Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2CA7
Title	:	CONKUNITZIN-S1 IS THE FIRST MEMBER OF A NEW KUNITZ-TYPE NEUROTOXIN FAMILY- STRUCTURAL AND FUNCTIONAL CHARACTERIZATION
Authors	:	Bayrhuber, M.; Vijayan, V.; Ferber, M.; Graf, R.; Korukottu, J.; Imperial, J.; Garrett, J.E.; Olivera, B.M.; Terlau, H.; Zweckstetter, M.; Becker, S.
Deposited on	:	2005-12-19

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

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

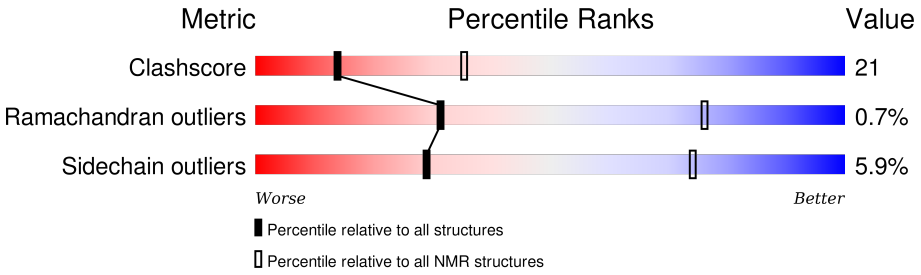
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 76%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	60	77% 18% 5%

2 Ensemble composition and analysis

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:4-A:60 (57)	0.36	1

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 785 atoms, of which 300 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CONKUNITZIN-S1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	60	785	293	300	92	96	4	0

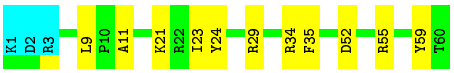
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: CONKUNITZIN-S1

Chain A:



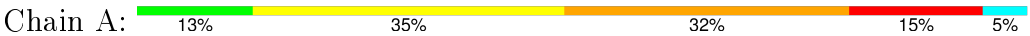
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: CONKUNITZIN-S1

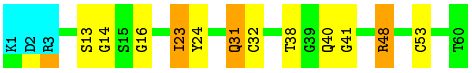
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: CONKUNITZIN-S1

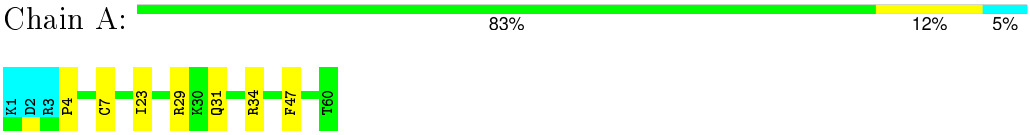
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: CONKUNITZIN-S1

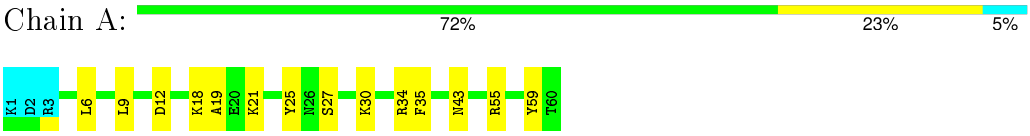
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: CONKUNITZIN-S1

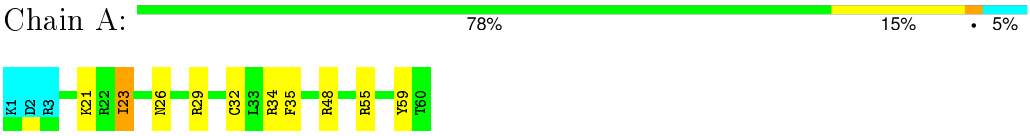
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: CONKUNITZIN-S1

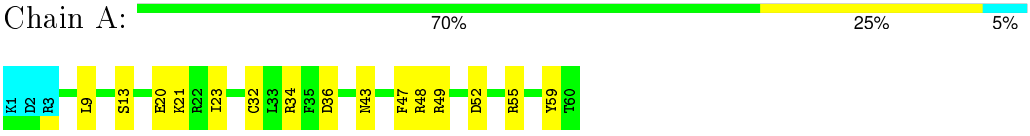
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: CONKUNITZIN-S1

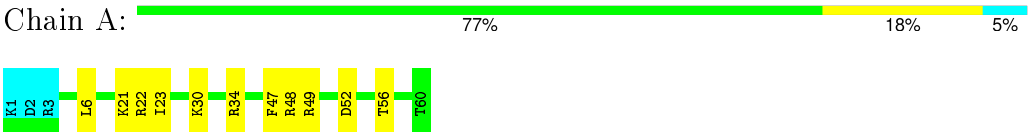
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: CONKUNITZIN-S1

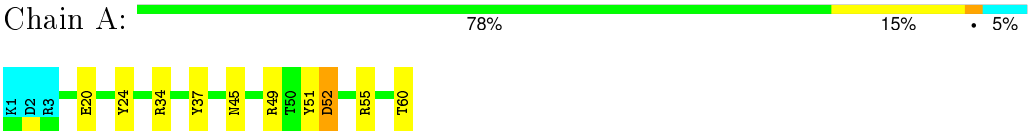
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: CONKUNITZIN-S1

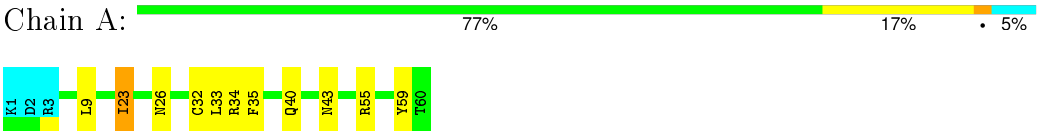
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: CONKUNITZIN-S1

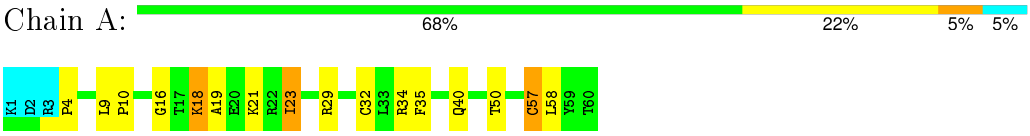
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: CONKUNITZIN-S1

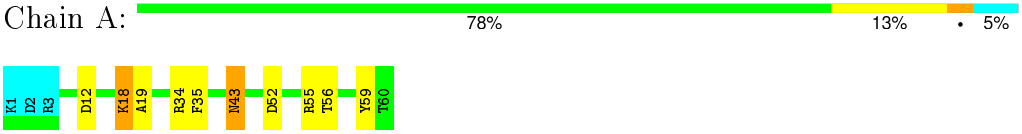
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: CONKUNITZIN-S1

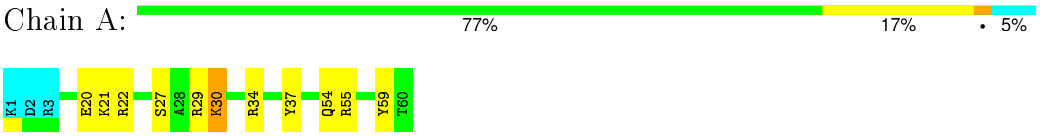
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: CONKUNITZIN-S1

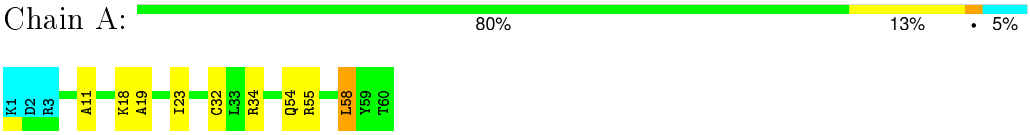
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: CONKUNITZIN-S1

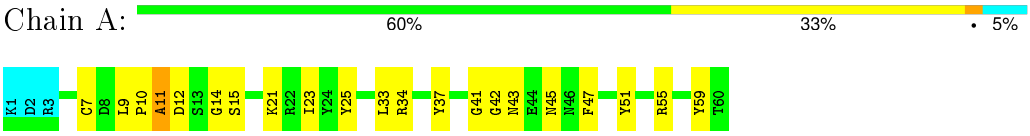
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: CONKUNITZIN-S1

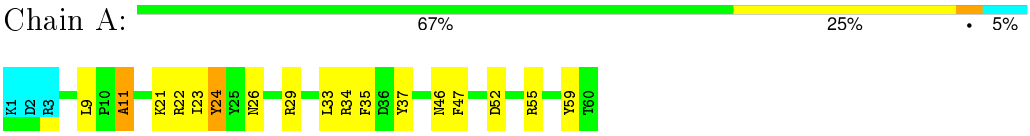
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: CONKUNITZIN-S1

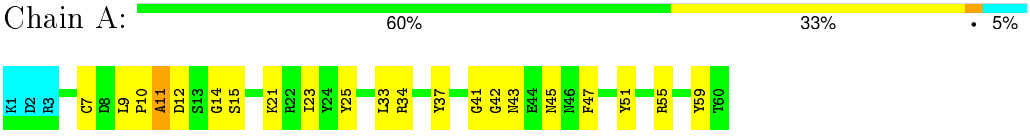
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: CONKUNITZIN-S1

