



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 05:37 AM UTC

PDB ID : 1C15 / pdb_00001c15
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.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

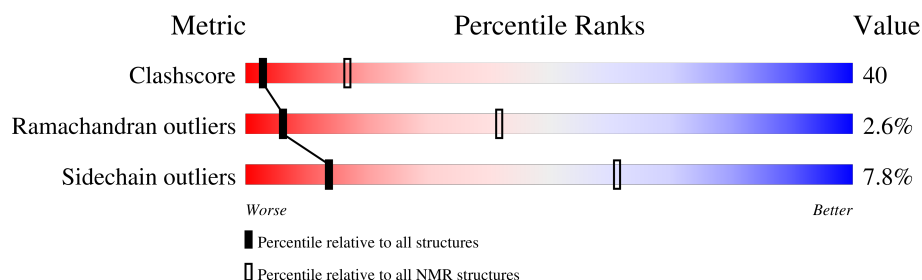
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	97	

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)	0.46	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
1	A	97	Total	C	H	N	O	S	0
			1553	485	778	133	151	6	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

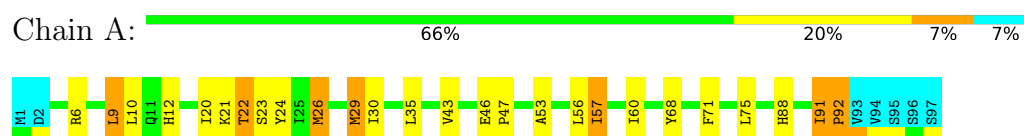


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

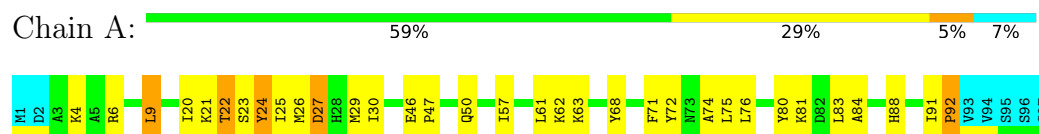
4.2.1 Score per residue for model 1

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1



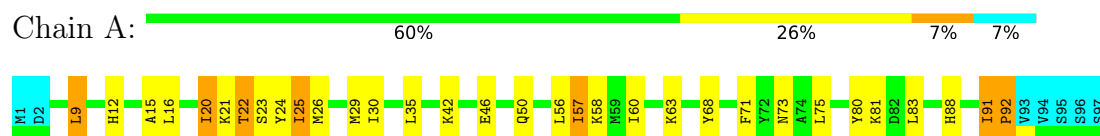
4.2.2 Score per residue for model 2

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1



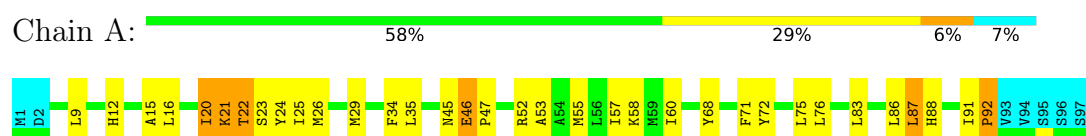
4.2.3 Score per residue for model 3

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1



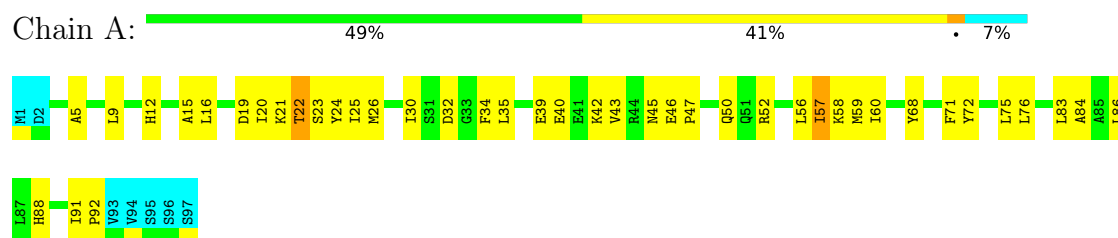
4.2.4 Score per residue for model 4

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1



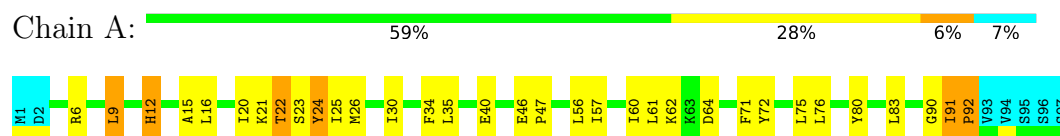
4.2.5 Score per residue for model 5

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1



4.2.6 Score per residue for model 6

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1



4.2.7 Score per residue for model 7

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1





4.2.8 Score per residue for model 8

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

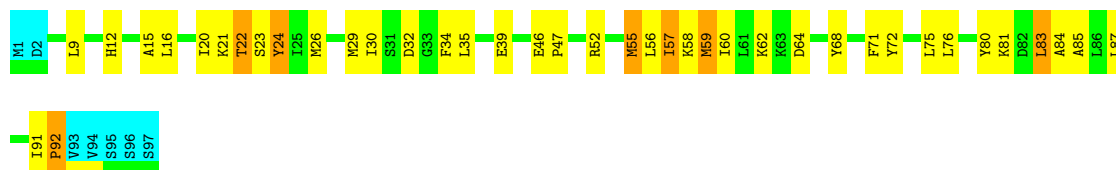
Chain A: 57% 30% 6% 7%



4.2.9 Score per residue for model 9

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

Chain A: 52% 34% 7% 7%



4.2.10 Score per residue for model 10

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

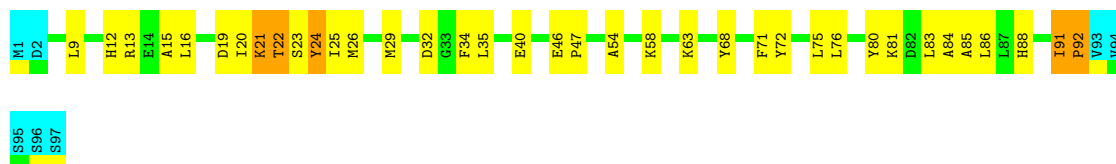
Chain A: 61% 23% 9% 7%



4.2.11 Score per residue for model 11

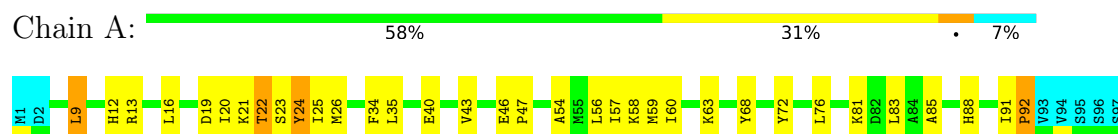
- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1

Chain A: 55% 33% 5% 7%



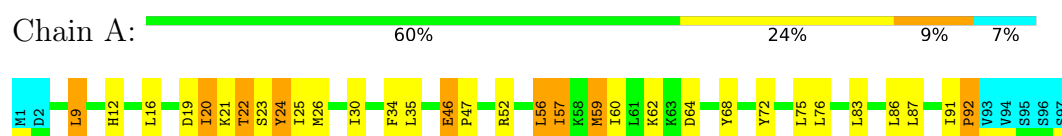
4.2.12 Score per residue for model 12

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1



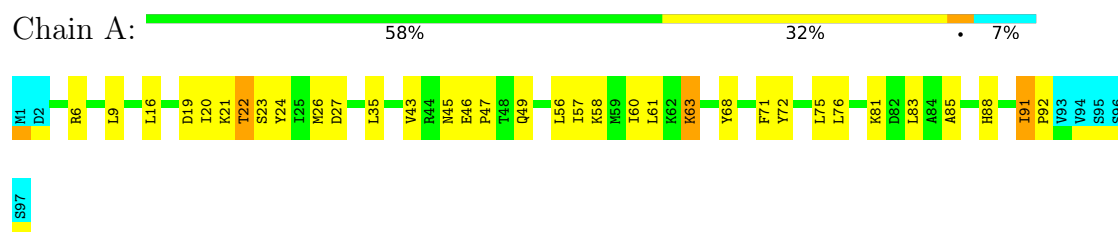
4.2.13 Score per residue for model 13

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1



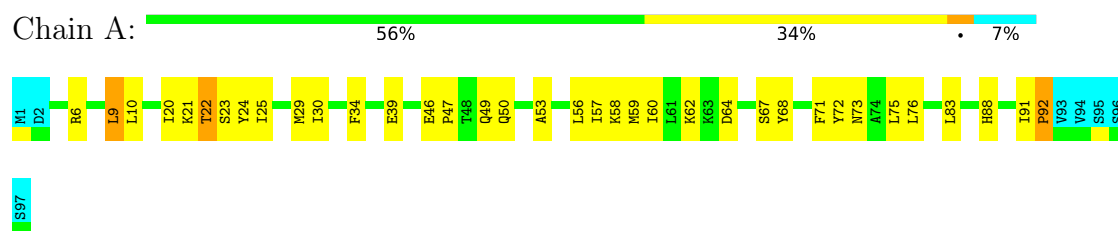
4.2.14 Score per residue for model 14

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1



4.2.15 Score per residue for model 15

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1



4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: APOPTOTIC PROTEASE ACTIVATING FACTOR 1



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

No chemical shift data was provided.

