Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 01:55 PM BST

PDB ID	:	1C15
Title	:	SOLUTION STRUCTURE OF APAF-1 CARD
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Deposited on	:	1999-07-20

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:

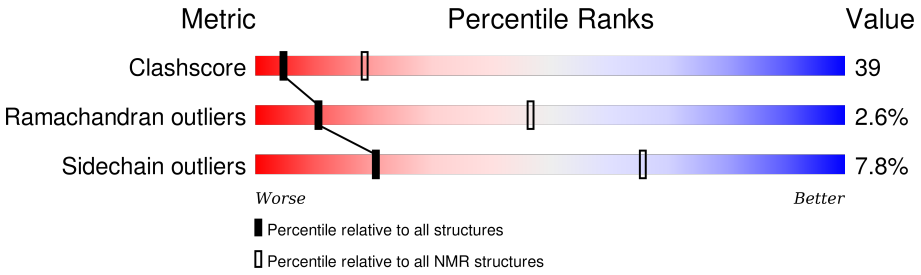
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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

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

The overall completeness of chemical shifts assignment is 61%.

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	97	58% 31% · 7%

2 Ensemble composition and analysis

This entry contains 16 models. Model 16 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:3-A:92 (90)	0.27	16

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, 4, 5, 9, 11, 12, 14, 15
2	3, 6, 7, 8, 10, 16
3	2, 13

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1553 atoms, of which 778 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called APOPTOTIC PROTEASE ACTIVATING FACTOR 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	97	1553	485	778	133	151	6	0

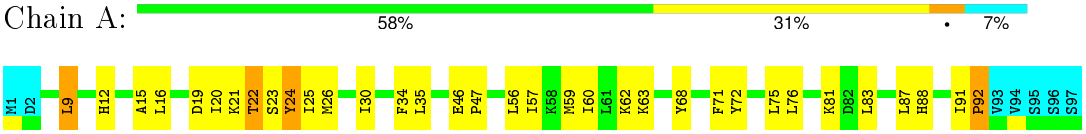
4 Residue-property plots (i)

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: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

Chain A:



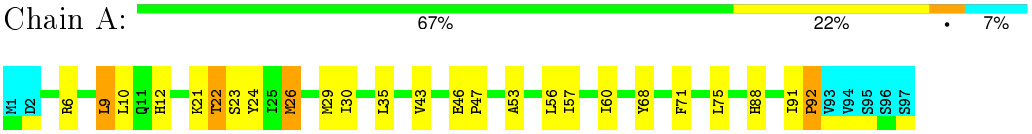
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

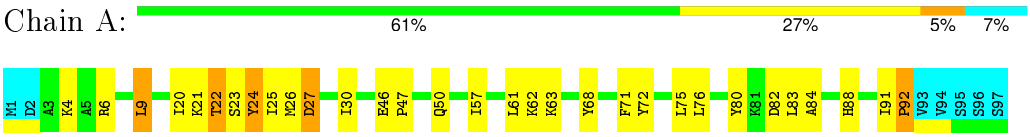
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

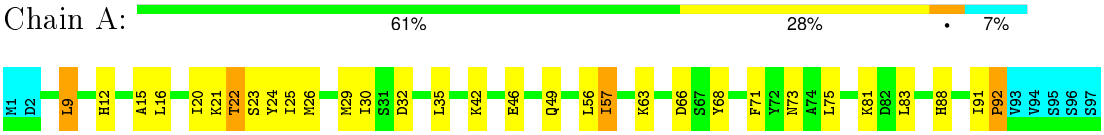
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

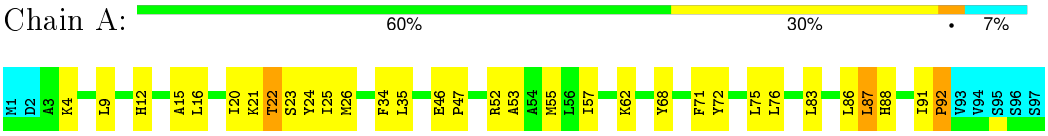
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

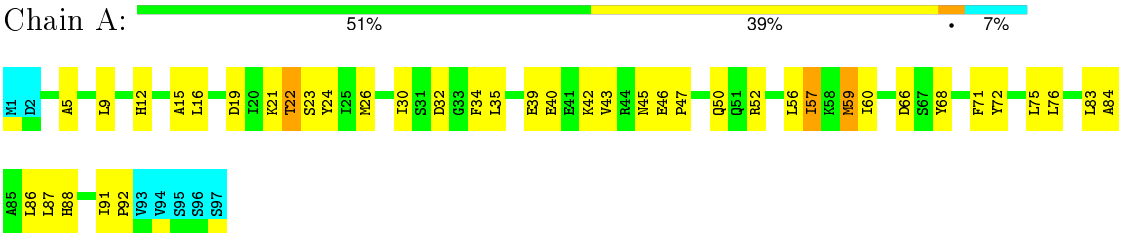
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

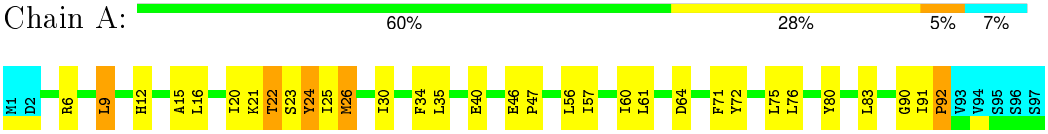
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

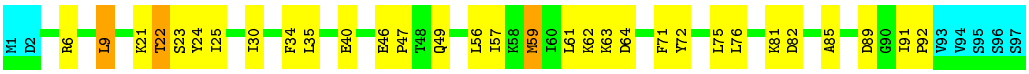
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

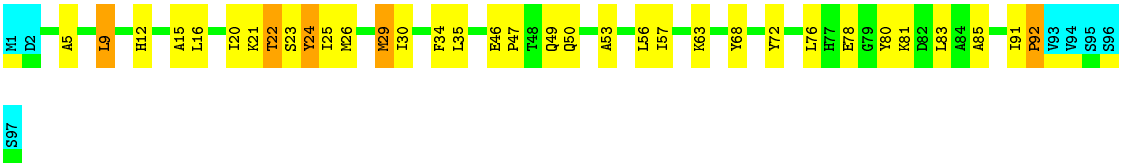
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

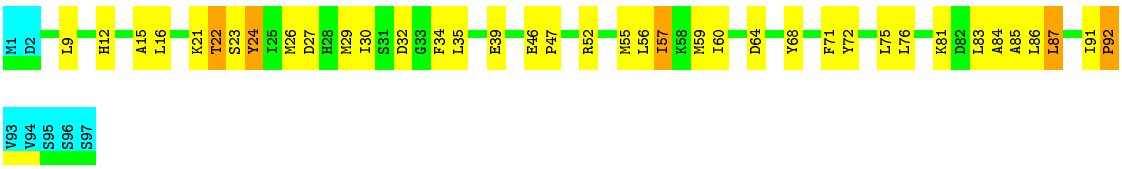
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

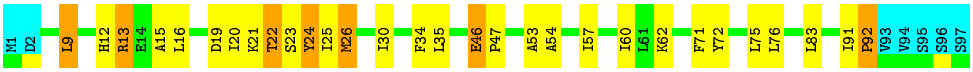
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

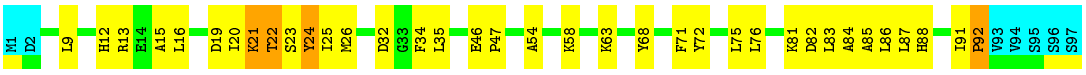
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

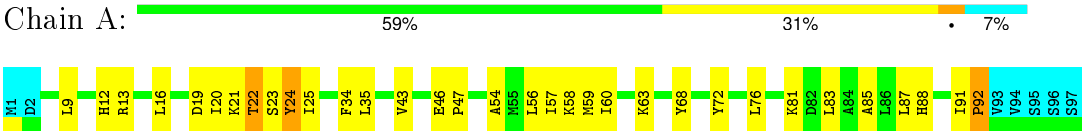
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

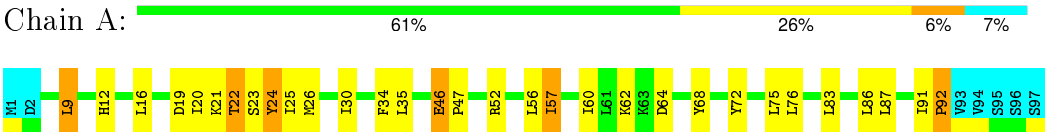
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

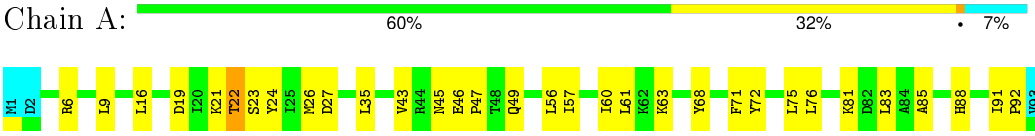
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

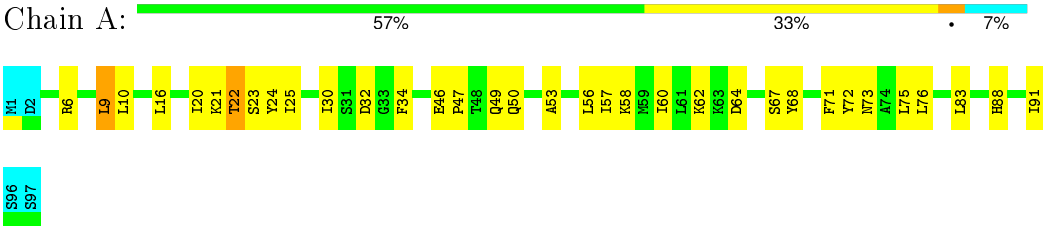
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

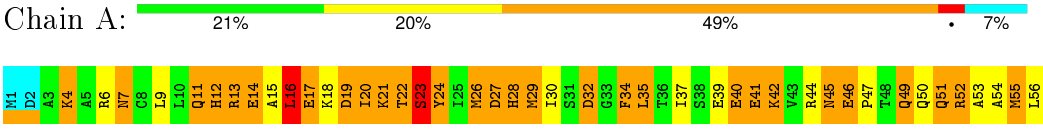
Chain A:

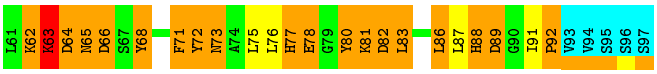


4.2.16 Score per residue for model 16 (medoid)

• Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

Chain A:




L61
K62
K63
D64
N65
D66
S67
Y68
F71
Y72
N73
A74
L75
L76
H77
E78
G79
Y80
K81
D82
L83
L86
L87
H88
D89
G90
I91
P92
V93
V94
S95
S96
S97

5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS*.

