



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 01:45 PM BST

PDB ID : 1BV8
Title : RECEPTOR DOMAIN FROM ALPHA-2-MACROGLOBULIN
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Deposited on : 1998-09-22

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

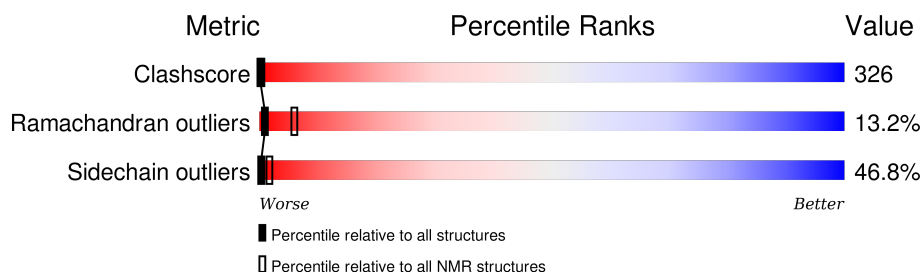
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	138	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

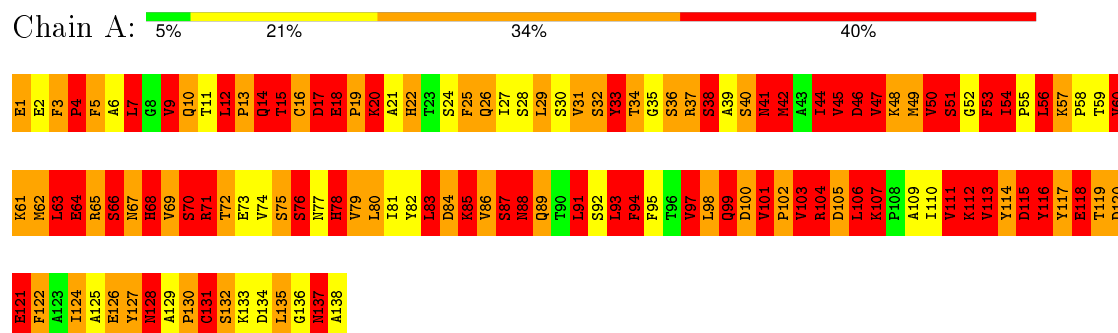
3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1986 atoms, of which 908 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ALPHA-2-MACROGLOBULIN.

Mol	Chain	Residues	Atoms						Trace
1	A	138	Total	C	H	N	O	S	0
			1986	688	908	174	211	5	

- Molecule 1: ALPHA-2-MACROGLOBULIN



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *DISTANCE GEOMETRY*.

Of the 20 calculated structures, 1 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
DYANA	structure solution	
DYANA	refinement	

No chemical shift data was provided. 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	24.24	593/1101 (53.9%)	16.34	526/1497 (35.1%)
All	All	24.24	593/1101 (53.9%)	16.34	526/1497 (35.1%)