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	2.35±3.39	10±39/738 (1.4± 5.2%)	2.27±2.97	14±48/992 (1.4± 4.8%)
All	All	4.13	160/11808 (1.4%)	3.74	217/15872 (1.4%)

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	28	HIS	CE1-NE2	-104.78	0.27	1.32	16	1
1	A	88	HIS	CE1-NE2	-99.91	0.32	1.32	16	1
1	A	77	HIS	CE1-NE2	-94.96	0.37	1.32	16	1
1	A	6	ARG	CZ-NH1	-67.18	0.38	1.32	16	1
1	A	13	ARG	CZ-NH1	-65.96	0.40	1.32	16	1
1	A	40	GLU	CD-OE1	-59.73	0.11	1.25	16	1
1	A	29	MET	SD-CE	-59.64	0.30	1.79	16	1
1	A	88	HIS	CG-ND1	-54.09	0.78	1.38	16	1
1	A	44	ARG	CZ-NH1	-53.87	0.57	1.32	16	1
1	A	28	HIS	CG-ND1	-52.69	0.80	1.38	16	1
1	A	12	HIS	CE1-NE2	-51.91	0.80	1.32	16	1
1	A	6	ARG	CZ-NH2	-51.38	0.66	1.33	16	1
1	A	46	GLU	CD-OE1	-50.84	0.28	1.25	16	1
1	A	44	ARG	CZ-NH2	-50.37	0.68	1.33	16	1
1	A	6	ARG	CD-NE	-49.23	0.77	1.46	16	1
1	A	64	ASP	CG-OD1	-48.92	0.32	1.25	16	1
1	A	77	HIS	CG-ND1	-48.85	0.84	1.38	16	1
1	A	44	ARG	CD-NE	-48.43	0.78	1.46	16	1
1	A	52	ARG	CZ-NH2	-48.24	0.70	1.33	16	1
1	A	52	ARG	CD-NE	-45.66	0.82	1.46	16	1
1	A	13	ARG	NE-CZ	-43.98	0.84	1.33	16	1
1	A	46	GLU	CD-OE2	-42.45	0.44	1.25	16	1
1	A	44	ARG	NE-CZ	-41.37	0.87	1.33	16	1
1	A	50	GLN	CD-OE1	-41.11	0.45	1.23	16	1
1	A	28	HIS	CG-CD2	-40.72	0.91	1.35	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	52	ARG	CZ-NH1	-40.39	0.76	1.32	16	1
1	A	77	HIS	CG-CD2	-40.35	0.91	1.35	16	1
1	A	41	GLU	CD-OE2	-39.57	0.50	1.25	16	1
1	A	88	HIS	CG-CD2	-38.26	0.93	1.35	16	1
1	A	6	ARG	NE-CZ	-37.49	0.91	1.33	16	1
1	A	49	GLN	CD-NE2	-36.98	0.55	1.33	16	1
1	A	17	GLU	CD-OE1	-36.79	0.55	1.25	16	1
1	A	40	GLU	CD-OE2	-36.73	0.55	1.25	16	1
1	A	12	HIS	CG-CD2	-36.72	0.95	1.35	16	1
1	A	14	GLU	CD-OE1	-36.37	0.56	1.25	16	1
1	A	66	ASP	CG-OD2	-35.28	0.58	1.25	16	1
1	A	46	GLU	CG-CD	-34.31	0.66	1.52	16	1
1	A	82	ASP	CG-OD1	-34.16	0.60	1.25	16	1
1	A	14	GLU	CD-OE2	-33.84	0.61	1.25	16	1
1	A	71	PHE	CG-CD2	-33.57	0.68	1.38	16	1
1	A	17	GLU	CD-OE2	-33.49	0.61	1.25	16	1
1	A	82	ASP	CG-OD2	-33.38	0.61	1.25	16	1
1	A	49	GLN	CD-OE1	-33.19	0.60	1.23	16	1
1	A	80	TYR	CG-CD2	-32.92	0.70	1.39	16	1
1	A	24	TYR	CG-CD1	-32.78	0.70	1.39	16	1
1	A	68	TYR	CG-CD1	-32.69	0.70	1.39	16	1
1	A	66	ASP	CG-OD1	-32.66	0.63	1.25	16	1
1	A	80	TYR	CG-CD1	-32.63	0.70	1.39	16	1
1	A	24	TYR	CG-CD2	-32.59	0.70	1.39	16	1
1	A	68	TYR	CG-CD2	-32.46	0.71	1.39	16	1
1	A	51	GLN	CD-OE1	-32.25	0.62	1.23	16	1
1	A	64	ASP	CG-OD2	-32.11	0.64	1.25	16	1
1	A	27	ASP	CG-OD1	-31.99	0.64	1.25	16	1
1	A	59	MET	CG-SD	-31.99	1.00	1.80	16	1
1	A	34	PHE	CG-CD2	-31.96	0.71	1.38	16	1
1	A	63	LYS	CG-CD	-31.91	0.56	1.52	16	1
1	A	23	SER	CB-OG	-31.83	0.78	1.42	16	1
1	A	45	ASN	CG-OD1	-31.55	0.63	1.23	16	1
1	A	34	PHE	CG-CD1	-31.51	0.72	1.38	16	1
1	A	71	PHE	CG-CD1	-31.20	0.73	1.38	16	1
1	A	72	TYR	CG-CD1	-31.11	0.74	1.39	16	1
1	A	4	LYS	CE-NZ	-30.99	0.56	1.49	16	1
1	A	19	ASP	CG-OD1	-30.98	0.66	1.25	16	1
1	A	55	MET	SD-CE	-30.78	1.02	1.79	16	1
1	A	72	TYR	CG-CD2	-30.74	0.74	1.39	16	1
1	A	7	ASN	CG-OD1	-30.47	0.65	1.23	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	89	ASP	CG-OD1	-30.47	0.67	1.25	16	1
1	A	32	ASP	CG-OD2	-30.15	0.68	1.25	16	1
1	A	11	GLN	CD-NE2	-30.06	0.70	1.33	16	1
1	A	27	ASP	CG-OD2	-30.04	0.68	1.25	16	1
1	A	41	GLU	CD-OE1	-29.77	0.68	1.25	16	1
1	A	89	ASP	CG-OD2	-29.63	0.69	1.25	16	1
1	A	78	GLU	CD-OE1	-28.75	0.70	1.25	16	1
1	A	80	TYR	CE1-CZ	-28.31	0.70	1.38	16	1
1	A	68	TYR	CE2-CZ	-28.25	0.70	1.38	16	1
1	A	7	ASN	CG-ND2	-28.17	0.74	1.33	16	1
1	A	24	TYR	CE2-CZ	-28.17	0.70	1.38	16	1
1	A	68	TYR	CE1-CZ	-28.04	0.70	1.38	16	1
1	A	80	TYR	CE2-CZ	-28.04	0.70	1.38	16	1
1	A	24	TYR	CE1-CZ	-28.02	0.71	1.38	16	1
1	A	35	LEU	CG-CD1	-27.73	0.61	1.52	16	1
1	A	51	GLN	CD-NE2	-27.67	0.75	1.33	16	1
1	A	19	ASP	CG-OD2	-27.54	0.73	1.25	16	1
1	A	63	LYS	CE-NZ	-27.47	0.67	1.49	16	1
1	A	32	ASP	CG-OD1	-27.08	0.73	1.25	16	1
1	A	50	GLN	CB-CG	-27.05	0.71	1.52	16	1
1	A	26	MET	CG-SD	-26.92	1.13	1.80	16	1
1	A	4	LYS	CD-CE	-26.89	0.71	1.52	16	1
1	A	72	TYR	CE2-CZ	-26.73	0.74	1.38	16	1
1	A	40	GLU	CG-CD	-26.66	0.85	1.52	16	1
1	A	72	TYR	CE1-CZ	-26.45	0.74	1.38	16	1
1	A	29	MET	CG-SD	-26.31	1.15	1.80	16	1
1	A	81	LYS	CD-CE	-26.14	0.74	1.52	16	1
1	A	35	LEU	CG-CD2	-25.89	0.67	1.52	16	1
1	A	78	GLU	CD-OE2	-25.39	0.77	1.25	16	1
1	A	11	GLN	CD-OE1	-25.33	0.75	1.23	16	1
1	A	73	ASN	CG-OD1	-24.76	0.76	1.23	16	1
1	A	73	ASN	CG-ND2	-24.68	0.81	1.33	16	1
1	A	16	LEU	CG-CD2	-24.26	0.72	1.52	16	1
1	A	26	MET	SD-CE	-24.09	1.19	1.79	16	1
1	A	39	GLU	CD-OE2	-23.90	0.80	1.25	16	1
1	A	71	PHE	CE1-CZ	-23.49	0.68	1.38	16	1
1	A	59	MET	SD-CE	-23.37	1.21	1.79	16	1
1	A	65	ASN	CG-OD1	-22.71	0.80	1.23	16	1
1	A	45	ASN	CG-ND2	-22.60	0.85	1.33	16	1
1	A	34	PHE	CE1-CZ	-22.44	0.71	1.38	16	1
1	A	16	LEU	CG-CD1	-22.34	0.78	1.52	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	-22.31	1.25	1.80	16	1
1	A	13	ARG	CZ-NH2	-22.25	1.04	1.33	16	1
1	A	34	PHE	CE2-CZ	-22.16	0.72	1.38	16	1
1	A	65	ASN	CG-ND2	-22.01	0.87	1.33	16	1
1	A	71	PHE	CE2-CZ	-21.81	0.73	1.38	16	1
1	A	83	LEU	CG-CD1	-21.55	0.81	1.52	16	1
1	A	86	LEU	CG-CD2	-21.54	0.81	1.52	16	1
1	A	62	LYS	CD-CE	-21.37	0.88	1.52	16	1
1	A	12	HIS	CG-ND1	-20.78	1.15	1.38	16	1
1	A	86	LEU	CG-CD1	-20.29	0.85	1.52	16	1
1	A	50	GLN	CG-CD	-19.99	1.02	1.52	16	1
1	A	21	LYS	CE-NZ	-19.74	0.90	1.49	16	1
1	A	21	LYS	CD-CE	-19.57	0.93	1.52	16	1
1	A	13	ARG	CD-NE	-18.76	1.20	1.46	16	1
1	A	58	LYS	CE-NZ	-18.51	0.93	1.49	16	1
1	A	58	LYS	CD-CE	-18.12	0.98	1.52	16	1
1	A	39	GLU	CD-OE1	-17.77	0.91	1.25	16	1
1	A	62	LYS	CE-NZ	-17.61	0.96	1.49	16	1
1	A	50	GLN	CD-NE2	-17.23	0.97	1.33	16	1
1	A	83	LEU	CG-CD2	-16.98	0.96	1.52	16	1
1	A	18	LYS	CE-NZ	-16.31	1.00	1.49	16	1
1	A	18	LYS	CD-CE	-15.33	1.06	1.52	16	1
1	A	78	GLU	CG-CD	-14.30	1.16	1.52	16	1