Of the 30 calculated structures, 16 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
DYANA	structure solution	1.5
X-PLOR	refinement	3.851

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 4661
Number of chemical shift lists	1
Total number of shifts	858
Number of shifts mapped to atoms	858
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	61%

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	2.00±3.78	9±36/738 (1.2±4.8%)	2.34±4.24	12±47/992 (1.2±4.8%)
All	All	4.27	147/11808 (1.2%)	4.84	195/15872 (1.2%)

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	40	GLU	CD-OE1	-103.44	0.11	1.25	16	1
1	A	46	GLU	CD-OE1	-88.08	0.28	1.25	16	1
1	A	46	GLU	CD-OE2	-73.61	0.44	1.25	16	1
1	A	6	ARG	CZ-NH1	-72.58	0.38	1.33	16	1
1	A	13	ARG	CZ-NH1	-71.27	0.40	1.33	16	1
1	A	41	GLU	CD-OE2	-68.62	0.50	1.25	16	1
1	A	17	GLU	CD-OE1	-63.82	0.55	1.25	16	1
1	A	40	GLU	CD-OE2	-63.71	0.55	1.25	16	1
1	A	14	GLU	CD-OE1	-63.09	0.56	1.25	16	1
1	A	14	GLU	CD-OE2	-58.72	0.61	1.25	16	1
1	A	44	ARG	CZ-NH1	-58.24	0.57	1.33	16	1
1	A	17	GLU	CD-OE2	-58.12	0.61	1.25	16	1
1	A	46	GLU	CG-CD	-57.12	0.66	1.51	16	1
1	A	80	TYR	CG-CD2	-53.02	0.70	1.39	16	1
1	A	24	TYR	CG-CD1	-52.80	0.70	1.39	16	1
1	A	68	TYR	CG-CD1	-52.65	0.70	1.39	16	1
1	A	80	TYR	CG-CD1	-52.56	0.70	1.39	16	1
1	A	80	TYR	CE1-CZ	-52.50	0.70	1.38	16	1
1	A	24	TYR	CG-CD2	-52.49	0.70	1.39	16	1
1	A	68	TYR	CE2-CZ	-52.39	0.70	1.38	16	1
1	A	68	TYR	CG-CD2	-52.29	0.71	1.39	16	1
1	A	24	TYR	CE2-CZ	-52.23	0.70	1.38	16	1
1	A	68	TYR	CE1-CZ	-52.00	0.70	1.38	16	1
1	A	80	TYR	CE2-CZ	-51.99	0.70	1.38	16	1
1	A	24	TYR	CE1-CZ	-51.96	0.71	1.38	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	41	GLU	CD-OE1	-51.70	0.68	1.25	16	1
1	A	6	ARG	CZ-NH2	-51.07	0.66	1.33	16	1
1	A	72	TYR	CG-CD1	-50.10	0.74	1.39	16	1
1	A	44	ARG	CZ-NH2	-50.06	0.68	1.33	16	1
1	A	78	GLU	CD-OE1	-49.92	0.70	1.25	16	1
1	A	72	TYR	CE2-CZ	-49.58	0.74	1.38	16	1
1	A	72	TYR	CG-CD2	-49.50	0.74	1.39	16	1
1	A	72	TYR	CE1-CZ	-49.05	0.74	1.38	16	1
1	A	23	SER	CB-OG	-49.04	0.78	1.42	16	1
1	A	52	ARG	CZ-NH2	-47.93	0.70	1.33	16	1
1	A	71	PHE	CG-CD2	-46.93	0.68	1.38	16	1
1	A	28	HIS	CE1-NE2	-45.60	0.27	1.32	16	1
1	A	34	PHE	CG-CD2	-44.67	0.71	1.38	16	1
1	A	40	GLU	CG-CD	-44.37	0.85	1.51	16	1
1	A	78	GLU	CD-OE2	-44.13	0.77	1.25	16	1
1	A	34	PHE	CG-CD1	-44.05	0.72	1.38	16	1
1	A	52	ARG	CZ-NH1	-43.72	0.76	1.33	16	1
1	A	71	PHE	CG-CD1	-43.61	0.73	1.38	16	1
1	A	88	HIS	CE1-NE2	-43.48	0.32	1.32	16	1
1	A	39	GLU	CD-OE2	-41.56	0.80	1.25	16	1
1	A	77	HIS	CE1-NE2	-41.33	0.37	1.32	16	1
1	A	6	ARG	CD-NE	-40.66	0.77	1.46	16	1
1	A	64	ASP	CG-OD1	-40.42	0.32	1.25	16	1
1	A	44	ARG	CD-NE	-40.00	0.78	1.46	16	1
1	A	52	ARG	CD-NE	-37.72	0.82	1.46	16	1
1	A	13	ARG	NE-CZ	-37.21	0.84	1.33	16	1
1	A	4	LYS	CE-NZ	-37.07	0.56	1.49	16	1
1	A	71	PHE	CE1-CZ	-36.40	0.68	1.37	16	1
1	A	50	GLN	CD-OE1	-35.69	0.45	1.24	16	1
1	A	44	ARG	NE-CZ	-35.01	0.87	1.33	16	1
1	A	34	PHE	CE1-CZ	-34.75	0.71	1.37	16	1
1	A	34	PHE	CE2-CZ	-34.30	0.72	1.37	16	1
1	A	71	PHE	CE2-CZ	-33.75	0.73	1.37	16	1
1	A	63	LYS	CE-NZ	-32.84	0.67	1.49	16	1
1	A	4	LYS	CD-CE	-31.79	0.71	1.51	16	1
1	A	6	ARG	NE-CZ	-31.72	0.91	1.33	16	1
1	A	39	GLU	CD-OE1	-30.96	0.91	1.25	16	1
1	A	59	MET	CG-SD	-30.91	1.00	1.81	16	1
1	A	49	GLN	CD-NE2	-30.91	0.55	1.32	16	1
1	A	81	LYS	CD-CE	-30.89	0.74	1.51	16	1
1	A	50	GLN	CB-CG	-30.09	0.71	1.52	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	66	ASP	CG-OD2	-29.14	0.58	1.25	16	1
1	A	49	GLN	CD-OE1	-28.84	0.60	1.24	16	1
1	A	82	ASP	CG-OD1	-28.22	0.60	1.25	16	1
1	A	63	LYS	CG-CD	-28.15	0.56	1.52	16	1
1	A	51	GLN	CD-OE1	-28.04	0.62	1.24	16	1
1	A	82	ASP	CG-OD2	-27.58	0.61	1.25	16	1
1	A	45	ASN	CG-OD1	-27.43	0.63	1.24	16	1
1	A	88	HIS	CG-ND1	-27.27	0.78	1.38	16	1
1	A	66	ASP	CG-OD1	-26.98	0.63	1.25	16	1
1	A	28	HIS	CG-ND1	-26.57	0.80	1.38	16	1
1	A	64	ASP	CG-OD2	-26.52	0.64	1.25	16	1
1	A	7	ASN	CG-OD1	-26.50	0.65	1.24	16	1
1	A	27	ASP	CG-OD1	-26.43	0.64	1.25	16	1
1	A	29	MET	SD-CE	-26.32	0.30	1.77	16	1
1	A	28	HIS	CG-CD2	-26.29	0.91	1.35	16	1
1	A	77	HIS	CG-CD2	-26.05	0.91	1.35	16	1
1	A	26	MET	CG-SD	-26.03	1.13	1.81	16	1
1	A	19	ASP	CG-OD1	-25.59	0.66	1.25	16	1
1	A	29	MET	CG-SD	-25.45	1.15	1.81	16	1
1	A	89	ASP	CG-OD1	-25.17	0.67	1.25	16	1
1	A	62	LYS	CD-CE	-25.17	0.88	1.51	16	1
1	A	11	GLN	CD-NE2	-25.09	0.70	1.32	16	1
1	A	32	ASP	CG-OD2	-24.91	0.68	1.25	16	1
1	A	27	ASP	CG-OD2	-24.81	0.68	1.25	16	1
1	A	88	HIS	CG-CD2	-24.70	0.93	1.35	16	1
1	A	77	HIS	CG-ND1	-24.66	0.84	1.38	16	1
1	A	35	LEU	CG-CD1	-24.54	0.61	1.51	16	1
1	A	89	ASP	CG-OD2	-24.48	0.69	1.25	16	1
1	A	78	GLU	CG-CD	-23.77	1.16	1.51	16	1
1	A	12	HIS	CG-CD2	-23.70	0.95	1.35	16	1
1	A	21	LYS	CE-NZ	-23.57	0.90	1.49	16	1
1	A	7	ASN	CG-ND2	-23.50	0.74	1.32	16	1
1	A	51	GLN	CD-NE2	-23.09	0.75	1.32	16	1
1	A	21	LYS	CD-CE	-23.01	0.93	1.51	16	1
1	A	35	LEU	CG-CD2	-22.90	0.67	1.51	16	1
1	A	19	ASP	CG-OD2	-22.75	0.73	1.25	16	1
1	A	12	HIS	CE1-NE2	-22.61	0.80	1.32	16	1
1	A	32	ASP	CG-OD1	-22.37	0.73	1.25	16	1
1	A	58	LYS	CE-NZ	-22.09	0.93	1.49	16	1
1	A	11	GLN	CD-OE1	-22.06	0.75	1.24	16	1
1	A	13	ARG	CZ-NH2	-21.94	1.04	1.33	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	55	MET	CG-SD	-21.61	1.25	1.81	16	1
1	A	73	ASN	CG-OD1	-21.57	0.76	1.24	16	1
1	A	16	LEU	CG-CD2	-21.45	0.72	1.51	16	1
1	A	50	GLN	CG-CD	-21.29	1.02	1.51	16	1
1	A	58	LYS	CD-CE	-21.27	0.98	1.51	16	1
1	A	62	LYS	CE-NZ	-21.02	0.96	1.49	16	1
1	A	73	ASN	CG-ND2	-20.57	0.81	1.32	16	1
1	A	65	ASN	CG-OD1	-19.79	0.80	1.24	16	1
1	A	16	LEU	CG-CD1	-19.73	0.78	1.51	16	1
1	A	18	LYS	CE-NZ	-19.45	1.00	1.49	16	1
1	A	83	LEU	CG-CD1	-19.03	0.81	1.51	16	1
1	A	86	LEU	CG-CD2	-19.02	0.81	1.51	16	1
1	A	45	ASN	CG-ND2	-18.83	0.85	1.32	16	1
1	A	65	ASN	CG-ND2	-18.32	0.87	1.32	16	1
1	A	18	LYS	CD-CE	-17.91	1.06	1.51	16	1
1	A	86	LEU	CG-CD1	-17.91	0.85	1.51	16	1
1	A	81	LYS	CE-NZ	-16.89	1.06	1.49	16	1
1	A	13	ARG	CD-NE	-15.57	1.20	1.46	16	1
1	A	83	LEU	CG-CD2	-14.96	0.96	1.51	16	1
1	A	50	GLN	CD-NE2	-14.31	0.97	1.32	16	1
1	A	55	MET	SD-CE	-13.44	1.02	1.77	16	1
1	A	49	GLN	CG-CD	-12.96	1.21	1.51	16	1
1	A	42	LYS	CE-NZ	-12.14	1.18	1.49	16	1
1	A	64	ASP	CB-CG	-11.34	1.27	1.51	16	1
1	A	12	HIS	CG-ND1	-10.62	1.15	1.38	16	1
1	A	26	MET	SD-CE	-10.45	1.19	1.77	16	1
1	A	59	MET	SD-CE	-10.13	1.21	1.77	16	1
1	A	49	GLN	CB-CG	-9.41	1.27	1.52	16	1
1	A	63	LYS	CD-CE	-9.09	1.28	1.51	16	1
1	A	52	ARG	NE-CZ	-8.66	1.21	1.33	16	1
1	A	42	LYS	CD-CE	-7.92	1.31	1.51	16	1
1	A	56	LEU	CG-CD2	-7.78	1.23	1.51	16	1
1	A	56	LEU	CG-CD1	-7.59	1.23	1.51	16	1
1	A	21	LYS	CG-CD	-6.72	1.29	1.52	16	1
1	A	20	ILE	C-O	-6.69	1.10	1.23	16	1
1	A	46	GLU	CB-CG	-6.59	1.39	1.52	16	1
1	A	58	LYS	CG-CD	-6.36	1.30	1.52	16	1
1	A	37	ILE	CG1-CD1	-6.26	1.07	1.50	16	1
1	A	30	ILE	CG1-CD1	-5.49	1.12	1.50	16	1
1	A	45	ASN	CB-CG	-5.39	1.38	1.51	16	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	80	TYR	CD1-CG-CD2	-96.22	12.06	117.90	16	1
1	A	68	TYR	CD1-CG-CD2	-95.92	12.39	117.90	16	1
1	A	24	TYR	CD1-CG-CD2	-95.30	13.07	117.90	16	1
1	A	13	ARG	NE-CZ-NH1	-94.84	72.88	120.30	16	1
1	A	68	TYR	CB-CG-CD1	88.32	173.99	121.00	16	1
1	A	80	TYR	CB-CG-CD2	88.29	173.97	121.00	16	1
1	A	80	TYR	CB-CG-CD1	88.28	173.97	121.00	16	1
1	A	24	TYR	CB-CG-CD1	88.17	173.90	121.00	16	1
1	A	68	TYR	CB-CG-CD2	87.69	173.62	121.00	16	1
1	A	24	TYR	CB-CG-CD2	86.69	173.01	121.00	16	1
1	A	71	PHE	CD1-CG-CD2	-81.50	12.36	118.30	16	1
1	A	14	GLU	OE1-CD-OE2	-77.40	30.41	123.30	16	1
1	A	6	ARG	NE-CZ-NH2	77.14	158.87	120.30	16	1
1	A	71	PHE	CB-CG-CD1	75.96	173.97	120.80	16	1
1	A	13	ARG	NE-CZ-NH2	75.91	158.26	120.30	16	1
1	A	71	PHE	CB-CG-CD2	75.52	173.67	120.80	16	1
1	A	17	GLU	OE1-CD-OE2	-74.77	33.58	123.30	16	1
1	A	72	TYR	CD1-CG-CD2	-72.45	38.21	117.90	16	1
1	A	34	PHE	CD1-CG-CD2	-70.57	26.55	118.30	16	1
1	A	41	GLU	OE1-CD-OE2	-70.39	38.84	123.30	16	1
1	A	80	TYR	CE1-CZ-CE2	-67.31	12.10	119.80	16	1
1	A	68	TYR	CE1-CZ-CE2	-67.11	12.43	119.80	16	1
1	A	24	TYR	CE1-CZ-CE2	-66.77	12.97	119.80	16	1
1	A	72	TYR	CB-CG-CD2	66.51	160.91	121.00	16	1
1	A	72	TYR	CB-CG-CD1	66.48	160.89	121.00	16	1
1	A	34	PHE	CB-CG-CD1	66.37	167.26	120.80	16	1
1	A	80	TYR	CG-CD1-CE1	65.92	174.04	121.30	16	1
1	A	80	TYR	CG-CD2-CE2	65.80	173.94	121.30	16	1
1	A	68	TYR	CG-CD2-CE2	65.77	173.91	121.30	16	1
1	A	68	TYR	CG-CD1-CE1	65.50	173.70	121.30	16	1
1	A	24	TYR	CG-CD2-CE2	65.22	173.48	121.30	16	1
1	A	24	TYR	CG-CD1-CE1	65.14	173.41	121.30	16	1
1	A	34	PHE	CB-CG-CD2	64.84	166.19	120.80	16	1
1	A	40	GLU	OE1-CD-OE2	-64.83	45.50	123.30	16	1
1	A	64	ASP	CB-CG-OD2	64.50	176.35	118.30	16	1
1	A	64	ASP	CB-CG-OD1	60.46	172.71	118.30	16	1
1	A	80	TYR	CZ-CE2-CD2	60.23	174.00	119.80	16	1
1	A	80	TYR	CD1-CE1-CZ	60.07	173.86	119.80	16	1
1	A	68	TYR	CZ-CE2-CD2	59.99	173.79	119.80	16	1
1	A	68	TYR	CD1-CE1-CZ	59.98	173.78	119.80	16	1
1	A	71	PHE	CE1-CZ-CE2	-59.81	12.34	120.00	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	24	TYR	CD1-CE1-CZ	59.72	173.54	119.80	16	1
1	A	24	TYR	CZ-CE2-CD2	59.69	173.52	119.80	16	1
1	A	64	ASP	OD1-CG-OD2	-59.14	10.94	123.30	16	1
1	A	28	HIS	ND1-CG-CD2	-56.08	27.49	106.00	16	1
1	A	52	ARG	NE-CZ-NH1	55.30	147.95	120.30	16	1
1	A	6	ARG	NH1-CZ-NH2	-54.54	59.41	119.40	16	1
1	A	88	HIS	ND1-CG-CD2	-52.98	31.83	106.00	16	1
1	A	34	PHE	CE1-CZ-CE2	-51.81	26.73	120.00	16	1
1	A	72	TYR	CE1-CZ-CE2	-51.00	38.20	119.80	16	1
1	A	72	TYR	CG-CD2-CE2	49.59	160.97	121.30	16	1
1	A	72	TYR	CG-CD1-CE1	49.42	160.83	121.30	16	1
1	A	52	ARG	NE-CZ-NH2	48.84	144.72	120.30	16	1
1	A	71	PHE	CG-CD1-CE1	48.49	174.14	120.80	16	1
1	A	66	ASP	CB-CG-OD1	48.19	161.67	118.30	16	1
1	A	71	PHE	CG-CD2-CE2	47.90	173.49	120.80	16	1
1	A	77	HIS	ND1-CG-CD2	-47.62	39.33	106.00	16	1
1	A	52	ARG	NH1-CZ-NH2	-47.34	67.33	119.40	16	1
1	A	66	ASP	CB-CG-OD2	46.49	160.14	118.30	16	1
1	A	82	ASP	CB-CG-OD2	45.85	159.57	118.30	16	1
1	A	72	TYR	CD1-CE1-CZ	45.73	160.96	119.80	16	1
1	A	72	TYR	CZ-CE2-CD2	45.59	160.83	119.80	16	1
1	A	82	ASP	CB-CG-OD1	45.08	158.87	118.30	16	1
1	A	71	PHE	CZ-CE2-CD2	44.96	174.05	120.10	16	1
1	A	66	ASP	OD1-CG-OD2	-44.79	38.19	123.30	16	1
1	A	71	PHE	CD1-CE1-CZ	44.61	173.63	120.10	16	1
1	A	82	ASP	OD1-CG-OD2	-43.02	41.56	123.30	16	1
1	A	6	ARG	NE-CZ-NH1	42.85	141.72	120.30	16	1
1	A	34	PHE	CG-CD2-CE2	41.80	166.78	120.80	16	1
1	A	34	PHE	CG-CD1-CE1	41.70	166.67	120.80	16	1
1	A	29	MET	CG-SD-CE	-41.66	33.54	100.20	16	1
1	A	34	PHE	CZ-CE2-CD2	38.84	166.70	120.10	16	1
1	A	34	PHE	CD1-CE1-CZ	38.71	166.56	120.10	16	1
1	A	28	HIS	CG-ND1-CE1	38.19	161.67	108.20	16	1
1	A	44	ARG	NE-CZ-NH2	37.85	139.22	120.30	16	1
1	A	88	HIS	CG-ND1-CE1	35.84	158.37	108.20	16	1
1	A	27	ASP	CB-CG-OD2	32.93	147.94	118.30	16	1
1	A	77	HIS	CG-ND1-CE1	32.77	154.07	108.20	16	1
1	A	89	ASP	CB-CG-OD2	32.21	147.29	118.30	16	1
1	A	89	ASP	CB-CG-OD1	31.09	146.28	118.30	16	1
1	A	7	ASN	OD1-CG-ND2	-30.93	50.76	121.90	16	1
1	A	19	ASP	CB-CG-OD2	30.82	146.03	118.30	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	51	GLN	OE1-CD-NE2	-30.59	51.55	121.90	16	1
1	A	27	ASP	CB-CG-OD1	30.54	145.79	118.30	16	1
1	A	27	ASP	OD1-CG-OD2	-30.01	66.27	123.30	16	1
1	A	89	ASP	OD1-CG-OD2	-29.93	66.42	123.30	16	1
1	A	28	HIS	CG-CD2-NE2	28.73	163.78	109.20	16	1
1	A	88	HIS	CG-CD2-NE2	27.63	161.69	109.20	16	1
1	A	40	GLU	CG-CD-OE2	27.16	172.61	118.30	16	1
1	A	19	ASP	OD1-CG-OD2	-27.07	71.86	123.30	16	1
1	A	26	MET	CG-SD-CE	26.77	143.03	100.20	16	1
1	A	19	ASP	CB-CG-OD1	26.45	142.10	118.30	16	1
1	A	49	GLN	OE1-CD-NE2	-26.43	61.10	121.90	16	1
1	A	59	MET	CG-SD-CE	26.28	142.25	100.20	16	1
1	A	32	ASP	CB-CG-OD1	26.25	141.93	118.30	16	1
1	A	4	LYS	CD-CE-NZ	25.84	171.14	111.70	16	1
1	A	35	LEU	CB-CG-CD2	25.80	154.87	111.00	16	1
1	A	44	ARG	NH1-CZ-NH2	-25.62	91.22	119.40	16	1
1	A	6	ARG	CD-NE-CZ	25.59	159.43	123.60	16	1
1	A	13	ARG	CD-NE-CZ	25.07	158.69	123.60	16	1
1	A	77	HIS	CG-CD2-NE2	24.81	156.34	109.20	16	1
1	A	35	LEU	CB-CG-CD1	24.60	152.82	111.00	16	1
1	A	14	GLU	CG-CD-OE2	23.54	165.38	118.30	16	1
1	A	11	GLN	OE1-CD-NE2	-23.05	68.89	121.90	16	1
1	A	14	GLU	CG-CD-OE1	22.95	164.21	118.30	16	1
1	A	17	GLU	CG-CD-OE2	22.94	164.17	118.30	16	1
1	A	32	ASP	OD1-CG-OD2	-22.73	80.12	123.30	16	1
1	A	41	GLU	CG-CD-OE1	22.71	163.73	118.30	16	1
1	A	17	GLU	CG-CD-OE1	21.98	162.25	118.30	16	1
1	A	35	LEU	CD1-CG-CD2	-21.96	44.62	110.50	16	1
1	A	32	ASP	CB-CG-OD2	21.84	137.96	118.30	16	1
1	A	46	GLU	OE1-CD-OE2	-21.33	97.70	123.30	16	1
1	A	73	ASN	OD1-CG-ND2	-20.58	74.57	121.90	16	1
1	A	39	GLU	OE1-CD-OE2	-20.18	99.08	123.30	16	1
1	A	63	LYS	CB-CG-CD	20.05	163.72	111.60	16	1
1	A	80	TYR	OH-CZ-CE2	19.98	174.04	120.10	16	1
1	A	80	TYR	CE1-CZ-OH	19.91	173.86	120.10	16	1
1	A	68	TYR	OH-CZ-CE2	19.90	173.83	120.10	16	1
1	A	68	TYR	CE1-CZ-OH	19.87	173.74	120.10	16	1
1	A	24	TYR	OH-CZ-CE2	19.79	173.54	120.10	16	1
1	A	24	TYR	CE1-CZ-OH	19.77	173.48	120.10	16	1
1	A	12	HIS	ND1-CG-CD2	-19.64	78.50	106.00	16	1
1	A	41	GLU	CG-CD-OE2	19.57	157.44	118.30	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	44	ARG	NE-CZ-NH1	18.52	129.56	120.30	16	1
1	A	45	ASN	OD1-CG-ND2	-18.27	79.87	121.90	16	1
1	A	63	LYS	CG-CD-CE	18.21	166.53	111.90	16	1
1	A	65	ASN	OD1-CG-ND2	-17.39	81.90	121.90	16	1
1	A	12	HIS	CG-ND1-CE1	17.17	132.24	108.20	16	1
1	A	16	LEU	CB-CG-CD1	16.85	139.64	111.00	16	1
1	A	28	HIS	CB-CG-ND1	16.50	164.45	123.20	16	1
1	A	88	HIS	CE1-NE2-CD2	-16.35	65.73	106.60	16	1
1	A	51	GLN	CG-CD-NE2	16.27	155.74	116.70	16	1
1	A	7	ASN	CB-CG-OD1	16.21	154.02	121.60	16	1
1	A	28	HIS	CE1-NE2-CD2	-16.06	66.45	106.60	16	1
1	A	7	ASN	CB-CG-ND2	16.05	155.22	116.70	16	1
1	A	52	ARG	CD-NE-CZ	15.93	145.90	123.60	16	1
1	A	51	GLN	CG-CD-OE1	15.56	152.71	121.60	16	1
1	A	63	LYS	CD-CE-NZ	15.37	147.04	111.70	16	1
1	A	88	HIS	CB-CG-ND1	15.35	161.57	123.20	16	1
1	A	46	GLU	CB-CG-CD	15.34	155.63	114.20	16	1
1	A	49	GLN	CG-CD-OE1	15.31	152.23	121.60	16	1
1	A	72	TYR	CE1-CZ-OH	15.14	160.97	120.10	16	1
1	A	72	TYR	OH-CZ-CE2	15.08	160.82	120.10	16	1
1	A	62	LYS	CD-CE-NZ	14.84	145.83	111.70	16	1
1	A	55	MET	CG-SD-CE	14.81	123.90	100.20	16	1
1	A	16	LEU	CB-CG-CD2	14.13	135.03	111.00	16	1
1	A	83	LEU	CB-CG-CD2	14.06	134.90	111.00	16	1
1	A	77	HIS	CB-CG-ND1	13.98	158.15	123.20	16	1
1	A	50	GLN	CG-CD-NE2	13.74	149.68	116.70	16	1
1	A	52	ARG	CG-CD-NE	13.74	140.65	111.80	16	1
1	A	11	GLN	CG-CD-OE1	13.54	148.67	121.60	16	1
1	A	46	GLU	CG-CD-OE2	13.53	145.37	118.30	16	1
1	A	50	GLN	CG-CD-OE1	-13.44	94.72	121.60	16	1
1	A	50	GLN	CB-CG-CD	13.42	146.49	111.60	16	1
1	A	16	LEU	CD1-CG-CD2	-12.96	71.63	110.50	16	1
1	A	78	GLU	OE1-CD-OE2	-12.93	107.79	123.30	16	1
1	A	4	LYS	CG-CD-CE	12.55	149.54	111.90	16	1
1	A	49	GLN	CG-CD-NE2	12.49	146.67	116.70	16	1
1	A	58	LYS	CD-CE-NZ	12.07	139.47	111.70	16	1
1	A	28	HIS	CB-CG-CD2	12.02	168.06	130.80	16	1
1	A	58	LYS	CG-CD-CE	11.98	147.84	111.90	16	1
1	A	45	ASN	CB-CG-ND2	11.85	145.14	116.70	16	1
1	A	40	GLU	CG-CD-OE1	11.79	141.89	118.30	16	1
1	A	44	ARG	CD-NE-CZ	11.79	140.11	123.60	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	88	HIS	CB-CG-CD2	11.55	166.60	130.80	16	1
1	A	81	LYS	CD-CE-NZ	11.24	137.56	111.70	16	1
1	A	77	HIS	CE1-NE2-CD2	-11.05	78.97	106.60	16	1
1	A	73	ASN	CB-CG-OD1	10.79	143.17	121.60	16	1
1	A	11	GLN	CG-CD-NE2	10.73	142.44	116.70	16	1
1	A	73	ASN	CB-CG-ND2	10.65	142.26	116.70	16	1
1	A	86	LEU	CB-CG-CD1	10.56	128.95	111.00	16	1
1	A	77	HIS	CB-CG-CD2	10.23	162.51	130.80	16	1
1	A	50	GLN	CA-CB-CG	9.86	135.09	113.40	16	1
1	A	65	ASN	CB-CG-ND2	9.27	138.95	116.70	16	1
1	A	12	HIS	CG-CD2-NE2	8.89	126.09	109.20	16	1
1	A	65	ASN	CB-CG-OD1	8.78	139.16	121.60	16	1
1	A	13	ARG	NH1-CZ-NH2	8.60	128.86	119.40	16	1
1	A	81	LYS	CG-CD-CE	8.56	137.58	111.90	16	1
1	A	39	GLU	CG-CD-OE1	8.34	134.97	118.30	16	1
1	A	62	LYS	CG-CD-CE	8.23	136.59	111.90	16	1
1	A	83	LEU	CD1-CG-CD2	-8.22	85.85	110.50	16	1
1	A	59	MET	CB-CG-SD	8.16	136.89	112.40	16	1
1	A	86	LEU	CB-CG-CD2	8.08	124.74	111.00	16	1
1	A	86	LEU	CD1-CG-CD2	-7.61	87.67	110.50	16	1
1	A	12	HIS	CB-CG-ND1	7.49	141.93	123.20	16	1
1	A	21	LYS	CG-CD-CE	6.88	132.53	111.90	16	1
1	A	45	ASN	CB-CG-OD1	6.70	135.00	121.60	16	1
1	A	6	ARG	CG-CD-NE	6.69	125.86	111.80	16	1
1	A	26	MET	CB-CG-SD	6.56	132.07	112.40	16	1
1	A	83	LEU	CB-CG-CD1	6.53	122.10	111.00	16	1
1	A	12	HIS	ND1-CE1-NE2	-6.41	95.81	109.90	16	1
1	A	23	SER	CA-CB-OG	6.13	127.76	111.20	16	1
1	A	88	HIS	ND1-CE1-NE2	5.67	122.37	109.90	16	1
1	A	21	LYS	CD-CE-NZ	5.64	124.66	111.70	16	1
1	A	78	GLU	CG-CD-OE2	5.57	129.45	118.30	16	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	726	730	724	56±93
All	All	11616	11680	11674	902

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LYS:CE	1:A:63:LYS:CG	1.53	1.83	16	1
1:A:49:GLN:CG	1:A:49:GLN:NE2	1.51	1.70	16	1
1:A:62:LYS:NZ	1:A:62:LYS:CD	1.47	1.76	16	1
1:A:78:GLU:OE1	1:A:78:GLU:CG	1.45	1.65	16	1
1:A:52:ARG:CZ	1:A:52:ARG:CD	1.45	1.95	16	1
1:A:88:HIS:CE1	1:A:88:HIS:CG	1.43	2.04	16	1
1:A:71:PHE:CD1	1:A:71:PHE:CZ	1.43	2.07	16	1
1:A:81:LYS:CD	1:A:81:LYS:NZ	1.42	1.68	16	1
1:A:80:TYR:CG	1:A:80:TYR:CE2	1.41	2.09	16	1
1:A:28:HIS:CE1	1:A:28:HIS:CG	1.41	2.06	16	1
1:A:80:TYR:CZ	1:A:80:TYR:CD2	1.40	2.10	16	1
1:A:71:PHE:CG	1:A:71:PHE:CE2	1.40	2.07	16	1
1:A:68:TYR:CD2	1:A:68:TYR:CZ	1.40	2.10	16	1
1:A:55:MET:CG	1:A:55:MET:CE	1.39	2.00	16	1
1:A:24:TYR:CD2	1:A:24:TYR:CZ	1.39	2.10	16	1
1:A:68:TYR:CE1	1:A:68:TYR:CG	1.39	2.10	16	1
1:A:24:TYR:CG	1:A:24:TYR:CE1	1.39	2.10	16	1
1:A:34:PHE:CD1	1:A:34:PHE:CZ	1.39	2.09	16	1
1:A:77:HIS:CG	1:A:77:HIS:CE1	1.39	2.07	16	1
1:A:80:TYR:CG	1:A:80:TYR:CE1	1.39	2.10	16	1
1:A:34:PHE:CG	1:A:34:PHE:CE2	1.38	2.09	16	1
1:A:34:PHE:CD2	1:A:34:PHE:CZ	1.38	2.09	16	1
1:A:34:PHE:CG	1:A:34:PHE:CE1	1.38	2.10	16	1
1:A:72:TYR:CE2	1:A:72:TYR:CG	1.37	2.11	16	1
1:A:72:TYR:CZ	1:A:72:TYR:CD1	1.36	2.11	16	1
1:A:72:TYR:CE1	1:A:72:TYR:CG	1.36	2.11	16	1
1:A:24:TYR:CG	1:A:24:TYR:CE2	1.36	2.10	16	1
1:A:72:TYR:CZ	1:A:72:TYR:CD2	1.36	2.11	16	1
1:A:80:TYR:CZ	1:A:80:TYR:CD1	1.36	2.09	16	1
1:A:24:TYR:CD1	1:A:24:TYR:CZ	1.36	2.10	16	1
1:A:63:LYS:CD	1:A:63:LYS:NZ	1.35	1.87	16	1
1:A:68:TYR:CG	1:A:68:TYR:CE2	1.35	2.10	16	1
1:A:29:MET:CB	1:A:29:MET:CE	1.34	2.04	16	1
1:A:68:TYR:CD1	1:A:68:TYR:CZ	1.34	2.10	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:PHE:CD2	1:A:71:PHE:CZ	1.33	2.12	16	1
1:A:29:MET:SD	1:A:29:MET:CB	1.32	2.15	16	1
1:A:63:LYS:CD	1:A:63:LYS:CB	1.31	2.07	16	1
1:A:71:PHE:CG	1:A:71:PHE:CE1	1.31	2.12	16	1
1:A:16:LEU:CB	1:A:16:LEU:CD2	1.31	2.08	16	1
1:A:49:GLN:CG	1:A:49:GLN:OE1	1.30	1.76	16	1
1:A:59:MET:SD	1:A:59:MET:CE	1.30	1.21	16	1
1:A:59:MET:CG	1:A:59:MET:CE	1.30	2.09	16	1
1:A:62:LYS:CE	1:A:62:LYS:CG	1.29	2.11	16	1
1:A:35:LEU:CD1	1:A:35:LEU:CB	1.29	2.08	16	1
1:A:78:GLU:CG	1:A:78:GLU:OE2	1.29	1.75	16	1
1:A:86:LEU:CD2	1:A:86:LEU:CB	1.28	2.09	16	1
1:A:26:MET:SD	1:A:26:MET:CE	1.28	1.19	16	1
1:A:46:GLU:CB	1:A:46:GLU:CD	1.27	2.01	16	1
1:A:29:MET:HE3	1:A:29:MET:CB	1.27	1.59	16	1
1:A:81:LYS:CG	1:A:81:LYS:CE	1.26	2.12	16	1
1:A:71:PHE:CD2	1:A:71:PHE:CB	1.26	2.19	16	1
1:A:52:ARG:NE	1:A:52:ARG:NH2	1.26	1.83	16	1
1:A:35:LEU:CD2	1:A:35:LEU:CB	1.25	2.14	16	1
1:A:4:LYS:CG	1:A:4:LYS:CE	1.25	2.13	16	1
1:A:80:TYR:CB	1:A:80:TYR:CD2	1.24	2.20	16	1
1:A:29:MET:SD	1:A:29:MET:CG	1.23	1.15	16	1
1:A:68:TYR:CB	1:A:68:TYR:CD1	1.23	2.21	16	1
1:A:16:LEU:CB	1:A:16:LEU:CD1	1.23	2.17	16	1
1:A:26:MET:SD	1:A:26:MET:CG	1.23	1.13	16	1
1:A:34:PHE:CD1	1:A:34:PHE:CB	1.22	2.22	16	1
1:A:68:TYR:CD2	1:A:68:TYR:CB	1.22	2.22	16	1
1:A:86:LEU:CD1	1:A:86:LEU:CB	1.21	2.16	16	1
1:A:34:PHE:CD2	1:A:34:PHE:CB	1.21	2.20	16	1
1:A:72:TYR:CB	1:A:72:TYR:CD1	1.20	2.22	16	1
1:A:45:ASN:CB	1:A:45:ASN:OD1	1.20	1.88	16	1
1:A:24:TYR:CD2	1:A:24:TYR:CB	1.19	2.21	16	1
1:A:72:TYR:CB	1:A:72:TYR:CD2	1.18	2.22	16	1
1:A:24:TYR:CD1	1:A:24:TYR:CB	1.18	2.21	16	1
1:A:64:ASP:CB	1:A:64:ASP:OD2	1.18	1.91	16	1
1:A:11:GLN:NE2	1:A:11:GLN:CG	1.18	2.05	16	1
1:A:26:MET:CE	1:A:26:MET:CG	1.17	2.20	16	1
1:A:40:GLU:CD	1:A:40:GLU:CB	1.16	2.12	16	1
1:A:80:TYR:CB	1:A:80:TYR:CD1	1.16	2.21	16	1
1:A:52:ARG:NH1	1:A:52:ARG:NE	1.15	1.90	16	1
1:A:59:MET:SD	1:A:59:MET:CB	1.14	2.36	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:GLU:CG	1:A:41:GLU:OE2	1.13	1.96	16	1
1:A:23:SER:HB3	1:A:23:SER:OG	1.12	1.39	16	1
1:A:55:MET:CE	1:A:55:MET:SD	1.12	1.02	16	1
1:A:46:GLU:OE1	1:A:46:GLU:CG	1.12	0.83	16	1
1:A:26:MET:HE3	1:A:26:MET:SD	1.10	1.77	16	1
1:A:59:MET:SD	1:A:59:MET:HE2	1.10	1.78	16	1
1:A:32:ASP:OD2	1:A:32:ASP:CB	1.10	2.00	16	1
1:A:59:MET:CG	1:A:59:MET:SD	1.09	1.00	16	1
1:A:59:MET:HE1	1:A:59:MET:SD	1.08	1.78	16	1
1:A:26:MET:HE2	1:A:26:MET:SD	1.08	1.77	16	1
1:A:80:TYR:OH	1:A:80:TYR:CE1	1.08	2.07	16	1
1:A:26:MET:SD	1:A:26:MET:CB	1.08	2.42	16	1
1:A:45:ASN:CB	1:A:45:ASN:ND2	1.07	2.14	16	1
1:A:23:SER:CB	1:A:23:SER:OG	1.07	0.78	16	1
1:A:77:HIS:CB	1:A:77:HIS:CD2	1.07	2.38	16	1
1:A:29:MET:SD	1:A:29:MET:HG2	1.07	1.71	16	1
1:A:68:TYR:OH	1:A:68:TYR:CE2	1.06	2.07	16	1
1:A:16:LEU:HG	1:A:16:LEU:CD1	1.06	1.60	16	1
1:A:26:MET:HE1	1:A:26:MET:SD	1.06	1.77	16	1
1:A:52:ARG:NE	1:A:52:ARG:CG	1.06	2.18	16	1
1:A:17:GLU:OE1	1:A:17:GLU:CG	1.06	2.02	16	1
1:A:24:TYR:OH	1:A:24:TYR:CE2	1.06	2.08	16	1
1:A:59:MET:HE3	1:A:59:MET:SD	1.06	1.78	16	1
1:A:16:LEU:CD2	1:A:16:LEU:HD12	1.05	1.80	16	1
1:A:23:SER:HB2	1:A:23:SER:OG	1.05	1.39	16	1
1:A:28:HIS:CD2	1:A:28:HIS:CB	1.05	2.39	16	1
1:A:68:TYR:OH	1:A:68:TYR:CE1	1.04	2.08	16	1
1:A:27:ASP:CB	1:A:27:ASP:OD1	1.04	2.04	16	1
1:A:16:LEU:CD1	1:A:16:LEU:HD23	1.04	1.81	16	1
1:A:51:GLN:CG	1:A:51:GLN:OE1	1.04	2.06	16	1
1:A:46:GLU:OE1	1:A:46:GLU:HG2	1.04	1.51	16	1
1:A:7:ASN:CB	1:A:7:ASN:ND2	1.04	2.21	16	1
1:A:14:GLU:OE1	1:A:14:GLU:CG	1.04	2.04	16	1
1:A:51:GLN:NE2	1:A:51:GLN:CG	1.03	2.19	16	1
1:A:29:MET:SD	1:A:29:MET:HG3	1.03	1.71	16	1
1:A:88:HIS:CD2	1:A:88:HIS:CB	1.03	2.41	16	1
1:A:24:TYR:OH	1:A:24:TYR:CE1	1.03	2.08	16	1
1:A:80:TYR:OH	1:A:80:TYR:CE2	1.03	2.08	16	1
1:A:26:MET:SD	1:A:26:MET:HG2	1.02	1.66	16	1
1:A:72:TYR:OH	1:A:72:TYR:CE2	1.02	2.09	16	1
1:A:27:ASP:CB	1:A:27:ASP:OD2	1.01	2.08	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:MET:HG3	1:A:26:MET:SD	1.01	1.66	16	1
1:A:19:ASP:OD1	1:A:19:ASP:CB	1.01	2.06	16	1
1:A:73:ASN:CB	1:A:73:ASN:ND2	1.01	2.21	16	1
1:A:40:GLU:CD	1:A:40:GLU:HG3	1.01	1.45	16	1
1:A:52:ARG:HD3	1:A:52:ARG:NE	1.01	1.39	16	1
1:A:17:GLU:OE2	1:A:17:GLU:CG	1.01	2.08	16	1
1:A:16:LEU:HG	1:A:16:LEU:CD2	1.00	1.58	16	1
1:A:82:ASP:CB	1:A:82:ASP:OD1	1.00	2.09	16	1
1:A:29:MET:CG	1:A:29:MET:HE1	1.00	1.58	16	1
1:A:72:TYR:OH	1:A:72:TYR:CE1	1.00	2.09	16	1
1:A:65:ASN:ND2	1:A:65:ASN:CB	1.00	2.25	16	1
1:A:66:ASP:CB	1:A:66:ASP:OD2	1.00	2.08	16	1
1:A:46:GLU:OE1	1:A:46:GLU:HG3	1.00	1.24	16	1
1:A:32:ASP:OD1	1:A:32:ASP:CB	1.00	2.07	16	1
1:A:14:GLU:OE2	1:A:14:GLU:CG	1.00	2.09	16	1
1:A:55:MET:HE1	1:A:55:MET:SD	0.99	1.63	16	1
1:A:40:GLU:CD	1:A:40:GLU:HG2	0.99	1.45	16	1
1:A:23:SER:CA	1:A:23:SER:OG	0.99	2.10	16	1
1:A:52:ARG:HD2	1:A:52:ARG:NE	0.99	1.39	16	1
1:A:82:ASP:CB	1:A:82:ASP:OD2	0.99	2.10	16	1
1:A:35:LEU:CD2	1:A:35:LEU:HG	0.98	1.59	16	1
1:A:89:ASP:CB	1:A:89:ASP:OD1	0.98	2.11	16	1
1:A:88:HIS:ND1	1:A:88:HIS:CB	0.98	2.25	16	1
1:A:55:MET:SD	1:A:55:MET:HE2	0.97	1.63	16	1
1:A:89:ASP:CB	1:A:89:ASP:OD2	0.97	2.12	16	1
1:A:52:ARG:CD	1:A:52:ARG:NE	0.96	0.82	16	1
1:A:7:ASN:CB	1:A:7:ASN:OD1	0.96	2.13	16	1
1:A:66:ASP:CB	1:A:66:ASP:OD1	0.96	2.13	16	1
1:A:19:ASP:OD2	1:A:19:ASP:CB	0.95	2.14	16	1
1:A:86:LEU:CG	1:A:86:LEU:HD11	0.95	1.49	16	1
1:A:40:GLU:CD	1:A:40:GLU:CG	0.94	0.85	16	1
1:A:46:GLU:OE1	1:A:46:GLU:CB	0.94	2.12	16	1
1:A:55:MET:SD	1:A:55:MET:HE3	0.94	1.63	16	1
1:A:41:GLU:CG	1:A:41:GLU:OE1	0.94	2.15	16	1
1:A:35:LEU:CD1	1:A:35:LEU:HG	0.93	1.54	16	1
1:A:86:LEU:CG	1:A:86:LEU:HD12	0.93	1.49	16	1
1:A:77:HIS:CG	1:A:77:HIS:NE2	0.92	2.17	16	1
1:A:73:ASN:CB	1:A:73:ASN:OD1	0.92	2.17	16	1
1:A:86:LEU:CG	1:A:86:LEU:HD13	0.92	1.49	16	1
1:A:86:LEU:CG	1:A:86:LEU:HD22	0.92	1.46	16	1
1:A:29:MET:CG	1:A:29:MET:CE	0.90	0.91	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:LEU:CG	1:A:86:LEU:HD21	0.90	1.46	16	1
1:A:62:LYS:HD3	1:A:62:LYS:CE	0.90	1.44	16	1
1:A:16:LEU:CG	1:A:16:LEU:HD11	0.90	1.44	16	1
1:A:59:MET:SD	1:A:59:MET:HG3	0.90	1.54	16	1
1:A:88:HIS:CD2	1:A:88:HIS:CG	0.90	0.93	16	1
1:A:86:LEU:CG	1:A:86:LEU:HD23	0.90	1.46	16	1
1:A:35:LEU:HD23	1:A:35:LEU:HD11	0.89	0.96	16	1
1:A:77:HIS:CG	1:A:77:HIS:CD2	0.89	0.91	16	1
1:A:59:MET:SD	1:A:59:MET:HG2	0.89	1.54	16	1
1:A:65:ASN:HD21	1:A:65:ASN:CG	0.89	1.49	16	1
1:A:29:MET:HE2	1:A:29:MET:CB	0.88	1.84	16	1
1:A:63:LYS:NZ	1:A:63:LYS:HE3	0.88	1.27	16	1
1:A:28:HIS:CG	1:A:28:HIS:CD2	0.88	0.91	16	1
1:A:41:GLU:CD	1:A:41:GLU:OE1	0.88	0.68	16	1
1:A:45:ASN:HD22	1:A:45:ASN:CG	0.88	1.48	16	1
1:A:62:LYS:HD2	1:A:62:LYS:CE	0.88	1.44	16	1
1:A:86:LEU:HG	1:A:86:LEU:CD2	0.88	1.58	16	1
1:A:29:MET:HG3	1:A:29:MET:CE	0.88	1.43	16	1
1:A:63:LYS:NZ	1:A:63:LYS:HE2	0.88	1.27	16	1
1:A:16:LEU:CD2	1:A:16:LEU:CD1	0.88	0.88	16	1
1:A:62:LYS:CD	1:A:62:LYS:CE	0.88	0.88	16	1
1:A:62:LYS:HE3	1:A:62:LYS:CD	0.87	1.42	16	1
1:A:86:LEU:HG	1:A:86:LEU:CD1	0.87	1.58	16	1
1:A:35:LEU:CD1	1:A:35:LEU:HD23	0.87	1.43	16	1
1:A:65:ASN:CB	1:A:65:ASN:OD1	0.87	2.19	16	1
1:A:16:LEU:CG	1:A:16:LEU:HD12	0.87	1.44	16	1
1:A:16:LEU:CG	1:A:16:LEU:HD13	0.87	1.44	16	1
1:A:35:LEU:CD2	1:A:35:LEU:HD12	0.86	1.42	16	1
1:A:28:HIS:CG	1:A:28:HIS:ND1	0.86	0.80	16	1
1:A:65:ASN:CG	1:A:65:ASN:HD22	0.86	1.49	16	1
1:A:62:LYS:HE2	1:A:62:LYS:CD	0.86	1.42	16	1
1:A:77:HIS:CG	1:A:77:HIS:ND1	0.85	0.84	16	1
1:A:7:ASN:CG	1:A:7:ASN:OD1	0.85	0.65	16	1
1:A:9:LEU:HD23	1:A:68:TYR:CE1	0.85	2.06	15	11
1:A:86:LEU:CG	1:A:86:LEU:CD1	0.85	0.85	16	1
1:A:29:MET:CG	1:A:29:MET:HE2	0.85	0.80	16	1
1:A:16:LEU:CG	1:A:16:LEU:HD23	0.85	1.39	16	1
1:A:71:PHE:CD1	1:A:71:PHE:CB	0.85	2.24	16	1
1:A:88:HIS:CG	1:A:88:HIS:ND1	0.84	0.78	16	1
1:A:16:LEU:CG	1:A:16:LEU:HD22	0.83	1.39	16	1
1:A:45:ASN:HD21	1:A:45:ASN:CG	0.83	1.48	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:HIS:CD2	1:A:15:ALA:HB3	0.83	2.07	16	5
1:A:30:ILE:HD11	1:A:56:LEU:HD21	0.82	1.51	15	2
1:A:16:LEU:CD1	1:A:16:LEU:HD22	0.82	1.37	16	1
1:A:11:GLN:OE1	1:A:11:GLN:CG	0.82	2.13	16	1
1:A:66:ASP:CG	1:A:66:ASP:OD1	0.82	0.63	16	1
1:A:16:LEU:CD2	1:A:16:LEU:HD13	0.82	1.36	16	1
1:A:34:PHE:CE2	1:A:34:PHE:HZ	0.81	1.64	16	1
1:A:71:PHE:HZ	1:A:71:PHE:CE1	0.81	1.60	16	1
1:A:51:GLN:CD	1:A:51:GLN:OE1	0.81	0.62	16	1
1:A:73:ASN:HD22	1:A:73:ASN:CG	0.81	1.45	16	1
1:A:65:ASN:CG	1:A:65:ASN:ND2	0.81	0.87	16	1
1:A:16:LEU:CG	1:A:16:LEU:HD21	0.81	1.39	16	1
1:A:82:ASP:CG	1:A:82:ASP:OD2	0.81	0.61	16	1
1:A:35:LEU:HD21	1:A:35:LEU:CG	0.81	1.35	16	1
1:A:86:LEU:CG	1:A:86:LEU:CD2	0.80	0.81	16	1
1:A:45:ASN:ND2	1:A:45:ASN:CG	0.80	0.85	16	1
1:A:35:LEU:HD22	1:A:35:LEU:CG	0.80	1.35	16	1
1:A:35:LEU:HD23	1:A:35:LEU:CG	0.80	1.35	16	1
1:A:81:LYS:CE	1:A:81:LYS:HD2	0.80	1.34	16	1
1:A:46:GLU:CD	1:A:46:GLU:HG3	0.80	1.24	16	1
1:A:16:LEU:HD21	1:A:26:MET:CE	0.79	2.07	11	1
1:A:46:GLU:HG2	1:A:46:GLU:CD	0.79	1.24	16	1
1:A:43:VAL:HG11	1:A:56:LEU:HD13	0.79	1.54	14	3
1:A:51:GLN:CD	1:A:51:GLN:NE2	0.79	0.75	16	1
1:A:82:ASP:CG	1:A:82:ASP:OD1	0.79	0.60	16	1
1:A:81:LYS:CD	1:A:81:LYS:HE2	0.79	1.34	16	1
1:A:81:LYS:CD	1:A:81:LYS:HE3	0.79	1.34	16	1
1:A:14:GLU:CD	1:A:14:GLU:OE2	0.79	0.61	16	1
1:A:73:ASN:HD21	1:A:73:ASN:CG	0.79	1.45	16	1
1:A:81:LYS:CE	1:A:81:LYS:HD3	0.78	1.34	16	1
1:A:17:GLU:OE2	1:A:17:GLU:CD	0.78	0.61	16	1
1:A:16:LEU:CG	1:A:16:LEU:CD1	0.78	0.78	16	1
1:A:63:LYS:CE	1:A:63:LYS:NZ	0.78	0.66	16	1
1:A:7:ASN:ND2	1:A:7:ASN:CG	0.78	0.74	16	1
1:A:66:ASP:CG	1:A:66:ASP:OD2	0.77	0.58	16	1
1:A:72:TYR:CE1	1:A:84:ALA:HB1	0.77	2.15	2	4
1:A:49:GLN:OE1	1:A:49:GLN:CD	0.77	0.60	16	1
1:A:51:GLN:CD	1:A:51:GLN:HE22	0.77	1.39	16	1
1:A:65:ASN:CG	1:A:65:ASN:OD1	0.76	0.80	16	1
1:A:35:LEU:HD13	1:A:35:LEU:CG	0.76	1.30	16	1
1:A:35:LEU:HD12	1:A:35:LEU:CG	0.76	1.30	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ASN:ND2	1:A:73:ASN:CG	0.76	0.81	16	1
1:A:7:ASN:HD22	1:A:7:ASN:CG	0.76	1.38	16	1
1:A:35:LEU:CG	1:A:35:LEU:HD11	0.75	1.30	16	1
1:A:51:GLN:CD	1:A:51:GLN:HE21	0.75	1.39	16	1
1:A:89:ASP:CG	1:A:89:ASP:OD1	0.75	0.67	16	1
1:A:4:LYS:HD2	1:A:4:LYS:CE	0.75	1.29	16	1
1:A:7:ASN:CG	1:A:7:ASN:HD21	0.75	1.38	16	1
1:A:34:PHE:CE1	1:A:34:PHE:HZ	0.74	1.63	16	1
1:A:4:LYS:HD3	1:A:4:LYS:CE	0.74	1.29	16	1
1:A:30:ILE:CD1	1:A:56:LEU:HD11	0.74	2.13	8	1
1:A:30:ILE:HG23	1:A:35:LEU:HB2	0.73	1.59	8	5
1:A:73:ASN:OD1	1:A:73:ASN:CG	0.73	0.76	16	1
1:A:81:LYS:CD	1:A:81:LYS:CE	0.73	0.74	16	1
1:A:16:LEU:CD1	1:A:16:LEU:HD21	0.73	0.97	16	1
1:A:49:GLN:CB	1:A:49:GLN:OE1	0.73	2.35	16	1
1:A:7:ASN:ND2	1:A:7:ASN:OD1	0.73	0.60	16	1
1:A:14:GLU:CD	1:A:14:GLU:OE1	0.73	0.56	16	1
1:A:11:GLN:HE21	1:A:11:GLN:CD	0.73	1.35	16	1
1:A:11:GLN:HE22	1:A:11:GLN:CD	0.73	1.35	16	1
1:A:51:GLN:NE2	1:A:51:GLN:OE1	0.73	0.60	16	1
1:A:17:GLU:OE1	1:A:17:GLU:CD	0.73	0.55	16	1
1:A:19:ASP:OD2	1:A:19:ASP:CG	0.73	0.73	16	1
1:A:19:ASP:OD1	1:A:19:ASP:CG	0.72	0.66	16	1
1:A:72:TYR:CZ	1:A:76:LEU:HD11	0.72	2.19	6	14
1:A:46:GLU:CG	1:A:46:GLU:CD	0.72	0.66	16	1
1:A:64:ASP:CG	1:A:64:ASP:OD2	0.72	0.64	16	1
1:A:49:GLN:OE1	1:A:49:GLN:NE2	0.72	0.59	16	1
1:A:16:LEU:CG	1:A:16:LEU:CD2	0.72	0.72	16	1
1:A:29:MET:HG3	1:A:29:MET:HE3	0.71	1.11	16	1
1:A:71:PHE:CE1	1:A:75:LEU:HD11	0.71	2.21	3	9
1:A:20:ILE:HD13	1:A:25:ILE:HG13	0.70	1.60	11	6
1:A:52:ARG:CZ	1:A:52:ARG:NH2	0.70	0.70	16	1
1:A:22:THR:HG22	1:A:56:LEU:HD22	0.70	1.64	6	4
1:A:52:ARG:HH11	1:A:52:ARG:CZ	0.69	1.40	16	1
1:A:4:LYS:CD	1:A:4:LYS:CE	0.69	0.71	16	1
1:A:27:ASP:CG	1:A:27:ASP:OD2	0.69	0.68	16	1
1:A:52:ARG:HH12	1:A:52:ARG:CZ	0.68	1.40	16	1
1:A:32:ASP:CG	1:A:32:ASP:OD2	0.68	0.68	16	1
1:A:53:ALA:O	1:A:57:ILE:HD12	0.68	1.89	10	3
1:A:77:HIS:CG	1:A:77:HIS:HD2	0.68	1.43	16	1
1:A:35:LEU:HD21	1:A:35:LEU:HD12	0.68	1.02	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:HIS:HA	1:A:91:ILE:HD12	0.68	1.66	3	8
1:A:72:TYR:CZ	1:A:72:TYR:CE1	0.68	0.74	16	1
1:A:41:GLU:OE2	1:A:41:GLU:CD	0.68	0.50	16	1
1:A:12:HIS:NE2	1:A:15:ALA:HB3	0.67	2.05	16	1
1:A:34:PHE:CE2	1:A:34:PHE:CZ	0.67	0.72	16	1
1:A:9:LEU:HD13	1:A:9:LEU:O	0.67	1.90	16	7
1:A:29:MET:HG2	1:A:29:MET:HE2	0.67	0.67	16	1
1:A:72:TYR:CG	1:A:72:TYR:CD2	0.67	0.74	16	1
1:A:9:LEU:O	1:A:9:LEU:HD13	0.67	1.89	5	9
1:A:35:LEU:CD2	1:A:35:LEU:CG	0.67	0.67	16	1
1:A:30:ILE:HD11	1:A:56:LEU:HD11	0.66	1.67	13	4
1:A:34:PHE:CE1	1:A:34:PHE:CZ	0.66	0.71	16	1
1:A:72:TYR:CZ	1:A:72:TYR:CE2	0.66	0.74	16	1
1:A:88:HIS:HD2	1:A:88:HIS:CG	0.66	1.42	16	1
1:A:71:PHE:CZ	1:A:71:PHE:CE1	0.66	0.68	16	1
1:A:72:TYR:CG	1:A:72:TYR:CD1	0.66	0.74	16	1
1:A:29:MET:SD	1:A:29:MET:HB2	0.66	2.28	16	1
1:A:16:LEU:HD22	1:A:16:LEU:HD13	0.65	1.04	16	1
1:A:20:ILE:HD11	1:A:80:TYR:CE2	0.65	2.25	8	1
1:A:89:ASP:CG	1:A:89:ASP:OD2	0.65	0.69	16	1
1:A:52:ARG:HE	1:A:52:ARG:CD	0.64	1.35	16	1
1:A:4:LYS:HE3	1:A:4:LYS:NZ	0.64	1.14	16	1
1:A:11:GLN:NE2	1:A:11:GLN:CD	0.64	0.70	16	1
1:A:6:ARG:O	1:A:10:LEU:HD12	0.64	1.92	1	1
1:A:11:GLN:OE1	1:A:11:GLN:CD	0.64	0.75	16	1
1:A:71:PHE:O	1:A:75:LEU:HD12	0.64	1.92	11	3
1:A:29:MET:HE3	1:A:29:MET:HB2	0.64	1.64	16	1
1:A:52:ARG:CZ	1:A:52:ARG:HH21	0.64	1.36	16	1
1:A:71:PHE:CZ	1:A:71:PHE:CE2	0.64	0.73	16	1
1:A:28:HIS:CG	1:A:28:HIS:HD2	0.64	1.39	16	1
1:A:72:TYR:CD1	1:A:84:ALA:HB1	0.63	2.28	11	3
1:A:72:TYR:CE1	1:A:76:LEU:HD11	0.63	2.28	16	11
1:A:4:LYS:CD	1:A:4:LYS:HE2	0.63	1.23	16	1
1:A:63:LYS:CD	1:A:63:LYS:HG3	0.63	1.16	16	1
1:A:16:LEU:CD2	1:A:16:LEU:HD11	0.63	1.06	16	1
1:A:30:ILE:HG21	1:A:40:GLU:OE1	0.62	1.94	5	1
1:A:30:ILE:CD1	1:A:56:LEU:HD21	0.62	2.23	13	1
1:A:63:LYS:CG	1:A:63:LYS:HD2	0.62	1.15	16	1
1:A:24:TYR:CE1	1:A:24:TYR:CZ	0.62	0.71	16	1
1:A:52:ARG:CZ	1:A:52:ARG:NH1	0.62	0.76	16	1
1:A:4:LYS:CD	1:A:4:LYS:HE3	0.62	1.23	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ILE:HD12	1:A:25:ILE:HG13	0.62	1.71	10	2
1:A:71:PHE:CE2	1:A:75:LEU:HD11	0.62	2.29	5	3
1:A:39:GLU:O	1:A:43:VAL:HG23	0.62	1.94	5	1
1:A:12:HIS:O	1:A:12:HIS:HD2	0.62	1.77	16	1
1:A:83:LEU:O	1:A:83:LEU:HD23	0.62	1.94	5	3
1:A:26:MET:HB3	1:A:56:LEU:HD21	0.61	1.70	9	2
1:A:49:GLN:HE22	1:A:49:GLN:CD	0.61	1.23	16	1
1:A:76:LEU:HD21	1:A:84:ALA:CB	0.61	2.23	5	2
1:A:49:GLN:HE21	1:A:49:GLN:CD	0.61	1.23	16	1
1:A:29:MET:CG	1:A:29:MET:HE3	0.61	0.96	16	1
1:A:23:SER:HG	1:A:23:SER:CB	0.61	1.32	16	1
1:A:35:LEU:HD22	1:A:39:GLU:OE1	0.61	1.95	9	1
1:A:34:PHE:CG	1:A:34:PHE:CD2	0.61	0.71	16	1
1:A:34:PHE:C	1:A:35:LEU:HD22	0.61	2.16	11	6
1:A:27:ASP:CG	1:A:27:ASP:OD1	0.60	0.64	16	1
1:A:86:LEU:O	1:A:86:LEU:HD13	0.60	1.97	11	3
1:A:68:TYR:CE2	1:A:68:TYR:CZ	0.60	0.70	16	1
1:A:35:LEU:CD1	1:A:35:LEU:CG	0.60	0.61	16	1
1:A:81:LYS:O	1:A:85:ALA:HB2	0.60	1.97	7	6
1:A:63:LYS:HG2	1:A:63:LYS:HD3	0.60	0.73	16	1
1:A:32:ASP:CG	1:A:32:ASP:OD1	0.60	0.73	16	1
1:A:68:TYR:CE1	1:A:68:TYR:CZ	0.60	0.70	16	1
1:A:5:ALA:CB	1:A:91:ILE:HG23	0.60	2.27	5	2
1:A:63:LYS:CG	1:A:63:LYS:HD3	0.60	1.15	16	1
1:A:16:LEU:C	1:A:16:LEU:HD13	0.60	2.18	11	1
1:A:63:LYS:CD	1:A:63:LYS:HG2	0.59	1.16	16	1
1:A:35:LEU:HD22	1:A:35:LEU:N	0.59	2.12	7	5
1:A:34:PHE:CG	1:A:34:PHE:CD1	0.59	0.72	16	1
1:A:72:TYR:CE2	1:A:76:LEU:HD11	0.59	2.31	16	3
1:A:80:TYR:CZ	1:A:80:TYR:CE2	0.59	0.71	16	1
1:A:12:HIS:NE2	1:A:15:ALA:CB	0.59	2.66	16	2
1:A:83:LEU:HD13	1:A:83:LEU:C	0.59	2.18	15	4
1:A:80:TYR:CZ	1:A:80:TYR:CE1	0.58	0.70	16	1
1:A:4:LYS:HE2	1:A:4:LYS:NZ	0.58	1.14	16	1
1:A:21:LYS:O	1:A:22:THR:C	0.58	2.42	15	16
1:A:26:MET:CB	1:A:56:LEU:HD21	0.58	2.27	9	1
1:A:46:GLU:HB3	1:A:47:PRO:HD3	0.58	1.76	16	13
1:A:83:LEU:C	1:A:83:LEU:HD13	0.58	2.18	3	3
1:A:20:ILE:HG21	1:A:26:MET:CE	0.58	2.29	6	2
1:A:35:LEU:N	1:A:35:LEU:HD22	0.58	2.13	11	1
1:A:24:TYR:CZ	1:A:24:TYR:CE2	0.58	0.70	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:HD13	1:A:16:LEU:C	0.58	2.19	13	3
1:A:22:THR:HG21	1:A:52:ARG:HG2	0.58	1.76	13	4
1:A:63:LYS:CE	1:A:63:LYS:HZ1	0.58	1.28	16	1
1:A:20:ILE:HD13	1:A:25:ILE:HG21	0.58	1.74	3	1
1:A:57:ILE:N	1:A:57:ILE:CD1	0.57	2.67	4	7
1:A:59:MET:HG2	1:A:59:MET:CE	0.57	2.22	16	1
1:A:16:LEU:HD13	1:A:57:ILE:CG1	0.57	2.30	14	1
1:A:34:PHE:C	1:A:35:LEU:HD12	0.57	2.19	12	1
1:A:21:LYS:O	1:A:23:SER:HB2	0.57	1.99	16	1
1:A:77:HIS:CG	1:A:77:HIS:HD1	0.57	1.33	16	1
1:A:22:THR:HG21	1:A:52:ARG:HD3	0.57	1.77	4	1
1:A:63:LYS:CE	1:A:63:LYS:HZ2	0.57	1.28	16	1
1:A:55:MET:CE	1:A:55:MET:HG3	0.56	2.22	16	1
1:A:71:PHE:CD1	1:A:71:PHE:CG	0.56	0.73	16	1
1:A:63:LYS:CE	1:A:63:LYS:HZ3	0.56	1.28	16	1
1:A:78:GLU:OE2	1:A:78:GLU:CD	0.56	0.77	16	1
1:A:12:HIS:O	1:A:12:HIS:CD2	0.56	2.59	16	3
1:A:9:LEU:HD23	1:A:68:TYR:HE1	0.56	1.59	13	7
1:A:16:LEU:HD22	1:A:57:ILE:HG12	0.56	1.77	8	2
1:A:13:ARG:HD2	1:A:54:ALA:HB2	0.56	1.78	16	3
1:A:46:GLU:OE1	1:A:46:GLU:OE2	0.56	0.56	16	1
1:A:16:LEU:HD23	1:A:57:ILE:HG13	0.56	1.77	3	1
1:A:57:ILE:CD1	1:A:57:ILE:N	0.55	2.69	13	2
1:A:16:LEU:HD22	1:A:57:ILE:CG1	0.55	2.32	6	2
1:A:49:GLN:CB	1:A:49:GLN:NE2	0.55	2.54	16	1
1:A:56:LEU:HD13	1:A:56:LEU:O	0.55	2.01	13	1
1:A:24:TYR:CD2	1:A:24:TYR:CG	0.55	0.70	16	1
1:A:68:TYR:CD1	1:A:68:TYR:CG	0.55	0.70	16	1
1:A:26:MET:SD	1:A:60:ILE:HD11	0.55	2.41	9	2
1:A:68:TYR:CZ	1:A:91:ILE:HD11	0.54	2.37	13	2
1:A:68:TYR:CD2	1:A:68:TYR:CG	0.54	0.71	16	1
1:A:57:ILE:N	1:A:57:ILE:HD12	0.54	2.16	6	2
1:A:75:LEU:HD23	1:A:80:TYR:CD2	0.54	2.37	6	1
1:A:6:ARG:HG3	1:A:61:LEU:HD12	0.54	1.79	14	4
1:A:71:PHE:CZ	1:A:75:LEU:HD11	0.54	2.37	3	10
1:A:80:TYR:CG	1:A:80:TYR:CD2	0.54	0.70	16	1
1:A:12:HIS:CD2	1:A:87:LEU:HD21	0.54	2.38	13	1
1:A:9:LEU:C	1:A:9:LEU:HD13	0.54	2.23	4	5
1:A:24:TYR:CD1	1:A:24:TYR:CG	0.54	0.70	16	1
1:A:86:LEU:C	1:A:86:LEU:HD13	0.54	2.23	5	3
1:A:49:GLN:NE2	1:A:49:GLN:CD	0.53	0.55	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ARG:HD2	1:A:54:ALA:CB	0.53	2.33	16	1
1:A:72:TYR:CZ	1:A:72:TYR:HE1	0.53	1.28	16	1
1:A:53:ALA:O	1:A:57:ILE:HD13	0.53	2.04	16	3
1:A:68:TYR:CE2	1:A:91:ILE:HD11	0.53	2.39	15	2
1:A:25:ILE:CG2	1:A:75:LEU:HD21	0.53	2.33	7	3
1:A:52:ARG:CZ	1:A:52:ARG:HH22	0.53	1.36	16	1
1:A:12:HIS:CE1	1:A:86:LEU:HD23	0.53	2.38	4	2
1:A:57:ILE:HA	1:A:60:ILE:HD12	0.53	1.80	12	8
1:A:72:TYR:CG	1:A:72:TYR:HD2	0.53	1.28	16	1
1:A:19:ASP:HB3	1:A:83:LEU:HD11	0.52	1.81	11	5
1:A:45:ASN:OD1	1:A:45:ASN:CG	0.52	0.63	16	1
1:A:91:ILE:N	1:A:92:PRO:HD2	0.52	2.19	3	12
1:A:71:PHE:CD2	1:A:71:PHE:CG	0.52	0.68	16	1
1:A:80:TYR:CG	1:A:80:TYR:CD1	0.52	0.70	16	1
1:A:22:THR:HG22	1:A:56:LEU:CD2	0.52	2.33	5	1
1:A:35:LEU:CD2	1:A:35:LEU:N	0.52	2.73	5	4
1:A:72:TYR:CZ	1:A:72:TYR:HE2	0.52	1.28	16	1
1:A:35:LEU:HD22	1:A:35:LEU:HD13	0.52	0.63	16	1
1:A:12:HIS:HD2	1:A:15:ALA:HB3	0.52	1.60	4	2
1:A:78:GLU:OE1	1:A:78:GLU:CD	0.52	0.70	16	1
1:A:91:ILE:HB	1:A:92:PRO:HD3	0.52	1.80	13	15
1:A:35:LEU:CD2	1:A:35:LEU:HD13	0.51	1.11	16	1
1:A:20:ILE:HG21	1:A:26:MET:HE1	0.51	1.83	6	1
1:A:26:MET:HE3	1:A:57:ILE:CD1	0.51	2.35	2	1
1:A:12:HIS:CE1	1:A:86:LEU:HD12	0.50	2.40	5	1
1:A:72:TYR:CG	1:A:72:TYR:HD1	0.50	1.28	16	1
1:A:16:LEU:HD13	1:A:16:LEU:O	0.50	2.06	11	3
1:A:19:ASP:CB	1:A:83:LEU:HD23	0.50	2.36	10	1
1:A:35:LEU:N	1:A:35:LEU:CD2	0.50	2.74	7	2
1:A:35:LEU:CD1	1:A:35:LEU:HD22	0.50	1.12	16	1
1:A:4:LYS:HZ1	1:A:4:LYS:CE	0.50	1.20	16	1
1:A:16:LEU:HD13	1:A:57:ILE:HG13	0.50	1.84	5	2
1:A:4:LYS:HZ2	1:A:4:LYS:CE	0.49	1.20	16	1
1:A:57:ILE:N	1:A:57:ILE:HD13	0.49	2.22	7	1
1:A:4:LYS:CE	1:A:4:LYS:HZ3	0.49	1.20	16	1
1:A:16:LEU:O	1:A:16:LEU:HD13	0.49	2.08	10	1
1:A:46:GLU:N	1:A:47:PRO:HD2	0.49	2.22	11	12
1:A:16:LEU:HD11	1:A:26:MET:HE2	0.49	1.84	5	1
1:A:62:LYS:HZ3	1:A:62:LYS:CD	0.49	2.06	16	1
1:A:71:PHE:CE1	1:A:87:LEU:HD22	0.49	2.43	9	1
1:A:63:LYS:CD	1:A:63:LYS:CA	0.49	2.89	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ILE:HD12	1:A:57:ILE:N	0.49	2.22	4	1
1:A:71:PHE:CZ	1:A:75:LEU:CD1	0.48	2.96	4	10
1:A:30:ILE:HD11	1:A:56:LEU:CD2	0.48	2.32	15	1
1:A:34:PHE:CG	1:A:34:PHE:HD1	0.48	1.24	16	1
1:A:16:LEU:HD11	1:A:26:MET:HE1	0.48	1.84	10	2
1:A:35:LEU:CD2	1:A:35:LEU:CD1	0.48	0.49	16	1
1:A:71:PHE:CE2	1:A:87:LEU:HD22	0.48	2.44	4	1
1:A:34:PHE:HB3	1:A:35:LEU:HD12	0.48	1.86	12	1
1:A:46:GLU:N	1:A:47:PRO:CD	0.48	2.77	15	11
1:A:34:PHE:CZ	1:A:34:PHE:HE2	0.48	1.24	16	1
1:A:57:ILE:HD13	1:A:57:ILE:N	0.48	2.24	3	1
1:A:45:ASN:OD1	1:A:45:ASN:CA	0.48	2.61	16	1
1:A:29:MET:SD	1:A:29:MET:HE3	0.47	1.11	16	1
1:A:72:TYR:O	1:A:76:LEU:HD12	0.47	2.08	2	1
1:A:62:LYS:HE3	1:A:62:LYS:CG	0.47	2.09	16	1
1:A:34:PHE:HD2	1:A:34:PHE:CG	0.47	1.24	16	1
1:A:9:LEU:HD13	1:A:9:LEU:C	0.47	2.29	14	9
1:A:29:MET:SD	1:A:29:MET:HE1	0.47	1.11	16	1
1:A:20:ILE:HD12	1:A:25:ILE:HG21	0.47	1.86	4	1
1:A:34:PHE:HE1	1:A:34:PHE:CZ	0.47	1.23	16	1
1:A:63:LYS:CD	1:A:63:LYS:CG	0.47	0.56	16	1
1:A:46:GLU:OE1	1:A:46:GLU:CD	0.47	0.28	16	1
1:A:20:ILE:HG21	1:A:25:ILE:HG21	0.47	1.87	10	1
1:A:59:MET:N	1:A:59:MET:SD	0.47	2.88	5	2
1:A:91:ILE:N	1:A:92:PRO:CD	0.47	2.78	3	5
1:A:16:LEU:HD11	1:A:26:MET:CE	0.47	2.40	9	6
1:A:30:ILE:HD13	1:A:35:LEU:HD13	0.47	1.87	3	1
1:A:27:ASP:HA	1:A:30:ILE:HD12	0.46	1.86	2	1
1:A:35:LEU:N	1:A:35:LEU:HD12	0.46	2.25	12	1
1:A:13:ARG:CD	1:A:54:ALA:HB1	0.46	2.41	12	1
1:A:20:ILE:HD11	1:A:80:TYR:CE1	0.46	2.45	2	1
1:A:12:HIS:HE1	1:A:86:LEU:HD23	0.46	1.69	16	1
1:A:16:LEU:CD1	1:A:16:LEU:C	0.46	2.84	11	2
1:A:19:ASP:CG	1:A:83:LEU:HD23	0.46	2.30	10	1
1:A:71:PHE:HD1	1:A:71:PHE:CG	0.46	1.21	16	1
1:A:23:SER:O	1:A:24:TYR:C	0.46	2.54	15	16
1:A:29:MET:HB2	1:A:29:MET:CE	0.46	2.26	16	1
1:A:83:LEU:C	1:A:83:LEU:HD23	0.45	2.31	14	3
1:A:25:ILE:HG23	1:A:75:LEU:HD21	0.45	1.89	7	2
1:A:68:TYR:CE2	1:A:91:ILE:CD1	0.45	2.99	15	2
1:A:71:PHE:HE2	1:A:71:PHE:CZ	0.45	1.21	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ILE:CD1	1:A:25:ILE:HG21	0.45	2.42	3	1
1:A:83:LEU:HD23	1:A:83:LEU:C	0.45	2.31	5	2
1:A:35:LEU:HD21	1:A:63:LYS:HB2	0.45	1.88	14	1
1:A:21:LYS:O	1:A:23:SER:N	0.45	2.50	10	5
1:A:34:PHE:O	1:A:63:LYS:HD3	0.45	2.11	16	1
1:A:68:TYR:HD2	1:A:68:TYR:CG	0.45	1.20	16	1
1:A:13:ARG:CD	1:A:54:ALA:HB2	0.45	2.42	10	1
1:A:24:TYR:CZ	1:A:24:TYR:HE1	0.45	1.20	16	1
1:A:68:TYR:HE1	1:A:68:TYR:CZ	0.45	1.20	16	1
1:A:23:SER:O	1:A:25:ILE:N	0.45	2.50	10	4
1:A:83:LEU:HD13	1:A:83:LEU:O	0.45	2.12	15	2
1:A:35:LEU:HD11	1:A:63:LYS:HB2	0.45	1.88	12	1
1:A:24:TYR:CG	1:A:24:TYR:HD1	0.45	1.20	16	1
1:A:91:ILE:HB	1:A:92:PRO:CD	0.44	2.42	13	6
1:A:56:LEU:HD13	1:A:56:LEU:C	0.44	2.31	13	1
1:A:68:TYR:HD1	1:A:68:TYR:CG	0.44	1.20	16	1
1:A:12:HIS:CE1	1:A:15:ALA:HB3	0.44	2.47	10	2
1:A:34:PHE:CB	1:A:35:LEU:HD12	0.44	2.43	10	2
1:A:12:HIS:CE1	1:A:15:ALA:CB	0.44	3.01	6	4
1:A:63:LYS:HZ3	1:A:63:LYS:HE2	0.44	1.13	16	1
1:A:80:TYR:HE2	1:A:80:TYR:CZ	0.44	1.20	16	1
1:A:80:TYR:HE1	1:A:80:TYR:CZ	0.44	1.19	16	1
1:A:24:TYR:HD2	1:A:24:TYR:CG	0.44	1.20	16	1
1:A:24:TYR:HE2	1:A:24:TYR:CZ	0.44	1.20	16	1
1:A:80:TYR:CG	1:A:80:TYR:HD1	0.44	1.20	16	1
1:A:76:LEU:HD21	1:A:84:ALA:HB3	0.44	1.89	2	1
1:A:4:LYS:CG	1:A:4:LYS:HE3	0.44	2.09	16	1
1:A:68:TYR:HE2	1:A:68:TYR:CZ	0.43	1.19	16	1
1:A:9:LEU:HD11	1:A:57:ILE:HG23	0.43	1.90	15	1
1:A:80:TYR:CG	1:A:80:TYR:HD2	0.43	1.19	16	1
1:A:12:HIS:CD2	1:A:16:LEU:N	0.43	2.86	9	1
1:A:35:LEU:CD2	1:A:35:LEU:HD11	0.43	0.73	16	1
1:A:42:LYS:O	1:A:46:GLU:HB2	0.43	2.13	16	1
1:A:82:ASP:OD1	1:A:82:ASP:OD2	0.43	0.43	16	1
1:A:34:PHE:CD1	1:A:34:PHE:N	0.43	2.85	11	1
1:A:26:MET:CE	1:A:60:ILE:HD11	0.43	2.44	1	1
1:A:68:TYR:OH	1:A:91:ILE:HD11	0.43	2.14	1	1
1:A:26:MET:SD	1:A:56:LEU:HD12	0.43	2.53	13	1
1:A:41:GLU:OE2	1:A:41:GLU:OE1	0.43	0.43	16	1
1:A:9:LEU:HD11	1:A:57:ILE:CG2	0.43	2.44	15	1
1:A:6:ARG:CZ	1:A:10:LEU:HD11	0.43	2.43	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ILE:HD13	1:A:56:LEU:HD11	0.42	1.89	8	1
1:A:16:LEU:HD21	1:A:26:MET:HE1	0.42	1.91	6	1
1:A:16:LEU:C	1:A:16:LEU:CD1	0.42	2.87	13	1
1:A:46:GLU:HB3	1:A:47:PRO:CD	0.42	2.45	16	1
1:A:86:LEU:CD1	1:A:86:LEU:C	0.42	2.88	5	1
1:A:13:ARG:HD2	1:A:54:ALA:HB1	0.42	1.92	12	1
1:A:71:PHE:CZ	1:A:71:PHE:HE1	0.42	1.18	16	1
1:A:20:ILE:HG22	1:A:21:LYS:N	0.42	2.29	15	2
1:A:71:PHE:HD2	1:A:71:PHE:CG	0.42	1.18	16	1
1:A:91:ILE:CB	1:A:92:PRO:CD	0.42	2.98	13	3
1:A:19:ASP:OD2	1:A:83:LEU:HD11	0.42	2.15	12	1
1:A:20:ILE:CG2	1:A:21:LYS:N	0.41	2.82	15	2
1:A:56:LEU:HD23	1:A:56:LEU:C	0.41	2.35	15	1
1:A:34:PHE:N	1:A:34:PHE:CD1	0.41	2.87	5	1
1:A:46:GLU:CB	1:A:47:PRO:CD	0.41	2.98	7	3
1:A:22:THR:HG23	1:A:53:ALA:HB2	0.41	1.92	8	1
1:A:86:LEU:C	1:A:86:LEU:CD1	0.41	2.89	11	2
1:A:26:MET:HE1	1:A:60:ILE:HD11	0.41	1.91	1	1
1:A:9:LEU:CD1	1:A:57:ILE:CG2	0.41	2.99	15	1
1:A:29:MET:O	1:A:34:PHE:CD2	0.41	2.73	9	1
1:A:20:ILE:CG2	1:A:26:MET:HE1	0.41	2.44	6	1
1:A:29:MET:O	1:A:34:PHE:CD1	0.41	2.74	8	1
1:A:4:LYS:NZ	1:A:4:LYS:CE	0.41	0.56	16	1
1:A:75:LEU:HD13	1:A:83:LEU:HD12	0.41	1.91	2	1
1:A:16:LEU:CD2	1:A:57:ILE:CG1	0.41	2.98	4	1
1:A:30:ILE:HD11	1:A:56:LEU:CD1	0.40	2.41	8	1
1:A:12:HIS:CD2	1:A:12:HIS:O	0.40	2.74	1	1
1:A:6:ARG:NH1	1:A:10:LEU:HD11	0.40	2.31	15	1
1:A:34:PHE:CD2	1:A:67:SER:OG	0.40	2.74	15	1
1:A:42:LYS:O	1:A:46:GLU:N	0.40	2.55	5	1
1:A:72:TYR:CE1	1:A:88:HIS:HB2	0.40	2.52	15	1
1:A:26:MET:CE	1:A:57:ILE:CD1	0.40	3.00	2	1
1:A:63:LYS:HZ1	1:A:63:LYS:HE3	0.40	1.14	16	1

6.3 Torsion angles

6.3.1 Protein backbone

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	90/97 (93%)	76±1 (85±1%)	12±1 (13±1%)	2±1 (3±1%)	11 47
All	All	1440/1552 (93%)	1219 (85%)	184 (13%)	37 (3%)	11 47

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	22	THR	16
1	A	92	PRO	13
1	A	24	TYR	8

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	79/86 (92%)	73±2 (92±3%)	6±2 (8±3%)	20 66
All	All	1264/1376 (92%)	1166 (92%)	98 (8%)	20 66

All 33 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	9	LEU	9
1	A	87	LEU	6
1	A	62	LYS	6
1	A	63	LYS	6
1	A	49	GLN	5
1	A	26	MET	5
1	A	32	ASP	5
1	A	64	ASP	5
1	A	57	ILE	5
1	A	50	GLN	4
1	A	59	MET	4
1	A	27	ASP	3
1	A	82	ASP	3
1	A	58	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	29	MET	3
1	A	46	GLU	3
1	A	66	ASP	2
1	A	40	GLU	2
1	A	45	ASN	2
1	A	16	LEU	2
1	A	73	ASN	2
1	A	55	MET	2
1	A	21	LYS	1
1	A	42	LYS	1
1	A	13	ARG	1
1	A	78	GLU	1
1	A	4	LYS	1
1	A	20	ILE	1
1	A	23	SER	1
1	A	86	LEU	1
1	A	81	LYS	1
1	A	89	ASP	1
1	A	83	LEU	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 61% for the well-defined parts and 61% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4661

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	858
Number of shifts mapped to atoms	858
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	87	-0.09 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	12	0.06 ± 0.41	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	90	0.97 ± 0.28	Should be applied

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 61%, i.e. 695 atoms were assigned a chemical shift out of a possible 1145. 10 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	337/446 (76%)	171/178 (96%)	82/180 (46%)	84/88 (95%)
Sidechain	328/621 (53%)	276/364 (76%)	52/229 (23%)	0/28 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	30/78 (38%)	30/42 (71%)	0/32 (0%)	0/4 (0%)
Overall	695/1145 (61%)	477/584 (82%)	134/441 (30%)	84/120 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 61%, i.e. 734 atoms were assigned a chemical shift out of a possible 1213. 10 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	360/481 (75%)	183/192 (95%)	87/194 (45%)	90/95 (95%)
Sidechain	344/654 (53%)	292/383 (76%)	52/243 (21%)	0/28 (0%)
Aromatic	30/78 (38%)	30/42 (71%)	0/32 (0%)	0/4 (0%)
Overall	734/1213 (61%)	505/617 (82%)	139/469 (30%)	90/127 (71%)

7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

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: