	1
1	A	24	HIS	CB-CG-ND1	7.32	133.68	122.70	21	1
1	A	74	GLU	CB-CG-CD	7.29	125.00	112.60	21	1
1	A	74	GLU	CG-CD-OE1	7.19	134.94	118.40	21	1
1	A	59	LEU	CB-CG-CD2	7.16	132.19	110.70	21	1
1	A	76	GLU	CG-CD-OE1	7.00	134.50	118.40	21	1
1	A	46	ASN	CB-CG-ND2	6.82	126.62	116.40	21	1
1	A	20	GLU	CA-CB-CG	6.74	127.58	114.10	21	1
1	A	101	LEU	CD1-CG-CD2	-6.61	96.26	110.80	21	1
1	A	59	LEU	CB-CG-CD1	6.45	130.06	110.70	21	1
1	A	31	HIS	CA-CB-CG	6.40	120.20	113.80	21	1
1	A	32	GLN	CB-CG-CD	-6.28	101.93	112.60	21	1
1	A	47	LYS	CB-CG-CD	6.17	125.49	111.30	21	1
1	A	32	GLN	OE1-CD-NE2	-6.11	116.49	122.60	21	1
1	A	56	ILE	CG1-CB-CG2	-6.10	92.40	110.70	21	1
1	A	117	GLN	CG-CD-OE1	-6.01	108.77	120.80	21	1
1	A	45	GLU	CA-CB-CG	5.93	125.97	114.10	21	1
1	A	31	HIS	ND1-CG-CD2	5.90	112.00	106.10	21	1
1	A	42	GLU	CA-CB-CG	5.89	125.89	114.10	21	1
1	A	24	HIS	ND1-CE1-NE2	-5.72	102.68	108.40	21	1
1	A	67	GLU	CB-CG-CD	5.62	122.15	112.60	21	1
1	A	101	LEU	CB-CG-CD2	5.62	127.55	110.70	21	1
1	A	98	LYS	CB-CG-CD	5.60	124.17	111.30	21	1
1	A	31	HIS	CB-CG-ND1	-5.48	114.48	122.70	21	1
1	A	28	LYS	CD-CE-NZ	5.41	129.22	111.90	21	1
1	A	24	HIS	CA-CB-CG	5.36	119.16	113.80	21	1
1	A	31	HIS	CG-ND1-CE1	-5.30	100.29	109.30	21	1
1	A	106	GLU	CB-CG-CD	5.30	121.61	112.60	21	1
1	A	102	LYS	CA-CB-CG	5.19	124.48	114.10	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	28	LYS	CB-CG-CD	5.12	123.09	111.30	21	1
1	A	24	HIS	CB-CG-CD2	5.10	137.83	131.20	21	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	788	803	803	37±83
All	All	16548	16863	16863	781

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:HIS:CG	1:A:38:HIS:CE1	1.63	1.82	21	1
1:A:36:LEU:CD2	1:A:36:LEU:CB	1.59	1.78	21	1
1:A:85:LEU:CD2	1:A:85:LEU:CB	1.55	1.84	21	1
1:A:18:LEU:CD1	1:A:18:LEU:CB	1.54	1.83	21	1
1:A:105:LYS:CG	1:A:105:LYS:CE	1.54	1.81	21	1
1:A:98:LYS:CE	1:A:98:LYS:CG	1.51	1.84	21	1
1:A:105:LYS:NZ	1:A:105:LYS:CD	1.51	1.70	21	1
1:A:40:LEU:CD2	1:A:40:LEU:CB	1.49	1.88	21	1
1:A:108:GLU:CB	1:A:108:GLU:CD	1.48	1.86	21	1
1:A:73:LEU:CD2	1:A:73:LEU:CB	1.48	1.88	21	1
1:A:73:LEU:CB	1:A:73:LEU:CD1	1.47	1.87	21	1
1:A:35:TYR:CZ	1:A:35:TYR:CD1	1.47	2.03	21	1
1:A:21:GLN:CG	1:A:21:GLN:NE2	1.45	1.72	21	1
1:A:35:TYR:CG	1:A:35:TYR:CE2	1.44	2.05	21	1
1:A:45:GLU:CD	1:A:45:GLU:CB	1.44	1.90	21	1
1:A:78:LYS:NZ	1:A:78:LYS:CD	1.43	1.82	21	1
1:A:21:GLN:CD	1:A:21:GLN:CB	1.43	1.92	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:GLU:CD	1:A:74:GLU:CB	1.43	1.91	21	1
1:A:43:LEU:CD2	1:A:43:LEU:CB	1.42	1.93	21	1
1:A:94:GLN:NE2	1:A:94:GLN:CG	1.42	1.81	21	1
1:A:50:GLU:CB	1:A:50:GLU:CD	1.41	1.92	21	1
1:A:94:GLN:CB	1:A:94:GLN:CD	1.41	1.93	21	1
1:A:88:PHE:CZ	1:A:88:PHE:CD1	1.41	2.06	21	1
1:A:90:TYR:CZ	1:A:90:TYR:CD1	1.40	2.08	21	1
1:A:88:PHE:CG	1:A:88:PHE:CE2	1.40	2.07	21	1
1:A:87:ARG:NE	1:A:87:ARG:CG	1.39	1.83	21	1
1:A:88:PHE:CG	1:A:88:PHE:CE1	1.39	2.11	21	1
1:A:50:GLU:OE1	1:A:50:GLU:CG	1.39	1.67	21	1
1:A:52:GLN:NE2	1:A:52:GLN:CG	1.38	1.86	21	1
1:A:90:TYR:CG	1:A:90:TYR:CE2	1.38	2.11	21	1
1:A:42:GLU:OE1	1:A:42:GLU:CG	1.36	1.70	21	1
1:A:92:GLU:OE1	1:A:92:GLU:CG	1.36	1.71	21	1
1:A:35:TYR:CZ	1:A:35:TYR:CD2	1.36	2.09	21	1
1:A:88:PHE:CZ	1:A:88:PHE:CD2	1.36	2.09	21	1
1:A:113:ASP:OD2	1:A:113:ASP:CB	1.35	1.73	21	1
1:A:90:TYR:CZ	1:A:90:TYR:CD2	1.35	2.11	21	1
1:A:35:TYR:CG	1:A:35:TYR:CE1	1.34	2.12	21	1
1:A:110:LYS:NZ	1:A:110:LYS:CD	1.34	1.87	21	1
1:A:30:GLU:OE2	1:A:30:GLU:CG	1.32	1.76	21	1
1:A:90:TYR:CG	1:A:90:TYR:CE1	1.32	2.14	21	1
1:A:70:GLN:CB	1:A:70:GLN:CD	1.31	2.03	21	1
1:A:103:ASP:OD2	1:A:103:ASP:CB	1.31	1.78	21	1
1:A:38:HIS:CG	1:A:38:HIS:NE2	1.30	1.93	21	1
1:A:117:GLN:O	1:A:117:GLN:CA	1.28	1.80	21	1
1:A:53:GLU:OE1	1:A:53:GLU:CG	1.27	1.81	21	1
