Full wwPDB NMR Structure Validation Report (i)

Dec 13, 2023 – 10:52 PM EST

PDB ID	:	2JMH
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 (i) 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 (i)) were used in the production of this report:

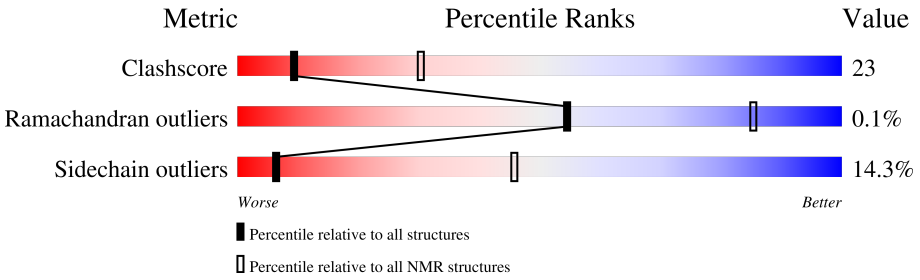
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	119	54% 27% 18% .

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
			Total	C	H	N	O	S	
1	A	117	1954	608	978	172	194	2	0

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

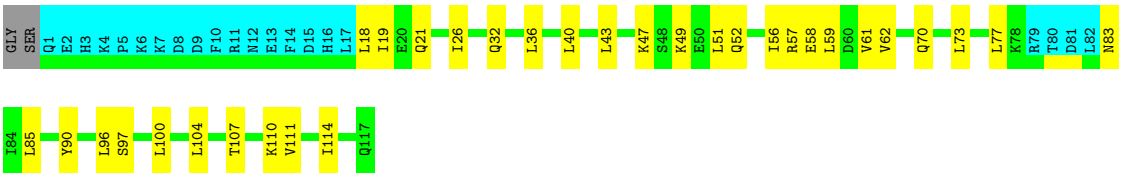
4 Residue-property plots

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

Chain A: 



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

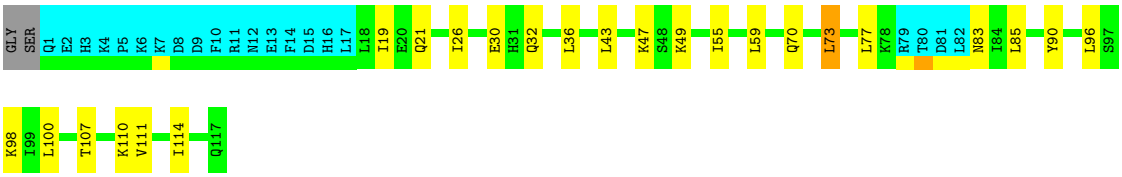
• Molecule 1: Mite allergen Blo t 5

Chain A: 

4.2.2 Score per residue for model 2

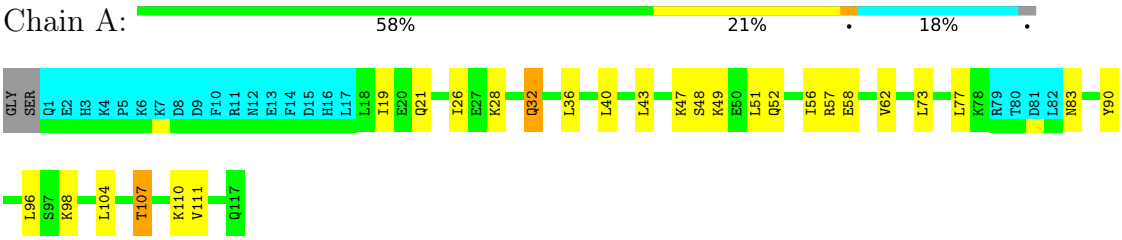
• Molecule 1: Mite allergen Blo t 5

Chain A: 