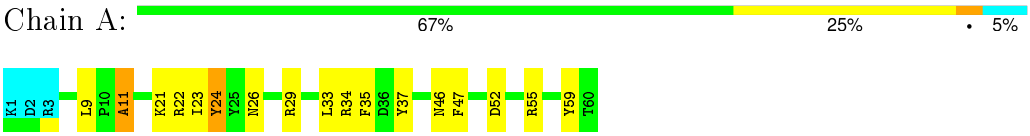
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: CONKUNITZIN-S1

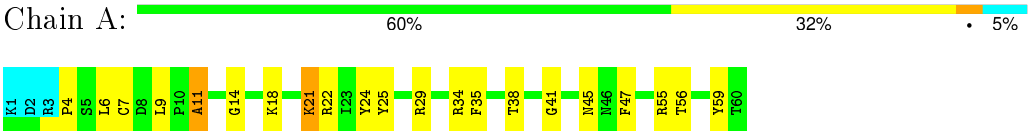
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: CONKUNITZIN-S1

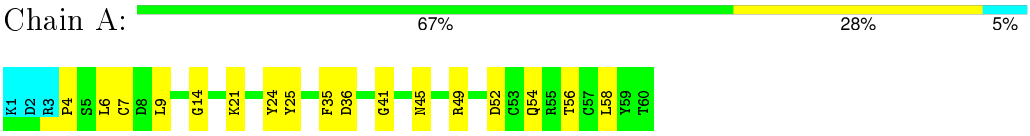
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: CONKUNITZIN-S1

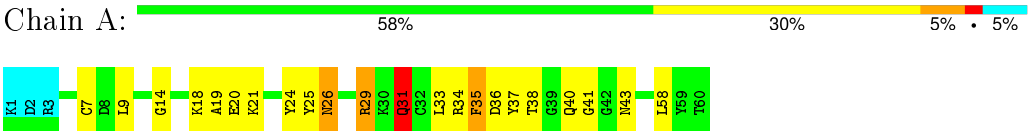
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: CONKUNITZIN-S1

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *MOLECULAR DYNAMICS, SIMULATED ANNEALING, TORSION ANGLE DYNAMICS.*

Of the 20 calculated structures, 20 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
X-PLOR NIH 2.9.7	refinement	
XWINNMR 3.5	structure solution	
NMRPIPE 97. 027.12.56	structure solution	
NMRDRAW 2.3 REV 2004.245.17.31	structure solution	
SPARKY 3. 110	structure solution	
ARIA2ALPHA	structure solution	
CYANA 2.0. 32	structure solution	
MARS 1.0	structure solution	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 6506
Number of chemical shift lists	1
Total number of shifts	566
Number of shifts mapped to atoms	566
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

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

6 Model quality

6.1 Standard geometry

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	1.76±3.92	7±32/465 (1.6±6.9%)	1.86±3.87	9±36/622 (1.4±5.8%)
All	All	4.29	149/9300 (1.6%)	4.30	179/12440 (1.4%)

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

Mol	Chain	Chirality	Planarity
1	A	0.1±0.4	0.2±0.4
All	All	2	5

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	44	GLU	CD-OE1	-80.22	0.37	1.25	1	1
1	A	44	GLU	CD-OE2	-73.64	0.44	1.25	1	1
1	A	48	ARG	CZ-NH2	-72.12	0.39	1.33	1	1
1	A	20	GLU	CD-OE2	-68.90	0.49	1.25	1	1
1	A	20	GLU	CD-OE1	-63.42	0.55	1.25	1	1
1	A	49	ARG	CZ-NH1	-61.20	0.53	1.33	1	1
1	A	29	ARG	CZ-NH1	-59.37	0.55	1.33	1	1
1	A	48	ARG	CD-NE	-57.34	0.48	1.46	1	1
1	A	48	ARG	CZ-NH1	-54.65	0.62	1.33	1	1
1	A	15	SER	CB-OG	-54.26	0.71	1.42	1	1
1	A	49	ARG	NE-CZ	-54.07	0.62	1.33	1	1
1	A	25	TYR	CE2-CZ	-53.74	0.68	1.38	1	1
1	A	51	TYR	CE1-CZ	-53.63	0.68	1.38	1	1
1	A	24	TYR	CE1-CZ	-53.59	0.68	1.38	1	1
1	A	27	SER	CB-OG	-52.94	0.73	1.42	1	1
1	A	51	TYR	CE2-CZ	-52.76	0.69	1.38	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	25	TYR	CE1-CZ	-52.26	0.70	1.38	1	1
1	A	51	TYR	CG-CD2	-51.87	0.71	1.39	1	1
1	A	24	TYR	CG-CD2	-51.82	0.71	1.39	1	1
1	A	25	TYR	CG-CD1	-51.67	0.71	1.39	1	1
1	A	51	TYR	CG-CD1	-51.06	0.72	1.39	1	1
1	A	59	TYR	CE1-CZ	-51.05	0.72	1.38	1	1
1	A	25	TYR	CG-CD2	-50.39	0.73	1.39	1	1
1	A	59	TYR	CG-CD2	-49.67	0.74	1.39	1	1
1	A	34	ARG	CZ-NH1	-49.28	0.69	1.33	1	1
1	A	44	GLU	CG-CD	-48.64	0.79	1.51	1	1
1	A	24	TYR	CE2-CZ	-47.52	0.76	1.38	1	1
1	A	59	TYR	CE2-CZ	-46.03	0.78	1.38	1	1
1	A	35	PHE	CG-CD1	-45.64	0.70	1.38	1	1
1	A	24	TYR	CG-CD1	-45.53	0.80	1.39	1	1
1	A	59	TYR	CG-CD1	-44.99	0.80	1.39	1	1
1	A	13	SER	CB-OG	-44.35	0.84	1.42	1	1
1	A	22	ARG	CZ-NH1	-43.97	0.75	1.33	1	1
1	A	49	ARG	CZ-NH2	-42.63	0.77	1.33	1	1
1	A	47	PHE	CG-CD1	-42.63	0.74	1.38	1	1
1	A	35	PHE	CG-CD2	-42.60	0.74	1.38	1	1
1	A	48	ARG	NE-CZ	-41.73	0.78	1.33	1	1
1	A	47	PHE	CG-CD2	-41.60	0.76	1.38	1	1
1	A	43	ASN	CB-CG	-40.73	0.57	1.51	1	1
1	A	43	ASN	CG-OD1	-39.48	0.37	1.24	1	1
1	A	17	THR	CB-OG1	-39.35	0.64	1.43	1	1
1	A	34	ARG	CZ-NH2	-38.26	0.83	1.33	1	1
1	A	50	THR	CB-OG1	-37.91	0.67	1.43	1	1
1	A	54	GLN	CD-NE2	-37.80	0.38	1.32	1	1
1	A	49	ARG	CD-NE	-36.61	0.84	1.46	1	1
1	A	40	GLN	CG-CD	-36.56	0.67	1.51	1	1
1	A	35	PHE	CE2-CZ	-36.36	0.68	1.37	1	1
1	A	29	ARG	CZ-NH2	-36.16	0.86	1.33	1	1
1	A	40	GLN	CD-OE1	-35.90	0.45	1.24	1	1
1	A	37	TYR	CE1-CZ	-35.37	0.92	1.38	1	1
1	A	36	ASP	CG-OD2	-34.49	0.46	1.25	1	1
1	A	37	TYR	CG-CD2	-34.24	0.94	1.39	1	1
1	A	8	ASP	CG-OD1	-34.09	0.47	1.25	1	1
1	A	35	PHE	CE1-CZ	-33.96	0.72	1.37	1	1
1	A	47	PHE	CE2-CZ	-33.68	0.73	1.37	1	1
1	A	30	LYS	CD-CE	-33.02	0.68	1.51	1	1
1	A	29	ARG	NE-CZ	-32.91	0.90	1.33	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	47	PHE	CE1-CZ	-32.80	0.75	1.37	1	1
1	A	37	TYR	CE2-CZ	-32.65	0.96	1.38	1	1
1	A	37	TYR	CG-CD1	-31.67	0.97	1.39	1	1
1	A	53	CYS	CB-SG	-31.40	1.28	1.82	1	1
1	A	60	THR	C-OXT	-30.37	0.65	1.23	1	1
1	A	34	ARG	CD-NE	-29.63	0.96	1.46	1	1
1	A	36	ASP	CG-OD1	-29.03	0.58	1.25	1	1
1	A	52	ASP	CG-OD2	-27.90	0.61	1.25	1	1
1	A	32	CYS	CB-SG	-27.04	1.36	1.82	1	1
1	A	21	LYS	CD-CE	-26.45	0.85	1.51	1	1
1	A	22	ARG	NE-CZ	-26.43	0.98	1.33	1	1
1	A	31	GLN	CD-OE1	-26.37	0.66	1.24	1	1
1	A	29	ARG	CD-NE	-26.30	1.01	1.46	1	1
1	A	17	THR	CB-CG2	-25.46	0.68	1.52	1	1
1	A	52	ASP	CG-OD1	-25.12	0.67	1.25	1	1
1	A	9	LEU	CG-CD1	-24.86	0.59	1.51	1	1
1	A	12	ASP	CG-OD2	-24.35	0.69	1.25	1	1
1	A	31	GLN	CB-CG	-23.89	0.88	1.52	1	1
1	A	9	LEU	CB-CG	-23.70	0.83	1.52	1	1
1	A	54	GLN	CD-OE1	-23.48	0.72	1.24	1	1
1	A	8	ASP	CG-OD2	-23.43	0.71	1.25	1	1
1	A	31	GLN	CD-NE2	-23.10	0.75	1.32	1	1
1	A	5	SER	CB-OG	-23.05	1.12	1.42	1	1
1	A	7	CYS	CB-SG	-22.80	1.43	1.82	1	1
1	A	21	LYS	CE-NZ	-22.52	0.92	1.49	1	1
1	A	9	LEU	CG-CD2	-22.46	0.68	1.51	1	1
1	A	48	ARG	CG-CD	-22.24	0.96	1.51	1	1
1	A	18	LYS	CG-CD	-22.23	0.76	1.52	1	1
1	A	30	LYS	CE-NZ	-21.59	0.95	1.49	1	1
1	A	43	ASN	CG-ND2	-21.00	0.80	1.32	1	1
1	A	33	LEU	CG-CD2	-21.00	0.74	1.51	1	1
1	A	18	LYS	CE-NZ	-20.51	0.97	1.49	1	1
1	A	6	LEU	CG-CD2	-20.37	0.76	1.51	1	1
1	A	50	THR	CB-CG2	-20.02	0.86	1.52	1	1
1	A	44	GLU	CB-CG	-19.97	1.14	1.52	1	1
1	A	60	THR	C-O	-19.86	0.85	1.23	1	1
1	A	49	ARG	CG-CD	-19.01	1.04	1.51	1	1
1	A	33	LEU	CG-CD1	-18.88	0.82	1.51	1	1
1	A	20	GLU	CG-CD	-18.79	1.23	1.51	1	1
1	A	34	ARG	NE-CZ	-18.75	1.08	1.33	1	1
1	A	57	CYS	CB-SG	-18.61	1.50	1.82	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	33	LEU	CB-CG	-18.56	0.98	1.52	1	1
1	A	29	ARG	CG-CD	-18.30	1.06	1.51	1	1
1	A	40	GLN	CD-NE2	-18.03	0.87	1.32	1	1
1	A	36	ASP	CB-CG	-17.69	1.14	1.51	1	1
1	A	58	LEU	CG-CD2	-17.47	0.87	1.51	1	1
1	A	21	LYS	CG-CD	-17.42	0.93	1.52	1	1
1	A	6	LEU	CB-CG	-17.38	1.02	1.52	1	1
1	A	55	ARG	CZ-NH1	-17.06	1.10	1.33	1	1
1	A	58	LEU	CG-CD1	-15.36	0.95	1.51	1	1
1	A	12	ASP	CG-OD1	-15.09	0.90	1.25	1	1
1	A	55	ARG	CZ-NH2	-14.98	1.13	1.33	1	1
1	A	31	GLN	CG-CD	-14.52	1.17	1.51	1	1
1	A	10	PRO	N-CD	-14.47	1.27	1.47	1	1
1	A	45	ASN	CG-ND2	-12.69	1.01	1.32	1	1
1	A	46	ASN	CG-ND2	-11.81	1.03	1.32	1	1
1	A	38	THR	CB-OG1	-11.78	1.19	1.43	1	1
1	A	55	ARG	CD-NE	-11.59	1.26	1.46	1	1
1	A	52	ASP	CB-CG	-10.97	1.28	1.51	1	1
1	A	30	LYS	CG-CD	-10.72	1.16	1.52	1	1
1	A	18	LYS	CD-CE	-10.64	1.24	1.51	1	1
1	A	6	LEU	CG-CD1	-10.31	1.13	1.51	1	1
1	A	10	PRO	CA-CB	-9.63	1.34	1.53	1	1
1	A	9	LEU	C-O	-9.38	1.05	1.23	1	1
1	A	45	ASN	CG-OD1	-8.92	1.04	1.24	1	1
1	A	54	GLN	CG-CD	-8.60	1.31	1.51	1	1
1	A	38	THR	C-N	-8.56	1.17	1.33	1	1
1	A	46	ASN	CG-OD1	-8.27	1.05	1.24	1	1
1	A	38	THR	C-O	-8.13	1.07	1.23	1	1
1	A	11	ALA	CA-CB	-7.56	1.36	1.52	1	1
1	A	10	PRO	CG-CD	-7.56	1.25	1.50	1	1
1	A	55	ARG	NE-CZ	-7.43	1.23	1.33	1	1
1	A	9	LEU	C-N	-7.04	1.20	1.34	1	1
1	A	59	TYR	CD2-CE2	-6.61	1.29	1.39	1	1
1	A	15	SER	CA-CB	-6.58	1.43	1.52	1	1
1	A	38	THR	CB-CG2	-6.49	1.30	1.52	1	1
1	A	60	THR	CA-CB	-6.47	1.36	1.53	1	1
1	A	59	TYR	CD1-CE1	-6.40	1.29	1.39	1	1
1	A	10	PRO	C-N	-6.25	1.19	1.34	1	1
1	A	10	PRO	N-CA	-6.25	1.36	1.47	1	1
1	A	60	THR	CA-C	-6.02	1.37	1.52	1	1
1	A	59	TYR	CB-CG	-5.94	1.42	1.51	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	60	THR	CB-CG2	-5.43	1.34	1.52	1	1
1	A	10	PRO	CA-C	-5.38	1.42	1.52	1	1
1	A	23	ILE	CG1-CD1	-5.18	1.14	1.50	1	1
1	A	8	ASP	CB-CG	-5.17	1.40	1.51	1	1
1	A	60	THR	N-CA	-5.15	1.36	1.46	1	1
1	A	11	ALA	N-CA	-5.15	1.36	1.46	1	2
1	A	22	ARG	CZ-NH2	-5.14	1.26	1.33	1	1
1	A	9	LEU	CA-C	-5.04	1.39	1.52	1	1
1	A	59	TYR	CZ-OH	-5.03	1.29	1.37	1	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	51	TYR	CD1-CG-CD2	-87.95	21.16	117.90	1	1
1	A	25	TYR	CD1-CG-CD2	-87.95	21.16	117.90	1	1
1	A	51	TYR	CB-CG-CD1	81.31	169.78	121.00	1	1
1	A	25	TYR	CB-CG-CD2	80.73	169.44	121.00	1	1
1	A	25	TYR	CB-CG-CD1	80.50	169.30	121.00	1	1
1	A	51	TYR	CB-CG-CD2	80.09	169.06	121.00	1	1
1	A	35	PHE	CD1-CG-CD2	-74.19	21.86	118.30	1	1
1	A	20	GLU	OE1-CD-OE2	-70.80	38.35	123.30	1	1
1	A	35	PHE	CB-CG-CD1	70.15	169.90	120.80	1	1
1	A	35	PHE	CB-CG-CD2	67.75	168.23	120.80	1	1
1	A	24	TYR	CD1-CG-CD2	-67.63	43.51	117.90	1	1
1	A	22	ARG	NE-CZ-NH1	-65.45	87.57	120.30	1	1
1	A	48	ARG	NE-CZ-NH1	63.65	152.12	120.30	1	1
1	A	24	TYR	CB-CG-CD1	62.17	158.30	121.00	1	1
1	A	24	TYR	CB-CG-CD2	61.93	158.16	121.00	1	1
1	A	51	TYR	CE1-CZ-CE2	-61.09	22.06	119.80	1	1
1	A	25	TYR	CE1-CZ-CE2	-61.06	22.11	119.80	1	1
1	A	25	TYR	CG-CD2-CE2	60.55	169.74	121.30	1	1
1	A	51	TYR	CG-CD1-CE1	60.33	169.56	121.30	1	1
1	A	51	TYR	CG-CD2-CE2	59.99	169.29	121.30	1	1
1	A	25	TYR	CG-CD1-CE1	59.73	169.09	121.30	1	1
1	A	47	PHE	CD1-CG-CD2	-59.31	41.20	118.30	1	1