1:A:61:VAL:CG1	1:A:61:VAL:CA	1.27	2.13	21	1
1:A:35:TYR:CD2	1:A:35:TYR:CB	1.26	2.18	21	1
1:A:61:VAL:CA	1:A:61:VAL:CG2	1.26	2.13	21	1
1:A:110:LYS:CG	1:A:110:LYS:CE	1.25	2.15	21	1
1:A:38:HIS:CD2	1:A:38:HIS:CB	1.24	2.20	21	1
1:A:113:ASP:CB	1:A:113:ASP:OD1	1.24	1.84	21	1
1:A:41:ASP:OD2	1:A:41:ASP:CB	1.24	1.84	21	1
1:A:39:GLN:NE2	1:A:39:GLN:CG	1.23	2.00	21	1
1:A:88:PHE:CD2	1:A:88:PHE:CB	1.23	2.19	21	1
1:A:21:GLN:CB	1:A:21:GLN:OE1	1.23	1.72	21	1
1:A:53:GLU:CG	1:A:53:GLU:OE2	1.23	1.84	21	1
1:A:59:LEU:CD1	1:A:59:LEU:CB	1.23	2.15	21	1
1:A:38:HIS:CB	1:A:38:HIS:ND1	1.22	2.03	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ASN:OD1	1:A:44:ASN:CB	1.22	1.87	21	1
1:A:59:LEU:CB	1:A:59:LEU:CD2	1.21	2.19	21	1
1:A:40:LEU:CB	1:A:40:LEU:CD1	1.20	2.16	21	1
1:A:43:LEU:CB	1:A:43:LEU:CD1	1.20	2.18	21	1
1:A:58:GLU:OE2	1:A:58:GLU:CG	1.20	1.89	21	1
1:A:63:CYS:CB	1:A:63:CYS:SG	1.20	1.11	21	1
1:A:90:TYR:CD2	1:A:90:TYR:CB	1.19	2.23	21	1
1:A:110:LYS:CD	1:A:110:LYS:CB	1.19	2.21	21	1
1:A:41:ASP:CB	1:A:41:ASP:OD1	1.18	1.92	21	1
1:A:18:LEU:CB	1:A:18:LEU:CD2	1.18	2.03	21	1
1:A:85:LEU:CB	1:A:85:LEU:CD1	1.18	2.19	21	1
1:A:94:GLN:CG	1:A:94:GLN:CA	1.18	2.20	21	1
1:A:105:LYS:CD	1:A:105:LYS:CB	1.18	2.20	21	1
1:A:54:LYS:CE	1:A:54:LYS:CG	1.17	2.22	21	1
1:A:76:GLU:CD	1:A:76:GLU:CB	1.17	2.16	21	1
1:A:58:GLU:CG	1:A:58:GLU:OE1	1.15	1.92	21	1
1:A:109:GLN:CD	1:A:109:GLN:CB	1.15	2.17	21	1
1:A:90:TYR:CD1	1:A:90:TYR:CB	1.15	2.27	21	1
1:A:108:GLU:CG	1:A:108:GLU:CA	1.14	2.25	21	1
1:A:84:ILE:CD1	1:A:84:ILE:CB	1.13	2.25	21	1
1:A:112:LYS:CG	1:A:112:LYS:CA	1.13	2.27	21	1
1:A:50:GLU:CG	1:A:50:GLU:CA	1.13	2.26	21	1
1:A:112:LYS:CB	1:A:112:LYS:CD	1.12	2.25	21	1
1:A:35:TYR:CE1	1:A:35:TYR:OH	1.12	2.02	21	1
1:A:61:VAL:CG1	1:A:61:VAL:HG23	1.11	1.70	21	1
1:A:70:GLN:CG	1:A:70:GLN:CA	1.10	2.29	21	1
1:A:88:PHE:CD1	1:A:88:PHE:CB	1.09	2.23	21	1
1:A:73:LEU:CD1	1:A:73:LEU:HG	1.08	1.63	21	1
1:A:43:LEU:CD2	1:A:43:LEU:HD12	1.07	1.66	21	1
1:A:61:VAL:CG2	1:A:61:VAL:HG12	1.06	1.70	21	1
1:A:63:CYS:SG	1:A:63:CYS:CA	1.06	2.43	21	1
1:A:90:TYR:CE1	1:A:90:TYR:OH	1.06	2.07	21	1
1:A:60:ASP:OD1	1:A:60:ASP:CB	1.05	2.02	21	1
1:A:43:LEU:CD1	1:A:43:LEU:HD23	1.04	1.67	21	1
1:A:73:LEU:CD2	1:A:73:LEU:HG	1.04	1.72	21	1
1:A:73:LEU:CD2	1:A:73:LEU:HD12	1.04	1.81	21	1
1:A:103:ASP:CB	1:A:103:ASP:OD1	1.04	2.05	21	1
1:A:44:ASN:CB	1:A:44:ASN:ND2	1.03	2.21	21	1
1:A:60:ASP:CB	1:A:60:ASP:OD2	1.02	2.07	21	1
1:A:61:VAL:CG2	1:A:61:VAL:HB	1.02	1.57	21	1
1:A:84:ILE:CG1	1:A:84:ILE:HD12	1.02	1.55	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:LEU:CD1	1:A:18:LEU:HG	1.01	1.62	21	1
1:A:39:GLN:CG	1:A:39:GLN:OE1	1.01	2.03	21	1
1:A:84:ILE:CG1	1:A:84:ILE:HD13	1.01	1.55	21	1
1:A:18:LEU:CD2	1:A:18:LEU:HG	1.01	1.61	21	1
1:A:40:LEU:HD22	1:A:107:THR:HG23	1.00	1.28	12	3
1:A:61:VAL:CG1	1:A:61:VAL:HB	0.99	1.57	21	1
1:A:73:LEU:CD1	1:A:73:LEU:HD23	0.98	1.79	21	1
1:A:84:ILE:CG1	1:A:84:ILE:HD11	0.98	1.55	21	1
1:A:90:TYR:CE2	1:A:90:TYR:OH	0.98	2.11	21	1
1:A:63:CYS:SG	1:A:63:CYS:HB3	0.98	1.64	21	1
1:A:109:GLN:CD	1:A:109:GLN:CG	0.98	0.94	21	1
1:A:18:LEU:CG	1:A:18:LEU:HD23	0.98	1.51	21	1
1:A:43:LEU:CD1	1:A:43:LEU:HG	0.97	1.57	21	1
1:A:18:LEU:CG	1:A:18:LEU:HD21	0.97	1.51	21	1
1:A:74:GLU:CD	1:A:74:GLU:HG2	0.97	1.46	21	1
1:A:63:CYS:SG	1:A:63:CYS:HB2	0.97	1.64	21	1
1:A:73:LEU:CG	1:A:73:LEU:HD21	0.96	1.49	21	1
1:A:74:GLU:CD	1:A:74:GLU:HG3	0.96	1.46	21	1
1:A:18:LEU:CG	1:A:18:LEU:HD22	0.95	1.51	21	1
1:A:70:GLN:CG	1:A:70:GLN:HB3	0.95	1.48	21	1
1:A:59:LEU:CD2	1:A:59:LEU:HG	0.95	1.62	21	1
1:A:73:LEU:CG	1:A:73:LEU:HD22	0.95	1.49	21	1
1:A:109:GLN:CD	1:A:109:GLN:HG3	0.95	1.43	21	1
1:A:84:ILE:CD1	1:A:84:ILE:HG12	0.94	1.50	21	1