1	A	81	LYS	CE-NZ	-14.17	1.06	1.49	16	1
1	A	20	ILE	C-O	-13.15	1.10	1.24	16	1
1	A	49	GLN	CG-CD	-12.32	1.21	1.52	16	1
1	A	37	ILE	CG1-CD1	-11.41	1.07	1.51	16	1
1	A	52	ARG	NE-CZ	-10.24	1.21	1.33	16	1
1	A	42	LYS	CE-NZ	-10.22	1.18	1.49	16	1
1	A	30	ILE	CG1-CD1	-10.04	1.12	1.51	16	1
1	A	12	HIS	ND1-CE1	-9.94	1.22	1.32	16	1
1	A	64	ASP	CB-CG	-9.64	1.27	1.52	16	1
1	A	56	LEU	CG-CD2	-8.94	1.23	1.52	16	1
1	A	56	LEU	CG-CD1	-8.72	1.23	1.52	16	1
1	A	49	GLN	CB-CG	-8.44	1.27	1.52	16	1
1	A	57	ILE	CG1-CD1	-8.19	1.19	1.51	16	1
1	A	63	LYS	CD-CE	-7.97	1.28	1.52	16	1
1	A	20	ILE	C-N	-7.73	1.22	1.33	16	1
1	A	21	LYS	CG-CD	-7.61	1.29	1.52	16	1
1	A	88	HIS	CD2-NE2	-7.54	1.29	1.37	16	1
1	A	58	LYS	CG-CD	-7.21	1.30	1.52	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	53	ALA	C-N	-7.13	1.24	1.33	16	1
1	A	42	LYS	CD-CE	-7.00	1.31	1.52	16	1
1	A	91	ILE	CG1-CD1	-6.94	1.24	1.51	16	1
1	A	53	ALA	C-O	-6.90	1.15	1.24	16	1
1	A	20	ILE	CG1-CD1	-6.70	1.25	1.51	16	1
1	A	28	HIS	CD2-NE2	-6.48	1.30	1.37	16	1
1	A	77	HIS	CD2-NE2	-6.19	1.31	1.37	16	1
1	A	29	MET	CB-CG	-5.51	1.35	1.52	16	1
1	A	92	PRO	C-N	-5.47	1.26	1.33	16	1
1	A	45	ASN	CB-CG	-5.36	1.38	1.52	16	1
1	A	11	GLN	C-O	-5.03	1.17	1.24	16	1
1	A	20	ILE	CA-CB	-5.00	1.48	1.54	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(°)	Ideal(°)	Models	
								Worst	Total
1	A	28	HIS	ND1-CG-CD2	-78.61	27.49	106.10	16	1
1	A	88	HIS	ND1-CG-CD2	-74.27	31.83	106.10	16	1
1	A	7	ASN	OD1-CG-ND2	-71.84	50.76	122.60	16	1
1	A	51	GLN	OE1-CD-NE2	-71.06	51.55	122.60	16	1
1	A	71	PHE	CD1-CG-CD2	-70.83	12.36	118.60	16	1
1	A	80	TYR	CD1-CG-CD2	-70.69	12.06	118.10	16	1
1	A	68	TYR	CD1-CG-CD2	-70.48	12.39	118.10	16	1
1	A	24	TYR	CD1-CG-CD2	-70.02	13.07	118.10	16	1
1	A	77	HIS	ND1-CG-CD2	-66.77	39.33	106.10	16	1
1	A	49	GLN	OE1-CD-NE2	-61.50	61.10	122.60	16	1
1	A	34	PHE	CD1-CG-CD2	-61.36	26.55	118.60	16	1
1	A	71	PHE	CE1-CZ-CE2	-59.81	12.34	120.00	16	1
1	A	28	HIS	CG-CD2-NE2	56.58	163.78	107.20	16	1
1	A	88	HIS	CG-CD2-NE2	54.49	161.69	107.20	16	1
1	A	80	TYR	CE1-CZ-CE2	-54.10	12.10	120.30	16	1
1	A	68	TYR	CE1-CZ-CE2	-53.94	12.43	120.30	16	1
1	A	11	GLN	OE1-CD-NE2	-53.71	68.89	122.60	16	1
1	A	24	TYR	CE1-CZ-CE2	-53.66	12.97	120.30	16	1
1	A	72	TYR	CD1-CG-CD2	-53.26	38.21	118.10	16	1
1	A	34	PHE	CE1-CZ-CE2	-51.81	26.73	120.00	16	1
1	A	77	HIS	CG-CD2-NE2	49.13	156.34	107.20	16	1
1	A	13	ARG	NE-CZ-NH1	-48.62	72.88	121.50	16	1
1	A	73	ASN	OD1-CG-ND2	-48.03	74.57	122.60	16	1
1	A	64	ASP	OD1-CG-OD2	-46.65	10.94	122.90	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	6	ARG	NH1-CZ-NH2	-46.07	59.41	119.30	16	1
1	A	6	ARG	NE-CZ-NH2	44.08	158.87	119.20	16	1
1	A	13	ARG	NE-CZ-NH2	43.40	158.26	119.20	16	1
1	A	88	HIS	CE1-NE2-CD2	-43.27	65.73	109.00	16	1
1	A	45	ASN	OD1-CG-ND2	-42.73	79.87	122.60	16	1
1	A	28	HIS	CE1-NE2-CD2	-42.55	66.45	109.00	16	1
1	A	72	TYR	CE1-CZ-CE2	-41.05	38.20	120.30	16	1
1	A	65	ASN	OD1-CG-ND2	-40.70	81.90	122.60	16	1
1	A	52	ARG	NH1-CZ-NH2	-39.98	67.33	119.30	16	1
1	A	14	GLU	OE1-CD-OE2	-38.53	30.41	122.90	16	1
1	A	17	GLU	OE1-CD-OE2	-37.22	33.58	122.90	16	1
1	A	68	TYR	CB-CG-CD1	35.46	173.99	120.80	16	1
1	A	80	TYR	CB-CG-CD2	35.45	173.97	120.80	16	1
1	A	80	TYR	CB-CG-CD1	35.45	173.97	120.80	16	1
1	A	24	TYR	CB-CG-CD1	35.40	173.90	120.80	16	1
1	A	66	ASP	OD1-CG-OD2	-35.30	38.19	122.90	16	1
1	A	80	TYR	CG-CD1-CE1	35.23	174.04	121.20	16	1
1	A	68	TYR	CB-CG-CD2	35.21	173.62	120.80	16	1
1	A	80	TYR	CG-CD2-CE2	35.16	173.94	121.20	16	1
1	A	68	TYR	CG-CD2-CE2	35.14	173.91	121.20	16	1
1	A	41	GLU	OE1-CD-OE2	-35.03	38.84	122.90	16	1
1	A	68	TYR	CG-CD1-CE1	35.00	173.70	121.20	16	1
1	A	24	TYR	CG-CD2-CE2	34.85	173.48	121.20	16	1
1	A	24	TYR	CB-CG-CD2	34.81	173.01	120.80	16	1
1	A	24	TYR	CG-CD1-CE1	34.81	173.41	121.20	16	1
1	A	82	ASP	OD1-CG-OD2	-33.89	41.56	122.90	16	1
1	A	40	GLU	OE1-CD-OE2	-32.25	45.50	122.90	16	1
1	A	71	PHE	CG-CD1-CE1	31.43	174.14	120.70	16	1
1	A	71	PHE	CB-CG-CD1	31.34	173.97	120.70	16	1
1	A	71	PHE	CB-CG-CD2	31.16	173.67	120.70	16	1
1	A	71	PHE	CG-CD2-CE2	31.05	173.49	120.70	16	1
1	A	28	HIS	CG-ND1-CE1	30.80	161.67	109.30	16	1
1	A	29	MET	CG-SD-CE	-30.62	33.54	100.90	16	1
1	A	80	TYR	CZ-CE2-CD2	30.22	174.00	119.60	16	1
1	A	80	TYR	CD1-CE1-CZ	30.15	173.86	119.60	16	1
1	A	68	TYR	CZ-CE2-CD2	30.11	173.79	119.60	16	1
1	A	68	TYR	CD1-CE1-CZ	30.10	173.78	119.60	16	1
1	A	35	LEU	CD1-CG-CD2	-30.08	44.62	110.80	16	1
1	A	77	HIS	CE1-NE2-CD2	-30.03	78.97	109.00	16	1
1	A	71	PHE	CZ-CE2-CD2	30.03	174.05	120.00	16	1
1	A	24	TYR	CD1-CE1-CZ	29.97	173.54	119.60	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	24	TYR	CZ-CE2-CD2	29.95	173.52	119.60	16	1
1	A	71	PHE	CD1-CE1-CZ	29.80	173.63	120.00	16	1
1	A	88	HIS	CG-ND1-CE1	28.87	158.37	109.30	16	1
1	A	52	ARG	NE-CZ-NH2	28.35	144.72	119.20	16	1
1	A	28	HIS	CB-CG-CD2	28.35	168.06	131.20	16	1
1	A	28	HIS	CB-CG-ND1	27.84	164.45	122.70	16	1
1	A	12	HIS	ND1-CG-CD2	-27.60	78.50	106.10	16	1
1	A	34	PHE	CB-CG-CD1	27.39	167.26	120.70	16	1
1	A	88	HIS	CB-CG-CD2	27.23	166.60	131.20	16	1
1	A	34	PHE	CG-CD2-CE2	27.11	166.78	120.70	16	1
1	A	34	PHE	CG-CD1-CE1	27.04	166.67	120.70	16	1
1	A	34	PHE	CB-CG-CD2	26.76	166.19	120.70	16	1
1	A	72	TYR	CB-CG-CD2	26.74	160.91	120.80	16	1
1	A	72	TYR	CB-CG-CD1	26.72	160.89	120.80	16	1
1	A	72	TYR	CG-CD2-CE2	26.51	160.97	121.20	16	1
1	A	52	ARG	NE-CZ-NH1	26.45	147.95	121.50	16	1
1	A	72	TYR	CG-CD1-CE1	26.42	160.83	121.20	16	1
1	A	77	HIS	CG-ND1-CE1	26.34	154.07	109.30	16	1
1	A	51	GLN	CG-CD-NE2	26.23	155.74	116.40	16	1
1	A	34	PHE	CZ-CE2-CD2	25.95	166.70	120.00	16	1
1	A	88	HIS	CB-CG-ND1	25.92	161.57	122.70	16	1
1	A	7	ASN	CB-CG-ND2	25.88	155.22	116.40	16	1
1	A	34	PHE	CD1-CE1-CZ	25.86	166.56	120.00	16	1