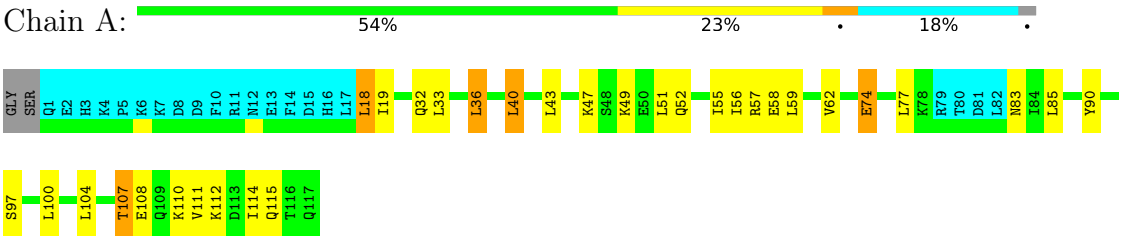
4.2.3 Score per residue for model 3

• Molecule 1: Mite allergen Blo t 5



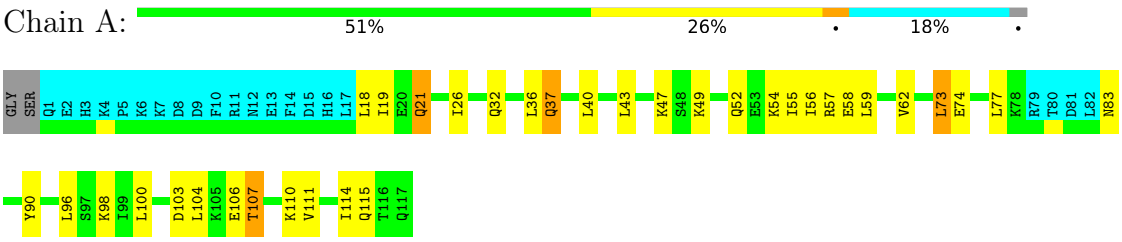
4.2.4 Score per residue for model 4

• Molecule 1: Mite allergen Blo t 5



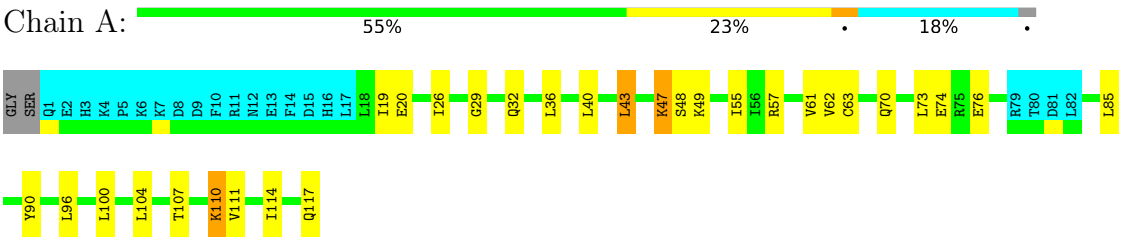
4.2.5 Score per residue for model 5

• Molecule 1: Mite allergen Blo t 5



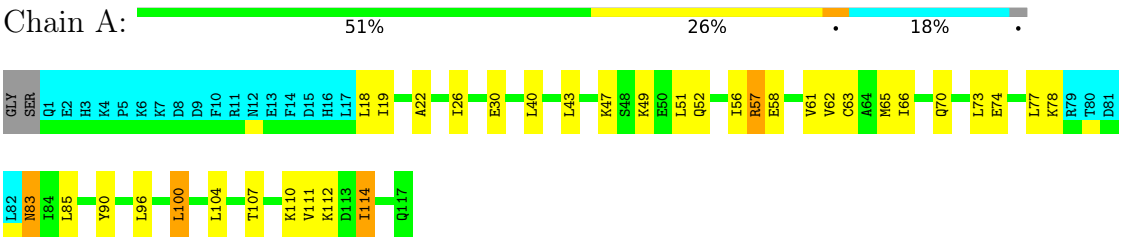
4.2.6 Score per residue for model 6

• Molecule 1: Mite allergen Blo t 5



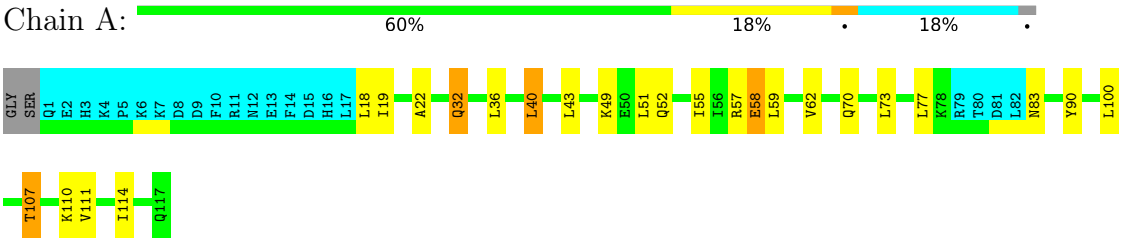
4.2.7 Score per residue for model 7

• Molecule 1: Mite allergen Blo t 5



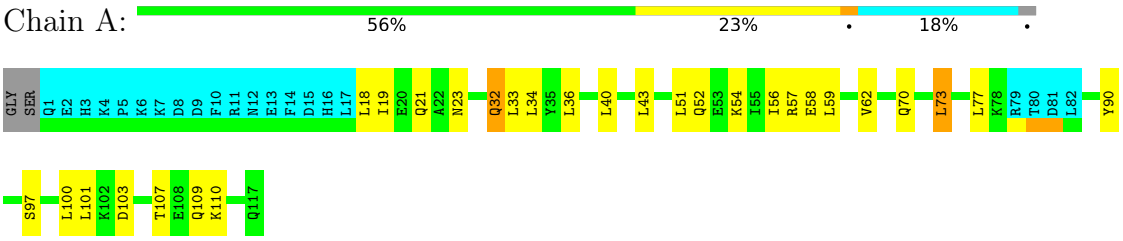
4.2.8 Score per residue for model 8

• Molecule 1: Mite allergen Blo t 5



4.2.9 Score per residue for model 9

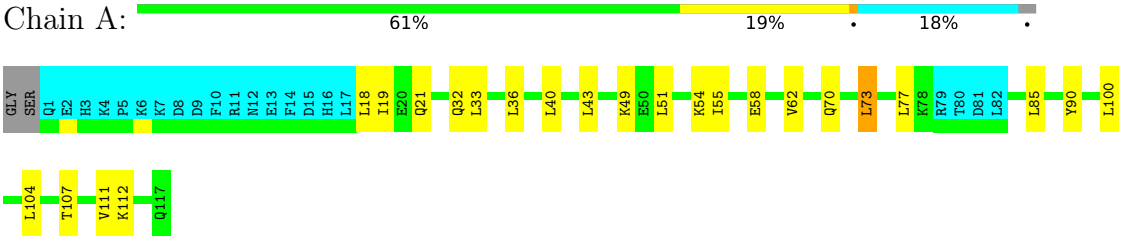
• Molecule 1: Mite allergen Blo t 5



4.2.10 Score per residue for model 10

• Molecule 1: Mite allergen Blo t 5

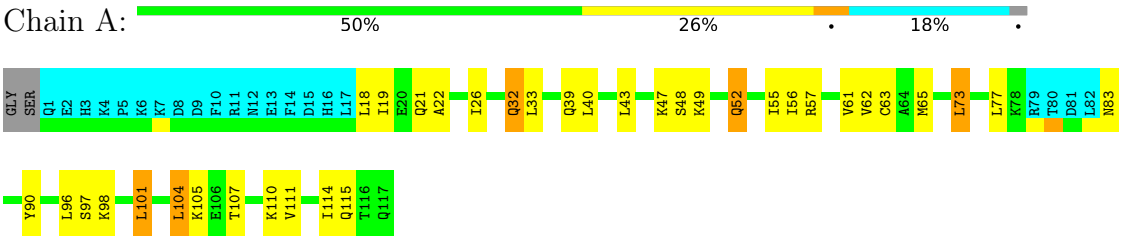
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Mite allergen Blo t 5

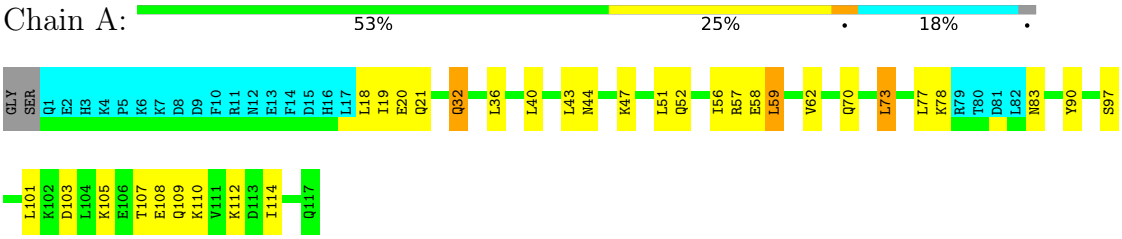
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Mite allergen Blo t 5

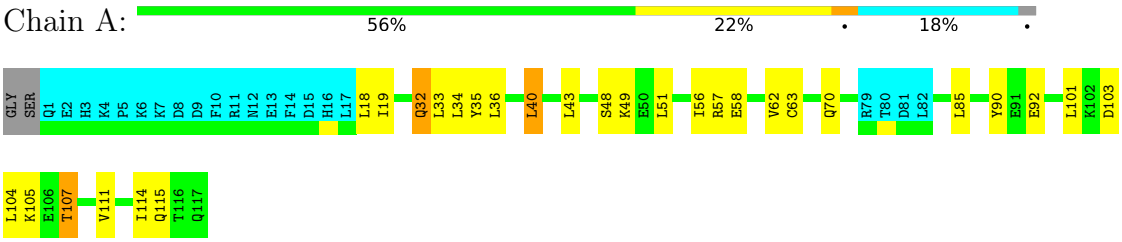
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Mite allergen Blo t 5

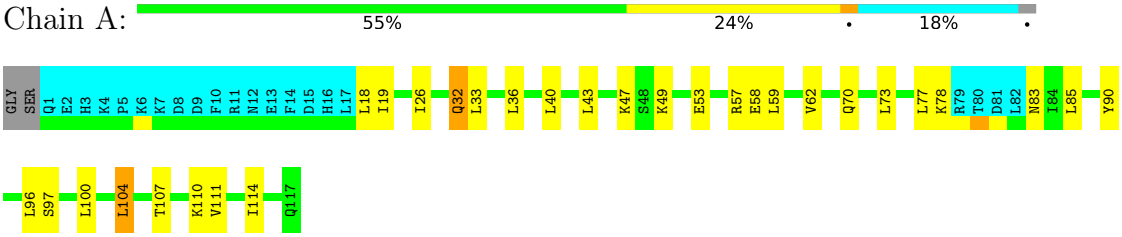
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Mite allergen Blo t 5

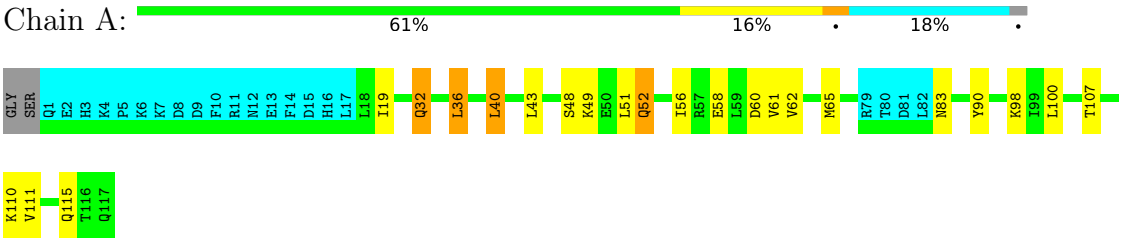
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Mite allergen Blo t 5

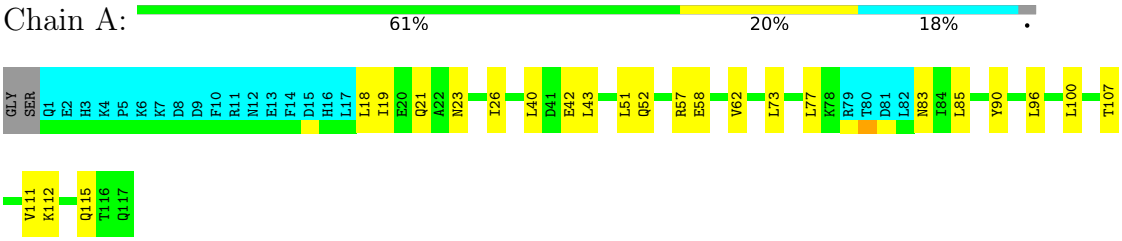
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Mite allergen Blo t 5

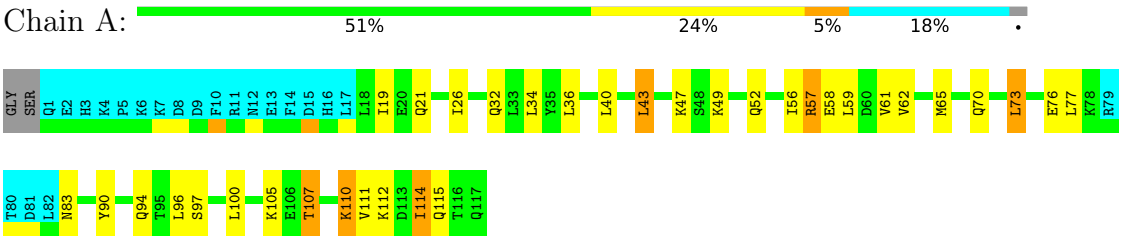
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Mite allergen Blo t 5

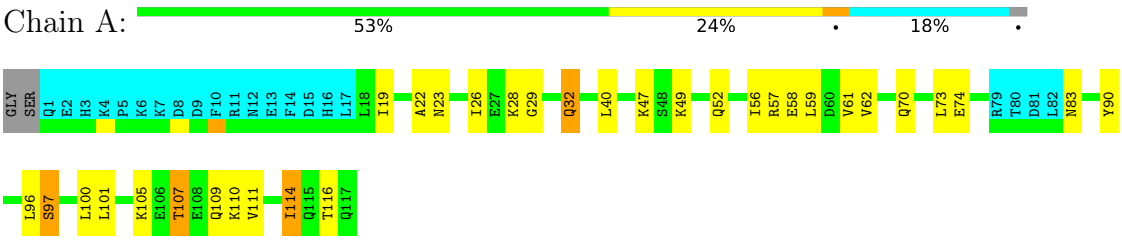
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Mite allergen Blo t 5