1:A:45:GLU:CD	1:A:45:GLU:HG2	0.94	1.43	21	1
1:A:50:GLU:CB	1:A:50:GLU:HG3	0.94	1.47	21	1
1:A:50:GLU:CB	1:A:50:GLU:HG2	0.94	1.47	21	1
1:A:109:GLN:CD	1:A:109:GLN:HG2	0.94	1.43	21	1
1:A:45:GLU:CD	1:A:45:GLU:HG3	0.94	1.43	21	1
1:A:84:ILE:CD1	1:A:84:ILE:HG13	0.94	1.50	21	1
1:A:117:GLN:O	1:A:117:GLN:C	0.94	0.69	21	1
1:A:59:LEU:CG	1:A:59:LEU:HD13	0.94	1.48	21	1
1:A:59:LEU:CG	1:A:59:LEU:HD23	0.93	1.49	21	1
1:A:38:HIS:CG	1:A:38:HIS:CD2	0.93	0.93	21	1
1:A:59:LEU:CG	1:A:59:LEU:HD22	0.93	1.49	21	1
1:A:105:LYS:CG	1:A:105:LYS:HD3	0.93	1.48	21	1
1:A:84:ILE:CD1	1:A:84:ILE:CG1	0.93	0.93	21	1
1:A:59:LEU:CG	1:A:59:LEU:HD21	0.93	1.49	21	1
1:A:98:LYS:NZ	1:A:98:LYS:HE2	0.93	1.34	21	1
1:A:105:LYS:CG	1:A:105:LYS:HD2	0.93	1.48	21	1
1:A:50:GLU:CG	1:A:50:GLU:HB2	0.93	1.48	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:GLU:CG	1:A:50:GLU:HB3	0.93	1.48	21	1
1:A:36:LEU:CD2	1:A:36:LEU:HG	0.93	1.57	21	1
1:A:73:LEU:HD23	1:A:73:LEU:CG	0.93	1.49	21	1
1:A:45:GLU:CD	1:A:45:GLU:CG	0.92	0.92	21	1
1:A:59:LEU:CG	1:A:59:LEU:HD12	0.92	1.48	21	1
1:A:70:GLN:CB	1:A:70:GLN:HG2	0.92	1.48	21	1
1:A:70:GLN:CB	1:A:70:GLN:CG	0.92	0.93	21	1
1:A:105:LYS:CG	1:A:105:LYS:CD	0.92	0.93	21	1
1:A:44:ASN:ND2	1:A:44:ASN:CG	0.92	0.82	21	1
1:A:70:GLN:CG	1:A:70:GLN:HB2	0.92	1.48	21	1
1:A:70:GLN:CB	1:A:70:GLN:HG3	0.92	1.48	21	1
1:A:87:ARG:NE	1:A:87:ARG:HD3	0.92	1.30	21	1
1:A:59:LEU:CD1	1:A:59:LEU:HG	0.91	1.62	21	1
1:A:98:LYS:NZ	1:A:98:LYS:HE3	0.91	1.34	21	1
1:A:50:GLU:CB	1:A:50:GLU:CG	0.91	0.91	21	1
1:A:73:LEU:CG	1:A:73:LEU:HD13	0.91	1.45	21	1
1:A:105:LYS:NZ	1:A:105:LYS:HE3	0.91	1.29	21	1
1:A:59:LEU:CG	1:A:59:LEU:HD11	0.90	1.48	21	1
1:A:74:GLU:CD	1:A:74:GLU:CG	0.90	0.86	21	1
1:A:78:LYS:NZ	1:A:78:LYS:HE2	0.90	1.28	21	1
1:A:98:LYS:CE	1:A:98:LYS:HD3	0.90	1.44	21	1
1:A:76:GLU:CD	1:A:76:GLU:CG	0.90	0.91	21	1
1:A:105:LYS:CG	1:A:105:LYS:HE3	0.90	1.95	21	1
1:A:105:LYS:CD	1:A:105:LYS:HG3	0.90	1.44	21	1
1:A:98:LYS:CE	1:A:98:LYS:HD2	0.89	1.44	21	1
1:A:103:ASP:OD1	1:A:103:ASP:CG	0.89	0.69	21	1
1:A:43:LEU:CD2	1:A:43:LEU:HG	0.89	1.46	21	1
1:A:98:LYS:HE2	1:A:98:LYS:CD	0.89	1.50	21	1
1:A:87:ARG:NE	1:A:87:ARG:HD2	0.89	1.30	21	1
1:A:73:LEU:HD12	1:A:73:LEU:CG	0.89	1.45	21	1
1:A:105:LYS:NZ	1:A:105:LYS:HE2	0.89	1.29	21	1
1:A:73:LEU:CG	1:A:73:LEU:HD11	0.89	1.45	21	1
1:A:105:LYS:CD	1:A:105:LYS:HG2	0.89	1.44	21	1
1:A:18:LEU:CG	1:A:18:LEU:HD11	0.88	1.42	21	1
1:A:18:LEU:CG	1:A:18:LEU:HD12	0.88	1.42	21	1
1:A:18:LEU:CG	1:A:18:LEU:HD13	0.88	1.42	21	1
1:A:78:LYS:NZ	1:A:78:LYS:HE3	0.88	1.28	21	1
1:A:43:LEU:HD12	1:A:43:LEU:CG	0.88	1.41	21	1
1:A:18:LEU:CD2	1:A:18:LEU:CG	0.88	0.88	21	1
1:A:76:GLU:CD	1:A:76:GLU:HG3	0.88	1.36	21	1
1:A:43:LEU:CG	1:A:43:LEU:HD11	0.87	1.41	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:GLN:O	1:A:117:GLN:CB	0.87	2.22	21	1
1:A:108:GLU:CG	1:A:108:GLU:HB3	0.87	1.41	21	1
1:A:85:LEU:CG	1:A:85:LEU:HD13	0.86	1.40	21	1
1:A:87:ARG:NE	1:A:87:ARG:CD	0.86	0.78	21	1
1:A:43:LEU:CG	1:A:43:LEU:HD13	0.86	1.41	21	1
1:A:98:LYS:CE	1:A:98:LYS:CD	0.86	0.86	21	1
1:A:85:LEU:CG	1:A:85:LEU:HD11	0.86	1.40	21	1
1:A:35:TYR:CD1	1:A:35:TYR:CB	0.86	2.25	21	1
1:A:85:LEU:CG	1:A:85:LEU:HD12	0.86	1.40	21	1
1:A:112:LYS:CG	1:A:112:LYS:HB2	0.86	1.39	21	1
1:A:59:LEU:CD2	1:A:59:LEU:CG	0.85	0.86	21	1
1:A:60:ASP:OD2	1:A:60:ASP:CG	0.85	0.63	21	1
1:A:76:GLU:CD	1:A:76:GLU:HG2	0.85	1.36	21	1
1:A:108:GLU:CG	1:A:108:GLU:HB2	0.85	1.41	21	1
1:A:112:LYS:CB	1:A:112:LYS:HG3	0.85	1.38	21	1
1:A:73:LEU:CD2	1:A:73:LEU:CD1	0.85	0.85	21	1
1:A:108:GLU:CB	1:A:108:GLU:CG	0.85	0.85	21	1
1:A:73:LEU:CD2	1:A:73:LEU:CG	0.85	0.85	21	1
1:A:61:VAL:CB	1:A:61:VAL:HG21	0.84	1.37	21	1
1:A:112:LYS:CB	1:A:112:LYS:HG2	0.84	1.38	21	1