1	A	46	GLU	CB-CG-CD	25.31	155.63	112.60	16	1
1	A	64	ASP	CB-CG-OD2	25.20	176.35	118.40	16	1
1	A	6	ARG	CD-NE-CZ	25.02	159.43	124.40	16	1
1	A	13	ARG	CD-NE-CZ	24.49	158.69	124.40	16	1
1	A	77	HIS	CB-CG-CD2	24.09	162.51	131.20	16	1
1	A	63	LYS	CG-CD-CE	24.01	166.53	111.30	16	1
1	A	77	HIS	CB-CG-ND1	23.63	158.15	122.70	16	1
1	A	64	ASP	CB-CG-OD1	23.61	172.71	118.40	16	1
1	A	27	ASP	OD1-CG-OD2	-23.59	66.27	122.90	16	1
1	A	40	GLU	CG-CD-OE2	23.57	172.61	118.40	16	1
1	A	89	ASP	OD1-CG-OD2	-23.53	66.42	122.90	16	1
1	A	72	TYR	CD1-CE1-CZ	22.98	160.96	119.60	16	1
1	A	72	TYR	CZ-CE2-CD2	22.91	160.83	119.60	16	1
1	A	63	LYS	CB-CG-CD	22.79	163.72	111.30	16	1
1	A	44	ARG	NE-CZ-NH2	22.25	139.22	119.20	16	1
1	A	50	GLN	CG-CD-NE2	22.18	149.68	116.40	16	1
1	A	44	ARG	NH1-CZ-NH2	-21.60	91.22	119.30	16	1
1	A	19	ASP	OD1-CG-OD2	-21.27	71.86	122.90	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	14	GLU	CG-CD-OE2	20.43	165.38	118.40	16	1
1	A	6	ARG	NE-CZ-NH1	20.23	141.72	121.50	16	1
1	A	49	GLN	CG-CD-NE2	20.18	146.67	116.40	16	1
1	A	50	GLN	CB-CG-CD	19.93	146.49	112.60	16	1
1	A	14	GLU	CG-CD-OE1	19.92	164.21	118.40	16	1
1	A	17	GLU	CG-CD-OE2	19.90	164.17	118.40	16	1
1	A	41	GLU	CG-CD-OE1	19.71	163.73	118.40	16	1
1	A	45	ASN	CB-CG-ND2	19.16	145.14	116.40	16	1
1	A	26	MET	CG-SD-CE	19.15	143.03	100.90	16	1
1	A	17	GLU	CG-CD-OE1	19.07	162.25	118.40	16	1
1	A	12	HIS	CG-CD2-NE2	18.89	126.09	107.20	16	1
1	A	66	ASP	CB-CG-OD1	18.81	161.67	118.40	16	1
1	A	59	MET	CG-SD-CE	18.80	142.25	100.90	16	1
1	A	4	LYS	CD-CE-NZ	18.51	171.14	111.90	16	1
1	A	66	ASP	CB-CG-OD2	18.15	160.14	118.40	16	1
1	A	80	TYR	OH-CZ-CE2	18.05	174.04	119.90	16	1
1	A	80	TYR	CE1-CZ-OH	17.99	173.86	119.90	16	1
1	A	68	TYR	OH-CZ-CE2	17.98	173.83	119.90	16	1
1	A	68	TYR	CE1-CZ-OH	17.95	173.74	119.90	16	1
1	A	82	ASP	CB-CG-OD2	17.90	159.57	118.40	16	1
1	A	24	TYR	OH-CZ-CE2	17.88	173.54	119.90	16	1
1	A	24	TYR	CE1-CZ-OH	17.86	173.48	119.90	16	1
1	A	32	ASP	OD1-CG-OD2	-17.83	80.12	122.90	16	1
1	A	16	LEU	CD1-CG-CD2	-17.80	71.63	110.80	16	1
1	A	82	ASP	CB-CG-OD1	17.60	158.87	118.40	16	1
1	A	11	GLN	CG-CD-NE2	17.36	142.44	116.40	16	1
1	A	73	ASN	CB-CG-ND2	17.24	142.26	116.40	16	1
1	A	41	GLU	CG-CD-OE2	16.97	157.44	118.40	16	1
1	A	4	LYS	CG-CD-CE	16.63	149.54	111.30	16	1
1	A	7	ASN	CB-CG-OD1	16.61	154.02	120.80	16	1
1	A	51	GLN	CG-CD-OE1	15.96	152.71	120.80	16	1
1	A	58	LYS	CG-CD-CE	15.89	147.84	111.30	16	1
1	A	49	GLN	CG-CD-OE1	15.71	152.23	120.80	16	1
1	A	52	ARG	CD-NE-CZ	15.35	145.90	124.40	16	1
1	A	65	ASN	CB-CG-ND2	15.03	138.95	116.40	16	1
1	A	35	LEU	CB-CG-CD2	14.72	154.87	110.70	16	1
1	A	35	LEU	CB-CG-CD1	14.04	152.82	110.70	16	1
1	A	88	HIS	ND1-CE1-NE2	13.97	122.37	108.40	16	1
1	A	11	GLN	CG-CD-OE1	13.94	148.67	120.80	16	1
1	A	72	TYR	CE1-CZ-OH	13.69	160.97	119.90	16	1
1	A	72	TYR	OH-CZ-CE2	13.64	160.82	119.90	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	12	HIS	CG-ND1-CE1	13.49	132.24	109.30	16	1
1	A	50	GLN	CG-CD-OE1	-13.04	94.72	120.80	16	1
1	A	52	ARG	CG-CD-NE	13.02	140.65	112.00	16	1
1	A	27	ASP	CB-CG-OD2	12.84	147.94	118.40	16	1
1	A	12	HIS	CB-CG-ND1	12.82	141.93	122.70	16	1
1	A	12	HIS	ND1-CE1-NE2	-12.59	95.81	108.40	16	1
1	A	89	ASP	CB-CG-OD2	12.56	147.29	118.40	16	1
1	A	28	HIS	ND1-CE1-NE2	12.21	120.61	108.40	16	1
1	A	89	ASP	CB-CG-OD1	12.12	146.28	118.40	16	1
1	A	19	ASP	CB-CG-OD2	12.02	146.03	118.40	16	1
1	A	27	ASP	CB-CG-OD1	11.91	145.79	118.40	16	1
1	A	46	GLU	CG-CD-OE2	11.72	145.37	118.40	16	1
1	A	81	LYS	CG-CD-CE	11.43	137.58	111.30	16	1
1	A	83	LEU	CD1-CG-CD2	-11.34	85.85	110.80	16	1
1	A	44	ARG	CD-NE-CZ	11.22	140.11	124.40	16	1
1	A	73	ASN	CB-CG-OD1	11.19	143.17	120.80	16	1
1	A	62	LYS	CG-CD-CE	11.00	136.59	111.30	16	1
1	A	63	LYS	CD-CE-NZ	10.98	147.04	111.90	16	1
1	A	62	LYS	CD-CE-NZ	10.60	145.83	111.90	16	1
1	A	86	LEU	CD1-CG-CD2	-10.51	87.67	110.80	16	1
1	A	46	GLU	OE1-CD-OE2	-10.50	97.70	122.90	16	1
1	A	50	GLN	CA-CB-CG	10.50	135.09	114.10	16	1
1	A	55	MET	CG-SD-CE	10.45	123.90	100.90	16	1
1	A	19	ASP	CB-CG-OD1	10.30	142.10	118.40	16	1
1	A	32	ASP	CB-CG-OD1	10.23	141.93	118.40	16	1
1	A	40	GLU	CG-CD-OE1	10.21	141.89	118.40	16	1
1	A	39	GLU	OE1-CD-OE2	-9.93	99.08	122.90	16	1
1	A	16	LEU	CB-CG-CD1	9.65	139.64	110.70	16	1
1	A	21	LYS	CG-CD-CE	9.23	132.53	111.30	16	1
1	A	65	ASN	CB-CG-OD1	9.18	139.16	120.80	16	1
1	A	58	LYS	CD-CE-NZ	8.61	139.47	111.90	16	1
1	A	32	ASP	CB-CG-OD2	8.50	137.96	118.40	16	1
1	A	23	SER	CA-CB-OG	8.33	127.76	111.10	16	1
1	A	16	LEU	CB-CG-CD2	8.11	135.03	110.70	16	1
1	A	83	LEU	CB-CG-CD2	8.07	134.90	110.70	16	1
1	A	59	MET	CB-CG-SD	8.06	136.89	112.70	16	1
1	A	44	ARG	NE-CZ-NH1	8.06	129.56	121.50	16	1
1	A	81	LYS	CD-CE-NZ	8.02	137.56	111.90	16	1
1	A	40	GLU	CB-CG-CD	7.75	125.77	112.60	16	1
1	A	13	ARG	NH1-CZ-NH2	7.36	128.86	119.30	16	1
1	A	39	GLU	CG-CD-OE1	7.21	134.97	118.40	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	45	ASN	CB-CG-OD1	7.10	135.00	120.80	16	1
1	A	50	GLN	OE1-CD-NE2	-7.00	115.60	122.60	16	1
1	A	91	ILE	N-CA-CB	-6.85	105.11	110.45	14	7
1	A	26	MET	CB-CG-SD	6.46	132.07	112.70	16	1
1	A	12	HIS	CB-CG-CD2	6.44	139.58	131.20	16	1
1	A	20	ILE	N-CA-CB	-6.32	104.87	112.07	10	8
1	A	6	ARG	CG-CD-NE	6.30	125.86	112.00	16	1
1	A	78	GLU	OE1-CD-OE2	-6.30	107.79	122.90	16	1
1	A	86	LEU	CB-CG-CD1	6.08	128.95	110.70	16	1
1	A	20	ILE	O-C-N	-5.93	116.77	123.18	16	1
1	A	12	HIS	CA-CB-CG	-5.92	107.88	113.80	16	1
1	A	57	ILE	CB-CG1-CD1	5.63	125.63	113.80	16	1
1	A	12	HIS	N-CA-CB	-5.61	105.06	111.79	6	1
1	A	25	ILE	N-CA-CB	-5.13	105.24	110.62	5	2
1	A	60	ILE	N-CA-CB	-5.08	105.08	110.62	3	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	726	730	724	58±93
All	All	11616	11680	11674	935