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

Mol	Chain	Chirality	Planarity
1	A	19	0
All	All	19	0

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	GLU	CD-OE1	-94.53	0.21	1.25
1	A	121	GLU	CD-OE1	-86.08	0.30	1.25
1	A	2	GLU	CD-OE2	-84.25	0.33	1.25
1	A	3	PHE	CG-CD2	-83.48	0.13	1.38
1	A	116	TYR	CE2-CZ	-82.38	0.31	1.38
1	A	1	GLU	CD-OE1	-81.00	0.36	1.25
1	A	116	TYR	CG-CD1	-80.54	0.34	1.39
1	A	73	GLU	CD-OE1	-79.07	0.38	1.25
1	A	71	ARG	CZ-NH1	-77.58	0.32	1.33
1	A	40	SER	CB-OG	-77.31	0.41	1.42
1	A	117	TYR	CE1-CZ	-75.55	0.40	1.38
1	A	53	PHE	CG-CD2	-75.02	0.26	1.38
1	A	117	TYR	CG-CD2	-74.99	0.41	1.39
1	A	118	GLU	CD-OE2	-74.89	0.43	1.25
1	A	37	ARG	CZ-NH2	-73.86	0.37	1.33
1	A	126	GLU	CD-OE2	-73.05	0.45	1.25
1	A	65	ARG	CZ-NH1	-69.97	0.42	1.33
1	A	37	ARG	CZ-NH1	-69.59	0.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	GLU	CD-OE1	-69.37	0.49	1.25
1	A	1	GLU	CD-OE2	-69.23	0.49	1.25
1	A	40	SER	CA-CB	-68.51	0.50	1.52
1	A	38	SER	CB-OG	-68.43	0.53	1.42
1	A	132	SER	CB-OG	-67.92	0.54	1.42
1	A	101	VAL	CB-CG2	-67.36	0.11	1.52
1	A	117	TYR	CE2-CZ	-66.14	0.52	1.38
1	A	51	SER	CB-OG	-65.40	0.57	1.42
1	A	117	TYR	CG-CD1	-65.31	0.54	1.39
1	A	3	PHE	CE1-CZ	-65.12	0.13	1.37
1	A	82	TYR	CE2-CZ	-65.00	0.54	1.38
1	A	64	GLU	CD-OE2	-64.53	0.54	1.25
1	A	82	TYR	CE1-CZ	-64.28	0.55	1.38
1	A	70	SER	CB-OG	-63.97	0.59	1.42
1	A	2	GLU	CG-CD	-63.97	0.56	1.51
1	A	82	TYR	CG-CD1	-63.04	0.57	1.39
1	A	18	GLU	CD-OE2	-62.35	0.57	1.25
1	A	82	TYR	CG-CD2	-62.34	0.58	1.39
1	A	138	ALA	CA-CB	-61.85	0.22	1.52
1	A	104	ARG	CZ-NH1	-61.43	0.53	1.33
1	A	36	SER	CB-OG	-61.28	0.62	1.42
1	A	87	SER	CB-OG	-60.94	0.63	1.42
1	A	64	GLU	CD-OE1	-60.77	0.58	1.25
1	A	33	TYR	CE2-CZ	-59.95	0.60	1.38
1	A	71	ARG	CZ-NH2	-59.92	0.55	1.33
1	A	126	GLU	CD-OE1	-59.29	0.60	1.25
1	A	136	GLY	C-O	-59.14	0.29	1.23
1	A	53	PHE	CE1-CZ	-58.49	0.26	1.37
1	A	37	ARG	CD-NE	-58.49	0.47	1.46
1	A	33	TYR	CG-CD1	-58.20	0.63	1.39
1	A	118	GLU	CG-CD	-57.97	0.65	1.51
1	A	5	PHE	CG-CD2	-57.80	0.52	1.38
1	A	121	GLU	CD-OE2	-57.74	0.62	1.25
1	A	104	ARG	CZ-NH2	-57.52	0.58	1.33
1	A	2	GLU	CB-CG	-57.03	0.43	1.52
1	A	137	ASN	C-O	-56.38	0.16	1.23
1	A	121	GLU	CG-CD	-54.75	0.69	1.51
1	A	2	GLU	C-O	-54.46	0.19	1.23
1	A	134	ASP	CB-CG	-54.37	0.37	1.51
1	A	114	TYR	CE2-CZ	-54.26	0.68	1.38
1	A	33	TYR	CE1-CZ	-53.77	0.68	1.38
1	A	114	TYR	CE1-CZ	-53.43	0.69	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	PHE	CG-CD2	-53.36	0.58	1.38
1	A	25	PHE	CG-CD2	-53.26	0.58	1.38
1	A	53	PHE	CG-CD1	-53.01	0.59	1.38
1	A	95	PHE	CG-CD2	-52.95	0.59	1.38
1	A	39	ALA	CA-CB	-52.92	0.41	1.52
1	A	114	TYR	CG-CD1	-52.25	0.71	1.39
1	A	134	ASP	CA-CB	-52.11	0.39	1.53
1	A	33	TYR	CG-CD2	-51.77	0.71	1.39
1	A	40	SER	C-O	-51.53	0.25	1.23
1	A	18	GLU	CD-OE1	-51.44	0.69	1.25
1	A	114	TYR	CG-CD2	-51.35	0.72	1.39
1	A	101	VAL	CB-CG1	-51.27	0.45	1.52
1	A	73	GLU	CD-OE2	-50.84	0.69	1.25
1	A	86	VAL	CA-CB	-50.66	0.48	1.54
1	A	116	TYR	CE1-CZ	-50.59	0.72	1.38
1	A	94	PHE	CG-CD1	-50.19	0.63	1.38
1	A	5	PHE	CG-CD1	-50.03	0.63	1.38
1	A	3	PHE	CG-CD1	-49.80	0.64	1.38
1	A	118	GLU	CA-CB	-49.68	0.44	1.53
1	A	86	VAL	C-O	-49.61	0.29	1.23
1	A	39	ALA	C-O	-49.61	0.29	1.23
1	A	117	TYR	CB-CG	-49.21	0.77	1.51
1	A	71	ARG	NE-CZ	-48.83	0.69	1.33
1	A	116	TYR	CG-CD2	-48.59	0.76	1.39
1	A	131	CYS	C-O	-48.56	0.31	1.23
1	A	68	HIS	CE1-NE2	-48.52	0.21	1.32
1	A	118	GLU	CB-CG	-48.43	0.60	1.52
1	A	15	THR	CB-OG1	-48.42	0.46	1.43
1	A	122	PHE	CG-CD1	-48.24	0.66	1.38
1	A	71	ARG	CD-NE	-47.68	0.65	1.46
1	A	65	ARG	NE-CZ	-47.57	0.71	1.33
1	A	25	PHE	CG-CD1	-47.22	0.68	1.38
1	A	137	ASN	CG-OD1	-47.17	0.20	1.24
1	A	41	ASN	CG-OD1	-47.05	0.20	1.24
1	A	104	ARG	NE-CZ	-46.53	0.72	1.33
1	A	119	THR	CB-OG1	-46.49	0.50	1.43
1	A	104	ARG	CD-NE	-46.44	0.67	1.46
1	A	134	ASP	C-O	-46.06	0.35	1.23
1	A	1	GLU	C-O	-46.05	0.35	1.23
1	A	117	TYR	CA-CB	-45.87	0.53	1.53
1	A	3	PHE	CB-CG	-45.76	0.73	1.51
1	A	5	PHE	CE1-CZ	-44.96	0.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ARG	NE-CZ	-44.67	0.74	1.33
1	A	88	ASN	CG-OD1	-44.57	0.25	1.24
1	A	85	LYS	C-O	-44.52	0.38	1.23
1	A	30	SER	CB-OG	-44.46	0.84	1.42
1	A	38	SER	CA-CB	-44.15	0.86	1.52
1	A	117	TYR	CD1-CE1	-44.05	0.73	1.39
1	A	117	TYR	CD2-CE2	-44.05	0.73	1.39
1	A	135	LEU	C-N	-43.70	0.54	1.33
1	A	99	GLN	CD-OE1	-43.68	0.27	1.24
1	A	103	VAL	CB-CG1	-43.30	0.61	1.52
1	A	45	VAL	CB-CG2	-43.00	0.62	1.52
1	A	2	GLU	CA-CB	-42.69	0.60	1.53
1	A	133	LYS	CE-NZ	-42.49	0.42	1.49
1	A	45	VAL	CB-CG1	-42.38	0.63	1.52
1	A	60	VAL	CB-CG2	-42.27	0.64	1.52
1	A	46	ASP	CG-OD1	-42.20	0.28	1.25
1	A	120	ASP	CG-OD1	-42.18	0.28	1.25
1	A	127	TYR	CE2-CZ	-41.95	0.84	1.38
1	A	137	ASN	CB-CG	-41.83	0.54	1.51
1	A	117	TYR	C-O	-41.64	0.44	1.23
1	A	119	THR	C-O	-41.51	0.44	1.23
1	A	113	VAL	CB-CG1	-41.45	0.65	1.52
1	A	122	PHE	CE1-CZ	-41.37	0.58	1.37
1	A	25	PHE	CE1-CZ	-41.28	0.58	1.37
1	A	41	ASN	C-O	-41.22	0.45	1.23
1	A	53	PHE	CE2-CZ	-41.13	0.59	1.37
1	A	95	PHE	CE1-CZ	-41.07	0.59	1.37
1	A	60	VAL	CB-CG1	-40.43	0.68	1.52
1	A	117	TYR	CZ-OH	-40.41	0.69	1.37
1	A	105	ASP	CG-OD1	-40.30	0.32	1.25
1	A	127	TYR	CG-CD1	-40.28	0.86	1.39
1	A	94	PHE	CG-CD2	-40.22	0.78	1.38
1	A	22	HIS	CG-CD2	-39.51	0.68	1.35
1	A	41	ASN	CB-CG	-39.50	0.60	1.51
1	A	1	GLU	CG-CD	-39.11	0.93	1.51
1	A	41	ASN	CA-CB	-38.95	0.51	1.53
1	A	94	PHE	CE2-CZ	-38.92	0.63	1.37
1	A	87	SER	CA-CB	-38.83	0.94	1.52
1	A	5	PHE	CE2-CZ	-38.77	0.63	1.37
1	A	115	ASP	CG-OD2	-38.62	0.36	1.25
1	A	3	PHE	CE2-CZ	-38.61	0.64	1.37
1	A	120	ASP	C-O	-38.47	0.50	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	VAL	CB-CG2	-38.13	0.72	1.52
1	A	135	LEU	CA-CB	-38.00	0.66	1.53
1	A	66	SER	C-O	-37.78	0.51	1.23
1	A	118	GLU	C-O	-37.75	0.51	1.23
1	A	127	TYR	CE1-CZ	-37.65	0.89	1.38
1	A	97	VAL	CB-CG1	-37.49	0.74	1.52
1	A	122	PHE	CE2-CZ	-37.37	0.66	1.37
1	A	68	HIS	CG-ND1	-37.32	0.56	1.38
1	A	115	ASP	CB-CG	-37.13	0.73	1.51
1	A	95	PHE	CG-CD1	-37.12	0.83	1.38
1	A	115	ASP	C-O	-36.76	0.53	1.23
1	A	86	VAL	CB-CG2	-36.72	0.75	1.52
1	A	25	PHE	CE2-CZ	-36.48	0.68	1.37
1	A	37	ARG	CB-CG	-36.37	0.54	1.52
1	A	134	ASP	CG-OD2	-36.30	0.41	1.25
1	A	121	GLU	CB-CG	-36.22	0.83	1.52
1	A	28	SER	CB-OG	-36.01	0.95	1.42
1	A	120	ASP	CG-OD2	-35.88	0.42	1.25
1	A	127	TYR	CG-CD2	-35.83	0.92	1.39
1	A	120	ASP	CB-CG	-35.80	0.76	1.51
1	A	97	VAL	CB-CG2	-35.72	0.77	1.52
1	A	84	ASP	CG-OD1	-35.71	0.43	1.25
1	A	37	ARG	C-O	-35.67	0.55	1.23
1	A	3	PHE	CD1-CE1	-35.51	0.68	1.39
1	A	53	PHE	CB-CG	-35.50	0.91	1.51
1	A	46	ASP	CB-CG	-35.48	0.77	1.51
1	A	3	PHE	CD2-CE2	-35.48	0.68	1.39
1	A	14	GLN	CD-OE1	-35.27	0.46	1.24
1	A	133	LYS	CD-CE	-35.27	0.63	1.51
1	A	100	ASP	C-N	-35.21	0.53	1.34
1	A	103	VAL	C-O	-35.06	0.56	1.23
1	A	138	ALA	N-CA	-34.98	0.76	1.46
1	A	4	PRO	N-CD	-34.83	0.99	1.47
1	A	22	HIS	CE1-NE2	-34.79	0.52	1.32
1	A	138	ALA	C-O	-34.60	0.57	1.23
1	A	31	VAL	CB-CG2	-34.60	0.80	1.52
1	A	112	LYS	CB-CG	-34.44	0.59	1.52
1	A	99	GLN	CD-NE2	-34.41	0.46	1.32
1	A	88	ASN	CB-CG	-34.36	0.72	1.51
1	A	105	ASP	CG-OD2	-34.19	0.46	1.25
1	A	100	ASP	C-O	-34.06	0.58	1.23
1	A	10	GLN	CD-OE1	-33.97	0.49	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	PRO	N-CD	-33.92	1.00	1.47
1	A	89	GLN	CD-OE1	-33.88	0.49	1.24
1	A	65	ARG	CZ-NH2	-33.75	0.89	1.33
1	A	136	GLY	CA-C	-33.44	0.98	1.51
1	A	73	GLU	CG-CD	-33.23	1.02	1.51
1	A	85	LYS	CE-NZ	-32.90	0.66	1.49
1	A	135	LEU	C-O	-32.86	0.60	1.23
1	A	137	ASN	CA-CB	-32.85	0.67	1.53
1	A	68	HIS	CG-CD2	-32.65	0.80	1.35
1	A	3	PHE	CA-CB	-32.58	0.82	1.53
1	A	31	VAL	CB-CG1	-32.27	0.85	1.52
1	A	1	GLU	CB-CG	-32.24	0.90	1.52
1	A	134	ASP	CG-OD1	-32.12	0.51	1.25
1	A	41	ASN	N-CA	-32.09	0.82	1.46
1	A	106	LEU	CB-CG	-31.80	0.60	1.52
1	A	116	TYR	C-O	-31.45	0.63	1.23
1	A	135	LEU	CB-CG	-31.41	0.61	1.52
1	A	41	ASN	CG-ND2	-31.14	0.55	1.32
1	A	94	PHE	CE1-CZ	-31.04	0.78	1.37
1	A	50	VAL	CB-CG2	-30.93	0.88	1.52
1	A	34	THR	CB-OG1	-30.84	0.81	1.43
1	A	4	PRO	N-CA	-30.72	0.95	1.47
1	A	47	VAL	CB-CG1	-30.70	0.88	1.52
1	A	120	ASP	CA-CB	-30.68	0.86	1.53
1	A	133	LYS	C-O	-30.57	0.65	1.23
1	A	119	THR	CB-CG2	-30.56	0.51	1.52
1	A	35	GLY	C-O	-30.39	0.75	1.23
1	A	130	PRO	N-CD	-30.36	1.05	1.47
1	A	106	LEU	CG-CD1	-29.89	0.41	1.51
1	A	137	ASN	CA-C	-29.74	0.75	1.52
1	A	132	SER	C-O	-29.55	0.67	1.23
1	A	9	VAL	CB-CG1	-29.33	0.91	1.52
1	A	84	ASP	CG-OD2	-29.03	0.58	1.25
1	A	133	LYS	CA-CB	-28.99	0.90	1.53
1	A	103	VAL	CB-CG2	-28.98	0.92	1.52
1	A	37	ARG	CG-CD	-28.97	0.79	1.51
1	A	20	LYS	CE-NZ	-28.96	0.76	1.49
1	A	110	ILE	CB-CG1	-28.93	0.73	1.54
1	A	88	ASN	CG-ND2	-28.87	0.60	1.32
1	A	9	VAL	CB-CG2	-28.80	0.92	1.52
1	A	12	LEU	CG-CD2	-28.59	0.46	1.51
1	A	95	PHE	CE2-CZ	-28.57	0.83	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	GLN	CG-CD	-28.48	0.85	1.51
1	A	137	ASN	C-N	-28.10	0.69	1.34
1	A	3	PHE	C-N	-28.06	0.81	1.34
1	A	47	VAL	CB-CG2	-27.92	0.94	1.52
1	A	40	SER	CA-C	-27.89	0.80	1.52
1	A	16	CYS	CB-SG	-27.84	1.34	1.82
1	A	32	SER	CB-OG	-27.76	1.06	1.42
1	A	107	LYS	CE-NZ	-27.73	0.79	1.49
1	A	22	HIS	CG-ND1	-27.68	0.77	1.38
1	A	132	SER	CA-CB	-27.66	1.11	1.52
1	A	134	ASP	C-N	-27.51	0.70	1.34
1	A	53	PHE	CD1-CE1	-27.40	0.84	1.39
1	A	57	LYS	CD-CE	-27.38	0.82	1.51
1	A	53	PHE	CD2-CE2	-27.37	0.84	1.39
1	A	89	GLN	CD-NE2	-27.06	0.65	1.32
1	A	14	GLN	CD-NE2	-27.03	0.65	1.32
1	A	133	LYS	CG-CD	-27.00	0.60	1.52
1	A	76	SER	CB-OG	-26.94	1.07	1.42
1	A	137	ASN	CG-ND2	-26.93	0.65	1.32
1	A	118	GLU	N-CA	-26.83	0.92	1.46
1	A	115	ASP	C-N	-26.78	0.72	1.34
1	A	102	PRO	CA-CB	-26.74	1.00	1.53
1	A	104	ARG	CB-CG	-26.51	0.81	1.52
1	A	100	ASP	CG-OD1	-26.45	0.64	1.25
1	A	66	SER	CB-OG	-26.43	1.07	1.42
1	A	99	GLN	CB-CG	-26.42	0.81	1.52
1	A	115	ASP	CG-OD1	-26.31	0.64	1.25
1	A	65	ARG	CD-NE	-26.30	1.01	1.46
1	A	103	VAL	CA-CB	-26.30	0.99	1.54
1	A	107	LYS	CB-CG	-26.30	0.81	1.52
1	A	135	LEU	CG-CD2	-26.25	0.54	1.51
1	A	1	GLU	CA-CB	-26.19	0.96	1.53
1	A	10	GLN	CD-NE2	-26.15	0.67	1.32
1	A	110	ILE	CB-CG2	-26.03	0.72	1.52
1	A	105	ASP	CB-CG	-25.86	0.97	1.51
1	A	106	LEU	CG-CD2	-25.84	0.56	1.51
1	A	15	THR	CB-CG2	-25.82	0.67	1.52
1	A	111	VAL	CB-CG1	-25.79	0.98	1.52
1	A	111	VAL	CB-CG2	-25.77	0.98	1.52
1	A	61	LYS	CE-NZ	-25.72	0.84	1.49
1	A	85	LYS	C-N	-25.70	0.74	1.34
1	A	88	ASN	CA-CB	-25.60	0.86	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	SER	C-N	-25.40	0.75	1.34
1	A	87	SER	C-O	-25.38	0.75	1.23
1	A	4	PRO	CA-CB	-25.26	1.03	1.53
1	A	17	ASP	CG-OD1	-25.22	0.67	1.25
1	A	117	TYR	C-N	-25.14	0.76	1.34
1	A	83	LEU	CB-CG	-24.92	0.80	1.52
1	A	29	LEU	CG-CD2	-24.73	0.60	1.51
1	A	130	PRO	C-N	-24.61	0.77	1.34
1	A	49	MET	CG-SD	-24.58	1.17	1.81
1	A	104	ARG	CG-CD	-24.56	0.90	1.51
1	A	57	LYS	CE-NZ	-24.54	0.87	1.49
1	A	2	GLU	N-CA	-24.45	0.97	1.46
1	A	17	ASP	CG-OD2	-24.27	0.69	1.25
1	A	118	GLU	C-N	-24.22	0.78	1.34
1	A	57	LYS	CB-CG	-24.20	0.87	1.52
1	A	119	THR	C-N	-24.18	0.78	1.34
1	A	86	VAL	C-N	-23.71	0.79	1.34
1	A	14	GLN	CB-CG	-23.69	0.88	1.52
1	A	78	HIS	CE1-NE2	-23.55	0.78	1.32
1	A	42	MET	CB-CG	-23.48	0.76	1.51