1	A	47	PHE	CB-CG-CD2	55.43	159.60	120.80	1	1
1	A	25	TYR	CZ-CE2-CD2	54.82	169.14	119.80	1	1
1	A	47	PHE	CB-CG-CD1	54.82	159.17	120.80	1	1
1	A	51	TYR	CZ-CE2-CD2	54.71	169.04	119.80	1	1
1	A	8	ASP	CB-CG-OD2	54.67	167.51	118.30	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	51	TYR	CD1-CE1-CZ	54.54	168.89	119.80	1	1
1	A	25	TYR	CD1-CE1-CZ	54.40	168.76	119.80	1	1
1	A	35	PHE	CE1-CZ-CE2	-54.10	22.63	120.00	1	1
1	A	59	TYR	CD1-CG-CD2	-52.24	60.44	117.90	1	1
1	A	49	ARG	NE-CZ-NH1	-52.18	94.21	120.30	1	1
1	A	59	TYR	CB-CG-CD1	51.27	151.76	121.00	1	1
1	A	8	ASP	OD1-CG-OD2	-48.28	31.57	123.30	1	1
1	A	24	TYR	CG-CD1-CE1	47.54	159.33	121.30	1	1
1	A	8	ASP	CB-CG-OD1	47.00	160.60	118.30	1	1
1	A	36	ASP	CB-CG-OD1	46.36	160.02	118.30	1	1
1	A	24	TYR	CE1-CZ-CE2	-46.31	45.71	119.80	1	1
1	A	24	TYR	CG-CD2-CE2	44.98	157.28	121.30	1	1
1	A	59	TYR	CB-CG-CD2	44.66	147.79	121.00	1	1
1	A	29	ARG	NE-CZ-NH2	44.43	142.51	120.30	1	1
1	A	35	PHE	CG-CD2-CE2	44.29	169.52	120.80	1	1
1	A	22	ARG	NE-CZ-NH2	43.98	142.29	120.30	1	1
1	A	35	PHE	CG-CD1-CE1	43.53	168.69	120.80	1	1
1	A	47	PHE	CE1-CZ-CE2	-43.26	42.13	120.00	1	1
1	A	24	TYR	CZ-CE2-CD2	42.78	158.30	119.80	1	1
1	A	35	PHE	CD1-CE1-CZ	40.79	169.05	120.10	1	1
1	A	35	PHE	CZ-CE2-CD2	40.13	168.25	120.10	1	1
1	A	24	TYR	CD1-CE1-CZ	40.08	155.87	119.80	1	1
1	A	36	ASP	OD1-CG-OD2	-39.39	48.47	123.30	1	1
1	A	44	GLU	OE1-CD-OE2	-38.20	77.46	123.30	1	1
1	A	34	ARG	NE-CZ-NH2	38.02	139.31	120.30	1	1
1	A	59	TYR	CG-CD1-CE1	37.66	151.43	121.30	1	1
1	A	48	ARG	NH1-CZ-NH2	-36.90	78.81	119.40	1	1
1	A	54	GLN	OE1-CD-NE2	-36.78	37.30	121.90	1	1
1	A	36	ASP	CB-CG-OD2	36.68	151.31	118.30	1	1
1	A	59	TYR	CE1-CZ-CE2	-35.70	62.68	119.80	1	1
1	A	47	PHE	CG-CD2-CE2	35.28	159.61	120.80	1	1
1	A	49	ARG	NE-CZ-NH2	35.10	137.85	120.30	1	1
1	A	47	PHE	CG-CD1-CE1	34.95	159.25	120.80	1	1
1	A	43	ASN	CB-CG-OD1	-33.87	53.87	121.60	1	1
1	A	59	TYR	CG-CD2-CE2	33.73	148.28	121.30	1	1
1	A	59	TYR	CZ-CE2-CD2	33.72	150.14	119.80	1	1
1	A	47	PHE	CD1-CE1-CZ	32.47	159.06	120.10	1	1
1	A	52	ASP	CB-CG-OD1	32.29	147.36	118.30	1	1
1	A	47	PHE	CZ-CE2-CD2	32.20	158.74	120.10	1	1
1	A	59	TYR	CD1-CE1-CZ	30.25	147.03	119.80	1	1
1	A	37	TYR	CD1-CG-CD2	-30.20	84.68	117.90	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	12	ASP	CB-CG-OD1	29.00	144.40	118.30	1	1
1	A	37	TYR	CB-CG-CD1	28.80	138.28	121.00	1	1
1	A	52	ASP	OD1-CG-OD2	-27.75	70.58	123.30	1	1
1	A	40	GLN	CG-CD-OE1	-27.27	67.05	121.60	1	1
1	A	37	TYR	CB-CG-CD2	26.73	137.04	121.00	1	1
1	A	34	ARG	NH1-CZ-NH2	-26.50	90.25	119.40	1	1
1	A	52	ASP	CB-CG-OD2	26.39	142.05	118.30	1	1
1	A	30	LYS	CD-CE-NZ	24.35	167.70	111.70	1	1
1	A	21	LYS	CD-CE-NZ	24.20	167.36	111.70	1	1
1	A	54	GLN	CG-CD-OE1	23.25	168.11	121.60	1	1
1	A	20	GLU	CG-CD-OE1	22.05	162.40	118.30	1	1
1	A	37	TYR	CG-CD1-CE1	21.89	138.81	121.30	1	1
1	A	12	ASP	OD1-CG-OD2	-20.90	83.60	123.30	1	1
1	A	50	THR	CA-CB-CG2	20.80	141.52	112.40	1	1
1	A	20	GLU	CG-CD-OE2	20.46	159.22	118.30	1	1
1	A	43	ASN	CA-CB-CG	20.46	158.41	113.40	1	1
1	A	37	TYR	CE1-CZ-CE2	-20.31	87.31	119.80	1	1
1	A	34	ARG	NE-CZ-NH1	20.25	130.42	120.30	1	1
1	A	17	THR	CA-CB-CG2	19.33	139.47	112.40	1	1
1	A	37	TYR	CZ-CE2-CD2	19.32	137.18	119.80	1	1
1	A	37	TYR	CG-CD2-CE2	19.27	136.72	121.30	1	1
1	A	33	LEU	CB-CG-CD2	18.87	143.09	111.00	1	1
1	A	33	LEU	CA-CB-CG	18.26	157.30	115.30	1	1
1	A	33	LEU	CB-CG-CD1	18.14	141.84	111.00	1	1
1	A	51	TYR	CE1-CZ-OH	18.12	169.03	120.10	1	1
1	A	25	TYR	CE1-CZ-OH	18.10	168.96	120.10	1	1
1	A	51	TYR	OH-CZ-CE2	18.08	168.91	120.10	1	1
1	A	25	TYR	OH-CZ-CE2	18.07	168.88	120.10	1	1
1	A	33	LEU	CD1-CG-CD2	-17.86	56.92	110.50	1	1
1	A	17	THR	OG1-CB-CG2	-17.80	69.06	110.00	1	1
1	A	48	ARG	NE-CZ-NH2	17.52	129.06	120.30	1	1
1	A	37	TYR	CD1-CE1-CZ	17.22	135.30	119.80	1	1
1	A	31	GLN	CA-CB-CG	16.73	150.21	113.40	1	1
1	A	18	LYS	CG-CD-CE	16.73	162.08	111.90	1	1
1	A	43	ASN	CB-CG-ND2	16.16	155.48	116.70	1	1
1	A	30	LYS	CG-CD-CE	16.07	160.10	111.90	1	1
1	A	54	GLN	CG-CD-NE2	15.79	154.58	116.70	1	1
1	A	29	ARG	NE-CZ-NH1	-15.77	112.41	120.30	1	1
1	A	18	LYS	CB-CG-CD	15.54	152.01	111.60	1	1
1	A	12	ASP	CB-CG-OD2	15.18	131.96	118.30	1	1
1	A	50	THR	OG1-CB-CG2	-14.60	76.42	110.00	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	49	ARG	CG-CD-NE	14.56	142.38	111.80	1	1
1	A	40	GLN	CB-CG-CD	14.36	148.95	111.60	1	1
1	A	24	TYR	OH-CZ-CE2	14.18	158.40	120.10	1	1
1	A	31	GLN	CB-CG-CD	14.08	148.22	111.60	1	1
1	A	22	ARG	CD-NE-CZ	14.02	143.22	123.60	1	1
1	A	44	GLU	CG-CD-OE2	13.85	146.00	118.30	1	1
1	A	34	ARG	CG-CD-NE	13.83	140.85	111.80	1	1
1	A	29	ARG	CD-NE-CZ	13.76	142.86	123.60	1	1
1	A	40	GLN	CG-CD-NE2	13.49	149.08	116.70	1	1
1	A	24	TYR	CE1-CZ-OH	13.26	155.90	120.10	1	1
1	A	17	THR	CA-CB-OG1	13.20	136.72	109.00	1	1
1	A	58	LEU	CB-CG-CD1	13.12	133.31	111.00	1	1
1	A	29	ARG	NH1-CZ-NH2	-13.03	105.07	119.40	1	1
1	A	34	ARG	CD-NE-CZ	12.65	141.31	123.60	1	1
1	A	43	ASN	OD1-CG-ND2	12.49	150.63	121.90	1	1
1	A	32	CYS	CA-CB-SG	12.47	136.45	114.00	1	1
1	A	9	LEU	CA-CB-CG	12.34	143.68	115.30	1	1
1	A	49	ARG	CD-NE-CZ	12.33	140.87	123.60	1	1
1	A	31	GLN	OE1-CD-NE2	-12.07	94.14	121.90	1	1
1	A	60	THR	CA-C-O	11.59	144.45	120.10	1	1
1	A	59	TYR	OH-CZ-CE2	11.14	150.19	120.10	1	1
1	A	21	LYS	CG-CD-CE	10.05	142.06	111.90	1	1
1	A	59	TYR	CE1-CZ-OH	10.01	147.13	120.10	1	1
1	A	29	ARG	CG-CD-NE	9.93	132.65	111.80	1	1
1	A	48	ARG	CD-NE-CZ	9.76	137.27	123.60	1	1
1	A	22	ARG	NH1-CZ-NH2	9.74	130.12	119.40	1	1
1	A	53	CYS	CA-CB-SG	9.72	131.50	114.00	1	1
1	A	40	GLN	OE1-CD-NE2	9.55	143.87	121.90	1	1
1	A	27	SER	CA-CB-OG	9.45	136.71	111.20	1	1
1	A	6	LEU	CA-CB-CG	9.42	136.97	115.30	1	1
1	A	29	ARG	CB-CG-CD	9.22	135.58	111.60	1	1
1	A	44	GLU	CG-CD-OE1	9.12	136.54	118.30	1	1
1	A	50	THR	CA-CB-OG1	8.81	127.50	109.00	1	1
1	A	9	LEU	CB-CG-CD2	8.59	125.61	111.00	1	1
1	A	44	GLU	CB-CG-CD	8.43	136.97	114.20	1	1
1	A	21	LYS	CB-CG-CD	8.38	133.39	111.60	1	1
1	A	18	LYS	CD-CE-NZ	8.08	130.28	111.70	1	1
1	A	49	ARG	NH1-CZ-NH2	7.76	127.94	119.40	1	1
1	A	37	TYR	C-N-CA	-7.69	102.47	121.70	20	1
1	A	55	ARG	NE-CZ-NH2	7.59	124.10	120.30	1	1
1	A	58	LEU	CD1-CG-CD2	-7.43	88.22	110.50	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	31	GLN	CG-CD-NE2	7.02	133.56	116.70	1	1
1	A	9	LEU	CD1-CG-CD2	-6.82	90.05	110.50	1	1
1	A	26	ASN	C-N-CA	-6.79	104.71	121.70	20	1
1	A	48	ARG	CG-CD-NE	6.64	125.75	111.80	1	1
1	A	36	ASP	CA-CB-CG	6.61	127.94	113.40	1	1
1	A	58	LEU	CB-CA-C	-6.50	97.85	110.20	10	1
1	A	37	TYR	OH-CZ-CE2	6.41	137.39	120.10	1	1
1	A	45	ASN	OD1-CG-ND2	-6.38	107.22	121.90	1	1
1	A	7	CYS	CA-CB-SG	6.37	125.47	114.00	1	1
1	A	9	LEU	CB-CG-CD1	6.19	121.52	111.00	1	1
1	A	38	THR	O-C-N	-6.09	112.85	123.20	1	1
1	A	6	LEU	CB-CG-CD1	5.99	121.19	111.00	1	1
1	A	11	ALA	N-CA-CB	5.97	118.46	110.10	13	1
1	A	45	ASN	CB-CG-OD1	5.96	133.52	121.60	1	1
1	A	29	ARG	CB-CA-C	-5.77	98.86	110.40	20	1
1	A	15	SER	CA-CB-OG	5.68	126.53	111.20	1	1
1	A	58	LEU	N-CA-CB	-5.67	99.05	110.40	13	2
1	A	37	TYR	CE1-CZ-OH	5.63	135.30	120.10	1	1
1	A	11	ALA	CA-C-N	-5.58	104.94	117.20	14	2
1	A	58	LEU	CB-CG-CD2	5.55	120.44	111.00	1	1
1	A	31	GLN	CA-C-N	-5.43	105.26	117.20	20	1
1	A	31	GLN	CG-CD-OE1	5.35	132.31	121.60	1	1
1	A	29	ARG	N-CA-CB	-5.34	100.99	110.60	20	1
1	A	46	ASN	OD1-CG-ND2	-5.26	109.80	121.90	1	1
1	A	15	SER	N-CA-CB	5.19	118.29	110.50	14	2
1	A	55	ARG	NH1-CZ-NH2	-5.00	113.89	119.40	1	1

All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	17	THR	CB	1
1	A	50	THR	CB	1

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	48	ARG	Sidechain	3
1	A	49	ARG	Sidechain	1
1	A	29	ARG	Sidechain	1

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	457	426	426	18±48
All	All	9140	8390	8515	363

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:TYR:CD1	1:A:59:TYR:CZ	1.56	1.93	1	1
1:A:59:TYR:CE2	1:A:59:TYR:CG	1.50	1.96	1	1
1:A:34:ARG:NE	1:A:34:ARG:NH1	1.49	1.61	1	1
1:A:24:TYR:CD1	1:A:24:TYR:CZ	1.48	1.99	1	1
1:A:59:TYR:CD2	1:A:59:TYR:CZ	1.48	2.01	1	1
1:A:21:LYS:CD	1:A:21:LYS:NZ	1.48	1.76	1	1
1:A:31:GLN:CG	1:A:31:GLN:NE2	1.48	1.77	1	1
1:A:44:GLU:CB	1:A:44:GLU:CD	1.47	1.79	1	1
1:A:59:TYR:CE1	1:A:59:TYR:CG	1.46	2.03	1	1
1:A:24:TYR:CG	1:A:24:TYR:CE2	1.46	2.02	1	1
1:A:51:TYR:CD1	1:A:51:TYR:CZ	1.44	2.04	1	1
1:A:35:PHE:CD2	1:A:35:PHE:CZ	1.43	2.04	1	1
1:A:25:TYR:CD2	1:A:25:TYR:CZ	1.42	2.04	1	1
1:A:47:PHE:CZ	1:A:47:PHE:CD2	1.42	2.07	1	1
1:A:25:TYR:CE1	1:A:25:TYR:CG	1.42	2.08	1	1
1:A:31:GLN:OE1	1:A:31:GLN:CG	1.42	1.68	1	1
1:A:51:TYR:CG	1:A:51:TYR:CE2	1.41	2.07	1	1
1:A:35:PHE:CG	1:A:35:PHE:CE1	1.41	2.06	1	1
1:A:47:PHE:CG	1:A:47:PHE:CE1	1.41	2.08	1	1
1:A:51:TYR:CD2	1:A:51:TYR:CZ	1.41	2.05	1	1
1:A:25:TYR:CD1	1:A:25:TYR:CZ	1.40	2.06	1	1
1:A:51:TYR:CG	1:A:51:TYR:CE1	1.40	2.08	1	1
1:A:35:PHE:CZ	1:A:35:PHE:CD1	1.40	2.09	1	1
1:A:20:GLU:OE2	1:A:20:GLU:CG	1.39	1.70	1	1
1:A:47:PHE:CZ	1:A:47:PHE:CD1	1.38	2.09	1	1
1:A:18:LYS:CE	1:A:18:LYS:CG	1.38	1.98	1	1
1:A:24:TYR:CD2	1:A:24:TYR:CZ	1.38	2.08	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:TYR:CG	1:A:25:TYR:CE2	1.38	2.09	1	1
1:A:36:ASP:OD1	1:A:36:ASP:CB	1.38	1.70	1	1
1:A:35:PHE:CE2	1:A:35:PHE:CG	1.38	2.11	1	1
1:A:47:PHE:CG	1:A:47:PHE:CE2	1.36	2.10	1	1
1:A:59:TYR:CD2	1:A:59:TYR:CB	1.36	2.09	1	1
1:A:24:TYR:CG	1:A:24:TYR:CE1	1.35	2.11	1	1
1:A:17:THR:CG2	1:A:17:THR:CA	1.34	2.06	1	1
1:A:20:GLU:CG	1:A:20:GLU:OE1	1.33	1.77	1	1
1:A:31:GLN:CD	1:A:31:GLN:CB	1.30	1.97	1	1
1:A:52:ASP:CB	1:A:52:ASP:OD2	1.28	1.80	1	1
1:A:24:TYR:CD2	1:A:24:TYR:CB	1.25	2.18	1	1
1:A:59:TYR:CD1	1:A:59:TYR:CB	1.24	2.16	1	1
1:A:43:ASN:CA	1:A:43:ASN:CG	1.24	2.06	1	1
1:A:47:PHE:CB	1:A:47:PHE:CD1	1.23	2.21	1	1
1:A:51:TYR:CD2	1:A:51:TYR:CB	1.23	2.21	1	1
1:A:8:ASP:OD1	1:A:8:ASP:CB	1.23	1.85	1	1
1:A:9:LEU:CG	1:A:9:LEU:CA	1.23	2.15	1	1
1:A:35:PHE:CB	1:A:35:PHE:CD1	1.21	2.21	1	1
1:A:25:TYR:CD1	1:A:25:TYR:CB	1.21	2.22	1	1
1:A:47:PHE:CB	1:A:47:PHE:CD2	1.20	2.23	1	1
1:A:51:TYR:CD1	1:A:51:TYR:CB	1.20	2.22	1	1
1:A:25:TYR:CD2	1:A:25:TYR:CB	1.19	2.24	1	1
1:A:18:LYS:CB	1:A:18:LYS:CD	1.18	2.21	1	1
1:A:59:TYR:OH	1:A:59:TYR:CE1	1.18	1.93	1	1
1:A:52:ASP:CB	1:A:52:ASP:OD1	1.14	1.88	1	1
1:A:24:TYR:CE1	1:A:24:TYR:OH	1.14	1.99	1	1
1:A:15:SER:CA	1:A:15:SER:OG	1.13	1.94	1	1
1:A:50:THR:CA	1:A:50:THR:CG2	1.13	2.27	1	1
1:A:21:LYS:CB	1:A:21:LYS:CD	1.12	2.26	1	1
1:A:34:ARG:NE	1:A:34:ARG:NH2	1.11	1.79	1	1
1:A:25:TYR:OH	1:A:25:TYR:CE2	1.10	2.04	1	1
1:A:51:TYR:OH	1:A:51:TYR:CE1	1.08	2.04	1	1
1:A:17:THR:OG1	1:A:17:THR:CA	1.07	2.01	1	1
1:A:31:GLN:CA	1:A:31:GLN:CG	1.06	2.33	1	1
1:A:24:TYR:CB	1:A:24:TYR:CD1	1.06	2.26	1	1
1:A:54:GLN:CG	1:A:54:GLN:OE1	1.06	2.02	1	1
1:A:50:THR:CA	1:A:50:THR:OG1	1.05	2.01	1	1
1:A:27:SER:OG	1:A:27:SER:HB3	1.05	1.34	1	1
1:A:27:SER:HB2	1:A:27:SER:OG	1.05	1.34	1	1
1:A:17:THR:CG2	1:A:17:THR:OG1	1.05	0.75	1	1
1:A:51:TYR:OH	1:A:51:TYR:CE2	1.04	2.05	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:SER:HB3	1:A:15:SER:OG	1.04	1.35	1	1
1:A:50:THR:CG2	1:A:50:THR:HB	1.04	1.61	1	1
1:A:17:THR:OG1	1:A:17:THR:HB	1.02	1.50	1	1
1:A:27:SER:OG	1:A:27:SER:CB	1.02	0.73	1	1
1:A:35:PHE:CD2	1:A:35:PHE:CB	1.02	2.25	1	1
1:A:15:SER:HB2	1:A:15:SER:OG	1.01	1.35	1	1
1:A:17:THR:HG23	1:A:17:THR:OG1	1.01	1.26	1	1
1:A:15:SER:CB	1:A:15:SER:OG	1.01	0.71	1	1
1:A:27:SER:OG	1:A:27:SER:CA	0.98	2.11	1	1
1:A:25:TYR:CE1	1:A:25:TYR:OH	0.98	2.06	1	1
1:A:59:TYR:CE2	1:A:59:TYR:OH	0.98	2.01	1	1
1:A:8:ASP:OD2	1:A:8:ASP:CB	0.97	2.10	1	1
1:A:17:THR:CG2	1:A:17:THR:HB	0.97	1.52	1	1
1:A:50:THR:CB	1:A:50:THR:HG21	0.96	1.49	1	1
1:A:50:THR:HG22	1:A:50:THR:CB	0.96	1.49	1	1
1:A:34:ARG:NH1	1:A:34:ARG:CD	0.96	2.27	1	1
1:A:21:LYS:CD	1:A:21:LYS:HG2	0.94	1.49	1	1
1:A:44:GLU:CD	1:A:44:GLU:HG3	0.94	1.38	1	1
1:A:17:THR:OG1	1:A:17:THR:CB	0.94	0.64	1	1
1:A:44:GLU:CD	1:A:44:GLU:HG2	0.94	1.38	1	1
1:A:21:LYS:CD	1:A:21:LYS:CG	0.93	0.93	1	1
1:A:21:LYS:HG3	1:A:21:LYS:CD	0.93	1.49	1	1
1:A:50:THR:HG23	1:A:50:THR:CB	0.93	1.49	1	1
1:A:23:ILE:HD11	1:A:32:CYS:HB3	0.91	1.41	5	3
1:A:8:ASP:OD2	1:A:8:ASP:CG	0.90	0.71	1	1
1:A:54:GLN:CD	1:A:54:GLN:OE1	0.88	0.72	1	1
1:A:44:GLU:CD	1:A:44:GLU:CG	0.87	0.79	1	1
1:A:31:GLN:CB	1:A:31:GLN:CG	0.87	0.88	1	1
1:A:24:TYR:CE2	1:A:24:TYR:OH	0.87	2.08	1	1
1:A:31:GLN:HG3	1:A:31:GLN:CB	0.86	1.41	1	1
1:A:31:GLN:HB3	1:A:31:GLN:CG	0.86	1.40	1	1
1:A:31:GLN:HB2	1:A:31:GLN:CG	0.86	1.40	1	1
1:A:9:LEU:HD13	1:A:45:ASN:HB3	0.86	1.44	18	1
1:A:50:THR:CG2	1:A:50:THR:CB	0.85	0.86	1	1
1:A:9:LEU:HB2	1:A:9:LEU:CG	0.85	1.39	1	1
1:A:31:GLN:HG2	1:A:31:GLN:CB	0.84	1.41	1	1
1:A:47:PHE:CE2	1:A:47:PHE:HZ	0.84	1.63	1	1
1:A:21:LYS:HD3	1:A:21:LYS:CE	0.83	1.41	1	1
1:A:9:LEU:HB3	1:A:9:LEU:CG	0.83	1.39	1	1
1:A:9:LEU:CG	1:A:9:LEU:HD23	0.83	1.36	1	1
1:A:17:THR:HG22	1:A:17:THR:CB	0.82	1.36	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LEU:CB	1:A:9:LEU:CG	0.82	0.83	1	1
1:A:21:LYS:HD2	1:A:21:LYS:CE	0.82	1.41	1	1
1:A:17:THR:HG21	1:A:17:THR:CB	0.82	1.36	1	1
1:A:9:LEU:HD22	1:A:9:LEU:CG	0.82	1.36	1	1
1:A:9:LEU:HD21	1:A:9:LEU:CG	0.81	1.36	1	1
1:A:17:THR:HG23	1:A:17:THR:CB	0.81	1.36	1	1
1:A:17:THR:CG2	1:A:17:THR:HG1	0.81	1.53	1	1
1:A:43:ASN:HD22	1:A:43:ASN:CG	0.80	1.44	1	1
1:A:43:ASN:HD21	1:A:43:ASN:CG	0.80	1.44	1	1
1:A:9:LEU:HB2	1:A:9:LEU:HG	0.80	0.94	1	1
1:A:21:LYS:HE3	1:A:21:LYS:CD	0.79	1.33	1	1
1:A:21:LYS:HE2	1:A:21:LYS:CD	0.79	1.33	1	1
1:A:35:PHE:CE2	1:A:35:PHE:HZ	0.79	1.60	1	1
1:A:21:LYS:HD2	1:A:21:LYS:CG	0.79	1.47	1	1
1:A:21:LYS:HD3	1:A:21:LYS:CG	0.78	1.47	1	1
1:A:18:LYS:HG3	1:A:18:LYS:CD	0.78	1.32	1	1
1:A:31:GLN:CD	1:A:31:GLN:HE22	0.78	1.39	1	1
1:A:47:PHE:HZ	1:A:47:PHE:CE1	0.78	1.65	1	1
1:A:18:LYS:HG2	1:A:18:LYS:CD	0.77	1.32	1	1
1:A:50:THR:CB	1:A:50:THR:OG1	0.76	0.67	1	1
1:A:31:GLN:CD	1:A:31:GLN:HE21	0.76	1.39	1	1
1:A:9:LEU:HD11	1:A:9:LEU:CG	0.76	1.30	1	1
1:A:18:LYS:HD3	1:A:18:LYS:CG	0.75	1.29	1	1
1:A:59:TYR:CD1	1:A:59:TYR:CG	0.75	0.80	1	1
1:A:18:LYS:HD2	1:A:18:LYS:CG	0.75	1.29	1	1
1:A:9:LEU:HD12	1:A:9:LEU:CG	0.75	1.30	1	1
1:A:17:THR:HG21	1:A:17:THR:OG1	0.75	0.98	1	1
1:A:18:LYS:CD	1:A:18:LYS:CG	0.75	0.76	1	1
1:A:9:LEU:CG	1:A:9:LEU:HD13	0.75	1.30	1	1
1:A:34:ARG:CZ	1:A:34:ARG:HH22	0.75	1.46	1	1
1:A:43:ASN:CG	1:A:43:ASN:ND2	0.74	0.80	1	1
1:A:24:TYR:CG	1:A:24:TYR:CD1	0.74	0.80	1	1
1:A:43:ASN:HB2	1:A:43:ASN:CG	0.74	1.18	1	1
1:A:9:LEU:HB3	1:A:45:ASN:HB2	0.74	1.59	19	3
1:A:59:TYR:CE2	1:A:59:TYR:CZ	0.74	0.78	1	1
1:A:34:ARG:CZ	1:A:34:ARG:HH21	0.73	1.46	1	1
1:A:43:ASN:HB3	1:A:43:ASN:CG	0.73	1.18	1	1
1:A:21:LYS:CD	1:A:21:LYS:CE	0.71	0.85	1	1
1:A:59:TYR:CD2	1:A:59:TYR:CG	0.70	0.74	1	1
1:A:24:TYR:CE2	1:A:24:TYR:CZ	0.70	0.76	1	1
1:A:47:PHE:CG	1:A:47:PHE:CD2	0.69	0.76	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:GLN:CD	1:A:31:GLN:NE2	0.69	0.75	1	1
1:A:12:ASP:HB3	1:A:43:ASN:HB3	0.69	1.62	4	3
1:A:59:TYR:CZ	1:A:59:TYR:CE1	0.69	0.72	1	1
1:A:17:THR:CG2	1:A:17:THR:CB	0.68	0.68	1	1
1:A:9:LEU:CG	1:A:9:LEU:CD2	0.68	0.68	1	1
1:A:34:ARG:CZ	1:A:34:ARG:NH2	0.68	0.83	1	1
1:A:47:PHE:CZ	1:A:47:PHE:CE1	0.67	0.75	1	1
1:A:54:GLN:O	1:A:58:LEU:HB3	0.67	1.88	1	2
1:A:9:LEU:HB3	1:A:43:ASN:HD21	0.67	1.50	9	2
1:A:31:GLN:OE1	1:A:31:GLN:HG2	0.67	1.86	1	1
1:A:36:ASP:OD1	1:A:36:ASP:CG	0.67	0.58	1	1
1:A:47:PHE:CZ	1:A:47:PHE:CE2	0.67	0.73	1	1
1:A:47:PHE:CG	1:A:47:PHE:CD1	0.67	0.74	1	1
1:A:21:LYS:HG3	1:A:34:ARG:HE	0.67	1.49	16	2
1:A:35:PHE:CE2	1:A:35:PHE:CZ	0.66	0.68	1	1
1:A:9:LEU:CB	1:A:9:LEU:HG	0.66	1.20	1	1
1:A:20:GLU:OE1	1:A:20:GLU:CD	0.66	0.55	1	1
1:A:35:PHE:CZ	1:A:35:PHE:CE1	0.65	0.72	1	1
1:A:24:TYR:CG	1:A:24:TYR:CD2	0.65	0.71	1	1
1:A:31:GLN:HA	1:A:31:GLN:HE21	0.64	1.51	2	1
1:A:9:LEU:CD1	1:A:9:LEU:HG	0.64	1.38	1	1
1:A:34:ARG:HH12	1:A:34:ARG:CZ	0.63	1.34	1	1
1:A:55:ARG:HA	1:A:59:TYR:CD1	0.63	2.29	18	3
1:A:34:ARG:CZ	1:A:34:ARG:HH11	0.62	1.34	1	1
1:A:43:ASN:CB	1:A:43:ASN:CG	0.62	0.57	1	1
1:A:24:TYR:CE1	1:A:24:TYR:CZ	0.62	0.68	1	1
1:A:12:ASP:HB3	1:A:43:ASN:HB2	0.62	1.72	11	1
1:A:24:TYR:CE1	1:A:35:PHE:HB3	0.62	2.30	18	1
1:A:59:TYR:HD1	1:A:59:TYR:CG	0.62	1.37	1	1
1:A:21:LYS:HE2	1:A:34:ARG:HG3	0.62	1.72	12	1
1:A:8:ASP:OD1	1:A:8:ASP:CG	0.62	0.46	1	1
1:A:35:PHE:CD2	1:A:35:PHE:CG	0.61	0.74	1	1
1:A:55:ARG:HA	1:A:59:TYR:CD2	0.61	2.30	5	6
1:A:20:GLU:OE2	1:A:20:GLU:CD	0.61	0.49	1	1
1:A:59:TYR:HE2	1:A:59:TYR:CZ	0.61	1.36	1	1
1:A:55:ARG:HA	1:A:59:TYR:HD2	0.60	1.57	6	5
1:A:23:ILE:HD11	1:A:32:CYS:SG	0.59	2.37	2	1
1:A:25:TYR:CD2	1:A:25:TYR:CG	0.59	0.73	1	1
1:A:20:GLU:HB3	1:A:37:TYR:O	0.59	1.98	8	2
1:A:4:PRO:HD2	1:A:57:CYS:SG	0.59	2.37	10	1
1:A:25:TYR:CD1	1:A:25:TYR:CG	0.59	0.72	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LEU:CD1	1:A:9:LEU:CG	0.59	0.59	1	1
1:A:54:GLN:NE2	1:A:54:GLN:OE1	0.59	0.48	1	1
1:A:59:TYR:HD2	1:A:59:TYR:CG	0.58	1.34	1	1
1:A:34:ARG:CZ	1:A:34:ARG:NH1	0.58	0.69	1	1
1:A:51:TYR:CG	1:A:51:TYR:CD1	0.58	0.72	1	1
1:A:44:GLU:HB3	1:A:44:GLU:CD	0.58	2.04	1	1
1:A:25:TYR:CZ	1:A:25:TYR:CE2	0.57	0.68	1	1
1:A:27:SER:CB	1:A:27:SER:HG	0.57	1.28	1	1
1:A:48:ARG:HH11	1:A:48:ARG:CZ	0.57	1.28	1	1
1:A:25:TYR:CE1	1:A:25:TYR:CZ	0.57	0.70	1	1
1:A:55:ARG:O	1:A:58:LEU:HB3	0.57	1.99	13	1
1:A:15:SER:CB	1:A:15:SER:HG	0.57	1.27	1	1
1:A:59:TYR:CZ	1:A:59:TYR:HE1	0.57	1.33	1	1
1:A:24:TYR:CG	1:A:24:TYR:HD1	0.57	1.33	1	1
1:A:23:ILE:HG12	1:A:32:CYS:SG	0.57	2.40	6	2
1:A:31:GLN:CB	1:A:31:GLN:NE2	0.56	2.44	1	1
1:A:51:TYR:CE1	1:A:51:TYR:CZ	0.56	0.68	1	1
1:A:35:PHE:CD1	1:A:35:PHE:CG	0.55	0.70	1	1
1:A:24:TYR:HE2	1:A:24:TYR:CZ	0.55	1.31	1	1
1:A:51:TYR:CE2	1:A:51:TYR:CZ	0.55	0.70	1	1
1:A:30:LYS:HD2	1:A:30:LYS:O	0.55	2.02	7	3
1:A:51:TYR:CG	1:A:51:TYR:CD2	0.54	0.71	1	1
1:A:47:PHE:CG	1:A:47:PHE:HD1	0.54	1.29	1	1
1:A:14:GLY:HA2	1:A:41:GLY:O	0.54	2.03	19	7
1:A:7:CYS:HB3	1:A:25:TYR:CD2	0.54	2.37	18	4
1:A:47:PHE:CG	1:A:47:PHE:HD2	0.54	1.30	1	1
1:A:47:PHE:CZ	1:A:47:PHE:HE1	0.53	1.29	1	1
1:A:47:PHE:CZ	1:A:47:PHE:HE2	0.53	1.28	1	1
1:A:50:THR:HG1	1:A:50:THR:CB	0.53	1.24	1	1
1:A:52:ASP:CG	1:A:52:ASP:OD1	0.53	0.67	1	1
1:A:9:LEU:HG	1:A:9:LEU:CD2	0.53	1.42	1	1
1:A:24:TYR:CG	1:A:24:TYR:HD2	0.53	1.28	1	1
1:A:16:GLY:CA	1:A:40:GLN:HB3	0.52	2.34	10	1
1:A:21:LYS:HD2	1:A:21:LYS:HE3	0.52	1.22	1	1
1:A:4:PRO:HD2	1:A:7:CYS:SG	0.52	2.45	3	2
1:A:24:TYR:HE1	1:A:24:TYR:CZ	0.51	1.26	1	1
1:A:9:LEU:HD21	1:A:24:TYR:HD2	0.51	1.66	18	1
1:A:11:ALA:HA	1:A:24:TYR:CE2	0.50	2.41	17	2
1:A:21:LYS:HD2	1:A:21:LYS:HG2	0.50	1.36	1	1
1:A:17:THR:HG1	1:A:17:THR:CB	0.50	1.21	1	1
1:A:34:ARG:HD2	1:A:35:PHE:N	0.50	2.20	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:O	1:A:9:LEU:HB3	0.50	2.06	18	1
1:A:9:LEU:HG	1:A:43:ASN:HB3	0.50	1.84	6	1
1:A:12:ASP:H	1:A:43:ASN:ND2	0.49	2.04	4	1
1:A:21:LYS:HD3	1:A:21:LYS:HG3	0.49	1.36	1	1
1:A:52:ASP:CG	1:A:52:ASP:OD2	0.49	0.61	1	1
1:A:18:LYS:HB3	1:A:38:THR:HG21	0.49	1.84	20	1
1:A:35:PHE:HD2	1:A:35:PHE:CG	0.49	1.24	1	1
1:A:49:ARG:HD3	1:A:52:ASP:OD1	0.49	2.06	6	1
1:A:54:GLN:O	1:A:58:LEU:HB2	0.49	2.08	13	1
1:A:18:LYS:HD3	1:A:19:ALA:N	0.48	2.23	10	2
1:A:29:ARG:HB3	1:A:31:GLN:HG3	0.48	1.85	20	1
1:A:23:ILE:O	1:A:47:PHE:HB2	0.48	2.09	6	4
1:A:13:SER:O	1:A:38:THR:HG22	0.47	2.09	2	1
1:A:25:TYR:HD2	1:A:25:TYR:CG	0.47	1.23	1	1
1:A:51:TYR:CG	1:A:51:TYR:HD2	0.47	1.22	1	1
1:A:31:GLN:HG3	1:A:31:GLN:HB2	0.47	1.31	1	1
1:A:24:TYR:HB2	1:A:45:ASN:OD1	0.47	2.09	8	1
1:A:25:TYR:CG	1:A:25:TYR:HD1	0.47	1.23	1	1
1:A:51:TYR:CG	1:A:51:TYR:HD1	0.47	1.23	1	1
1:A:21:LYS:HG3	1:A:34:ARG:HD3	0.47	1.84	6	1
1:A:35:PHE:HE1	1:A:35:PHE:CZ	0.47	1.23	1	1
1:A:21:LYS:HE3	1:A:34:ARG:HD2	0.46	1.86	7	1
1:A:48:ARG:NH1	1:A:48:ARG:CZ	0.46	0.62	1	1
1:A:35:PHE:HD1	1:A:35:PHE:CG	0.46	1.22	1	1
1:A:25:TYR:CZ	1:A:25:TYR:HE1	0.46	1.22	1	1
1:A:51:TYR:HE2	1:A:51:TYR:CZ	0.46	1.21	1	1
1:A:29:ARG:N	1:A:29:ARG:HD2	0.46	2.26	12	1
1:A:51:TYR:HE1	1:A:51:TYR:CZ	0.46	1.21	1	1
1:A:18:LYS:HG2	1:A:19:ALA:N	0.46	2.26	4	3
1:A:35:PHE:CE2	1:A:37:TYR:HB2	0.46	2.46	17	2
1:A:52:ASP:O	1:A:56:THR:HG22	0.45	2.10	11	3
1:A:31:GLN:OE1	1:A:31:GLN:CD	0.45	0.65	1	1
1:A:25:TYR:CZ	1:A:25:TYR:HE2	0.45	1.20	1	1
1:A:18:LYS:O	1:A:38:THR:HA	0.45	2.12	18	1
1:A:26:ASN:HB2	1:A:33:LEU:HD22	0.45	1.86	17	2
1:A:21:LYS:HD3	1:A:34:ARG:HD3	0.45	1.87	5	1
1:A:35:PHE:CZ	1:A:35:PHE:HE2	0.45	1.21	1	1
1:A:16:GLY:H	1:A:38:THR:HG23	0.45	1.72	2	1
1:A:23:ILE:HG23	1:A:47:PHE:HB2	0.44	1.88	7	3
1:A:22:ARG:HD2	1:A:46:ASN:OD1	0.44	2.12	17	2
1:A:23:ILE:HG21	1:A:49:ARG:C	0.44	2.33	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ASP:OD1	1:A:36:ASP:OD2	0.44	0.44	1	1
1:A:24:TYR:HD2	1:A:35:PHE:CD1	0.44	2.31	19	1
1:A:34:ARG:NH1	1:A:34:ARG:HD3	0.44	2.19	1	1
1:A:21:LYS:HG2	1:A:34:ARG:HD3	0.44	1.90	18	1
1:A:23:ILE:CD1	1:A:32:CYS:SG	0.44	3.06	2	1
1:A:6:LEU:HA	1:A:9:LEU:HD23	0.43	1.88	4	1
1:A:23:ILE:HG13	1:A:33:LEU:C	0.43	2.33	16	2
1:A:22:ARG:HB3	1:A:47:PHE:O	0.43	2.13	18	1
1:A:25:TYR:CE2	1:A:27:SER:HA	0.43	2.48	4	1
1:A:20:GLU:O	1:A:36:ASP:HA	0.43	2.13	6	2
1:A:49:ARG:HD3	1:A:52:ASP:OD2	0.43	2.13	8	1
1:A:9:LEU:HD12	1:A:10:PRO:HD2	0.43	1.89	10	1
1:A:37:TYR:CE1	1:A:42:GLY:HA3	0.43	2.48	16	2
1:A:13:SER:HA	1:A:36:ASP:O	0.43	2.12	6	1
1:A:21:LYS:HA	1:A:34:ARG:NH1	0.43	2.29	20	1
1:A:12:ASP:CB	1:A:43:ASN:HD22	0.42	2.27	1	1
1:A:29:ARG:O	1:A:31:GLN:HG3	0.42	2.14	3	1
1:A:21:LYS:CE	1:A:34:ARG:HG3	0.42	2.43	12	1
1:A:26:ASN:OD1	1:A:29:ARG:HG2	0.42	2.14	5	1
1:A:4:PRO:HB2	1:A:6:LEU:CD2	0.42	2.44	19	1
1:A:51:TYR:CE2	1:A:55:ARG:HD2	0.42	2.50	8	3
1:A:47:PHE:CZ	1:A:56:THR:HG21	0.42	2.50	18	1
1:A:24:TYR:HD1	1:A:35:PHE:CD1	0.41	2.33	20	1
1:A:24:TYR:CE2	1:A:26:ASN:HB2	0.41	2.49	20	1
1:A:22:ARG:HD2	1:A:48:ARG:HA	0.41	1.91	7	1
1:A:7:CYS:SG	1:A:25:TYR:CD1	0.41	3.13	20	1
1:A:6:LEU:O	1:A:45:ASN:HB2	0.41	2.15	18	1
1:A:26:ASN:OD1	1:A:29:ARG:HD3	0.41	2.14	17	2
1:A:22:ARG:HG3	1:A:37:TYR:HB3	0.41	1.91	12	1
1:A:29:ARG:HD2	1:A:29:ARG:N	0.41	2.31	10	1
1:A:21:LYS:HA	1:A:34:ARG:CZ	0.40	2.45	20	1
1:A:21:LYS:CD	1:A:34:ARG:HD3	0.40	2.46	5	1
1:A:23:ILE:HD13	1:A:24:TYR:N	0.40	2.31	2	1
1:A:26:ASN:HD22	1:A:33:LEU:HD12	0.40	1.76	9	1
1:A:58:LEU:HD13	1:A:58:LEU:O	0.40	2.17	20	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	56/60 (93%)	54±1 (96±2%)	2±1 (3±2%)	0±1 (1±1%)	31 76
All	All	1120/1200 (93%)	1078 (96%)	34 (3%)	8 (1%)	31 76

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	11	ALA	5
1	A	10	PRO	2
1	A	6	LEU	1

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	49/52 (94%)	46±3 (94±6%)	3±3 (6±6%)	29 74
All	All	980/1040 (94%)	922 (94%)	58 (6%)	29 74

All 23 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	34	ARG	9
1	A	21	LYS	7
1	A	35	PHE	5
1	A	52	ASP	4
1	A	23	ILE	4
1	A	40	GLN	3
1	A	31	GLN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	9	LEU	3
1	A	48	ARG	2
1	A	53	CYS	2
1	A	18	LYS	2
1	A	24	TYR	2
1	A	36	ASP	2
1	A	27	SER	1
1	A	50	THR	1
1	A	57	CYS	1
1	A	33	LEU	1
1	A	29	ARG	1
1	A	54	GLN	1
1	A	43	ASN	1
1	A	6	LEU	1
1	A	30	LYS	1
1	A	17	THR	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 carbohydrates 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

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6506

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	566
Number of shifts mapped to atoms	566
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	58	0.53 ± 0.19	Should be applied
$^{13}C_{\beta}$	54	-0.16 ± 0.50	None needed (< 0.5 ppm)
$^{13}C'$	55	0.42 ± 0.19	None needed (< 0.5 ppm)
^{15}N	55	-0.13 ± 0.86	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 539 atoms were assigned a chemical shift out of a possible 708. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	269/281 (96%)	107/112 (96%)	109/114 (96%)	53/55 (96%)
Sidechain	249/369 (67%)	162/220 (74%)	87/121 (72%)	0/28 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	21/58 (36%)	20/30 (67%)	1/28 (4%)	0/0 (—%)
Overall	539/708 (76%)	289/362 (80%)	197/263 (75%)	53/83 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 565 atoms were assigned a chemical shift out of a possible 758. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	279/296 (94%)	111/118 (94%)	113/120 (94%)	55/58 (95%)
Sidechain	265/404 (66%)	172/241 (71%)	93/131 (71%)	0/32 (0%)
Aromatic	21/58 (36%)	20/30 (67%)	1/28 (4%)	0/0 (—%)
Overall	565/758 (75%)	303/389 (78%)	207/279 (74%)	55/90 (61%)

7.1.4 Statistically unusual chemical shifts (i)

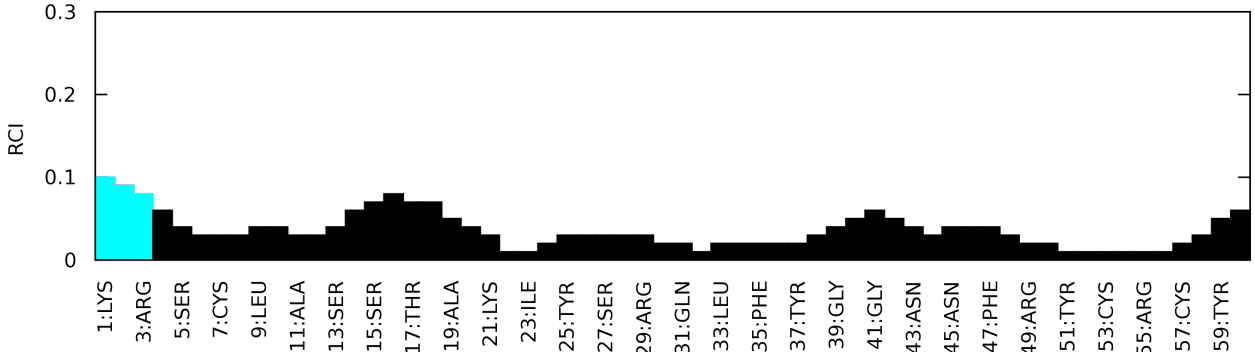
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	24	TYR	CD1	54.99	139.11 – 126.41	-61.2
1	A	11	ALA	HB1	-0.40	2.61 – 0.11	-7.0
1	A	11	ALA	HB3	-0.40	2.61 – 0.11	-7.0
1	A	11	ALA	HB2	-0.40	2.61 – 0.11	-7.0

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:


RCI
0.3
0.2
0.1
0
1:LYS
3:ARG
5:SER
7:CYS
9:LEU
11:ALA
13:SER
15:SER
17:THR
19:ALA
21:LYS
23:ILE
25:TYR
27:SER
29:ARG
31:GLN
33:LEU
35:PHE
37:TYR
39:GLY
41:GLY
43:ASN
45:ASN
47:PHE
49:ARG
51:TYR
53:CYS
55:ARG
57:CYS
59:TYR