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 40.

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:CG	1:A:63:LYS:CE	1.53	1.83	16	1
1:A:49:GLN:NE2	1:A:49:GLN:CG	1.51	1.70	16	1
1:A:62:LYS:CD	1:A:62:LYS:NZ	1.47	1.76	16	1
1:A:78:GLU:OE1	1:A:78:GLU:CG	1.45	1.65	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ARG:CD	1:A:52:ARG:CZ	1.45	1.95	16	1
1:A:88:HIS:CG	1:A:88:HIS:CE1	1.43	2.04	16	1
1:A:71:PHE:CZ	1:A:71:PHE:CD1	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:CG	1:A:28:HIS:CE1	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:CZ	1:A:68:TYR:CD2	1.40	2.10	16	1
1:A:55:MET:CE	1:A:55:MET:CG	1.39	2.00	16	1
1:A:24:TYR:CZ	1:A:24:TYR:CD2	1.39	2.10	16	1
1:A:68:TYR:CG	1:A:68:TYR:CE1	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:CZ	1:A:34:PHE:CD1	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:29:MET:HE3	1:A:29:MET:CB	1.38	1.47	16	1
1:A:34:PHE:CZ	1:A:34:PHE:CD2	1.38	2.09	16	1
1:A:34:PHE:CG	1:A:34:PHE:CE2	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:CG	1:A:72:TYR:CE2	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:CG	1:A:72:TYR:CE1	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:CZ	1:A:24:TYR:CD1	1.36	2.10	16	1
1:A:63:LYS:NZ	1:A:63:LYS:CD	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:CZ	1:A:68:TYR:CD1	1.34	2.10	16	1
1:A:71:PHE:CZ	1:A:71:PHE:CD2	1.33	2.12	16	1
1:A:29:MET:CB	1:A:29:MET:SD	1.32	2.15	16	1
1:A:46:GLU:CD	1:A:46:GLU:CB	1.32	2.01	16	1
1:A:63:LYS:CD	1:A:63:LYS:CB	1.31	2.07	16	1
1:A:16:LEU:CD2	1:A:16:LEU:CB	1.31	2.08	16	1
1:A:71:PHE:CG	1:A:71:PHE:CE1	1.31	2.12	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:CE	1:A:59:MET:CG	1.30	2.09	16	1
1:A:35:LEU:CD1	1:A:35:LEU:CB	1.29	2.08	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:LYS:CE	1:A:62:LYS:CG	1.29	2.11	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:81:LYS:CE	1:A:81:LYS:CG	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:NH2	1:A:52:ARG:NE	1.26	1.83	16	1
1:A:35:LEU:CB	1:A:35:LEU:CD2	1.25	2.14	16	1
1:A:4:LYS:CE	1:A:4:LYS:CG	1.25	2.13	16	1
1:A:80:TYR:CD2	1:A:80:TYR:CB	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:CD1	1:A:68:TYR:CB	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:CB	1:A:86:LEU:CD1	1.21	2.16	16	1
1:A:40:GLU:CD	1:A:40:GLU:CB	1.21	2.12	16	1
1:A:34:PHE:CD2	1:A:34:PHE:CB	1.21	2.20	16	1
1:A:72:TYR:CD1	1:A:72:TYR:CB	1.20	2.22	16	1
1:A:45:ASN:OD1	1:A:45:ASN:CB	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:CD2	1:A:72:TYR:CB	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:OD2	1:A:64:ASP:CB	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:80:TYR:CD1	1:A:80:TYR:CB	1.16	2.21	16	1
1:A:52:ARG:NE	1:A:52:ARG:NH1	1.15	1.90	16	1
1:A:59:MET:SD	1:A:59:MET:CB	1.14	2.36	16	1
1:A:41:GLU:OE2	1:A:41:GLU:CG	1.13	1.96	16	1
1:A:23:SER:OG	1:A:23:SER:HB3	1.12	1.39	16	1
1:A:46:GLU:OE1	1:A:46:GLU:CG	1.12	0.83	16	1
1:A:55:MET:CE	1:A:55:MET:SD	1.12	1.02	16	1
1:A:59:MET:SD	1:A:59:MET:HE2	1.11	1.78	16	1
1:A:32:ASP:OD2	1:A:32:ASP:CB	1.10	2.00	16	1
1:A:59:MET:SD	1:A:59:MET:CG	1.09	1.00	16	1
1:A:59:MET:SD	1:A:59:MET:HE3	1.08	1.78	16	1
1:A:59:MET:SD	1:A:59:MET:HE1	1.08	1.78	16	1
1:A:26:MET:SD	1:A:26:MET:HE2	1.08	1.77	16	1
1:A:26:MET:SD	1:A:26:MET:CB	1.08	2.42	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:TYR:CE1	1:A:80:TYR:OH	1.08	2.07	16	1
1:A:45:ASN:CB	1:A:45:ASN:ND2	1.07	2.14	16	1
1:A:23:SER:OG	1:A:23:SER:CB	1.07	0.78	16	1
1:A:29:MET:SD	1:A:29:MET:HG2	1.07	1.71	16	1
1:A:77:HIS:CD2	1:A:77:HIS:CB	1.07	2.38	16	1
1:A:16:LEU:CD1	1:A:16:LEU:HG	1.06	1.60	16	1
1:A:68:TYR:CE2	1:A:68:TYR:OH	1.06	2.07	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:26:MET:SD	1:A:26:MET:HE3	1.06	1.77	16	1
1:A:24:TYR:CE2	1:A:24:TYR:OH	1.06	2.08	16	1
1:A:16:LEU:CD2	1:A:16:LEU:HD12	1.05	1.80	16	1
1:A:23:SER:OG	1:A:23:SER:HB2	1.05	1.39	16	1
1:A:28:HIS:CD2	1:A:28:HIS:CB	1.05	2.39	16	1
1:A:27:ASP:OD1	1:A:27:ASP:CB	1.04	2.04	16	1
1:A:68:TYR:CE1	1:A:68:TYR:OH	1.04	2.08	16	1
1:A:16:LEU:CD1	1:A:16:LEU:HD23	1.04	1.81	16	1
1:A:51:GLN:OE1	1:A:51:GLN:CG	1.04	2.06	16	1
1:A:7:ASN:ND2	1:A:7:ASN:CB	1.04	2.21	16	1
1:A:46:GLU:OE1	1:A:46:GLU:HG2	1.04	1.51	16	1
1:A:14:GLU:OE1	1:A:14:GLU:CG	1.04	2.04	16	1
1:A:51:GLN:CG	1:A:51:GLN:NE2	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:CE1	1:A:24:TYR:OH	1.03	2.08	16	1
1:A:26:MET:SD	1:A:26:MET:HE1	1.03	1.77	16	1
1:A:80:TYR:CE2	1:A:80:TYR:OH	1.03	2.08	16	1
1:A:29:MET:CG	1:A:29:MET:HE1	1.03	1.58	16	1
1:A:26:MET:SD	1:A:26:MET:HG2	1.02	1.66	16	1
1:A:72:TYR:CE2	1:A:72:TYR:OH	1.02	2.09	16	1
1:A:27:ASP:CB	1:A:27:ASP:OD2	1.01	2.08	16	1
1:A:19:ASP:OD1	1:A:19:ASP:CB	1.01	2.06	16	1
1:A:26:MET:SD	1:A:26:MET:HG3	1.01	1.66	16	1
1:A:73:ASN:ND2	1:A:73:ASN:CB	1.01	2.21	16	1
1:A:17:GLU:CG	1:A:17:GLU:OE2	1.01	2.08	16	1
1:A:52:ARG:NE	1:A:52:ARG:HD3	1.01	1.39	16	1
1:A:16:LEU:CD2	1:A:16:LEU:HG	1.00	1.58	16	1
1:A:82:ASP:OD1	1:A:82:ASP:CB	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:OD2	1:A:66:ASP:CB	1.00	2.08	16	1
1:A:72:TYR:CE1	1:A:72:TYR:OH	1.00	2.09	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:GLU:CG	1:A:14:GLU:OE2	1.00	2.09	16	1
1:A:32:ASP:CB	1:A:32:ASP:OD1	1.00	2.07	16	1
1:A:46:GLU:OE1	1:A:46:GLU:HG3	1.00	1.24	16	1
1:A:55:MET:SD	1:A:55:MET:HE2	1.00	1.63	16	1
1:A:23:SER:OG	1:A:23:SER:CA	0.99	2.10	16	1
1:A:52:ARG:NE	1:A:52:ARG:HD2	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:OD1	1:A:89:ASP:CB	0.98	2.11	16	1
1:A:88:HIS:CB	1:A:88:HIS:ND1	0.98	2.25	16	1
1:A:55:MET:SD	1:A:55:MET:HE1	0.98	1.63	16	1
1:A:89:ASP:CB	1:A:89:ASP:OD2	0.97	2.12	16	1
1:A:40:GLU:CD	1:A:40:GLU:HG3	0.96	1.45	16	1
1:A:40:GLU:CD	1:A:40:GLU:HG2	0.96	1.45	16	1
1:A:52:ARG:CD	1:A:52:ARG:NE	0.96	0.82	16	1
1:A:55:MET:SD	1:A:55:MET:HE3	0.96	1.63	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:CB	1:A:19:ASP:OD2	0.95	2.14	16	1
1:A:86:LEU:CG	1:A:86:LEU:HD11	0.95	1.49	16	1
1:A:46:GLU:CB	1:A:46:GLU:OE1	0.94	2.12	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:41:GLU:OE1	1:A:41:GLU:CD	0.93	0.68	16	1
1:A:73:ASN:CB	1:A:73:ASN:OD1	0.92	2.17	16	1
1:A:77:HIS:CG	1:A:77:HIS:NE2	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:CE	1:A:29:MET:CG	0.90	0.91	16	1
1:A:86:LEU:CG	1:A:86:LEU:HD21	0.90	1.46	16	1
1:A:16:LEU:CG	1:A:16:LEU:HD11	0.90	1.44	16	1
1:A:62:LYS:CE	1:A:62:LYS:HD3	0.90	1.44	16	1
1:A:7:ASN:OD1	1:A:7:ASN:CG	0.90	0.65	16	1
1:A:59:MET:SD	1:A:59:MET:HG3	0.90	1.54	16	1
1:A:40:GLU:CD	1:A:40:GLU:CG	0.90	0.85	16	1
1:A:88:HIS:CG	1:A:88:HIS:CD2	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:HD11	1:A:35:LEU:HD23	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:HIS:CG	1:A:28:HIS:CD2	0.88	0.91	16	1
1:A:63:LYS:NZ	1:A:63:LYS:HE3	0.88	1.27	16	1
1:A:62:LYS:CE	1:A:62:LYS:HD2	0.88	1.44	16	1
1:A:86:LEU:CD2	1:A:86:LEU:HG	0.88	1.58	16	1
1:A:29:MET:CE	1:A:29:MET:HG3	0.88	1.43	16	1
1:A:16:LEU:CD2	1:A:16:LEU:CD1	0.88	0.88	16	1
1:A:63:LYS:NZ	1:A:63:LYS:HE2	0.88	1.27	16	1
1:A:62:LYS:CD	1:A:62:LYS:CE	0.88	0.88	16	1
1:A:66:ASP:OD1	1:A:66:ASP:CG	0.87	0.63	16	1
1:A:62:LYS:CD	1:A:62:LYS:HE3	0.87	1.42	16	1
1:A:86:LEU:CD1	1:A:86:LEU:HG	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:HD12	1:A:16:LEU:CG	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:51:GLN:OE1	1:A:51:GLN:CD	0.86	0.62	16	1
1:A:28:HIS:CG	1:A:28:HIS:ND1	0.86	0.80	16	1
1:A:82:ASP:OD2	1:A:82:ASP:CG	0.86	0.61	16	1