1	A	102	PRO	C-O	-23.44	0.76	1.23
1	A	50	VAL	CB-CG1	-23.30	1.03	1.52
1	A	62	MET	CG-SD	-23.12	1.21	1.81
1	A	130	PRO	CA-CB	-23.04	1.07	1.53
1	A	78	HIS	CG-CD2	-23.01	0.96	1.35
1	A	48	LYS	CD-CE	-22.90	0.94	1.51
1	A	83	LEU	CG-CD2	-22.88	0.67	1.51
1	A	100	ASP	CG-OD2	-22.87	0.72	1.25
1	A	22	HIS	CB-CG	-22.75	1.09	1.50
1	A	112	LYS	CD-CE	-22.69	0.94	1.51
1	A	12	LEU	CG-CD1	-22.67	0.68	1.51
1	A	135	LEU	N-CA	-22.57	1.01	1.46
1	A	95	PHE	CB-CG	-22.57	1.12	1.51
1	A	34	THR	C-O	-22.55	0.80	1.23
1	A	117	TYR	CA-C	-22.52	0.94	1.52
1	A	137	ASN	N-CA	-22.50	1.01	1.46
1	A	40	SER	C-N	-22.48	0.82	1.34
1	A	34	THR	C-N	-22.46	0.92	1.33
1	A	37	ARG	CA-CB	-22.46	1.04	1.53
1	A	119	THR	CA-CB	-22.40	0.95	1.53
1	A	116	TYR	CB-CG	-21.86	1.18	1.51
1	A	121	GLU	C-O	-21.78	0.81	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	GLU	N-CA	-21.75	1.02	1.46
1	A	83	LEU	CG-CD1	-21.68	0.71	1.51
1	A	41	ASN	C-N	-21.67	0.84	1.34
1	A	1	GLU	CA-C	-21.56	0.96	1.52
1	A	99	GLN	C-O	-21.54	0.82	1.23
1	A	121	GLU	CA-CB	-21.54	1.06	1.53
1	A	87	SER	N-CA	-21.38	1.03	1.46
1	A	128	ASN	CG-OD1	-21.28	0.77	1.24
1	A	38	SER	C-O	-21.25	0.82	1.23
1	A	64	GLU	CB-CG	-21.24	1.11	1.52
1	A	136	GLY	N-CA	-20.87	1.14	1.46
1	A	112	LYS	CE-NZ	-20.83	0.96	1.49
1	A	3	PHE	C-O	-20.76	0.83	1.23
1	A	46	ASP	CG-OD2	-20.62	0.78	1.25
1	A	135	LEU	CG-CD1	-20.35	0.76	1.51
1	A	131	CYS	CB-SG	-20.25	1.47	1.82
1	A	101	VAL	C-O	-20.09	0.85	1.23
1	A	39	ALA	N-CA	-19.90	1.06	1.46
1	A	82	TYR	CB-CG	-19.84	1.21	1.51
1	A	128	ASN	CG-ND2	-19.76	0.83	1.32
1	A	3	PHE	CA-C	-19.72	1.01	1.52
1	A	138	ALA	CA-C	-19.67	1.01	1.52
1	A	84	ASP	CB-CG	-19.66	1.10	1.51
1	A	36	SER	C-O	-19.66	0.85	1.23
1	A	39	ALA	C-N	-19.60	0.89	1.34
1	A	22	HIS	CD2-NE2	-19.60	0.94	1.38
1	A	67	ASN	CG-OD1	-19.49	0.81	1.24
1	A	120	ASP	CA-C	-19.39	1.02	1.52
1	A	29	LEU	CG-CD1	-19.35	0.80	1.51
1	A	91	LEU	CB-CG	-19.35	0.96	1.52
1	A	86	VAL	CB-CG1	-19.18	1.12	1.52
1	A	56	LEU	CG-CD2	-19.14	0.81	1.51
1	A	56	LEU	CG-CD1	-19.12	0.81	1.51
1	A	1	GLU	C-N	-19.04	0.90	1.34
1	A	85	LYS	CD-CE	-19.00	1.03	1.51
1	A	50	VAL	C-N	-18.99	0.90	1.34
1	A	134	ASP	CA-C	-18.93	1.03	1.52
1	A	116	TYR	CZ-OH	-18.88	1.05	1.37
1	A	37	ARG	C-N	-18.85	0.90	1.34
1	A	4	PRO	CG-CD	-18.75	0.88	1.50
1	A	104	ARG	CA-CB	-18.74	1.12	1.53
1	A	18	GLU	CG-CD	-18.62	1.24	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	PHE	CB-CG	-18.55	1.19	1.51
1	A	133	LYS	CB-CG	-18.54	1.02	1.52
1	A	86	VAL	CA-C	-18.51	1.04	1.52
1	A	66	SER	C-N	-18.42	0.91	1.34
1	A	93	LEU	CG-CD2	-18.33	0.84	1.51
1	A	116	TYR	CD2-CE2	-18.28	1.11	1.39
1	A	26	GLN	CD-NE2	-18.26	0.87	1.32
1	A	116	TYR	CD1-CE1	-18.24	1.11	1.39
1	A	38	SER	C-N	-18.08	0.92	1.34
1	A	68	HIS	CD2-NE2	-18.01	0.98	1.38
1	A	26	GLN	CD-OE1	-17.99	0.84	1.24
1	A	129	ALA	C-O	-17.94	0.89	1.23
1	A	107	LYS	CD-CE	-17.93	1.06	1.51
1	A	103	VAL	C-N	-17.88	0.93	1.34
1	A	34	THR	CB-CG2	-17.60	0.94	1.52
1	A	101	VAL	CA-CB	-17.55	1.18	1.54
1	A	22	HIS	ND1-CE1	-17.54	0.91	1.34
1	A	101	VAL	C-N	-17.33	1.01	1.34
1	A	82	TYR	CZ-OH	-17.31	1.08	1.37
1	A	131	CYS	C-N	-17.20	0.94	1.34
1	A	50	VAL	CA-CB	-17.17	1.18	1.54
1	A	95	PHE	CD1-CE1	-17.16	1.04	1.39
1	A	95	PHE	CD2-CE2	-17.12	1.05	1.39
1	A	130	PRO	C-O	-17.11	0.89	1.23
1	A	121	GLU	C-N	-17.05	0.94	1.34
1	A	88	ASN	N-CA	-16.88	1.12	1.46
1	A	3	PHE	N-CA	-16.87	1.12	1.46
1	A	126	GLU	CB-CG	-16.75	1.20	1.52
1	A	20	LYS	CG-CD	-16.47	0.96	1.52
1	A	15	THR	C-O	-16.45	0.92	1.23
1	A	82	TYR	CD1-CE1	-16.43	1.14	1.39
1	A	84	ASP	C-O	-16.42	0.92	1.23
1	A	82	TYR	CD2-CE2	-16.39	1.14	1.39
1	A	62	MET	SD-CE	-16.37	0.86	1.77
1	A	2	GLU	CA-C	-16.36	1.10	1.52
1	A	14	GLN	CG-CD	-16.19	1.13	1.51
1	A	71	ARG	CA-CB	-16.18	1.18	1.53
1	A	24	SER	CB-OG	-16.16	1.21	1.42
1	A	70	SER	CA-CB	-16.11	1.28	1.52
1	A	38	SER	CA-C	-15.91	1.11	1.52
1	A	61	LYS	CD-CE	-15.88	1.11	1.51
1	A	10	GLN	CG-CD	-15.79	1.14	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ASN	CG-ND2	-15.64	0.93	1.32
1	A	120	ASP	N-CA	-15.46	1.15	1.46
1	A	42	MET	CG-SD	-15.24	1.41	1.81
1	A	129	ALA	C-N	-15.21	1.05	1.34
1	A	51	SER	CA-CB	-15.21	1.30	1.52
1	A	77	ASN	CG-OD1	-15.18	0.90	1.24
1	A	40	SER	N-CA	-15.04	1.16	1.46
1	A	124	ILE	CB-CG1	-15.03	1.11	1.54
1	A	126	GLU	CG-CD	-15.01	1.29	1.51
1	A	78	HIS	CG-ND1	-15.00	1.05	1.38
1	A	110	ILE	CG1-CD1	-14.96	0.47	1.50
1	A	89	GLN	CG-CD	-14.79	1.17	1.51
1	A	35	GLY	C-N	-14.79	1.00	1.34
1	A	120	ASP	C-N	-14.57	1.00	1.34
1	A	116	TYR	C-N	-14.48	1.00	1.34
1	A	48	LYS	CE-NZ	-14.48	1.12	1.49
1	A	51	SER	C-N	-14.46	1.07	1.33
1	A	49	MET	CB-CG	-14.44	1.05	1.51
1	A	54	ILE	CG1-CD1	-14.41	0.51	1.50
1	A	89	GLN	CB-CG	-14.41	1.13	1.52
1	A	77	ASN	CG-ND2	-14.40	0.96	1.32
1	A	124	ILE	CB-CG2	-14.38	1.08	1.52
1	A	106	LEU	CA-CB	-14.35	1.20	1.53
1	A	89	GLN	CA-CB	-14.34	1.22	1.53
1	A	68	HIS	CB-CG	-14.31	1.24	1.50
1	A	93	LEU	CB-CG	-14.30	1.11	1.52
1	A	88	ASN	C-N	-14.28	1.01	1.34
1	A	33	TYR	CB-CG	-14.25	1.30	1.51
1	A	38	SER	N-CA	-14.16	1.18	1.46
1	A	20	LYS	CB-CG	-14.07	1.14	1.52
1	A	50	VAL	C-O	-14.07	0.96	1.23
1	A	25	PHE	CD1-CE1	-14.05	1.11	1.39
1	A	25	PHE	CD2-CE2	-14.05	1.11	1.39
1	A	91	LEU	CG-CD2	-13.96	1.00	1.51
1	A	132	SER	C-N	-13.92	1.02	1.34
1	A	102	PRO	CA-C	-13.90	1.25	1.52
1	A	5	PHE	CB-CG	-13.74	1.27	1.51
1	A	15	THR	C-N	-13.66	1.02	1.34
1	A	39	ALA	CA-C	-13.61	1.17	1.52
1	A	71	ARG	CG-CD	-13.58	1.18	1.51
1	A	104	ARG	C-O	-13.46	0.97	1.23
1	A	134	ASP	N-CA	-13.41	1.19	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	TYR	CA-CB	-13.27	1.24	1.53
1	A	69	VAL	CB-CG1	-13.21	1.25	1.52
1	A	105	ASP	C-O	-13.15	0.98	1.23
1	A	57	LYS	CG-CD	-13.09	1.07	1.52
1	A	100	ASP	CB-CG	-13.08	1.24	1.51
1	A	119	THR	CA-C	-13.07	1.19	1.52
1	A	69	VAL	CA-CB	-13.00	1.27	1.54
1	A	87	SER	CA-C	-12.99	1.19	1.52
1	A	33	TYR	CZ-OH	-12.94	1.15	1.37
1	A	36	SER	CA-CB	-12.88	1.33	1.52
1	A	89	GLN	N-CA	-12.78	1.20	1.46
1	A	99	GLN	C-N	-12.76	1.04	1.34
1	A	13	PRO	C-N	-12.69	1.04	1.34
1	A	71	ARG	CB-CG	-12.63	1.18	1.52
1	A	64	GLU	CG-CD	-12.54	1.33	1.51
1	A	104	ARG	N-CA	-12.51	1.21	1.46
1	A	88	ASN	C-O	-12.50	0.99	1.23
1	A	37	ARG	CA-C	-12.31	1.21	1.52
1	A	133	LYS	CA-C	-12.29	1.21	1.52
1	A	136	GLY	C-N	-12.28	1.05	1.34
1	A	77	ASN	CB-CG	-12.25	1.22	1.51
1	A	65	ARG	CG-CD	-12.24	1.21	1.51
1	A	71	ARG	N-CA	-12.12	1.22	1.46
1	A	13	PRO	C-O	-12.10	0.99	1.23
1	A	103	VAL	N-CA	-12.08	1.22	1.46
1	A	135	LEU	CA-C	-12.03	1.21	1.52
1	A	54	ILE	CB-CG1	-11.99	1.20	1.54
1	A	124	ILE	CG1-CD1	-11.89	0.68	1.50
1	A	63	LEU	CG-CD1	-11.83	1.08	1.51
1	A	104	ARG	C-N	-11.81	1.06	1.34
1	A	85	LYS	CB-CG	-11.80	1.20	1.52
1	A	51	SER	C-O	-11.78	1.00	1.23
1	A	49	MET	SD-CE	-11.72	1.12	1.77
1	A	61	LYS	CG-CD	-11.69	1.12	1.52
1	A	2	GLU	C-N	-11.64	1.07	1.34
1	A	44	ILE	CB-CG1	-11.55	1.21	1.54
1	A	105	ASP	CA-CB	-11.54	1.28	1.53
1	A	84	ASP	C-N	-11.46	1.07	1.34
1	A	68	HIS	C-O	-11.45	1.01	1.23
1	A	76	SER	C-O	-11.42	1.01	1.23
1	A	133	LYS	N-CA	-11.41	1.23	1.46
1	A	117	TYR	N-CA	-11.38	1.23	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLN	CB-CG	-11.37	1.21	1.52
1	A	85	LYS	CG-CD	-11.34	1.13	1.52
1	A	100	ASP	CA-CB	-11.28	1.29	1.53
1	A	51	SER	N-CA	-11.26	1.23	1.46
1	A	33	TYR	CD2-CE2	-11.16	1.22	1.39
1	A	33	TYR	CD1-CE1	-11.13	1.22	1.39
1	A	85	LYS	CA-CB	-11.10	1.29	1.53
1	A	119	THR	N-CA	-11.05	1.24	1.46
1	A	7	LEU	CG-CD2	-11.05	1.10	1.51
1	A	103	VAL	CA-C	-10.97	1.24	1.52
1	A	79	VAL	CB-CG2	-10.93	1.29	1.52
1	A	86	VAL	N-CA	-10.93	1.24	1.46
1	A	68	HIS	ND1-CE1	-10.86	1.07	1.34
1	A	102	PRO	C-N	-10.78	1.09	1.34
1	A	106	LEU	C-O	-10.71	1.03	1.23
1	A	44	ILE	CB-CG2	-10.68	1.19	1.52
1	A	130	PRO	N-CA	-10.59	1.29	1.47
1	A	36	SER	C-N	-10.58	1.09	1.34
1	A	133	LYS	C-N	-10.54	1.09	1.34
1	A	4	PRO	CB-CG	-10.34	0.98	1.50
1	A	5	PHE	CD2-CE2	-10.23	1.18	1.39
1	A	5	PHE	CD1-CE1	-10.18	1.18	1.39
1	A	116	TYR	CA-C	-10.14	1.26	1.52
1	A	37	ARG	N-CA	-10.13	1.26	1.46
1	A	54	ILE	CB-CG2	-10.11	1.21	1.52
1	A	79	VAL	CB-CG1	-10.06	1.31	1.52
1	A	132	SER	CA-C	-10.05	1.26	1.52
1	A	7	LEU	CG-CD1	-9.95	1.15	1.51
1	A	26	GLN	CG-CD	-9.88	1.28	1.51
1	A	131	CYS	CA-CB	-9.71	1.32	1.53
1	A	17	ASP	C-O	-9.61	1.05	1.23
1	A	88	ASN	CA-C	-9.59	1.28	1.52
1	A	63	LEU	CG-CD2	-9.57	1.16	1.51
1	A	85	LYS	CA-C	-9.42	1.28	1.52
1	A	70	SER	CA-C	-9.38	1.28	1.52
1	A	112	LYS	CG-CD	-9.38	1.20	1.52
1	A	75	SER	CB-OG	-9.33	1.30	1.42
1	A	118	GLU	CA-C	-9.28	1.28	1.52
1	A	42	MET	SD-CE	-9.09	1.26	1.77
1	A	105	ASP	C-N	-9.07	1.13	1.34
1	A	102	PRO	N-CA	-8.99	1.31	1.47
1	A	89	GLN	C-O	-8.87	1.06	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	THR	CB-OG1	-8.63	1.25	1.43
1	A	36	SER	CA-C	-8.61	1.30	1.52
1	A	102	PRO	CG-CD	-8.55	1.22	1.50
1	A	92	SER	CB-OG	-8.54	1.31	1.42
1	A	67	ASN	CB-CG	-8.50	1.31	1.51
1	A	130	PRO	CG-CD	-8.49	1.22	1.50
1	A	122	PHE	CB-CG	-8.48	1.36	1.51
1	A	69	VAL	C-O	-8.44	1.07	1.23
1	A	62	MET	CB-CG	-8.38	1.24	1.51
1	A	49	MET	C-O	-8.20	1.07	1.23
1	A	131	CYS	N-CA	-8.12	1.30	1.46
1	A	80	LEU	CG-CD2	-8.09	1.22	1.51
1	A	14	GLN	C-N	-8.03	1.15	1.34
1	A	50	VAL	CA-C	-8.00	1.32	1.52
1	A	114	TYR	CZ-OH	-7.95	1.24	1.37
1	A	114	TYR	CB-CG	-7.93	1.39	1.51
1	A	106	LEU	N-CA	-7.90	1.30	1.46
1	A	132	SER	N-CA	-7.88	1.30	1.46
1	A	131	CYS	CA-C	-7.82	1.32	1.52
1	A	68	HIS	C-N	-7.81	1.16	1.34
1	A	98	LEU	C-O	-7.73	1.08	1.23
1	A	70	SER	N-CA	-7.71	1.30	1.46
1	A	14	GLN	C-O	-7.64	1.08	1.23
1	A	48	LYS	CB-CG	-7.60	1.32	1.52
1	A	98	LEU	C-N	-7.41	1.17	1.34
1	A	76	SER	C-N	-7.31	1.17	1.34
1	A	129	ALA	CA-CB	-7.29	1.37	1.52
1	A	89	GLN	C-N	-7.14	1.17	1.34
1	A	67	ASN	C-O	-7.06	1.09	1.23
1	A	17	ASP	C-N	-7.04	1.17	1.34
1	A	99	GLN	CA-CB	-7.01	1.38	1.53
1	A	7	LEU	CB-CG	-6.97	1.32	1.52
1	A	107	LYS	N-CA	-6.96	1.32	1.46
1	A	130	PRO	CA-C	-6.92	1.39	1.52
1	A	101	VAL	N-CA	-6.90	1.32	1.46
1	A	129	ALA	CA-C	-6.79	1.35	1.52
1	A	70	SER	C-N	-6.75	1.18	1.34
1	A	17	ASP	CB-CG	-6.72	1.37	1.51
1	A	122	PHE	N-CA	-6.67	1.33	1.46
1	A	69	VAL	CA-C	-6.61	1.35	1.52
1	A	107	LYS	CA-CB	-6.61	1.39	1.53
1	A	70	SER	C-O	-6.57	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	THR	CA-CB	-6.50	1.36	1.53
1	A	106	LEU	C-N	-6.48	1.19	1.34
1	A	100	ASP	N-CA	-6.46	1.33	1.46
1	A	16	CYS	N-CA	-6.34	1.33	1.46
1	A	35	GLY	CA-C	-6.33	1.41	1.51
1	A	105	ASP	CA-C	-6.32	1.36	1.52
1	A	73	GLU	CB-CG	-6.24	1.40	1.52
1	A	130	PRO	CB-CG	-6.16	1.19	1.50
1	A	65	ARG	CB-CG	-6.15	1.35	1.52
1	A	122	PHE	CD1-CE1	-6.08	1.27	1.39
1	A	122	PHE	CD2-CE2	-6.04	1.27	1.39
1	A	16	CYS	CA-CB	-5.89	1.41	1.53
1	A	102	PRO	CB-CG	-5.86	1.20	1.50
1	A	78	HIS	CD2-NE2	-5.82	1.25	1.38
1	A	48	LYS	CG-CD	-5.78	1.32	1.52
1	A	66	SER	CA-CB	-5.66	1.44	1.52
1	A	101	VAL	CA-C	-5.66	1.38	1.52
1	A	106	LEU	CA-C	-5.66	1.38	1.52
1	A	84	ASP	CA-CB	-5.52	1.41	1.53
1	A	99	GLN	CA-C	-5.51	1.38	1.52
1	A	128	ASN	C-O	-5.46	1.12	1.23
1	A	78	HIS	ND1-CE1	-5.39	1.21	1.34
1	A	19	PRO	N-CD	-5.35	1.40	1.47
1	A	69	VAL	CB-CG2	-5.26	1.41	1.52
1	A	121	GLU	CA-C	-5.21	1.39	1.52
1	A	61	LYS	CB-CG	-5.20	1.38	1.52
1	A	49	MET	CA-CB	-5.12	1.42	1.53
1	A	114	TYR	CD2-CE2	-5.12	1.31	1.39
1	A	114	TYR	CD1-CE1	-5.12	1.31	1.39