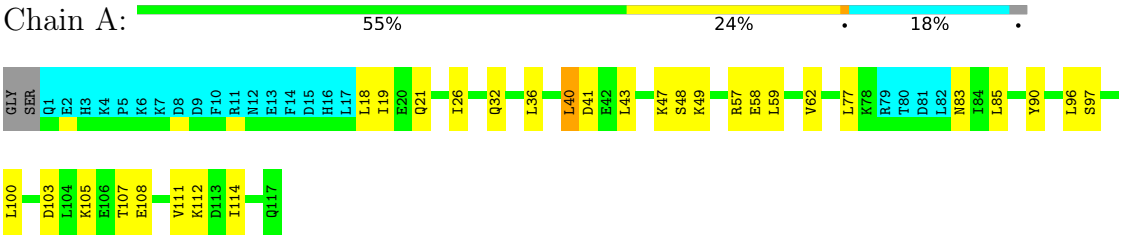
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Mite allergen Blo t 5

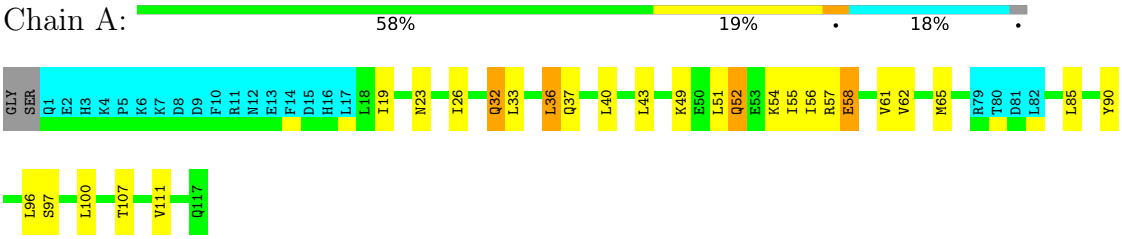
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Mite allergen Blo t 5

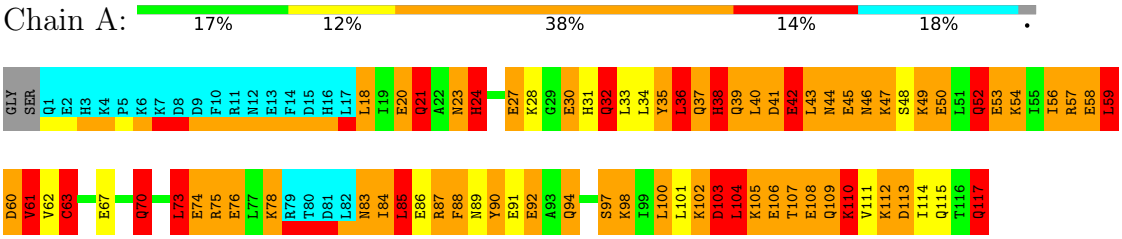
Chain A:



4.2.21 Score per residue for model 21 (medoid)

• Molecule 1: Mite allergen Blo t 5

Chain A:



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	1.13±4.15	11±49/793 (1.4± 6.2%)	1.01±3.18	11±48/1061 (1.0± 4.5%)
All	All	4.30	232/16653 (1.4%)	3.34	225/22281 (1.0%)