1:A:62:LYS:CD	1:A:62:LYS:HE2	0.86	1.42	16	1
1:A:17:GLU:OE2	1:A:17:GLU:CD	0.85	0.61	16	1
1:A:77:HIS:CG	1:A:77:HIS:ND1	0.85	0.84	16	1
1:A:9:LEU:HD23	1:A:68:TYR:CE1	0.85	2.06	15	11
1:A:86:LEU:CD1	1:A:86:LEU:CG	0.85	0.85	16	1
1:A:16:LEU:HD23	1:A:16:LEU:CG	0.85	1.39	16	1
1:A:65:ASN:ND2	1:A:65:ASN:CG	0.85	0.87	16	1
1:A:71:PHE:CD1	1:A:71:PHE:CB	0.85	2.24	16	1
1:A:65:ASN:OD1	1:A:65:ASN:CG	0.84	0.80	16	1
1:A:88:HIS:CG	1:A:88:HIS:ND1	0.84	0.78	16	1
1:A:65:ASN:CG	1:A:65:ASN:HD21	0.84	1.49	16	1
1:A:51:GLN:NE2	1:A:51:GLN:CD	0.84	0.75	16	1
1:A:82:ASP:OD1	1:A:82:ASP:CG	0.84	0.60	16	1
1:A:14:GLU:OE2	1:A:14:GLU:CD	0.84	0.61	16	1
1:A:16:LEU:CG	1:A:16:LEU:HD22	0.83	1.39	16	1
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:7:ASN:ND2	1:A:7:ASN:CG	0.82	0.74	16	1
1:A:45:ASN:CG	1:A:45:ASN:HD22	0.82	1.48	16	1
1:A:16:LEU:CD1	1:A:16:LEU:HD22	0.82	1.37	16	1
1:A:11:GLN:CG	1:A:11:GLN:OE1	0.82	2.13	16	1
1:A:66:ASP:OD2	1:A:66:ASP:CG	0.82	0.58	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:CD2	1:A:16:LEU:HD13	0.82	1.36	16	1
1:A:29:MET:CG	1:A:29:MET:HE2	0.82	0.88	16	1
1:A:49:GLN:OE1	1:A:49:GLN:CD	0.82	0.60	16	1
1:A:34:PHE:CE2	1:A:34:PHE:HZ	0.81	1.64	16	1
1:A:71:PHE:CE1	1:A:71:PHE:HZ	0.81	1.60	16	1
1:A:16:LEU:CG	1:A:16:LEU:HD21	0.81	1.39	16	1
1:A:35:LEU:CG	1:A:35:LEU:HD21	0.81	1.35	16	1
1:A:86:LEU:CD2	1:A:86:LEU:CG	0.80	0.81	16	1
1:A:19:ASP:OD2	1:A:19:ASP:CG	0.80	0.73	16	1
1:A:35:LEU:CG	1:A:35:LEU:HD22	0.80	1.35	16	1
1:A:35:LEU:HD23	1:A:35:LEU:CG	0.80	1.35	16	1
1:A:65:ASN:CG	1:A:65:ASN:HD22	0.80	1.49	16	1
1:A:81:LYS:CE	1:A:81:LYS:HD2	0.80	1.34	16	1
1:A:16:LEU:HD21	1:A:26:MET:CE	0.79	2.07	11	1
1:A:89:ASP:OD1	1:A:89:ASP:CG	0.79	0.67	16	1
1:A:45:ASN:CG	1:A:45:ASN:HD21	0.79	1.48	16	1
1:A:29:MET:HE3	1:A:29:MET:CG	0.79	0.88	16	1
1:A:43:VAL:HG11	1:A:56:LEU:HD13	0.79	1.54	14	3
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:81:LYS:CE	1:A:81:LYS:HD3	0.78	1.34	16	1
1:A:16:LEU:CD1	1:A:16:LEU:CG	0.78	0.78	16	1
1:A:73:ASN:OD1	1:A:73:ASN:CG	0.78	0.76	16	1
1:A:63:LYS:CE	1:A:63:LYS:NZ	0.78	0.66	16	1
1:A:14:GLU:OE1	1:A:14:GLU:CD	0.78	0.56	16	1
1:A:64:ASP:OD2	1:A:64:ASP:CG	0.78	0.64	16	1
1:A:89:ASP:OD2	1:A:89:ASP:CG	0.77	0.69	16	1
1:A:17:GLU:OE1	1:A:17:GLU:CD	0.77	0.55	16	1
1:A:19:ASP:OD1	1:A:19:ASP:CG	0.77	0.66	16	1
1:A:73:ASN:CG	1:A:73:ASN:HD22	0.77	1.45	16	1
1:A:72:TYR:CE1	1:A:84:ALA:HB1	0.77	2.15	2	4
1:A:73:ASN:CG	1:A:73:ASN:HD21	0.77	1.45	16	1
1:A:32:ASP:OD1	1:A:32:ASP:CG	0.77	0.73	16	1
1:A:73:ASN:ND2	1:A:73:ASN:CG	0.76	0.81	16	1
1:A:35:LEU:CG	1:A:35:LEU:HD13	0.76	1.30	16	1
1:A:29:MET:HE3	1:A:29:MET:HB2	0.76	1.55	16	1
1:A:35:LEU:HD12	1:A:35:LEU:CG	0.76	1.30	16	1
1:A:45:ASN:ND2	1:A:45:ASN:CG	0.75	0.85	16	1
1:A:20:ILE:HG21	1:A:26:MET:HE1	0.75	1.57	6	1
1:A:46:GLU:CD	1:A:46:GLU:HG3	0.75	1.24	16	1
1:A:35:LEU:HD11	1:A:35:LEU:CG	0.75	1.30	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:GLU:CD	1:A:46:GLU:HG2	0.75	1.24	16	1
1:A:4:LYS:CE	1:A:4:LYS:HD2	0.75	1.29	16	1
1:A:4:LYS:CE	1:A:4:LYS:HD3	0.74	1.29	16	1
1:A:34:PHE:CE1	1:A:34:PHE:HZ	0.74	1.63	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:16:LEU:CD1	1:A:16:LEU:HD21	0.73	0.97	16	1
1:A:81:LYS:CD	1:A:81:LYS:CE	0.73	0.74	16	1
1:A:49:GLN:OE1	1:A:49:GLN:CB	0.73	2.35	16	1
1:A:7:ASN:ND2	1:A:7:ASN:OD1	0.73	0.60	16	1
1:A:27:ASP:OD2	1:A:27:ASP:CG	0.73	0.68	16	1
1:A:32:ASP:OD2	1:A:32:ASP:CG	0.73	0.68	16	1
1:A:51:GLN:OE1	1:A:51:GLN:NE2	0.73	0.60	16	1
1:A:41:GLU:OE2	1:A:41:GLU:CD	0.72	0.50	16	1
1:A:51:GLN:CD	1:A:51:GLN:HE22	0.72	1.39	16	1
1:A:72:TYR:CZ	1:A:76:LEU:HD11	0.72	2.19	6	14
1:A:49:GLN:NE2	1:A:49:GLN:OE1	0.72	0.59	16	1
1:A:16:LEU:CD2	1:A:16:LEU:CG	0.72	0.72	16	1
1:A:51:GLN:CD	1:A:51:GLN:HE21	0.71	1.39	16	1
1:A:71:PHE:CE1	1:A:75:LEU:HD11	0.71	2.21	3	9
1:A:7:ASN:CG	1:A:7:ASN:HD22	0.70	1.38	16	1
1:A:20:ILE:HD13	1:A:25:ILE:HG13	0.70	1.60	11	6
1:A:7:ASN:CG	1:A:7:ASN:HD21	0.70	1.38	16	1
1:A:52:ARG:CZ	1:A:52:ARG:NH2	0.70	0.70	16	1
1:A:11:GLN:NE2	1:A:11:GLN:CD	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:CZ	1:A:52:ARG:HH11	0.69	1.40	16	1
1:A:11:GLN:CD	1:A:11:GLN:HE22	0.69	1.35	16	1
1:A:4:LYS:CE	1:A:4:LYS:CD	0.69	0.71	16	1
1:A:11:GLN:OE1	1:A:11:GLN:CD	0.69	0.75	16	1
1:A:26:MET:HE3	1:A:56:LEU:HD23	0.69	1.64	7	1
1:A:11:GLN:CD	1:A:11:GLN:HE21	0.68	1.35	16	1
1:A:52:ARG:CZ	1:A:52:ARG:HH12	0.68	1.40	16	1
1:A:55:MET:HG2	1:A:59:MET:HE1	0.68	1.62	9	1
1:A:26:MET:HE1	1:A:60:ILE:HD11	0.68	1.65	1	1
1:A:53:ALA:O	1:A:57:ILE:HD12	0.68	1.89	10	3
1:A:27:ASP:OD1	1:A:27:ASP:CG	0.68	0.64	16	1
1:A:77:HIS:CG	1:A:77:HIS:HD2	0.68	1.43	16	1
1:A:35:LEU:HD12	1:A:35:LEU:HD21	0.68	1.02	16	1
1:A:88:HIS:HA	1:A:91:ILE:HD12	0.68	1.66	3	8
1:A:29:MET:HG2	1:A:29:MET:HE2	0.68	0.69	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:TYR:CZ	1:A:72:TYR:CE1	0.68	0.74	16	1
1:A:39:GLU:OE1	1:A:59:MET:HE1	0.67	1.88	15	1
1:A:12:HIS:NE2	1:A:15:ALA:HB3	0.67	2.05	16	1
1:A:34:PHE:CZ	1:A:34:PHE:CE2	0.67	0.72	16	1
1:A:9:LEU:HD13	1:A:9:LEU:O	0.67	1.90	16	16
1:A:72:TYR:CG	1:A:72:TYR:CD2	0.67	0.74	16	1
1:A:46:GLU:CD	1:A:46:GLU:CG	0.67	0.66	16	1
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:CZ	1:A:34:PHE:CE1	0.66	0.71	16	1
1:A:72:TYR:CE2	1:A:72:TYR:CZ	0.66	0.74	16	1
1:A:71:PHE:CZ	1:A:71:PHE:CE1	0.66	0.68	16	1
1:A:88:HIS:CG	1:A:88:HIS:HD2	0.66	1.42	16	1
1:A:72:TYR:CG	1:A:72:TYR:CD1	0.66	0.74	16	1
1:A:34:PHE:C	1:A:35:LEU:HD22	0.66	2.16	11	6
1:A:29:MET:SD	1:A:29:MET:HB2	0.66	2.28	16	1
1:A:16:LEU:HD13	1:A:16:LEU:HD22	0.65	1.04	16	1
1:A:29:MET:HE3	1:A:29:MET:HG3	0.65	1.12	16	1
1:A:20:ILE:HD11	1:A:80:TYR:CE2	0.65	2.25	8	1
1:A:4:LYS:NZ	1:A:4:LYS:HE3	0.64	1.14	16	1
1:A:52:ARG:CD	1:A:52:ARG:HE	0.64	1.35	16	1
1:A:16:LEU:C	1:A:16:LEU:HD13	0.64	2.18	11	4
1:A:6:ARG:O	1:A:10:LEU:HD12	0.64	1.92	1	1
1:A:71:PHE:O	1:A:75:LEU:HD12	0.64	1.92	11	3
1:A:26:MET:HE3	1:A:57:ILE:HD12	0.64	1.68	12	1
1:A:52:ARG:CZ	1:A:52:ARG:HH21	0.64	1.36	16	1
1:A:16:LEU:HD11	1:A:26:MET:HE2	0.64	1.68	5	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:83:LEU:HD13	1:A:83:LEU:C	0.63	2.18	15	7
1:A:72:TYR:CE1	1:A:76:LEU:HD11	0.63	2.28	16	11
1:A:21:LYS:O	1:A:22:THR:C	0.63	2.42	15	16
1:A:4:LYS:CD	1:A:4:LYS:HE2	0.63	1.23	16	1
1:A:16:LEU:CD2	1:A:16:LEU:HD11	0.63	1.06	16	1
1:A:63:LYS:CD	1:A:63:LYS:HG3	0.63	1.16	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:45:ASN:OD1	1:A:45:ASN:CG	0.62	0.63	16	1
1:A:63:LYS:CG	1:A:63:LYS:HD2	0.62	1.15	16	1
1:A:24:TYR:CZ	1:A:24:TYR:CE1	0.62	0.71	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:71:PHE:CE2	1:A:75:LEU:HD11	0.62	2.29	5	3
1:A:20:ILE:HD12	1:A:25:ILE:HG13	0.62	1.71	10	2
1:A:39:GLU:O	1:A:43:VAL:HG23	0.62	1.94	5	1
1:A:12:HIS:HD2	1:A:12:HIS:O	0.62	1.77	16	1
1:A:34:PHE:C	1:A:35:LEU:HD12	0.62	2.19	12	1
1:A:83:LEU:O	1:A:83:LEU:HD23	0.62	1.94	5	2
1:A:26:MET:HB3	1:A:56:LEU:HD21	0.61	1.70	9	2
1:A:76:LEU:HD21	1:A:84:ALA:CB	0.61	2.23	5	2
1:A:49:GLN:NE2	1:A:49:GLN:CD	0.61	0.55	16	1
1:A:23:SER:CB	1:A:23:SER:HG	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:78:GLU:OE2	1:A:78:GLU:CD	0.60	0.77	16	1
1:A:86:LEU:O	1:A:86:LEU:HD13	0.60	1.97	11	1
1:A:68:TYR:CZ	1:A:68:TYR:CE2	0.60	0.70	16	1
1:A:29:MET:HE1	1:A:60:ILE:HG12	0.60	1.73	4	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:HD3	1:A:63:LYS:HG2	0.60	0.73	16	1
1:A:68:TYR:CZ	1:A:68:TYR:CE1	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:63:LYS:CD	1:A:63:LYS:HG2	0.59	1.16	16	1