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	NE-CZ-NH1	-88.29	76.15	120.30
1	A	116	TYR	CB-CG-CD2	84.23	171.54	121.00
1	A	116	TYR	CD1-CG-CD2	-82.21	27.47	117.90
1	A	37	ARG	NE-CZ-NH1	78.96	159.78	120.30
1	A	5	PHE	CD1-CG-CD2	-77.94	16.98	118.30
1	A	82	TYR	CD1-CG-CD2	-76.77	33.45	117.90
1	A	5	PHE	CB-CG-CD1	73.69	172.38	120.80
1	A	37	ARG	NE-CZ-NH2	72.67	156.64	120.30
1	A	122	PHE	CD1-CG-CD2	-72.47	24.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	PHE	CB-CG-CD2	71.19	170.63	120.80
1	A	82	TYR	CB-CG-CD2	70.69	163.41	121.00
1	A	82	TYR	CB-CG-CD1	70.22	163.13	121.00
1	A	37	ARG	NH1-CZ-NH2	-68.93	43.58	119.40
1	A	122	PHE	CB-CG-CD1	68.37	168.66	120.80
1	A	53	PHE	CB-CG-CD1	68.36	168.65	120.80
1	A	3	PHE	CB-CG-CD1	67.89	168.32	120.80
1	A	126	GLU	OE1-CD-OE2	-67.04	42.85	123.30
1	A	116	TYR	CB-CG-CD1	66.65	160.99	121.00
1	A	122	PHE	CB-CG-CD2	66.36	167.25	120.80
1	A	65	ARG	NE-CZ-NH2	65.91	153.25	120.30
1	A	71	ARG	NE-CZ-NH2	64.94	152.77	120.30
1	A	116	TYR	CG-CD2-CE2	62.84	171.57	121.30
1	A	53	PHE	CD1-CG-CD2	-61.63	38.19	118.30
1	A	94	PHE	CD1-CG-CD2	-61.34	38.56	118.30
1	A	68	HIS	ND1-CG-CD2	-61.09	20.48	106.00
1	A	100	ASP	O-C-N	-60.97	25.14	122.70
1	A	94	PHE	CB-CG-CD2	60.16	162.91	120.80
1	A	45	VAL	CG1-CB-CG2	-59.05	16.41	110.90
1	A	64	GLU	OE1-CD-OE2	-58.97	52.54	123.30
1	A	5	PHE	CE1-CZ-CE2	-57.25	16.95	120.00
1	A	116	TYR	CD1-CE1-CZ	57.02	171.12	119.80
1	A	116	TYR	CE1-CZ-CE2	-56.26	29.78	119.80
1	A	114	TYR	CD1-CG-CD2	-55.63	56.70	117.90
1	A	105	ASP	CB-CG-OD2	54.23	167.11	118.30
1	A	94	PHE	CB-CG-CD1	53.89	158.52	120.80
1	A	33	TYR	CD1-CG-CD2	-53.56	58.99	117.90
1	A	122	PHE	CE1-CZ-CE2	-53.22	24.20	120.00
1	A	82	TYR	CE1-CZ-CE2	-52.72	35.45	119.80
1	A	82	TYR	CG-CD2-CE2	52.64	163.41	121.30
1	A	33	TYR	CB-CG-CD2	52.38	152.43	121.00
1	A	82	TYR	CG-CD1-CE1	52.29	163.13	121.30
1	A	114	TYR	CB-CG-CD2	51.42	151.85	121.00
1	A	114	TYR	CB-CG-CD1	50.74	151.45	121.00
1	A	46	ASP	CB-CG-OD1	-50.68	72.69	118.30
1	A	115	ASP	O-C-N	-50.36	42.12	122.70
1	A	105	ASP	CB-CG-OD1	50.17	163.46	118.30
1	A	116	TYR	CG-CD1-CE1	49.60	160.98	121.30
1	A	105	ASP	OD1-CG-OD2	-49.40	29.44	123.30
1	A	101	VAL	CG1-CB-CG2	-48.14	33.88	110.90
1	A	82	TYR	CD1-CE1-CZ	47.44	162.50	119.80
1	A	1	GLU	OE1-CD-OE2	-47.31	66.53	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	TYR	CZ-CE2-CD2	46.96	162.06	119.80
1	A	5	PHE	CG-CD1-CE1	46.91	172.40	120.80
1	A	53	PHE	CB-CG-CD2	46.23	153.16	120.80
1	A	33	TYR	CB-CG-CD1	45.98	148.59	121.00
1	A	53	PHE	CE1-CZ-CE2	-45.40	38.27	120.00
1	A	94	PHE	CE1-CZ-CE2	-45.28	38.50	120.00
1	A	5	PHE	CG-CD2-CE2	45.27	170.59	120.80
1	A	137	ASN	CB-CA-C	-45.23	19.94	110.40
1	A	134	ASP	CB-CG-OD2	-44.87	77.91	118.30
1	A	46	ASP	CB-CG-OD2	44.00	157.90	118.30
1	A	116	TYR	CZ-CE2-CD2	43.63	159.07	119.80
1	A	5	PHE	CZ-CE2-CD2	43.61	172.44	120.10
1	A	122	PHE	CG-CD1-CE1	43.56	168.72	120.80
1	A	53	PHE	CG-CD1-CE1	43.51	168.67	120.80
1	A	3	PHE	CG-CD1-CE1	43.24	168.36	120.80
1	A	85	LYS	O-C-N	-42.95	53.98	122.70
1	A	122	PHE	CG-CD2-CE2	42.23	167.25	120.80
1	A	5	PHE	CD1-CE1-CZ	42.11	170.64	120.10
1	A	25	PHE	CB-CG-CD1	41.63	149.94	120.80
1	A	41	ASN	O-C-N	-41.50	56.30	122.70
1	A	68	HIS	CG-ND1-CE1	40.98	165.57	108.20
1	A	25	PHE	CD1-CG-CD2	-40.61	65.50	118.30
1	A	122	PHE	CZ-CE2-CD2	40.41	168.60	120.10
1	A	53	PHE	CZ-CE2-CD2	40.35	168.52	120.10
1	A	3	PHE	CZ-CE2-CD2	40.22	168.37	120.10
1	A	136	GLY	CA-C-O	-40.18	48.28	120.60
1	A	101	VAL	CA-CB-CG1	40.10	171.05	110.90
1	A	45	VAL	CA-CB-CG1	39.83	170.64	110.90
1	A	45	VAL	CA-CB-CG2	39.80	170.60	110.90
1	A	137	ASN	CB-CG-OD1	-39.35	42.89	121.60
1	A	122	PHE	CD1-CE1-CZ	39.21	167.15	120.10
1	A	120	ASP	CB-CG-OD2	39.06	153.45	118.30
1	A	33	TYR	CG-CD2-CE2	38.97	152.47	121.30
1	A	117	TYR	CB-CG-CD1	38.42	144.05	121.00
1	A	94	PHE	CG-CD2-CE2	38.25	162.88	120.80
1	A	114	TYR	CG-CD2-CE2	38.20	151.86	121.30
1	A	114	TYR	CG-CD1-CE1	37.67	151.44	121.30
1	A	84	ASP	CB-CG-OD2	37.62	152.16	118.30
1	A	114	TYR	CE1-CZ-CE2	-37.58	59.68	119.80
1	A	33	TYR	CE1-CZ-CE2	-36.00	62.20	119.80
1	A	94	PHE	CD1-CE1-CZ	35.64	162.87	120.10
1	A	71	ARG	NH1-CZ-NH2	-35.48	80.38	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	VAL	CG1-CB-CG2	-34.96	54.96	110.90
1	A	33	TYR	CD1-CE1-CZ	34.79	151.11	119.80
1	A	118	GLU	OE1-CD-OE2	-34.78	81.56	123.30
1	A	115	ASP	CB-CG-OD1	34.52	149.37	118.30
1	A	94	PHE	CG-CD1-CE1	34.29	158.52	120.80
1	A	2	GLU	CA-C-O	-34.12	48.45	120.10
1	A	33	TYR	CG-CD1-CE1	34.10	148.58	121.30
1	A	114	TYR	CD1-CE1-CZ	34.05	150.44	119.80
1	A	25	PHE	CB-CG-CD2	33.93	144.55	120.80
1	A	42	MET	CA-CB-CG	33.58	170.38	113.30
1	A	115	ASP	CB-CG-OD2	-33.56	88.10	118.30
1	A	114	TYR	CZ-CE2-CD2	33.42	149.88	119.80
1	A	95	PHE	CB-CG-CD1	33.19	144.03	120.80
1	A	18	GLU	OE1-CD-OE2	-32.78	83.96	123.30
1	A	99	GLN	OE1-CD-NE2	-32.52	47.10	121.90
1	A	94	PHE	CZ-CE2-CD2	32.14	158.66	120.10
1	A	137	ASN	N-CA-CB	31.66	167.60	110.60
1	A	12	LEU	CB-CG-CD1	31.61	164.73	111.00
1	A	84	ASP	OD1-CG-OD2	-31.57	63.32	123.30
1	A	68	HIS	CG-CD2-NE2	31.43	168.92	109.20
1	A	131	CYS	O-C-N	-31.32	72.58	122.70
1	A	135	LEU	O-C-N	-31.31	69.98	123.20
1	A	120	ASP	OD1-CG-OD2	-30.77	64.85	123.30
1	A	113	VAL	CG1-CB-CG2	-30.75	61.70	110.90
1	A	127	TYR	CB-CG-CD2	30.70	139.42	121.00
1	A	25	PHE	CE1-CZ-CE2	-30.34	65.39	120.00
1	A	127	TYR	CD1-CG-CD2	-30.18	84.70	117.90
1	A	33	TYR	CZ-CE2-CD2	29.83	146.65	119.80
1	A	137	ASN	CA-CB-CG	29.79	178.94	113.40
1	A	53	PHE	CG-CD2-CE2	29.46	153.21	120.80
1	A	40	SER	CB-CA-C	-29.39	54.27	110.10
1	A	84	ASP	CB-CG-OD1	29.13	144.52	118.30
1	A	66	SER	O-C-N	-28.90	76.45	122.70
1	A	117	TYR	CD1-CG-CD2	-28.78	86.24	117.90
1	A	117	TYR	CG-CD1-CE1	28.35	143.98	121.30
1	A	73	GLU	OE1-CD-OE2	-28.11	89.57	123.30
1	A	118	GLU	O-C-N	-27.96	77.96	122.70
1	A	17	ASP	CB-CG-OD1	27.55	143.09	118.30
1	A	53	PHE	CD1-CE1-CZ	27.54	153.15	120.10
1	A	112	LYS	CA-CB-CG	27.42	173.72	113.40
1	A	101	VAL	CA-CB-CG2	27.32	151.87	110.90
1	A	41	ASN	N-CA-CB	-26.98	62.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	CD-NE-CZ	26.54	160.76	123.60
1	A	25	PHE	CG-CD1-CE1	26.49	149.94	120.80
1	A	135	LEU	N-CA-CB	-26.34	57.71	110.40
1	A	3	PHE	CB-CG-CD2	-26.29	102.40	120.80
1	A	120	ASP	CB-CG-OD1	26.00	141.70	118.30
1	A	40	SER	CA-C-O	-25.90	65.71	120.10
1	A	104	ARG	NE-CZ-NH2	25.68	133.14	120.30
1	A	60	VAL	CA-CB-CG1	25.65	149.37	110.90
1	A	12	LEU	CD1-CG-CD2	-25.60	33.69	110.50
1	A	22	HIS	ND1-CG-CD2	-25.55	70.24	106.00
1	A	117	TYR	CZ-CE2-CD2	25.52	142.77	119.80
1	A	49	MET	CG-SD-CE	25.42	140.87	100.20
1	A	12	LEU	CB-CG-CD2	25.39	154.16	111.00
1	A	119	THR	O-C-N	-25.37	82.11	122.70
1	A	134	ASP	O-C-N	-25.25	82.29	122.70
1	A	97	VAL	CG1-CB-CG2	-24.98	70.94	110.90
1	A	25	PHE	CZ-CE2-CD2	24.86	149.94	120.10
1	A	127	TYR	CB-CG-CD1	24.79	135.88	121.00
1	A	106	LEU	CB-CG-CD2	24.62	152.85	111.00
1	A	2	GLU	CA-C-N	24.53	171.17	117.20
1	A	17	ASP	OD1-CG-OD2	-24.44	76.86	123.30
1	A	17	ASP	CB-CG-OD2	24.16	140.04	118.30
1	A	60	VAL	CA-CB-CG2	24.15	147.12	110.90
1	A	136	GLY	N-CA-C	24.14	173.45	113.10
1	A	39	ALA	N-CA-CB	-23.99	76.52	110.10
1	A	113	VAL	CA-CB-CG2	23.78	146.57	110.90
1	A	68	HIS	CE1-NE2-CD2	-23.77	47.19	106.60
1	A	39	ALA	O-C-N	-23.65	84.85	122.70
1	A	83	LEU	CA-CB-CG	23.37	169.06	115.30
1	A	100	ASP	CA-C-O	23.24	168.90	120.10
1	A	57	LYS	CD-CE-NZ	23.19	165.04	111.70
1	A	71	ARG	CD-NE-CZ	23.04	155.86	123.60
1	A	127	TYR	CG-CD2-CE2	22.63	139.41	121.30
1	A	65	ARG	CD-NE-CZ	22.61	155.25	123.60
1	A	136	GLY	CA-C-N	22.52	166.75	117.20
1	A	3	PHE	CD1-CG-CD2	-22.32	89.28	118.30
1	A	126	GLU	CG-CD-OE1	22.23	162.76	118.30
1	A	100	ASP	CA-C-N	22.16	165.96	117.20
1	A	137	ASN	CA-C-N	21.92	165.42	117.20
1	A	106	LEU	CA-CB-CG	21.91	165.69	115.30
1	A	14	GLN	OE1-CD-NE2	-21.85	71.65	121.90
1	A	89	GLN	OE1-CD-NE2	-21.83	71.69	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	LYS	CD-CE-NZ	21.71	161.63	111.70
1	A	86	VAL	O-C-N	-21.70	87.98	122.70
1	A	25	PHE	CG-CD2-CE2	21.60	144.56	120.80
1	A	137	ASN	N-CA-C	21.39	168.76	111.00
1	A	86	VAL	CG1-CB-CG2	21.10	144.66	110.90
1	A	95	PHE	CG-CD1-CE1	21.07	143.98	120.80
1	A	137	ASN	CA-C-O	-21.00	75.99	120.10
1	A	113	VAL	CA-CB-CG1	20.98	142.37	110.90
1	A	83	LEU	CB-CG-CD2	20.82	146.40	111.00
1	A	22	HIS	CG-ND1-CE1	20.62	137.07	108.20
1	A	78	HIS	ND1-CG-CD2	-20.61	77.15	106.00
1	A	87	SER	CA-CB-OG	20.60	166.82	111.20
1	A	137	ASN	CB-CG-ND2	20.59	166.11	116.70
1	A	29	LEU	CB-CG-CD1	20.58	145.98	111.00
1	A	95	PHE	CD1-CG-CD2	-20.56	91.57	118.30
1	A	131	CYS	CA-C-N	20.54	162.40	117.20
1	A	25	PHE	CD1-CE1-CZ	20.48	144.68	120.10
1	A	42	MET	CG-SD-CE	20.45	132.92	100.20
1	A	40	SER	N-CA-CB	20.36	141.04	110.50
1	A	112	LYS	CB-CG-CD	20.32	164.43	111.60
1	A	40	SER	CA-C-N	20.28	161.81	117.20
1	A	2	GLU	C-N-CA	20.22	172.24	121.70
1	A	20	LYS	CB-CG-CD	19.96	163.50	111.60
1	A	95	PHE	CZ-CE2-CD2	19.95	144.03	120.10
1	A	115	ASP	CA-C-N	19.88	160.94	117.20
1	A	127	TYR	CD1-CE1-CZ	19.87	137.69	119.80
1	A	138	ALA	N-CA-C	19.75	164.34	111.00
1	A	127	TYR	CE1-CZ-CE2	-19.72	88.25	119.80
1	A	85	LYS	CA-C-N	19.70	160.55	117.20
1	A	39	ALA	CA-C-N	19.69	160.51	117.20
1	A	110	ILE	CG1-CB-CG2	-19.53	68.44	111.40
1	A	97	VAL	CA-CB-CG2	19.39	139.99	110.90
1	A	100	ASP	CB-CG-OD2	19.32	135.69	118.30
1	A	10	GLN	OE1-CD-NE2	-19.20	77.74	121.90
1	A	41	ASN	CA-C-N	19.18	159.40	117.20
1	A	48	LYS	CD-CE-NZ	19.00	155.39	111.70
1	A	116	TYR	CE1-CZ-OH	18.91	171.15	120.10
1	A	64	GLU	CG-CD-OE1	18.87	156.03	118.30
1	A	117	TYR	CE1-CZ-CE2	-18.78	89.75	119.80
1	A	40	SER	N-CA-C	18.71	161.52	111.00
1	A	136	GLY	C-N-CA	18.71	168.47	121.70
1	A	57	LYS	CG-CD-CE	18.52	167.48	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	VAL	CA-C-N	18.51	157.93	117.20
1	A	99	GLN	CG-CD-NE2	18.43	160.92	116.70
1	A	14	GLN	CB-CG-CD	18.26	159.09	111.60
1	A	127	TYR	CG-CD1-CE1	18.26	135.91	121.30
1	A	31	VAL	CG1-CB-CG2	-18.23	81.73	110.90
1	A	137	ASN	C-N-CA	18.17	167.13	121.70
1	A	126	GLU	CG-CD-OE2	18.04	154.39	118.30
1	A	100	ASP	C-N-CA	17.99	166.67	121.70
1	A	97	VAL	CA-CB-CG1	17.89	137.74	110.90
1	A	100	ASP	CB-CG-OD1	17.72	134.25	118.30
1	A	68	HIS	CB-CG-ND1	17.71	167.48	123.20
1	A	118	GLU	CG-CD-OE2	17.69	153.68	118.30
1	A	115	ASP	CA-C-O	17.54	156.94	120.10
1	A	100	ASP	OD1-CG-OD2	-17.49	90.07	123.30
1	A	134	ASP	CB-CG-OD1	17.49	134.04	118.30
1	A	49	MET	CA-CB-CG	17.39	142.86	113.30
1	A	46	ASP	CA-CB-CG	17.37	151.62	113.40
1	A	104	ARG	NH1-CZ-NH2	-17.35	100.32	119.40
1	A	39	ALA	N-CA-C	17.22	157.50	111.00
1	A	112	LYS	CG-CD-CE	17.18	163.43	111.90
1	A	2	GLU	N-CA-CB	-17.14	79.75	110.60
1	A	99	GLN	CB-CG-CD	17.11	156.08	111.60
1	A	134	ASP	N-CA-C	17.11	157.19	111.00
1	A	3	PHE	CE1-CZ-CE2	-17.10	89.22	120.00
1	A	40	SER	C-N-CA	16.96	164.10	121.70
1	A	131	CYS	C-N-CA	16.92	164.01	121.70
1	A	118	GLU	N-CA-CB	-16.87	80.23	110.60
1	A	121	GLU	CB-CG-CD	16.86	159.72	114.20
1	A	78	HIS	CG-ND1-CE1	16.83	131.76	108.20
1	A	3	PHE	CG-CD2-CE2	-16.74	102.39	120.80
1	A	64	GLU	CG-CD-OE2	16.57	151.43	118.30
1	A	1	GLU	CA-C-N	16.53	153.56	117.20
1	A	9	VAL	CG1-CB-CG2	-16.41	84.65	110.90
1	A	41	ASN	N-CA-C	16.38	155.23	111.00
1	A	1	GLU	CG-CD-OE2	16.35	151.00	118.30
1	A	39	ALA	C-N-CA	16.26	162.35	121.70
1	A	115	ASP	C-N-CA	16.17	162.12	121.70
1	A	85	LYS	C-N-CA	16.14	162.04	121.70
1	A	134	ASP	CA-C-N	15.95	152.28	117.20
1	A	106	LEU	CB-CG-CD1	15.89	138.02	111.00
1	A	95	PHE	CE1-CZ-CE2	-15.85	91.47	120.00
1	A	127	TYR	CZ-CE2-CD2	15.83	134.05	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ILE	CA-CB-CG1	15.77	140.96	111.00
1	A	86	VAL	N-CA-C	15.72	153.44	111.00
1	A	66	SER	CA-C-N	15.71	151.76	117.20
1	A	82	TYR	CE1-CZ-OH	15.69	162.47	120.10
1	A	41	ASN	C-N-CA	15.69	160.92	121.70
1	A	41	ASN	CB-CG-ND2	15.69	154.35	116.70
1	A	135	LEU	CB-CA-C	15.57	139.78	110.20
1	A	82	TYR	OH-CZ-CE2	15.55	162.08	120.10
1	A	31	VAL	CA-CB-CG1	15.49	134.13	110.90
1	A	73	GLU	CG-CD-OE2	15.42	149.14	118.30
1	A	86	VAL	C-N-CA	15.35	160.08	121.70
1	A	56	LEU	CB-CG-CD2	15.29	137.00	111.00
1	A	118	GLU	N-CA-C	15.23	152.12	111.00
1	A	135	LEU	N-CA-C	15.22	152.08	111.00
1	A	119	THR	CA-CB-OG1	15.21	140.94	109.00
1	A	99	GLN	CG-CD-OE1	15.19	151.98	121.60
1	A	34	THR	O-C-N	-15.10	97.52	123.20
1	A	1	GLU	CA-CB-CG	14.91	146.21	113.40
1	A	56	LEU	CB-CG-CD1	14.88	136.30	111.00
1	A	119	THR	CA-C-N	14.83	149.84	117.20
1	A	134	ASP	N-CA-CB	-14.82	83.92	110.60
1	A	110	ILE	CA-CB-CG2	14.77	140.45	110.90
1	A	3	PHE	CD1-CE1-CZ	-14.76	102.39	120.10
1	A	1	GLU	CA-C-O	-14.67	89.28	120.10
1	A	121	GLU	CG-CD-OE2	14.58	147.46	118.30
1	A	47	VAL	CG1-CB-CG2	-14.56	87.61	110.90
1	A	117	TYR	CB-CG-CD2	14.51	129.71	121.00
1	A	88	ASN	CB-CG-ND2	14.46	151.40	116.70
1	A	116	TYR	OH-CZ-CE2	14.43	159.07	120.10
1	A	117	TYR	N-CA-C	14.39	149.86	111.00
1	A	103	VAL	O-C-N	-14.23	99.93	122.70
1	A	135	LEU	CA-C-O	14.14	149.80	120.10
1	A	2	GLU	N-CA-C	14.06	148.97	111.00
1	A	106	LEU	CD1-CG-CD2	-14.05	68.36	110.50
1	A	41	ASN	CA-CB-CG	13.97	144.14	113.40
1	A	1	GLU	C-N-CA	13.92	156.51	121.70
1	A	136	GLY	O-C-N	13.92	144.97	122.70
1	A	133	LYS	CB-CG-CD	13.90	147.74	111.60
1	A	118	GLU	CA-C-N	13.87	147.72	117.20
1	A	41	ASN	CB-CG-OD1	-13.85	93.91	121.60
1	A	37	ARG	O-C-N	-13.81	100.60	122.70
1	A	130	PRO	O-C-N	-13.79	100.64	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PHE	CB-CA-C	-13.51	83.37	110.40
1	A	128	ASN	OD1-CG-ND2	-13.44	90.99	121.90
1	A	120	ASP	CA-C-O	-13.40	91.96	120.10
1	A	18	GLU	CG-CD-OE1	13.35	145.00	118.30
1	A	68	HIS	CB-CG-CD2	13.30	172.04	130.80
1	A	47	VAL	CA-CB-CG2	13.29	130.84	110.90
1	A	35	GLY	O-C-N	-13.29	101.44	122.70
1	A	134	ASP	C-N-CA	13.20	154.70	121.70
1	A	9	VAL	CA-CB-CG2	13.16	130.64	110.90
1	A	29	LEU	CD1-CG-CD2	-13.12	71.15	110.50
1	A	71	ARG	NE-CZ-NH1	13.11	126.85	120.30
1	A	14	GLN	CG-CD-NE2	13.07	148.06	116.70
1	A	138	ALA	CB-CA-C	-13.06	90.51	110.10
1	A	134	ASP	OD1-CG-OD2	13.03	148.05	123.30
1	A	93	LEU	CB-CG-CD1	12.98	133.07	111.00
1	A	120	ASP	CA-C-N	12.98	145.75	117.20
1	A	133	LYS	CD-CE-NZ	12.97	141.52	111.70
1	A	66	SER	C-N-CA	12.92	154.01	121.70
1	A	48	LYS	CG-CD-CE	12.82	150.35	111.90
1	A	29	LEU	CB-CG-CD2	12.76	132.69	111.00
1	A	4	PRO	N-CA-CB	-12.72	88.04	103.30
1	A	68	HIS	ND1-CE1-NE2	12.70	137.85	109.90
1	A	31	VAL	CA-CB-CG2	12.69	129.93	110.90
1	A	137	ASN	OD1-CG-ND2	12.65	151.00	121.90
1	A	9	VAL	CA-CB-CG1	12.54	129.72	110.90
1	A	22	HIS	CG-CD2-NE2	12.51	132.98	109.20
1	A	104	ARG	NE-CZ-NH1	12.49	126.54	120.30
1	A	89	GLN	CG-CD-NE2	12.44	146.55	116.70
1	A	1	GLU	CB-CG-CD	12.41	147.71	114.20
1	A	2	GLU	CG-CD-OE2	-12.40	93.49	118.30
1	A	119	THR	C-N-CA	12.25	152.32	121.70
1	A	37	ARG	CG-CD-NE	12.23	137.49	111.80
1	A	20	LYS	CD-CE-NZ	12.19	139.73	111.70
1	A	2	GLU	CG-CD-OE1	12.13	142.56	118.30
1	A	1	GLU	CG-CD-OE1	12.09	142.47	118.30
1	A	85	LYS	CA-C-O	12.08	145.47	120.10
1	A	37	ARG	CA-CB-CG	-12.07	86.85	113.40
1	A	107	LYS	CD-CE-NZ	12.04	139.39	111.70
1	A	135	LEU	CA-C-N	12.01	140.22	116.20
1	A	86	VAL	CA-CB-CG1	-11.94	92.99	110.90
1	A	15	THR	CA-CB-CG2	11.93	129.09	112.40
1	A	111	VAL	CG1-CB-CG2	-11.91	91.84	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	GLU	CB-CA-C	11.85	134.10	110.40
1	A	131	CYS	CA-CB-SG	11.81	135.26	114.00
1	A	56	LEU	CD1-CG-CD2	-11.79	75.14	110.50
1	A	115	ASP	CA-CB-CG	11.72	139.18	113.40
1	A	121	GLU	O-C-N	-11.70	103.99	122.70
1	A	10	GLN	CG-CD-NE2	11.69	144.74	116.70
1	A	87	SER	N-CA-CB	-11.54	93.19	110.50
1	A	41	ASN	CA-C-O	11.52	144.30	120.10
1	A	33	TYR	CE1-CZ-OH	11.51	151.18	120.10
1	A	87	SER	O-C-N	-11.49	104.32	122.70
1	A	41	ASN	CB-CA-C	11.48	133.35	110.40
1	A	117	TYR	CA-C-N	11.42	142.32	117.20
1	A	103	VAL	CA-C-N	11.41	142.31	117.20
1	A	118	GLU	C-N-CA	11.39	150.17	121.70
1	A	37	ARG	CA-C-N	11.33	142.13	117.20
1	A	121	GLU	CG-CD-OE1	-11.27	95.75	118.30
1	A	114	TYR	CE1-CZ-OH	11.24	150.44	120.10
1	A	120	ASP	C-N-CA	11.20	149.70	121.70
1	A	117	TYR	CB-CA-C	-11.20	88.00	110.40
1	A	95	PHE	CA-CB-CG	11.17	140.71	113.90
1	A	133	LYS	CG-CD-CE	11.12	145.27	111.90
1	A	34	THR	CA-CB-CG2	11.10	127.94	112.40
1	A	2	GLU	O-C-N	11.05	140.38	122.70
1	A	114	TYR	OH-CZ-CE2	11.03	149.88	120.10
1	A	16	CYS	CA-CB-SG	11.02	133.83	114.00
1	A	71	ARG	CB-CG-CD	10.94	140.05	111.60
1	A	65	ARG	CG-CD-NE	10.77	134.42	111.80
1	A	138	ALA	CA-C-O	10.77	142.71	120.10
1	A	3	PHE	CA-CB-CG	-10.74	88.12	113.90
1	A	91	LEU	CA-CB-CG	10.68	139.87	115.30
1	A	117	TYR	CG-CD2-CE2	10.50	129.70	121.30
1	A	30	SER	CA-CB-OG	10.45	139.41	111.20
1	A	49	MET	CB-CG-SD	10.40	143.60	112.40
1	A	121	GLU	N-CA-CB	-10.36	91.95	110.60
1	A	104	ARG	CD-NE-CZ	10.31	138.03	123.60
1	A	78	HIS	CG-CD2-NE2	10.27	128.71	109.20
1	A	47	VAL	CA-CB-CG1	10.19	126.19	110.90
1	A	104	ARG	CA-CB-CG	10.18	135.80	113.40
1	A	65	ARG	NH1-CZ-NH2	10.17	130.59	119.40
1	A	117	TYR	O-C-N	-10.13	106.49	122.70
1	A	89	GLN	CG-CD-OE1	10.08	141.76	121.60
1	A	133	LYS	CA-C-N	10.00	139.20	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	TYR	CA-C-N	9.94	139.08	117.20
1	A	83	LEU	CD1-CG-CD2	-9.91	80.76	110.50
1	A	57	LYS	CB-CG-CD	9.87	137.25	111.60
1	A	33	TYR	OH-CZ-CE2	9.82	146.62	120.10
1	A	111	VAL	CA-CB-CG1	9.78	125.56	110.90
1	A	111	VAL	CA-CB-CG2	9.77	125.56	110.90
1	A	42	MET	CB-CG-SD	9.72	141.55	112.40
1	A	117	TYR	C-N-CA	9.71	145.98	121.70
1	A	103	VAL	C-N-CA	9.62	145.75	121.70
1	A	116	TYR	O-C-N	-9.59	107.36	122.70
1	A	135	LEU	C-N-CA	9.56	142.38	122.30
1	A	132	SER	CA-CB-OG	9.56	137.00	111.20
1	A	107	LYS	CB-CG-CD	9.55	136.44	111.60
1	A	37	ARG	C-N-CA	9.51	145.48	121.70
1	A	44	ILE	CB-CG1-CD1	9.49	140.47	113.90
1	A	14	GLN	CG-CD-OE1	9.35	140.29	121.60
1	A	54	ILE	CB-CG1-CD1	9.26	139.84	113.90
1	A	118	GLU	CA-CB-CG	9.26	133.78	113.40
1	A	135	LEU	CB-CG-CD2	9.25	126.73	111.00
1	A	119	THR	OG1-CB-CG2	-9.23	88.78	110.00
1	A	34	THR	OG1-CB-CG2	-9.22	88.79	110.00
1	A	120	ASP	CA-CB-CG	9.10	133.42	113.40
1	A	61	LYS	CD-CE-NZ	9.03	132.47	111.70
1	A	132	SER	CA-C-N	9.01	137.03	117.20
1	A	99	GLN	CA-CB-CG	8.80	132.76	113.40
1	A	134	ASP	CA-CB-CG	8.78	132.71	113.40
1	A	133	LYS	C-N-CA	8.73	143.53	121.70
1	A	38	SER	N-CA-C	8.72	134.54	111.00
1	A	22	HIS	CB-CG-ND1	8.71	144.97	123.20
1	A	3	PHE	N-CA-C	8.70	134.48	111.00
1	A	103	VAL	CA-CB-CG2	8.69	123.94	110.90
1	A	117	TYR	CD1-CE1-CZ	8.62	127.56	119.80
1	A	83	LEU	CB-CG-CD1	8.50	125.45	111.00
1	A	116	TYR	C-N-CA	8.50	142.95	121.70
1	A	102	PRO	N-CD-CG	-8.45	90.52	103.20
1	A	13	PRO	O-C-N	-8.42	109.23	122.70
1	A	99	GLN	O-C-N	-8.39	109.28	122.70
1	A	117	TYR	OH-CZ-CE2	8.37	142.69	120.10
1	A	70	SER	CA-CB-OG	8.36	133.76	111.20
1	A	132	SER	O-C-N	-8.33	109.37	122.70
1	A	36	SER	CA-CB-OG	8.25	133.48	111.20
1	A	88	ASN	OD1-CG-ND2	-8.21	103.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	PHE	CA-CB-CG	8.20	133.57	113.90
1	A	35	GLY	CA-C-N	8.12	135.06	117.20
1	A	88	ASN	CB-CG-OD1	-8.01	105.58	121.60
1	A	10	GLN	CG-CD-OE1	7.96	137.52	121.60
1	A	133	LYS	CA-C-O	-7.95	103.41	120.10
1	A	57	LYS	CA-CB-CG	7.94	130.87	113.40
1	A	104	ARG	CG-CD-NE	7.92	128.44	111.80
1	A	22	HIS	ND1-CE1-NE2	-7.92	92.49	109.90
1	A	34	THR	CA-C-N	7.79	131.78	116.20
1	A	132	SER	C-N-CA	7.76	141.09	121.70
1	A	130	PRO	CA-C-O	7.74	138.76	120.20
1	A	128	ASN	CB-CG-OD1	7.68	136.96	121.60
1	A	51	SER	CA-CB-OG	7.58	131.68	111.20
1	A	71	ARG	CG-CD-NE	-7.57	95.91	111.80
1	A	88	ASN	N-CA-C	7.56	131.41	111.00
1	A	85	LYS	CB-CG-CD	7.53	131.17	111.60
1	A	110	ILE	CB-CG1-CD1	7.50	134.89	113.90
1	A	50	VAL	CA-CB-CG2	-7.38	99.83	110.90
1	A	133	LYS	N-CA-C	7.26	130.61	111.00
1	A	121	GLU	CA-CB-CG	7.20	129.23	113.40
1	A	2	GLU	CA-CB-CG	7.18	129.20	113.40
1	A	117	TYR	CA-CB-CG	7.17	127.03	113.40
1	A	15	THR	OG1-CB-CG2	-7.12	93.62	110.00
1	A	86	VAL	CB-CA-C	-7.10	97.91	111.40
1	A	25	PHE	CA-CB-CG	7.09	130.92	113.90
1	A	138	ALA	N-CA-CB	-7.09	100.17	110.10
1	A	78	HIS	CB-CG-ND1	7.01	140.72	123.20
1	A	15	THR	O-C-N	-6.99	111.52	122.70
1	A	118	GLU	CB-CG-CD	6.99	133.07	114.20
1	A	4	PRO	CA-N-CD	6.85	121.29	111.70
1	A	35	GLY	C-N-CA	6.84	138.81	121.70
1	A	102	PRO	CA-C-N	6.81	132.18	117.20
1	A	63	LEU	CB-CG-CD2	6.80	122.56	111.00
1	A	101	VAL	O-C-N	-6.80	108.18	121.10
1	A	93	LEU	CB-CG-CD2	-6.79	99.45	111.00
1	A	118	GLU	CA-C-O	6.77	134.32	120.10
1	A	80	LEU	CB-CG-CD1	6.76	122.50	111.00
1	A	84	ASP	O-C-N	-6.75	111.89	122.70
1	A	133	LYS	N-CA-CB	-6.67	98.59	110.60
1	A	51	SER	O-C-N	-6.63	111.93	123.20
1	A	3	PHE	N-CA-CB	6.62	122.52	110.60
1	A	119	THR	N-CA-C	6.60	128.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	LEU	CA-CB-CG	6.59	130.45	115.30
1	A	61	LYS	CG-CD-CE	6.53	131.50	111.90
1	A	127	TYR	CE1-CZ-OH	6.52	137.70	120.10
1	A	87	SER	N-CA-C	6.40	128.28	111.00
1	A	22	HIS	CA-CB-CG	6.40	124.48	113.60
1	A	128	ASN	CB-CG-ND2	6.40	132.05	116.70
1	A	18	GLU	CG-CD-OE2	6.37	131.04	118.30
1	A	67	ASN	OD1-CG-ND2	-6.32	107.37	121.90
1	A	40	SER	CA-CB-OG	6.30	128.21	111.20
1	A	34	THR	C-N-CA	6.23	135.38	122.30
1	A	4	PRO	CA-CB-CG	6.21	116.61	104.80
1	A	78	HIS	ND1-CE1-NE2	-6.19	96.28	109.90
1	A	85	LYS	CD-CE-NZ	6.18	125.91	111.70
1	A	102	PRO	C-N-CA	6.12	136.99	121.70
1	A	40	SER	O-C-N	6.11	132.48	122.70
1	A	102	PRO	N-CA-C	6.07	127.89	112.10
1	A	28	SER	CA-CB-OG	6.06	127.56	111.20
1	A	38	SER	CB-CA-C	-5.98	98.74	110.10
1	A	64	GLU	CB-CG-CD	5.97	130.31	114.20
1	A	104	ARG	O-C-N	-5.87	113.30	122.70
1	A	91	LEU	CB-CG-CD2	-5.85	101.06	111.00
1	A	14	GLN	CA-CB-CG	5.84	126.25	113.40
1	A	99	GLN	CA-C-N	5.83	130.03	117.20
1	A	86	VAL	N-CA-CB	-5.82	98.70	111.50
1	A	104	ARG	N-CA-CB	-5.81	100.14	110.60
1	A	26	GLN	OE1-CD-NE2	-5.79	108.58	121.90
1	A	130	PRO	N-CA-C	5.79	127.14	112.10
1	A	87	SER	CA-C-O	5.78	132.24	120.10
1	A	124	ILE	CA-CB-CG1	5.78	121.98	111.00
1	A	124	ILE	CB-CG1-CD1	5.74	129.96	113.90
1	A	121	GLU	CB-CA-C	5.68	121.76	110.40
1	A	120	ASP	N-CA-C	5.68	126.33	111.00
1	A	10	GLN	CB-CG-CD	5.65	126.29	111.60
1	A	4	PRO	CB-CA-C	5.64	126.09	112.00
1	A	91	LEU	CD1-CG-CD2	5.62	127.35	110.50
1	A	66	SER	CA-C-O	5.56	131.78	120.10
1	A	62	MET	CG-SD-CE	5.55	109.08	100.20
1	A	135	LEU	CD1-CG-CD2	-5.52	93.94	110.50
1	A	34	THR	CA-CB-OG1	5.44	120.42	109.00
1	A	121	GLU	OE1-CD-OE2	-5.42	116.79	123.30
1	A	50	VAL	CA-CB-CG1	5.39	118.99	110.90
1	A	87	SER	CB-CA-C	5.39	120.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	LEU	CB-CG-CD1	5.36	120.11	111.00
1	A	50	VAL	CA-C-O	5.32	131.28	120.10
1	A	82	TYR	CA-CB-CG	5.24	123.35	113.40
1	A	121	GLU	CA-C-N	5.22	128.69	117.20
1	A	50	VAL	O-C-N	-5.22	114.35	122.70
1	A	127	TYR	OH-CZ-CE2	5.16	134.04	120.10
1	A	84	ASP	CA-CB-CG	5.16	124.75	113.40
1	A	95	PHE	CB-CG-CD2	5.14	124.40	120.80
1	A	119	THR	N-CA-CB	-5.09	100.62	110.30
1	A	102	PRO	CA-N-CD	5.07	118.80	111.70
1	A	99	GLN	C-N-CA	5.06	134.35	121.70
1	A	34	THR	CA-C-O	5.04	130.69	120.10
1	A	7	LEU	CB-CG-CD1	5.02	119.54	111.00