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	76	GLU	CD-OE1	-97.95	0.17	1.25	21	1
1	A	67	GLU	CD-OE1	-91.27	0.25	1.25	21	1
1	A	30	GLU	CD-OE1	-87.99	0.28	1.25	21	1
1	A	108	GLU	CD-OE2	-86.36	0.30	1.25	21	1
1	A	87	ARG	CZ-NH1	-85.92	0.21	1.33	21	1
1	A	92	GLU	CD-OE2	-82.25	0.35	1.25	21	1
1	A	91	GLU	CD-OE2	-81.37	0.36	1.25	21	1
1	A	106	GLU	CD-OE2	-79.17	0.38	1.25	21	1
1	A	27	GLU	CD-OE2	-78.40	0.39	1.25	21	1
1	A	86	GLU	CD-OE2	-78.08	0.39	1.25	21	1
1	A	20	GLU	CD-OE2	-76.95	0.41	1.25	21	1
1	A	45	GLU	CD-OE1	-75.90	0.42	1.25	21	1
1	A	50	GLU	CD-OE2	-74.98	0.43	1.25	21	1
1	A	20	GLU	CD-OE1	-74.63	0.43	1.25	21	1
1	A	27	GLU	CD-OE1	-74.03	0.44	1.25	21	1
1	A	106	GLU	CD-OE1	-73.64	0.44	1.25	21	1
1	A	42	GLU	CD-OE2	-70.94	0.47	1.25	21	1
1	A	74	GLU	CD-OE2	-69.77	0.48	1.25	21	1
1	A	45	GLU	CD-OE2	-67.89	0.51	1.25	21	1
1	A	91	GLU	CD-OE1	-66.67	0.52	1.25	21	1
1	A	86	GLU	CD-OE1	-66.35	0.52	1.25	21	1
1	A	50	GLU	CD-OE1	-66.11	0.53	1.25	21	1
1	A	42	GLU	CD-OE1	-64.33	0.54	1.25	21	1
1	A	53	GLU	CD-OE1	-63.79	0.55	1.25	21	1
1	A	57	ARG	CZ-NH1	-63.59	0.50	1.33	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	74	GLU	CD-OE1	-62.24	0.57	1.25	21	1
1	A	108	GLU	CD-OE1	-62.03	0.57	1.25	21	1
1	A	53	GLU	CD-OE2	-61.60	0.57	1.25	21	1
1	A	92	GLU	CD-OE1	-60.24	0.59	1.25	21	1
1	A	75	ARG	CZ-NH1	-59.90	0.55	1.33	21	1
1	A	76	GLU	CD-OE2	-59.08	0.60	1.25	21	1
1	A	35	TYR	CE1-CZ	-55.50	0.66	1.38	21	1
1	A	58	GLU	CD-OE2	-54.58	0.65	1.25	21	1
1	A	30	GLU	CD-OE2	-54.36	0.65	1.25	21	1
1	A	35	TYR	CG-CD2	-53.84	0.69	1.39	21	1
1	A	58	GLU	CD-OE1	-52.54	0.67	1.25	21	1
1	A	35	TYR	CE2-CZ	-50.37	0.73	1.38	21	1
1	A	87	ARG	CZ-NH2	-50.30	0.67	1.33	21	1
1	A	75	ARG	CZ-NH2	-49.22	0.69	1.33	21	1
1	A	35	TYR	CG-CD1	-48.68	0.75	1.39	21	1
1	A	90	TYR	CE1-CZ	-47.93	0.76	1.38	21	1
1	A	90	TYR	CG-CD2	-46.57	0.78	1.39	21	1
1	A	88	PHE	CG-CD2	-45.68	0.70	1.38	21	1
1	A	90	TYR	CE2-CZ	-45.47	0.79	1.38	21	1
1	A	52	GLN	CD-OE1	-44.92	0.25	1.24	21	1
1	A	97	SER	CB-OG	-44.91	0.83	1.42	21	1
1	A	90	TYR	CG-CD1	-44.05	0.81	1.39	21	1
1	A	74	GLU	CG-CD	-43.71	0.86	1.51	21	1
1	A	67	GLU	CD-OE2	-43.58	0.77	1.25	21	1
1	A	88	PHE	CG-CD1	-43.39	0.73	1.38	21	1
1	A	63	CYS	CB-SG	-41.71	1.11	1.82	21	1
1	A	76	GLU	CG-CD	-40.35	0.91	1.51	21	1
1	A	87	ARG	CD-NE	-40.16	0.78	1.46	21	1
1	A	21	GLN	CD-OE1	-39.97	0.36	1.24	21	1
1	A	45	GLU	CG-CD	-39.85	0.92	1.51	21	1
1	A	75	ARG	CD-NE	-39.59	0.79	1.46	21	1
1	A	61	VAL	CB-CG1	-39.23	0.70	1.52	21	1
1	A	61	VAL	CB-CG2	-39.13	0.70	1.52	21	1
1	A	117	GLN	CD-OE1	-38.28	0.39	1.24	21	1
1	A	87	ARG	NE-CZ	-37.69	0.84	1.33	21	1
1	A	94	GLN	CD-OE1	-37.17	0.42	1.24	21	1
1	A	103	ASP	CG-OD2	-36.26	0.41	1.25	21	1
1	A	88	PHE	CE1-CZ	-36.04	0.68	1.37	21	1
1	A	28	LYS	CE-NZ	-35.96	0.59	1.49	21	1
1	A	27	GLU	CG-CD	-35.51	0.98	1.51	21	1
1	A	20	GLU	CG-CD	-35.23	0.99	1.51	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	108	GLU	CB-CG	-35.07	0.85	1.52	21	1
1	A	70	GLN	CD-OE1	-34.84	0.47	1.24	21	1
1	A	106	GLU	CG-CD	-34.77	0.99	1.51	21	1
1	A	113	ASP	CG-OD2	-34.24	0.46	1.25	21	1
1	A	88	PHE	CE2-CZ	-34.23	0.72	1.37	21	1
1	A	110	LYS	CE-NZ	-33.99	0.64	1.49	21	1
1	A	91	GLU	CG-CD	-33.78	1.01	1.51	21	1
1	A	44	ASN	CG-OD1	-33.68	0.49	1.24	21	1
1	A	78	LYS	CE-NZ	-33.31	0.65	1.49	21	1
1	A	48	SER	CB-OG	-33.25	0.99	1.42	21	1
1	A	98	LYS	CE-NZ	-33.16	0.66	1.49	21	1
1	A	41	ASP	CG-OD2	-32.63	0.50	1.25	21	1
1	A	21	GLN	CG-CD	-32.28	0.76	1.51	21	1
1	A	37	GLN	CD-OE1	-32.22	0.53	1.24	21	1
1	A	50	GLU	CB-CG	-31.82	0.91	1.52	21	1
1	A	38	HIS	CE1-NE2	-31.65	0.59	1.32	21	1
1	A	117	GLN	CG-CD	-30.87	0.80	1.51	21	1
1	A	85	LEU	CG-CD2	-30.25	0.40	1.51	21	1
1	A	75	ARG	NE-CZ	-30.14	0.93	1.33	21	1
1	A	105	LYS	CE-NZ	-30.00	0.74	1.49	21	1
1	A	108	GLU	CG-CD	-29.99	1.06	1.51	21	1
1	A	32	GLN	CD-OE1	-29.68	0.58	1.24	21	1
1	A	113	ASP	CG-OD1	-29.55	0.57	1.25	21	1
1	A	40	LEU	CG-CD2	-29.40	0.43	1.51	21	1
1	A	41	ASP	CG-OD1	-29.36	0.57	1.25	21	1
1	A	60	ASP	CG-OD1	-29.06	0.58	1.25	21	1
1	A	94	GLN	CD-NE2	-28.66	0.61	1.32	21	1
1	A	117	GLN	C-O	-28.50	0.69	1.23	21	1
1	A	54	LYS	CD-CE	-28.33	0.80	1.51	21	1
1	A	86	GLU	CG-CD	-28.20	1.09	1.51	21	1
1	A	60	ASP	CG-OD2	-26.98	0.63	1.25	21	1
1	A	94	GLN	CB-CG	-26.96	0.79	1.52	21	1
1	A	30	GLU	CG-CD	-26.30	1.12	1.51	21	1
1	A	54	LYS	CE-NZ	-26.06	0.83	1.49	21	1
1	A	43	LEU	CG-CD2	-25.89	0.56	1.51	21	1
1	A	38	HIS	CG-ND1	-25.89	0.81	1.38	21	1
1	A	67	GLU	CG-CD	-25.86	1.13	1.51	21	1
1	A	20	GLU	CB-CG	-25.78	1.03	1.52	21	1
1	A	98	LYS	CD-CE	-25.77	0.86	1.51	21	1
1	A	92	GLU	CG-CD	-25.64	1.13	1.51	21	1
1	A	117	GLN	CD-NE2	-25.57	0.69	1.32	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	24	HIS	CG-CD2	-25.22	0.92	1.35	21	1
1	A	112	LYS	CB-CG	-25.18	0.84	1.52	21	1
1	A	45	GLU	CB-CG	-24.98	1.04	1.52	21	1
1	A	115	GLN	CD-OE1	-24.96	0.69	1.24	21	1
1	A	109	GLN	CG-CD	-24.70	0.94	1.51	21	1
1	A	38	HIS	CG-CD2	-24.68	0.93	1.35	21	1
1	A	103	ASP	CG-OD1	-24.47	0.69	1.25	21	1
1	A	37	GLN	CG-CD	-24.21	0.95	1.51	21	1
1	A	57	ARG	NE-CZ	-23.99	1.01	1.33	21	1
1	A	47	LYS	CE-NZ	-23.77	0.89	1.49	21	1
1	A	50	GLU	CG-CD	-23.70	1.16	1.51	21	1
1	A	36	LEU	CG-CD1	-23.39	0.65	1.51	21	1
1	A	36	LEU	CG-CD2	-23.15	0.66	1.51	21	1
1	A	39	GLN	CD-NE2	-23.15	0.74	1.32	21	1
1	A	57	ARG	CZ-NH2	-22.85	1.03	1.33	21	1
1	A	24	HIS	CE1-NE2	-22.79	0.80	1.32	21	1
1	A	39	GLN	CD-OE1	-22.51	0.74	1.24	21	1
1	A	52	GLN	CD-NE2	-22.39	0.76	1.32	21	1
1	A	42	GLU	CG-CD	-22.31	1.18	1.51	21	1
1	A	100	LEU	CG-CD2	-22.27	0.69	1.51	21	1
1	A	40	LEU	CG-CD1	-22.03	0.70	1.51	21	1
1	A	70	GLN	CB-CG	-21.94	0.93	1.52	21	1
1	A	109	GLN	CD-OE1	-21.74	0.76	1.24	21	1
1	A	42	GLU	CB-CG	-21.59	1.11	1.52	21	1
1	A	112	LYS	CE-NZ	-21.41	0.95	1.49	21	1
1	A	85	LEU	CG-CD1	-20.96	0.74	1.51	21	1
1	A	28	LYS	CD-CE	-20.58	0.99	1.51	21	1
1	A	43	LEU	CG-CD1	-20.50	0.76	1.51	21	1
1	A	117	GLN	CB-CG	-20.29	0.97	1.52	21	1
1	A	105	LYS	CD-CE	-20.27	1.00	1.51	21	1
1	A	18	LEU	CG-CD1	-20.23	0.77	1.51	21	1
1	A	44	ASN	CG-ND2	-20.17	0.82	1.32	21	1
1	A	109	GLN	CD-NE2	-19.72	0.83	1.32	21	1
1	A	56	ILE	CB-CG1	-19.62	0.99	1.54	21	1
1	A	73	LEU	CG-CD1	-19.35	0.80	1.51	21	1
1	A	110	LYS	CG-CD	-19.30	0.86	1.52	21	1
1	A	24	HIS	CG-ND1	-18.85	0.97	1.38	21	1
1	A	89	ASN	CG-OD1	-18.38	0.83	1.24	21	1
1	A	59	LEU	CG-CD1	-18.36	0.83	1.51	21	1
1	A	73	LEU	CG-CD2	-17.90	0.85	1.51	21	1
1	A	59	LEU	CG-CD2	-17.73	0.86	1.51	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	104	LEU	CG-CD1	-17.68	0.86	1.51	21	1
1	A	57	ARG	CD-NE	-17.65	1.16	1.46	21	1
1	A	87	ARG	CG-CD	-17.52	1.08	1.51	21	1
1	A	52	GLN	CG-CD	-17.45	1.10	1.51	21	1
1	A	27	GLU	CB-CG	-17.36	1.19	1.52	21	1
1	A	115	GLN	CD-NE2	-17.28	0.89	1.32	21	1
1	A	105	LYS	CG-CD	-17.25	0.93	1.52	21	1
1	A	18	LEU	CG-CD2	-17.24	0.88	1.51	21	1
1	A	56	ILE	CB-CG2	-17.17	0.99	1.52	21	1
1	A	89	ASN	CG-ND2	-16.91	0.90	1.32	21	1
1	A	31	HIS	CB-CG	-16.79	1.19	1.50	21	1
1	A	102	LYS	CB-CG	-16.25	1.08	1.52	21	1
1	A	49	LYS	CE-NZ	-16.24	1.08	1.49	21	1
1	A	83	ASN	CG-OD1	-15.43	0.90	1.24	21	1
1	A	46	ASN	CB-CG	-15.43	1.15	1.51	21	1
1	A	70	GLN	CD-NE2	-15.29	0.94	1.32	21	1
1	A	31	HIS	CD2-NE2	-14.93	1.05	1.38	21	1
1	A	115	GLN	CG-CD	-14.80	1.17	1.51	21	1
1	A	104	LEU	CG-CD2	-14.80	0.97	1.51	21	1
1	A	24	HIS	CB-CG	-14.62	1.23	1.50	21	1
1	A	100	LEU	CG-CD1	-14.56	0.97	1.51	21	1
1	A	101	LEU	CG-CD1	-14.49	0.98	1.51	21	1
1	A	117	GLN	CA-CB	-14.28	1.22	1.53	21	1
1	A	32	GLN	CG-CD	-14.23	1.18	1.51	21	1
1	A	53	GLU	CG-CD	-14.22	1.30	1.51	21	1
1	A	102	LYS	CE-NZ	-13.93	1.14	1.49	21	1
1	A	21	GLN	CD-NE2	-13.79	0.98	1.32	21	1
1	A	75	ARG	CB-CG	-13.68	1.15	1.52	21	1
1	A	76	GLU	CB-CG	-13.47	1.26	1.52	21	1
1	A	46	ASN	CG-OD1	-13.44	0.94	1.24	21	1
1	A	111	VAL	CB-CG2	-13.39	1.24	1.52	21	1
1	A	75	ARG	CG-CD	-13.37	1.18	1.51	21	1
1	A	31	HIS	CG-ND1	-13.23	1.09	1.38	21	1
1	A	36	LEU	CB-CG	-13.01	1.14	1.52	21	1
1	A	100	LEU	CB-CG	-12.99	1.14	1.52	21	1
1	A	94	GLN	CG-CD	-12.84	1.21	1.51	21	1
1	A	107	THR	CB-OG1	-12.72	1.17	1.43	21	1
1	A	111	VAL	CB-CG1	-12.66	1.26	1.52	21	1
1	A	32	GLN	CB-CG	-12.52	1.18	1.52	21	1
1	A	74	GLU	CB-CG	-12.10	1.29	1.52	21	1
1	A	73	LEU	CB-CG	-12.09	1.17	1.52	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	58	GLU	CG-CD	-12.07	1.33	1.51	21	1
1	A	24	HIS	CD2-NE2	-12.02	1.11	1.38	21	1
1	A	117	GLN	CA-C	-11.87	1.22	1.52	21	1
1	A	21	GLN	CB-CG	-11.78	1.20	1.52	21	1
1	A	91	GLU	CB-CG	-11.72	1.29	1.52	21	1
1	A	70	GLN	CG-CD	-11.57	1.24	1.51	21	1
1	A	98	LYS	CG-CD	-11.37	1.13	1.52	21	1
1	A	102	LYS	CD-CE	-11.33	1.23	1.51	21	1
1	A	24	HIS	ND1-CE1	-11.31	1.06	1.34	21	1
1	A	38	HIS	CD2-NE2	-11.20	1.13	1.38	21	1
1	A	113	ASP	CB-CG	-11.16	1.28	1.51	21	1
1	A	87	ARG	CB-CG	-10.80	1.23	1.52	21	1
1	A	101	LEU	CG-CD2	-10.56	1.12	1.51	21	1
1	A	30	GLU	CB-CG	-10.48	1.32	1.52	21	1
1	A	34	LEU	CB-CG	-10.15	1.23	1.52	21	1
1	A	31	HIS	ND1-CE1	-9.89	1.10	1.34	21	1
1	A	28	LYS	CG-CD	-9.70	1.19	1.52	21	1
1	A	38	HIS	CB-CG	-9.13	1.33	1.50	21	1
1	A	109	GLN	CB-CG	-8.94	1.28	1.52	21	1
1	A	78	LYS	CD-CE	-8.87	1.29	1.51	21	1
1	A	18	LEU	CB-CG	-8.50	1.27	1.52	21	1
1	A	32	GLN	CD-NE2	-8.26	1.12	1.32	21	1
1	A	110	LYS	CD-CE	-8.22	1.30	1.51	21	1
1	A	84	ILE	CG1-CD1	-8.22	0.93	1.50	21	1
1	A	52	GLN	CB-CG	-8.20	1.30	1.52	21	1
1	A	31	HIS	CG-CD2	-8.18	1.21	1.35	21	1
1	A	107	THR	CB-CG2	-8.17	1.25	1.52	21	1
1	A	41	ASP	CB-CG	-7.84	1.35	1.51	21	1
1	A	104	LEU	CB-CG	-7.65	1.30	1.52	21	1
1	A	112	LYS	CD-CE	-7.53	1.32	1.51	21	1
1	A	23	ASN	CG-OD1	-7.49	1.07	1.24	21	1
1	A	38	HIS	ND1-CE1	-7.38	1.16	1.34	21	1
1	A	58	GLU	CB-CG	-7.34	1.38	1.52	21	1
1	A	34	LEU	CG-CD2	-7.21	1.25	1.51	21	1
1	A	106	GLU	CB-CG	-7.12	1.38	1.52	21	1
1	A	105	LYS	CB-CG	-7.00	1.33	1.52	21	1
1	A	31	HIS	CE1-NE2	-7.00	1.16	1.32	21	1
1	A	103	ASP	CB-CG	-6.66	1.37	1.51	21	1
1	A	110	LYS	CB-CG	-6.28	1.35	1.52	21	1
1	A	83	ASN	CG-ND2	-6.23	1.17	1.32	21	1
1	A	56	ILE	CG1-CD1	-5.87	1.09	1.50	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	-5.66	1.37	1.52	21	1
1	A	37	GLN	CD-NE2	-5.62	1.18	1.32	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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	87	ARG	NE-CZ-NH2	100.03	170.32	120.30	21	1
1	A	35	TYR	CD1-CG-CD2	-89.34	19.63	117.90	21	1
1	A	35	TYR	CB-CG-CD1	82.58	170.55	121.00	21	1
1	A	35	TYR	CB-CG-CD2	81.37	169.82	121.00	21	1
1	A	88	PHE	CD1-CG-CD2	-76.02	19.48	118.30	21	1
1	A	50	GLU	OE1-CD-OE2	-73.27	35.38	123.30	21	1
1	A	108	GLU	OE1-CD-OE2	-73.00	35.70	123.30	21	1
1	A	88	PHE	CB-CG-CD1	71.02	170.52	120.80	21	1
1	A	106	GLU	OE1-CD-OE2	-70.61	38.57	123.30	21	1
1	A	88	PHE	CB-CG-CD2	70.29	170.00	120.80	21	1
1	A	87	ARG	NH1-CZ-NH2	-69.87	42.54	119.40	21	1