1:A:112:LYS:CG	1:A:112:LYS:HB3	0.84	1.39	21	1
1:A:112:LYS:CG	1:A:112:LYS:CB	0.84	0.84	21	1
1:A:61:VAL:HG12	1:A:61:VAL:CB	0.84	1.37	21	1
1:A:110:LYS:NZ	1:A:110:LYS:HE3	0.84	1.25	21	1
1:A:94:GLN:CG	1:A:94:GLN:HB2	0.84	1.37	21	1
1:A:40:LEU:CG	1:A:40:LEU:HD12	0.83	1.37	21	1
1:A:110:LYS:NZ	1:A:110:LYS:HE2	0.83	1.25	21	1
1:A:59:LEU:CD1	1:A:59:LEU:CG	0.83	0.83	21	1
1:A:54:LYS:CD	1:A:54:LYS:HE2	0.83	1.38	21	1
1:A:61:VAL:HG23	1:A:61:VAL:CB	0.83	1.37	21	1
1:A:40:LEU:CG	1:A:40:LEU:HD13	0.83	1.37	21	1
1:A:94:GLN:CG	1:A:94:GLN:HB3	0.83	1.37	21	1
1:A:36:LEU:CD2	1:A:36:LEU:HD12	0.83	1.38	21	1
1:A:40:LEU:CG	1:A:40:LEU:HD11	0.83	1.37	21	1
1:A:61:VAL:CB	1:A:61:VAL:HG11	0.83	1.37	21	1
1:A:108:GLU:CB	1:A:108:GLU:HG2	0.83	1.38	21	1
1:A:61:VAL:CB	1:A:61:VAL:HG13	0.83	1.37	21	1
1:A:88:PHE:CE1	1:A:88:PHE:HZ	0.83	1.61	21	1
1:A:108:GLU:CB	1:A:108:GLU:HG3	0.83	1.38	21	1
1:A:73:LEU:HD23	1:A:77:LEU:HD23	0.83	1.49	2	6
1:A:61:VAL:CB	1:A:61:VAL:HG22	0.83	1.37	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:LYS:HE3	1:A:98:LYS:CD	0.82	1.50	21	1
1:A:105:LYS:CE	1:A:105:LYS:NZ	0.82	0.74	21	1
1:A:54:LYS:NZ	1:A:54:LYS:HE3	0.82	1.40	21	1
1:A:94:GLN:CB	1:A:94:GLN:HG3	0.82	1.35	21	1
1:A:30:GLU:OE2	1:A:30:GLU:CD	0.81	0.65	21	1
1:A:110:LYS:CG	1:A:110:LYS:HD2	0.81	1.35	21	1
1:A:94:GLN:CB	1:A:94:GLN:HG2	0.81	1.35	21	1
1:A:44:ASN:OD1	1:A:44:ASN:ND2	0.81	0.67	21	1
1:A:54:LYS:CD	1:A:54:LYS:HE3	0.81	1.38	21	1
1:A:110:LYS:CG	1:A:110:LYS:HD3	0.81	1.35	21	1
1:A:21:GLN:CD	1:A:21:GLN:HG2	0.80	1.31	21	1
1:A:78:LYS:NZ	1:A:78:LYS:CE	0.80	0.65	21	1
1:A:22:ALA:HB2	1:A:73:LEU:HD22	0.80	1.53	11	1
1:A:60:ASP:OD1	1:A:60:ASP:CG	0.80	0.58	21	1
1:A:110:LYS:CD	1:A:110:LYS:HG2	0.80	1.33	21	1
1:A:53:GLU:OE2	1:A:53:GLU:CD	0.80	0.57	21	1
1:A:36:LEU:CG	1:A:36:LEU:HD23	0.80	1.34	21	1
1:A:110:LYS:CD	1:A:110:LYS:CG	0.80	0.86	21	1
1:A:73:LEU:CD1	1:A:73:LEU:CG	0.79	0.80	21	1
1:A:105:LYS:CG	1:A:105:LYS:HE2	0.79	2.03	21	1
1:A:73:LEU:CD2	1:A:73:LEU:HB3	0.79	2.07	21	1
1:A:110:LYS:CD	1:A:110:LYS:HG3	0.79	1.33	21	1
1:A:94:GLN:CG	1:A:94:GLN:CB	0.79	0.79	21	1
1:A:109:GLN:CD	1:A:109:GLN:HE22	0.79	1.46	21	1
1:A:109:GLN:CD	1:A:109:GLN:HE21	0.79	1.46	21	1
1:A:44:ASN:CG	1:A:44:ASN:HD21	0.79	1.45	21	1
1:A:90:TYR:CD1	1:A:90:TYR:CG	0.78	0.81	21	1
1:A:40:LEU:HD23	1:A:107:THR:HG22	0.78	1.55	3	1
1:A:61:VAL:CG1	1:A:61:VAL:HG22	0.77	1.31	21	1
1:A:61:VAL:CG2	1:A:61:VAL:HG13	0.77	1.31	21	1
1:A:53:GLU:OE1	1:A:53:GLU:CD	0.77	0.55	21	1
1:A:98:LYS:CE	1:A:98:LYS:HG3	0.77	2.03	21	1
1:A:36:LEU:HD12	1:A:36:LEU:HD21	0.77	0.99	21	1
1:A:54:LYS:CE	1:A:54:LYS:HD2	0.77	1.31	21	1
1:A:61:VAL:CG1	1:A:61:VAL:CG2	0.77	0.78	21	1
1:A:54:LYS:CE	1:A:54:LYS:HD3	0.77	1.31	21	1
1:A:110:LYS:NZ	1:A:110:LYS:CE	0.77	0.64	21	1
1:A:43:LEU:CD1	1:A:43:LEU:HD22	0.77	1.30	21	1
1:A:110:LYS:HD3	1:A:110:LYS:HG2	0.77	1.01	21	1
1:A:40:LEU:HD13	1:A:111:VAL:HG22	0.76	1.57	3	1
1:A:18:LEU:CD1	1:A:18:LEU:CG	0.76	0.77	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LEU:CD2	1:A:43:LEU:HD13	0.76	1.30	21	1
1:A:40:LEU:HD22	1:A:107:THR:HG22	0.76	1.56	1	1
1:A:43:LEU:CD1	1:A:43:LEU:CG	0.76	0.76	21	1
1:A:54:LYS:CE	1:A:54:LYS:CD	0.75	0.80	21	1
1:A:38:HIS:CG	1:A:38:HIS:HD2	0.75	1.53	21	1
1:A:43:LEU:CD2	1:A:43:LEU:CD1	0.75	0.75	21	1
1:A:90:TYR:CG	1:A:90:TYR:CD2	0.75	0.78	21	1
1:A:90:TYR:CZ	1:A:90:TYR:CE2	0.75	0.79	21	1
1:A:44:ASN:CG	1:A:44:ASN:HD22	0.75	1.45	21	1
1:A:92:GLU:OE1	1:A:92:GLU:CD	0.75	0.59	21	1
1:A:41:ASP:OD1	1:A:41:ASP:CG	0.74	0.57	21	1
1:A:18:LEU:CD1	1:A:18:LEU:HB2	0.74	2.06	21	1
1:A:63:CYS:CB	1:A:63:CYS:HG	0.74	1.89	21	1
1:A:113:ASP:OD1	1:A:113:ASP:CG	0.74	0.57	21	1
1:A:35:TYR:CE2	1:A:35:TYR:OH	0.74	2.09	21	1
1:A:21:GLN:CG	1:A:21:GLN:CD	0.74	0.76	21	1
1:A:39:GLN:CD	1:A:39:GLN:HE21	0.74	1.39	21	1
1:A:26:ILE:HD12	1:A:96:LEU:HD12	0.74	1.59	16	10
1:A:73:LEU:CD1	1:A:73:LEU:HD22	0.74	1.31	21	1
1:A:42:GLU:OE1	1:A:42:GLU:CD	0.74	0.54	21	1
1:A:85:LEU:CD1	1:A:85:LEU:CG	0.73	0.74	21	1
1:A:36:LEU:HD23	1:A:36:LEU:HD11	0.73	0.99	21	1
1:A:43:LEU:CG	1:A:43:LEU:HD22	0.73	1.27	21	1
1:A:43:LEU:HD23	1:A:43:LEU:CG	0.73	1.27	21	1
1:A:54:LYS:HE2	1:A:54:LYS:NZ	0.73	1.40	21	1
1:A:52:GLN:CD	1:A:52:GLN:HE22	0.73	1.41	21	1
1:A:21:GLN:OE1	1:A:21:GLN:HG3	0.73	0.98	21	1
1:A:44:ASN:OD1	1:A:44:ASN:CG	0.73	0.49	21	1
1:A:109:GLN:CD	1:A:109:GLN:NE2	0.73	0.83	21	1
1:A:52:GLN:CD	1:A:52:GLN:HE21	0.72	1.41	21	1
1:A:52:GLN:NE2	1:A:52:GLN:CD	0.72	0.76	21	1
1:A:39:GLN:CD	1:A:39:GLN:HE22	0.72	1.39	21	1
1:A:61:VAL:HG13	1:A:61:VAL:HG22	0.71	1.00	21	1
1:A:21:GLN:CG	1:A:21:GLN:OE1	0.71	0.58	21	1
1:A:90:TYR:CZ	1:A:90:TYR:CE1	0.71	0.76	21	1
1:A:19:ILE:HD11	1:A:90:TYR:CD1	0.71	2.20	11	20
1:A:74:GLU:CD	1:A:74:GLU:HB3	0.71	2.09	21	1
1:A:40:LEU:HD12	1:A:111:VAL:HG23	0.71	1.63	17	3
1:A:54:LYS:CE	1:A:54:LYS:HZ2	0.71	1.41	21	1
1:A:73:LEU:HD22	1:A:73:LEU:HD13	0.71	0.77	21	1
1:A:61:VAL:CG2	1:A:61:VAL:CB	0.70	0.70	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:VAL:CG1	1:A:61:VAL:CB	0.70	0.70	21	1
1:A:40:LEU:CD1	1:A:40:LEU:CG	0.70	0.70	21	1
1:A:73:LEU:CD1	1:A:73:LEU:HB2	0.70	2.11	21	1
1:A:54:LYS:CE	1:A:54:LYS:HZ1	0.69	1.41	21	1
1:A:36:LEU:HD11	1:A:55:ILE:HG23	0.69	1.62	20	4
1:A:39:GLN:OE1	1:A:39:GLN:CD	0.69	0.74	21	1
1:A:50:GLU:CD	1:A:50:GLU:OE1	0.69	0.52	21	1
1:A:54:LYS:CE	1:A:54:LYS:HZ3	0.68	1.41	21	1
1:A:54:LYS:CE	1:A:54:LYS:NZ	0.68	0.83	21	1
1:A:32:GLN:CD	1:A:62:VAL:HG11	0.68	2.13	6	7
1:A:58:GLU:OE2	1:A:58:GLU:CD	0.68	0.65	21	1
1:A:110:LYS:NZ	1:A:110:LYS:HD3	0.67	2.02	21	1
1:A:41:ASP:OD2	1:A:41:ASP:CG	0.67	0.50	21	1
1:A:38:HIS:CG	1:A:38:HIS:ND1	0.67	0.81	21	1
1:A:43:LEU:CD1	1:A:43:LEU:HD21	0.67	0.76	21	1
1:A:43:LEU:CG	1:A:43:LEU:HD21	0.67	1.27	21	1
1:A:42:GLU:OE1	1:A:42:GLU:CB	0.67	2.35	21	1
1:A:88:PHE:CZ	1:A:88:PHE:CE2	0.66	0.72	21	1
1:A:88:PHE:CZ	1:A:88:PHE:CE1	0.66	0.68	21	1
1:A:40:LEU:HD13	1:A:107:THR:HG23	0.65	1.66	19	2
1:A:40:LEU:CG	1:A:40:LEU:HD23	0.65	1.18	21	1
1:A:117:GLN:O	1:A:117:GLN:HB3	0.65	1.90	21	1
1:A:73:LEU:CD2	1:A:73:LEU:HD13	0.64	1.21	21	1
1:A:39:GLN:NE2	1:A:39:GLN:CD	0.64	0.75	21	1
1:A:58:GLU:OE1	1:A:58:GLU:CD	0.64	0.67	21	1
1:A:33:LEU:HD11	1:A:103:ASP:CG	0.64	2.17	9	2
1:A:36:LEU:HD13	1:A:59:LEU:CD1	0.64	2.23	9	2
1:A:38:HIS:CG	1:A:38:HIS:HD1	0.64	1.39	21	1
1:A:40:LEU:CG	1:A:40:LEU:HD22	0.64	1.18	21	1
1:A:40:LEU:HD22	1:A:107:THR:CG2	0.64	2.23	1	3
1:A:73:LEU:CD2	1:A:73:LEU:HD11	0.64	1.02	21	1
1:A:43:LEU:HD13	1:A:43:LEU:HD22	0.63	0.99	21	1
1:A:40:LEU:HD13	1:A:107:THR:CG2	0.63	2.23	15	2
1:A:61:VAL:CG1	1:A:61:VAL:HG21	0.63	0.92	21	1
1:A:40:LEU:CG	1:A:40:LEU:HD21	0.63	1.18	21	1
1:A:87:ARG:CZ	1:A:87:ARG:HH22	0.63	1.33	21	1
1:A:85:LEU:CG	1:A:85:LEU:HD23	0.62	1.16	21	1
1:A:105:LYS:CE	1:A:105:LYS:HZ1	0.62	1.33	21	1
1:A:113:ASP:OD2	1:A:113:ASP:CG	0.62	0.46	21	1
1:A:21:GLN:CB	1:A:73:LEU:HD11	0.62	2.23	9	4
1:A:73:LEU:CD1	1:A:73:LEU:HD21	0.62	1.01	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ILE:HD12	1:A:96:LEU:CD1	0.62	2.23	7	8
1:A:36:LEU:HD22	1:A:107:THR:HG21	0.62	1.71	14	2
1:A:85:LEU:CG	1:A:85:LEU:HD22	0.62	1.16	21	1
1:A:87:ARG:CZ	1:A:87:ARG:HH21	0.62	1.33	21	1
1:A:105:LYS:CE	1:A:105:LYS:HZ2	0.62	1.33	21	1
1:A:18:LEU:HD23	1:A:77:LEU:HB3	0.62	1.71	5	1
1:A:98:LYS:CE	1:A:98:LYS:NZ	0.62	0.66	21	1
1:A:110:LYS:O	1:A:114:ILE:HD12	0.62	1.95	17	9
1:A:43:LEU:HD21	1:A:111:VAL:HG23	0.61	1.72	8	2
1:A:40:LEU:HD13	1:A:107:THR:HG22	0.61	1.70	13	3
1:A:94:GLN:CD	1:A:94:GLN:HE21	0.61	1.28	21	1
1:A:85:LEU:CD1	1:A:85:LEU:HD23	0.61	1.16	21	1
1:A:105:LYS:CE	1:A:105:LYS:HZ3	0.61	1.33	21	1
1:A:32:GLN:NE2	1:A:62:VAL:HG11	0.61	2.11	11	8
1:A:21:GLN:HB3	1:A:73:LEU:HD11	0.61	1.71	3	5
1:A:35:TYR:CD1	1:A:35:TYR:CG	0.61	0.75	21	1
1:A:107:THR:O	1:A:111:VAL:HG23	0.61	1.95	13	8
1:A:43:LEU:CD2	1:A:114:ILE:HD13	0.61	2.25	17	1
1:A:105:LYS:HE3	1:A:105:LYS:HG2	0.61	1.60	21	1
1:A:52:GLN:OE1	1:A:111:VAL:HG22	0.60	1.96	18	1
1:A:90:TYR:CG	1:A:90:TYR:HD1	0.60	1.37	21	1
1:A:61:VAL:HG22	1:A:65:MET:CE	0.60	2.26	11	3
1:A:33:LEU:HD23	1:A:104:LEU:HD12	0.60	1.74	10	3
1:A:40:LEU:HD12	1:A:111:VAL:CG2	0.59	2.27	15	2
1:A:35:TYR:CZ	1:A:35:TYR:CE1	0.59	0.66	21	1
1:A:40:LEU:HD23	1:A:111:VAL:HG22	0.59	1.74	10	2
1:A:63:CYS:HB2	1:A:104:LEU:HD23	0.59	1.74	21	1
1:A:90:TYR:CG	1:A:90:TYR:HD2	0.59	1.35	21	1
1:A:43:LEU:CD2	1:A:111:VAL:HG23	0.59	2.28	20	2
1:A:26:ILE:HD12	1:A:96:LEU:HB2	0.59	1.75	20	1
1:A:90:TYR:CZ	1:A:90:TYR:HE2	0.59	1.35	21	1
1:A:35:TYR:CZ	1:A:35:TYR:CE2	0.59	0.73	21	1
1:A:30:GLU:CB	1:A:100:LEU:HD21	0.58	2.28	7	1
1:A:88:PHE:CD1	1:A:88:PHE:CG	0.58	0.73	21	1
1:A:73:LEU:CD1	1:A:77:LEU:HD23	0.58	2.29	12	1
1:A:22:ALA:HB2	1:A:73:LEU:HD13	0.58	1.75	18	1
1:A:103:ASP:OD2	1:A:103:ASP:CG	0.58	0.42	21	1
1:A:40:LEU:CD1	1:A:40:LEU:HD23	0.58	1.15	21	1
1:A:61:VAL:CG2	1:A:61:VAL:HG11	0.57	0.92	21	1
1:A:36:LEU:HD13	1:A:59:LEU:HD13	0.57	1.77	9	3
1:A:94:GLN:NE2	1:A:94:GLN:CD	0.57	0.61	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:LYS:CE	1:A:98:LYS:HZ2	0.57	1.27	21	1
1:A:88:PHE:CG	1:A:88:PHE:CD2	0.57	0.70	21	1
1:A:98:LYS:CE	1:A:98:LYS:HZ1	0.57	1.27	21	1
1:A:98:LYS:CE	1:A:98:LYS:HZ3	0.57	1.27	21	1
1:A:90:TYR:CZ	1:A:90:TYR:HE1	0.56	1.34	21	1
1:A:52:GLN:O	1:A:56:ILE:HG22	0.56	2.01	3	10
1:A:39:GLN:HB3	1:A:55:ILE:HD11	0.56	1.77	11	1
1:A:78:LYS:CE	1:A:78:LYS:HZ3	0.56	1.27	21	1
1:A:40:LEU:HD23	1:A:111:VAL:CG2	0.56	2.31	10	3
1:A:36:LEU:O	1:A:36:LEU:HD23	0.56	1.99	14	2
1:A:57:ARG:O	1:A:61:VAL:HG23	0.56	2.01	6	4
1:A:43:LEU:CD2	1:A:43:LEU:CG	0.56	0.56	21	1
1:A:78:LYS:CE	1:A:78:LYS:HZ1	0.56	1.27	21	1
1:A:110:LYS:CE	1:A:110:LYS:HZ1	0.56	1.25	21	1
1:A:43:LEU:HD13	1:A:43:LEU:O	0.55	2.01	1	5
1:A:78:LYS:CE	1:A:78:LYS:HZ2	0.55	1.27	21	1
1:A:101:LEU:HA	1:A:104:LEU:HD23	0.55	1.79	11	1
1:A:110:LYS:CE	1:A:110:LYS:HZ2	0.55	1.25	21	1
1:A:40:LEU:HD13	1:A:111:VAL:CG2	0.55	2.28	3	1
1:A:19:ILE:HD11	1:A:90:TYR:CE1	0.55	2.37	11	10
1:A:63:CYS:SG	1:A:104:LEU:HD13	0.55	2.42	11	1
1:A:32:GLN:OE1	1:A:62:VAL:HG21	0.55	2.01	13	1
1:A:40:LEU:HG	1:A:107:THR:HG23	0.54	1.79	16	4
1:A:36:LEU:HD11	1:A:107:THR:HG21	0.54	1.78	15	1
1:A:85:LEU:HD11	1:A:85:LEU:HD23	0.54	0.71	21	1
1:A:110:LYS:CE	1:A:110:LYS:HZ3	0.54	1.26	21	1
1:A:35:TYR:CG	1:A:35:TYR:CD2	0.54	0.69	21	1
1:A:43:LEU:HD13	1:A:51:LEU:HG	0.54	1.78	15	6
1:A:85:LEU:CG	1:A:85:LEU:HD21	0.54	1.16	21	1
1:A:63:CYS:SG	1:A:63:CYS:C	0.54	2.91	21	1
1:A:40:LEU:CD2	1:A:107:THR:HG23	0.53	2.27	9	2
1:A:40:LEU:HD11	1:A:110:LYS:HB3	0.53	1.80	17	3
1:A:85:LEU:HD13	1:A:85:LEU:HD22	0.53	0.55	21	1
1:A:47:LYS:CD	1:A:114:ILE:HG23	0.53	2.33	1	12
1:A:112:LYS:HG2	1:A:112:LYS:HB3	0.53	1.23	21	1
1:A:58:GLU:O	1:A:62:VAL:HG23	0.52	2.04	20	17
1:A:18:LEU:HD22	1:A:77:LEU:HB3	0.52	1.82	19	5
1:A:36:LEU:CD2	1:A:36:LEU:CG	0.52	0.66	21	1
1:A:87:ARG:CZ	1:A:87:ARG:NH2	0.52	0.67	21	1
1:A:59:LEU:O	1:A:63:CYS:HB3	0.52	2.05	21	1
1:A:73:LEU:CD2	1:A:77:LEU:HD23	0.52	2.34	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:LEU:CD2	1:A:85:LEU:HD13	0.52	1.15	21	1
1:A:97:SER:O	1:A:101:LEU:HD23	0.51	2.05	18	1
1:A:85:LEU:CD2	1:A:85:LEU:HD11	0.51	1.06	21	1
1:A:32:GLN:NE2	1:A:62:VAL:HG21	0.51	2.20	15	1
1:A:36:LEU:HD23	1:A:36:LEU:CD1	0.51	1.42	21	1
1:A:21:GLN:HB2	1:A:73:LEU:HD11	0.51	1.83	10	3
1:A:18:LEU:HD11	1:A:77:LEU:HD23	0.51	1.81	14	1
1:A:74:GLU:OE1	1:A:77:LEU:HD21	0.51	2.06	4	1
1:A:40:LEU:HD11	1:A:40:LEU:HD23	0.51	0.65	21	1
1:A:63:CYS:SG	1:A:104:LEU:HD22	0.50	2.47	6	1
1:A:43:LEU:CD2	1:A:43:LEU:HD11	0.50	1.08	21	1
1:A:109:GLN:CD	1:A:109:GLN:OE1	0.50	0.76	21	1
1:A:52:GLN:CD	1:A:56:ILE:HD11	0.50	2.31	18	2
1:A:34:LEU:HD12	1:A:35:TYR:N	0.50	2.21	13	1
1:A:36:LEU:HD23	1:A:55:ILE:HG23	0.50	1.84	4	1
1:A:59:LEU:HD21	1:A:104:LEU:HG	0.50	1.84	5	2
1:A:32:GLN:O	1:A:36:LEU:HD23	0.50	2.07	6	1
1:A:30:GLU:HA	1:A:100:LEU:HD11	0.50	1.83	7	1
1:A:59:LEU:HD23	1:A:108:GLU:CB	0.49	2.37	19	1
1:A:32:GLN:O	1:A:36:LEU:HB2	0.49	2.07	21	1
1:A:33:LEU:HD11	1:A:103:ASP:OD1	0.49	2.07	1	1
1:A:32:GLN:O	1:A:36:LEU:HD12	0.49	2.08	9	2
1:A:61:VAL:HG12	1:A:65:MET:CE	0.49	2.37	17	2
1:A:37:GLN:OE1	1:A:107:THR:HG23	0.49	2.07	5	1
1:A:36:LEU:O	1:A:36:LEU:HD13	0.49	2.08	20	1
1:A:43:LEU:HD23	1:A:51:LEU:HB3	0.49	1.84	3	5
1:A:59:LEU:O	1:A:59:LEU:HD23	0.49	2.08	5	4
1:A:33:LEU:HD11	1:A:103:ASP:OD2	0.48	2.08	9	1
1:A:35:TYR:CG	1:A:35:TYR:HD1	0.48	1.24	21	1
1:A:73:LEU:O	1:A:73:LEU:HD13	0.48	2.09	12	1
1:A:26:ILE:HD12	1:A:96:LEU:HD13	0.48	1.86	19	1
1:A:18:LEU:HD13	1:A:90:TYR:OH	0.48	2.09	4	1
1:A:42:GLU:O	1:A:46:ASN:HB2	0.48	2.08	21	1
1:A:53:GLU:OE1	1:A:53:GLU:OE2	0.48	0.48	21	1
1:A:43:LEU:HD13	1:A:43:LEU:C	0.48	2.34	16	5
1:A:77:LEU:HD13	1:A:90:TYR:CE2	0.48	2.44	5	2
1:A:22:ALA:HB2	1:A:73:LEU:CD2	0.48	2.31	11	1
1:A:29:GLY:HA3	1:A:100:LEU:HD21	0.47	1.85	18	2
1:A:88:PHE:CG	1:A:88:PHE:HD1	0.47	1.23	21	1
1:A:33:LEU:C	1:A:33:LEU:HD13	0.47	2.34	20	21
1:A:40:LEU:HD13	1:A:40:LEU:C	0.47	2.35	20	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:LEU:HD13	1:A:100:LEU:C	0.47	2.34	14	5
1:A:30:GLU:HB2	1:A:100:LEU:HD21	0.47	1.87	2	1
1:A:70:GLN:OE1	1:A:101:LEU:HD21	0.47	2.10	9	1
1:A:85:LEU:HD13	1:A:85:LEU:C	0.47	2.34	10	1
1:A:40:LEU:CD2	1:A:40:LEU:HD11	0.47	1.01	21	1
1:A:36:LEU:CD2	1:A:107:THR:HG21	0.47	2.40	12	1
1:A:77:LEU:HD12	1:A:78:LYS:N	0.47	2.25	12	2
1:A:36:LEU:HD22	1:A:36:LEU:HD13	0.47	0.48	21	1
1:A:22:ALA:HB2	1:A:73:LEU:HD21	0.47	1.86	8	2
1:A:43:LEU:O	1:A:43:LEU:HD13	0.47	2.10	12	1
1:A:100:LEU:C	1:A:100:LEU:HD13	0.46	2.34	5	3
1:A:59:LEU:HD13	1:A:108:GLU:HG2	0.46	1.87	12	1
1:A:35:TYR:CZ	1:A:35:TYR:HE2	0.46	1.23	21	1
1:A:43:LEU:C	1:A:43:LEU:HD13	0.46	2.35	7	2
1:A:18:LEU:HD12	1:A:19:ILE:HG12	0.46	1.87	4	1
1:A:40:LEU:C	1:A:40:LEU:HD13	0.46	2.36	11	2
1:A:18:LEU:HD13	1:A:77:LEU:CB	0.46	2.41	7	1
1:A:21:GLN:CD	1:A:21:GLN:HG3	0.46	1.31	21	1
1:A:40:LEU:HG	1:A:107:THR:HG22	0.46	1.87	8	2
1:A:88:PHE:CZ	1:A:88:PHE:HE2	0.46	1.22	21	1
1:A:59:LEU:C	1:A:59:LEU:HD13	0.45	2.37	2	1
1:A:94:GLN:NE2	1:A:94:GLN:OE1	0.45	0.33	21	1
1:A:73:LEU:HD13	1:A:77:LEU:HD23	0.45	1.87	12	1
1:A:36:LEU:C	1:A:36:LEU:HD13	0.45	2.36	13	1
1:A:88:PHE:CG	1:A:88:PHE:HD2	0.45	1.21	21	1
1:A:36:LEU:CD2	1:A:36:LEU:CD1	0.45	0.46	21	1
1:A:53:GLU:O	1:A:57:ARG:HD3	0.45	2.12	21	1
1:A:88:PHE:CZ	1:A:88:PHE:HE1	0.45	1.20	21	1
1:A:19:ILE:HD11	1:A:90:TYR:HD1	0.45	1.69	19	4
1:A:100:LEU:C	1:A:100:LEU:HD12	0.45	2.37	20	1
1:A:40:LEU:HD13	1:A:40:LEU:HD22	0.45	0.50	21	1
1:A:40:LEU:CD2	1:A:55:ILE:HG21	0.45	2.41	8	1
1:A:35:TYR:CG	1:A:35:TYR:HD2	0.45	1.20	21	1
1:A:108:GLU:CA	1:A:108:GLU:HG3	0.45	2.19	21	1
1:A:32:GLN:O	1:A:36:LEU:HD13	0.44	2.12	3	1
1:A:40:LEU:HD11	1:A:110:LYS:HD2	0.44	1.89	5	1
1:A:23:ASN:O	1:A:27:GLU:HB2	0.44	2.12	21	1
1:A:73:LEU:HD12	1:A:74:GLU:N	0.44	2.27	6	2
1:A:73:LEU:HD22	1:A:77:LEU:HD23	0.44	1.88	16	1
1:A:33:LEU:O	1:A:33:LEU:HD22	0.44	2.11	20	1
1:A:40:LEU:HD12	1:A:40:LEU:O	0.44	2.13	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:LEU:C	1:A:104:LEU:HD12	0.43	2.38	11	1
1:A:70:GLN:OE1	1:A:101:LEU:HD11	0.43	2.13	13	1
1:A:36:LEU:HD13	1:A:36:LEU:O	0.43	2.13	13	1
1:A:36:LEU:HD11	1:A:55:ILE:CG2	0.43	2.39	20	1
1:A:85:LEU:CD1	1:A:85:LEU:HD22	0.43	1.00	21	1
1:A:56:ILE:HD13	1:A:112:LYS:HG3	0.43	1.89	4	1
1:A:105:LYS:HD2	1:A:105:LYS:HG3	0.43	1.39	21	1
1:A:47:LYS:HD2	1:A:114:ILE:HG23	0.43	1.91	21	3
1:A:63:CYS:CB	1:A:104:LEU:HD23	0.43	2.43	7	2
1:A:40:LEU:CD2	1:A:40:LEU:HD13	0.43	1.11	21	1
1:A:110:LYS:O	1:A:114:ILE:HD13	0.43	2.14	14	2
1:A:50:GLU:CG	1:A:50:GLU:N	0.43	2.81	21	1
1:A:33:LEU:HD23	1:A:104:LEU:CD1	0.43	2.43	13	1
1:A:35:TYR:CZ	1:A:35:TYR:HE1	0.43	1.19	21	1
1:A:97:SER:HA	1:A:100:LEU:HD23	0.42	1.91	1	1
1:A:56:ILE:HG13	1:A:111:VAL:HG11	0.42	1.91	13	1
1:A:42:GLU:OE1	1:A:42:GLU:OE2	0.42	0.43	21	1
1:A:47:LYS:HD3	1:A:114:ILE:HG23	0.42	1.91	12	2
1:A:36:LEU:HD11	1:A:107:THR:CG2	0.42	2.45	15	1
1:A:100:LEU:HD12	1:A:100:LEU:C	0.41	2.40	9	1
1:A:116:THR:O	1:A:117:GLN:C	0.41	2.64	20	1
1:A:24:HIS:CD2	1:A:24:HIS:HA	0.41	2.50	21	1
1:A:77:LEU:HD12	1:A:77:LEU:C	0.41	2.40	12	1
1:A:40:LEU:HD23	1:A:41:ASP:N	0.41	2.30	19	1
1:A:47:LYS:O	1:A:116:THR:HG22	0.41	2.16	18	1
1:A:54:LYS:HE2	1:A:54:LYS:HD3	0.41	1.26	21	1
1:A:43:LEU:CD1	1:A:55:ILE:HD12	0.41	2.46	6	1
1:A:65:MET:HG3	1:A:66:ILE:HD12	0.41	1.93	7	1
1:A:59:LEU:HD22	1:A:108:GLU:HB3	0.41	1.93	4	1
1:A:30:GLU:CA	1:A:100:LEU:HD21	0.41	2.46	7	1
1:A:40:LEU:HD11	1:A:111:VAL:CG2	0.41	2.46	13	1
1:A:40:LEU:O	1:A:40:LEU:HD22	0.40	2.16	10	1
1:A:59:LEU:HD22	1:A:108:GLU:CG	0.40	2.46	12	1
1:A:36:LEU:CD2	1:A:36:LEU:HD13	0.40	1.14	21	1
1:A:84:ILE:CD1	1:A:84:ILE:CG2	0.40	2.95	21	1
1:A:85:LEU:C	1:A:85:LEU:HD23	0.40	2.41	9	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/119 (80%)	93±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	49	83
All	All	1995/2499 (80%)	1953 (98%)	40 (2%)	2 (0%)	49	83

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	18	LEU	2

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	87/109 (80%)	74±5 (85±6%)	13±5 (15±6%)	5	41
All	All	1827/2289 (80%)	1545 (85%)	282 (15%)	5	41

All 55 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	32	GLN	16
1	A	83	ASN	16
1	A	49	LYS	16
1	A	114	ILE	13
1	A	85	LEU	11
1	A	57	ARG	11
1	A	73	LEU	10
1	A	97	SER	10
1	A	107	THR	9
1	A	54	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	115	GLN	8
1	A	37	GLN	8
1	A	48	SER	7
1	A	70	GLN	7
1	A	98	LYS	7
1	A	23	ASN	6
1	A	100	LEU	6
1	A	40	LEU	6
1	A	43	LEU	6
1	A	110	LYS	6
1	A	105	LYS	6
1	A	78	LYS	5
1	A	104	LEU	5
1	A	18	LEU	5
1	A	36	LEU	5
1	A	112	LYS	5
1	A	103	ASP	5
1	A	52	GLN	5
1	A	21	GLN	4
1	A	58	GLU	4
1	A	101	LEU	3
1	A	28	LYS	3
1	A	74	GLU	3
1	A	59	LEU	3
1	A	44	ASN	2
1	A	108	GLU	2
1	A	106	GLU	2
1	A	76	GLU	2
1	A	117	GLN	2
1	A	102	LYS	2
1	A	34	LEU	2
1	A	33	LEU	2
1	A	20	GLU	2
1	A	94	GLN	2
1	A	109	GLN	2
1	A	42	GLU	2
1	A	30	GLU	1
1	A	53	GLU	1
1	A	60	ASP	1
1	A	24	HIS	1
1	A	38	HIS	1
1	A	56	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	61	VAL	1
1	A	63	CYS	1
1	A	75	ARG	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	21-A	17

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
21	A	81:ASP	C	82:LEU	N	1.04
21	A	16:HIS	C	17:LEU	N	0.93
21	A	3:HIS	C	4:LYS	N	0.83
21	A	5:PRO	C	6:LYS	N	0.81

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
21	A	7:LYS	C	8:ASP	N	0.81
21	A	11:ARG	C	12:ASN	N	0.77
21	A	15:ASP	C	16:HIS	N	0.69
21	A	2:GLU	C	3:HIS	N	0.65
21	A	6:LYS	C	7:LYS	N	0.65
21	A	12:ASN	C	13:GLU	N	0.65
21	A	14:PHE	C	15:ASP	N	0.60
21	A	4:LYS	C	5:PRO	N	0.55
21	A	13:GLU	C	14:PHE	N	0.54
21	A	10:PHE	C	11:ARG	N	0.49
21	A	1:GLN	C	2:GLU	N	0.46
21	A	9:ASP	C	10:PHE	N	0.39
21	A	8:ASP	C	9:ASP	N	0.33

7 Chemical shift validation

No chemical shift data were provided