1:A:55:MET:HE2	1:A:59:MET:HE1	0.59	1.73	7	1
1:A:35:LEU:HD22	1:A:35:LEU:N	0.59	2.12	7	6
1:A:34:PHE:CD1	1:A:34:PHE:CG	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:CE2	1:A:80:TYR:CZ	0.59	0.71	16	1
1:A:12:HIS:NE2	1:A:15:ALA:CB	0.59	2.66	16	2
1:A:55:MET:CG	1:A:59:MET:HE1	0.59	2.27	9	1
1:A:9:LEU:HD13	1:A:9:LEU:C	0.58	2.23	4	16
1:A:86:LEU:C	1:A:86:LEU:HD13	0.58	2.23	5	2
1:A:4:LYS:NZ	1:A:4:LYS:HE2	0.58	1.14	16	1
1:A:80:TYR:CZ	1:A:80:TYR:CE1	0.58	0.70	16	1
1:A:26:MET:HE3	1:A:57:ILE:CD1	0.58	2.27	12	1
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:20:ILE:HG21	1:A:26:MET:CE	0.58	2.29	6	2
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:20:ILE:HD13	1:A:25:ILE:HG21	0.58	1.74	3	1
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:HZ2	0.57	1.28	16	1
1:A:57:ILE:CD1	1:A:57:ILE:N	0.57	2.67	4	6
1:A:59:MET:CE	1:A:59:MET:HG2	0.57	2.22	16	1
1:A:63:LYS:CE	1:A:63:LYS:HZ1	0.57	1.28	16	1
1:A:49:GLN:CD	1:A:49:GLN:HE21	0.57	1.23	16	1
1:A:16:LEU:HD13	1:A:57:ILE:CG1	0.57	2.30	14	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:86:LEU:HD13	1:A:86:LEU:C	0.57	2.24	11	1
1:A:49:GLN:CD	1:A:49:GLN:HE22	0.57	1.23	16	1
1:A:22:THR:HG21	1:A:52:ARG:HD3	0.57	1.77	4	1
1:A:55:MET:CE	1:A:55:MET:HG3	0.56	2.22	16	1
1:A:78:GLU:OE1	1:A:78:GLU:CD	0.56	0.70	16	1
1:A:71:PHE:CD1	1:A:71:PHE:CG	0.56	0.73	16	1
1:A:20:ILE:CG2	1:A:26:MET:HE1	0.56	2.29	6	2
1:A:63:LYS:CE	1:A:63:LYS:HZ3	0.56	1.28	16	1
1:A:12:HIS:CD2	1:A:12:HIS:O	0.56	2.59	16	4
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:16:LEU:HD23	1:A:57:ILE:HG13	0.56	1.77	3	1
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:HD22	1:A:57:ILE:CG1	0.55	2.32	6	2
1:A:56:LEU:HD13	1:A:56:LEU:O	0.55	2.01	13	1
1:A:86:LEU:HD13	1:A:86:LEU:O	0.55	2.02	5	2
1:A:24:TYR:CD2	1:A:24:TYR:CG	0.55	0.70	16	1
1:A:68:TYR:CG	1:A:68:TYR:CD1	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:16:LEU:HD11	1:A:26:MET:HE3	0.54	1.77	16	1
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	3
1:A:75:LEU:HD23	1:A:80:TYR:CD2	0.54	2.37	6	1
1:A:39:GLU:CD	1:A:59:MET:HE1	0.54	2.27	15	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:26:MET:HE1	1:A:57:ILE:CD1	0.54	2.32	7	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:TYR:CG	1:A:24:TYR:CD1	0.54	0.70	16	1
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:26:MET:HE1	1:A:57:ILE:HD11	0.53	1.81	7	1
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:91:ILE:N	1:A:92:PRO:HD2	0.52	2.19	3	12
1:A:71:PHE:CG	1:A:71:PHE:CD2	0.52	0.68	16	1
1:A:80:TYR:CG	1:A:80:TYR:CD1	0.52	0.70	16	1
1:A:35:LEU:N	1:A:35:LEU:CD2	0.52	2.73	5	6
1:A:22:THR:HG22	1:A:56:LEU:CD2	0.52	2.33	5	1
1:A:35:LEU:HD22	1:A:35:LEU:HD13	0.52	0.63	16	1
1:A:72:TYR:CZ	1:A:72:TYR:HE2	0.52	1.28	16	1
1:A:12:HIS:HD2	1:A:15:ALA:HB3	0.52	1.60	4	2
1:A:46:GLU:CD	1:A:46:GLU:OE1	0.52	0.28	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:19:ASP:CG	1:A:83:LEU:HD23	0.51	2.30	10	1
1:A:16:LEU:HD21	1:A:26:MET:HE3	0.51	1.82	16	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:23:SER:O	1:A:24:TYR:C	0.50	2.54	15	16
1:A:29:MET:HE2	1:A:74:ALA:CB	0.50	2.36	2	1
1:A:16:LEU:HD13	1:A:16:LEU:O	0.50	2.06	11	4
1:A:19:ASP:CB	1:A:83:LEU:HD23	0.50	2.36	10	1
1:A:83:LEU:C	1:A:83:LEU:HD23	0.50	2.31	14	4
1:A:56:LEU:HD13	1:A:56:LEU:C	0.50	2.31	13	1
1:A:16:LEU:C	1:A:16:LEU:CD1	0.50	2.84	11	3
1:A:83:LEU:HD23	1:A:83:LEU:C	0.50	2.31	5	2
1:A:35:LEU:CD1	1:A:35:LEU:HD22	0.50	1.12	16	1
1:A:4:LYS:CE	1:A:4:LYS:HZ1	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:CE	1:A:4:LYS:HZ2	0.49	1.20	16	1
1:A:57:ILE:HD13	1:A:57:ILE:N	0.49	2.22	7	2
1:A:4:LYS:CE	1:A:4:LYS:HZ3	0.49	1.20	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:GLU:N	1:A:47:PRO:HD2	0.49	2.22	11	12
1:A:62:LYS:CD	1:A:62:LYS:HZ3	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
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:35:LEU:CD1	1:A:35:LEU:CD2	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:29:MET:HE3	1:A:29:MET:HA	0.48	1.85	1	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:29:MET:HE3	1:A:29:MET:SD	0.48	1.11	16	1
1:A:45:ASN:OD1	1:A:45:ASN:CA	0.48	2.61	16	1
1:A:57:ILE:N	1:A:57:ILE:CD1	0.47	2.77	3	3
1:A:26:MET:HE1	1:A:57:ILE:HG13	0.47	1.86	8	1
1:A:72:TYR:O	1:A:76:LEU:HD12	0.47	2.08	2	1
1:A:62:LYS:CG	1:A:62:LYS:HE3	0.47	2.09	16	1
1:A:34:PHE:CG	1:A:34:PHE:HD2	0.47	1.24	16	1
1:A:86:LEU:C	1:A:86:LEU:CD1	0.47	2.88	5	3
1:A:59:MET:HA	1:A:59:MET:HE2	0.47	1.86	13	1
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:CZ	1:A:34:PHE:HE1	0.47	1.23	16	1
1:A:63:LYS:CG	1:A:63:LYS:CD	0.47	0.56	16	1
1:A:91:ILE:N	1:A:92:PRO:CD	0.47	2.78	3	5
1:A:59:MET:N	1:A:59:MET:SD	0.47	2.88	5	2
1:A:20:ILE:HG21	1:A:25:ILE:HG21	0.47	1.87	10	1
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:20:ILE:HD11	1:A:80:TYR:CE1	0.46	2.45	2	1
1:A:13:ARG:CD	1:A:54:ALA:HB1	0.46	2.41	12	1
1:A:35:LEU:HD12	1:A:35:LEU:N	0.46	2.25	12	1
1:A:12:HIS:HE1	1:A:86:LEU:HD23	0.46	1.69	16	1
1:A:56:LEU:C	1:A:56:LEU:HD23	0.46	2.35	15	1
1:A:71:PHE:CG	1:A:71:PHE:HD1	0.46	1.21	16	1
1:A:25:ILE:HG23	1:A:75:LEU:HD21	0.45	1.89	7	2
1:A:20:ILE:CD1	1:A:25:ILE:HG21	0.45	2.42	3	1
1:A:68:TYR:CE2	1:A:91:ILE:CD1	0.45	2.99	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:PHE:CZ	1:A:71:PHE:HE2	0.45	1.21	16	1
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:83:LEU:C	1:A:83:LEU:CD1	0.45	2.90	3	5
1:A:68:TYR:CG	1:A:68:TYR:HD2	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:CZ	1:A:68:TYR:HE1	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:68:TYR:CG	1:A:68:TYR:HD1	0.44	1.20	16	1
1:A:12:HIS:CE1	1:A:15:ALA:HB3	0.44	2.47	10	2
1:A:12:HIS:CE1	1:A:15:ALA:CB	0.44	3.01	6	4
1:A:34:PHE:CB	1:A:35:LEU:HD12	0.44	2.43	10	2
1:A:80:TYR:CZ	1:A:80:TYR:HE2	0.44	1.20	16	1
1:A:80:TYR:CZ	1:A:80:TYR:HE1	0.44	1.19	16	1
1:A:24:TYR:CZ	1:A:24:TYR:HE2	0.44	1.20	16	1
1:A:24:TYR:CG	1:A:24:TYR:HD2	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:CZ	1:A:68:TYR:HE2	0.43	1.19	16	1
1:A:71:PHE:CD1	1:A:71:PHE:C	0.43	2.96	5	2
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:N	1:A:34:PHE:CD1	0.43	2.85	11	2
1:A:68:TYR:OH	1:A:91:ILE:HD11	0.43	2.14	1	1
1:A:29:MET:HE1	1:A:71:PHE:HB2	0.43	1.89	11	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:6:ARG:CZ	1:A:10:LEU:HD11	0.43	2.43	15	1
1:A:9:LEU:HD11	1:A:57:ILE:CG2	0.43	2.44	15	1
1:A:30:ILE:HD13	1:A:56:LEU:HD11	0.42	1.89	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:GLU:HB3	1:A:47:PRO:CD	0.42	2.45	16	1
1:A:56:LEU:C	1:A:56:LEU:CD1	0.42	2.92	13	1
1:A:29:MET:HA	1:A:29:MET:HE2	0.42	1.91	15	1
1:A:13:ARG:HD2	1:A:54:ALA:HB1	0.42	1.92	12	1
1:A:29:MET:SD	1:A:29:MET:HE2	0.42	1.11	16	1
1:A:71:PHE:CZ	1:A:71:PHE:HE1	0.42	1.18	16	1
1:A:80:TYR:O	1:A:81:LYS:C	0.42	2.61	9	6
1:A:20:ILE:HG22	1:A:21:LYS:N	0.42	2.29	15	2
1:A:9:LEU:C	1:A:9:LEU:CD1	0.42	2.92	4	3
1:A:71:PHE:CG	1:A:71:PHE:HD2	0.42	1.18	16	1
1:A:29:MET:HE3	1:A:34:PHE:HD2	0.42	1.74	4	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:83:LEU:HD23	1:A:83:LEU:O	0.42	2.15	14	1
1:A:20:ILE:CG2	1:A:21:LYS:N	0.41	2.82	15	2
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:29:MET:O	1:A:34:PHE:CD2	0.41	2.73	9	1
1:A:19:ASP:CG	1:A:83:LEU:HD11	0.41	2.41	12	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:CD1	0.41	2.74	8	1
1:A:4:LYS:CE	1:A:4:LYS:NZ	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: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