1	A	92	GLU	OE1-CD-OE2	-69.46	39.95	123.30	21	1
1	A	86	GLU	OE1-CD-OE2	-67.57	42.22	123.30	21	1
1	A	27	GLU	OE1-CD-OE2	-66.81	43.12	123.30	21	1
1	A	30	GLU	OE1-CD-OE2	-65.53	44.67	123.30	21	1
1	A	20	GLU	OE1-CD-OE2	-65.19	45.07	123.30	21	1
1	A	57	ARG	NE-CZ-NH2	62.63	151.62	120.30	21	1
1	A	35	TYR	CE1-CZ-CE2	-62.01	20.58	119.80	21	1
1	A	42	GLU	OE1-CD-OE2	-61.68	49.28	123.30	21	1
1	A	35	TYR	CG-CD1-CE1	61.64	170.61	121.30	21	1
1	A	53	GLU	OE1-CD-OE2	-60.86	50.27	123.30	21	1
1	A	35	TYR	CG-CD2-CE2	60.67	169.84	121.30	21	1
1	A	91	GLU	OE1-CD-OE2	-58.95	52.56	123.30	21	1
1	A	90	TYR	CD1-CG-CD2	-58.74	53.28	117.90	21	1
1	A	41	ASP	CB-CG-OD1	58.14	170.62	118.30	21	1
1	A	103	ASP	CB-CG-OD1	57.67	170.20	118.30	21	1
1	A	41	ASP	CB-CG-OD2	56.50	169.15	118.30	21	1
1	A	35	TYR	CZ-CE2-CD2	55.93	170.14	119.80	21	1
1	A	88	PHE	CE1-CZ-CE2	-55.63	19.86	120.00	21	1
1	A	90	TYR	CB-CG-CD1	54.96	153.98	121.00	21	1
1	A	35	TYR	CD1-CE1-CZ	54.90	169.21	119.80	21	1
1	A	113	ASP	CB-CG-OD1	54.86	167.68	118.30	21	1
1	A	76	GLU	OE1-CD-OE2	-54.82	57.52	123.30	21	1
1	A	41	ASP	OD1-CG-OD2	-54.25	20.23	123.30	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	87	ARG	NE-CZ-NH1	53.69	147.14	120.30	21	1
1	A	90	TYR	CB-CG-CD2	52.90	152.74	121.00	21	1
1	A	113	ASP	CB-CG-OD2	51.64	164.77	118.30	21	1
1	A	103	ASP	OD1-CG-OD2	-51.21	25.99	123.30	21	1
1	A	103	ASP	CB-CG-OD2	50.56	163.81	118.30	21	1
1	A	113	ASP	OD1-CG-OD2	-50.39	27.55	123.30	21	1
1	A	60	ASP	CB-CG-OD2	49.13	162.52	118.30	21	1
1	A	75	ARG	NE-CZ-NH2	48.44	144.52	120.30	21	1
1	A	60	ASP	CB-CG-OD1	47.31	160.88	118.30	21	1
1	A	60	ASP	OD1-CG-OD2	-45.63	36.60	123.30	21	1
1	A	88	PHE	CG-CD1-CE1	45.21	170.53	120.80	21	1
1	A	88	PHE	CG-CD2-CE2	44.72	169.99	120.80	21	1
1	A	67	GLU	OE1-CD-OE2	-42.88	71.85	123.30	21	1
1	A	88	PHE	CZ-CE2-CD2	41.86	170.33	120.10	21	1
1	A	88	PHE	CD1-CE1-CZ	41.42	169.81	120.10	21	1
1	A	90	TYR	CG-CD1-CE1	40.93	154.04	121.30	21	1
1	A	90	TYR	CE1-CZ-CE2	-40.25	55.40	119.80	21	1
1	A	94	GLN	OE1-CD-NE2	-39.79	30.39	121.90	21	1
1	A	58	GLU	OE1-CD-OE2	-39.45	75.97	123.30	21	1
1	A	90	TYR	CG-CD2-CE2	39.42	152.84	121.30	21	1
1	A	21	GLN	CG-CD-OE1	-37.72	46.17	121.60	21	1
1	A	45	GLU	OE1-CD-OE2	-37.63	78.14	123.30	21	1
1	A	90	TYR	CZ-CE2-CD2	36.73	152.86	119.80	21	1
1	A	90	TYR	CD1-CE1-CZ	35.31	151.58	119.80	21	1
1	A	57	ARG	NE-CZ-NH1	-34.90	102.85	120.30	21	1
1	A	85	LEU	CB-CG-CD1	34.78	170.13	111.00	21	1
1	A	40	LEU	CB-CG-CD1	34.69	169.97	111.00	21	1
1	A	75	ARG	NH1-CZ-NH2	-34.18	81.81	119.40	21	1
1	A	87	ARG	CD-NE-CZ	33.96	171.15	123.60	21	1
1	A	85	LEU	CB-CG-CD2	31.13	163.92	111.00	21	1
1	A	40	LEU	CB-CG-CD2	31.10	163.87	111.00	21	1
1	A	36	LEU	CB-CG-CD2	29.64	161.39	111.00	21	1
1	A	44	ASN	OD1-CG-ND2	-29.24	54.65	121.90	21	1
1	A	85	LEU	CD1-CG-CD2	-29.15	23.05	110.50	21	1
1	A	40	LEU	CD1-CG-CD2	-29.11	23.15	110.50	21	1
1	A	52	GLN	OE1-CD-NE2	-29.00	55.21	121.90	21	1
1	A	38	HIS	ND1-CG-CD2	-27.46	67.55	106.00	21	1
1	A	37	GLN	CG-CD-OE1	-27.44	66.72	121.60	21	1
1	A	61	VAL	CG1-CB-CG2	-27.38	67.09	110.90	21	1
1	A	75	ARG	NE-CZ-NH1	26.75	133.68	120.30	21	1
1	A	76	GLU	CG-CD-OE2	24.84	167.99	118.30	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	108	GLU	CG-CD-OE1	24.74	167.78	118.30	21	1
1	A	30	GLU	CG-CD-OE2	24.30	166.89	118.30	21	1
1	A	92	GLU	CG-CD-OE1	23.50	165.31	118.30	21	1
1	A	36	LEU	CD1-CG-CD2	-23.13	41.12	110.50	21	1
1	A	67	GLU	CG-CD-OE2	23.08	164.45	118.30	21	1
1	A	87	ARG	CG-CD-NE	22.95	160.00	111.80	21	1
1	A	50	GLU	CG-CD-OE1	22.91	164.11	118.30	21	1
1	A	110	LYS	CB-CG-CD	22.32	169.62	111.60	21	1
1	A	36	LEU	CB-CG-CD1	22.16	148.66	111.00	21	1
1	A	106	GLU	CG-CD-OE1	21.98	162.27	118.30	21	1
1	A	86	GLU	CG-CD-OE1	21.90	162.11	118.30	21	1
1	A	57	ARG	CD-NE-CZ	21.35	153.49	123.60	21	1
1	A	43	LEU	CB-CG-CD1	21.27	147.16	111.00	21	1
1	A	76	GLU	CB-CG-CD	21.17	171.36	114.20	21	1
1	A	50	GLU	CG-CD-OE2	21.10	160.51	118.30	21	1
1	A	94	GLN	CG-CD-NE2	20.85	166.75	116.70	21	1
1	A	27	GLU	CG-CD-OE1	20.76	159.82	118.30	21	1
1	A	94	GLN	CG-CD-OE1	20.63	162.87	121.60	21	1
1	A	52	GLN	CG-CD-NE2	20.60	166.14	116.70	21	1
1	A	106	GLU	CG-CD-OE2	20.43	159.16	118.30	21	1
1	A	91	GLU	CG-CD-OE1	20.37	159.04	118.30	21	1
1	A	61	VAL	CA-CB-CG2	20.17	141.16	110.90	21	1
1	A	61	VAL	CA-CB-CG1	20.07	141.00	110.90	21	1
1	A	20	GLU	CG-CD-OE1	19.91	158.12	118.30	21	1
1	A	42	GLU	CG-CD-OE1	19.48	157.26	118.30	21	1
1	A	27	GLU	CG-CD-OE2	19.38	157.05	118.30	21	1
1	A	20	GLU	CG-CD-OE2	19.26	156.81	118.30	21	1
1	A	21	GLN	CG-CD-NE2	19.23	162.87	116.70	21	1
1	A	100	LEU	CB-CG-CD1	19.11	143.49	111.00	21	1
1	A	108	GLU	CG-CD-OE2	19.11	156.52	118.30	21	1
1	A	105	LYS	CD-CE-NZ	18.73	154.79	111.70	21	1
1	A	38	HIS	CG-ND1-CE1	18.73	134.42	108.20	21	1
1	A	86	GLU	CG-CD-OE2	18.69	155.68	118.30	21	1
1	A	53	GLU	CG-CD-OE2	18.63	155.56	118.30	21	1
1	A	73	LEU	CB-CG-CD1	18.63	142.66	111.00	21	1
1	A	35	TYR	OH-CZ-CE2	18.55	170.19	120.10	21	1
1	A	74	GLU	OE1-CD-OE2	-18.45	101.15	123.30	21	1
1	A	92	GLU	CG-CD-OE2	18.22	154.75	118.30	21	1
1	A	35	TYR	CE1-CZ-OH	18.20	169.23	120.10	21	1
1	A	53	GLU	CG-CD-OE1	17.94	154.17	118.30	21	1
1	A	39	GLN	OE1-CD-NE2	-17.64	81.34	121.90	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	110	LYS	CG-CD-CE	17.64	164.81	111.90	21	1