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	2	GLU	CA
1	A	3	PHE	CA
1	A	15	THR	CB
1	A	34	THR	CB
1	A	38	SER	CA
1	A	39	ALA	CA
1	A	40	SER	CA
1	A	41	ASN	CA
1	A	86	VAL	CA
1	A	87	SER	CA
1	A	110	ILE	CB
1	A	117	TYR	CA
1	A	118	GLU	CA
1	A	119	THR	CB
1	A	120	ASP	CA
1	A	134	ASP	CA
1	A	135	LEU	CA
1	A	137	ASN	CA
1	A	138	ALA	CA

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	1078	908	1010	681
All	All	1078	908	1010	681

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 326.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:33:TYR:CZ	1:A:33:TYR:CD1	1.64	1.85
1:A:33:TYR:CE1	1:A:33:TYR:CG	1.61	1.79
1:A:33:TYR:CZ	1:A:33:TYR:CD2	1.61	1.76
1:A:1:GLU:CG	1:A:1:GLU:CA	1.59	1.78
1:A:122:PHE:CD1	1:A:122:PHE:CZ	1.59	1.84
1:A:122:PHE:CG	1:A:122:PHE:CE2	1.59	1.84
1:A:33:TYR:CE2	1:A:33:TYR:CG	1.58	1.88
1:A:106:LEU:CA	1:A:106:LEU:HG	1.58	1.08
1:A:114:TYR:CZ	1:A:114:TYR:CD2	1.57	1.93
1:A:112:LYS:CD	1:A:112:LYS:CB	1.56	1.78
1:A:57:LYS:CD	1:A:57:LYS:CB	1.56	1.81
1:A:104:ARG:CA	1:A:104:ARG:CG	1.56	1.79
1:A:122:PHE:CD2	1:A:122:PHE:CZ	1.55	1.92
1:A:12:LEU:CB	1:A:12:LEU:CD2	1.52	1.83
1:A:33:TYR:CB	1:A:33:TYR:CD1	1.51	1.87
1:A:1:GLU:CD	1:A:1:GLU:CB	1.51	1.76
1:A:107:LYS:NZ	1:A:107:LYS:CD	1.51	1.74
1:A:114:TYR:CE1	1:A:114:TYR:CG	1.51	1.96
1:A:10:GLN:CG	1:A:10:GLN:NE2	1.51	1.73
1:A:114:TYR:CD1	1:A:114:TYR:CZ	1.50	1.94
1:A:94:PHE:CZ	1:A:94:PHE:CD2	1.50	1.99
1:A:57:LYS:CG	1:A:57:LYS:CE	1.49	1.89
1:A:122:PHE:CE1	1:A:122:PHE:CG	1.49	1.92
1:A:114:TYR:CE2	1:A:114:TYR:CG	1.49	1.98
1:A:14:GLN:CG	1:A:14:GLN:NE2	1.49	1.72
1:A:122:PHE:CB	1:A:122:PHE:CD2	1.47	1.94
1:A:94:PHE:CG	1:A:94:PHE:CE1	1.47	1.99
1:A:61:LYS:NZ	1:A:61:LYS:CD	1.45	1.79