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%)	6	42
All	All	1440/1552 (93%)	1219 (85%)	184 (13%)	37 (3%)	6	42

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 ⓘ

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±2%)	6±2 (8±2%)	14	61
All	All	1264/1376 (92%)	1165 (92%)	99 (8%)	14	61

All 29 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	10
1	A	58	LYS	9
1	A	62	LYS	7
1	A	63	LYS	7
1	A	57	ILE	6
1	A	46	GLU	6
1	A	50	GLN	5
1	A	26	MET	4
1	A	29	MET	4
1	A	40	GLU	4
1	A	64	ASP	4
1	A	49	GLN	4
1	A	45	ASN	3
1	A	32	ASP	3
1	A	59	MET	3

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Mol	Chain	Res	Type	Models (Total)
1	A	27	ASP	2
1	A	73	ASN	2
1	A	21	LYS	2
1	A	55	MET	2
1	A	4	LYS	2
1	A	83	LEU	2
1	A	42	LYS	1
1	A	87	LEU	1
1	A	78	GLU	1
1	A	13	ARG	1
1	A	56	LEU	1
1	A	16	LEU	1
1	A	20	ILE	1
1	A	23	SER	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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	16-A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
16	A	1:MET	C	2:ASP	N	1.13
16	A	94:VAL	C	95:SER	N	1.12
16	A	96:SER	C	97:SER	N	0.68
16	A	95:SER	C	96:SER	N	0.49

7 Chemical shift validation

No chemical shift data were provided