1	A	42	GLU	CG-CD-OE2	17.58	153.46	118.30	21	1
1	A	18	LEU	CB-CG-CD2	17.53	140.81	111.00	21	1
1	A	44	ASN	CB-CG-ND2	17.38	158.40	116.70	21	1
1	A	75	ARG	CD-NE-CZ	17.23	147.73	123.60	21	1
1	A	54	LYS	CG-CD-CE	17.10	163.19	111.90	21	1
1	A	109	GLN	CB-CG-CD	16.71	155.03	111.60	21	1
1	A	75	ARG	CB-CG-CD	16.69	154.99	111.60	21	1
1	A	21	GLN	CB-CG-CD	16.61	154.78	111.60	21	1
1	A	27	GLU	CB-CG-CD	16.20	157.95	114.20	21	1
1	A	73	LEU	CD1-CG-CD2	-16.07	62.30	110.50	21	1
1	A	38	HIS	CG-CD2-NE2	15.57	138.78	109.20	21	1
1	A	110	LYS	CD-CE-NZ	15.51	147.38	111.70	21	1
1	A	105	LYS	CB-CG-CD	15.16	151.03	111.60	21	1
1	A	30	GLU	CG-CD-OE1	15.07	148.44	118.30	21	1
1	A	91	GLU	CG-CD-OE2	15.05	148.40	118.30	21	1
1	A	37	GLN	CG-CD-NE2	14.98	152.64	116.70	21	1
1	A	73	LEU	CB-CG-CD2	14.70	135.99	111.00	21	1
1	A	112	LYS	CA-CB-CG	14.37	145.02	113.40	21	1
1	A	108	GLU	CB-CG-CD	14.35	152.95	114.20	21	1
1	A	112	LYS	CB-CG-CD	14.33	148.86	111.60	21	1
1	A	94	GLN	CB-CG-CD	14.27	148.71	111.60	21	1
1	A	104	LEU	CB-CG-CD2	14.11	134.98	111.00	21	1
1	A	43	LEU	CD1-CG-CD2	-14.10	68.19	110.50	21	1
1	A	70	GLN	CG-CD-NE2	14.04	150.39	116.70	21	1
1	A	45	GLU	CB-CG-CD	13.87	151.65	114.20	21	1
1	A	104	LEU	CB-CG-CD1	13.59	134.10	111.00	21	1
1	A	45	GLU	CG-CD-OE2	13.56	145.42	118.30	21	1
1	A	89	ASN	OD1-CG-ND2	-13.38	91.13	121.90	21	1
1	A	43	LEU	CB-CG-CD2	13.31	133.62	111.00	21	1
1	A	70	GLN	OE1-CD-NE2	-13.15	91.64	121.90	21	1
1	A	75	ARG	CG-CD-NE	12.82	138.71	111.80	21	1
1	A	44	ASN	CB-CG-OD1	12.68	146.96	121.60	21	1
1	A	87	ARG	CB-CG-CD	12.64	144.47	111.60	21	1
1	A	21	GLN	OE1-CD-NE2	12.64	150.97	121.90	21	1
1	A	57	ARG	NH1-CZ-NH2	-12.60	105.54	119.40	21	1
1	A	94	GLN	CA-CB-CG	12.55	141.01	113.40	21	1
1	A	24	HIS	ND1-CG-CD2	-12.50	88.50	106.00	21	1
1	A	59	LEU	CB-CG-CD2	12.46	132.19	111.00	21	1
1	A	112	LYS	CD-CE-NZ	12.46	140.36	111.70	21	1
1	A	54	LYS	CD-CE-NZ	12.41	140.24	111.70	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	58	GLU	CG-CD-OE1	12.28	142.86	118.30	21	1
1	A	104	LEU	CD1-CG-CD2	-12.18	73.97	110.50	21	1
1	A	90	TYR	OH-CZ-CE2	12.17	152.96	120.10	21	1
1	A	108	GLU	CA-CB-CG	12.14	140.11	113.40	21	1
1	A	52	GLN	CB-CG-CD	11.82	142.34	111.60	21	1
1	A	90	TYR	CE1-CZ-OH	11.68	151.64	120.10	21	1
1	A	32	GLN	CG-CD-NE2	11.67	144.72	116.70	21	1
1	A	47	LYS	CD-CE-NZ	11.59	138.37	111.70	21	1
1	A	58	GLU	CG-CD-OE2	11.44	141.17	118.30	21	1
1	A	32	GLN	CG-CD-OE1	-11.40	98.80	121.60	21	1
1	A	59	LEU	CB-CG-CD1	11.21	130.06	111.00	21	1
1	A	37	GLN	CB-CG-CD	11.10	140.46	111.60	21	1
1	A	63	CYS	CA-CB-SG	10.89	133.61	114.00	21	1
1	A	24	HIS	CG-ND1-CE1	10.82	123.35	108.20	21	1
1	A	18	LEU	CD1-CG-CD2	-10.75	78.25	110.50	21	1
1	A	117	GLN	CG-CD-NE2	10.72	142.42	116.70	21	1
1	A	78	LYS	CD-CE-NZ	10.67	136.24	111.70	21	1
1	A	70	GLN	CA-CB-CG	10.41	136.30	113.40	21	1
1	A	39	GLN	CG-CD-OE1	10.24	142.08	121.60	21	1
1	A	70	GLN	CB-CG-CD	10.08	137.80	111.60	21	1
1	A	46	ASN	CB-CG-OD1	-9.81	101.97	121.60	21	1
1	A	101	LEU	CB-CG-CD2	9.73	127.55	111.00	21	1
1	A	91	GLU	CB-CG-CD	9.61	140.13	114.20	21	1
1	A	50	GLU	CA-CB-CG	9.55	134.42	113.40	21	1
1	A	117	GLN	CA-C-O	9.53	140.11	120.10	21	1
1	A	59	LEU	CD1-CG-CD2	-9.26	82.73	110.50	21	1
1	A	45	GLU	CG-CD-OE1	9.07	136.44	118.30	21	1
1	A	105	LYS	CG-CD-CE	8.96	138.77	111.90	21	1
1	A	56	ILE	CG1-CB-CG2	-8.64	92.40	111.40	21	1
1	A	18	LEU	CB-CG-CD1	8.53	125.50	111.00	21	1
1	A	52	GLN	CG-CD-OE1	8.53	138.65	121.60	21	1
1	A	74	GLU	CG-CD-OE1	8.32	134.94	118.30	21	1
1	A	39	GLN	CG-CD-NE2	8.29	136.58	116.70	21	1
1	A	37	GLN	OE1-CD-NE2	8.14	140.63	121.90	21	1
1	A	76	GLU	CG-CD-OE1	8.10	134.50	118.30	21	1
1	A	50	GLU	CB-CG-CD	8.04	135.90	114.20	21	1
1	A	28	LYS	CD-CE-NZ	7.62	129.22	111.70	21	1
1	A	56	ILE	CB-CG1-CD1	7.49	134.86	113.90	21	1
1	A	98	LYS	CG-CD-CE	7.25	133.65	111.90	21	1
1	A	38	HIS	CB-CG-ND1	7.24	141.29	123.20	21	1
1	A	100	LEU	CD1-CG-CD2	-7.10	89.21	110.50	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	56	ILE	CA-CB-CG2	7.04	124.97	110.90	21	1
1	A	89	ASN	CB-CG-OD1	6.98	135.56	121.60	21	1
1	A	38	HIS	CE1-NE2-CD2	-6.95	89.23	106.60	21	1
1	A	89	ASN	CB-CG-ND2	6.92	133.31	116.70	21	1
1	A	56	ILE	CA-CB-CG1	6.91	124.12	111.00	21	1
1	A	115	GLN	OE1-CD-NE2	-6.76	106.34	121.90	21	1
1	A	38	HIS	CB-CG-CD2	6.57	151.16	130.80	21	1
1	A	115	GLN	CG-CD-NE2	6.50	132.30	116.70	21	1
1	A	20	GLU	CA-CB-CG	6.45	127.58	113.40	21	1
1	A	117	GLN	CG-CD-OE1	-6.41	108.77	121.60	21	1
1	A	117	GLN	CB-CG-CD	6.39	128.22	111.60	21	1
1	A	20	GLU	CB-CG-CD	6.33	131.28	114.20	21	1
1	A	97	SER	CA-CB-OG	6.19	127.91	111.20	21	1
1	A	84	ILE	CB-CG1-CD1	6.00	130.70	113.90	21	1
1	A	24	HIS	CG-CD2-NE2	5.87	120.35	109.20	21	1
1	A	83	ASN	CB-CG-ND2	5.86	130.76	116.70	21	1
1	A	102	LYS	CG-CD-CE	5.84	129.41	111.90	21	1
1	A	45	GLU	CA-CB-CG	5.71	125.97	113.40	21	1
1	A	117	GLN	OE1-CD-NE2	-5.69	108.81	121.90	21	1
1	A	42	GLU	CA-CB-CG	5.68	125.89	113.40	21	1
1	A	30	GLU	CB-CG-CD	5.48	129.00	114.20	21	1
1	A	73	LEU	CA-CB-CG	5.42	127.77	115.30	21	1
1	A	100	LEU	CA-CB-CG	5.42	127.77	115.30	21	1
1	A	47	LYS	CB-CG-CD	5.34	125.49	111.60	21	1
1	A	36	LEU	CA-CB-CG	5.15	127.15	115.30	21	1
1	A	102	LYS	CA-CB-CG	5.04	124.48	113.40	21	1
1	A	57	ARG	CG-CD-NE	5.02	122.34	111.80	21	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	788	803	803	36±83

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	16548	16863	16863	754

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: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:108:GLU:CB	1:A:108:GLU:CD	1.43	1.86	21	1
1:A:78:LYS:NZ	1:A:78:LYS:CD	1.43	1.82	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: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:45:GLU:CD	1:A:45:GLU:CB	1.39	1.90	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:21:GLN:CD	1:A:21:GLN:CB	1.38	1.92	21	1
1:A:74:GLU:CD	1:A:74:GLU:CB	1.38	1.91	21	1
1:A:21:GLN:CB	1:A:21:GLN:OE1	1.38	1.72	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:50:GLU:CB	1:A:50:GLU:CD	1.36	1.92	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:GLN:CB	1:A:94:GLN:CD	1.36	1.93	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: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:70:GLN:CB	1:A:70:GLN:CD	1.26	2.03	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: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
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:58:GLU:CG	1:A:58:GLU:OE1	1.15	1.92	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:76:GLU:CD	1:A:76:GLU:CB	1.10	2.16	21	1
1:A:109:GLN:CD	1:A:109:GLN:CB	1.10	2.17	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:109:GLN:CD	1:A:109:GLN:CG	1.03	0.94	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:74:GLU:CD	1:A:74:GLU:HG2	1.02	1.46	21	1
1:A:84:ILE:CG1	1:A:84:ILE:HD12	1.02	1.55	21	1
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:74:GLU:CD	1:A:74:GLU:HG3	1.00	1.46	21	1
1:A:61:VAL:CG1	1:A:61:VAL:HB	0.99	1.57	21	1
1:A:109:GLN:CD	1:A:109:GLN:HG3	0.99	1.43	21	1
1:A:45:GLU:CD	1:A:45:GLU:HG2	0.99	1.43	21	1
1:A:109:GLN:CD	1:A:109:GLN:HG2	0.99	1.43	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:18:LEU:CG	1:A:18:LEU:HD23	0.98	1.51	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:45:GLU:CD	1:A:45:GLU:HG3	0.97	1.43	21	1
1:A:45:GLU:CD	1:A:45:GLU:CG	0.97	0.92	21	1
1:A:76:GLU:CD	1:A:76:GLU:CG	0.97	0.91	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: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:74:GLU:CD	1:A:74:GLU:CG	0.95	0.86	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:84:ILE:CD1	1:A:84:ILE:HG12	0.94	1.50	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:84:ILE:CD1	1:A:84:ILE:HG13	0.94	1.50	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
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:59:LEU:CG	1:A:59:LEU:HD12	0.92	1.48	21	1
1:A:70:GLN:CB	1:A:70:GLN:CG	0.92	0.93	21	1
1:A:70:GLN:CB	1:A:70:GLN:HG2	0.92	1.48	21	1
1:A:76:GLU:CD	1:A:76:GLU:HG3	0.92	1.36	21	1
1:A:105:LYS:CG	1:A:105:LYS:CD	0.92	0.93	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:CG	1:A:50:GLU:CB	0.91	0.91	21	1
1:A:73:LEU:CG	1:A:73:LEU:HD13	0.91	1.45	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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:76:GLU:CD	1:A:76:GLU:HG2	0.90	1.36	21	1
1:A:98:LYS:CE	1:A:98:LYS:HD2	0.89	1.44	21	1
1:A:43:LEU:CD2	1:A:43:LEU:HG	0.89	1.46	21	1
1:A:117:GLN:O	1:A:117:GLN:C	0.89	0.69	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:43:LEU:CG	1:A:43:LEU:HD11	0.87	1.41	21	1
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: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:21:GLN:CD	1:A:21:GLN:HG2	0.85	1.31	21	1
1:A:44:ASN:ND2	1:A:44:ASN:CG	0.84	0.82	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ASN:CG	1:A:44:ASN:HD21	0.84	1.45	21	1
1:A:103:ASP:OD1	1:A:103:ASP:CG	0.84	0.69	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:109:GLN:CD	1:A:109:GLN:HE22	0.83	1.46	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:109:GLN:CD	1:A:109:GLN:HE21	0.83	1.46	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
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:110:LYS:CG	1:A:110:LYS:HD2	0.81	1.35	21	1
1:A:44:ASN:CG	1:A:44:ASN:HD22	0.81	1.45	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:60:ASP:OD2	1:A:60:ASP:CG	0.81	0.63	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:110:LYS:CD	1:A:110:LYS:HG2	0.80	1.33	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:GLN:CG	1:A:21:GLN:CD	0.80	0.76	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:39:GLN:CD	1:A:39:GLN:HE21	0.79	1.39	21	1
1:A:52:GLN:CD	1:A:52:GLN:HE21	0.78	1.41	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:63:CYS:CB	1:A:63:CYS:HG	0.78	1.89	21	1
1:A:109:GLN:CD	1:A:109:GLN:NE2	0.78	0.83	21	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: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
1:A:39:GLN:CD	1:A:39:GLN:HE22	0.76	1.39	21	1
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:30:GLU:OE2	1:A:30:GLU:CD	0.76	0.65	21	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:60:ASP:OD1	1:A:60:ASP:CG	0.75	0.58	21	1
1:A:90:TYR:CZ	1:A:90:TYR:CE2	0.75	0.79	21	1
1:A:18:LEU:CD1	1:A:18:LEU:HB2	0.74	2.06	21	1
1:A:35:TYR:CE2	1:A:35:TYR:OH	0.74	2.09	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:GLU:OE2	1:A:53:GLU:CD	0.74	0.57	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:21:GLN:OE1	1:A:21:GLN:HG3	0.73	0.98	21	1
1:A:21:GLN:CG	1:A:21:GLN:OE1	0.72	0.58	21	1
1:A:61:VAL:HG13	1:A:61:VAL:HG22	0.71	1.00	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:40:LEU:HD12	1:A:111:VAL:HG23	0.71	1.63	17	3
1:A:52:GLN:NE2	1:A:52:GLN:CD	0.71	0.76	21	1
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
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:53:GLU:OE1	1:A:53:GLU:CD	0.70	0.55	21	1
1:A:54:LYS:CE	1:A:54:LYS:HZ1	0.69	1.41	21	1
1:A:39:GLN:NE2	1:A:39:GLN:CD	0.69	0.75	21	1
1:A:36:LEU:HD11	1:A:55:ILE:HG23	0.69	1.62	20	4
1:A:54:LYS:CE	1:A:54:LYS:HZ3	0.68	1.41	21	1
1:A:44:ASN:OD1	1:A:44:ASN:CG	0.68	0.49	21	1
1:A:92:GLU:OE1	1:A:92:GLU:CD	0.68	0.59	21	1
1:A:54:LYS:CE	1:A:54:LYS:NZ	0.68	0.83	21	1
1:A:110:LYS:NZ	1:A:110:LYS:HD3	0.67	2.02	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:42:GLU:OE1	1:A:42:GLU:CD	0.66	0.54	21	1
1:A:88:PHE:CZ	1:A:88:PHE:CE1	0.66	0.68	21	1
1:A:41:ASP:OD1	1:A:41:ASP:CG	0.66	0.57	21	1
1:A:94:GLN:CD	1:A:94:GLN:HE21	0.66	1.28	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:52:GLN:CD	1:A:52:GLN:HE22	0.65	1.41	21	1
1:A:113:ASP:OD1	1:A:113:ASP:CG	0.65	0.57	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: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:36:LEU:HD13	1:A:59:LEU:CD1	0.64	2.23	9	2
1:A:39:GLN:OE1	1:A:39:GLN:CD	0.64	0.74	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: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
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:32:GLN:CD	1:A:62:VAL:HG11	0.62	2.13	6	4
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:50:GLU:OE1	1:A:50:GLU:CD	0.61	0.52	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:41:ASP:OD2	1:A:41:ASP:CG	0.59	0.50	21	1
1:A:58:GLU:OE1	1:A:58:GLU:CD	0.59	0.67	21	1
1:A:63:CYS:HB2	1:A:104:LEU:HD23	0.59	1.74	21	1
1:A:33:LEU:HD11	1:A:103:ASP:CG	0.59	2.17	9	2
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:40:LEU:CD1	1:A:40:LEU:HD23	0.58	1.15	21	1
1:A:113:ASP:OD2	1:A:113:ASP:CG	0.57	0.46	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: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:78:LYS:CE	1:A:78:LYS:HZ3	0.56	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:40:LEU:HD23	1:A:111:VAL:CG2	0.56	2.31	10	3
1:A:78:LYS:CE	1:A:78:LYS:HZ1	0.56	1.27	21	1
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: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	6
1:A:78:LYS:CE	1:A:78:LYS:HZ2	0.55	1.27	21	1
1:A:109:GLN:CD	1:A:109:GLN:OE1	0.55	0.76	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:GLN:OE1	1:A:62:VAL:HG21	0.55	2.01	13	1
1:A:58:GLU:OE2	1:A:58:GLU:CD	0.55	0.65	21	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:40:LEU:CD2	1:A:107:THR:HG23	0.53	2.27	9	2
1:A:74:GLU:CD	1:A:74:GLU:HB3	0.53	2.09	21	1
1:A:103:ASP:OD2	1:A:103:ASP:CG	0.53	0.42	21	1
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
1:A:85:LEU:CD2	1:A:85:LEU:HD13	0.52	1.15	21	1
1:A:94:GLN:NE2	1:A:94:GLN:CD	0.52	0.61	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	2
1:A:63:CYS:SG	1:A:63:CYS:C	0.49	2.91	21	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: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: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: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:94:GLN:NE2	1:A:94:GLN:OE1	0.47	0.33	21	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: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:18:LEU:HD12	1:A:19:ILE:HG12	0.46	1.87	4	1
1:A:18:LEU:HD13	1:A:77:LEU:CB	0.46	2.41	7	1
1:A:40:LEU:HG	1:A:107:THR:HG22	0.46	1.87	8	2
1:A:52:GLN:CD	1:A:56:ILE:HD11	0.46	2.31	18	1
1:A:88:PHE:CZ	1:A:88:PHE:HE2	0.46	1.22	21	1
1:A:73:LEU:HD13	1:A:77:LEU:HD23	0.45	1.87	12	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:40:LEU:HD13	1:A:40:LEU:HD22	0.45	0.50	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:30:GLU:OE2	1:A:30:GLU:OE1	0.44	0.49	21	1
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
1:A:33:LEU:C	1:A:33:LEU:HD13	0.43	2.34	20	4
1:A:70:GLN:OE1	1:A:101:LEU:HD11	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:61:VAL:HG22	1:A:65:MET:HE2	0.43	1.91	11	1
1:A:40:LEU:CD2	1:A:40:LEU:HD13	0.43	1.11	21	1
1:A:43:LEU:HD13	1:A:43:LEU:C	0.43	2.34	16	6
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:42:GLU:OE1	1:A:42:GLU:OE2	0.43	0.43	21	1
1:A:40:LEU:HD13	1:A:40:LEU:C	0.43	2.35	20	3
1:A:35:TYR:CZ	1:A:35:TYR:HE1	0.43	1.19	21	1
1:A:100:LEU:HD13	1:A:100:LEU:C	0.42	2.34	14	7
1:A:97:SER:HA	1:A:100:LEU:HD23	0.42	1.91	1	1
1:A:85:LEU:HD13	1:A:85:LEU:C	0.42	2.34	10	1
1:A:56:ILE:HG13	1:A:111:VAL:HG11	0.42	1.91	13	1
1:A:43:LEU:C	1:A:43:LEU:HD13	0.42	2.35	7	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:40:LEU:C	1:A:40:LEU:HD13	0.42	2.36	11	2
1:A:61:VAL:HG12	1:A:65:MET:HE2	0.42	1.91	20	1
1:A:100:LEU:C	1:A:100:LEU:HD13	0.42	2.36	17	1
1:A:24:HIS:CD2	1:A:24:HIS:HA	0.41	2.50	21	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LYS:HE2	1:A:54:LYS:HD3	0.41	1.26	21	1
1:A:59:LEU:HD13	1:A:59:LEU:C	0.41	2.37	2	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:36:LEU:HD13	1:A:36:LEU:C	0.41	2.36	13	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:33:LEU:HD13	1:A:33:LEU:C	0.40	2.37	21	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

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%)	54	85
All	All	1995/2499 (80%)	1953 (98%)	40 (2%)	2 (0%)	54	85

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%)	75±4 (86±5%)	12±4 (14±5%)	6 46
All	All	1827/2289 (80%)	1566 (86%)	261 (14%)	6 46

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	17
1	A	49	LYS	17
1	A	83	ASN	16
1	A	57	ARG	14
1	A	70	GLN	11
1	A	85	LEU	11
1	A	97	SER	11
1	A	73	LEU	10
1	A	107	THR	9
1	A	48	SER	7
1	A	115	GLN	7
1	A	100	LEU	6
1	A	110	LYS	6
1	A	43	LEU	6
1	A	112	LYS	6
1	A	52	GLN	6
1	A	105	LYS	6
1	A	98	LYS	5
1	A	36	LEU	5
1	A	40	LEU	5
1	A	103	ASP	5
1	A	104	LEU	4
1	A	21	GLN	4
1	A	54	LYS	4
1	A	114	ILE	4
1	A	23	ASN	4
1	A	28	LYS	3
1	A	101	LEU	3
1	A	47	LYS	3
1	A	18	LEU	3
1	A	74	GLU	3
1	A	37	GLN	3
1	A	20	GLU	3
1	A	58	GLU	3
1	A	109	GLN	3
1	A	59	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	44	ASN	2
1	A	106	GLU	2
1	A	76	GLU	2
1	A	117	GLN	2
1	A	34	LEU	2
1	A	42	GLU	2
1	A	108	GLU	1
1	A	78	LYS	1
1	A	92	GLU	1
1	A	53	GLU	1
1	A	60	ASP	1
1	A	94	GLN	1
1	A	24	HIS	1
1	A	38	HIS	1
1	A	56	ILE	1
1	A	61	VAL	1
1	A	63	CYS	1
1	A	75	ARG	1
1	A	102	LYS	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

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
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 (i)

No chemical shift data were provided