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:57:LYS:CD	1:A:57:LYS:NZ	1.45	1.68
1:A:89:GLN:NE2	1:A:89:GLN:CG	1.45	1.74
1:A:84:ASP:CB	1:A:84:ASP:OD2	1.44	1.64
1:A:127:TYR:CZ	1:A:127:TYR:CD2	1.43	2.05
1:A:107:LYS:CA	1:A:107:LYS:CG	1.42	1.96
1:A:42:MET:CB	1:A:42:MET:SD	1.42	2.06
1:A:29:LEU:CB	1:A:29:LEU:CD2	1.42	1.93
1:A:102:PRO:CA	1:A:102:PRO:O	1.42	1.67
1:A:100:ASP:C	1:A:101:VAL:CA	1.42	1.84
1:A:18:GLU:CG	1:A:18:GLU:OE2	1.41	1.66
1:A:114:TYR:CD1	1:A:114:TYR:CB	1.41	2.04
1:A:115:ASP:O	1:A:116:TYR:CA	1.39	1.69
1:A:127:TYR:CE1	1:A:127:TYR:CG	1.39	2.09
1:A:118:GLU:CA	1:A:118:GLU:O	1.38	1.68
1:A:49:MET:CB	1:A:49:MET:SD	1.37	2.10
1:A:126:GLU:CG	1:A:126:GLU:OE2	1.37	1.71
1:A:107:LYS:CD	1:A:107:LYS:CB	1.36	2.04
1:A:114:TYR:CD2	1:A:114:TYR:CB	1.36	2.06
1:A:99:GLN:CG	1:A:99:GLN:CA	1.36	2.02
1:A:127:TYR:CZ	1:A:127:TYR:CD1	1.35	2.12
1:A:51:SER:CA	1:A:51:SER:OG	1.35	1.73
1:A:70:SER:CA	1:A:70:SER:OG	1.35	1.74
1:A:94:PHE:CG	1:A:94:PHE:CE2	1.35	2.15
1:A:94:PHE:CB	1:A:94:PHE:CD1	1.35	2.10
1:A:100:ASP:CB	1:A:100:ASP:OD1	1.35	1.75
1:A:94:PHE:CD1	1:A:94:PHE:CZ	1.34	2.15
1:A:102:PRO:O	1:A:103:VAL:N	1.34	1.59
1:A:60:VAL:CA	1:A:60:VAL:CG2	1.33	2.05
1:A:12:LEU:CD1	1:A:12:LEU:CB	1.33	2.07
1:A:118:GLU:C	1:A:119:THR:CA	1.32	1.95
1:A:106:LEU:CG	1:A:106:LEU:CA	1.32	1.79
1:A:100:ASP:CA	1:A:101:VAL:N	1.31	1.91
1:A:113:VAL:CG1	1:A:113:VAL:CA	1.31	2.08
1:A:127:TYR:CE2	1:A:127:TYR:CG	1.31	2.16
1:A:62:MET:CB	1:A:62:MET:SD	1.31	2.18
1:A:14:GLN:CD	1:A:14:GLN:CB	1.29	1.98
1:A:60:VAL:CG1	1:A:60:VAL:CA	1.28	2.09
1:A:97:VAL:CG1	1:A:97:VAL:CA	1.28	2.12
1:A:41:ASN:CA	1:A:41:ASN:O	1.27	1.82
1:A:100:ASP:CB	1:A:100:ASP:OD2	1.27	1.83
1:A:31:VAL:CG2	1:A:31:VAL:CA	1.27	2.11
1:A:34:THR:CG2	1:A:34:THR:CA	1.26	2.11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:112:LYS:CG	1:A:112:LYS:CA	1.26	2.11
1:A:36:SER:OG	1:A:36:SER:CA	1.26	1.82
1:A:49:MET:CG	1:A:49:MET:SD	1.26	1.17
1:A:45:VAL:CA	1:A:45:VAL:CG2	1.26	2.13
1:A:33:TYR:OH	1:A:33:TYR:CE2	1.25	1.69
1:A:127:TYR:CB	1:A:127:TYR:CD1	1.25	2.17
1:A:68:HIS:CD2	1:A:68:HIS:CB	1.25	2.03
1:A:33:TYR:CB	1:A:33:TYR:CD2	1.25	1.96
1:A:45:VAL:CA	1:A:45:VAL:CG1	1.25	2.14
1:A:64:GLU:OE2	1:A:64:GLU:CG	1.25	1.82
1:A:14:GLN:CG	1:A:14:GLN:CA	1.24	2.14
1:A:49:MET:CE	1:A:49:MET:CG	1.24	2.15
1:A:47:VAL:CA	1:A:47:VAL:CG1	1.24	2.16
1:A:56:LEU:CB	1:A:56:LEU:CD2	1.24	2.16
1:A:56:LEU:CD1	1:A:56:LEU:CB	1.23	2.16
1:A:113:VAL:CG2	1:A:113:VAL:CA	1.23	2.16
1:A:97:VAL:CG2	1:A:97:VAL:CA	1.22	2.16
1:A:48:LYS:CD	1:A:48:LYS:NZ	1.22	2.01
1:A:64:GLU:OE1	1:A:64:GLU:CG	1.22	1.88
1:A:57:LYS:CA	1:A:57:LYS:CG	1.22	2.18
1:A:49:MET:CE	1:A:49:MET:SD	1.21	1.12
1:A:126:GLU:CG	1:A:126:GLU:OE1	1.21	1.87
1:A:115:ASP:CG	1:A:115:ASP:CA	1.21	2.10
1:A:114:TYR:CE2	1:A:114:TYR:OH	1.20	1.85
1:A:29:LEU:CB	1:A:29:LEU:CD1	1.20	2.18
1:A:127:TYR:CB	1:A:127:TYR:CD2	1.19	2.24
1:A:42:MET:CA	1:A:42:MET:CG	1.19	2.20
1:A:48:LYS:CE	1:A:48:LYS:CG	1.19	2.19
1:A:20:LYS:NZ	1:A:20:LYS:CD	1.18	2.04
1:A:41:ASN:O	1:A:42:MET:CA	1.18	1.91
1:A:115:ASP:C	1:A:116:TYR:CA	1.17	2.12
1:A:9:VAL:CG2	1:A:9:VAL:CA	1.17	2.23
1:A:9:VAL:CG1	1:A:9:VAL:CA	1.16	2.21
1:A:31:VAL:CA	1:A:31:VAL:CG1	1.16	2.19
1:A:128:ASN:CB	1:A:128:ASN:ND2	1.16	2.08
1:A:34:THR:OG1	1:A:34:THR:CA	1.15	1.95
1:A:127:TYR:OH	1:A:127:TYR:CE2	1.14	1.97
1:A:17:ASP:OD2	1:A:17:ASP:CB	1.14	1.95
1:A:47:VAL:CA	1:A:47:VAL:CG2	1.14	2.25
1:A:17:ASP:OD1	1:A:17:ASP:CB	1.13	1.95
1:A:18:GLU:CG	1:A:18:GLU:OE1	1.12	1.84
1:A:114:TYR:CE1	1:A:114:TYR:OH	1.12	1.87

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:118:GLU:CA	1:A:119:THR:N	1.11	1.99
1:A:62:MET:SD	1:A:62:MET:CG	1.10	1.21
1:A:83:LEU:CG	1:A:83:LEU:CA	1.10	2.29
1:A:118:GLU:CB	1:A:119:THR:N	1.09	2.15
1:A:83:LEU:CD1	1:A:91:LEU:CD2	1.09	2.28
1:A:115:ASP:O	1:A:115:ASP:CA	1.09	1.99
1:A:41:ASN:C	1:A:42:MET:CA	1.08	2.20
1:A:62:MET:HG3	1:A:62:MET:SD	1.07	1.74
1:A:29:LEU:HD23	1:A:29:LEU:CD1	1.07	1.74
1:A:29:LEU:HD12	1:A:29:LEU:CD2	1.06	1.73
1:A:127:TYR:OH	1:A:127:TYR:CE1	1.06	2.05
1:A:46:ASP:CG	1:A:46:ASP:CA	1.06	2.22
1:A:118:GLU:HA	1:A:118:GLU:O	1.05	1.35
1:A:34:THR:HB	1:A:34:THR:CG2	1.05	1.63
1:A:9:VAL:CG2	1:A:9:VAL:HB	1.05	1.67
1:A:12:LEU:CD1	1:A:12:LEU:HG	1.05	1.60
1:A:41:ASN:HA	1:A:41:ASN:O	1.05	1.48
1:A:72:THR:HG21	1:A:93:LEU:HD13	1.05	1.07
1:A:56:LEU:HG	1:A:56:LEU:CD1	1.05	1.63
1:A:115:ASP:CA	1:A:116:TYR:N	1.05	2.18
1:A:97:VAL:HB	1:A:97:VAL:CG2	1.05	1.61
1:A:61:LYS:NZ	1:A:61:LYS:HE3	1.04	1.43
1:A:62:MET:HG2	1:A:62:MET:SD	1.04	1.74
1:A:31:VAL:CG1	1:A:31:VAL:HB	1.04	1.61
1:A:118:GLU:HB3	1:A:119:THR:N	1.03	1.57
1:A:69:VAL:HG22	1:A:70:SER:H	1.03	1.10
1:A:113:VAL:CG1	1:A:113:VAL:HG23	1.03	1.63
1:A:33:TYR:OH	1:A:33:TYR:CE1	1.03	1.78
1:A:113:VAL:HG12	1:A:113:VAL:CG2	1.03	1.63
1:A:97:VAL:HB	1:A:97:VAL:CG1	1.03	1.59
1:A:29:LEU:HG	1:A:29:LEU:CD1	1.02	1.59
1:A:41:ASN:HA	1:A:42:MET:N	1.02	1.63
1:A:49:MET:HE3	1:A:49:MET:SD	1.02	1.71
1:A:113:VAL:CG2	1:A:113:VAL:HB	1.02	1.59
1:A:1:GLU:CD	1:A:1:GLU:HG2	1.01	1.45
1:A:61:LYS:NZ	1:A:61:LYS:HE2	1.01	1.43
1:A:70:SER:HB2	1:A:70:SER:OG	1.01	1.25
1:A:60:VAL:HB	1:A:60:VAL:CG2	1.01	1.55
1:A:49:MET:HG2	1:A:49:MET:SD	1.01	1.65
1:A:9:VAL:CB	1:A:9:VAL:HG22	1.01	1.54
1:A:83:LEU:HD11	1:A:91:LEU:HD23	1.01	1.27
1:A:97:VAL:HG12	1:A:97:VAL:CG2	1.01	1.80

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:128:ASN:OD1	1:A:128:ASN:CB	1.01	2.06
1:A:9:VAL:CG1	1:A:9:VAL:HB	1.00	1.67
1:A:49:MET:HE1	1:A:49:MET:SD	1.00	1.71
1:A:9:VAL:HG11	1:A:9:VAL:CB	1.00	1.53
1:A:97:VAL:CG1	1:A:97:VAL:HG23	1.00	1.79
1:A:31:VAL:CG2	1:A:31:VAL:HB	1.00	1.60
1:A:49:MET:HG3	1:A:49:MET:SD	1.00	1.65
1:A:83:LEU:HD13	1:A:91:LEU:HD21	1.00	1.28
1:A:49:MET:HE2	1:A:49:MET:SD	0.99	1.71
1:A:47:VAL:CB	1:A:47:VAL:HG23	0.99	1.56
1:A:34:THR:HG21	1:A:34:THR:CB	0.99	1.56
1:A:61:LYS:NZ	1:A:61:LYS:CE	0.99	0.84
1:A:113:VAL:HB	1:A:113:VAL:CG1	0.99	1.55
1:A:33:TYR:CZ	1:A:115:ASP:OD1	0.99	2.15
1:A:9:VAL:HG23	1:A:9:VAL:CB	0.99	1.54
1:A:47:VAL:CB	1:A:47:VAL:HG22	0.99	1.56
1:A:99:GLN:C	1:A:99:GLN:HG3	0.99	1.78
1:A:1:GLU:CG	1:A:1:GLU:CD	0.99	0.93
1:A:41:ASN:CA	1:A:42:MET:N	0.99	2.25
1:A:47:VAL:CB	1:A:47:VAL:HG21	0.99	1.56
1:A:122:PHE:CB	1:A:122:PHE:CD1	0.99	2.02
1:A:1:GLU:CD	1:A:1:GLU:HG3	0.98	1.45
1:A:34:THR:HG22	1:A:34:THR:CB	0.98	1.56
1:A:9:VAL:CB	1:A:9:VAL:HG13	0.98	1.53
1:A:34:THR:HG23	1:A:34:THR:CB	0.98	1.56
1:A:36:SER:HB2	1:A:36:SER:OG	0.98	1.27
1:A:36:SER:HB3	1:A:36:SER:OG	0.98	1.27
1:A:60:VAL:CG1	1:A:60:VAL:HB	0.98	1.57
1:A:9:VAL:CB	1:A:9:VAL:HG12	0.97	1.53
1:A:51:SER:HB2	1:A:51:SER:OG	0.97	1.24
1:A:70:SER:HB3	1:A:70:SER:OG	0.97	1.25
1:A:107:LYS:HE3	1:A:107:LYS:NZ	0.97	1.37
1:A:51:SER:HB3	1:A:51:SER:OG	0.97	1.24
1:A:60:VAL:HG12	1:A:60:VAL:CG2	0.97	1.54
1:A:47:VAL:CB	1:A:47:VAL:HG12	0.97	1.51
1:A:102:PRO:CB	1:A:102:PRO:O	0.97	2.12
1:A:72:THR:CG2	1:A:93:LEU:HD13	0.96	1.89
1:A:47:VAL:CG2	1:A:47:VAL:HB	0.96	1.65
1:A:107:LYS:HE2	1:A:107:LYS:NZ	0.96	1.37
1:A:56:LEU:HG	1:A:56:LEU:CD2	0.96	1.63
1:A:47:VAL:CB	1:A:47:VAL:HG13	0.96	1.51
1:A:9:VAL:HG21	1:A:9:VAL:CB	0.96	1.54

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:33:TYR:CE1	1:A:115:ASP:CG	0.96	2.38
1:A:60:VAL:CG1	1:A:60:VAL:HG23	0.96	1.54
1:A:20:LYS:NZ	1:A:20:LYS:HE3	0.95	1.35
1:A:20:LYS:NZ	1:A:20:LYS:HE2	0.95	1.35
1:A:81:ILE:HG12	1:A:93:LEU:HD11	0.95	1.36
1:A:102:PRO:O	1:A:102:PRO:C	0.95	0.76
1:A:47:VAL:CB	1:A:47:VAL:HG11	0.94	1.51
1:A:31:VAL:HG11	1:A:31:VAL:CB	0.94	1.48
1:A:107:LYS:NZ	1:A:107:LYS:CE	0.94	0.79
1:A:57:LYS:HD3	1:A:57:LYS:CB	0.94	1.88
1:A:14:GLN:CG	1:A:14:GLN:HB3	0.94	1.48
1:A:31:VAL:HG13	1:A:31:VAL:CB	0.94	1.49
1:A:47:VAL:CB	1:A:47:VAL:CG2	0.93	0.94
1:A:48:LYS:CE	1:A:48:LYS:CD	0.93	0.94
1:A:33:TYR:CE1	1:A:115:ASP:OD2	0.93	2.20
1:A:83:LEU:CA	1:A:83:LEU:HG	0.93	1.89
1:A:14:GLN:HB2	1:A:14:GLN:CG	0.93	1.48
1:A:34:THR:CB	1:A:34:THR:CG2	0.93	0.94
1:A:29:LEU:HG	1:A:29:LEU:CD2	0.93	1.50
1:A:115:ASP:O	1:A:116:TYR:CB	0.93	2.16
1:A:31:VAL:HG12	1:A:31:VAL:CB	0.93	1.49
1:A:50:VAL:O	1:A:52:GLY:N	0.93	2.01
1:A:33:TYR:CE1	1:A:115:ASP:OD1	0.92	2.22
1:A:47:VAL:CG1	1:A:47:VAL:HB	0.92	1.65
1:A:127:TYR:CD2	1:A:127:TYR:CG	0.92	0.92
1:A:56:LEU:HD22	1:A:56:LEU:CG	0.92	1.45
1:A:56:LEU:HD13	1:A:56:LEU:CG	0.92	1.45
1:A:36:SER:OG	1:A:36:SER:CB	0.92	0.62
1:A:9:VAL:CG2	1:A:9:VAL:CB	0.92	0.92
1:A:56:LEU:HD11	1:A:56:LEU:CG	0.91	1.45
1:A:56:LEU:CG	1:A:56:LEU:HD23	0.91	1.45
1:A:81:ILE:CG1	1:A:93:LEU:HD11	0.91	1.94
1:A:31:VAL:CB	1:A:31:VAL:HG23	0.91	1.45
1:A:48:LYS:CE	1:A:48:LYS:HD3	0.91	1.45
1:A:57:LYS:CG	1:A:57:LYS:HB3	0.91	1.45
1:A:29:LEU:HD11	1:A:29:LEU:CG	0.91	1.45
1:A:31:VAL:CB	1:A:31:VAL:HG22	0.91	1.45
1:A:20:LYS:NZ	1:A:20:LYS:CE	0.91	0.76
1:A:9:VAL:CG1	1:A:9:VAL:CB	0.91	0.91
1:A:48:LYS:CE	1:A:48:LYS:HD2	0.90	1.45
1:A:29:LEU:HD12	1:A:29:LEU:CG	0.90	1.45
1:A:9:VAL:HG11	1:A:111:VAL:HG11	0.90	1.41

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:29:LEU:HD13	1:A:29:LEU:CG	0.90	1.45
1:A:1:GLU:CG	1:A:1:GLU:HB3	0.90	1.44
1:A:57:LYS:CG	1:A:57:LYS:HB2	0.90	1.45
1:A:56:LEU:HD21	1:A:56:LEU:CG	0.90	1.45
1:A:56:LEU:HD12	1:A:56:LEU:CG	0.90	1.45
1:A:1:GLU:CB	1:A:1:GLU:HG2	0.90	1.43
1:A:127:TYR:CZ	1:A:127:TYR:CE1	0.89	0.89
1:A:115:ASP:CG	1:A:115:ASP:HB3	0.89	1.33
1:A:31:VAL:CB	1:A:31:VAL:HG21	0.89	1.45
1:A:41:ASN:C	1:A:42:MET:N	0.89	0.84
1:A:97:VAL:CB	1:A:97:VAL:HG22	0.89	1.43
1:A:1:GLU:CB	1:A:1:GLU:HG3	0.89	1.43
1:A:70:SER:CB	1:A:70:SER:OG	0.89	0.59
1:A:57:LYS:CB	1:A:57:LYS:HG2	0.89	1.44
1:A:97:VAL:HG21	1:A:97:VAL:CB	0.89	1.43
1:A:107:LYS:HB3	1:A:107:LYS:CG	0.88	1.43
1:A:57:LYS:CB	1:A:57:LYS:HG3	0.88	1.43
1:A:107:LYS:HB2	1:A:107:LYS:CG	0.88	1.43
1:A:104:ARG:CG	1:A:104:ARG:N	0.88	2.36
1:A:46:ASP:CG	1:A:46:ASP:HB3	0.88	1.32
1:A:115:ASP:CG	1:A:115:ASP:HB2	0.88	1.33
1:A:48:LYS:CD	1:A:48:LYS:HE2	0.88	1.43
1:A:46:ASP:HB2	1:A:46:ASP:CG	0.88	1.32
1:A:33:TYR:CE2	1:A:115:ASP:OD1	0.88	2.27
1:A:48:LYS:CD	1:A:48:LYS:HE3	0.88	1.43
1:A:33:TYR:CE2	1:A:115:ASP:CG	0.88	2.47
1:A:47:VAL:CB	1:A:47:VAL:CG1	0.88	0.88
1:A:97:VAL:CG1	1:A:97:VAL:CG2	0.88	0.88
1:A:14:GLN:CG	1:A:14:GLN:CB	0.88	0.88
1:A:1:GLU:CG	1:A:1:GLU:HB2	0.87	1.44
1:A:83:LEU:HD13	1:A:91:LEU:CD2	0.87	1.96
1:A:99:GLN:HB3	1:A:99:GLN:CG	0.87	1.40
1:A:62:MET:SD	1:A:62:MET:CE	0.87	0.86
1:A:104:ARG:CB	1:A:104:ARG:HG2	0.87	1.43
1:A:97:VAL:CB	1:A:97:VAL:HG23	0.86	1.43
1:A:33:TYR:CZ	1:A:115:ASP:CG	0.86	2.47
1:A:57:LYS:CG	1:A:57:LYS:CB	0.86	0.87
1:A:51:SER:CB	1:A:51:SER:OG	0.86	0.57
1:A:127:TYR:CD1	1:A:127:TYR:CG	0.86	0.86
1:A:104:ARG:CB	1:A:104:ARG:HG3	0.86	1.43
1:A:99:GLN:HB2	1:A:99:GLN:CG	0.86	1.40
1:A:62:MET:SD	1:A:62:MET:HE3	0.86	1.49

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:1:GLU:CG	1:A:1:GLU:CB	0.86	0.90
1:A:106:LEU:C	1:A:106:LEU:HG	0.86	1.90
1:A:107:LYS:CB	1:A:107:LYS:HG3	0.86	1.40
1:A:113:VAL:HG23	1:A:113:VAL:CB	0.86	1.39
1:A:46:ASP:CG	1:A:46:ASP:CB	0.86	0.77
1:A:128:ASN:HD21	1:A:128:ASN:CG	0.86	1.46
1:A:104:ARG:CG	1:A:104:ARG:HB3	0.86	1.39
1:A:97:VAL:HG13	1:A:97:VAL:CB	0.85	1.40
1:A:14:GLN:CB	1:A:14:GLN:HG3	0.85	1.38
1:A:62:MET:SD	1:A:62:MET:HE2	0.84	1.49
1:A:31:VAL:CG1	1:A:31:VAL:CB	0.84	0.85
1:A:41:ASN:O	1:A:42:MET:N	0.84	0.70
1:A:83:LEU:CG	1:A:83:LEU:HD12	0.84	1.38
1:A:97:VAL:CB	1:A:97:VAL:HG12	0.84	1.40
1:A:97:VAL:HG13	1:A:97:VAL:CG2	0.84	1.39
1:A:107:LYS:CB	1:A:107:LYS:HG2	0.84	1.39
1:A:128:ASN:CG	1:A:128:ASN:HD22	0.84	1.46
1:A:14:GLN:O	1:A:15:THR:HB	0.84	1.73
1:A:62:MET:HE1	1:A:62:MET:SD	0.84	1.49
1:A:113:VAL:HG21	1:A:113:VAL:CB	0.84	1.39
1:A:112:LYS:HD3	1:A:112:LYS:CB	0.84	2.02
1:A:69:VAL:HG22	1:A:70:SER:N	0.84	1.80
1:A:33:TYR:CE2	1:A:115:ASP:OD2	0.83	2.30
1:A:118:GLU:C	1:A:119:THR:HB	0.83	1.93
1:A:113:VAL:HG22	1:A:113:VAL:CB	0.83	1.39
1:A:97:VAL:CG1	1:A:97:VAL:HG22	0.83	1.38
1:A:127:TYR:CZ	1:A:127:TYR:CE2	0.83	0.84
1:A:14:GLN:CB	1:A:14:GLN:HG2	0.83	1.38
1:A:29:LEU:CD1	1:A:29:LEU:HD22	0.83	1.37
1:A:83:LEU:CG	1:A:83:LEU:HD11	0.83	1.38
1:A:115:ASP:CB	1:A:115:ASP:CG	0.83	0.73
1:A:29:LEU:HD13	1:A:29:LEU:CD2	0.83	1.36
1:A:83:LEU:CG	1:A:83:LEU:HD13	0.83	1.38
1:A:29:LEU:CD2	1:A:29:LEU:CD1	0.82	0.83
1:A:60:VAL:HG11	1:A:60:VAL:CB	0.82	1.35
1:A:12:LEU:CG	1:A:12:LEU:HD11	0.82	1.35
1:A:60:VAL:HG13	1:A:60:VAL:CB	0.82	1.35
1:A:83:LEU:HD22	1:A:83:LEU:CG	0.82	1.35
1:A:60:VAL:HG12	1:A:60:VAL:CB	0.82	1.35
1:A:83:LEU:CD1	1:A:91:LEU:HD23	0.82	1.92
1:A:12:LEU:CG	1:A:12:LEU:HD13	0.81	1.35
1:A:83:LEU:CG	1:A:83:LEU:HD23	0.81	1.35

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:104:ARG:CG	1:A:104:ARG:HB2	0.81	1.39
1:A:34:THR:OG1	1:A:34:THR:CB	0.81	0.81
1:A:107:LYS:CG	1:A:107:LYS:CB	0.81	0.81
1:A:60:VAL:HG12	1:A:60:VAL:HG21	0.81	1.18
1:A:84:ASP:O	1:A:85:LYS:HB2	0.81	1.74
1:A:42:MET:HG2	1:A:42:MET:CB	0.81	1.34
1:A:12:LEU:CG	1:A:12:LEU:HD12	0.81	1.35
1:A:99:GLN:CB	1:A:99:GLN:CG	0.81	0.81
1:A:83:LEU:CG	1:A:83:LEU:HD21	0.81	1.35
1:A:94:PHE:CB	1:A:94:PHE:CD2	0.81	2.25
1:A:14:GLN:NE2	1:A:14:GLN:HG3	0.81	1.89
1:A:42:MET:HG3	1:A:42:MET:CB	0.81	1.34
1:A:56:LEU:CD2	1:A:56:LEU:CG	0.81	0.81
1:A:56:LEU:CD1	1:A:56:LEU:CG	0.80	0.81
1:A:113:VAL:CB	1:A:113:VAL:HG11	0.80	1.34
1:A:113:VAL:HG13	1:A:113:VAL:CB	0.80	1.34
1:A:97:VAL:HG11	1:A:97:VAL:CB	0.80	1.40
1:A:72:THR:HG21	1:A:93:LEU:CD1	0.80	2.01
1:A:106:LEU:CG	1:A:106:LEU:N	0.80	2.43
1:A:104:ARG:CB	1:A:104:ARG:CG	0.80	0.81
1:A:29:LEU:CD1	1:A:29:LEU:CG	0.80	0.80
1:A:102:PRO:O	1:A:103:VAL:HG12	0.80	1.77
1:A:31:VAL:CG2	1:A:31:VAL:CB	0.80	0.80
1:A:60:VAL:CB	1:A:60:VAL:HG22	0.79	1.33
1:A:57:LYS:HD2	1:A:57:LYS:CB	0.79	2.01
1:A:60:VAL:CB	1:A:60:VAL:HG21	0.79	1.33
1:A:45:VAL:HG13	1:A:45:VAL:CB	0.79	1.32
1:A:113:VAL:HG12	1:A:113:VAL:CB	0.79	1.34
1:A:45:VAL:HG11	1:A:45:VAL:CB	0.79	1.32
1:A:60:VAL:HG23	1:A:60:VAL:CB	0.79	1.33
1:A:99:GLN:CB	1:A:99:GLN:HG2	0.79	1.34
1:A:94:PHE:CE2	1:A:94:PHE:HZ	0.79	1.54
1:A:1:GLU:CD	1:A:1:GLU:HB3	0.78	1.97
1:A:45:VAL:HG12	1:A:45:VAL:CB	0.78	1.32
1:A:42:MET:HB2	1:A:42:MET:SD	0.78	1.96
1:A:57:LYS:CD	1:A:57:LYS:HE2	0.78	1.32
1:A:83:LEU:CD1	1:A:91:LEU:HD21	0.78	1.94
1:A:57:LYS:HE3	1:A:57:LYS:CD	0.78	1.32
1:A:45:VAL:CB	1:A:45:VAL:HG21	0.78	1.31
1:A:57:LYS:CE	1:A:57:LYS:HD2	0.78	1.31
1:A:33:TYR:CD1	1:A:115:ASP:OD2	0.78	2.37
1:A:118:GLU:C	1:A:119:THR:CB	0.78	2.46

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:128:ASN:CG	1:A:128:ASN:ND2	0.77	0.83
1:A:45:VAL:HG22	1:A:45:VAL:CB	0.77	1.32
1:A:88:ASN:O	1:A:89:GLN:HG3	0.77	1.80
1:A:99:GLN:CA	1:A:99:GLN:HG3	0.77	1.88
1:A:97:VAL:CB	1:A:97:VAL:CG2	0.77	0.77
1:A:57:LYS:CE	1:A:57:LYS:HD3	0.77	1.31
1:A:29:LEU:CG	1:A:29:LEU:HD22	0.77	1.30
1:A:45:VAL:CB	1:A:45:VAL:HG23	0.77	1.31
1:A:29:LEU:HD23	1:A:29:LEU:CG	0.77	1.30
1:A:7:LEU:HD21	1:A:125:ALA:CB	0.76	2.11
1:A:34:THR:HB	1:A:34:THR:OG1	0.76	1.58
1:A:127:TYR:HD2	1:A:127:TYR:CG	0.75	1.52
1:A:127:TYR:HE1	1:A:127:TYR:CZ	0.75	1.50
1:A:33:TYR:CZ	1:A:115:ASP:OD2	0.75	2.38
1:A:57:LYS:N	1:A:58:PRO:CD	0.75	2.50
1:A:100:ASP:C	1:A:101:VAL:CB	0.75	2.51
1:A:83:LEU:CG	1:A:83:LEU:HB3	0.74	1.29
1:A:115:ASP:C	1:A:116:TYR:N	0.74	0.72
1:A:64:GLU:CD	1:A:64:GLU:OE1	0.74	0.58
1:A:99:GLN:C	1:A:99:GLN:CG	0.74	2.48
1:A:70:SER:C	1:A:71:ARG:HD3	0.74	2.03
1:A:106:LEU:CG	1:A:106:LEU:HD21	0.74	1.27
1:A:42:MET:CB	1:A:42:MET:CG	0.74	0.76
1:A:99:GLN:CB	1:A:99:GLN:HG3	0.74	1.34
1:A:102:PRO:O	1:A:103:VAL:CA	0.74	2.33
1:A:126:GLU:OE1	1:A:126:GLU:CD	0.74	0.60
1:A:83:LEU:CD2	1:A:91:LEU:HD23	0.74	2.12
1:A:113:VAL:HG13	1:A:113:VAL:CG2	0.74	1.27
1:A:97:VAL:CG1	1:A:97:VAL:CB	0.74	0.74
1:A:14:GLN:CA	1:A:14:GLN:HG3	0.73	1.97
1:A:106:LEU:CG	1:A:106:LEU:HD23	0.73	1.27
1:A:12:LEU:CD1	1:A:12:LEU:HD23	0.73	1.26
1:A:29:LEU:HD21	1:A:29:LEU:CD1	0.73	0.80
1:A:42:MET:HB3	1:A:42:MET:CG	0.73	1.26
1:A:33:TYR:CD2	1:A:115:ASP:OD2	0.73	2.41
1:A:122:PHE:CE1	1:A:122:PHE:HZ	0.73	1.50
1:A:106:LEU:CG	1:A:106:LEU:HD22	0.73	1.27
1:A:107:LYS:CA	1:A:107:LYS:HG3	0.73	1.85
1:A:113:VAL:CG1	1:A:113:VAL:HG22	0.72	1.27
1:A:84:ASP:CG	1:A:84:ASP:OD2	0.72	0.58
1:A:9:VAL:HG21	1:A:111:VAL:HG11	0.72	1.61
1:A:83:LEU:CG	1:A:83:LEU:CB	0.72	0.80

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:113:VAL:CG2	1:A:113:VAL:CB	0.72	0.72
1:A:42:MET:CG	1:A:42:MET:HB2	0.72	1.26
1:A:10:GLN:CD	1:A:10:GLN:HE21	0.72	1.33
1:A:127:TYR:HD1	1:A:127:TYR:CG	0.71	1.49
1:A:115:ASP:C	1:A:115:ASP:O	0.71	0.53
1:A:61:LYS:HZ2	1:A:61:LYS:CE	0.71	1.42
1:A:83:LEU:CG	1:A:83:LEU:CD1	0.71	0.71
1:A:94:PHE:CE1	1:A:94:PHE:CZ	0.71	0.78
1:A:113:VAL:CG2	1:A:113:VAL:CG1	0.71	0.71
1:A:64:GLU:CD	1:A:64:GLU:OE2	0.71	0.54
1:A:88:ASN:O	1:A:89:GLN:CG	0.71	2.38
1:A:57:LYS:CD	1:A:57:LYS:CE	0.70	0.82
1:A:5:PHE:CE2	1:A:122:PHE:O	0.70	2.44
1:A:12:LEU:CD2	1:A:12:LEU:HG	0.70	1.42
1:A:60:VAL:HG23	1:A:60:VAL:HG11	0.70	1.21
1:A:97:VAL:HG11	1:A:97:VAL:CG2	0.70	0.96
1:A:112:LYS:HD2	1:A:112:LYS:CB	0.70	2.11
1:A:107:LYS:CG	1:A:107:LYS:N	0.70	2.55
1:A:61:LYS:HZ1	1:A:61:LYS:CE	0.70	1.42
1:A:127:TYR:HE2	1:A:127:TYR:CZ	0.70	1.47
1:A:49:MET:HB2	1:A:49:MET:SD	0.70	2.22
1:A:61:LYS:HZ3	1:A:61:LYS:CE	0.69	1.42
1:A:69:VAL:CG2	1:A:70:SER:H	0.69	1.95
1:A:12:LEU:HD21	1:A:12:LEU:HD12	0.69	0.69
1:A:99:GLN:HG2	1:A:99:GLN:CD	0.69	1.37
1:A:83:LEU:HD11	1:A:91:LEU:CD2	0.69	2.00
1:A:14:GLN:CD	1:A:14:GLN:HE21	0.69	1.31
1:A:89:GLN:CD	1:A:89:GLN:HE21	0.69	1.31
1:A:99:GLN:HG3	1:A:99:GLN:CD	0.69	1.37
1:A:94:PHE:CG	1:A:94:PHE:CD2	0.68	0.78
1:A:69:VAL:C	1:A:71:ARG:HD3	0.68	2.08
1:A:57:LYS:HD3	1:A:57:LYS:HE2	0.68	1.03
1:A:9:VAL:HG21	1:A:111:VAL:HG21	0.68	1.63
1:A:83:LEU:HB2	1:A:83:LEU:HG	0.68	0.69
1:A:69:VAL:O	1:A:71:ARG:HD3	0.68	1.89
1:A:12:LEU:HD23	1:A:12:LEU:HD11	0.68	0.92
1:A:60:VAL:CG1	1:A:60:VAL:CB	0.68	0.68
1:A:12:LEU:CD1	1:A:12:LEU:CG	0.67	0.68
1:A:114:TYR:CD2	1:A:114:TYR:CG	0.67	0.72
1:A:107:LYS:CE	1:A:107:LYS:HZ1	0.67	1.38
1:A:114:TYR:CD1	1:A:114:TYR:CG	0.67	0.71
1:A:12:LEU:CG	1:A:12:LEU:HD23	0.67	1.20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:60:VAL:CG1	1:A:60:VAL:HG22	0.67	1.20
1:A:12:LEU:CG	1:A:12:LEU:HD22	0.67	1.20
1:A:10:GLN:CD	1:A:10:GLN:NE2	0.67	0.67
1:A:7:LEU:HB2	1:A:113:VAL:HG21	0.66	1.64
1:A:83:LEU:CG	1:A:83:LEU:CD2	0.66	0.67
1:A:88:ASN:HD22	1:A:88:ASN:CG	0.66	1.27
1:A:60:VAL:HG13	1:A:60:VAL:CG2	0.66	1.20
1:A:33:TYR:CD1	1:A:115:ASP:CG	0.66	2.67
1:A:88:ASN:HD21	1:A:88:ASN:CG	0.66	1.27
1:A:12:LEU:CG	1:A:12:LEU:HD21	0.66	1.20
1:A:107:LYS:CE	1:A:107:LYS:HZ2	0.66	1.38
1:A:83:LEU:HG	1:A:83:LEU:CB	0.66	0.82
1:A:107:LYS:CE	1:A:107:LYS:HZ3	0.65	1.38
1:A:113:VAL:CG1	1:A:113:VAL:CB	0.65	0.65
1:A:41:ASN:HB2	1:A:41:ASN:O	0.65	1.92
1:A:97:VAL:HG13	1:A:97:VAL:HG22	0.65	1.11
1:A:14:GLN:CD	1:A:14:GLN:NE2	0.65	0.65
1:A:83:LEU:CG	1:A:83:LEU:HB2	0.65	1.29
1:A:89:GLN:CD	1:A:89:GLN:NE2	0.64	0.65
1:A:56:LEU:CB	1:A:59:THR:HB	0.64	2.23
1:A:20:LYS:HZ2	1:A:20:LYS:CE	0.64	1.35
1:A:112:LYS:CB	1:A:112:LYS:HG2	0.64	1.18
1:A:29:LEU:HD13	1:A:29:LEU:HD22	0.64	1.12
1:A:33:TYR:CD2	1:A:115:ASP:CG	0.64	2.71
1:A:106:LEU:CG	1:A:106:LEU:HD12	0.64	1.17
1:A:91:LEU:N	1:A:91:LEU:CD1	0.64	2.58
1:A:106:LEU:CG	1:A:106:LEU:HB2	0.64	1.18
1:A:112:LYS:HG3	1:A:112:LYS:CB	0.64	1.18
1:A:106:LEU:CG	1:A:106:LEU:HD13	0.64	1.17
1:A:56:LEU:HB3	1:A:59:THR:HB	0.64	1.68
1:A:113:VAL:HG13	1:A:113:VAL:HG22	0.64	0.95
1:A:33:TYR:CD2	1:A:33:TYR:CG	0.64	0.71
1:A:20:LYS:HZ3	1:A:20:LYS:CE	0.64	1.35
1:A:106:LEU:CG	1:A:106:LEU:HD11	0.63	1.17
1:A:45:VAL:CG1	1:A:45:VAL:CB	0.63	0.63
1:A:60:VAL:CB	1:A:60:VAL:CG2	0.63	0.64
1:A:60:VAL:HG21	1:A:74:VAL:HG12	0.63	1.71
1:A:115:ASP:O	1:A:116:TYR:N	0.63	0.48
1:A:113:VAL:HG12	1:A:113:VAL:HG21	0.63	1.38
1:A:85:LYS:C	1:A:86:VAL:CA	0.63	1.96
1:A:34:THR:CB	1:A:34:THR:HG1	0.63	1.35
1:A:114:TYR:CZ	1:A:114:TYR:CE1	0.63	0.69

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:113:VAL:HG23	1:A:113:VAL:HG11	0.63	1.33
1:A:5:PHE:CD2	1:A:122:PHE:O	0.63	2.51
1:A:41:ASN:C	1:A:41:ASN:O	0.63	0.45
1:A:113:VAL:CG2	1:A:113:VAL:HG11	0.63	0.81
1:A:20:LYS:HZ1	1:A:20:LYS:CE	0.63	1.35
1:A:17:ASP:CG	1:A:17:ASP:OD2	0.63	0.69
1:A:100:ASP:CB	1:A:101:VAL:N	0.62	2.59
1:A:97:VAL:CG1	1:A:97:VAL:HG21	0.62	1.01
1:A:94:PHE:CE2	1:A:94:PHE:CZ	0.62	0.63
1:A:112:LYS:CG	1:A:112:LYS:HB3	0.62	1.15
1:A:29:LEU:HD11	1:A:47:VAL:HG11	0.62	1.72
1:A:60:VAL:HG13	1:A:60:VAL:HG22	0.62	0.83
1:A:57:LYS:HD3	1:A:57:LYS:HB3	0.62	1.56
1:A:45:VAL:CG2	1:A:45:VAL:CB	0.62	0.62
1:A:5:PHE:CD1	1:A:122:PHE:O	0.62	2.52
1:A:33:TYR:CZ	1:A:33:TYR:CE1	0.62	0.68
1:A:112:LYS:CG	1:A:112:LYS:HB2	0.61	1.15
1:A:13:PRO:O	1:A:15:THR:N	0.61	2.33
1:A:100:ASP:CA	1:A:100:ASP:OD1	0.61	2.42
1:A:107:LYS:HA	1:A:107:LYS:HG3	0.61	1.72
1:A:12:LEU:CD2	1:A:12:LEU:HD12	0.61	1.32
1:A:114:TYR:CE2	1:A:114:TYR:CZ	0.61	0.68
1:A:87:SER:HB3	1:A:87:SER:O	0.61	1.70
1:A:115:ASP:O	1:A:116:TYR:HB2	0.60	1.93
1:A:126:GLU:CB	1:A:126:GLU:OE1	0.60	2.45
1:A:60:VAL:CG1	1:A:60:VAL:CG2	0.60	0.61
1:A:7:LEU:HD21	1:A:125:ALA:HB3	0.60	1.73
1:A:107:LYS:HD2	1:A:107:LYS:NZ	0.60	2.01
1:A:29:LEU:CD2	1:A:29:LEU:CG	0.60	0.60
1:A:57:LYS:N	1:A:58:PRO:HD2	0.59	2.11
1:A:106:LEU:HG	1:A:106:LEU:HB3	0.59	0.66
1:A:102:PRO:HB2	1:A:102:PRO:O	0.59	1.95
1:A:70:SER:C	1:A:71:ARG:CD	0.59	2.71
1:A:60:VAL:CG1	1:A:74:VAL:HG12	0.59	2.28
1:A:10:GLN:OE1	1:A:10:GLN:NE2	0.58	0.74
1:A:126:GLU:OE2	1:A:126:GLU:CD	0.58	0.45
1:A:51:SER:OG	1:A:51:SER:N	0.58	2.30
1:A:70:SER:O	1:A:71:ARG:HD3	0.58	1.99
1:A:33:TYR:CD1	1:A:33:TYR:CG	0.58	0.63
1:A:69:VAL:HA	1:A:71:ARG:NH1	0.58	2.13
1:A:122:PHE:CE1	1:A:122:PHE:CZ	0.57	0.58
1:A:56:LEU:O	1:A:59:THR:HG22	0.57	1.99

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:29:LEU:CA	1:A:29:LEU:CD2	0.57	2.79
1:A:7:LEU:HB2	1:A:113:VAL:HG11	0.57	1.75
1:A:128:ASN:OD1	1:A:128:ASN:CG	0.57	0.77
1:A:59:THR:CG2	1:A:60:VAL:N	0.57	2.67
1:A:60:VAL:CG1	1:A:74:VAL:CG1	0.57	2.82
1:A:83:LEU:CD2	1:A:91:LEU:CD2	0.57	2.73
1:A:122:PHE:CE2	1:A:122:PHE:CZ	0.57	0.66
1:A:11:THR:HG23	1:A:127:TYR:OH	0.57	1.98
1:A:41:ASN:CB	1:A:41:ASN:O	0.57	2.16
1:A:17:ASP:CG	1:A:17:ASP:OD1	0.57	0.67
1:A:46:ASP:OD2	1:A:46:ASP:CG	0.57	0.77
1:A:7:LEU:HD21	1:A:125:ALA:HB2	0.57	1.76
1:A:49:MET:O	1:A:51:SER:N	0.56	2.38
1:A:118:GLU:C	1:A:119:THR:N	0.56	0.78
1:A:99:GLN:HE21	1:A:99:GLN:CD	0.56	1.16
1:A:33:TYR:CE2	1:A:33:TYR:CZ	0.56	0.60
1:A:53:PHE:CG	1:A:53:PHE:N	0.56	2.66
1:A:115:ASP:C	1:A:116:TYR:CB	0.56	2.69
1:A:106:LEU:CG	1:A:106:LEU:CD2	0.56	0.56
1:A:61:LYS:NZ	1:A:61:LYS:HD2	0.56	2.05
1:A:33:TYR:C	1:A:33:TYR:CD1	0.55	2.79
1:A:94:PHE:CG	1:A:94:PHE:CD1	0.55	0.63
1:A:60:VAL:HG11	1:A:74:VAL:HG12	0.55	1.79
1:A:33:TYR:HD2	1:A:33:TYR:CG	0.55	1.30
1:A:89:GLN:OE1	1:A:89:GLN:NE2	0.55	0.68
1:A:88:ASN:CG	1:A:88:ASN:ND2	0.55	0.60
1:A:106:LEU:CG	1:A:106:LEU:HB3	0.55	1.18
1:A:99:GLN:HE22	1:A:99:GLN:CD	0.55	1.16
1:A:114:TYR:CG	1:A:114:TYR:HD2	0.55	1.31
1:A:68:HIS:CD2	1:A:68:HIS:CG	0.55	0.80
1:A:94:PHE:CZ	1:A:94:PHE:HE1	0.55	1.30
1:A:94:PHE:CG	1:A:94:PHE:HD2	0.54	1.30
1:A:34:THR:C	1:A:34:THR:CG2	0.54	2.75
1:A:69:VAL:C	1:A:71:ARG:CD	0.54	2.76
1:A:69:VAL:HA	1:A:71:ARG:CZ	0.54	2.29
1:A:122:PHE:CA	1:A:122:PHE:CD1	0.54	2.82
1:A:112:LYS:HB2	1:A:112:LYS:HD3	0.54	1.71
1:A:83:LEU:HD21	1:A:91:LEU:HD23	0.54	1.46
1:A:84:ASP:OD1	1:A:84:ASP:OD2	0.54	0.55
1:A:114:TYR:HD1	1:A:114:TYR:CG	0.53	1.30
1:A:48:LYS:HD3	1:A:48:LYS:HE2	0.53	1.24
1:A:115:ASP:C	1:A:115:ASP:CG	0.53	2.65

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:33:TYR:CA	1:A:33:TYR:CD1	0.53	2.84
1:A:33:TYR:HE1	1:A:33:TYR:CZ	0.53	1.28
1:A:100:ASP:CG	1:A:100:ASP:OD1	0.53	0.64
1:A:99:GLN:HG3	1:A:100:ASP:N	0.53	2.12
1:A:91:LEU:HD12	1:A:91:LEU:N	0.53	2.17
1:A:107:LYS:HB3	1:A:107:LYS:HG2	0.53	1.31
1:A:114:TYR:CZ	1:A:114:TYR:HE1	0.53	1.29
1:A:29:LEU:HD11	1:A:29:LEU:CD2	0.53	1.10
1:A:14:GLN:NE2	1:A:14:GLN:OE1	0.53	0.67
1:A:71:ARG:CZ	1:A:71:ARG:HH21	0.53	1.23
1:A:60:VAL:HG21	1:A:74:VAL:CG1	0.53	2.33
1:A:42:MET:HG2	1:A:42:MET:HB3	0.52	1.22
1:A:60:VAL:CG1	1:A:60:VAL:HG21	0.52	0.78
1:A:113:VAL:CG1	1:A:113:VAL:HG21	0.52	0.92
1:A:128:ASN:O	1:A:130:PRO:HD3	0.52	2.05
1:A:114:TYR:CZ	1:A:114:TYR:HE2	0.52	1.28
1:A:47:VAL:CG1	1:A:47:VAL:N	0.52	2.69
1:A:100:ASP:CG	1:A:100:ASP:OD2	0.52	0.72
1:A:46:ASP:HB2	1:A:80:LEU:CD1	0.52	2.34
1:A:5:PHE:CE1	1:A:122:PHE:O	0.52	2.51
1:A:3:PHE:O	1:A:4:PRO:O	0.52	2.21
1:A:106:LEU:O	1:A:107:LYS:HG3	0.51	2.05
1:A:14:GLN:O	1:A:15:THR:CB	0.51	2.46
1:A:118:GLU:C	1:A:118:GLU:O	0.51	0.51
1:A:49:MET:CE	1:A:49:MET:HG3	0.51	2.24
1:A:33:TYR:HD1	1:A:33:TYR:CG	0.50	1.26
1:A:7:LEU:CD2	1:A:125:ALA:HB2	0.50	2.36
1:A:9:VAL:HG11	1:A:111:VAL:HG21	0.50	1.73
1:A:54:ILE:O	1:A:54:ILE:HG22	0.50	2.04
1:A:36:SER:HG	1:A:36:SER:CB	0.50	1.20
1:A:64:GLU:OE2	1:A:64:GLU:OE1	0.50	0.50
1:A:106:LEU:HG	1:A:106:LEU:HB2	0.50	1.06
1:A:33:TYR:CG	1:A:115:ASP:OD2	0.49	2.64
1:A:122:PHE:CG	1:A:122:PHE:CD1	0.49	0.66
1:A:33:TYR:HE2	1:A:33:TYR:CZ	0.49	1.24
1:A:18:GLU:CD	1:A:18:GLU:OE1	0.49	0.69
1:A:51:SER:HG	1:A:51:SER:N	0.49	2.03
1:A:106:LEU:O	1:A:107:LYS:HD2	0.48	2.08
1:A:18:GLU:CD	1:A:18:GLU:OE2	0.48	0.57
1:A:68:HIS:CG	1:A:68:HIS:HD2	0.48	1.28
1:A:81:ILE:HG13	1:A:93:LEU:HD11	0.48	1.79
1:A:106:LEU:O	1:A:107:LYS:CG	0.48	2.61

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:112:LYS:HB3	1:A:112:LYS:HG2	0.48	0.98
1:A:60:VAL:CG1	1:A:60:VAL:N	0.48	2.73
1:A:63:LEU:O	1:A:66:SER:HB2	0.48	2.09
1:A:135:LEU:HD23	1:A:135:LEU:O	0.48	1.54
1:A:6:ALA:N	1:A:32:SER:O	0.47	2.46
1:A:100:ASP:C	1:A:101:VAL:N	0.47	0.53
1:A:14:GLN:HG2	1:A:14:GLN:HB3	0.47	1.27
1:A:106:LEU:C	1:A:107:LYS:CG	0.47	2.83
1:A:102:PRO:O	1:A:102:PRO:CG	0.47	2.57
1:A:69:VAL:O	1:A:70:SER:O	0.47	2.32
1:A:118:GLU:CD	1:A:119:THR:N	0.47	2.63
1:A:85:LYS:C	1:A:86:VAL:N	0.46	0.74
1:A:70:SER:HG	1:A:70:SER:CB	0.46	1.17
1:A:79:VAL:O	1:A:80:LEU:HD13	0.46	2.11
1:A:36:SER:OG	1:A:36:SER:O	0.46	2.32
1:A:9:VAL:CG2	1:A:9:VAL:N	0.46	2.75
1:A:94:PHE:HE2	1:A:94:PHE:CZ	0.46	1.22
1:A:37:ARG:CZ	1:A:37:ARG:HG3	0.46	1.89
1:A:97:VAL:N	1:A:97:VAL:CG2	0.46	2.77
1:A:94:PHE:CG	1:A:94:PHE:HD1	0.46	1.22
1:A:51:SER:CB	1:A:51:SER:HG	0.46	1.16
1:A:12:LEU:CD2	1:A:12:LEU:HD11	0.45	0.99
1:A:60:VAL:CG2	1:A:60:VAL:C	0.45	2.81
1:A:29:LEU:HD21	1:A:47:VAL:HG11	0.45	1.89
1:A:99:GLN:HB3	1:A:99:GLN:HG2	0.45	1.25
1:A:106:LEU:O	1:A:107:LYS:CD	0.45	2.65
1:A:112:LYS:CG	1:A:112:LYS:CB	0.45	0.59
1:A:14:GLN:C	1:A:15:THR:HG22	0.45	2.27
1:A:107:LYS:HD3	1:A:107:LYS:CB	0.45	2.27
1:A:12:LEU:CG	1:A:12:LEU:CD2	0.44	0.46
1:A:115:ASP:OD1	1:A:115:ASP:CG	0.44	0.64
1:A:116:TYR:HD2	1:A:116:TYR:CG	0.44	1.24
1:A:69:VAL:C	1:A:71:ARG:CZ	0.44	2.85
1:A:7:LEU:HB2	1:A:113:VAL:CG1	0.44	2.39
1:A:122:PHE:HD1	1:A:122:PHE:CG	0.44	1.19
1:A:122:PHE:CZ	1:A:122:PHE:HE2	0.44	1.19
1:A:102:PRO:N	1:A:102:PRO:O	0.44	2.38
1:A:48:LYS:HG3	1:A:78:HIS:HB3	0.43	1.90
1:A:33:TYR:C	1:A:33:TYR:CD2	0.43	2.90
1:A:69:VAL:HG13	1:A:70:SER:N	0.43	2.24
1:A:60:VAL:CG2	1:A:74:VAL:HG12	0.42	2.41
1:A:27:ILE:HD11	1:A:97:VAL:HG22	0.42	1.90

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:13:PRO:O	1:A:14:GLN:CB	0.42	2.52
1:A:49:MET:HA	1:A:109:ALA:CB	0.42	2.45
1:A:60:VAL:HG11	1:A:60:VAL:CG2	0.42	0.85
1:A:113:VAL:C	1:A:113:VAL:CG1	0.42	2.82
1:A:44:ILE:CD1	1:A:44:ILE:C	0.42	2.88
1:A:70:SER:HB3	1:A:70:SER:HG	0.42	1.23
1:A:122:PHE:CD2	1:A:122:PHE:CG	0.41	0.58
1:A:94:PHE:CD1	1:A:94:PHE:N	0.41	2.88
1:A:71:ARG:HE	1:A:71:ARG:N	0.41	1.97
1:A:71:ARG:CD	1:A:71:ARG:N	0.41	2.65
1:A:1:GLU:CD	1:A:1:GLU:HB2	0.41	2.07
1:A:9:VAL:CG1	1:A:111:VAL:HG11	0.41	2.30
1:A:99:GLN:NE2	1:A:99:GLN:CD	0.41	0.46
1:A:126:GLU:OE2	1:A:126:GLU:OE1	0.41	0.41
1:A:5:PHE:CZ	1:A:122:PHE:O	0.41	2.66
1:A:106:LEU:CD1	1:A:106:LEU:CG	0.41	0.41
1:A:12:LEU:CD2	1:A:12:LEU:HD13	0.41	1.07
1:A:80:LEU:HD22	1:A:80:LEU:N	0.41	2.31
1:A:19:PRO:C	1:A:21:ALA:N	0.41	2.74
1:A:55:PRO:HG2	1:A:76:SER:HA	0.40	1.92
1:A:12:LEU:HD22	1:A:12:LEU:HD13	0.40	0.43
1:A:41:ASN:O	1:A:42:MET:CB	0.40	2.61
1:A:59:THR:O	1:A:62:MET:HB2	0.40	2.17

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	136/138 (99%)	102 (75%)	16 (12%)	18 (13%)	1	6
All	All	136/138 (99%)	102 (75%)	16 (12%)	18 (13%)	1	6

All 18 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	40	SER
1	A	131	CYS
1	A	17	ASP
1	A	41	ASN
1	A	120	ASP
1	A	118	GLU
1	A	137	ASN
1	A	85	LYS
1	A	15	THR
1	A	38	SER
1	A	116	TYR
1	A	4	PRO
1	A	70	SER
1	A	121	GLU
1	A	51	SER
1	A	50	VAL
1	A	67	ASN
1	A	88	ASN

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	124/125 (99%)	66 (53%)	58 (47%)	0	2
All	All	124/125 (99%)	66 (53%)	58 (47%)	0	2

All 58 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	117	TYR
1	A	132	SER
1	A	66	SER
1	A	91	LEU
1	A	137	ASN
1	A	25	PHE
1	A	64	GLU
1	A	63	LEU

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Mol	Chain	Res	Type
1	A	7	LEU
1	A	14	GLN
1	A	97	VAL
1	A	38	SER
1	A	88	ASN
1	A	33	TYR
1	A	111	VAL
1	A	128	ASN
1	A	75	SER
1	A	9	VAL
1	A	56	LEU
1	A	113	VAL
1	A	93	LEU
1	A	105	ASP
1	A	44	ILE
1	A	54	ILE
1	A	68	HIS
1	A	112	LYS
1	A	18	GLU
1	A	12	LEU
1	A	106	LEU
1	A	107	LYS
1	A	101	VAL
1	A	22	HIS
1	A	76	SER
1	A	71	ARG
1	A	131	CYS
1	A	15	THR
1	A	99	GLN
1	A	87	SER
1	A	47	VAL
1	A	94	PHE
1	A	50	VAL
1	A	20	LYS
1	A	42	MET
1	A	26	GLN
1	A	104	ARG
1	A	53	PHE
1	A	46	ASP
1	A	103	VAL
1	A	124	ILE
1	A	115	ASP

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Mol	Chain	Res	Type
1	A	65	ARG
1	A	16	CYS
1	A	83	LEU
1	A	45	VAL
1	A	78	HIS
1	A	121	GLU
1	A	98	LEU
1	A	60	VAL

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided