



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 01:01 AM UTC

PDB ID : 5JB1 / pdb_00005jb1
EMDB ID : EMD-8147
Title : Pseudo-atomic structure of Human Papillomavirus Type 59 L1 Virus-like Particle
Authors : Li, Z.H.; Yan, X.D.; Yu, H.; Zheng, Q.B.; Gu, Y.; Li, S.W.
Deposited on : 2016-04-13
Resolution : 6.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

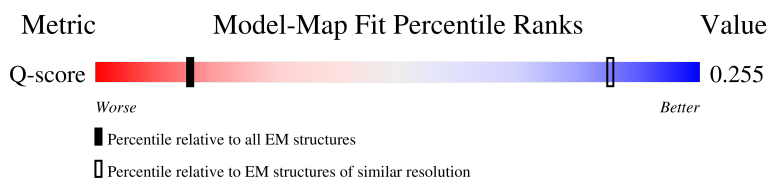
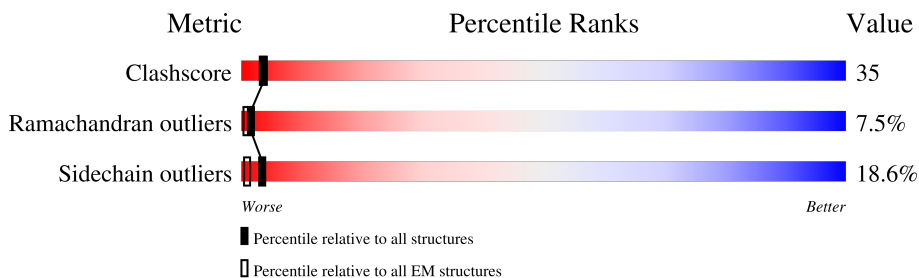
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.00 Å.

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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	525 (5.50 - 6.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	15% 18% 31% 31% 11% 9%
1	B	500	16% 19% 33% 30% 10% 7%
1	C	500	17% 19% 31% 31% 10% 9%
1	D	500	15% 16% 33% 29% 12% 9%

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Mol	Chain	Length	Quality of chain
1	E	500	13% 16% 30% 33% 12% 9%
1	F	500	17% 19% 31% 31% 13% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21696 atoms, of which 0 are hydrogens and 0 are deuteriums.

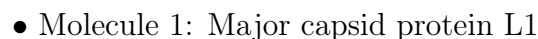
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

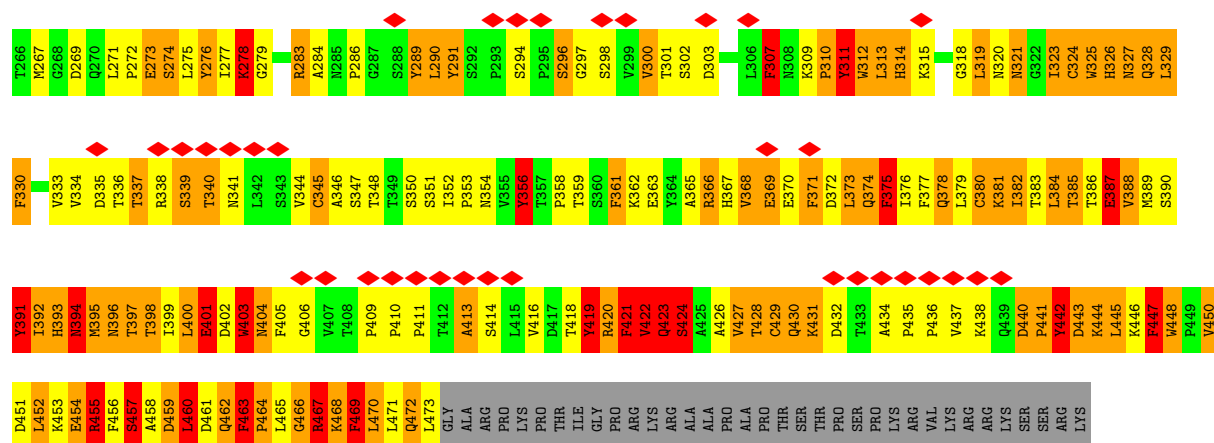
- Molecule 1 is a protein called Major capsid protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	456	Total	C	N	O	S	0	0
			3598	2289	604	686	19		
1	B	464	Total	C	N	O	S	0	0
			3661	2333	613	696	19		
1	C	457	Total	C	N	O	S	0	0
			3604	2292	605	688	19		
1	D	454	Total	C	N	O	S	0	0
			3586	2281	602	684	19		
1	E	454	Total	C	N	O	S	0	0
			3586	2281	602	684	19		
1	F	464	Total	C	N	O	S	0	0
			3661	2333	613	696	19		

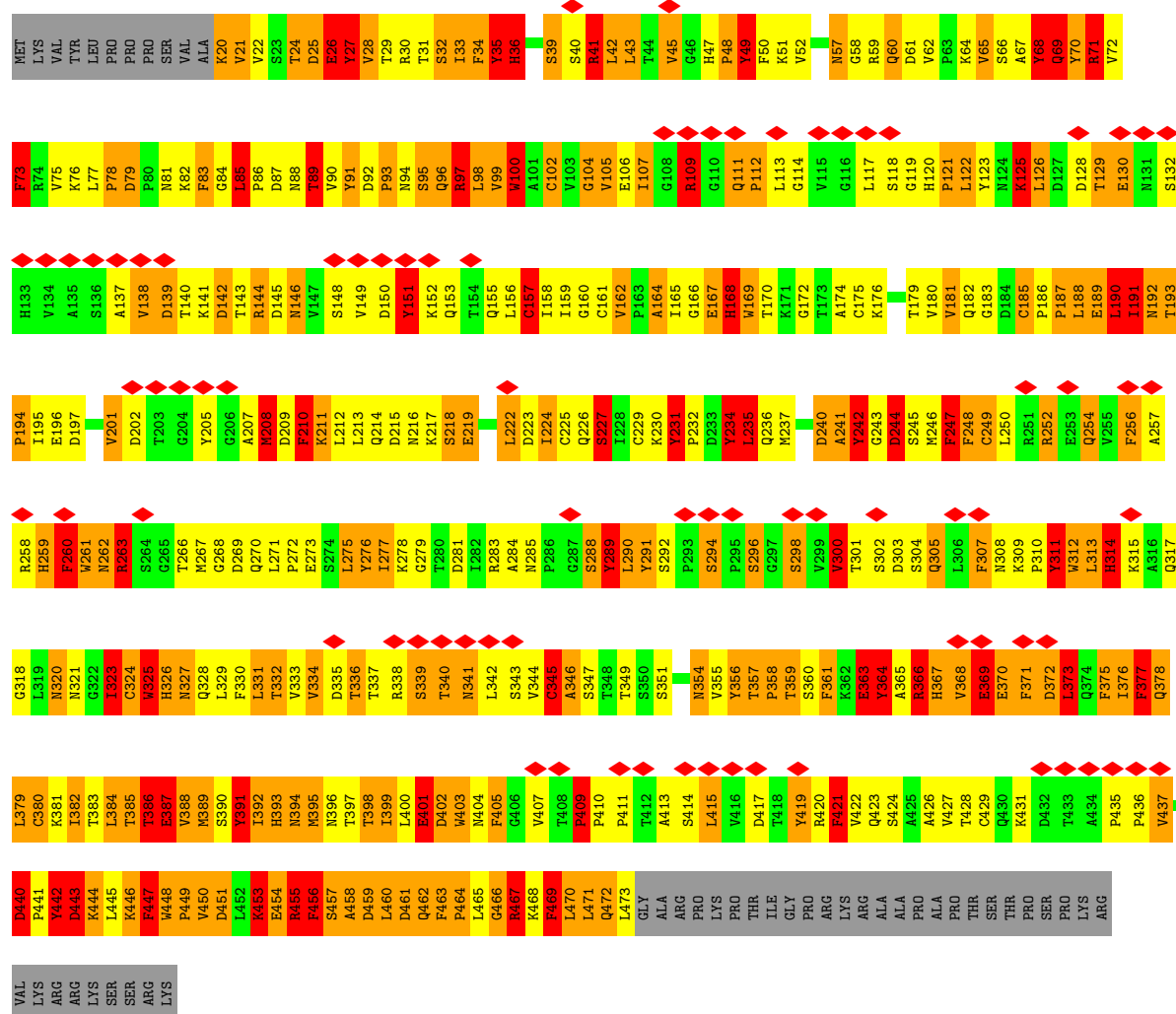
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP Q81971
B	9	MET	-	initiating methionine	UNP Q81971
C	9	MET	-	initiating methionine	UNP Q81971
D	9	MET	-	initiating methionine	UNP Q81971
E	9	MET	-	initiating methionine	UNP Q81971
F	9	MET	-	initiating methionine	UNP Q81971

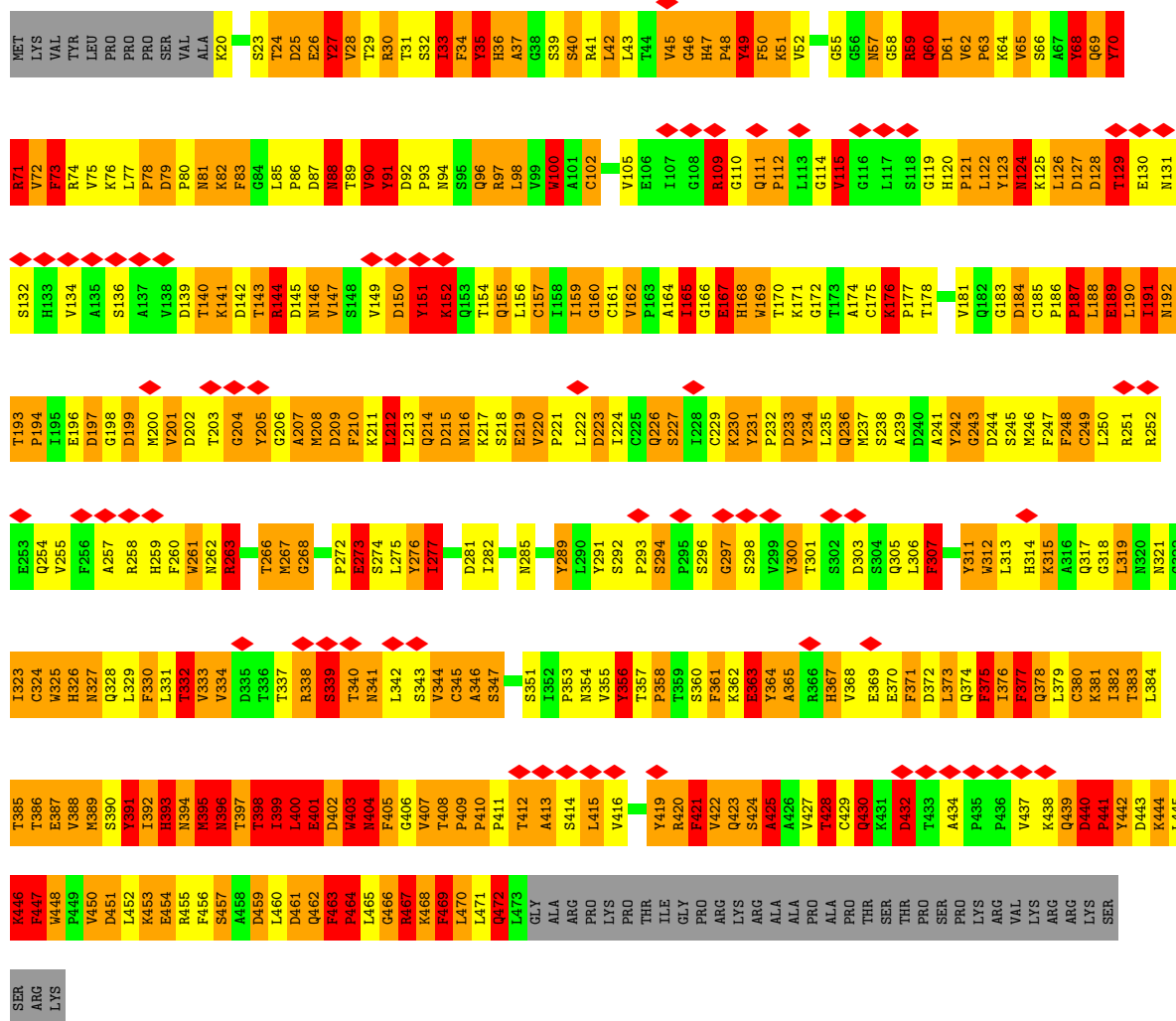




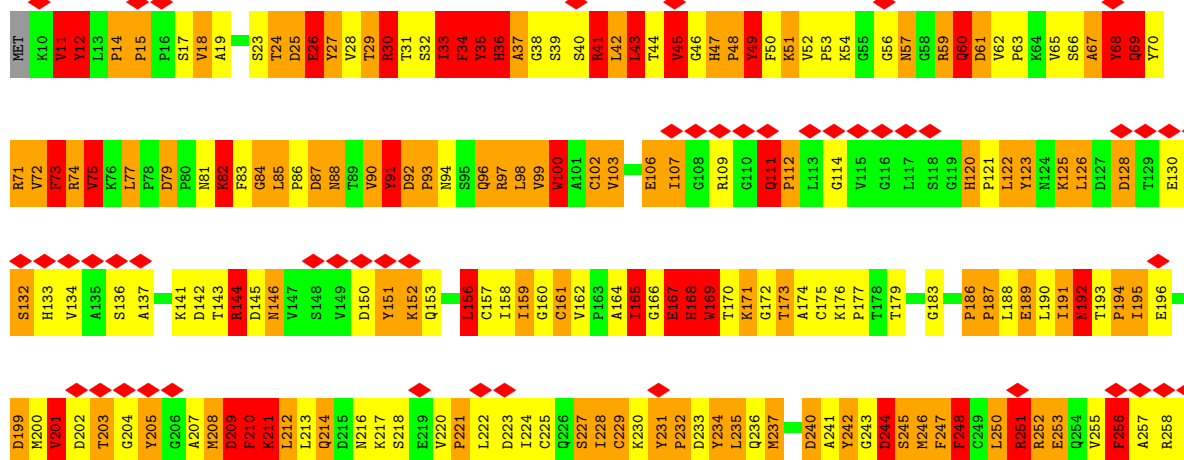
• Molecule 1: Major capsid protein L1



• Molecule 1: Major capsid protein L1



• Molecule 1: Major capsid protein L1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3100	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	14.133	Depositor
Minimum map value	-6.758	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.25	Depositor
Map size (Å)	910.2, 910.2, 910.2	wwPDB
Map dimensions	820, 820, 820	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 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 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	2.31	192/3694 (5.2%)	2.49	258/5036 (5.1%)
1	B	2.25	178/3761 (4.7%)	2.41	241/5130 (4.7%)
1	C	2.31	193/3700 (5.2%)	2.46	246/5044 (4.9%)
1	D	2.34	193/3682 (5.2%)	2.41	245/5019 (4.9%)
1	E	3.01	195/3682 (5.3%)	2.48	267/5019 (5.3%)
1	F	2.32	215/3761 (5.7%)	2.41	265/5130 (5.2%)
All	All	2.44	1166/22280 (5.2%)	2.44	1522/30378 (5.0%)

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 outliers	#Planarity outliers
1	A	0	35
1	B	0	45
1	C	0	46
1	D	0	43
1	E	0	37
1	F	0	47
All	All	0	253

All (1166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	405	PHE	N-CA	119.81	3.00	1.46
1	A	219	GLU	CA-C	-17.43	1.44	1.52
1	A	463	PHE	CA-C	-14.09	1.41	1.52
1	F	463	PHE	CA-C	-13.77	1.37	1.52
1	A	447	PHE	CA-C	-12.69	1.36	1.52
1	D	463	PHE	CA-C	-12.60	1.42	1.52
1	D	52	VAL	N-CA	-11.51	1.38	1.46
1	D	311	TYR	CA-C	-11.39	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	314	HIS	CA-C	-11.30	1.43	1.52
1	F	33	ILE	CA-C	-11.14	1.40	1.52
1	D	52	VAL	CA-C	-11.11	1.44	1.53
1	E	244	ASP	CA-C	-10.99	1.45	1.52
1	C	463	PHE	CA-C	-10.96	1.43	1.52
1	D	78	PRO	CA-C	-10.85	1.40	1.52
1	C	62	VAL	CA-C	-10.81	1.45	1.52
1	D	325	TRP	CA-C	-10.80	1.39	1.52
1	B	311	TYR	CA-C	-10.75	1.39	1.52
1	D	447	PHE	CA-C	-10.70	1.38	1.52
1	B	398	THR	CA-C	-10.53	1.38	1.52
1	B	463	PHE	CA-C	-10.40	1.41	1.52
1	D	351	SER	CA-C	-10.29	1.48	1.53
1	B	388	VAL	CA-C	-10.23	1.40	1.52
1	C	388	VAL	CA-C	-10.19	1.40	1.52
1	F	392	ILE	N-CA	-10.18	1.33	1.46
1	C	447	PHE	CA-C	-10.14	1.40	1.52
1	A	310	PRO	CA-C	-10.11	1.41	1.52
1	D	310	PRO	CA-C	-10.02	1.41	1.52
1	F	391	TYR	CA-C	-9.97	1.39	1.52
1	C	82	LYS	CA-C	-9.86	1.42	1.53
1	D	33	ILE	CA-C	-9.74	1.41	1.52
1	B	33	ILE	CA-C	-9.74	1.41	1.52
1	B	447	PHE	CA-C	-9.68	1.40	1.52
1	A	385	THR	CA-C	-9.66	1.41	1.52
1	A	33	ILE	CA-C	-9.62	1.41	1.52
1	F	388	VAL	CA-C	-9.55	1.40	1.52
1	F	403	TRP	CA-C	-9.53	1.40	1.52
1	B	42	LEU	CA-C	-9.50	1.41	1.52
1	A	440	ASP	C-N	-9.45	1.22	1.33
1	D	403	TRP	CA-C	-9.44	1.39	1.52
1	B	314	HIS	CA-C	-9.44	1.41	1.52
1	B	201	VAL	CA-C	-9.42	1.44	1.52
1	F	447	PHE	CA-C	-9.37	1.41	1.52
1	B	35	TYR	CA-C	-9.35	1.41	1.52
1	A	52	VAL	N-CA	-9.34	1.39	1.46
1	F	469	PHE	N-CA	-9.28	1.34	1.46
1	A	62	VAL	CA-C	-9.22	1.44	1.52
1	C	313	LEU	CA-C	-9.21	1.41	1.52
1	C	52	VAL	CA-C	-9.14	1.45	1.53
1	F	465	LEU	CA-C	-8.96	1.41	1.52
1	C	62	VAL	CA-CB	-8.95	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	PRO	CA-C	-8.87	1.43	1.52
1	E	62	VAL	CA-C	-8.86	1.45	1.53
1	D	28	VAL	CA-CB	-8.80	1.45	1.54
1	A	69	GLN	N-CA	-8.78	1.34	1.45
1	A	311	TYR	CA-C	-8.78	1.42	1.52
1	C	311	TYR	CA-C	-8.72	1.42	1.52
1	E	97	ARG	CA-C	-8.68	1.42	1.52
1	E	469	PHE	N-CA	-8.64	1.35	1.46
1	C	390	SER	CA-C	-8.57	1.41	1.52
1	A	428	THR	CA-C	-8.49	1.42	1.52
1	F	307	PHE	CA-C	-8.47	1.41	1.53
1	F	325	TRP	CA-C	-8.47	1.42	1.52
1	D	442	TYR	CA-C	-8.45	1.42	1.53
1	C	403	TRP	CA-C	-8.43	1.42	1.52
1	A	69	GLN	CA-C	-8.42	1.42	1.52
1	C	62	VAL	N-CA	-8.40	1.38	1.46
1	C	61	ASP	N-CA	-8.38	1.36	1.46
1	D	29	THR	CA-C	-8.35	1.42	1.52
1	D	469	PHE	N-CA	-8.33	1.36	1.46
1	D	91	TYR	N-CA	-8.32	1.36	1.46
1	F	381	LYS	CA-C	-8.31	1.42	1.52
1	D	92	ASP	N-CA	-8.30	1.37	1.46
1	C	125	LYS	N-CA	-8.30	1.36	1.46
1	B	98	LEU	CA-C	-8.30	1.42	1.52
1	D	224	ILE	CA-CB	-8.29	1.45	1.54
1	D	388	VAL	CA-C	-8.28	1.42	1.52
1	F	192	ASN	CA-C	-8.28	1.42	1.52
1	D	315	LYS	CA-C	-8.26	1.42	1.52
1	B	52	VAL	N-CA	-8.26	1.40	1.46
1	D	377	PHE	CA-C	-8.26	1.42	1.52
1	C	303	ASP	CA-C	-8.25	1.42	1.52
1	F	311	TYR	CA-C	-8.25	1.42	1.52
1	E	466	GLY	CA-C	-8.23	1.43	1.52
1	E	392	ILE	CA-C	-8.22	1.42	1.52
1	E	315	LYS	CA-C	-8.21	1.43	1.52
1	E	430	GLN	CA-C	-8.20	1.42	1.53
1	D	450	VAL	CA-C	-8.19	1.46	1.53
1	E	344	VAL	CA-C	-8.19	1.42	1.52
1	F	467	ARG	CA-C	-8.18	1.42	1.52
1	E	405	PHE	CA-CB	8.17	1.67	1.53
1	E	214	GLN	CA-C	-8.15	1.42	1.52
1	F	34	PHE	CA-C	-8.13	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	VAL	CA-C	-8.13	1.46	1.53
1	D	90	VAL	CA-C	-8.13	1.42	1.52
1	B	214	GLN	CA-C	-8.12	1.42	1.52
1	C	470	LEU	CA-C	-8.10	1.42	1.52
1	C	47	HIS	C-N	-8.10	1.25	1.34
1	E	33	ILE	CA-C	-8.09	1.43	1.52
1	A	277	ILE	CA-C	-8.09	1.43	1.52
1	F	440	ASP	N-CA	-8.08	1.37	1.46
1	C	375	PHE	CA-C	-8.08	1.42	1.52
1	E	392	ILE	CA-CB	-8.07	1.44	1.54
1	B	235	LEU	CA-C	-8.03	1.42	1.52
1	D	328	GLN	N-CA	-8.02	1.36	1.46
1	B	470	LEU	CA-C	-8.02	1.42	1.52
1	E	75	VAL	CA-CB	-8.02	1.44	1.54
1	D	459	ASP	CA-C	-8.01	1.43	1.53
1	D	26	GLU	CA-C	-7.98	1.42	1.52
1	B	236	GLN	CA-C	-7.97	1.42	1.52
1	B	52	VAL	CA-C	-7.96	1.46	1.53
1	E	392	ILE	N-CA	-7.96	1.37	1.46
1	C	443	ASP	N-CA	-7.96	1.36	1.46
1	A	328	GLN	CA-C	-7.96	1.43	1.52
1	D	96	GLN	CA-C	-7.95	1.43	1.52
1	E	52	VAL	CA-C	-7.95	1.44	1.52
1	C	224	ILE	CA-CB	-7.93	1.45	1.54
1	A	326	HIS	CA-C	-7.93	1.40	1.52
1	F	234	TYR	CA-C	-7.90	1.42	1.52
1	C	466	GLY	CA-C	-7.90	1.43	1.52
1	C	49	TYR	CA-C	-7.89	1.42	1.52
1	D	390	SER	CA-C	-7.87	1.43	1.52
1	B	352	ILE	CA-C	-7.85	1.45	1.52
1	B	69	GLN	CA-C	-7.85	1.43	1.52
1	B	26	GLU	N-CA	-7.85	1.37	1.46
1	D	327	ASN	CA-C	-7.84	1.43	1.53
1	E	388	VAL	N-CA	-7.83	1.37	1.46
1	B	328	GLN	CA-C	-7.83	1.43	1.52
1	B	143	THR	CA-C	-7.83	1.45	1.53
1	F	231	TYR	C-N	-7.80	1.24	1.33
1	F	392	ILE	CA-CB	-7.80	1.43	1.54
1	D	91	TYR	CA-C	-7.79	1.43	1.52
1	F	466	GLY	CA-C	-7.79	1.43	1.52
1	D	448	TRP	N-CA	-7.78	1.34	1.46
1	F	428	THR	CA-C	-7.78	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	386	THR	CA-C	-7.77	1.42	1.52
1	C	60	GLN	CA-C	-7.76	1.44	1.53
1	B	75	VAL	CA-CB	-7.75	1.44	1.53
1	D	328	GLN	CA-C	-7.73	1.43	1.52
1	D	392	ILE	CA-C	-7.73	1.42	1.52
1	B	96	GLN	CA-C	-7.72	1.42	1.52
1	E	390	SER	CA-C	-7.72	1.43	1.52
1	D	162	VAL	CA-C	-7.72	1.44	1.52
1	B	99	VAL	CA-C	-7.70	1.43	1.52
1	E	91	TYR	CA-C	-7.70	1.43	1.52
1	E	447	PHE	CA-C	-7.69	1.43	1.52
1	F	471	LEU	CA-C	-7.68	1.42	1.52
1	C	448	TRP	N-CA	-7.67	1.36	1.46
1	E	98	LEU	CA-C	-7.67	1.43	1.52
1	C	450	VAL	CA-C	-7.67	1.46	1.53
1	E	311	TYR	CA-C	-7.67	1.43	1.52
1	C	325	TRP	CA-C	-7.66	1.43	1.52
1	F	386	THR	CA-C	-7.65	1.42	1.52
1	E	325	TRP	CA-C	-7.63	1.43	1.52
1	C	400	LEU	CA-C	-7.63	1.43	1.52
1	F	201	VAL	CA-C	-7.63	1.43	1.52
1	E	459	ASP	CA-C	-7.61	1.42	1.52
1	C	33	ILE	CA-C	-7.61	1.43	1.52
1	F	393	HIS	CA-C	-7.61	1.42	1.52
1	F	144	ARG	N-CA	-7.60	1.36	1.46
1	F	391	TYR	C-N	-7.60	1.24	1.34
1	C	388	VAL	CA-CB	-7.59	1.45	1.54
1	F	315	LYS	CA-C	-7.59	1.43	1.52
1	C	228	ILE	CA-C	-7.58	1.43	1.52
1	C	25	ASP	N-CA	-7.56	1.36	1.46
1	D	466	GLY	CA-C	-7.56	1.43	1.52
1	F	303	ASP	CA-C	-7.55	1.43	1.52
1	A	52	VAL	C-N	-7.54	1.24	1.33
1	F	389	MET	CA-C	-7.52	1.43	1.52
1	C	235	LEU	CA-C	-7.51	1.43	1.52
1	D	82	LYS	CA-C	-7.51	1.42	1.52
1	A	398	THR	CA-C	-7.50	1.43	1.52
1	D	388	VAL	CA-CB	-7.50	1.45	1.54
1	B	385	THR	CA-C	-7.49	1.43	1.52
1	F	52	VAL	CA-C	-7.48	1.47	1.53
1	F	62	VAL	CA-C	-7.47	1.46	1.53
1	F	26	GLU	CA-C	-7.46	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	VAL	CA-CB	-7.45	1.47	1.54
1	A	446	LYS	CA-C	-7.44	1.43	1.52
1	E	162	VAL	CA-C	-7.43	1.45	1.52
1	D	338	ARG	N-CA	-7.42	1.37	1.45
1	E	35	TYR	CA-C	-7.42	1.43	1.52
1	C	388	VAL	N-CA	-7.42	1.37	1.46
1	E	419	TYR	CA-C	-7.40	1.43	1.52
1	C	50	PHE	CA-C	-7.38	1.43	1.52
1	B	386	THR	CA-C	-7.38	1.43	1.52
1	D	97	ARG	CA-C	-7.37	1.43	1.52
1	C	378	GLN	N-CA	-7.36	1.37	1.46
1	B	352	ILE	N-CA	-7.36	1.39	1.46
1	D	52	VAL	CA-CB	-7.35	1.46	1.53
1	E	235	LEU	CA-C	-7.34	1.43	1.52
1	F	380	CYS	CA-C	-7.34	1.43	1.52
1	C	214	GLN	CA-C	-7.33	1.43	1.52
1	C	469	PHE	N-CA	-7.32	1.37	1.46
1	B	192	ASN	CA-C	-7.32	1.43	1.52
1	A	459	ASP	CA-C	-7.32	1.43	1.52
1	B	392	ILE	CA-CB	-7.32	1.45	1.54
1	B	375	PHE	CA-C	-7.31	1.43	1.52
1	E	94	ASN	CA-C	-7.30	1.43	1.53
1	E	465	LEU	CA-C	-7.30	1.43	1.52
1	E	125	LYS	CA-C	-7.29	1.44	1.52
1	E	467	ARG	CA-C	-7.28	1.43	1.52
1	A	471	LEU	N-CA	-7.28	1.37	1.46
1	D	262	ASN	N-CA	-7.27	1.36	1.46
1	D	236	GLN	CA-C	-7.26	1.43	1.52
1	A	29	THR	CA-C	-7.26	1.43	1.52
1	D	332	THR	CA-C	-7.25	1.43	1.52
1	F	385	THR	CA-C	-7.25	1.43	1.52
1	B	50	PHE	CA-C	-7.25	1.43	1.52
1	E	389	MET	CA-C	-7.24	1.43	1.52
1	C	28	VAL	CA-C	-7.24	1.44	1.52
1	A	391	TYR	CA-C	-7.23	1.43	1.52
1	C	310	PRO	CA-C	-7.23	1.42	1.52
1	B	92	ASP	C-N	-7.23	1.27	1.34
1	F	49	TYR	CA-C	-7.23	1.42	1.52
1	E	471	LEU	N-CA	-7.22	1.37	1.46
1	C	387	GLU	CA-C	-7.22	1.42	1.52
1	B	95	SER	CA-C	-7.22	1.42	1.52
1	F	470	LEU	CA-C	-7.22	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	446	LYS	CA-C	-7.21	1.43	1.52
1	B	463	PHE	N-CA	-7.21	1.36	1.46
1	A	450	VAL	CA-C	-7.19	1.43	1.52
1	D	392	ILE	CA-CB	-7.19	1.45	1.54
1	C	162	VAL	CA-C	-7.19	1.45	1.52
1	C	461	ASP	N-CA	-7.19	1.37	1.46
1	B	82	LYS	CA-C	-7.18	1.43	1.52
1	B	457	SER	CA-C	-7.17	1.43	1.52
1	D	167	GLU	CA-C	-7.16	1.43	1.52
1	B	236	GLN	N-CA	-7.16	1.37	1.46
1	D	234	TYR	CA-C	-7.16	1.43	1.52
1	C	172	GLY	CA-C	-7.15	1.45	1.52
1	E	427	VAL	CA-C	-7.15	1.43	1.52
1	A	392	ILE	CA-CB	-7.14	1.44	1.54
1	B	325	TRP	CA-C	-7.14	1.43	1.52
1	E	85	LEU	C-N	-7.12	1.27	1.33
1	D	323	ILE	CA-CB	-7.12	1.45	1.54
1	E	313	LEU	CA-C	-7.11	1.43	1.52
1	D	33	ILE	N-CA	-7.11	1.38	1.46
1	D	281	ASP	CA-C	-7.11	1.47	1.53
1	C	231	TYR	C-N	-7.10	1.25	1.33
1	A	162	VAL	CA-C	-7.09	1.45	1.52
1	F	390	SER	CA-C	-7.09	1.43	1.52
1	B	390	SER	CA-C	-7.08	1.42	1.52
1	B	352	ILE	CA-CB	-7.08	1.48	1.54
1	E	397	THR	CA-C	-7.08	1.42	1.52
1	B	401	GLU	CA-C	-7.07	1.43	1.52
1	E	448	TRP	C-N	-7.07	1.25	1.33
1	A	392	ILE	CA-C	-7.07	1.42	1.52
1	A	214	GLN	CA-C	-7.07	1.43	1.53
1	C	460	LEU	C-N	-7.07	1.24	1.34
1	D	33	ILE	CA-CB	-7.06	1.45	1.54
1	F	167	GLU	CA-C	-7.06	1.43	1.52
1	A	127	ASP	CA-C	-7.06	1.44	1.52
1	F	388	VAL	N-CA	-7.05	1.37	1.46
1	A	104	GLY	CA-C	-7.05	1.45	1.51
1	A	245	SER	CA-C	-7.05	1.43	1.52
1	E	41	ARG	CA-C	-7.04	1.43	1.52
1	F	395	MET	N-CA	-7.03	1.37	1.46
1	D	395	MET	CA-C	-7.02	1.44	1.53
1	C	125	LYS	CA-C	-7.01	1.44	1.52
1	D	388	VAL	N-CA	-7.01	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	35	TYR	CA-C	-7.00	1.44	1.52
1	D	62	VAL	CA-CB	-7.00	1.48	1.54
1	E	49	TYR	CA-C	-7.00	1.43	1.52
1	F	382	ILE	CA-C	-6.99	1.43	1.52
1	A	377	PHE	CA-C	-6.99	1.44	1.52
1	C	431	LYS	N-CA	-6.98	1.37	1.46
1	B	468	LYS	CA-C	-6.97	1.43	1.52
1	B	224	ILE	CA-CB	-6.96	1.45	1.54
1	B	382	ILE	CA-C	-6.96	1.43	1.52
1	D	98	LEU	CA-C	-6.96	1.44	1.52
1	F	235	LEU	CA-C	-6.96	1.43	1.52
1	C	471	LEU	N-CA	-6.95	1.38	1.46
1	E	224	ILE	CA-CB	-6.95	1.47	1.54
1	D	471	LEU	CA-C	-6.95	1.43	1.52
1	E	78	PRO	CA-C	-6.94	1.44	1.52
1	B	49	TYR	CA-C	-6.93	1.43	1.52
1	B	162	VAL	N-CA	-6.93	1.38	1.46
1	C	398	THR	CA-C	-6.93	1.43	1.52
1	A	401	GLU	CA-C	-6.92	1.43	1.52
1	C	395	MET	N-CA	-6.92	1.38	1.46
1	D	381	LYS	CA-C	-6.92	1.44	1.52
1	B	310	PRO	CA-C	-6.92	1.43	1.52
1	D	62	VAL	CA-C	-6.92	1.46	1.52
1	E	403	TRP	CA-C	-6.91	1.45	1.53
1	D	451	ASP	CA-C	-6.91	1.44	1.52
1	A	390	SER	CA-C	-6.90	1.43	1.52
1	B	52	VAL	CA-CB	-6.90	1.46	1.53
1	C	465	LEU	CA-C	-6.90	1.43	1.52
1	C	450	VAL	CA-CB	-6.89	1.46	1.53
1	E	26	GLU	N-CA	-6.89	1.38	1.46
1	F	392	ILE	CA-C	-6.89	1.43	1.52
1	E	36	HIS	CA-C	-6.88	1.44	1.52
1	D	385	THR	CA-C	-6.88	1.44	1.52
1	A	165	ILE	CA-C	-6.86	1.44	1.52
1	C	392	ILE	N-CA	-6.85	1.37	1.46
1	D	201	VAL	CA-C	-6.85	1.45	1.52
1	E	274	SER	CA-C	-6.85	1.43	1.52
1	E	381	LYS	CA-C	-6.85	1.44	1.52
1	C	24	THR	CA-C	-6.83	1.43	1.52
1	D	470	LEU	CA-C	-6.83	1.43	1.52
1	F	337	THR	CA-C	-6.83	1.43	1.52
1	E	388	VAL	CA-C	-6.83	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	ASN	N-CA	-6.82	1.37	1.46
1	C	36	HIS	N-CA	-6.82	1.37	1.45
1	A	321	ASN	N-CA	-6.82	1.37	1.46
1	A	403	TRP	CA-C	-6.81	1.43	1.52
1	A	158	ILE	N-CA	-6.81	1.38	1.46
1	A	301	THR	CA-C	-6.81	1.44	1.52
1	A	469	PHE	N-CA	-6.80	1.38	1.46
1	E	391	TYR	CA-C	-6.80	1.43	1.52
1	B	392	ILE	N-CA	-6.80	1.38	1.46
1	D	51	LYS	C-N	-6.79	1.27	1.33
1	E	383	THR	CA-C	-6.79	1.44	1.52
1	A	329	LEU	CA-C	-6.77	1.44	1.52
1	B	162	VAL	CA-C	-6.77	1.45	1.52
1	E	439	GLN	CA-C	-6.77	1.44	1.53
1	D	61	ASP	N-CA	-6.76	1.38	1.46
1	B	389	MET	CA-C	-6.76	1.43	1.52
1	D	104	GLY	CA-C	-6.76	1.45	1.51
1	B	394	ASN	CA-C	-6.75	1.43	1.52
1	C	28	VAL	CA-CB	-6.75	1.46	1.54
1	E	160	GLY	CA-C	-6.75	1.44	1.51
1	D	235	LEU	N-CA	-6.75	1.38	1.46
1	F	36	HIS	CA-C	-6.74	1.44	1.52
1	B	391	TYR	CA-C	-6.74	1.43	1.52
1	F	125	LYS	CA-C	-6.74	1.43	1.52
1	B	61	ASP	N-CA	-6.74	1.38	1.46
1	B	396	ASN	N-CA	-6.74	1.38	1.46
1	D	159	ILE	CA-CB	-6.73	1.46	1.54
1	E	62	VAL	N-CA	-6.73	1.41	1.46
1	E	401	GLU	N-CA	-6.73	1.37	1.46
1	C	399	ILE	N-CA	-6.72	1.38	1.46
1	B	448	TRP	N-CA	-6.72	1.38	1.46
1	C	352	ILE	N-CA	-6.71	1.40	1.47
1	F	97	ARG	CA-C	-6.71	1.44	1.52
1	D	49	TYR	CA-C	-6.71	1.43	1.52
1	E	314	HIS	CA-C	-6.71	1.44	1.52
1	B	171	LYS	CA-C	-6.71	1.44	1.52
1	C	236	GLN	CA-C	-6.70	1.44	1.52
1	B	469	PHE	N-CA	-6.70	1.38	1.46
1	B	391	TYR	N-CA	-6.70	1.37	1.46
1	E	387	GLU	N-CA	-6.69	1.38	1.46
1	C	457	SER	CA-C	-6.69	1.44	1.52
1	E	345	CYS	CA-C	-6.69	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	300	VAL	CA-C	-6.68	1.44	1.52
1	D	52	VAL	C-N	-6.68	1.25	1.33
1	A	450	VAL	CA-CB	-6.67	1.46	1.54
1	C	307	PHE	CA-C	-6.67	1.43	1.52
1	C	391	TYR	N-CA	-6.66	1.37	1.46
1	D	392	ILE	N-CA	-6.64	1.38	1.46
1	F	468	LYS	CA-C	-6.64	1.44	1.52
1	A	320	ASN	CA-C	-6.63	1.44	1.52
1	D	391	TYR	N-CA	-6.62	1.37	1.46
1	F	255	VAL	CA-CB	-6.62	1.50	1.55
1	D	391	TYR	C-N	-6.62	1.25	1.33
1	A	68	TYR	CA-C	-6.62	1.46	1.53
1	F	48	PRO	CA-C	-6.61	1.43	1.52
1	C	52	VAL	N-CA	-6.61	1.41	1.46
1	E	246	MET	CA-C	-6.60	1.44	1.52
1	C	33	ILE	CA-CB	-6.60	1.46	1.54
1	B	388	VAL	N-CA	-6.60	1.38	1.46
1	A	62	VAL	N-CA	-6.60	1.40	1.46
1	D	398	THR	CA-C	-6.60	1.44	1.52
1	C	34	PHE	CA-C	-6.59	1.44	1.52
1	A	200	MET	CA-C	-6.59	1.44	1.52
1	F	102	CYS	CA-C	-6.58	1.44	1.52
1	B	262	ASN	N-CA	-6.58	1.37	1.45
1	F	224	ILE	CA-CB	-6.57	1.46	1.54
1	B	168	HIS	CB-CG	-6.57	1.41	1.50
1	A	126	LEU	CA-C	-6.57	1.46	1.53
1	C	311	TYR	N-CA	-6.57	1.38	1.46
1	F	471	LEU	N-CA	-6.56	1.38	1.46
1	F	158	ILE	N-CA	-6.56	1.38	1.46
1	C	440	ASP	C-N	-6.56	1.26	1.34
1	C	394	ASN	CA-C	-6.56	1.43	1.52
1	C	92	ASP	N-CA	-6.55	1.36	1.46
1	E	420	ARG	CA-C	-6.54	1.44	1.52
1	F	41	ARG	CA-C	-6.54	1.44	1.52
1	B	443	ASP	N-CA	-6.53	1.38	1.46
1	B	221	PRO	CA-C	-6.53	1.45	1.52
1	A	367	HIS	CA-C	-6.53	1.44	1.52
1	C	75	VAL	CA-C	-6.52	1.44	1.52
1	B	323	ILE	CA-CB	-6.52	1.46	1.54
1	E	231	TYR	C-N	-6.51	1.26	1.33
1	A	389	MET	CA-C	-6.51	1.44	1.52
1	B	75	VAL	CA-C	-6.51	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	235	LEU	N-CA	-6.50	1.38	1.46
1	A	468	LYS	CA-C	-6.50	1.43	1.52
1	F	312	TRP	N-CA	-6.50	1.37	1.45
1	A	75	VAL	CA-C	-6.50	1.44	1.52
1	C	162	VAL	C-N	-6.50	1.25	1.33
1	D	86	PRO	CA-C	-6.49	1.45	1.53
1	F	26	GLU	N-CA	-6.49	1.38	1.46
1	A	41	ARG	CA-C	-6.49	1.44	1.52
1	E	427	VAL	CA-CB	-6.48	1.47	1.54
1	A	25	ASP	N-CA	-6.48	1.37	1.46
1	B	311	TYR	N-CA	-6.48	1.38	1.46
1	D	303	ASP	CA-C	-6.48	1.44	1.52
1	E	382	ILE	CA-C	-6.47	1.44	1.52
1	A	201	VAL	CA-C	-6.47	1.45	1.52
1	C	98	LEU	CA-C	-6.47	1.45	1.52
1	E	92	ASP	C-N	-6.47	1.26	1.34
1	A	230	LYS	CA-C	-6.46	1.44	1.52
1	A	125	LYS	CA-C	-6.46	1.44	1.52
1	C	99	VAL	CA-C	-6.46	1.44	1.52
1	C	395	MET	CA-C	-6.46	1.45	1.53
1	F	279	GLY	N-CA	-6.46	1.40	1.45
1	B	261	TRP	CA-C	-6.46	1.44	1.52
1	B	306	LEU	CA-C	-6.45	1.43	1.52
1	C	87	ASP	CA-C	-6.45	1.44	1.53
1	E	400	LEU	CA-C	-6.45	1.44	1.52
1	C	122	LEU	CA-C	-6.45	1.44	1.53
1	D	28	VAL	N-CA	-6.44	1.37	1.46
1	A	395	MET	N-CA	-6.44	1.38	1.46
1	C	61	ASP	C-N	-6.44	1.28	1.33
1	F	103	VAL	N-CA	-6.44	1.39	1.46
1	B	62	VAL	CA-CB	-6.43	1.49	1.54
1	E	121	PRO	CA-C	-6.43	1.43	1.52
1	A	466	GLY	CA-C	-6.42	1.44	1.52
1	D	300	VAL	CA-C	-6.42	1.47	1.52
1	C	399	ILE	CA-CB	-6.42	1.46	1.54
1	D	387	GLU	N-CA	-6.42	1.38	1.46
1	D	248	PHE	CA-C	-6.41	1.44	1.52
1	E	266	THR	CA-C	-6.41	1.44	1.52
1	C	381	LYS	CA-C	-6.40	1.45	1.52
1	A	246	MET	N-CA	-6.40	1.38	1.46
1	C	318	GLY	CA-C	-6.40	1.45	1.52
1	E	391	TYR	C-N	-6.40	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	471	LEU	CA-C	-6.40	1.44	1.52
1	A	122	LEU	CA-C	-6.40	1.44	1.53
1	D	261	TRP	CA-C	-6.40	1.44	1.52
1	C	75	VAL	CA-CB	-6.39	1.46	1.53
1	D	34	PHE	CA-C	-6.39	1.44	1.52
1	A	24	THR	C-N	-6.38	1.25	1.33
1	E	224	ILE	N-CA	-6.38	1.39	1.46
1	D	162	VAL	N-CA	-6.38	1.38	1.46
1	E	64	LYS	CA-C	-6.38	1.45	1.52
1	B	465	LEU	CA-C	-6.38	1.44	1.52
1	F	387	GLU	N-CA	-6.37	1.38	1.46
1	F	146	ASN	N-CA	-6.36	1.38	1.46
1	F	75	VAL	CA-CB	-6.36	1.46	1.53
1	A	465	LEU	CA-C	-6.36	1.44	1.52
1	A	331	LEU	CA-C	-6.35	1.44	1.52
1	A	400	LEU	CA-C	-6.35	1.44	1.52
1	C	383	THR	CA-C	-6.35	1.44	1.52
1	A	314	HIS	CA-C	-6.33	1.44	1.52
1	F	35	TYR	CA-C	-6.33	1.44	1.52
1	A	450	VAL	N-CA	-6.33	1.38	1.46
1	A	218	SER	CA-C	-6.33	1.45	1.52
1	E	395	MET	CA-C	-6.33	1.44	1.52
1	D	114	GLY	CA-C	-6.32	1.45	1.51
1	D	465	LEU	CA-C	-6.32	1.44	1.52
1	D	98	LEU	N-CA	-6.32	1.38	1.46
1	E	191	ILE	CA-CB	-6.32	1.46	1.54
1	F	172	GLY	CA-C	-6.32	1.43	1.52
1	A	148	SER	C-N	6.31	1.37	1.33
1	F	65	VAL	CA-C	-6.31	1.44	1.52
1	B	195	ILE	N-CA	-6.31	1.38	1.46
1	C	471	LEU	CA-C	-6.31	1.44	1.52
1	C	451	ASP	CA-C	-6.31	1.45	1.52
1	C	467	ARG	N-CA	-6.30	1.38	1.46
1	F	112	PRO	CA-C	-6.30	1.46	1.53
1	C	469	PHE	CA-C	-6.30	1.44	1.52
1	E	199	ASP	CA-C	-6.30	1.44	1.52
1	E	424	SER	CA-C	-6.30	1.45	1.52
1	D	79	ASP	CA-C	-6.29	1.45	1.52
1	C	124	ASN	CA-C	-6.28	1.44	1.52
1	E	354	ASN	CA-C	-6.28	1.44	1.52
1	C	389	MET	CA-C	-6.27	1.44	1.52
1	A	192	ASN	CA-C	-6.27	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	173	THR	CA-C	-6.27	1.44	1.52
1	F	427	VAL	CA-CB	-6.26	1.47	1.54
1	B	385	THR	C-N	-6.25	1.25	1.33
1	A	246	MET	CA-C	-6.25	1.45	1.52
1	E	406	GLY	CA-C	-6.25	1.46	1.52
1	B	395	MET	N-CA	-6.24	1.38	1.46
1	C	219	GLU	CA-C	-6.23	1.44	1.52
1	F	73	PHE	CA-C	-6.23	1.45	1.52
1	D	313	LEU	CA-C	-6.23	1.44	1.52
1	D	463	PHE	C-N	-6.23	1.25	1.33
1	C	384	LEU	N-CA	-6.23	1.38	1.46
1	C	300	VAL	CA-C	-6.23	1.45	1.52
1	B	51	LYS	CA-C	-6.22	1.44	1.52
1	D	401	GLU	N-CA	-6.22	1.38	1.46
1	E	275	LEU	N-CA	-6.22	1.37	1.46
1	C	94	ASN	CA-C	-6.22	1.44	1.52
1	F	61	ASP	N-CA	-6.21	1.38	1.46
1	F	404	ASN	N-CA	-6.21	1.38	1.45
1	C	395	MET	CA-CB	-6.21	1.44	1.53
1	F	122	LEU	CA-C	-6.21	1.44	1.52
1	E	422	VAL	CA-CB	-6.20	1.46	1.54
1	E	83	PHE	CA-C	-6.20	1.44	1.52
1	A	176	LYS	N-CA	-6.20	1.38	1.45
1	D	358	PRO	CA-C	-6.20	1.43	1.52
1	A	399	ILE	CA-C	-6.20	1.45	1.52
1	F	162	VAL	CA-C	-6.20	1.46	1.52
1	B	226	GLN	CA-C	-6.19	1.46	1.53
1	A	275	LEU	N-CA	-6.19	1.37	1.45
1	E	201	VAL	CA-C	-6.19	1.46	1.53
1	E	385	THR	CA-C	-6.19	1.44	1.52
1	B	68	TYR	CA-C	-6.19	1.46	1.53
1	D	219	GLU	CA-C	-6.19	1.44	1.52
1	A	226	GLN	CA-C	-6.18	1.46	1.53
1	F	67	ALA	CA-C	-6.18	1.45	1.53
1	F	24	THR	C-N	-6.17	1.25	1.33
1	D	467	ARG	N-CA	-6.17	1.39	1.46
1	A	400	LEU	N-CA	-6.17	1.38	1.46
1	A	381	LYS	CA-C	-6.16	1.45	1.52
1	E	387	GLU	CA-C	-6.16	1.44	1.52
1	B	231	TYR	C-N	-6.16	1.26	1.33
1	C	179	THR	CA-C	-6.15	1.44	1.53
1	B	457	SER	N-CA	-6.14	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	394	ASN	C-N	-6.13	1.25	1.33
1	E	399	ILE	N-CA	-6.13	1.38	1.46
1	A	226	GLN	N-CA	-6.13	1.39	1.46
1	A	70	TYR	N-CA	-6.12	1.38	1.46
1	B	377	PHE	CA-C	-6.12	1.45	1.52
1	F	74	ARG	CA-C	-6.12	1.45	1.52
1	E	168	HIS	CA-C	-6.12	1.45	1.52
1	F	248	PHE	N-CA	-6.12	1.38	1.46
1	A	64	LYS	N-CA	-6.11	1.37	1.45
1	A	392	ILE	N-CA	-6.11	1.38	1.46
1	E	340	THR	CA-C	-6.11	1.45	1.52
1	B	280	THR	CA-C	-6.11	1.45	1.52
1	C	315	LYS	CA-C	-6.10	1.44	1.52
1	B	328	GLN	N-CA	-6.10	1.39	1.46
1	C	448	TRP	CA-C	-6.10	1.45	1.52
1	A	329	LEU	N-CA	-6.10	1.38	1.46
1	C	462	GLN	CA-C	-6.09	1.44	1.52
1	F	29	THR	CA-C	-6.09	1.45	1.52
1	F	191	ILE	CA-CB	-6.08	1.46	1.54
1	E	470	LEU	CA-C	-6.08	1.44	1.52
1	A	188	LEU	CA-C	-6.08	1.45	1.52
1	C	61	ASP	CA-C	-6.08	1.45	1.52
1	C	302	SER	C-N	-6.08	1.25	1.33
1	E	429	CYS	CA-C	-6.08	1.45	1.53
1	B	329	LEU	CA-C	-6.07	1.45	1.52
1	E	324	CYS	CA-C	-6.07	1.46	1.53
1	C	452	LEU	CA-C	-6.07	1.44	1.52
1	D	314	HIS	CA-C	-6.07	1.44	1.52
1	F	96	GLN	N-CA	-6.06	1.38	1.45
1	D	351	SER	N-CA	-6.06	1.41	1.46
1	B	78	PRO	CA-C	-6.05	1.43	1.52
1	C	261	TRP	CA-C	-6.05	1.44	1.52
1	B	471	LEU	N-CA	-6.05	1.39	1.46
1	D	90	VAL	CA-CB	-6.05	1.47	1.54
1	D	314	HIS	N-CA	-6.05	1.38	1.46
1	B	36	HIS	N-CA	-6.04	1.38	1.46
1	C	36	HIS	CA-C	-6.04	1.45	1.52
1	D	236	GLN	N-CA	-6.04	1.39	1.46
1	D	449	PRO	CA-C	-6.04	1.45	1.52
1	F	345	CYS	CA-C	-6.04	1.45	1.52
1	B	210	PHE	N-CA	-6.03	1.38	1.46
1	D	245	SER	N-CA	-6.03	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	378	GLN	N-CA	-6.03	1.39	1.46
1	B	276	TYR	CA-C	-6.03	1.45	1.52
1	D	68	TYR	CA-C	-6.03	1.44	1.52
1	C	39	SER	CA-C	-6.02	1.45	1.52
1	F	92	ASP	C-N	-6.02	1.26	1.33
1	D	460	LEU	C-N	-6.02	1.25	1.33
1	B	400	LEU	CA-C	-6.01	1.45	1.52
1	D	89	THR	CA-C	-6.01	1.44	1.52
1	A	195	ILE	CA-CB	-6.00	1.47	1.54
1	D	378	GLN	N-CA	-5.99	1.39	1.46
1	D	460	LEU	CA-C	-5.99	1.44	1.52
1	D	92	ASP	C-N	-5.99	1.26	1.33
1	D	285	ASN	CA-C	-5.99	1.45	1.52
1	F	98	LEU	CA-C	-5.99	1.45	1.52
1	D	65	VAL	CA-C	-5.98	1.45	1.52
1	C	169	TRP	CA-C	-5.98	1.45	1.52
1	F	106	GLU	CA-C	-5.98	1.45	1.52
1	F	456	PHE	N-CA	-5.98	1.38	1.46
1	D	73	PHE	CA-C	-5.97	1.45	1.52
1	A	445	LEU	N-CA	-5.97	1.38	1.45
1	E	303	ASP	CA-C	-5.97	1.45	1.52
1	F	382	ILE	N-CA	-5.97	1.37	1.46
1	F	224	ILE	CA-C	-5.96	1.43	1.52
1	A	61	ASP	N-CA	-5.96	1.38	1.46
1	A	165	ILE	CA-CB	-5.96	1.47	1.54
1	D	276	TYR	CA-C	-5.96	1.45	1.52
1	D	25	ASP	N-CA	-5.95	1.38	1.46
1	A	30	ARG	CA-C	-5.95	1.45	1.53
1	B	448	TRP	C-N	-5.95	1.27	1.33
1	C	444	LYS	CA-C	-5.95	1.44	1.52
1	C	463	PHE	C-N	-5.94	1.25	1.33
1	C	314	HIS	CA-C	-5.94	1.45	1.52
1	C	448	TRP	C-N	-5.94	1.26	1.33
1	A	49	TYR	CA-C	-5.93	1.44	1.52
1	F	386	THR	C-N	-5.93	1.25	1.33
1	F	462	GLN	N-CA	-5.93	1.38	1.46
1	A	326	HIS	CB-CG	-5.93	1.41	1.50
1	C	224	ILE	CA-C	-5.93	1.43	1.52
1	F	25	ASP	N-CA	-5.93	1.38	1.46
1	E	441	PRO	CA-C	-5.93	1.44	1.52
1	D	311	TYR	N-CA	-5.93	1.39	1.46
1	F	162	VAL	N-CA	-5.93	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	378	GLN	CA-C	-5.92	1.45	1.52
1	D	382	ILE	CA-C	-5.92	1.45	1.52
1	F	442	TYR	CA-C	-5.92	1.44	1.52
1	B	404	ASN	N-CA	-5.92	1.38	1.46
1	D	469	PHE	CA-C	-5.92	1.45	1.52
1	A	234	TYR	CA-C	-5.92	1.45	1.52
1	F	387	GLU	CA-C	-5.92	1.44	1.52
1	A	448	TRP	N-CA	-5.92	1.37	1.46
1	B	470	LEU	N-CA	-5.90	1.39	1.46
1	D	260	PHE	CA-C	-5.90	1.45	1.52
1	C	445	LEU	CA-C	-5.90	1.45	1.52
1	D	457	SER	CA-C	-5.90	1.45	1.52
1	F	162	VAL	CA-CB	-5.90	1.46	1.54
1	F	467	ARG	N-CA	-5.90	1.39	1.46
1	E	402	ASP	CA-C	-5.89	1.45	1.52
1	F	212	LEU	CA-C	-5.89	1.44	1.52
1	C	31	THR	CA-C	-5.89	1.44	1.52
1	C	348	THR	CA-C	-5.88	1.44	1.52
1	E	248	PHE	CA-C	-5.88	1.45	1.52
1	A	162	VAL	N-CA	-5.88	1.39	1.46
1	D	470	LEU	N-CA	-5.88	1.39	1.46
1	E	464	PRO	CA-C	-5.88	1.43	1.52
1	C	303	ASP	N-CA	-5.88	1.39	1.46
1	C	386	THR	N-CA	-5.88	1.39	1.46
1	F	281	ASP	CA-C	-5.88	1.48	1.53
1	A	311	TYR	N-CA	-5.87	1.39	1.46
1	D	461	ASP	N-CA	-5.87	1.38	1.46
1	E	26	GLU	CA-C	-5.87	1.45	1.52
1	D	338	ARG	CA-C	-5.87	1.45	1.52
1	A	236	GLN	CA-C	-5.87	1.45	1.52
1	D	450	VAL	CA-CB	-5.86	1.47	1.53
1	A	285	ASN	CA-C	-5.86	1.45	1.52
1	F	123	TYR	CA-C	-5.86	1.45	1.52
1	B	396	ASN	CA-C	-5.85	1.46	1.52
1	E	384	LEU	N-CA	-5.85	1.38	1.46
1	F	168	HIS	N-CA	-5.85	1.38	1.46
1	B	326	HIS	CA-C	-5.85	1.43	1.52
1	A	52	VAL	CA-CB	-5.85	1.47	1.53
1	F	328	GLN	N-CA	-5.85	1.38	1.46
1	A	470	LEU	N-CA	-5.84	1.39	1.46
1	D	344	VAL	CA-C	-5.84	1.45	1.52
1	A	396	ASN	CA-C	-5.84	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	409	PRO	C-N	-5.84	1.28	1.33
1	A	334	VAL	CA-CB	-5.84	1.47	1.54
1	D	60	GLN	CA-C	-5.84	1.45	1.52
1	C	463	PHE	N-CA	-5.83	1.39	1.46
1	A	22	VAL	N-CA	-5.83	1.39	1.46
1	F	69	GLN	N-CA	-5.82	1.38	1.46
1	A	300	VAL	CA-C	-5.82	1.45	1.52
1	A	280	THR	CA-C	-5.82	1.45	1.52
1	F	91	TYR	N-CA	-5.82	1.39	1.46
1	F	146	ASN	CA-C	-5.82	1.45	1.52
1	E	457	SER	CA-C	-5.81	1.45	1.52
1	A	313	LEU	CA-C	-5.81	1.45	1.52
1	C	328	GLN	N-CA	-5.81	1.39	1.46
1	F	93	PRO	N-CA	-5.80	1.40	1.47
1	F	394	ASN	CA-C	-5.80	1.44	1.52
1	D	95	SER	CA-C	-5.80	1.45	1.52
1	B	455	ARG	CA-C	-5.80	1.44	1.52
1	C	210	PHE	CA-C	-5.80	1.45	1.52
1	D	168	HIS	N-CA	-5.80	1.39	1.46
1	F	384	LEU	N-CA	-5.79	1.39	1.46
1	C	200	MET	CA-C	-5.79	1.45	1.52
1	C	180	VAL	CA-C	-5.79	1.45	1.52
1	F	236	GLN	N-CA	-5.79	1.39	1.46
1	C	96	GLN	CA-C	-5.79	1.45	1.52
1	E	191	ILE	N-CA	-5.79	1.39	1.46
1	F	50	PHE	CA-C	-5.79	1.45	1.52
1	E	386	THR	C-N	-5.78	1.26	1.33
1	E	446	LYS	CA-C	-5.78	1.45	1.52
1	C	52	VAL	CA-CB	-5.78	1.47	1.53
1	A	213	LEU	CA-C	-5.78	1.45	1.52
1	F	341	ASN	N-CA	-5.78	1.38	1.45
1	F	424	SER	N-CA	-5.78	1.38	1.46
1	F	230	LYS	CA-C	-5.77	1.45	1.52
1	F	347	SER	CA-C	-5.77	1.45	1.52
1	B	464	PRO	N-CA	-5.77	1.40	1.47
1	F	326	HIS	CA-C	-5.77	1.43	1.52
1	F	344	VAL	CA-C	-5.77	1.45	1.52
1	E	380	CYS	CA-C	-5.76	1.45	1.52
1	B	120	HIS	N-CA	-5.75	1.38	1.46
1	F	36	HIS	N-CA	-5.75	1.39	1.45
1	D	100	TRP	CA-C	-5.75	1.45	1.52
1	E	112	PRO	CA-C	-5.74	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	277	ILE	CA-C	-5.74	1.46	1.52
1	A	26	GLU	N-CA	-5.73	1.38	1.46
1	F	88	ASN	N-CA	-5.73	1.38	1.46
1	A	318	GLY	CA-C	-5.73	1.46	1.52
1	E	328	GLN	N-CA	-5.72	1.39	1.46
1	E	398	THR	CA-CB	-5.72	1.43	1.53
1	D	215	ASP	CA-C	-5.72	1.44	1.52
1	F	240	ASP	N-CA	-5.72	1.38	1.46
1	D	27	TYR	CA-C	-5.72	1.45	1.52
1	D	79	ASP	C-N	-5.71	1.26	1.34
1	C	190	LEU	CA-C	-5.71	1.45	1.52
1	D	181	VAL	CA-C	-5.71	1.47	1.53
1	D	24	THR	C-N	-5.71	1.26	1.33
1	A	454	GLU	N-CA	-5.71	1.38	1.46
1	D	304	SER	N-CA	-5.70	1.38	1.46
1	F	357	THR	CA-C	-5.70	1.46	1.52
1	D	76	LYS	CA-C	-5.70	1.45	1.52
1	F	250	LEU	CA-C	-5.70	1.45	1.52
1	A	451	ASP	CA-C	-5.70	1.45	1.52
1	F	141	LYS	CA-C	-5.70	1.45	1.52
1	D	231	TYR	C-N	-5.70	1.26	1.33
1	F	43	LEU	CA-C	-5.70	1.45	1.52
1	F	68	TYR	CA-C	-5.69	1.44	1.52
1	E	327	ASN	CA-C	-5.69	1.45	1.53
1	B	53	PRO	CA-C	-5.68	1.45	1.52
1	C	393	HIS	C-N	-5.68	1.25	1.33
1	C	389	MET	N-CA	-5.68	1.39	1.46
1	F	189	GLU	CA-C	5.68	1.59	1.52
1	B	97	ARG	CA-C	-5.68	1.45	1.52
1	B	388	VAL	CA-CB	-5.68	1.47	1.54
1	B	403	TRP	CA-C	-5.68	1.45	1.52
1	E	70	TYR	CA-C	-5.68	1.45	1.52
1	E	377	PHE	CA-C	-5.67	1.46	1.52
1	A	78	PRO	CA-C	-5.67	1.44	1.52
1	E	73	PHE	CA-C	-5.67	1.45	1.52
1	D	89	THR	N-CA	-5.67	1.38	1.46
1	D	250	LEU	CA-C	-5.67	1.45	1.52
1	E	346	ALA	CA-C	-5.67	1.45	1.52
1	A	157	CYS	CA-C	-5.67	1.45	1.52
1	E	239	ALA	N-CA	-5.67	1.39	1.46
1	F	159	ILE	CA-CB	-5.66	1.46	1.54
1	D	29	THR	N-CA	-5.66	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	102	CYS	C-N	-5.66	1.27	1.33
1	A	25	ASP	CA-C	-5.66	1.44	1.52
1	B	461	ASP	CA-C	-5.66	1.44	1.52
1	F	396	ASN	N-CA	-5.66	1.39	1.46
1	B	466	GLY	CA-C	-5.66	1.45	1.52
1	B	357	THR	C-N	-5.66	1.27	1.34
1	D	456	PHE	N-CA	-5.66	1.39	1.46
1	E	454	GLU	CA-C	-5.66	1.45	1.52
1	F	85	LEU	C-N	-5.65	1.28	1.34
1	D	266	THR	CA-C	-5.65	1.45	1.52
1	E	315	LYS	N-CA	-5.65	1.39	1.46
1	F	106	GLU	N-CA	-5.65	1.39	1.46
1	B	462	GLN	CA-C	-5.65	1.45	1.52
1	E	388	VAL	CA-CB	-5.65	1.47	1.54
1	E	390	SER	N-CA	-5.65	1.39	1.46
1	C	180	VAL	N-CA	-5.65	1.39	1.46
1	C	216	ASN	N-CA	-5.64	1.42	1.47
1	A	106	GLU	N-CA	-5.64	1.39	1.46
1	A	461	ASP	N-CA	-5.64	1.39	1.46
1	E	468	LYS	CA-C	-5.64	1.45	1.52
1	F	107	ILE	N-CA	-5.64	1.40	1.46
1	D	342	LEU	N-CA	-5.63	1.39	1.46
1	F	120	HIS	CA-C	-5.63	1.45	1.52
1	D	180	VAL	CA-C	-5.62	1.46	1.52
1	B	194	PRO	CA-C	-5.62	1.45	1.52
1	F	277	ILE	CA-C	-5.62	1.46	1.52
1	C	345	CYS	CA-C	-5.62	1.46	1.52
1	A	224	ILE	CA-CB	-5.62	1.47	1.54
1	C	41	ARG	CA-C	-5.62	1.45	1.52
1	E	100	TRP	CA-C	-5.62	1.45	1.52
1	E	356	TYR	N-CA	-5.61	1.39	1.46
1	B	277	ILE	CA-C	-5.61	1.46	1.52
1	E	123	TYR	N-CA	-5.61	1.39	1.46
1	A	407	VAL	CA-C	-5.61	1.45	1.52
1	B	312	TRP	N-CA	-5.61	1.38	1.46
1	E	294	SER	CA-C	-5.61	1.45	1.52
1	E	391	TYR	N-CA	-5.61	1.39	1.46
1	E	210	PHE	CA-C	-5.61	1.45	1.52
1	F	61	ASP	CA-C	-5.61	1.46	1.52
1	A	383	THR	CA-C	-5.60	1.45	1.52
1	D	162	VAL	CA-CB	-5.60	1.47	1.54
1	D	312	TRP	N-CA	-5.60	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	301	THR	CA-C	-5.60	1.45	1.52
1	E	394	ASN	CA-C	-5.60	1.44	1.52
1	B	191	ILE	CA-CB	-5.60	1.47	1.54
1	C	82	LYS	CA-CB	-5.60	1.48	1.53
1	D	50	PHE	CA-C	-5.60	1.46	1.52
1	A	300	VAL	CA-CB	-5.59	1.47	1.54
1	D	467	ARG	CA-C	-5.59	1.45	1.52
1	C	468	LYS	CA-C	-5.59	1.45	1.52
1	E	462	GLN	CA-C	-5.59	1.44	1.52
1	E	323	ILE	CA-CB	-5.59	1.47	1.54
1	A	345	CYS	CA-C	-5.59	1.45	1.52
1	A	127	ASP	N-CA	-5.59	1.39	1.46
1	A	187	PRO	CA-C	-5.59	1.46	1.52
1	B	22	VAL	CA-C	-5.59	1.46	1.52
1	B	279	GLY	CA-C	-5.59	1.45	1.52
1	D	126	LEU	CA-C	-5.59	1.45	1.52
1	B	34	PHE	CA-C	-5.58	1.45	1.52
1	C	73	PHE	CA-C	-5.58	1.46	1.52
1	D	326	HIS	CA-C	-5.58	1.44	1.52
1	A	28	VAL	CA-C	-5.58	1.46	1.52
1	F	33	ILE	CA-CB	-5.58	1.47	1.54
1	F	229	CYS	CA-C	-5.58	1.45	1.53
1	F	385	THR	C-N	-5.57	1.26	1.33
1	B	43	LEU	N-CA	-5.57	1.39	1.46
1	C	423	GLN	CA-C	-5.57	1.45	1.52
1	E	393	HIS	N-CA	-5.57	1.39	1.46
1	A	352	ILE	N-CA	-5.57	1.42	1.46
1	E	249	CYS	N-CA	-5.57	1.39	1.46
1	B	378	GLN	N-CA	-5.57	1.40	1.46
1	B	389	MET	N-CA	-5.57	1.39	1.46
1	C	353	PRO	CA-C	-5.57	1.45	1.52
1	E	471	LEU	CA-C	-5.57	1.45	1.52
1	C	23	SER	CA-C	-5.56	1.45	1.52
1	A	278	LYS	CA-C	-5.56	1.45	1.53
1	F	389	MET	N-CA	-5.56	1.39	1.46
1	B	69	GLN	N-CA	-5.56	1.39	1.45
1	F	398	THR	CA-C	-5.56	1.45	1.52
1	D	320	ASN	CA-C	-5.56	1.45	1.52
1	D	125	LYS	N-CA	-5.55	1.39	1.46
1	F	248	PHE	CA-C	-5.55	1.45	1.52
1	A	149	VAL	CA-CB	-5.55	1.51	1.55
1	A	300	VAL	N-CA	-5.55	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	LEU	CA-C	-5.55	1.45	1.52
1	B	353	PRO	CA-C	-5.55	1.45	1.52
1	B	230	LYS	CA-C	-5.55	1.45	1.52
1	B	384	LEU	N-CA	-5.55	1.39	1.46
1	C	170	THR	CA-C	-5.55	1.45	1.52
1	D	468	LYS	CA-C	-5.55	1.45	1.52
1	E	463	PHE	CA-C	-5.55	1.46	1.52
1	F	111	GLN	CA-C	-5.55	1.45	1.52
1	B	29	THR	CA-C	-5.55	1.45	1.52
1	B	79	ASP	C-N	-5.55	1.27	1.34
1	E	102	CYS	CA-C	-5.54	1.45	1.52
1	F	62	VAL	CA-CB	-5.54	1.47	1.54
1	A	107	ILE	CA-CB	-5.54	1.47	1.54
1	C	141	LYS	CA-C	-5.54	1.45	1.52
1	B	424	SER	N-CA	-5.54	1.39	1.46
1	C	382	ILE	CA-C	-5.54	1.45	1.52
1	D	31	THR	CA-C	-5.53	1.45	1.52
1	D	190	LEU	CA-C	-5.53	1.46	1.52
1	A	61	ASP	CA-C	-5.53	1.45	1.52
1	B	275	LEU	N-CA	-5.53	1.39	1.46
1	D	394	ASN	N-CA	-5.53	1.38	1.46
1	A	93	PRO	CA-C	-5.53	1.42	1.52
1	F	120	HIS	N-CA	-5.53	1.38	1.46
1	F	156	LEU	CA-C	-5.53	1.46	1.52
1	A	168	HIS	CB-CG	-5.53	1.42	1.50
1	B	467	ARG	N-CA	-5.53	1.39	1.46
1	B	172	GLY	CA-C	-5.52	1.44	1.52
1	C	396	ASN	N-CA	-5.52	1.40	1.46
1	E	42	LEU	CA-C	-5.52	1.46	1.52
1	C	442	TYR	CA-C	-5.52	1.44	1.52
1	F	34	PHE	N-CA	-5.52	1.39	1.46
1	F	320	ASN	CA-C	-5.52	1.45	1.52
1	B	195	ILE	CA-CB	-5.52	1.47	1.54
1	F	63	PRO	CA-C	-5.52	1.45	1.52
1	A	73	PHE	CA-C	-5.51	1.46	1.52
1	A	235	LEU	N-CA	-5.51	1.39	1.46
1	D	229	CYS	CA-C	-5.51	1.46	1.52
1	A	89	THR	CA-C	-5.51	1.45	1.52
1	A	247	PHE	CA-C	-5.51	1.45	1.52
1	E	470	LEU	N-CA	-5.50	1.39	1.46
1	F	35	TYR	N-CA	-5.50	1.38	1.45
1	B	250	LEU	CA-C	-5.50	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	VAL	CA-CB	-5.50	1.47	1.54
1	D	384	LEU	CA-C	-5.50	1.45	1.52
1	D	443	ASP	CA-C	-5.50	1.45	1.52
1	E	300	VAL	CA-C	-5.50	1.45	1.52
1	C	33	ILE	C-O	-5.49	1.18	1.24
1	B	355	VAL	N-CA	-5.49	1.39	1.46
1	B	381	LYS	CA-C	-5.49	1.46	1.52
1	F	383	THR	CA-C	-5.49	1.45	1.52
1	C	401	GLU	N-CA	-5.49	1.39	1.46
1	E	226	GLN	CA-C	-5.49	1.46	1.53
1	B	472	GLN	N-CA	-5.48	1.39	1.46
1	A	90	VAL	N-CA	-5.47	1.39	1.46
1	C	90	VAL	CA-C	-5.47	1.45	1.52
1	F	90	VAL	CA-C	-5.47	1.45	1.52
1	B	464	PRO	CA-C	-5.47	1.44	1.52
1	C	177	PRO	CA-C	-5.47	1.44	1.52
1	F	275	LEU	N-CA	-5.47	1.39	1.46
1	F	280	THR	CA-C	-5.47	1.46	1.52
1	C	392	ILE	CA-C	-5.47	1.45	1.52
1	A	86	PRO	N-CA	-5.47	1.40	1.47
1	A	221	PRO	CA-C	-5.46	1.46	1.52
1	F	236	GLN	CA-C	-5.46	1.46	1.52
1	E	230	LYS	N-CA	-5.46	1.39	1.46
1	E	393	HIS	CB-CG	-5.46	1.42	1.50
1	B	173	THR	CA-C	-5.46	1.45	1.52
1	C	385	THR	CA-C	-5.46	1.46	1.52
1	D	389	MET	CA-C	-5.46	1.45	1.52
1	D	263	ARG	CA-C	-5.45	1.46	1.52
1	A	397	THR	N-CA	-5.45	1.39	1.46
1	B	390	SER	C-N	-5.44	1.25	1.33
1	D	384	LEU	N-CA	-5.44	1.39	1.46
1	E	96	GLN	CA-C	-5.44	1.46	1.52
1	E	332	THR	CA-CB	-5.44	1.45	1.53
1	E	328	GLN	CA-C	-5.43	1.46	1.52
1	F	145	ASP	CA-C	-5.43	1.46	1.52
1	D	304	SER	CA-C	-5.43	1.44	1.52
1	F	332	THR	CA-CB	-5.43	1.45	1.53
1	A	60	GLN	CA-C	-5.43	1.45	1.52
1	C	65	VAL	CA-C	-5.43	1.45	1.52
1	F	385	THR	CA-CB	-5.42	1.45	1.53
1	A	359	THR	CA-C	-5.42	1.45	1.52
1	A	394	ASN	CA-C	-5.42	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	VAL	CA-C	-5.42	1.45	1.52
1	E	307	PHE	CA-C	-5.42	1.46	1.53
1	F	304	SER	N-CA	-5.42	1.38	1.46
1	B	357	THR	CA-C	-5.42	1.47	1.52
1	D	169	TRP	N-CA	-5.42	1.39	1.46
1	C	197	ASP	CA-C	-5.41	1.45	1.52
1	D	383	THR	CA-CB	-5.41	1.46	1.53
1	B	315	LYS	N-CA	-5.41	1.39	1.46
1	A	86	PRO	CA-C	-5.40	1.44	1.52
1	E	47	HIS	CA-C	-5.40	1.47	1.53
1	C	300	VAL	N-CA	-5.40	1.39	1.46
1	B	391	TYR	C-N	-5.40	1.27	1.33
1	E	312	TRP	N-CA	-5.40	1.38	1.46
1	C	162	VAL	N-CA	-5.39	1.40	1.46
1	D	69	GLN	N-CA	-5.39	1.39	1.45
1	F	25	ASP	CA-C	-5.39	1.45	1.52
1	F	164	ALA	CA-C	-5.39	1.46	1.52
1	C	159	ILE	CA-CB	-5.39	1.47	1.54
1	A	432	ASP	CA-C	-5.38	1.46	1.53
1	C	28	VAL	N-CA	-5.38	1.39	1.46
1	B	95	SER	N-CA	-5.38	1.39	1.46
1	F	396	ASN	C-N	-5.38	1.26	1.34
1	A	46	GLY	CA-C	-5.38	1.45	1.51
1	F	463	PHE	N-CA	-5.38	1.38	1.46
1	A	36	HIS	CA-C	-5.38	1.46	1.52
1	C	24	THR	C-N	-5.38	1.26	1.33
1	D	349	THR	CA-C	-5.38	1.46	1.52
1	A	457	SER	N-CA	-5.37	1.40	1.46
1	C	121	PRO	CA-C	-5.36	1.43	1.52
1	F	201	VAL	N-CA	-5.36	1.39	1.46
1	F	312	TRP	CA-C	-5.36	1.45	1.52
1	F	376	ILE	CA-C	-5.36	1.45	1.52
1	C	51	LYS	CA-C	-5.36	1.45	1.52
1	C	79	ASP	CA-C	-5.35	1.47	1.53
1	A	403	TRP	CA-CB	-5.35	1.46	1.54
1	A	380	CYS	CA-C	-5.35	1.46	1.52
1	D	402	ASP	CA-C	-5.35	1.45	1.52
1	E	65	VAL	N-CA	-5.35	1.40	1.46
1	D	75	VAL	CA-CB	-5.34	1.47	1.53
1	E	263	ARG	CA-C	-5.34	1.45	1.53
1	A	352	ILE	CA-CB	-5.34	1.48	1.53
1	D	450	VAL	N-CA	-5.34	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	194	PRO	CA-C	-5.34	1.46	1.52
1	F	448	TRP	C-N	-5.34	1.27	1.33
1	C	401	GLU	CA-C	-5.34	1.45	1.52
1	F	228	ILE	CA-C	-5.34	1.46	1.52
1	F	313	LEU	CA-C	-5.34	1.46	1.52
1	D	462	GLN	CA-C	-5.33	1.44	1.52
1	B	85	LEU	CA-C	-5.33	1.47	1.53
1	B	350	SER	CA-C	-5.33	1.46	1.52
1	D	48	PRO	CA-C	-5.33	1.44	1.52
1	F	169	TRP	N-CA	-5.33	1.39	1.46
1	D	275	LEU	N-CA	-5.32	1.39	1.46
1	A	159	ILE	N-CA	-5.32	1.40	1.46
1	E	145	ASP	CA-C	-5.32	1.46	1.52
1	F	359	THR	N-CA	-5.32	1.39	1.46
1	F	123	TYR	N-CA	-5.32	1.39	1.46
1	C	423	GLN	N-CA	-5.31	1.39	1.46
1	E	301	THR	CA-C	-5.31	1.46	1.52
1	D	35	TYR	CA-C	-5.31	1.46	1.52
1	E	321	ASN	N-CA	-5.31	1.39	1.46
1	F	62	VAL	N-CA	-5.31	1.41	1.46
1	F	353	PRO	N-CA	-5.31	1.40	1.47
1	F	394	ASN	N-CA	-5.31	1.39	1.46
1	E	450	VAL	CA-CB	-5.31	1.46	1.53
1	A	81	ASN	N-CA	-5.30	1.39	1.46
1	F	167	GLU	N-CA	-5.30	1.39	1.45
1	C	91	TYR	N-CA	-5.30	1.39	1.46
1	A	307	PHE	CA-C	-5.30	1.46	1.52
1	A	347	SER	CA-C	-5.30	1.45	1.52
1	B	169	TRP	CA-C	-5.30	1.46	1.52
1	B	302	SER	CA-C	-5.30	1.45	1.52
1	E	144	ARG	CA-C	-5.30	1.45	1.52
1	A	469	PHE	C-N	-5.29	1.27	1.33
1	B	21	VAL	CA-C	-5.29	1.46	1.52
1	C	377	PHE	N-CA	-5.29	1.39	1.45
1	D	244	ASP	CA-C	-5.29	1.45	1.52
1	E	236	GLN	CA-C	-5.29	1.45	1.52
1	A	231	TYR	C-N	-5.29	1.27	1.33
1	F	266	THR	CA-C	-5.29	1.46	1.52
1	E	355	VAL	CA-C	-5.29	1.46	1.52
1	E	194	PRO	CA-C	-5.29	1.45	1.52
1	E	50	PHE	CA-C	-5.28	1.46	1.52
1	F	301	THR	N-CA	-5.28	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	402	ASP	N-CA	-5.28	1.39	1.46
1	A	211	LYS	N-CA	-5.28	1.40	1.46
1	C	319	LEU	CA-C	-5.27	1.45	1.52
1	D	393	HIS	CA-C	-5.27	1.46	1.52
1	B	99	VAL	N-CA	-5.27	1.40	1.46
1	F	96	GLN	CA-C	-5.27	1.46	1.52
1	E	60	GLN	CA-C	-5.27	1.45	1.52
1	E	65	VAL	CA-C	-5.27	1.46	1.52
1	F	93	PRO	C-N	-5.27	1.25	1.33
1	B	71	ARG	CA-C	-5.26	1.46	1.52
1	B	229	CYS	CA-C	-5.26	1.46	1.52
1	C	77	LEU	CA-C	-5.26	1.46	1.52
1	D	321	ASN	N-CA	-5.26	1.39	1.46
1	A	355	VAL	CA-CB	-5.26	1.48	1.54
1	F	37	ALA	N-CA	-5.25	1.39	1.45
1	B	168	HIS	N-CA	-5.25	1.40	1.46
1	D	176	LYS	C-N	-5.25	1.28	1.34
1	A	159	ILE	CA-CB	-5.25	1.48	1.54
1	E	246	MET	N-CA	-5.25	1.40	1.46
1	E	306	LEU	N-CA	-5.25	1.40	1.46
1	F	300	VAL	N-CA	-5.25	1.40	1.46
1	C	246	MET	CA-C	-5.25	1.46	1.52
1	F	262	ASN	N-CA	-5.25	1.39	1.46
1	F	100	TRP	CA-C	-5.24	1.46	1.52
1	F	141	LYS	N-CA	-5.24	1.39	1.46
1	F	461	ASP	N-CA	-5.24	1.39	1.46
1	E	397	THR	N-CA	-5.24	1.38	1.46
1	C	467	ARG	CA-C	-5.24	1.46	1.52
1	E	127	ASP	N-CA	-5.24	1.39	1.46
1	E	197	ASP	N-CA	-5.24	1.39	1.46
1	E	468	LYS	C-N	-5.24	1.26	1.33
1	A	390	SER	N-CA	-5.23	1.39	1.46
1	C	29	THR	N-CA	-5.23	1.39	1.46
1	F	246	MET	CA-C	-5.23	1.46	1.52
1	A	168	HIS	CA-C	-5.23	1.46	1.52
1	D	248	PHE	N-CA	-5.23	1.39	1.45
1	A	42	LEU	CA-C	-5.23	1.46	1.52
1	B	73	PHE	CA-C	-5.23	1.46	1.52
1	D	448	TRP	C-N	-5.23	1.27	1.33
1	F	429	CYS	CA-C	-5.23	1.45	1.52
1	D	214	GLN	CA-C	-5.22	1.46	1.52
1	A	220	VAL	N-CA	-5.22	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	93	PRO	CA-C	-5.22	1.43	1.52
1	F	87	ASP	CA-C	-5.22	1.45	1.52
1	E	396	ASN	N-CA	-5.21	1.39	1.46
1	A	71	ARG	CA-C	-5.21	1.46	1.52
1	F	327	ASN	CA-C	-5.21	1.46	1.53
1	C	398	THR	C-N	-5.21	1.27	1.33
1	E	378	GLN	N-CA	-5.21	1.40	1.46
1	C	159	ILE	CA-C	-5.21	1.46	1.52
1	E	102	CYS	C-N	-5.21	1.26	1.33
1	B	65	VAL	CA-C	-5.20	1.46	1.52
1	E	61	ASP	N-CA	-5.20	1.40	1.46
1	B	51	LYS	N-CA	-5.20	1.39	1.46
1	E	146	ASN	CA-C	-5.20	1.46	1.52
1	F	158	ILE	CA-C	-5.20	1.46	1.52
1	C	26	GLU	CA-C	-5.20	1.46	1.52
1	B	400	LEU	N-CA	-5.20	1.40	1.46
1	B	468	LYS	N-CA	-5.20	1.39	1.46
1	F	195	ILE	CA-CB	-5.20	1.47	1.54
1	B	274	SER	CA-C	-5.19	1.45	1.52
1	F	60	GLN	CA-C	-5.19	1.45	1.52
1	C	320	ASN	CA-C	-5.19	1.46	1.52
1	D	324	CYS	CA-C	-5.19	1.45	1.52
1	E	52	VAL	N-CA	-5.19	1.40	1.46
1	F	114	GLY	CA-C	-5.19	1.45	1.51
1	C	461	ASP	CA-C	-5.19	1.45	1.52
1	F	446	LYS	CA-C	-5.19	1.46	1.52
1	E	68	TYR	CA-C	-5.19	1.44	1.52
1	A	428	THR	CA-CB	-5.18	1.45	1.53
1	A	356	TYR	N-CA	-5.18	1.39	1.46
1	B	394	ASN	N-CA	-5.18	1.39	1.46
1	B	252	ARG	CA-C	-5.18	1.46	1.52
1	B	321	ASN	CA-C	-5.18	1.47	1.53
1	C	97	ARG	CA-C	-5.18	1.46	1.52
1	E	451	ASP	CA-C	-5.18	1.46	1.52
1	B	232	PRO	CA-C	-5.17	1.46	1.52
1	B	273	GLU	CA-C	-5.17	1.45	1.52
1	B	344	VAL	CA-C	-5.17	1.46	1.52
1	C	93	PRO	CA-C	-5.17	1.45	1.52
1	E	29	THR	CA-C	-5.17	1.46	1.52
1	C	396	ASN	C-N	-5.17	1.26	1.33
1	B	392	ILE	CA-C	-5.16	1.46	1.52
1	F	454	GLU	CA-C	-5.16	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	452	LEU	N-CA	-5.16	1.41	1.46
1	B	226	GLN	N-CA	-5.16	1.40	1.46
1	A	469	PHE	CA-C	-5.16	1.46	1.52
1	D	454	GLU	N-CA	-5.16	1.39	1.46
1	F	71	ARG	CA-C	-5.16	1.46	1.53
1	A	456	PHE	CA-C	-5.16	1.45	1.52
1	A	262	ASN	N-CA	-5.16	1.39	1.46
1	C	181	VAL	CA-CB	-5.16	1.49	1.54
1	B	94	ASN	CA-C	-5.15	1.45	1.52
1	D	290	LEU	CA-C	-5.15	1.45	1.52
1	F	340	THR	CA-C	-5.15	1.46	1.52
1	A	443	ASP	N-CA	-5.15	1.40	1.46
1	E	402	ASP	N-CA	-5.15	1.40	1.46
1	F	92	ASP	N-CA	-5.15	1.39	1.46
1	B	321	ASN	N-CA	-5.15	1.39	1.46
1	D	380	CYS	CA-C	-5.14	1.46	1.52
1	E	383	THR	CA-CB	-5.13	1.45	1.53
1	B	120	HIS	CB-CG	-5.13	1.43	1.50
1	E	75	VAL	CA-C	-5.13	1.46	1.52
1	E	159	ILE	N-CA	-5.13	1.40	1.46
1	F	375	PHE	CA-C	-5.13	1.46	1.52
1	C	123	TYR	CA-C	-5.12	1.46	1.52
1	A	37	ALA	CA-C	-5.12	1.46	1.52
1	D	64	LYS	CA-C	-5.12	1.46	1.52
1	A	467	ARG	CA-C	-5.12	1.46	1.52
1	F	316	ALA	N-CA	-5.12	1.39	1.45
1	C	460	LEU	CA-C	-5.12	1.46	1.52
1	C	470	LEU	N-CA	-5.12	1.40	1.46
1	B	278	LYS	CA-C	-5.12	1.46	1.53
1	E	147	VAL	N-CA	-5.12	1.40	1.46
1	F	195	ILE	N-CA	-5.12	1.40	1.46
1	B	77	LEU	N-CA	-5.11	1.41	1.46
1	B	378	GLN	CA-C	-5.11	1.46	1.52
1	E	454	GLU	N-CA	-5.11	1.39	1.45
1	F	451	ASP	CA-C	-5.11	1.46	1.52
1	D	444	LYS	N-CA	-5.10	1.39	1.46
1	E	28	VAL	CA-CB	-5.09	1.48	1.53
1	A	99	VAL	CA-C	-5.09	1.46	1.52
1	A	312	TRP	CA-C	-5.09	1.46	1.52
1	C	445	LEU	N-CA	-5.09	1.39	1.45
1	F	53	PRO	CA-C	-5.09	1.47	1.52
1	E	123	TYR	CA-C	-5.09	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	ARG	CA-C	-5.09	1.46	1.53
1	E	197	ASP	CA-C	-5.09	1.46	1.52
1	D	241	ALA	N-CA	-5.09	1.40	1.46
1	A	303	ASP	N-CA	-5.08	1.40	1.46
1	E	37	ALA	N-CA	-5.08	1.39	1.45
1	E	34	PHE	CA-C	-5.08	1.46	1.52
1	A	327	ASN	N-CA	-5.08	1.38	1.46
1	B	355	VAL	CA-C	-5.08	1.46	1.52
1	C	71	ARG	CA-C	-5.08	1.46	1.52
1	B	255	VAL	CA-CB	-5.07	1.50	1.55
1	D	113	LEU	CA-C	-5.07	1.46	1.53
1	B	266	THR	CA-C	-5.07	1.46	1.52
1	F	311	TYR	C-N	-5.07	1.26	1.33
1	A	422	VAL	CA-C	-5.07	1.46	1.52
1	D	391	TYR	C-O	-5.07	1.17	1.24
1	B	244	ASP	CA-C	-5.07	1.45	1.52
1	C	48	PRO	CA-C	-5.07	1.43	1.52
1	F	450	VAL	CA-CB	-5.07	1.46	1.53
1	D	279	GLY	CA-C	-5.06	1.44	1.51
1	A	307	PHE	N-CA	-5.06	1.39	1.46
1	C	248	PHE	N-CA	-5.06	1.39	1.45
1	A	449	PRO	CA-C	-5.06	1.45	1.52
1	C	427	VAL	N-CA	-5.06	1.40	1.46
1	C	35	TYR	N-CA	-5.05	1.39	1.45
1	D	99	VAL	N-CA	-5.05	1.40	1.46
1	E	351	SER	N-CA	-5.05	1.39	1.45
1	E	462	GLN	N-CA	-5.05	1.39	1.46
1	C	146	ASN	CA-C	-5.05	1.46	1.52
1	F	42	LEU	N-CA	-5.05	1.40	1.46
1	F	211	LYS	CA-C	-5.05	1.46	1.52
1	A	391	TYR	N-CA	-5.05	1.40	1.46
1	E	100	TRP	N-CA	-5.05	1.39	1.46
1	C	462	GLN	N-CA	-5.04	1.40	1.46
1	D	463	PHE	N-CA	-5.04	1.40	1.46
1	E	212	LEU	N-CA	-5.04	1.39	1.46
1	E	161	CYS	CA-C	-5.04	1.46	1.52
1	F	159	ILE	CA-C	-5.04	1.46	1.52
1	B	25	ASP	CA-C	-5.04	1.45	1.52
1	E	62	VAL	CA-CB	-5.04	1.48	1.53
1	A	51	LYS	N-CA	-5.04	1.40	1.46
1	F	221	PRO	CA-C	-5.03	1.46	1.52
1	A	464	PRO	CA-C	-5.03	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	468	LYS	C-N	-5.03	1.27	1.33
1	C	162	VAL	CA-CB	-5.03	1.47	1.54
1	B	399	ILE	N-CA	-5.03	1.40	1.46
1	C	382	ILE	CA-CB	-5.03	1.47	1.54
1	C	391	TYR	C-N	-5.03	1.27	1.34
1	A	460	LEU	C-N	-5.02	1.27	1.33
1	D	386	THR	CA-C	-5.02	1.46	1.52
1	E	337	THR	CA-C	-5.02	1.46	1.53
1	E	176	LYS	N-CA	-5.02	1.40	1.46
1	E	358	PRO	CA-C	-5.02	1.44	1.52
1	A	51	LYS	CA-C	-5.02	1.46	1.52
1	E	347	SER	CA-C	-5.02	1.46	1.52
1	A	167	GLU	CA-C	-5.02	1.46	1.52
1	A	193	THR	CA-C	-5.01	1.47	1.52
1	B	332	THR	CA-C	-5.01	1.46	1.52
1	D	208	MET	CA-C	-5.01	1.46	1.52
1	D	399	ILE	CA-C	-5.01	1.46	1.52
1	E	218	SER	CA-C	-5.01	1.48	1.52
1	B	465	LEU	N-CA	-5.01	1.40	1.46
1	C	358	PRO	CA-C	-5.01	1.45	1.52
1	A	63	PRO	CA-C	-5.01	1.45	1.52
1	B	207	ALA	CA-C	-5.01	1.46	1.52
1	F	98	LEU	N-CA	-5.00	1.39	1.45
1	E	440	ASP	CA-C	-5.00	1.46	1.52

All (1522) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	THR	N-CA-C	27.06	146.38	111.75
1	F	463	PHE	CA-CB-CG	-17.36	96.44	113.80
1	A	447	PHE	CA-CB-CG	-16.38	97.42	113.80
1	D	447	PHE	CA-CB-CG	-16.17	97.63	113.80
1	B	447	PHE	CA-CB-CG	-16.00	97.80	113.80
1	B	40	SER	N-CA-C	15.56	130.15	111.33
1	C	447	PHE	CA-CB-CG	-15.53	98.27	113.80
1	F	447	PHE	CA-CB-CG	-15.45	98.35	113.80
1	C	421	PHE	CA-CB-CG	15.00	128.80	113.80
1	E	447	PHE	CA-CB-CG	-14.58	99.22	113.80
1	C	375	PHE	CA-CB-CG	-14.39	99.41	113.80
1	D	459	ASP	CA-CB-CG	-14.20	98.40	112.60
1	C	87	ASP	CA-CB-CG	-14.18	98.42	112.60
1	A	192	ASN	CA-CB-CG	-14.08	98.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	87	ASP	CA-CB-CG	-13.97	98.63	112.60
1	B	314	HIS	CA-CB-CG	-13.89	99.91	113.80
1	F	34	PHE	CA-CB-CG	-13.70	100.10	113.80
1	F	314	HIS	CA-CB-CG	-13.63	100.17	113.80
1	A	387	GLU	N-CA-C	-13.45	95.53	112.88
1	A	307	PHE	CA-CB-CG	-13.38	100.42	113.80
1	E	463	PHE	CA-CB-CG	-13.35	100.45	113.80
1	A	394	ASN	CA-CB-CG	-13.31	99.29	112.60
1	B	375	PHE	CA-CB-CG	-13.31	100.49	113.80
1	C	210	PHE	CA-CB-CG	-13.19	100.61	113.80
1	C	192	ASN	CA-CB-CG	-13.14	99.46	112.60
1	F	73	PHE	CA-CB-CG	-13.09	100.71	113.80
1	A	463	PHE	CA-CB-CG	-13.09	100.72	113.80
1	E	73	PHE	CA-CB-CG	-13.03	100.77	113.80
1	C	81	ASN	CA-CB-CG	-13.01	99.59	112.60
1	C	73	PHE	CA-CB-CG	-12.88	100.92	113.80
1	E	404	ASN	CA-C-N	12.83	146.05	121.54
1	E	404	ASN	C-N-CA	12.83	146.05	121.54
1	C	460	LEU	CA-C-N	12.76	138.66	120.28
1	C	460	LEU	C-N-CA	12.76	138.66	120.28
1	B	327	ASN	CA-CB-CG	-12.69	99.92	112.60
1	F	354	ASN	CA-CB-CG	-12.66	99.94	112.60
1	C	330	PHE	CA-CB-CG	-12.56	101.24	113.80
1	B	404	ASN	CA-CB-CG	-12.50	100.10	112.60
1	A	371	PHE	N-CA-C	12.49	128.60	108.99
1	D	463	PHE	CA-CB-CG	-12.48	101.32	113.80
1	B	73	PHE	CA-CB-CG	-12.46	101.34	113.80
1	A	248	PHE	CA-CB-CG	-12.44	101.36	113.80
1	D	73	PHE	CA-CB-CG	-12.41	101.39	113.80
1	D	202	ASP	CA-CB-CG	-12.37	100.23	112.60
1	A	73	PHE	CA-CB-CG	-12.35	101.45	113.80
1	A	387	GLU	N-CA-CB	-12.15	91.89	110.73
1	E	371	PHE	CA-CB-CG	-12.10	101.70	113.80
1	C	463	PHE	CA-CB-CG	-12.02	101.78	113.80
1	A	469	PHE	CA-CB-CG	-11.94	101.86	113.80
1	A	459	ASP	CA-CB-CG	-11.90	100.70	112.60
1	E	83	PHE	CA-CB-CG	-11.87	101.93	113.80
1	D	354	ASN	CA-CB-CG	-11.78	100.82	112.60
1	B	330	PHE	CA-CB-CG	-11.73	102.07	113.80
1	D	92	ASP	CA-CB-CG	-11.68	100.92	112.60
1	A	432	ASP	CA-CB-CG	-11.58	101.02	112.60
1	B	57	ASN	CA-CB-CG	-11.57	101.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	307	PHE	CA-CB-CG	-11.55	102.25	113.80
1	D	244	ASP	CA-C-N	11.48	135.66	120.28
1	D	244	ASP	C-N-CA	11.48	135.66	120.28
1	A	88	ASN	CA-CB-CG	11.47	124.07	112.60
1	D	330	PHE	CA-CB-CG	-11.46	102.33	113.80
1	C	62	VAL	N-CA-C	-11.46	93.97	107.61
1	E	354	ASN	CA-CB-CG	-11.31	101.29	112.60
1	A	94	ASN	CA-CB-CG	-11.30	101.30	112.60
1	C	307	PHE	CA-CB-CG	-11.29	102.51	113.80
1	E	405	PHE	N-CA-CB	11.26	129.51	110.49
1	C	431	LYS	N-CA-C	-11.10	91.32	108.42
1	C	422	VAL	CA-C-N	11.06	135.53	120.38
1	C	422	VAL	C-N-CA	11.06	135.53	120.38
1	E	94	ASN	CA-CB-CG	-11.03	101.57	112.60
1	F	303	ASP	CA-CB-CG	-10.95	101.65	112.60
1	B	463	PHE	CA-CB-CG	-10.94	102.86	113.80
1	F	375	PHE	CA-CB-CG	-10.90	102.90	113.80
1	B	326	HIS	CA-CB-CG	-10.84	102.96	113.80
1	C	258	ARG	N-CA-C	10.83	123.05	111.03
1	D	34	PHE	CA-CB-CG	-10.81	102.99	113.80
1	E	443	ASP	CA-CB-CG	-10.78	101.82	112.60
1	A	285	ASN	CA-CB-CG	-10.77	101.83	112.60
1	B	94	ASN	CA-CB-CG	-10.67	101.93	112.60
1	C	24	THR	CA-C-N	10.67	137.67	120.60
1	C	24	THR	C-N-CA	10.67	137.67	120.60
1	E	448	TRP	N-CA-CB	10.63	123.67	110.17
1	F	341	ASN	CA-CB-CG	-10.60	102.00	112.60
1	C	303	ASP	CA-CB-CG	-10.57	102.03	112.60
1	D	258	ARG	N-CA-C	10.50	122.69	111.03
1	E	239	ALA	N-CA-C	-10.48	100.77	112.72
1	B	371	PHE	N-CA-C	10.37	125.26	108.99
1	E	314	HIS	CA-CB-CG	-10.35	103.45	113.80
1	F	455	ARG	CA-C-N	10.30	136.08	121.24
1	F	455	ARG	C-N-CA	10.30	136.08	121.24
1	A	456	PHE	CA-CB-CG	-10.30	103.50	113.80
1	E	169	TRP	CB-CG-CD2	-10.29	112.40	126.80
1	F	248	PHE	CA-CB-CG	-10.28	103.52	113.80
1	C	40	SER	N-CA-C	10.26	123.75	111.33
1	A	459	ASP	CA-C-N	10.24	133.75	120.44
1	A	459	ASP	C-N-CA	10.24	133.75	120.44
1	F	391	TYR	N-CA-C	-10.23	99.10	111.69
1	B	372	ASP	N-CA-C	10.22	125.10	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	396	ASN	CA-CB-CG	-10.21	102.39	112.60
1	B	192	ASN	CA-CB-CG	-10.21	102.39	112.60
1	C	419	TYR	CA-C-N	10.20	140.05	121.70
1	C	419	TYR	C-N-CA	10.20	140.05	121.70
1	E	459	ASP	CA-CB-CG	10.18	122.78	112.60
1	F	131	ASN	CA-CB-CG	-10.15	102.45	112.60
1	A	39	SER	N-CA-C	10.13	124.38	108.67
1	E	24	THR	N-CA-C	10.13	125.00	112.23
1	B	240	ASP	CA-CB-CG	10.10	122.70	112.60
1	D	469	PHE	CA-CB-CG	-10.07	103.73	113.80
1	B	354	ASN	CA-CB-CG	-10.05	102.55	112.60
1	E	272	PRO	CA-C-N	10.00	133.44	120.44
1	E	272	PRO	C-N-CA	10.00	133.44	120.44
1	B	18	VAL	CA-C-N	9.98	139.67	121.70
1	B	18	VAL	C-N-CA	9.98	139.67	121.70
1	D	314	HIS	CA-CB-CG	-9.98	103.82	113.80
1	E	330	PHE	CA-CB-CG	-9.97	103.83	113.80
1	E	124	ASN	CA-CB-CG	9.95	122.55	112.60
1	A	176	LYS	N-CA-C	-9.94	93.12	109.82
1	D	40	SER	N-CA-C	9.90	131.89	110.80
1	C	451	ASP	CA-CB-CG	-9.87	102.73	112.60
1	F	102	CYS	N-CA-CB	9.86	126.21	110.23
1	F	433	THR	N-CA-C	9.86	125.31	113.28
1	D	440	ASP	O-C-N	-9.84	110.00	121.32
1	A	330	PHE	CA-CB-CG	-9.84	103.96	113.80
1	B	311	TYR	CA-CB-CG	-9.82	96.23	113.90
1	D	43	LEU	N-CA-C	9.80	124.42	109.23
1	A	164	ALA	CA-C-N	9.79	135.33	123.19
1	A	164	ALA	C-N-CA	9.79	135.33	123.19
1	B	191	ILE	N-CA-C	9.78	121.81	108.11
1	A	126	LEU	N-CA-C	-9.74	98.22	111.96
1	F	40	SER	N-CA-C	9.68	123.04	111.33
1	E	405	PHE	CB-CA-C	-9.68	91.16	110.42
1	F	82	LYS	N-CA-C	9.65	121.56	111.14
1	E	209	ASP	CA-C-N	9.64	132.97	120.44
1	E	209	ASP	C-N-CA	9.64	132.97	120.44
1	D	285	ASN	CA-CB-CG	-9.59	103.01	112.60
1	E	26	GLU	N-CA-C	-9.59	100.81	111.07
1	B	120	HIS	CA-CB-CG	-9.58	104.22	113.80
1	A	326	HIS	CA-CB-CG	-9.57	104.23	113.80
1	D	321	ASN	CA-CB-CG	-9.50	103.10	112.60
1	D	94	ASN	CA-CB-CG	-9.48	103.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ASP	CA-CB-CG	-9.43	103.17	112.60
1	F	462	GLN	N-CA-C	-9.35	100.82	112.88
1	A	354	ASN	CA-CB-CG	-9.35	103.25	112.60
1	F	405	PHE	CA-CB-CG	-9.34	104.46	113.80
1	A	391	TYR	N-CA-C	-9.33	100.21	111.69
1	C	88	ASN	CA-CB-CG	-9.31	103.29	112.60
1	A	339	SER	N-CA-C	9.31	125.39	108.17
1	E	413	ALA	CA-C-N	9.29	138.42	121.70
1	E	413	ALA	C-N-CA	9.29	138.42	121.70
1	F	72	VAL	N-CA-C	9.29	122.05	107.28
1	D	303	ASP	CA-CB-CG	-9.27	103.33	112.60
1	A	365	ALA	N-CA-C	9.26	124.22	108.02
1	B	446	LYS	CB-CA-C	-9.20	96.91	110.16
1	E	373	LEU	CB-CA-C	9.18	124.90	109.48
1	B	107	ILE	CB-CA-C	-9.17	101.33	111.23
1	C	109	ARG	CD-NE-CZ	-9.16	111.57	124.40
1	B	262	ASN	N-CA-C	-9.13	95.07	109.50
1	E	373	LEU	N-CA-CB	-9.13	95.45	110.52
1	C	395	MET	N-CA-CB	-9.10	95.94	110.14
1	D	222	LEU	CA-C-N	9.09	132.46	120.28
1	D	222	LEU	C-N-CA	9.09	132.46	120.28
1	A	375	PHE	CA-CB-CG	-9.08	104.72	113.80
1	F	430	GLN	N-CA-C	-9.07	92.03	107.99
1	C	92	ASP	CA-CB-CG	-9.06	103.54	112.60
1	D	125	LYS	N-CA-C	-9.06	91.49	110.80
1	A	34	PHE	CA-CB-CG	-9.06	104.74	113.80
1	C	111	GLN	N-CA-C	9.04	122.41	109.84
1	E	375	PHE	CA-CB-CG	-9.04	104.76	113.80
1	F	258	ARG	N-CA-C	9.02	121.04	111.03
1	D	317	GLN	CA-C-N	9.02	128.58	119.92
1	D	317	GLN	C-N-CA	9.02	128.58	119.92
1	F	404	ASN	N-CA-C	-9.01	96.57	110.17
1	E	405	PHE	N-CA-C	8.98	129.92	110.80
1	C	49	TYR	CA-CB-CG	-8.97	97.76	113.90
1	E	189	GLU	N-CA-C	8.96	124.01	109.59
1	A	124	ASN	CA-CB-CG	8.95	121.55	112.60
1	F	456	PHE	N-CA-CB	-8.94	95.94	109.71
1	B	270	GLN	N-CA-C	8.93	124.00	109.72
1	A	57	ASN	CA-CB-CG	-8.91	103.69	112.60
1	D	409	PRO	N-CA-C	-8.88	99.87	110.70
1	B	39	SER	N-CA-C	8.88	122.70	108.41
1	B	450	VAL	N-CA-C	8.87	122.41	106.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311	TYR	CA-CB-CG	-8.84	97.98	113.90
1	A	314	HIS	CA-CB-CG	-8.84	104.96	113.80
1	B	459	ASP	CA-CB-CG	-8.84	103.76	112.60
1	E	365	ALA	N-CA-C	8.84	123.63	107.99
1	E	25	ASP	CA-C-N	8.83	131.92	120.44
1	E	25	ASP	C-N-CA	8.83	131.92	120.44
1	E	102	CYS	N-CA-CB	8.83	123.71	110.29
1	E	72	VAL	N-CA-C	8.82	121.31	107.28
1	C	340	THR	N-CA-C	8.81	121.47	108.60
1	A	361	PHE	CA-CB-CG	-8.80	105.00	113.80
1	F	381	LYS	N-CA-CB	8.77	124.35	110.85
1	C	354	ASN	CA-CB-CG	-8.70	103.91	112.60
1	E	192	ASN	CA-CB-CG	-8.69	103.91	112.60
1	D	459	ASP	CA-C-N	8.68	138.11	121.54
1	D	459	ASP	C-N-CA	8.68	138.11	121.54
1	D	248	PHE	CA-CB-CG	-8.66	105.14	113.80
1	E	127	ASP	CA-C-N	8.66	138.08	121.54
1	E	127	ASP	C-N-CA	8.66	138.08	121.54
1	C	264	SER	N-CA-C	8.65	122.58	112.72
1	E	222	LEU	CA-C-N	8.62	132.69	120.28
1	E	222	LEU	C-N-CA	8.62	132.69	120.28
1	B	443	ASP	N-CA-CB	-8.61	96.96	110.22
1	E	89	THR	N-CA-C	-8.61	101.90	111.28
1	E	440	ASP	CA-CB-CG	-8.60	104.00	112.60
1	C	420	ARG	NE-CZ-NH2	8.59	126.93	119.20
1	E	207	ALA	CA-C-N	8.59	137.94	121.54
1	E	207	ALA	C-N-CA	8.59	137.94	121.54
1	F	469	PHE	CA-CB-CG	-8.59	105.21	113.80
1	A	325	TRP	CB-CG-CD2	-8.58	114.79	126.80
1	D	87	ASP	CA-C-N	8.57	132.89	120.38
1	D	87	ASP	C-N-CA	8.57	132.89	120.38
1	B	345	CYS	N-CA-C	-8.55	94.58	108.52
1	B	189	GLU	N-CA-C	8.53	123.30	109.40
1	B	92	ASP	CB-CA-C	8.52	120.73	109.65
1	E	341	ASN	N-CA-C	-8.52	95.87	109.59
1	F	87	ASP	CA-CB-CG	-8.52	104.08	112.60
1	E	459	ASP	N-CA-C	-8.52	97.88	110.48
1	C	125	LYS	N-CA-C	-8.49	93.19	108.48
1	D	262	ASN	N-CA-C	-8.48	95.07	109.24
1	F	386	THR	N-CA-C	8.48	120.52	111.28
1	C	413	ALA	CA-C-N	8.44	136.89	121.70
1	C	413	ALA	C-N-CA	8.44	136.89	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	61	ASP	N-CA-C	-8.43	95.32	108.14
1	E	312	TRP	N-CA-C	-8.42	95.81	109.96
1	A	342	LEU	N-CA-C	8.39	123.52	109.76
1	B	273	GLU	CA-C-N	8.38	137.54	121.54
1	B	273	GLU	C-N-CA	8.38	137.54	121.54
1	C	244	ASP	CA-CB-CG	-8.37	104.23	112.60
1	C	68	TYR	N-CA-C	-8.36	100.40	110.44
1	E	136	SER	N-CA-C	8.34	119.99	111.07
1	E	34	PHE	CA-CB-CG	-8.33	105.47	113.80
1	C	94	ASN	CA-CB-CG	-8.32	104.28	112.60
1	C	430	GLN	N-CA-CB	8.31	123.24	109.94
1	E	423	GLN	N-CA-C	-8.31	103.14	113.28
1	E	386	THR	CA-C-N	8.31	131.77	120.38
1	E	386	THR	C-N-CA	8.31	131.77	120.38
1	C	102	CYS	N-CA-CB	8.28	122.56	110.06
1	A	52	VAL	N-CA-C	-8.26	99.37	107.55
1	E	79	ASP	CA-CB-CG	-8.26	104.34	112.60
1	F	314	HIS	N-CA-C	-8.25	99.04	111.34
1	E	456	PHE	CA-CB-CG	-8.25	105.55	113.80
1	E	92	ASP	CA-CB-CG	-8.24	104.36	112.60
1	A	371	PHE	CA-CB-CG	-8.23	105.57	113.80
1	E	127	ASP	CA-CB-CG	-8.22	104.38	112.60
1	E	224	ILE	N-CA-CB	-8.22	103.17	112.21
1	C	421	PHE	N-CA-CB	-8.21	96.61	110.49
1	E	461	ASP	CA-CB-CG	-8.20	104.40	112.60
1	A	333	VAL	CA-C-N	8.16	134.33	122.99
1	A	333	VAL	C-N-CA	8.16	134.33	122.99
1	E	463	PHE	N-CA-C	-8.16	96.35	109.40
1	F	86	PRO	CA-C-N	8.16	132.03	120.28
1	F	86	PRO	C-N-CA	8.16	132.03	120.28
1	F	24	THR	CA-C-O	8.13	129.39	119.79
1	B	18	VAL	O-C-N	-8.13	112.41	122.57
1	B	448	TRP	CB-CG-CD2	-8.11	115.45	126.80
1	F	91	TYR	N-CA-C	8.11	122.45	109.24
1	E	469	PHE	CA-CB-CG	-8.09	105.71	113.80
1	B	233	ASP	CA-CB-CG	-8.09	104.51	112.60
1	C	391	TYR	N-CA-C	-8.09	101.21	112.45
1	A	102	CYS	N-CA-CB	8.09	123.59	110.41
1	A	333	VAL	N-CA-C	8.09	119.98	108.42
1	C	302	SER	CA-C-N	8.09	131.11	120.28
1	C	302	SER	C-N-CA	8.09	131.11	120.28
1	D	25	ASP	CA-C-N	8.08	131.43	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	25	ASP	C-N-CA	8.08	131.43	120.44
1	A	311	TYR	N-CA-C	-8.07	93.90	108.02
1	F	424	SER	N-CA-C	-8.07	96.25	108.52
1	E	25	ASP	CA-C-O	8.05	129.24	119.10
1	B	149	VAL	N-CA-C	8.04	118.98	107.88
1	F	192	ASN	N-CA-CB	8.01	123.21	110.23
1	F	146	ASN	CA-CB-CG	-8.01	104.59	112.60
1	C	361	PHE	CA-CB-CG	-8.00	105.80	113.80
1	F	373	LEU	CB-CA-C	7.99	122.70	109.53
1	F	68	TYR	CA-CB-CG	-7.98	99.54	113.90
1	B	72	VAL	N-CA-C	7.98	119.97	107.28
1	E	169	TRP	N-CA-C	7.96	122.60	109.95
1	B	361	PHE	CA-CB-CG	-7.93	105.87	113.80
1	A	363	GLU	CB-CA-C	7.92	123.43	109.72
1	B	394	ASN	CA-CB-CG	-7.92	104.68	112.60
1	B	259	HIS	N-CA-C	7.91	121.49	109.23
1	E	149	VAL	N-CA-C	7.91	120.70	108.44
1	C	458	ALA	CA-C-N	7.90	136.62	121.54
1	C	458	ALA	C-N-CA	7.90	136.62	121.54
1	D	68	TYR	CA-CB-CG	-7.90	99.68	113.90
1	C	259	HIS	N-CA-C	7.88	121.45	109.23
1	E	203	THR	N-CA-CB	7.88	123.65	110.41
1	A	245	SER	CA-C-N	7.87	134.07	123.05
1	A	245	SER	C-N-CA	7.87	134.07	123.05
1	D	188	LEU	N-CA-C	7.87	121.24	108.41
1	F	389	MET	CG-SD-CE	7.86	118.20	100.90
1	B	164	ALA	CA-C-N	7.86	132.94	123.19
1	B	164	ALA	C-N-CA	7.86	132.94	123.19
1	B	461	ASP	CA-CB-CG	-7.86	104.74	112.60
1	B	244	ASP	CA-CB-CG	-7.84	104.76	112.60
1	E	102	CYS	N-CA-C	-7.84	98.87	110.48
1	D	386	THR	CA-C-N	7.84	132.57	120.82
1	D	386	THR	C-N-CA	7.84	132.57	120.82
1	F	397	THR	N-CA-C	7.84	120.91	111.82
1	B	396	ASN	CA-CB-CG	-7.83	104.77	112.60
1	A	149	VAL	N-CA-C	7.82	117.25	107.70
1	F	450	VAL	N-CA-C	7.82	120.53	106.61
1	E	450	VAL	N-CA-C	7.81	120.51	106.61
1	E	459	ASP	N-CA-CB	7.81	122.16	110.29
1	B	303	ASP	N-CA-CB	-7.79	98.66	110.12
1	C	405	PHE	CA-CB-CG	-7.79	106.01	113.80
1	D	361	PHE	CA-CB-CG	-7.79	106.01	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	462	GLN	N-CA-C	-7.79	103.60	113.72
1	D	102	CYS	N-CA-C	-7.78	98.36	110.42
1	C	443	ASP	N-CA-CB	-7.76	98.28	109.85
1	B	25	ASP	CA-C-N	7.76	130.52	120.44
1	B	25	ASP	C-N-CA	7.76	130.52	120.44
1	A	87	ASP	N-CA-C	-7.75	103.28	112.89
1	C	232	PRO	N-CA-C	7.73	122.48	110.80
1	E	351	SER	N-CA-C	-7.73	97.32	109.07
1	D	281	ASP	CA-CB-CG	-7.71	104.89	112.60
1	A	386	THR	CB-CA-C	-7.71	95.51	110.46
1	C	154	THR	N-CA-C	7.71	122.16	109.06
1	F	103	VAL	N-CA-C	-7.70	105.65	112.12
1	F	311	TYR	CA-CB-CG	-7.69	100.05	113.90
1	F	75	VAL	N-CA-C	7.69	118.97	107.51
1	C	72	VAL	N-CA-C	7.68	119.49	107.28
1	C	69	GLN	CB-CG-CD	7.68	125.65	112.60
1	A	338	ARG	N-CA-C	7.66	120.19	110.61
1	A	222	LEU	CA-C-N	7.66	131.31	120.28
1	A	222	LEU	C-N-CA	7.66	131.31	120.28
1	B	369	GLU	CA-C-N	7.66	134.43	122.94
1	B	369	GLU	C-N-CA	7.66	134.43	122.94
1	D	102	CYS	N-CA-CB	7.65	122.49	110.56
1	F	443	ASP	CA-CB-CG	-7.64	104.96	112.60
1	C	441	PRO	N-CA-C	-7.63	103.57	114.18
1	A	403	TRP	CB-CG-CD2	-7.62	116.13	126.80
1	C	139	ASP	CA-CB-CG	-7.61	104.99	112.60
1	C	459	ASP	N-CA-C	7.61	127.00	110.80
1	F	143	THR	N-CA-C	-7.61	104.02	113.38
1	B	25	ASP	CA-CB-CG	-7.60	105.00	112.60
1	A	99	VAL	N-CA-C	7.58	118.35	108.35
1	F	363	GLU	N-CA-C	7.58	121.79	109.59
1	B	102	CYS	N-CA-CB	7.57	122.74	110.41
1	C	432	ASP	CA-CB-CG	-7.57	105.03	112.60
1	D	446	LYS	CB-CA-C	-7.56	94.92	109.37
1	A	136	SER	N-CA-C	7.55	119.30	111.14
1	E	331	LEU	N-CA-C	7.55	121.04	108.73
1	A	363	GLU	CB-CG-CD	7.54	125.42	112.60
1	F	232	PRO	N-CA-C	7.53	122.63	111.03
1	F	460	LEU	CA-C-O	7.53	127.35	118.69
1	E	92	ASP	N-CA-C	-7.52	98.78	109.24
1	D	240	ASP	CA-C-N	7.52	131.11	120.28
1	D	240	ASP	C-N-CA	7.52	131.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	248	PHE	CA-CB-CG	-7.52	106.28	113.80
1	C	24	THR	CA-C-O	7.51	128.62	119.31
1	E	273	GLU	CA-C-N	7.51	131.34	120.38
1	E	273	GLU	C-N-CA	7.51	131.34	120.38
1	D	365	ALA	N-CA-C	7.50	120.75	108.52
1	E	193	THR	O-C-N	-7.50	116.55	121.88
1	C	146	ASN	CA-CB-CG	-7.50	105.10	112.60
1	D	451	ASP	N-CA-CB	7.50	122.53	110.16
1	C	311	TYR	N-CA-C	-7.49	94.91	108.02
1	E	35	TYR	CA-CB-CG	-7.48	100.43	113.90
1	A	389	MET	CA-C-O	7.47	128.34	120.42
1	F	361	PHE	CA-CB-CG	-7.47	106.33	113.80
1	F	25	ASP	CA-C-N	7.47	130.60	120.44
1	F	25	ASP	C-N-CA	7.47	130.60	120.44
1	A	33	ILE	CB-CA-C	-7.47	101.44	111.15
1	A	40	SER	N-CA-C	7.46	126.69	110.80
1	B	386	THR	N-CA-C	7.46	119.41	111.28
1	B	413	ALA	N-CA-C	7.46	119.49	108.60
1	B	169	TRP	N-CA-C	7.45	121.98	109.76
1	C	329	LEU	N-CA-C	7.45	121.54	109.40
1	C	393	HIS	N-CA-CB	-7.45	99.18	110.12
1	F	262	ASN	N-CA-C	-7.43	97.28	109.40
1	F	330	PHE	CA-CB-CG	-7.43	106.37	113.80
1	F	440	ASP	N-CA-C	-7.42	93.65	109.01
1	D	448	TRP	CB-CG-CD2	-7.42	116.42	126.80
1	B	209	ASP	CA-C-N	7.41	133.09	120.71
1	B	209	ASP	C-N-CA	7.41	133.09	120.71
1	D	372	ASP	N-CA-CB	7.41	122.46	110.90
1	A	148	SER	CA-C-N	7.40	129.37	121.97
1	A	148	SER	C-N-CA	7.40	129.37	121.97
1	A	376	ILE	CB-CA-C	-7.38	101.94	110.73
1	B	169	TRP	CB-CG-CD2	-7.38	116.46	126.80
1	C	100	TRP	N-CA-C	-7.38	98.54	110.20
1	D	79	ASP	CA-CB-CG	-7.38	105.22	112.60
1	F	244	ASP	CA-C-N	7.37	132.91	121.19
1	F	244	ASP	C-N-CA	7.37	132.91	121.19
1	C	58	GLY	O-C-N	-7.36	114.03	122.42
1	D	142	ASP	CA-CB-CG	7.36	119.96	112.60
1	E	332	THR	N-CA-C	7.35	121.22	109.24
1	C	222	LEU	CA-C-N	7.35	130.13	120.28
1	C	222	LEU	C-N-CA	7.35	130.13	120.28
1	F	12	TYR	CA-CB-CG	-7.34	100.68	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	143	THR	CA-C-N	7.34	135.56	121.54
1	E	143	THR	C-N-CA	7.34	135.56	121.54
1	C	393	HIS	CA-C-O	7.33	128.32	120.55
1	E	469	PHE	N-CA-CB	-7.32	99.33	110.16
1	E	424	SER	CA-C-N	7.31	134.86	121.70
1	E	424	SER	C-N-CA	7.31	134.86	121.70
1	F	434	ALA	N-CA-C	7.31	120.00	109.84
1	C	42	LEU	CA-C-O	-7.29	112.82	120.70
1	D	106	GLU	CA-C-N	7.29	131.61	122.43
1	D	106	GLU	C-N-CA	7.29	131.61	122.43
1	E	78	PRO	CA-C-O	-7.28	113.44	121.23
1	F	256	PHE	CA-CB-CG	-7.28	106.52	113.80
1	F	217	LYS	CB-CA-C	-7.27	101.57	111.89
1	A	269	ASP	CA-CB-CG	-7.26	105.34	112.60
1	D	51	LYS	CA-C-N	7.26	127.54	122.60
1	D	51	LYS	C-N-CA	7.26	127.54	122.60
1	C	35	TYR	CA-CB-CG	-7.25	100.84	113.90
1	D	52	VAL	N-CA-C	-7.25	100.96	107.56
1	E	62	VAL	N-CA-C	-7.25	99.84	107.60
1	E	210	PHE	CA-CB-CG	-7.24	106.56	113.80
1	B	144	ARG	CA-C-N	7.24	131.14	120.87
1	B	144	ARG	C-N-CA	7.24	131.14	120.87
1	D	259	HIS	N-CA-C	7.23	120.93	109.50
1	A	137	ALA	N-CA-C	7.23	120.06	111.02
1	D	261	TRP	CB-CG-CD2	-7.23	116.68	126.80
1	C	396	ASN	CA-C-O	7.23	128.80	119.98
1	F	36	HIS	N-CA-C	-7.22	98.47	109.95
1	C	233	ASP	CB-CA-C	-7.22	100.28	111.83
1	F	137	ALA	CA-C-N	7.21	130.93	120.91
1	F	137	ALA	C-N-CA	7.21	130.93	120.91
1	C	236	GLN	N-CA-CB	7.21	120.52	110.07
1	B	79	ASP	N-CA-C	-7.20	100.58	109.65
1	A	72	VAL	N-CA-C	7.20	118.72	107.28
1	F	57	ASN	CA-CB-CG	-7.18	105.42	112.60
1	C	365	ALA	N-CA-C	7.18	120.22	108.52
1	F	395	MET	N-CA-C	-7.18	100.58	111.56
1	E	75	VAL	N-CA-C	7.17	118.46	107.99
1	A	24	THR	CA-C-O	7.17	130.76	120.51
1	A	146	ASN	CA-CB-CG	-7.17	105.43	112.60
1	A	216	ASN	N-CA-C	7.16	119.95	111.71
1	F	469	PHE	N-CA-CB	-7.16	99.56	110.16
1	C	57	ASN	CA-CB-CG	-7.16	105.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	457	SER	N-CA-C	-7.15	97.30	109.24
1	E	311	TYR	CA-CB-CG	-7.15	101.03	113.90
1	B	247	PHE	CA-CB-CG	-7.15	106.65	113.80
1	B	460	LEU	N-CA-CB	-7.15	101.50	111.00
1	D	39	SER	N-CA-C	7.15	119.92	108.41
1	F	189	GLU	O-C-N	-7.15	113.94	123.23
1	C	279	GLY	N-CA-C	-7.14	96.26	113.18
1	E	165	ILE	N-CA-C	7.14	118.88	108.53
1	C	58	GLY	CA-C-N	7.12	134.52	121.70
1	C	58	GLY	C-N-CA	7.12	134.52	121.70
1	F	35	TYR	CA-CB-CG	-7.12	101.08	113.90
1	F	165	ILE	N-CA-CB	7.12	120.93	111.25
1	A	317	GLN	CA-C-N	7.11	126.75	119.92
1	A	317	GLN	C-N-CA	7.11	126.75	119.92
1	A	395	MET	N-CA-C	-7.10	100.69	111.56
1	D	340	THR	N-CA-C	7.10	119.66	108.79
1	D	407	VAL	CA-C-N	7.10	134.48	121.70
1	D	407	VAL	C-N-CA	7.10	134.48	121.70
1	F	296	SER	O-C-N	-7.09	115.72	123.52
1	F	92	ASP	CA-CB-CG	-7.09	105.51	112.60
1	B	331	LEU	N-CA-C	7.08	120.28	108.73
1	C	202	ASP	CA-CB-CG	-7.08	105.52	112.60
1	A	258	ARG	N-CA-C	7.08	118.89	111.03
1	B	111	GLN	N-CA-C	7.08	125.45	109.81
1	B	45	VAL	O-C-N	-7.08	115.02	123.02
1	A	460	LEU	CA-C-N	7.07	131.42	120.82
1	A	460	LEU	C-N-CA	7.07	131.42	120.82
1	F	103	VAL	CB-CA-C	7.05	117.82	110.91
1	E	303	ASP	CA-CB-CG	-7.04	105.56	112.60
1	D	62	VAL	N-CA-C	-7.04	96.59	107.71
1	E	167	GLU	CB-CG-CD	7.04	124.56	112.60
1	E	358	PRO	CA-C-N	7.04	130.02	120.38
1	E	358	PRO	C-N-CA	7.04	130.02	120.38
1	F	394	ASN	CA-CB-CG	-7.04	105.56	112.60
1	E	425	ALA	N-CA-CB	7.04	120.95	110.40
1	B	377	PHE	CB-CA-C	-7.03	96.50	109.37
1	E	46	GLY	O-C-N	-7.03	117.17	123.92
1	C	253	GLU	N-CA-C	7.03	121.01	109.06
1	F	210	PHE	CA-CB-CG	-7.02	106.78	113.80
1	B	426	ALA	CA-C-N	7.02	134.34	121.70
1	B	426	ALA	C-N-CA	7.02	134.34	121.70
1	D	298	SER	CA-C-N	7.02	130.11	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	298	SER	C-N-CA	7.02	130.11	120.35
1	F	459	ASP	CA-CB-CG	-7.02	105.58	112.60
1	B	469	PHE	N-CA-CB	-7.02	99.78	110.16
1	C	135	ALA	CA-C-N	7.01	134.32	121.70
1	C	135	ALA	C-N-CA	7.01	134.32	121.70
1	E	58	GLY	N-CA-C	-7.01	96.57	113.18
1	B	414	SER	N-CA-C	7.01	119.88	110.35
1	B	168	HIS	CB-CG-CD2	-7.00	122.10	131.20
1	A	49	TYR	CA-CB-CG	-6.99	101.31	113.90
1	C	356	TYR	N-CA-C	6.98	120.35	110.23
1	B	333	VAL	N-CA-C	6.98	118.40	108.42
1	E	68	TYR	CA-CB-CG	-6.98	101.34	113.90
1	B	88	ASN	CB-CA-C	-6.97	107.49	115.79
1	A	262	ASN	N-CA-C	-6.97	97.60	109.24
1	F	169	TRP	CB-CG-CD2	-6.95	117.07	126.80
1	A	273	GLU	CB-CA-C	-6.95	99.03	110.85
1	B	49	TYR	N-CA-C	6.95	118.86	111.28
1	F	455	ARG	CA-C-O	6.94	128.14	119.95
1	A	343	SER	CA-C-O	6.94	127.76	120.54
1	F	311	TYR	CA-C-N	6.93	132.90	121.39
1	F	311	TYR	C-N-CA	6.93	132.90	121.39
1	B	413	ALA	CA-C-N	6.93	131.21	120.75
1	B	413	ALA	C-N-CA	6.93	131.21	120.75
1	D	244	ASP	CA-C-O	6.93	127.89	120.55
1	A	366	ARG	N-CA-C	6.93	120.83	109.06
1	C	461	ASP	N-CA-CB	-6.92	99.56	110.22
1	D	122	LEU	N-CA-C	-6.92	102.02	110.88
1	A	189	GLU	CB-CG-CD	6.92	124.37	112.60
1	A	253	GLU	N-CA-C	6.92	120.82	109.06
1	E	244	ASP	CA-CB-CG	-6.92	105.68	112.60
1	F	234	TYR	CB-CA-C	-6.92	98.92	110.68
1	A	451	ASP	CA-CB-CG	-6.91	105.69	112.60
1	E	258	ARG	N-CA-C	6.91	118.70	111.03
1	A	448	TRP	N-CA-C	-6.90	101.09	109.72
1	B	165	ILE	N-CA-C	6.89	117.81	108.17
1	C	371	PHE	CA-C-O	-6.89	113.28	120.99
1	C	377	PHE	CA-CB-CG	-6.88	106.92	113.80
1	B	188	LEU	N-CA-CB	-6.88	99.92	110.65
1	A	169	TRP	CB-CG-CD2	-6.87	117.18	126.80
1	F	191	ILE	N-CA-C	6.87	118.02	108.12
1	A	345	CYS	N-CA-C	-6.85	95.86	107.99
1	E	73	PHE	N-CA-C	6.85	119.90	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	451	ASP	CA-CB-CG	-6.85	105.75	112.60
1	B	145	ASP	N-CA-C	6.84	120.41	110.28
1	F	358	PRO	CA-C-N	6.84	129.75	120.38
1	F	358	PRO	C-N-CA	6.84	129.75	120.38
1	D	149	VAL	N-CA-C	6.83	119.87	108.81
1	A	145	ASP	CA-CB-CG	-6.83	105.77	112.60
1	D	393	HIS	CA-C-O	6.83	127.79	120.55
1	F	326	HIS	CA-CB-CG	-6.83	106.97	113.80
1	A	62	VAL	N-CA-C	-6.82	96.93	107.71
1	F	400	LEU	CA-C-N	6.82	129.42	120.28
1	F	400	LEU	C-N-CA	6.82	129.42	120.28
1	D	396	ASN	CA-C-N	6.82	131.04	120.82
1	D	396	ASN	C-N-CA	6.82	131.04	120.82
1	B	35	TYR	CA-CB-CG	-6.81	101.64	113.90
1	E	397	THR	N-CA-CB	-6.81	101.94	111.00
1	A	139	ASP	CA-CB-CG	-6.81	105.79	112.60
1	B	145	ASP	CA-CB-CG	-6.81	105.79	112.60
1	D	269	ASP	CA-CB-CG	-6.80	105.80	112.60
1	C	188	LEU	N-CA-C	6.79	119.97	108.90
1	F	365	ALA	N-CA-C	6.79	120.00	107.99
1	A	420	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	A	109	ARG	CD-NE-CZ	-6.78	114.91	124.40
1	C	399	ILE	N-CA-CB	-6.78	102.61	110.55
1	C	169	TRP	CB-CG-CD2	-6.78	117.31	126.80
1	D	383	THR	CA-C-N	6.76	130.41	120.95
1	D	383	THR	C-N-CA	6.76	130.41	120.95
1	D	25	ASP	N-CA-CB	-6.76	98.83	110.32
1	A	76	LYS	N-CA-C	6.76	120.68	109.46
1	C	141	LYS	N-CA-C	-6.76	99.05	109.52
1	B	103	VAL	N-CA-CB	-6.75	102.65	111.90
1	D	189	GLU	N-CA-CB	-6.75	99.12	110.80
1	D	191	ILE	N-CA-C	6.75	117.83	108.12
1	D	440	ASP	CA-C-O	-6.75	110.92	120.16
1	B	345	CYS	N-CA-CB	6.74	121.14	110.55
1	A	127	ASP	CA-C-N	6.74	134.41	121.54
1	A	127	ASP	C-N-CA	6.74	134.41	121.54
1	D	189	GLU	CB-CG-CD	-6.74	101.14	112.60
1	E	83	PHE	N-CA-C	6.74	120.86	110.42
1	C	373	LEU	N-CA-CB	-6.73	99.06	110.16
1	E	396	ASN	N-CA-C	-6.73	96.47	110.80
1	A	153	GLN	N-CA-CB	-6.72	99.37	109.71
1	A	316	ALA	CA-C-N	6.71	129.58	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ALA	C-N-CA	6.71	129.58	120.38
1	D	151	TYR	CA-C-N	6.71	131.31	121.31
1	D	151	TYR	C-N-CA	6.71	131.31	121.31
1	D	119	GLY	N-CA-C	6.71	119.17	110.45
1	E	39	SER	CA-C-N	6.71	129.57	120.38
1	E	39	SER	C-N-CA	6.71	129.57	120.38
1	B	77	LEU	N-CA-C	-6.70	102.10	108.07
1	C	248	PHE	CA-CB-CG	-6.70	107.10	113.80
1	E	421	PHE	CA-C-N	6.70	134.03	121.97
1	E	421	PHE	C-N-CA	6.70	134.03	121.97
1	B	189	GLU	N-CA-CB	-6.70	99.18	110.83
1	C	256	PHE	CA-CB-CG	-6.69	107.11	113.80
1	B	222	LEU	N-CA-C	6.69	118.57	111.28
1	B	463	PHE	N-CA-C	-6.69	96.28	108.85
1	C	88	ASN	CA-C-N	6.68	129.91	120.28
1	C	88	ASN	C-N-CA	6.68	129.91	120.28
1	E	39	SER	N-CA-CB	6.68	120.63	109.94
1	B	154	THR	N-CA-C	6.68	120.51	108.48
1	E	307	PHE	CA-CB-CG	-6.68	107.12	113.80
1	B	355	VAL	N-CA-C	-6.67	98.77	108.11
1	C	175	CYS	N-CA-C	-6.67	105.43	113.97
1	E	125	LYS	N-CA-CB	6.67	121.33	110.32
1	D	247	PHE	N-CA-C	-6.67	105.18	113.38
1	D	49	TYR	CA-CB-CG	-6.66	101.90	113.90
1	A	88	ASN	CB-CA-C	6.66	122.22	111.36
1	D	369	GLU	N-CA-C	6.65	120.12	108.75
1	F	440	ASP	CB-CA-C	6.64	117.11	110.33
1	C	107	ILE	CB-CA-C	-6.64	104.06	111.23
1	B	26	GLU	N-CA-CB	-6.63	100.39	110.01
1	B	129	THR	N-CA-C	-6.63	104.51	112.59
1	B	332	THR	CB-CA-C	-6.63	98.82	109.75
1	C	395	MET	CB-CA-C	6.62	123.42	111.03
1	C	260	PHE	N-CA-C	6.62	119.72	109.07
1	B	67	ALA	N-CA-C	6.62	124.89	110.80
1	C	430	GLN	N-CA-C	-6.61	98.43	108.67
1	E	268	GLY	N-CA-C	-6.61	106.46	114.66
1	F	260	PHE	CA-CB-CG	-6.61	107.19	113.80
1	B	179	THR	N-CA-CB	6.60	121.65	110.49
1	B	437	VAL	CA-C-N	6.60	133.57	121.70
1	B	437	VAL	C-N-CA	6.60	133.57	121.70
1	C	460	LEU	CA-C-O	6.59	129.93	120.51
1	B	192	ASN	CB-CA-C	-6.59	98.66	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	277	ILE	CB-CA-C	-6.58	102.19	111.21
1	E	314	HIS	CA-C-N	-6.58	110.92	121.58
1	E	314	HIS	C-N-CA	-6.58	110.92	121.58
1	F	102	CYS	N-CA-C	-6.58	98.90	109.96
1	A	68	TYR	CA-CB-CG	-6.58	102.06	113.90
1	B	428	THR	N-CA-C	6.58	119.78	110.50
1	F	26	GLU	N-CA-C	-6.58	104.03	111.14
1	E	371	PHE	N-CA-C	6.58	119.42	109.23
1	E	177	PRO	CA-C-N	6.58	130.68	120.75
1	E	177	PRO	C-N-CA	6.58	130.68	120.75
1	C	344	VAL	CA-C-O	-6.57	114.83	121.59
1	E	430	GLN	N-CA-C	6.56	119.41	109.63
1	E	71	ARG	N-CA-CB	-6.56	99.37	110.46
1	C	369	GLU	N-CA-C	6.56	120.30	108.69
1	C	440	ASP	O-C-N	-6.56	115.46	121.30
1	D	24	THR	CA-C-O	6.55	127.52	119.79
1	E	434	ALA	N-CA-C	6.55	117.96	109.64
1	F	240	ASP	CA-CB-CG	-6.55	106.05	112.60
1	D	24	THR	CA-C-N	6.55	131.08	120.60
1	D	24	THR	C-N-CA	6.55	131.08	120.60
1	D	57	ASN	CA-CB-CG	-6.55	106.05	112.60
1	C	223	ASP	N-CA-CB	-6.55	100.49	110.12
1	C	435	PRO	N-CA-C	6.55	118.69	110.70
1	F	340	THR	N-CA-CB	6.54	119.59	110.17
1	D	394	ASN	CA-CB-CG	-6.54	106.06	112.60
1	B	81	ASN	CA-CB-CG	-6.54	106.06	112.60
1	F	439	GLN	CA-C-O	6.53	127.39	119.49
1	A	61	ASP	N-CA-C	-6.53	98.37	108.42
1	F	120	HIS	CA-CB-CG	-6.53	107.27	113.80
1	B	258	ARG	N-CA-C	6.52	118.26	111.03
1	B	399	ILE	CB-CA-C	-6.52	103.50	112.04
1	D	377	PHE	CA-CB-CG	-6.52	107.28	113.80
1	A	154	THR	N-CA-C	6.50	120.18	108.48
1	D	455	ARG	CA-C-N	6.50	130.56	120.75
1	D	455	ARG	C-N-CA	6.50	130.56	120.75
1	C	39	SER	N-CA-C	6.50	118.87	108.41
1	C	136	SER	CA-C-N	6.50	133.39	121.70
1	C	136	SER	C-N-CA	6.50	133.39	121.70
1	F	25	ASP	CA-CB-CG	-6.49	106.11	112.60
1	A	244	ASP	CA-C-N	6.48	133.92	121.54
1	A	244	ASP	C-N-CA	6.48	133.92	121.54
1	C	419	TYR	CA-CB-CG	-6.47	102.25	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	GLN	CB-CG-CD	-6.46	101.62	112.60
1	A	377	PHE	CA-CB-CG	-6.45	107.35	113.80
1	A	396	ASN	CA-CB-CG	-6.45	106.15	112.60
1	B	235	LEU	CB-CA-C	-6.45	100.08	110.79
1	F	366	ARG	N-CA-C	6.45	119.69	109.50
1	E	367	HIS	CB-CA-C	-6.44	97.16	109.66
1	E	339	SER	N-CA-C	6.44	124.52	110.80
1	F	312	TRP	N-CA-C	-6.44	100.95	110.48
1	B	201	VAL	N-CA-CB	-6.44	104.73	112.07
1	C	345	CYS	N-CA-CB	6.44	120.62	110.84
1	D	379	LEU	N-CA-CB	6.43	119.43	110.17
1	B	91	TYR	N-CA-C	-6.43	97.11	110.80
1	A	256	PHE	CA-CB-CG	-6.42	107.38	113.80
1	B	285	ASN	N-CA-C	-6.42	100.63	110.32
1	E	115	VAL	CA-C-N	6.42	129.83	121.23
1	E	115	VAL	C-N-CA	6.42	129.83	121.23
1	E	332	THR	CB-CA-C	-6.42	99.17	109.75
1	D	164	ALA	N-CA-C	6.41	119.19	110.35
1	E	176	LYS	N-CA-C	-6.40	96.88	109.10
1	A	252	ARG	N-CA-CB	-6.40	100.92	110.71
1	C	294	SER	N-CA-C	6.40	118.89	109.62
1	C	298	SER	CA-C-N	6.39	129.24	120.35
1	C	298	SER	C-N-CA	6.39	129.24	120.35
1	C	312	TRP	N-CA-C	-6.39	99.22	109.96
1	B	391	TYR	N-CA-CB	-6.38	100.75	110.26
1	D	210	PHE	CA-CB-CG	-6.38	107.42	113.80
1	B	333	VAL	CA-C-N	6.38	131.81	122.94
1	B	333	VAL	C-N-CA	6.38	131.81	122.94
1	D	279	GLY	N-CA-C	-6.38	98.07	113.18
1	A	375	PHE	N-CA-C	6.37	119.11	109.23
1	B	426	ALA	O-C-N	-6.37	115.29	122.93
1	A	217	LYS	CB-CA-C	-6.36	102.52	111.80
1	D	231	TYR	O-C-N	-6.36	116.87	121.83
1	B	90	VAL	CA-C-N	6.35	133.66	121.54
1	B	90	VAL	C-N-CA	6.35	133.66	121.54
1	D	469	PHE	N-CA-CB	-6.34	100.77	110.16
1	D	42	LEU	N-CA-CB	-6.34	100.03	110.68
1	D	189	GLU	N-CA-C	6.33	119.46	108.76
1	B	437	VAL	O-C-N	-6.33	116.00	123.03
1	A	367	HIS	CA-C-N	6.33	131.82	122.71
1	A	367	HIS	C-N-CA	6.33	131.82	122.71
1	E	214	GLN	CB-CA-C	-6.33	100.54	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	HIS	CA-C-O	6.33	127.26	120.55
1	E	376	ILE	O-C-N	-6.32	116.60	123.18
1	E	460	LEU	CA-C-O	6.32	125.79	118.77
1	A	253	GLU	O-C-N	-6.32	115.69	123.33
1	A	260	PHE	N-CA-C	6.31	119.75	109.59
1	E	24	THR	CA-C-N	6.31	132.73	120.99
1	E	24	THR	C-N-CA	6.31	132.73	120.99
1	F	273	GLU	CA-C-N	6.30	133.58	121.54
1	F	273	GLU	C-N-CA	6.30	133.58	121.54
1	C	134	VAL	N-CA-C	6.30	122.45	109.34
1	A	202	ASP	N-CA-C	-6.30	101.16	110.48
1	A	438	LYS	N-CA-C	-6.29	104.35	111.14
1	A	398	THR	N-CA-C	6.29	118.21	111.36
1	C	314	HIS	CA-CB-CG	-6.29	107.51	113.80
1	F	387	GLU	N-CA-CB	-6.28	100.63	110.30
1	A	327	ASN	CA-CB-CG	-6.28	106.32	112.60
1	F	209	ASP	CA-CB-CG	-6.27	106.33	112.60
1	F	444	LYS	N-CA-C	-6.27	105.20	112.92
1	D	112	PRO	N-CA-C	-6.27	99.55	112.47
1	B	307	PHE	N-CA-C	6.27	116.27	108.19
1	B	101	ALA	N-CA-C	-6.26	98.18	108.76
1	C	145	ASP	N-CA-C	6.26	117.69	108.86
1	E	294	SER	CB-CA-C	-6.26	99.75	109.08
1	D	363	GLU	N-CA-C	6.25	119.65	109.59
1	D	87	ASP	N-CA-C	6.25	118.10	110.41
1	B	377	PHE	CA-CB-CG	-6.24	107.56	113.80
1	F	448	TRP	CB-CA-C	6.24	117.25	110.08
1	E	327	ASN	CA-CB-CG	-6.24	106.36	112.60
1	A	191	ILE	N-CA-C	6.23	116.84	108.11
1	B	414	SER	CA-C-N	6.23	132.92	121.70
1	B	414	SER	C-N-CA	6.23	132.92	121.70
1	C	296	SER	O-C-N	-6.23	116.66	123.52
1	E	131	ASN	CA-C-N	6.23	133.44	121.54
1	E	131	ASN	C-N-CA	6.23	133.44	121.54
1	C	41	ARG	N-CA-C	6.23	118.64	108.55
1	F	353	PRO	N-CA-C	-6.23	99.64	112.47
1	B	123	TYR	N-CA-C	6.22	119.30	109.96
1	F	345	CYS	N-CA-C	-6.22	98.27	108.41
1	E	223	ASP	CA-CB-CG	-6.22	106.38	112.60
1	E	79	ASP	CA-C-N	6.21	125.90	119.56
1	E	79	ASP	C-N-CA	6.21	125.90	119.56
1	F	165	ILE	CA-C-N	6.19	129.38	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	165	ILE	C-N-CA	6.19	129.38	122.69
1	C	284	ALA	N-CA-C	-6.19	103.85	111.40
1	F	144	ARG	CB-CA-C	6.19	121.51	111.05
1	D	455	ARG	CA-C-O	6.18	126.78	119.48
1	D	257	ALA	N-CA-C	6.18	118.36	108.41
1	F	24	THR	CA-C-N	6.18	130.48	120.60
1	F	24	THR	C-N-CA	6.18	130.48	120.60
1	D	459	ASP	N-CA-C	6.17	118.84	107.73
1	E	468	LYS	CA-C-O	6.17	127.09	120.55
1	D	88	ASN	CA-C-N	6.17	133.32	121.54
1	D	88	ASN	C-N-CA	6.17	133.32	121.54
1	B	446	LYS	N-CA-CB	6.17	119.26	109.51
1	A	72	VAL	CA-C-O	6.17	127.26	120.48
1	D	143	THR	N-CA-C	-6.17	103.83	113.02
1	A	372	ASP	CB-CA-C	-6.17	100.28	110.14
1	D	27	TYR	CA-C-O	6.16	127.29	120.82
1	E	392	ILE	N-CA-CB	-6.16	102.17	110.54
1	C	62	VAL	CB-CA-C	-6.15	104.16	110.13
1	D	370	GLU	N-CA-C	6.15	119.43	109.40
1	B	383	THR	CA-C-N	6.15	129.50	120.82
1	B	383	THR	C-N-CA	6.15	129.50	120.82
1	C	421	PHE	N-CA-C	6.14	123.89	110.80
1	E	420	ARG	CA-C-O	-6.14	114.87	121.56
1	D	428	THR	CA-C-N	6.14	128.51	120.28
1	D	428	THR	C-N-CA	6.14	128.51	120.28
1	E	39	SER	CB-CA-C	-6.14	100.52	110.77
1	A	227	SER	CA-C-N	6.13	131.88	122.25
1	A	227	SER	C-N-CA	6.13	131.88	122.25
1	F	412	THR	N-CA-C	6.13	117.20	108.74
1	A	398	THR	CA-C-N	6.13	128.86	120.46
1	A	398	THR	C-N-CA	6.13	128.86	120.46
1	B	169	TRP	CA-CB-CG	-6.13	101.95	113.60
1	F	327	ASN	CA-CB-CG	-6.13	106.47	112.60
1	B	49	TYR	CB-CA-C	-6.12	100.62	110.79
1	D	72	VAL	N-CA-C	6.12	117.02	107.28
1	C	419	TYR	O-C-N	-6.12	114.12	122.81
1	D	156	LEU	N-CA-C	6.11	118.70	109.23
1	A	56	GLY	O-C-N	-6.10	116.76	123.05
1	C	372	ASP	CB-CA-C	-6.10	100.38	110.14
1	C	327	ASN	CA-CB-CG	-6.10	106.50	112.60
1	D	442	TYR	N-CA-C	-6.10	103.27	111.87
1	C	33	ILE	CB-CA-C	-6.09	103.59	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	VAL	N-CA-CB	6.09	121.28	111.23
1	B	451	ASP	N-CA-CB	6.09	120.41	110.17
1	F	189	GLU	CB-CA-C	6.09	121.00	109.37
1	E	136	SER	O-C-N	-6.09	115.80	122.07
1	F	72	VAL	CA-C-O	6.09	127.18	120.48
1	F	380	CYS	CA-CB-SG	-6.08	100.41	114.40
1	D	364	TYR	N-CA-C	6.08	119.11	109.50
1	A	440	ASP	CB-CA-C	6.08	116.78	109.85
1	D	345	CYS	N-CA-C	-6.08	98.50	108.41
1	D	351	SER	N-CA-C	-6.08	102.92	108.75
1	B	460	LEU	CA-C-O	6.07	125.47	118.55
1	E	49	TYR	CA-CB-CG	-6.06	102.99	113.90
1	E	233	ASP	N-CA-C	6.06	118.66	107.99
1	D	373	LEU	CB-CA-C	6.05	119.86	109.51
1	F	193	THR	O-C-N	-6.05	115.58	121.94
1	C	378	GLN	CB-CA-C	-6.05	101.48	110.62
1	B	365	ALA	N-CA-C	6.05	118.61	108.02
1	F	93	PRO	N-CA-C	-6.05	99.77	111.69
1	F	384	LEU	N-CA-CB	-6.05	100.38	110.42
1	F	257	ALA	N-CA-C	6.05	118.15	108.41
1	C	372	ASP	N-CA-C	6.04	118.25	108.34
1	F	228	ILE	N-CA-CB	6.04	121.20	111.23
1	B	75	VAL	N-CA-C	6.04	116.51	107.51
1	C	144	ARG	N-CA-CB	-6.04	100.28	110.49
1	A	471	LEU	N-CA-CB	-6.04	101.24	110.12
1	A	373	LEU	CA-C-O	-6.04	113.98	120.92
1	B	68	TYR	CA-CB-CG	-6.04	103.03	113.90
1	C	294	SER	CB-CA-C	-6.04	101.88	109.31
1	C	51	LYS	N-CA-C	-6.04	100.72	110.32
1	D	169	TRP	CB-CG-CD2	-6.02	118.37	126.80
1	A	273	GLU	CA-C-N	6.02	133.04	121.54
1	A	273	GLU	C-N-CA	6.02	133.04	121.54
1	B	339	SER	N-CA-C	6.02	123.62	110.80
1	F	17	SER	CA-C-N	6.02	132.81	121.97
1	F	17	SER	C-N-CA	6.02	132.81	121.97
1	A	458	ALA	N-CA-C	-6.02	103.65	111.71
1	A	98	LEU	N-CA-C	6.01	119.27	109.59
1	A	312	TRP	N-CA-C	-6.01	99.86	109.96
1	D	314	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	B	379	LEU	N-CA-CB	-6.01	101.21	110.04
1	C	371	PHE	CA-C-N	6.00	131.24	122.77
1	C	371	PHE	C-N-CA	6.00	131.24	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	187	PRO	CA-C-O	-6.00	114.67	122.12
1	B	34	PHE	CA-CB-CG	-6.00	107.80	113.80
1	D	468	LYS	CB-CA-C	-6.00	100.48	110.68
1	D	326	HIS	CA-CB-CG	-6.00	107.80	113.80
1	D	227	SER	N-CA-C	5.99	123.57	110.80
1	A	273	GLU	CB-CG-CD	-5.99	102.41	112.60
1	A	254	GLN	N-CA-C	5.99	118.39	108.99
1	F	383	THR	N-CA-CB	5.99	119.63	109.87
1	E	188	LEU	N-CA-CB	-5.99	101.31	110.65
1	A	392	ILE	CB-CA-C	-5.98	102.89	112.16
1	B	279	GLY	N-CA-C	-5.98	102.88	111.20
1	E	363	GLU	N-CA-C	5.98	119.22	109.59
1	B	94	ASN	N-CA-C	-5.98	105.64	113.17
1	B	340	THR	N-CA-C	5.97	117.93	108.79
1	D	109	ARG	CD-NE-CZ	-5.97	116.04	124.40
1	F	174	ALA	CA-C-N	5.97	128.56	120.38
1	F	174	ALA	C-N-CA	5.97	128.56	120.38
1	A	219	GLU	CA-C-O	5.97	123.17	119.77
1	A	21	VAL	CA-C-N	5.96	128.19	120.56
1	A	21	VAL	C-N-CA	5.96	128.19	120.56
1	B	442	TYR	CA-C-N	5.96	128.86	120.28
1	B	442	TYR	C-N-CA	5.96	128.86	120.28
1	A	343	SER	N-CA-C	5.96	118.39	108.20
1	C	442	TYR	CA-C-O	5.96	126.64	119.43
1	F	408	THR	N-CA-CB	5.95	119.81	109.57
1	C	249	CYS	N-CA-CB	-5.95	100.36	111.13
1	C	250	LEU	N-CA-C	5.95	118.92	108.75
1	B	191	ILE	N-CA-CB	-5.94	103.21	111.41
1	A	42	LEU	CA-C-O	-5.93	114.42	120.71
1	C	52	VAL	N-CA-C	-5.93	101.68	107.55
1	D	217	LYS	CB-CA-C	-5.93	103.14	111.80
1	A	88	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	D	129	THR	N-CA-C	-5.93	105.96	112.72
1	D	243	GLY	CA-C-O	5.92	125.70	119.06
1	F	426	ALA	N-CA-C	-5.92	103.12	110.41
1	D	405	PHE	CA-CB-CG	-5.92	107.88	113.80
1	C	216	ASN	CA-CB-CG	-5.92	106.68	112.60
1	E	71	ARG	CD-NE-CZ	-5.92	116.11	124.40
1	E	187	PRO	CB-CA-C	5.92	118.77	110.60
1	F	168	HIS	CB-CG-CD2	-5.92	123.51	131.20
1	F	189	GLU	CB-CG-CD	5.92	122.66	112.60
1	B	461	ASP	CA-C-N	5.91	131.66	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	461	ASP	C-N-CA	5.91	131.66	122.26
1	D	391	TYR	O-C-N	-5.91	115.46	122.20
1	E	432	ASP	CA-C-N	5.91	132.33	121.70
1	E	432	ASP	C-N-CA	5.91	132.33	121.70
1	F	39	SER	N-CA-C	5.91	117.83	108.67
1	F	393	HIS	CB-CA-C	-5.91	100.98	110.79
1	F	125	LYS	N-CA-C	-5.91	98.22	110.80
1	E	122	LEU	N-CA-C	-5.90	106.71	112.97
1	F	99	VAL	N-CA-C	5.90	116.14	108.35
1	F	168	HIS	CA-CB-CG	-5.90	107.90	113.80
1	F	403	TRP	CB-CG-CD2	-5.90	118.54	126.80
1	D	375	PHE	CA-CB-CG	-5.89	107.91	113.80
1	E	145	ASP	CA-CB-CG	-5.89	106.71	112.60
1	C	321	ASN	CA-CB-CG	-5.89	106.71	112.60
1	A	460	LEU	CA-C-O	5.89	127.00	120.82
1	A	179	THR	N-CA-C	-5.89	101.21	109.69
1	F	49	TYR	N-CA-C	5.88	118.47	111.71
1	B	42	LEU	CA-C-N	-5.88	112.26	122.37
1	B	42	LEU	C-N-CA	-5.88	112.26	122.37
1	B	369	GLU	N-CA-C	5.88	119.05	109.06
1	C	404	ASN	CB-CA-C	5.88	119.74	111.86
1	B	271	LEU	N-CA-C	5.88	121.41	109.60
1	E	454	GLU	N-CA-C	-5.87	106.45	113.97
1	A	146	ASN	N-CA-C	5.87	117.86	108.41
1	C	396	ASN	CA-CB-CG	-5.87	106.73	112.60
1	F	183	GLY	N-CA-C	-5.87	103.84	114.46
1	C	420	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	A	111	GLN	N-CA-C	5.86	122.75	109.81
1	A	234	TYR	CB-CA-C	-5.86	101.07	110.79
1	D	312	TRP	N-CA-C	-5.86	100.12	109.96
1	B	201	VAL	N-CA-C	5.86	117.54	109.46
1	C	106	GLU	N-CA-CB	5.85	119.74	110.84
1	E	260	PHE	CA-CB-CG	-5.85	107.95	113.80
1	B	204	GLY	N-CA-C	-5.85	99.32	113.18
1	B	426	ALA	N-CA-C	-5.85	99.00	108.41
1	B	261	TRP	CB-CG-CD2	-5.85	118.61	126.80
1	A	340	THR	N-CA-C	5.84	118.74	108.75
1	B	393	HIS	CA-C-O	5.84	126.74	120.55
1	C	122	LEU	N-CA-C	-5.84	103.63	111.87
1	B	367	HIS	N-CA-CB	-5.84	101.09	111.08
1	B	463	PHE	CB-CA-C	5.84	117.95	110.13
1	A	370	GLU	N-CA-C	5.84	118.91	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	378	GLN	CA-C-O	5.83	126.42	120.24
1	D	218	SER	N-CA-C	-5.83	103.87	113.50
1	D	409	PRO	N-CA-CB	-5.83	97.42	103.08
1	F	261	TRP	CB-CG-CD2	-5.83	118.63	126.80
1	E	472	GLN	CB-CG-CD	-5.83	102.69	112.60
1	D	424	SER	CA-C-N	5.83	132.19	121.70
1	D	424	SER	C-N-CA	5.83	132.19	121.70
1	E	227	SER	CA-C-N	5.83	132.46	121.97
1	E	227	SER	C-N-CA	5.83	132.46	121.97
1	A	202	ASP	CA-C-N	5.83	131.38	122.23
1	A	202	ASP	C-N-CA	5.83	131.38	122.23
1	D	368	VAL	N-CA-C	5.83	117.07	108.45
1	D	338	ARG	N-CA-C	-5.82	101.40	110.42
1	F	209	ASP	CA-C-N	5.82	132.66	121.54
1	F	209	ASP	C-N-CA	5.82	132.66	121.54
1	C	250	LEU	CB-CA-C	-5.82	98.16	109.68
1	A	193	THR	O-C-N	-5.81	117.75	121.88
1	F	397	THR	CA-C-N	-5.81	111.47	120.31
1	F	397	THR	C-N-CA	-5.81	111.47	120.31
1	A	144	ARG	CG-CD-NE	-5.81	99.22	112.00
1	A	226	GLN	N-CA-C	-5.81	103.33	110.65
1	D	357	THR	N-CA-C	-5.81	98.82	108.23
1	D	327	ASN	CA-CB-CG	-5.80	106.80	112.60
1	E	395	MET	CB-CA-C	-5.80	100.99	110.85
1	F	106	GLU	N-CA-CB	5.80	119.65	110.84
1	A	437	VAL	N-CA-C	5.79	121.39	109.34
1	C	372	ASP	N-CA-CB	5.79	119.86	110.77
1	E	376	ILE	N-CA-C	5.79	116.34	107.77
1	D	334	VAL	CA-C-N	5.79	131.62	122.36
1	D	334	VAL	C-N-CA	5.79	131.62	122.36
1	F	263	ARG	N-CA-CB	5.79	119.54	109.18
1	B	312	TRP	N-CA-C	-5.79	100.24	109.96
1	C	233	ASP	N-CA-CB	5.79	118.91	110.58
1	E	382	ILE	CA-C-N	-5.79	113.23	121.50
1	E	382	ILE	C-N-CA	-5.79	113.23	121.50
1	A	310	PRO	CA-C-N	-5.78	114.63	123.07
1	A	310	PRO	C-N-CA	-5.78	114.63	123.07
1	F	61	ASP	N-CA-CB	-5.78	102.56	111.46
1	D	468	LYS	CA-C-O	5.78	126.87	120.63
1	F	325	TRP	CB-CA-C	-5.78	100.13	109.72
1	A	22	VAL	N-CA-CB	-5.77	103.18	110.57
1	B	72	VAL	CA-C-O	5.77	126.83	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	82	LYS	CB-CA-C	-5.77	101.73	111.02
1	F	214	GLN	CA-C-N	5.77	128.32	120.54
1	F	214	GLN	C-N-CA	5.77	128.32	120.54
1	B	469	PHE	CA-CB-CG	-5.77	108.03	113.80
1	B	414	SER	O-C-N	-5.76	115.72	122.81
1	C	34	PHE	CA-CB-CG	-5.76	108.03	113.80
1	F	423	GLN	CB-CA-C	-5.76	101.79	110.90
1	C	67	ALA	N-CA-C	5.76	123.07	110.80
1	C	110	GLY	N-CA-C	5.76	126.83	113.18
1	C	455	ARG	NE-CZ-NH1	5.76	127.26	121.50
1	A	396	ASN	CA-C-N	5.75	130.33	120.72
1	A	396	ASN	C-N-CA	5.75	130.33	120.72
1	A	41	ARG	N-CA-CB	5.75	120.21	110.49
1	F	176	LYS	N-CA-C	-5.75	100.30	109.04
1	C	386	THR	N-CA-C	5.75	117.55	111.28
1	D	189	GLU	O-C-N	-5.74	116.59	123.31
1	E	233	ASP	CA-CB-CG	-5.74	106.86	112.60
1	A	375	PHE	CB-CA-C	-5.74	96.81	109.56
1	B	376	ILE	CB-CA-C	-5.74	103.90	110.73
1	D	174	ALA	CA-C-N	5.74	132.50	121.54
1	D	174	ALA	C-N-CA	5.74	132.50	121.54
1	F	416	VAL	CA-C-N	5.74	132.50	121.54
1	F	416	VAL	C-N-CA	5.74	132.50	121.54
1	D	39	SER	O-C-N	-5.73	116.05	122.93
1	D	460	LEU	CA-C-N	5.73	132.49	121.54
1	D	460	LEU	C-N-CA	5.73	132.49	121.54
1	C	257	ALA	N-CA-C	5.72	118.06	108.96
1	D	152	LYS	N-CA-C	5.72	118.35	110.35
1	A	469	PHE	CA-C-O	5.71	126.48	120.42
1	E	262	ASN	CA-CB-CG	-5.71	106.89	112.60
1	F	355	VAL	N-CA-C	-5.71	99.32	107.77
1	B	26	GLU	N-CA-C	-5.70	104.97	111.07
1	C	430	GLN	CA-C-N	5.70	133.48	121.91
1	C	430	GLN	C-N-CA	5.70	133.48	121.91
1	E	144	ARG	N-CA-C	5.70	122.94	110.80
1	A	379	LEU	CA-C-O	-5.70	114.78	121.16
1	B	211	LYS	CA-C-N	5.70	129.37	120.82
1	B	211	LYS	C-N-CA	5.70	129.37	120.82
1	C	262	ASN	N-CA-C	-5.70	100.50	109.50
1	D	168	HIS	CB-CG-CD2	-5.70	123.80	131.20
1	E	448	TRP	CB-CG-CD2	-5.70	118.83	126.80
1	F	256	PHE	O-C-N	-5.70	116.76	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	THR	N-CA-C	5.69	122.92	110.80
1	D	333	VAL	N-CA-C	5.69	116.56	108.42
1	D	395	MET	CG-SD-CE	-5.69	88.38	100.90
1	F	460	LEU	N-CA-CB	-5.69	103.47	110.98
1	A	372	ASP	N-CA-CB	5.69	119.70	110.77
1	B	25	ASP	CA-C-O	5.68	126.26	119.10
1	D	421	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	65	VAL	N-CA-CB	5.68	120.60	111.23
1	C	368	VAL	N-CA-CB	-5.68	102.13	111.44
1	A	236	GLN	N-CA-C	-5.67	105.18	111.36
1	B	190	LEU	CB-CA-C	-5.67	100.50	109.80
1	B	445	LEU	N-CA-CB	-5.67	101.69	111.55
1	E	372	ASP	CA-C-O	5.67	128.40	120.52
1	D	288	SER	N-CA-C	5.67	118.45	110.23
1	A	311	TYR	CA-CB-CG	-5.66	103.71	113.90
1	A	372	ASP	N-CA-C	5.66	117.62	108.34
1	C	424	SER	N-CA-CB	5.66	120.06	110.49
1	D	346	ALA	O-C-N	-5.66	116.56	123.30
1	C	383	THR	N-CA-CB	5.65	118.98	109.94
1	E	257	ALA	O-C-N	-5.65	116.15	122.93
1	E	380	CYS	N-CA-C	-5.65	100.58	109.50
1	A	341	ASN	N-CA-C	-5.64	100.50	109.59
1	D	462	GLN	N-CA-C	-5.64	105.98	112.92
1	E	208	MET	CG-SD-CE	-5.64	88.49	100.90
1	E	198	GLY	N-CA-C	-5.63	107.87	115.36
1	E	69	GLN	N-CA-C	-5.63	100.61	109.50
1	D	41	ARG	CA-C-N	-5.63	115.05	122.99
1	D	41	ARG	C-N-CA	-5.63	115.05	122.99
1	B	49	TYR	N-CA-CB	5.62	118.39	110.12
1	C	395	MET	CB-CG-SD	-5.62	95.83	112.70
1	F	342	LEU	CA-C-N	5.62	130.15	122.84
1	F	342	LEU	C-N-CA	5.62	130.15	122.84
1	D	146	ASN	CA-CB-CG	-5.61	106.99	112.60
1	D	194	PRO	N-CA-C	-5.61	100.91	112.47
1	E	446	LYS	N-CA-C	5.61	118.70	109.72
1	C	261	TRP	CA-CB-CG	-5.60	102.95	113.60
1	C	129	THR	N-CA-C	-5.60	105.79	113.30
1	C	470	LEU	CA-C-O	5.60	126.49	120.55
1	A	314	HIS	N-CA-C	-5.60	98.87	110.80
1	F	12	TYR	CA-C-N	5.60	131.77	121.70
1	F	12	TYR	C-N-CA	5.60	131.77	121.70
1	B	396	ASN	CA-C-O	5.59	126.53	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	105	VAL	N-CA-C	5.59	115.93	108.27
1	A	389	MET	CB-CA-C	-5.59	101.35	110.85
1	C	233	ASP	CA-CB-CG	-5.59	107.01	112.60
1	D	27	TYR	CA-C-N	5.59	128.12	120.35
1	D	27	TYR	C-N-CA	5.59	128.12	120.35
1	F	69	GLN	CA-C-N	5.59	128.64	120.71
1	F	69	GLN	C-N-CA	5.59	128.64	120.71
1	D	26	GLU	N-CA-C	-5.58	105.11	111.14
1	D	58	GLY	O-C-N	-5.58	115.44	122.70
1	E	334	VAL	N-CA-C	5.58	116.71	108.45
1	F	431	LYS	N-CA-C	-5.58	98.91	110.80
1	A	439	GLN	N-CA-CB	5.58	119.92	110.49
1	C	429	CYS	N-CA-CB	5.58	118.70	110.33
1	F	466	GLY	N-CA-C	-5.58	106.04	112.73
1	B	49	TYR	CA-CB-CG	-5.58	103.86	113.90
1	B	378	GLN	CA-C-N	5.58	129.17	120.75
1	B	378	GLN	C-N-CA	5.58	129.17	120.75
1	A	451	ASP	N-CA-C	-5.57	100.88	109.52
1	A	62	VAL	CA-C-O	-5.57	115.19	119.98
1	A	461	ASP	N-CA-CB	-5.57	100.70	109.78
1	D	461	ASP	N-CA-CB	-5.57	101.08	110.49
1	F	422	VAL	CA-C-N	-5.57	112.87	120.44
1	F	422	VAL	C-N-CA	-5.57	112.87	120.44
1	D	229	CYS	N-CA-C	5.57	117.80	108.73
1	D	291	TYR	CA-CB-CG	-5.57	103.88	113.90
1	D	256	PHE	O-C-N	-5.57	116.91	123.25
1	A	187	PRO	N-CA-C	-5.56	101.77	112.01
1	B	323	ILE	CA-C-N	5.56	130.44	122.21
1	B	323	ILE	C-N-CA	5.56	130.44	122.21
1	F	69	GLN	N-CA-C	-5.56	99.95	109.24
1	F	399	ILE	CA-C-O	5.56	126.73	120.95
1	C	459	ASP	CA-C-N	5.56	132.16	121.54
1	C	459	ASP	C-N-CA	5.56	132.16	121.54
1	E	40	SER	N-CA-C	5.56	118.06	111.33
1	E	462	GLN	CA-CB-CG	-5.56	102.98	114.10
1	E	469	PHE	CA-C-O	5.56	126.31	120.42
1	C	34	PHE	N-CA-C	5.56	118.28	109.50
1	B	270	GLN	CA-C-N	5.55	133.68	121.63
1	B	270	GLN	C-N-CA	5.55	133.68	121.63
1	F	420	ARG	N-CA-C	5.55	122.63	110.80
1	E	338	ARG	CA-C-N	5.55	132.15	121.54
1	E	338	ARG	C-N-CA	5.55	132.15	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	185	CYS	N-CA-C	-5.55	102.63	110.29
1	D	296	SER	O-C-N	-5.55	117.41	123.52
1	D	453	LYS	N-CA-C	5.55	122.62	110.80
1	E	31	THR	CA-C-N	5.55	131.67	122.73
1	E	31	THR	C-N-CA	5.55	131.67	122.73
1	A	275	LEU	N-CA-C	-5.55	106.50	113.72
1	F	260	PHE	N-CA-C	5.54	118.52	109.59
1	C	61	ASP	N-CA-C	-5.54	99.72	108.14
1	F	367	HIS	N-CA-CB	5.54	120.18	111.20
1	F	381	LYS	N-CA-C	-5.54	101.56	110.14
1	A	91	TYR	N-CA-C	5.54	117.51	108.76
1	A	428	THR	N-CA-C	-5.53	98.53	108.48
1	D	40	SER	CA-C-O	-5.52	112.61	120.51
1	E	45	VAL	O-C-N	-5.52	116.70	123.00
1	F	56	GLY	O-C-N	-5.52	115.53	122.70
1	B	232	PRO	CB-CA-C	-5.51	104.54	111.71
1	F	455	ARG	N-CA-C	-5.51	105.87	112.59
1	B	181	VAL	CB-CA-C	-5.51	102.98	111.08
1	C	83	PHE	N-CA-C	-5.51	102.73	110.50
1	B	24	THR	CA-C-N	5.51	131.23	120.99
1	B	24	THR	C-N-CA	5.51	131.23	120.99
1	E	128	ASP	N-CA-CB	-5.51	101.18	110.49
1	F	463	PHE	N-CA-C	-5.50	98.50	108.85
1	A	79	ASP	CA-CB-CG	-5.50	107.10	112.60
1	C	138	VAL	N-CA-C	5.50	120.79	109.34
1	F	451	ASP	N-CA-CB	5.50	118.84	109.87
1	A	416	VAL	CA-C-N	5.50	132.05	121.54
1	A	416	VAL	C-N-CA	5.50	132.05	121.54
1	E	411	PRO	CA-C-N	5.50	131.60	121.70
1	E	411	PRO	C-N-CA	5.50	131.60	121.70
1	E	37	ALA	N-CA-C	-5.50	100.36	108.99
1	B	96	GLN	CB-CG-CD	-5.50	103.26	112.60
1	F	202	ASP	CA-CB-CG	-5.50	107.10	112.60
1	A	85	LEU	N-CA-CB	5.50	120.15	110.37
1	C	145	ASP	CA-CB-CG	-5.50	107.11	112.60
1	E	33	ILE	CA-C-N	-5.49	113.83	122.73
1	E	33	ILE	C-N-CA	-5.49	113.83	122.73
1	E	193	THR	CA-C-N	5.49	125.42	119.76
1	E	193	THR	C-N-CA	5.49	125.42	119.76
1	A	297	GLY	N-CA-C	5.49	120.43	113.24
1	B	58	GLY	CA-C-N	5.49	131.58	121.70
1	B	58	GLY	C-N-CA	5.49	131.58	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	152	LYS	N-CA-C	5.49	122.48	110.80
1	A	342	LEU	CA-C-N	5.48	129.97	122.84
1	A	342	LEU	C-N-CA	5.48	129.97	122.84
1	E	209	ASP	CA-C-O	5.48	126.41	120.43
1	D	52	VAL	O-C-N	-5.48	117.66	121.55
1	F	186	PRO	N-CA-C	5.48	117.38	110.70
1	C	258	ARG	N-CA-CB	-5.47	102.04	109.98
1	D	250	LEU	CB-CA-C	-5.47	100.50	109.80
1	B	237	MET	CB-CA-C	5.47	121.73	110.31
1	C	169	TRP	CA-CB-CG	-5.47	103.22	113.60
1	B	404	ASN	CA-C-N	5.46	128.36	120.38
1	B	404	ASN	C-N-CA	5.46	128.36	120.38
1	B	41	ARG	N-CA-C	-5.46	99.17	110.80
1	B	418	THR	CB-CA-C	-5.46	99.55	110.42
1	E	169	TRP	CA-CB-CG	-5.46	103.22	113.60
1	E	378	GLN	CA-C-N	5.46	129.00	120.75
1	E	378	GLN	C-N-CA	5.46	129.00	120.75
1	B	425	ALA	N-CA-CB	5.46	117.93	110.01
1	E	109	ARG	CD-NE-CZ	-5.46	116.75	124.40
1	E	202	ASP	CA-CB-CG	-5.46	107.14	112.60
1	B	262	ASN	CB-CA-C	5.46	120.79	109.38
1	F	388	VAL	CA-CB-CG1	5.45	119.67	110.40
1	C	398	THR	CA-C-O	5.45	126.23	119.97
1	A	377	PHE	CB-CA-C	-5.45	99.91	109.71
1	A	398	THR	CB-CA-C	-5.45	101.59	110.85
1	B	178	THR	N-CA-C	-5.45	105.80	113.20
1	D	261	TRP	CA-CB-CG	-5.45	103.25	113.60
1	D	364	TYR	CA-C-N	5.45	130.67	123.05
1	D	364	TYR	C-N-CA	5.45	130.67	123.05
1	A	369	GLU	N-CA-C	5.44	118.33	108.69
1	D	161	CYS	N-CA-C	-5.44	105.86	112.88
1	E	238	SER	N-CA-C	-5.44	105.65	114.09
1	E	66	SER	O-C-N	-5.44	117.18	123.33
1	F	404	ASN	O-C-N	-5.44	115.57	122.43
1	F	299	VAL	N-CA-C	5.44	120.65	109.34
1	C	333	VAL	N-CA-C	5.44	116.19	108.42
1	D	419	TYR	CA-C-N	5.44	131.49	121.70
1	D	419	TYR	C-N-CA	5.44	131.49	121.70
1	F	213	LEU	N-CA-CB	-5.44	102.43	110.53
1	D	303	ASP	CA-C-O	5.43	126.31	120.55
1	B	83	PHE	CA-CB-CG	-5.43	108.37	113.80
1	C	226	GLN	CA-C-N	5.43	131.91	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	226	GLN	C-N-CA	5.43	131.91	121.54
1	D	356	TYR	N-CA-C	5.43	117.70	110.53
1	B	151	TYR	CA-C-N	5.43	131.91	121.54
1	B	151	TYR	C-N-CA	5.43	131.91	121.54
1	E	222	LEU	CA-C-O	5.43	126.30	120.55
1	C	50	PHE	N-CA-C	-5.42	100.23	107.88
1	A	326	HIS	CB-CA-C	-5.42	102.52	111.36
1	E	424	SER	N-CA-CB	5.42	117.63	109.34
1	B	445	LEU	CA-C-N	5.42	129.03	121.02
1	B	445	LEU	C-N-CA	5.42	129.03	121.02
1	E	345	CYS	N-CA-C	-5.41	98.55	108.02
1	F	35	TYR	CA-C-N	5.41	131.58	122.87
1	F	35	TYR	C-N-CA	5.41	131.58	122.87
1	F	194	PRO	N-CA-C	5.41	119.36	111.03
1	D	98	LEU	N-CA-C	-5.41	100.89	109.76
1	A	69	GLN	CA-C-N	5.41	128.45	120.82
1	A	69	GLN	C-N-CA	5.41	128.45	120.82
1	F	136	SER	N-CA-C	5.41	118.09	110.14
1	F	277	ILE	N-CA-CB	5.41	116.43	110.53
1	C	383	THR	CB-CA-C	-5.41	101.74	110.77
1	F	73	PHE	CB-CA-C	5.40	118.94	110.19
1	C	359	THR	N-CA-C	-5.40	105.55	111.82
1	A	421	PHE	CA-C-N	5.40	131.69	121.97
1	A	421	PHE	C-N-CA	5.40	131.69	121.97
1	D	43	LEU	CA-C-O	5.40	127.33	121.06
1	D	213	LEU	N-CA-CB	-5.40	102.59	110.53
1	F	42	LEU	N-CA-CB	-5.40	101.61	110.68
1	C	157	CYS	N-CA-CB	5.39	120.89	111.13
1	E	27	TYR	N-CA-C	-5.39	106.71	113.72
1	E	460	LEU	N-CA-CB	-5.39	103.72	110.90
1	F	189	GLU	N-CA-C	5.39	118.19	109.40
1	A	357	THR	CA-C-N	5.39	125.20	119.28
1	A	357	THR	C-N-CA	5.39	125.20	119.28
1	B	376	ILE	O-C-N	-5.39	117.81	123.03
1	F	62	VAL	N-CA-C	-5.39	101.59	107.73
1	A	169	TRP	N-CA-C	5.38	118.70	110.36
1	E	30	ARG	N-CA-C	5.38	117.82	110.55
1	E	364	TYR	N-CA-C	5.38	118.01	109.50
1	C	206	GLY	CA-C-N	5.38	131.82	121.54
1	C	206	GLY	C-N-CA	5.38	131.82	121.54
1	B	314	HIS	N-CA-C	-5.38	106.65	113.43
1	E	247	PHE	N-CA-C	-5.38	107.37	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	45	VAL	N-CA-C	5.38	117.52	108.81
1	A	58	GLY	CA-C-N	5.38	131.38	121.70
1	A	58	GLY	C-N-CA	5.38	131.38	121.70
1	C	351	SER	N-CA-C	-5.38	101.95	109.69
1	C	25	ASP	N-CA-C	-5.36	105.84	112.38
1	D	42	LEU	N-CA-C	5.36	117.64	108.90
1	E	296	SER	N-CA-C	5.36	116.56	108.46
1	E	394	ASN	CB-CA-C	-5.36	99.10	110.31
1	B	411	PRO	N-CA-C	-5.36	101.43	112.47
1	D	277	ILE	N-CA-CB	5.36	117.95	110.56
1	C	414	SER	N-CA-CB	5.35	119.60	110.50
1	C	427	VAL	CB-CA-C	-5.35	104.16	111.33
1	E	164	ALA	CA-C-N	5.35	130.00	123.10
1	E	164	ALA	C-N-CA	5.35	130.00	123.10
1	C	471	LEU	N-CA-CB	-5.35	102.25	110.12
1	A	223	ASP	CA-CB-CG	-5.35	107.25	112.60
1	A	470	LEU	CA-C-O	5.35	126.22	120.55
1	A	213	LEU	N-CA-C	5.34	117.11	111.28
1	F	203	THR	CB-CA-C	-5.34	99.46	109.72
1	B	41	ARG	NE-CZ-NH1	5.34	126.84	121.50
1	F	66	SER	N-CA-C	-5.34	99.43	110.80
1	B	144	ARG	CB-CG-CD	5.34	123.58	111.30
1	D	243	GLY	CA-C-N	5.34	127.43	120.28
1	D	243	GLY	C-N-CA	5.34	127.43	120.28
1	F	169	TRP	N-CA-CB	-5.33	101.72	110.52
1	C	374	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	D	42	LEU	CA-C-N	5.33	131.08	122.29
1	D	42	LEU	C-N-CA	5.33	131.08	122.29
1	D	444	LYS	N-CA-C	-5.33	106.62	113.01
1	C	36	HIS	N-CA-C	-5.33	101.20	109.72
1	B	41	ARG	CA-C-N	-5.33	115.48	122.99
1	B	41	ARG	C-N-CA	-5.33	115.48	122.99
1	C	135	ALA	O-C-N	-5.33	117.41	123.48
1	D	417	ASP	CA-C-O	5.33	126.39	119.95
1	F	77	LEU	O-C-N	-5.33	116.82	121.35
1	F	165	ILE	CB-CA-C	-5.33	102.89	110.83
1	F	377	PHE	CA-CB-CG	-5.33	108.47	113.80
1	F	370	GLU	N-CA-C	5.32	118.08	109.40
1	E	68	TYR	N-CA-C	-5.32	104.07	110.88
1	F	274	SER	CA-C-N	5.32	131.70	121.54
1	F	274	SER	C-N-CA	5.32	131.70	121.54
1	E	154	THR	N-CA-C	5.32	118.06	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ASN	N-CA-C	-5.32	106.37	112.86
1	A	462	GLN	CB-CG-CD	5.32	121.64	112.60
1	A	403	TRP	CB-CG-CD1	5.32	134.87	126.90
1	C	337	THR	CA-C-O	5.31	126.17	120.70
1	A	81	ASN	N-CA-C	-5.31	101.99	109.96
1	C	92	ASP	N-CA-C	-5.31	98.08	109.81
1	F	247	PHE	N-CA-C	-5.31	106.19	113.30
1	E	412	THR	N-CA-CB	5.31	120.52	111.50
1	F	343	SER	CA-C-O	5.31	126.06	120.54
1	F	446	LYS	CB-CA-C	-5.31	101.40	109.89
1	C	233	ASP	N-CA-C	5.31	117.75	108.52
1	B	243	GLY	CA-C-O	5.30	124.86	118.97
1	C	434	ALA	N-CA-C	5.30	118.46	109.87
1	A	455	ARG	CA-C-N	5.30	131.67	121.54
1	A	455	ARG	C-N-CA	5.30	131.67	121.54
1	D	234	TYR	CB-CA-C	-5.30	100.82	110.63
1	E	79	ASP	N-CA-CB	5.30	119.81	110.37
1	A	440	ASP	N-CA-C	-5.30	100.99	109.04
1	D	29	THR	CB-CA-C	-5.30	102.21	110.74
1	E	319	LEU	CA-C-O	5.30	126.04	119.79
1	F	137	ALA	N-CA-C	5.30	115.53	108.38
1	F	363	GLU	CB-CG-CD	5.29	121.60	112.60
1	E	193	THR	N-CA-C	5.29	117.77	108.82
1	C	269	ASP	CA-CB-CG	-5.29	107.31	112.60
1	B	162	VAL	N-CA-CB	-5.28	103.81	111.21
1	B	217	LYS	CB-CA-C	-5.28	104.39	111.89
1	A	100	TRP	CB-CG-CD2	-5.28	119.41	126.80
1	A	307	PHE	N-CA-C	5.28	117.88	110.23
1	F	15	PRO	N-CA-C	5.28	117.14	110.70
1	B	91	TYR	CB-CG-CD2	-5.28	112.89	120.80
1	D	229	CYS	CA-CB-SG	-5.28	102.26	114.40
1	D	60	GLN	CA-C-N	5.27	131.90	122.09
1	D	60	GLN	C-N-CA	5.27	131.90	122.09
1	F	14	PRO	CA-C-N	5.27	125.81	120.38
1	F	14	PRO	C-N-CA	5.27	125.81	120.38
1	C	154	THR	CA-C-N	5.27	130.43	123.00
1	C	154	THR	C-N-CA	5.27	130.43	123.00
1	E	169	TRP	CB-CG-CD1	5.27	134.80	126.90
1	F	209	ASP	N-CA-C	5.27	117.31	107.99
1	B	260	PHE	N-CA-CB	5.26	119.16	110.69
1	E	325	TRP	CA-CB-CG	-5.26	103.60	113.60
1	F	240	ASP	CA-C-N	5.26	127.86	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	240	ASP	C-N-CA	5.26	127.86	120.28
1	F	253	GLU	N-CA-C	5.26	118.01	109.06
1	A	33	ILE	CA-C-O	-5.26	114.85	120.85
1	A	309	LYS	O-C-N	-5.26	117.07	121.54
1	C	91	TYR	CB-CG-CD2	-5.26	112.91	120.80
1	A	70	TYR	CB-CA-C	5.26	118.10	109.90
1	C	155	GLN	CB-CA-C	-5.26	101.44	110.16
1	C	405	PHE	N-CA-C	-5.26	101.19	109.50
1	A	26	GLU	N-CA-C	-5.25	106.71	113.02
1	C	469	PHE	CA-CB-CG	-5.25	108.55	113.80
1	E	151	TYR	CA-C-N	5.25	131.57	121.54
1	E	151	TYR	C-N-CA	5.25	131.57	121.54
1	E	333	VAL	N-CA-C	5.25	115.93	108.42
1	A	383	THR	N-CA-C	5.25	117.28	109.25
1	A	442	TYR	N-CA-C	-5.25	106.90	113.15
1	C	168	HIS	CA-C-O	5.25	126.94	121.38
1	E	188	LEU	N-CA-C	5.25	116.97	108.41
1	F	79	ASP	CA-CB-CG	-5.25	107.35	112.60
1	A	35	TYR	CA-CB-CG	-5.25	104.46	113.90
1	B	64	LYS	N-CA-C	-5.24	101.16	109.76
1	D	92	ASP	N-CA-C	-5.24	98.15	109.01
1	D	351	SER	CA-C-O	5.24	121.63	118.33
1	D	403	TRP	CA-CB-CG	-5.24	103.64	113.60
1	C	434	ALA	CA-C-N	5.24	125.78	120.38
1	C	434	ALA	C-N-CA	5.24	125.78	120.38
1	F	161	CYS	N-CA-C	-5.24	106.94	113.38
1	C	302	SER	CA-C-O	5.24	125.86	119.05
1	B	377	PHE	N-CA-CB	5.23	119.22	110.85
1	E	86	PRO	N-CA-C	-5.23	108.69	114.92
1	A	35	TYR	N-CA-C	5.23	117.14	109.24
1	C	222	LEU	CB-CA-C	-5.23	101.79	110.68
1	F	417	ASP	N-CA-CB	5.23	119.33	110.49
1	F	171	LYS	CA-C-N	5.23	127.45	122.27
1	F	171	LYS	C-N-CA	5.23	127.45	122.27
1	C	245	SER	CA-C-N	5.23	130.28	122.86
1	C	245	SER	C-N-CA	5.23	130.28	122.86
1	C	277	ILE	CB-CA-C	-5.22	104.20	110.99
1	D	453	LYS	CA-CB-CG	-5.22	103.65	114.10
1	C	273	GLU	CB-CG-CD	5.22	121.48	112.60
1	C	378	GLN	N-CA-CB	5.22	118.78	110.84
1	D	347	SER	N-CA-C	5.22	117.86	110.50
1	F	373	LEU	O-C-N	-5.22	117.10	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	LEU	N-CA-C	-5.22	106.59	113.17
1	B	33	ILE	CA-CB-CG1	-5.22	101.53	110.40
1	D	331	LEU	N-CA-C	5.22	117.12	108.20
1	F	84	GLY	CA-C-N	5.22	131.09	121.70
1	F	84	GLY	C-N-CA	5.22	131.09	121.70
1	F	445	LEU	CA-C-N	5.22	128.25	120.95
1	F	445	LEU	C-N-CA	5.22	128.25	120.95
1	F	447	PHE	CB-CA-C	-5.22	99.24	110.45
1	E	399	ILE	O-C-N	-5.21	116.05	122.57
1	B	391	TYR	N-CA-C	-5.21	105.20	112.45
1	D	366	ARG	O-C-N	-5.21	116.83	123.24
1	E	416	VAL	CB-CA-C	-5.21	102.75	111.29
1	D	403	TRP	CB-CG-CD2	-5.21	119.51	126.80
1	F	187	PRO	N-CA-C	-5.21	101.75	112.47
1	A	70	TYR	N-CA-CB	-5.20	101.73	109.69
1	A	122	LEU	N-CA-C	-5.20	104.54	111.87
1	A	127	ASP	CA-CB-CG	-5.20	107.40	112.60
1	A	399	ILE	CA-C-O	5.20	126.36	120.95
1	E	272	PRO	CA-C-O	5.20	127.72	121.48
1	B	354	ASN	N-CA-C	-5.20	106.18	112.88
1	C	106	GLU	CA-C-O	5.20	125.94	120.33
1	F	298	SER	CA-C-N	5.20	131.32	121.97
1	F	298	SER	C-N-CA	5.20	131.32	121.97
1	C	185	CYS	N-CA-C	5.19	116.23	109.64
1	A	423	GLN	N-CA-C	-5.19	99.74	110.80
1	C	80	PRO	N-CA-C	-5.19	101.78	112.47
1	C	376	ILE	CB-CA-C	-5.19	103.42	110.42
1	B	87	ASP	N-CA-C	-5.19	101.03	108.60
1	A	39	SER	CB-CA-C	-5.18	102.11	110.77
1	A	259	HIS	N-CA-C	5.18	117.26	109.23
1	A	294	SER	CA-C-N	5.18	125.65	120.52
1	A	294	SER	C-N-CA	5.18	125.65	120.52
1	A	396	ASN	N-CA-C	-5.18	99.76	110.80
1	F	420	ARG	CG-CD-NE	-5.18	100.60	112.00
1	F	311	TYR	CB-CA-C	-5.18	102.40	110.74
1	B	427	VAL	N-CA-C	-5.18	96.50	111.00
1	C	467	ARG	CA-CB-CG	-5.18	103.74	114.10
1	D	357	THR	O-C-N	-5.18	118.22	121.85
1	F	320	ASN	CA-C-N	-5.18	114.06	122.34
1	F	320	ASN	C-N-CA	-5.18	114.06	122.34
1	C	429	CYS	N-CA-C	-5.18	106.12	112.90
1	D	367	HIS	CA-C-O	-5.18	115.26	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	261	TRP	CB-CG-CD2	-5.18	119.55	126.80
1	E	210	PHE	CA-C-O	5.17	126.25	120.82
1	C	88	ASN	CA-C-O	5.17	125.54	119.28
1	D	83	PHE	N-CA-C	-5.17	101.70	109.15
1	F	245	SER	N-CA-C	-5.17	102.89	111.37
1	A	420	ARG	N-CA-C	-5.17	99.79	110.80
1	A	181	VAL	N-CA-C	5.17	120.09	109.34
1	B	44	THR	CB-CA-C	5.17	119.17	109.86
1	A	143	THR	N-CA-C	-5.17	105.66	112.94
1	B	460	LEU	N-CA-C	5.17	121.12	114.56
1	D	61	ASP	CA-CB-CG	-5.17	107.43	112.60
1	F	44	THR	CB-CA-C	5.17	119.91	109.68
1	F	199	ASP	CA-C-N	-5.16	114.04	121.42
1	F	199	ASP	C-N-CA	-5.16	114.04	121.42
1	F	468	LYS	CB-CA-C	-5.16	102.22	110.79
1	B	165	ILE	CB-CA-C	-5.16	103.14	110.83
1	F	229	CYS	CA-CB-SG	-5.16	102.53	114.40
1	E	324	CYS	CA-C-N	-5.16	113.39	120.71
1	E	324	CYS	C-N-CA	-5.16	113.39	120.71
1	E	422	VAL	N-CA-C	5.16	120.07	109.34
1	D	21	VAL	N-CA-C	5.16	117.93	109.78
1	C	453	LYS	CB-CA-C	5.15	118.97	110.88
1	C	226	GLN	CB-CG-CD	5.15	121.36	112.60
1	E	205	TYR	CA-C-N	5.15	131.50	121.41
1	E	205	TYR	C-N-CA	5.15	131.50	121.41
1	F	448	TRP	CA-C-O	5.15	122.64	119.29
1	C	380	CYS	CA-CB-SG	-5.15	102.56	114.40
1	A	191	ILE	O-C-N	-5.15	117.70	123.26
1	F	45	VAL	O-C-N	-5.15	117.13	123.00
1	F	251	ARG	CD-NE-CZ	-5.15	117.20	124.40
1	E	361	PHE	N-CA-C	5.14	117.80	108.69
1	E	215	ASP	CA-C-N	5.14	127.17	120.28
1	E	215	ASP	C-N-CA	5.14	127.17	120.28
1	A	438	LYS	CA-C-N	5.14	131.36	121.54
1	A	438	LYS	C-N-CA	5.14	131.36	121.54
1	B	128	ASP	CA-CB-CG	5.14	117.74	112.60
1	E	85	LEU	N-CA-CB	5.14	119.52	110.37
1	E	199	ASP	CA-CB-CG	-5.14	107.46	112.60
1	F	451	ASP	CB-CA-C	-5.14	101.86	110.29
1	E	297	GLY	CA-C-N	5.14	131.35	121.54
1	E	297	GLY	C-N-CA	5.14	131.35	121.54
1	A	248	PHE	N-CA-C	5.13	117.19	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	107	ILE	N-CA-C	5.13	115.74	107.73
1	E	231	TYR	CA-C-N	5.13	125.29	119.90
1	E	231	TYR	C-N-CA	5.13	125.29	119.90
1	E	415	LEU	N-CA-C	5.13	121.73	110.80
1	B	261	TRP	CA-CB-CG	-5.13	103.86	113.60
1	D	35	TYR	CA-CB-CG	-5.13	104.67	113.90
1	F	107	ILE	CB-CA-C	-5.13	105.69	111.23
1	D	139	ASP	CA-C-N	5.13	131.33	121.54
1	D	139	ASP	C-N-CA	5.13	131.33	121.54
1	E	69	GLN	CB-CA-C	5.13	120.09	109.38
1	D	157	CYS	N-CA-CB	5.12	120.41	111.13
1	A	103	VAL	CA-C-O	5.12	125.00	120.34
1	C	448	TRP	CA-CB-CG	-5.12	103.87	113.60
1	D	263	ARG	N-CA-CB	5.12	118.73	111.05
1	C	324	CYS	CA-C-N	5.12	127.98	120.71
1	C	324	CYS	C-N-CA	5.12	127.98	120.71
1	C	453	LYS	N-CA-CB	-5.12	102.59	110.01
1	A	371	PHE	CA-C-N	5.11	129.98	122.77
1	A	371	PHE	C-N-CA	5.11	129.98	122.77
1	B	18	VAL	N-CA-C	5.11	119.97	109.34
1	C	222	LEU	CA-C-O	5.11	126.15	120.63
1	D	318	GLY	N-CA-C	5.11	117.34	111.36
1	D	325	TRP	CB-CA-C	-5.11	100.47	109.62
1	E	28	VAL	N-CA-CB	-5.11	105.02	111.41
1	D	60	GLN	CA-C-O	5.11	127.82	120.51
1	F	455	ARG	CD-NE-CZ	-5.11	117.24	124.40
1	D	376	ILE	O-C-N	-5.11	117.87	123.18
1	E	176	LYS	CA-C-N	5.11	125.79	120.12
1	E	176	LYS	C-N-CA	5.11	125.79	120.12
1	C	252	ARG	N-CA-CB	-5.10	102.17	110.59
1	B	146	ASN	CA-C-N	5.10	130.08	122.99
1	B	146	ASN	C-N-CA	5.10	130.08	122.99
1	D	387	GLU	N-CA-CB	-5.10	101.47	109.78
1	F	319	LEU	CA-C-N	-5.10	114.33	121.72
1	F	319	LEU	C-N-CA	-5.10	114.33	121.72
1	A	81	ASN	CB-CA-C	5.10	118.05	109.89
1	E	372	ASP	N-CA-C	5.10	118.36	107.70
1	A	44	THR	N-CA-C	5.09	116.81	108.76
1	A	234	TYR	N-CA-CB	5.09	117.61	110.12
1	B	256	PHE	CA-CB-CG	-5.09	108.70	113.80
1	F	144	ARG	CG-CD-NE	-5.09	100.80	112.00
1	D	167	GLU	N-CA-C	-5.09	100.78	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	SER	N-CA-CB	5.09	118.30	110.21
1	E	441	PRO	N-CA-C	-5.09	101.99	112.47
1	C	403	TRP	CA-CB-CG	-5.08	103.94	113.60
1	A	166	GLY	N-CA-C	-5.08	102.85	112.10
1	A	291	TYR	CA-CB-CG	-5.07	104.77	113.90
1	C	72	VAL	CA-C-O	5.07	126.06	120.48
1	C	215	ASP	N-CA-C	-5.07	104.56	111.56
1	C	127	ASP	CA-CB-CG	-5.07	107.53	112.60
1	E	90	VAL	CA-C-N	-5.07	113.43	122.45
1	E	90	VAL	C-N-CA	-5.07	113.43	122.45
1	A	334	VAL	CA-C-N	5.07	129.41	121.76
1	A	334	VAL	C-N-CA	5.07	129.41	121.76
1	F	281	ASP	CB-CA-C	-5.06	110.76	116.63
1	C	265	GLY	N-CA-C	5.06	119.84	112.60
1	C	421	PHE	CA-C-N	5.06	131.08	121.97
1	C	421	PHE	C-N-CA	5.06	131.08	121.97
1	E	446	LYS	CB-CA-C	-5.06	99.36	109.33
1	B	383	THR	N-CA-CB	5.06	118.11	109.87
1	E	413	ALA	CB-CA-C	5.06	118.08	110.50
1	F	436	PRO	CA-C-N	5.06	130.80	121.70
1	F	436	PRO	C-N-CA	5.06	130.80	121.70
1	B	91	TYR	CB-CG-CD1	5.05	128.38	120.80
1	F	133	HIS	CA-CB-CG	5.05	118.85	113.80
1	B	93	PRO	N-CA-C	-5.05	108.14	114.20
1	D	25	ASP	CB-CA-C	5.05	120.98	110.32
1	D	187	PRO	N-CA-C	-5.05	103.89	111.57
1	D	440	ASP	CB-CA-C	5.05	120.12	110.17
1	E	184	ASP	N-CA-CB	-5.05	103.02	111.20
1	F	53	PRO	N-CA-C	-5.05	102.72	112.01
1	B	388	VAL	N-CA-C	-5.05	105.78	110.53
1	D	270	GLN	N-CA-C	5.05	116.62	108.34
1	D	337	THR	CA-C-O	5.05	125.81	120.10
1	F	303	ASP	CA-C-O	5.05	125.90	120.55
1	F	373	LEU	N-CA-CB	-5.05	102.05	110.23
1	A	246	MET	N-CA-C	-5.05	100.29	108.52
1	A	295	PRO	CB-CA-C	-5.05	103.28	110.75
1	B	102	CYS	N-CA-C	-5.05	102.30	110.32
1	C	189	GLU	N-CA-C	5.05	117.62	109.40
1	B	261	TRP	N-CA-CB	5.04	119.19	111.22
1	F	428	THR	CB-CA-C	-5.04	102.27	110.85
1	B	368	VAL	N-CA-C	5.04	115.91	108.45
1	B	323	ILE	CA-C-O	5.04	125.68	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	381	LYS	N-CA-C	-5.04	101.93	109.95
1	F	106	GLU	CA-C-O	5.04	125.78	120.33
1	E	141	LYS	N-CA-CB	-5.04	101.25	110.27
1	E	187	PRO	N-CA-C	-5.04	103.91	111.57
1	E	469	PHE	CB-CA-C	5.04	119.41	110.85
1	E	306	LEU	N-CA-C	5.04	116.46	111.07
1	D	245	SER	N-CA-CB	-5.04	102.72	110.12
1	C	353	PRO	N-CA-C	-5.03	103.86	111.41
1	E	51	LYS	N-CA-C	-5.03	102.34	110.14
1	F	428	THR	N-CA-CB	5.03	117.61	110.16
1	C	459	ASP	CA-CB-CG	-5.03	107.57	112.60
1	E	88	ASN	CA-C-N	5.03	127.02	120.28
1	E	88	ASN	C-N-CA	5.03	127.02	120.28
1	A	50	PHE	N-CA-C	5.03	121.50	110.80
1	A	338	ARG	O-C-N	-5.03	115.76	121.99
1	D	219	GLU	CB-CG-CD	-5.03	104.06	112.60
1	C	68	TYR	CA-CB-CG	-5.02	104.86	113.90
1	B	383	THR	CA-C-O	5.02	126.31	120.49
1	F	47	HIS	CB-CA-C	-5.02	101.70	108.68
1	D	436	PRO	CA-C-N	5.01	131.00	121.97
1	D	436	PRO	C-N-CA	5.01	131.00	121.97
1	E	131	ASN	N-CA-C	-5.01	107.00	113.02
1	E	144	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	E	383	THR	N-CA-CB	5.01	117.72	109.95
1	D	355	VAL	N-CA-C	-5.01	101.26	108.48
1	B	364	TYR	N-CA-CB	-5.01	102.25	111.37
1	B	417	ASP	CA-CB-CG	-5.01	107.59	112.60
1	B	343	SER	N-CA-C	5.01	116.68	108.52
1	B	455	ARG	CG-CD-NE	-5.01	100.98	112.00
1	A	159	ILE	N-CA-CB	-5.01	104.50	111.41
1	F	386	THR	N-CA-CB	-5.00	102.76	110.12
1	B	453	LYS	N-CA-C	5.00	117.11	111.11
1	C	406	GLY	CA-C-N	5.00	130.71	121.70
1	C	406	GLY	C-N-CA	5.00	130.71	121.70
1	D	455	ARG	N-CA-C	-5.00	105.89	112.94
1	F	46	GLY	O-C-N	-5.00	119.13	123.88
1	F	72	VAL	N-CA-CB	5.00	118.20	111.90
1	F	469	PHE	CB-CA-C	5.00	119.35	110.85

There are no chirality outliers.

All (253) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	144	ARG	Sidechain
1	A	234	TYR	Sidechain
1	A	242	TYR	Sidechain
1	A	248	PHE	Sidechain
1	A	258	ARG	Sidechain
1	A	263	ARG	Sidechain
1	A	283	ARG	Sidechain
1	A	289	TYR	Sidechain
1	A	307	PHE	Sidechain
1	A	314	HIS	Sidechain
1	A	319	LEU	Peptide,Mainchain
1	A	35	TYR	Sidechain
1	A	361	PHE	Sidechain
1	A	366	ARG	Sidechain
1	A	375	PHE	Sidechain
1	A	391	TYR	Sidechain
1	A	405	PHE	Sidechain
1	A	41	ARG	Sidechain
1	A	420	ARG	Sidechain
1	A	442	TYR	Sidechain
1	A	447	PHE	Sidechain
1	A	456	PHE	Sidechain
1	A	463	PHE	Sidechain
1	A	469	PHE	Sidechain
1	A	49	TYR	Sidechain
1	A	68	TYR	Sidechain
1	A	70	TYR	Sidechain
1	A	71	ARG	Sidechain
1	A	73	PHE	Sidechain
1	A	74	ARG	Sidechain
1	A	86	PRO	Mainchain
1	A	91	TYR	Sidechain
1	A	97	ARG	Sidechain
1	B	120	HIS	Sidechain
1	B	123	TYR	Sidechain
1	B	151	TYR	Sidechain
1	B	168	HIS	Sidechain
1	B	203	THR	Mainchain
1	B	205	TYR	Sidechain
1	B	234	TYR	Sidechain
1	B	244	ASP	Mainchain
1	B	274	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	B	283	ARG	Sidechain
1	B	289	TYR	Sidechain
1	B	291	TYR	Sidechain
1	B	303	ASP	Peptide,Mainchain
1	B	311	TYR	Sidechain
1	B	35	TYR	Mainchain,Sidechain
1	B	364	TYR	Sidechain
1	B	375	PHE	Sidechain
1	B	377	PHE	Mainchain
1	B	385	THR	Peptide,Mainchain
1	B	393	HIS	Sidechain
1	B	403	TRP	Mainchain
1	B	419	TYR	Sidechain
1	B	420	ARG	Sidechain
1	B	421	PHE	Sidechain
1	B	425	ALA	Mainchain
1	B	442	TYR	Mainchain,Sidechain
1	B	447	PHE	Sidechain
1	B	455	ARG	Sidechain
1	B	459	ASP	Peptide,Mainchain
1	B	460	LEU	Mainchain
1	B	467	ARG	Sidechain
1	B	469	PHE	Sidechain
1	B	49	TYR	Sidechain
1	B	59	ARG	Sidechain
1	B	68	TYR	Sidechain
1	B	71	ARG	Sidechain
1	B	73	PHE	Sidechain
1	B	78	PRO	Mainchain
1	B	91	TYR	Mainchain
1	B	95	SER	Mainchain
1	C	109	ARG	Sidechain
1	C	144	ARG	Sidechain
1	C	151	TYR	Sidechain
1	C	168	HIS	Sidechain
1	C	174	ALA	Peptide
1	C	205	TYR	Sidechain
1	C	210	PHE	Sidechain
1	C	234	TYR	Sidechain
1	C	242	TYR	Sidechain
1	C	248	PHE	Sidechain
1	C	256	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	C	263	ARG	Sidechain
1	C	27	TYR	Sidechain
1	C	276	TYR	Sidechain
1	C	291	TYR	Sidechain
1	C	307	PHE	Sidechain
1	C	311	TYR	Sidechain
1	C	323	ILE	Mainchain
1	C	330	PHE	Sidechain
1	C	338	ARG	Sidechain
1	C	34	PHE	Sidechain
1	C	35	TYR	Sidechain
1	C	356	TYR	Sidechain
1	C	366	ARG	Sidechain
1	C	375	PHE	Sidechain
1	C	385	THR	Peptide,Mainchain
1	C	403	TRP	Mainchain
1	C	41	ARG	Sidechain
1	C	419	TYR	Sidechain
1	C	42	LEU	Mainchain
1	C	421	PHE	Sidechain
1	C	442	TYR	Sidechain
1	C	447	PHE	Sidechain
1	C	455	ARG	Sidechain
1	C	463	PHE	Sidechain
1	C	467	ARG	Sidechain
1	C	469	PHE	Sidechain
1	C	49	TYR	Sidechain
1	C	68	TYR	Sidechain
1	C	71	ARG	Sidechain
1	C	73	PHE	Sidechain
1	C	74	ARG	Sidechain
1	C	87	ASP	Mainchain
1	C	88	ASN	Mainchain
1	C	91	TYR	Mainchain
1	D	100	TRP	Peptide,Mainchain
1	D	109	ARG	Sidechain
1	D	144	ARG	Mainchain,Sidechain
1	D	151	TYR	Sidechain
1	D	157	CYS	Mainchain
1	D	168	HIS	Sidechain
1	D	205	TYR	Sidechain
1	D	210	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	D	231	TYR	Sidechain
1	D	242	TYR	Sidechain
1	D	252	ARG	Sidechain
1	D	263	ARG	Sidechain
1	D	283	ARG	Sidechain
1	D	289	TYR	Sidechain
1	D	311	TYR	Sidechain
1	D	314	HIS	Sidechain
1	D	323	ILE	Peptide,Mainchain
1	D	35	TYR	Sidechain
1	D	354	ASN	Mainchain
1	D	36	HIS	Sidechain
1	D	364	TYR	Sidechain
1	D	366	ARG	Sidechain
1	D	371	PHE	Sidechain
1	D	377	PHE	Sidechain
1	D	391	TYR	Sidechain
1	D	419	TYR	Sidechain
1	D	442	TYR	Sidechain
1	D	443	ASP	Mainchain
1	D	447	PHE	Sidechain
1	D	455	ARG	Sidechain
1	D	456	PHE	Sidechain
1	D	458	ALA	Mainchain
1	D	467	ARG	Sidechain
1	D	469	PHE	Sidechain
1	D	49	TYR	Sidechain
1	D	68	TYR	Sidechain
1	D	70	TYR	Sidechain
1	D	71	ARG	Sidechain
1	D	73	PHE	Sidechain
1	D	97	ARG	Sidechain
1	E	100	TRP	Mainchain
1	E	109	ARG	Sidechain
1	E	144	ARG	Sidechain
1	E	151	TYR	Sidechain
1	E	187	PRO	Mainchain
1	E	234	TYR	Sidechain
1	E	243	GLY	Mainchain
1	E	263	ARG	Sidechain
1	E	276	TYR	Sidechain
1	E	289	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	E	311	TYR	Peptide,Mainchain,Sidechain
1	E	35	TYR	Sidechain
1	E	356	TYR	Sidechain
1	E	375	PHE	Sidechain
1	E	377	PHE	Sidechain
1	E	381	LYS	Mainchain
1	E	391	TYR	Sidechain
1	E	393	HIS	Sidechain
1	E	398	THR	Mainchain
1	E	407	VAL	Mainchain
1	E	430	GLN	Mainchain
1	E	440	ASP	Mainchain
1	E	442	TYR	Sidechain
1	E	447	PHE	Sidechain
1	E	463	PHE	Sidechain
1	E	467	ARG	Sidechain
1	E	469	PHE	Sidechain
1	E	49	TYR	Sidechain
1	E	59	ARG	Mainchain,Sidechain
1	E	68	TYR	Sidechain
1	E	70	TYR	Sidechain
1	E	71	ARG	Sidechain
1	E	73	PHE	Sidechain
1	E	88	ASN	Mainchain
1	F	100	TRP	Mainchain
1	F	109	ARG	Sidechain
1	F	12	TYR	Sidechain
1	F	144	ARG	Sidechain
1	F	151	TYR	Sidechain
1	F	168	HIS	Sidechain
1	F	203	THR	Mainchain
1	F	209	ASP	Peptide,Mainchain
1	F	242	TYR	Sidechain
1	F	244	ASP	Mainchain
1	F	245	SER	Peptide,Mainchain
1	F	248	PHE	Sidechain
1	F	251	ARG	Sidechain
1	F	256	PHE	Sidechain
1	F	260	PHE	Sidechain
1	F	27	TYR	Sidechain
1	F	276	TYR	Sidechain
1	F	283	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	291	TYR	Sidechain
1	F	30	ARG	Sidechain
1	F	307	PHE	Sidechain
1	F	311	TYR	Sidechain
1	F	314	HIS	Sidechain
1	F	32	SER	Mainchain
1	F	34	PHE	Sidechain
1	F	356	TYR	Sidechain
1	F	364	TYR	Sidechain
1	F	391	TYR	Sidechain
1	F	397	THR	Peptide,Mainchain
1	F	41	ARG	Sidechain
1	F	417	ASP	Mainchain
1	F	420	ARG	Sidechain
1	F	429	CYS	Mainchain
1	F	442	TYR	Sidechain
1	F	447	PHE	Sidechain
1	F	455	ARG	Sidechain
1	F	469	PHE	Sidechain
1	F	49	TYR	Sidechain
1	F	59	ARG	Sidechain
1	F	60	GLN	Mainchain
1	F	68	TYR	Sidechain
1	F	73	PHE	Sidechain
1	F	91	TYR	Sidechain
1	F	92	ASP	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3598	0	3503	288	0
1	B	3661	0	3571	254	0
1	C	3604	0	3508	242	0
1	D	3586	0	3489	252	0
1	E	3586	0	3489	271	0
1	F	3661	0	3571	249	0
All	All	21696	0	21131	1494	0

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 35.

All (1494) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:THR:HG22	1:A:386:THR:O	1.56	1.06
1:D:169:TRP:CD1	1:D:190:LEU:HD13	2.06	0.90
1:B:169:TRP:CE2	1:B:190:LEU:HD13	2.05	0.90
1:A:70:TYR:CD1	1:A:201:VAL:HG12	2.07	0.90
1:F:169:TRP:CD1	1:F:190:LEU:HD13	2.11	0.85
1:A:386:THR:O	1:A:386:THR:CG2	2.25	0.84
1:D:120:HIS:CD2	1:D:122:LEU:H	1.97	0.83
1:F:70:TYR:CD1	1:F:201:VAL:HG12	2.13	0.83
1:E:70:TYR:CD1	1:E:201:VAL:HG12	2.13	0.83
1:E:47:HIS:CD2	1:E:48:PRO:HD2	2.13	0.82
1:E:40:SER:H	1:E:455:ARG:HH12	1.23	0.81
1:F:168:HIS:CE1	1:F:191:ILE:HB	2.20	0.77
1:D:168:HIS:CE1	1:D:191:ILE:HG23	2.20	0.76
1:A:22:VAL:HG12	1:A:27:TYR:CE1	2.21	0.76
1:A:47:HIS:CD2	1:A:48:PRO:HD2	2.21	0.75
1:A:97:ARG:HB3	1:A:403:TRP:CE2	2.21	0.75
1:F:94:ASN:O	1:F:384:LEU:HD12	1.87	0.75
1:D:313:LEU:HD12	1:D:314:HIS:H	1.53	0.74
1:C:171:LYS:H	1:C:212:LEU:HD21	1.52	0.74
1:C:325:TRP:H	1:C:325:TRP:CD1	2.03	0.73
1:E:171:LYS:H	1:E:212:LEU:HD23	1.54	0.73
1:D:47:HIS:CE1	1:D:49:TYR:H	2.06	0.73
1:F:91:TYR:CD2	1:F:98:LEU:HD21	2.24	0.72
1:B:387:GLU:H	1:B:387:GLU:CD	1.97	0.72
1:F:467:ARG:HA	1:F:470:LEU:HD12	1.70	0.71
1:A:120:HIS:CD2	1:A:122:LEU:H	2.07	0.71
1:B:341:ASN:HD21	1:B:367:HIS:CD2	2.08	0.71
1:A:460:LEU:HB2	1:A:470:LEU:HD11	1.73	0.71
1:E:47:HIS:CG	1:E:48:PRO:HD2	2.25	0.71
1:F:387:GLU:CD	1:F:387:GLU:H	1.98	0.71
1:F:422:VAL:HG23	1:F:426:ALA:H	1.55	0.71
1:A:38:GLY:H	1:A:455:ARG:HB3	1.56	0.71
1:F:325:TRP:H	1:F:325:TRP:CD1	2.09	0.70
1:C:169:TRP:CZ2	1:C:190:LEU:HD13	2.26	0.70
1:B:167:GLU:HG3	1:B:190:LEU:HD11	1.74	0.70
1:F:107:ILE:HD12	1:F:107:ILE:H	1.56	0.70
1:D:91:TYR:CD2	1:D:98:LEU:HD21	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:VAL:O	1:A:391:TYR:CD2	2.44	0.70
1:C:387:GLU:CD	1:C:387:GLU:H	2.00	0.69
1:C:393:HIS:O	1:C:397:THR:HG23	1.92	0.69
1:D:35:TYR:CE2	1:D:458:ALA:HB2	2.27	0.69
1:C:467:ARG:HA	1:C:470:LEU:HD12	1.75	0.69
1:F:47:HIS:CE1	1:F:49:TYR:HB2	2.28	0.68
1:B:365:ALA:C	1:B:366:ARG:HE	2.00	0.68
1:E:47:HIS:CE1	1:E:49:TYR:H	2.11	0.68
1:A:167:GLU:HG2	1:A:190:LEU:HD11	1.75	0.68
1:B:120:HIS:CE1	1:B:222:LEU:HD21	2.29	0.68
1:E:45:VAL:HG13	1:E:367:HIS:O	1.94	0.68
1:A:398:THR:HA	1:A:401:GLU:CD	2.18	0.68
1:B:120:HIS:CG	1:B:123:TYR:CD1	2.81	0.68
1:A:416:VAL:HG23	1:A:417:ASP:H	1.57	0.67
1:F:74:ARG:HB2	1:F:447:PHE:CG	2.29	0.67
1:C:47:HIS:CE1	1:C:49:TYR:H	2.12	0.67
1:F:167:GLU:HA	1:F:192:ASN:HA	1.77	0.67
1:A:120:HIS:CD2	1:A:222:LEU:HD21	2.30	0.66
1:A:169:TRP:NE1	1:A:190:LEU:HD13	2.11	0.66
1:B:196:GLU:CD	1:B:446:LYS:H	2.03	0.66
1:B:101:ALA:HB3	1:B:378:GLN:O	1.95	0.66
1:D:235:LEU:H	1:D:235:LEU:HD12	1.60	0.66
1:F:36:HIS:CD2	1:F:463:PHE:CD1	2.83	0.66
1:A:171:LYS:H	1:A:212:LEU:HD21	1.62	0.65
1:A:388:VAL:O	1:A:392:ILE:HG13	1.95	0.65
1:D:262:ASN:HA	1:D:290:LEU:O	1.97	0.65
1:F:120:HIS:CD2	1:F:222:LEU:HD21	2.31	0.65
1:A:190:LEU:HD12	1:A:191:ILE:H	1.60	0.65
1:B:120:HIS:CD2	1:B:120:HIS:C	2.74	0.65
1:A:259:HIS:CG	1:B:131:ASN:HD21	2.14	0.65
1:A:170:THR:HB	1:A:191:ILE:HD11	1.77	0.65
1:B:42:LEU:H	1:B:371:PHE:H	1.45	0.65
1:C:169:TRP:CH2	1:C:190:LEU:HD13	2.32	0.65
1:A:169:TRP:CD1	1:A:190:LEU:HD13	2.32	0.64
1:A:165:ILE:HA	1:A:194:PRO:HA	1.78	0.64
1:A:83:PHE:CE2	1:F:83:PHE:HA	2.33	0.64
1:A:91:TYR:CD2	1:A:98:LEU:HD21	2.33	0.64
1:B:305:GLN:CD	1:B:307:PHE:H	2.05	0.64
1:D:36:HIS:CG	1:D:463:PHE:CE2	2.86	0.64
1:E:123:TYR:CD2	1:E:147:VAL:HG21	2.32	0.64
1:C:273:GLU:HG2	1:C:276:TYR:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:THR:O	1:F:28:VAL:HG23	1.98	0.64
1:F:70:TYR:CZ	1:F:201:VAL:HA	2.33	0.64
1:C:30:ARG:HH11	1:C:30:ARG:HB3	1.63	0.64
1:D:107:ILE:H	1:D:107:ILE:HD12	1.61	0.64
1:D:462:GLN:C	1:D:467:ARG:HH21	2.06	0.64
1:D:67:ALA:HB3	1:D:68:TYR:CE2	2.33	0.63
1:E:197:ASP:HB2	1:E:447:PHE:HA	1.80	0.63
1:B:66:SER:HA	1:B:367:HIS:CD2	2.32	0.63
1:D:219:GLU:HA	1:D:263:ARG:HH22	1.62	0.63
1:C:97:ARG:HG2	1:C:384:LEU:HD11	1.81	0.63
1:D:70:TYR:CD1	1:D:201:VAL:HG12	2.33	0.63
1:A:356:TYR:CE1	1:A:361:PHE:CE2	2.87	0.63
1:A:444:LYS:C	1:A:445:LEU:HD12	2.24	0.63
1:A:211:LYS:HB3	1:A:211:LYS:HZ3	1.64	0.63
1:C:442:TYR:HA	1:C:445:LEU:HD12	1.80	0.63
1:E:190:LEU:HD12	1:E:191:ILE:H	1.64	0.63
1:F:70:TYR:CE1	1:F:201:VAL:HG12	2.33	0.63
1:A:42:LEU:O	1:A:370:GLU:HA	1.99	0.63
1:C:24:THR:HA	1:C:27:TYR:CZ	2.33	0.63
1:A:30:ARG:HA	1:A:380:CYS:SG	2.39	0.62
1:A:47:HIS:CE1	1:A:49:TYR:HB2	2.34	0.62
1:B:97:ARG:HB3	1:B:403:TRP:CE2	2.34	0.62
1:B:120:HIS:CD2	1:B:123:TYR:CD1	2.88	0.62
1:E:234:TYR:CZ	1:E:249:CYS:HB2	2.34	0.62
1:F:121:PRO:HD2	1:F:222:LEU:HD11	1.81	0.62
1:A:168:HIS:HB3	1:A:230:LYS:HA	1.81	0.62
1:B:47:HIS:CE1	1:B:50:PHE:H	2.18	0.62
1:C:168:HIS:CD2	1:C:191:ILE:O	2.53	0.62
1:D:448:TRP:HA	1:D:448:TRP:CE3	2.34	0.62
1:F:81:ASN:HA	1:F:98:LEU:HD12	1.81	0.62
1:F:169:TRP:NE1	1:F:190:LEU:HD13	2.15	0.62
1:A:70:TYR:CE2	1:A:201:VAL:HA	2.35	0.61
1:A:91:TYR:CE2	1:A:98:LEU:HD21	2.35	0.61
1:F:367:HIS:CG	1:F:368:VAL:H	2.18	0.61
1:E:74:ARG:HB2	1:E:447:PHE:CG	2.35	0.61
1:F:234:TYR:HA	1:F:237:MET:HE2	1.82	0.61
1:A:391:TYR:CD1	1:A:391:TYR:C	2.78	0.61
1:D:66:SER:HA	1:D:367:HIS:CD2	2.36	0.61
1:D:84:GLY:C	1:D:85:LEU:HD23	2.24	0.61
1:F:99:VAL:O	1:F:379:LEU:HD12	2.00	0.61
1:B:341:ASN:HD21	1:B:367:HIS:CG	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLU:H	1:C:199:ASP:CG	2.09	0.61
1:D:271:LEU:HD12	1:D:275:LEU:HD22	1.83	0.61
1:B:35:TYR:HB2	1:B:377:PHE:H	1.66	0.61
1:D:167:GLU:HA	1:D:192:ASN:HA	1.81	0.61
1:A:329:LEU:HD23	1:A:330:PHE:N	2.15	0.61
1:D:100:TRP:CZ3	1:D:377:PHE:HB3	2.35	0.61
1:D:460:LEU:HB2	1:D:470:LEU:HD11	1.80	0.61
1:B:220:VAL:HG22	1:B:225:CYS:HA	1.83	0.61
1:E:172:GLY:HA2	1:E:189:GLU:CD	2.26	0.60
1:B:421:PHE:CE1	1:B:422:VAL:HG12	2.36	0.60
1:E:24:THR:HA	1:E:27:TYR:CZ	2.37	0.60
1:E:377:PHE:N	1:E:377:PHE:CD2	2.68	0.60
1:A:169:TRP:CE2	1:A:190:LEU:HD13	2.37	0.60
1:E:121:PRO:HA	1:E:146:ASN:HA	1.82	0.60
1:B:13:LEU:H	1:B:393:HIS:CE1	2.20	0.60
1:B:41:ARG:HB3	1:B:43:LEU:HD11	1.84	0.60
1:C:70:TYR:CE2	1:C:201:VAL:HA	2.36	0.60
1:C:120:HIS:HB2	1:C:221:PRO:HA	1.84	0.60
1:F:161:CYS:HG	1:F:325:TRP:CD1	2.20	0.60
1:C:208:MET:HB2	1:C:213:LEU:HD21	1.83	0.60
1:F:30:ARG:HA	1:F:380:CYS:SG	2.42	0.60
1:A:399:ILE:HD12	1:A:399:ILE:H	1.67	0.60
1:B:169:TRP:CH2	1:B:190:LEU:HB2	2.37	0.60
1:C:24:THR:HA	1:C:27:TYR:CE2	2.36	0.60
1:F:214:GLN:HB3	1:F:216:ASN:HD21	1.66	0.60
1:F:442:TYR:HA	1:F:445:LEU:HD12	1.82	0.60
1:A:171:LYS:HE3	1:A:213:LEU:HA	1.84	0.59
1:D:79:ASP:CA	1:D:327:ASN:HD21	2.15	0.59
1:E:214:GLN:CD	1:E:219:GLU:HB2	2.27	0.59
1:E:424:SER:HA	1:E:425:ALA:HB3	1.85	0.59
1:E:40:SER:H	1:E:455:ARG:NH1	1.98	0.59
1:F:168:HIS:C	1:F:168:HIS:CD2	2.81	0.59
1:B:169:TRP:NE1	1:B:190:LEU:HD13	2.16	0.59
1:B:24:THR:HA	1:B:27:TYR:CE2	2.37	0.59
1:B:89:THR:C	1:B:91:TYR:H	2.09	0.59
1:B:123:TYR:CE1	1:B:219:GLU:HA	2.37	0.59
1:D:169:TRP:NE1	1:D:190:LEU:HD13	2.16	0.59
1:E:172:GLY:H	1:E:188:LEU:HA	1.67	0.59
1:E:57:ASN:HD21	1:E:61:ASP:HB3	1.68	0.59
1:E:168:HIS:HB3	1:E:230:LYS:HA	1.85	0.59
1:F:45:VAL:HG12	1:F:368:VAL:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:GLN:C	1:A:467:ARG:HH21	2.11	0.59
1:E:190:LEU:HD12	1:E:191:ILE:N	2.18	0.59
1:C:469:PHE:C	1:C:469:PHE:CD2	2.81	0.59
1:F:97:ARG:O	1:F:382:ILE:HD12	2.03	0.59
1:A:273:GLU:C	1:A:275:LEU:H	2.11	0.58
1:C:42:LEU:O	1:C:370:GLU:HA	2.03	0.58
1:F:107:ILE:HG23	1:F:373:LEU:HD22	1.83	0.58
1:A:181:VAL:HB	1:A:184:ASP:HB2	1.85	0.58
1:A:442:TYR:CD1	1:A:442:TYR:N	2.71	0.58
1:E:273:GLU:CD	1:E:273:GLU:H	2.10	0.58
1:F:173:THR:HB	1:F:175:CYS:SG	2.43	0.58
1:F:312:TRP:H	1:F:312:TRP:CD1	2.11	0.58
1:D:300:VAL:HG12	1:D:301:THR:H	1.67	0.58
1:E:30:ARG:HA	1:E:380:CYS:SG	2.44	0.58
1:B:356:TYR:CD2	1:C:142:ASP:HB3	2.39	0.58
1:B:121:PRO:HA	1:B:146:ASN:HA	1.84	0.58
1:D:36:HIS:CG	1:D:463:PHE:CD2	2.90	0.58
1:D:73:PHE:CE2	1:D:448:TRP:HB3	2.38	0.58
1:E:392:ILE:HA	1:E:395:MET:SD	2.44	0.58
1:F:35:TYR:CE1	1:F:456:PHE:CD2	2.92	0.58
1:B:152:LYS:HA	1:B:297:GLY:HA2	1.85	0.58
1:D:73:PHE:HB3	1:D:450:VAL:HG21	1.85	0.58
1:C:168:HIS:HA	1:C:207:ALA:HB1	1.86	0.58
1:F:24:THR:HA	1:F:27:TYR:CE1	2.38	0.58
1:A:47:HIS:CE1	1:A:49:TYR:H	2.21	0.58
1:B:120:HIS:CD2	1:B:122:LEU:H	2.22	0.58
1:C:47:HIS:CE1	1:C:49:TYR:HB2	2.39	0.58
1:B:454:GLU:H	1:B:454:GLU:CD	2.11	0.58
1:C:169:TRP:CZ3	1:C:190:LEU:HA	2.39	0.58
1:C:169:TRP:HA	1:C:169:TRP:CE3	2.38	0.58
1:B:396:ASN:HD21	1:B:398:THR:HB	1.69	0.57
1:C:233:ASP:CG	1:C:236:GLN:H	2.12	0.57
1:D:97:ARG:HG3	1:D:403:TRP:CD2	2.39	0.57
1:B:344:VAL:HB	1:B:364:TYR:HB2	1.86	0.57
1:B:393:HIS:CE1	1:B:394:ASN:OD1	2.57	0.57
1:F:152:LYS:HA	1:F:297:GLY:HA2	1.87	0.57
1:F:256:PHE:CE1	1:F:296:SER:HB3	2.39	0.57
1:D:41:ARG:HH22	1:E:233:ASP:CG	2.12	0.57
1:A:367:HIS:CG	1:A:368:VAL:H	2.22	0.57
1:B:120:HIS:CD2	1:B:123:TYR:HD1	2.22	0.57
1:B:248:PHE:CD1	1:B:248:PHE:C	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:ARG:HG2	1:F:384:LEU:HD11	1.86	0.57
1:B:156:LEU:HD23	1:B:157:CYS:N	2.20	0.57
1:B:164:ALA:HB1	1:B:237:MET:SD	2.45	0.57
1:B:248:PHE:CZ	1:B:250:LEU:HB2	2.39	0.57
1:F:356:TYR:CE1	1:F:361:PHE:CE2	2.91	0.57
1:B:99:VAL:O	1:B:379:LEU:HD22	2.04	0.57
1:B:398:THR:HA	1:B:401:GLU:CD	2.30	0.57
1:C:91:TYR:CE2	1:C:93:PRO:HA	2.39	0.57
1:D:196:GLU:CD	1:D:446:LYS:H	2.12	0.57
1:B:30:ARG:HA	1:B:380:CYS:SG	2.45	0.57
1:E:74:ARG:CZ	1:E:442:TYR:HB2	2.34	0.57
1:F:325:TRP:HB2	1:F:326:HIS:CD2	2.40	0.57
1:A:342:LEU:O	1:A:365:ALA:HA	2.04	0.56
1:A:387:GLU:HG2	1:A:388:VAL:HG23	1.87	0.56
1:B:220:VAL:CG2	1:B:225:CYS:HA	2.34	0.56
1:B:420:ARG:HH22	1:B:427:VAL:H	1.52	0.56
1:F:404:ASN:HB2	1:F:405:PHE:CE1	2.40	0.56
1:A:243:GLY:HA3	1:A:319:LEU:HD22	1.87	0.56
1:B:395:MET:HE2	1:F:408:THR:HG21	1.86	0.56
1:D:91:TYR:CZ	1:D:93:PRO:HA	2.40	0.56
1:F:31:THR:H	1:F:378:GLN:NE2	2.03	0.56
1:A:48:PRO:HG2	1:A:49:TYR:CE2	2.39	0.56
1:A:344:VAL:O	1:A:363:GLU:HA	2.05	0.56
1:B:105:VAL:HG13	1:B:375:PHE:CE1	2.41	0.56
1:C:48:PRO:HB2	1:C:49:TYR:CE2	2.40	0.56
1:D:26:GLU:CD	1:D:26:GLU:H	2.09	0.56
1:E:259:HIS:HB2	1:E:261:TRP:CZ2	2.40	0.56
1:A:196:GLU:CD	1:A:446:LYS:H	2.12	0.56
1:B:234:TYR:CZ	1:B:249:CYS:HB2	2.40	0.56
1:C:120:HIS:CE1	1:C:122:LEU:C	2.83	0.56
1:C:326:HIS:HB2	1:C:328:GLN:HE21	1.70	0.56
1:D:24:THR:HA	1:D:27:TYR:CE2	2.39	0.56
1:B:47:HIS:CE1	1:B:49:TYR:CD2	2.93	0.56
1:C:278:LYS:H	1:C:278:LYS:HZ2	1.53	0.56
1:A:276:TYR:CD2	1:E:122:LEU:HD12	2.41	0.56
1:B:133:HIS:CD2	1:B:134:VAL:HA	2.41	0.56
1:E:59:ARG:NE	1:E:60:GLN:HE22	2.04	0.56
1:E:97:ARG:HB2	1:E:382:ILE:HD12	1.87	0.56
1:F:120:HIS:CD2	1:F:122:LEU:H	2.23	0.56
1:F:422:VAL:HG23	1:F:426:ALA:N	2.21	0.56
1:A:91:TYR:CZ	1:A:98:LEU:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:VAL:HG13	1:C:375:PHE:CE1	2.40	0.56
1:C:391:TYR:HA	1:C:394:ASN:HD21	1.70	0.56
1:C:440:ASP:O	1:C:443:ASP:HB2	2.06	0.56
1:F:123:TYR:C	1:F:144:ARG:HA	2.31	0.56
1:F:126:LEU:H	1:F:263:ARG:HA	1.71	0.56
1:A:259:HIS:HB2	1:A:261:TRP:CZ3	2.41	0.56
1:B:67:ALA:H	1:B:367:HIS:CE1	2.24	0.56
1:C:71:ARG:HH21	1:C:197:ASP:CG	2.14	0.56
1:E:454:GLU:CD	1:E:454:GLU:N	2.64	0.56
1:E:120:HIS:HB3	1:E:123:TYR:HB2	1.87	0.56
1:E:400:LEU:HD11	1:E:405:PHE:CE1	2.41	0.56
1:B:167:GLU:CG	1:B:190:LEU:HD11	2.35	0.55
1:E:91:TYR:CE2	1:E:98:LEU:HG	2.41	0.55
1:C:454:GLU:CD	1:C:454:GLU:H	2.13	0.55
1:D:377:PHE:N	1:D:377:PHE:CD2	2.73	0.55
1:E:47:HIS:CE1	1:E:50:PHE:CE1	2.95	0.55
1:E:428:THR:HG23	1:E:430:GLN:HE21	1.71	0.55
1:A:36:HIS:CG	1:A:37:ALA:N	2.74	0.55
1:F:252:ARG:HH21	1:F:253:GLU:C	2.14	0.55
1:A:47:HIS:CG	1:A:48:PRO:HD2	2.41	0.55
1:A:168:HIS:O	1:A:190:LEU:HD12	2.06	0.55
1:E:469:PHE:HA	1:E:472:GLN:OE1	2.06	0.55
1:E:441:PRO:HD2	1:E:442:TYR:CE1	2.42	0.55
1:F:49:TYR:HA	1:F:223:ASP:OD2	2.07	0.55
1:F:422:VAL:HA	1:F:426:ALA:HB3	1.89	0.55
1:C:41:ARG:HA	1:C:371:PHE:O	2.06	0.55
1:C:115:VAL:HG22	1:C:116:GLY:H	1.72	0.55
1:F:121:PRO:HA	1:F:146:ASN:HA	1.89	0.55
1:F:427:VAL:HG13	1:F:429:CYS:SG	2.47	0.55
1:A:69:GLN:CA	1:A:201:VAL:HG13	2.37	0.55
1:A:391:TYR:CZ	1:A:392:ILE:HA	2.41	0.55
1:E:109:ARG:HA	1:E:371:PHE:CE1	2.42	0.55
1:E:323:ILE:HB	1:E:325:TRP:CE2	2.42	0.55
1:F:312:TRP:HB2	1:F:314:HIS:CE1	2.42	0.55
1:A:48:PRO:HB2	1:A:49:TYR:CZ	2.42	0.55
1:A:467:ARG:HA	1:A:470:LEU:HD12	1.88	0.55
1:B:30:ARG:HH11	1:B:378:GLN:CD	2.14	0.55
1:C:124:ASN:HA	1:C:144:ARG:CB	2.37	0.55
1:C:325:TRP:O	1:C:326:HIS:CD2	2.59	0.55
1:E:102:CYS:HA	1:E:377:PHE:CD1	2.42	0.55
1:E:273:GLU:HA	1:E:276:TYR:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:O	1:A:378:GLN:HA	2.07	0.55
1:B:85:LEU:HD23	1:B:86:PRO:N	2.21	0.55
1:B:78:PRO:HD3	1:B:456:PHE:CE1	2.42	0.55
1:C:301:THR:HA	1:D:254:GLN:HA	1.89	0.55
1:C:420:ARG:HB2	1:C:423:GLN:HE22	1.72	0.55
1:A:70:TYR:CZ	1:A:201:VAL:HA	2.42	0.54
1:E:169:TRP:H	1:E:207:ALA:C	2.15	0.54
1:A:26:GLU:N	1:A:26:GLU:CD	2.66	0.54
1:A:172:GLY:HA3	1:A:189:GLU:CD	2.32	0.54
1:B:80:PRO:HA	1:B:83:PHE:HB2	1.89	0.54
1:C:190:LEU:HD12	1:C:191:ILE:N	2.22	0.54
1:D:128:ASP:HA	1:D:261:TRP:HA	1.90	0.54
1:A:169:TRP:HB2	1:A:208:MET:HB3	1.88	0.54
1:A:169:TRP:CZ2	1:A:190:LEU:HB2	2.42	0.54
1:E:100:TRP:HB2	1:E:324:CYS:SG	2.47	0.54
1:E:402:ASP:HB2	1:E:403:TRP:CD2	2.42	0.54
1:B:76:LYS:HB2	1:B:451:ASP:HA	1.89	0.54
1:E:152:LYS:HA	1:E:297:GLY:HA2	1.89	0.54
1:E:165:ILE:HD11	1:E:192:ASN:HB3	1.89	0.54
1:E:236:GLN:HE21	1:E:237:MET:HG3	1.72	0.54
1:B:99:VAL:C	1:B:379:LEU:HD22	2.33	0.54
1:B:123:TYR:CD2	1:B:263:ARG:NH2	2.76	0.54
1:E:357:THR:HG22	1:E:358:PRO:HD2	1.90	0.54
1:F:35:TYR:CE1	1:F:457:SER:C	2.86	0.54
1:F:100:TRP:CZ3	1:F:377:PHE:HB3	2.42	0.54
1:F:340:THR:O	1:F:367:HIS:CE1	2.61	0.54
1:B:262:ASN:HA	1:B:290:LEU:O	2.07	0.54
1:F:168:HIS:O	1:F:190:LEU:HD12	2.08	0.54
1:F:387:GLU:CD	1:F:387:GLU:N	2.66	0.54
1:A:168:HIS:CE1	1:A:191:ILE:HB	2.42	0.54
1:D:346:ALA:HB1	1:E:183:GLY:C	2.33	0.54
1:F:107:ILE:CG2	1:F:373:LEU:HD22	2.38	0.54
1:A:81:ASN:HA	1:A:98:LEU:HD12	1.90	0.53
1:B:186:PRO:HG2	1:B:188:LEU:HD21	1.89	0.53
1:E:49:TYR:HB2	1:E:50:PHE:CD2	2.43	0.53
1:E:393:HIS:CD2	1:E:397:THR:HG22	2.44	0.53
1:A:77:LEU:H	1:A:327:ASN:HB3	1.72	0.53
1:A:185:CYS:HB2	1:E:364:TYR:CD2	2.44	0.53
1:B:107:ILE:H	1:B:107:ILE:HD12	1.71	0.53
1:B:190:LEU:HD12	1:B:191:ILE:N	2.24	0.53
1:C:150:ASP:HA	1:C:151:TYR:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:ILE:HG21	1:C:400:LEU:HD21	1.89	0.53
1:D:334:VAL:HG12	1:D:335:ASP:H	1.72	0.53
1:D:391:TYR:O	1:D:395:MET:SD	2.66	0.53
1:D:448:TRP:CD2	1:D:449:PRO:HD2	2.43	0.53
1:F:371:PHE:CD2	1:F:371:PHE:N	2.76	0.53
1:A:22:VAL:HG21	1:A:391:TYR:CZ	2.43	0.53
1:D:426:ALA:HB3	1:D:427:VAL:C	2.34	0.53
1:F:235:LEU:HD12	1:F:235:LEU:H	1.72	0.53
1:C:43:LEU:HA	1:C:369:GLU:O	2.08	0.53
1:D:45:VAL:HA	1:D:367:HIS:O	2.08	0.53
1:E:88:ASN:HA	1:E:90:VAL:HB	1.90	0.53
1:D:472:GLN:CD	1:D:472:GLN:C	2.77	0.53
1:A:190:LEU:HD12	1:A:191:ILE:N	2.21	0.53
1:B:51:LYS:HG2	1:B:63:PRO:HA	1.91	0.53
1:B:123:TYR:HB2	1:B:145:ASP:O	2.08	0.53
1:D:77:LEU:H	1:D:327:ASN:HB3	1.73	0.53
1:D:130:GLU:HA	1:D:260:PHE:CD2	2.43	0.53
1:D:273:GLU:HA	1:D:276:TYR:CE1	2.44	0.53
1:A:73:PHE:CD2	1:A:448:TRP:HB3	2.43	0.53
1:A:367:HIS:CG	1:A:368:VAL:N	2.76	0.53
1:B:169:TRP:HB2	1:B:208:MET:HB3	1.90	0.53
1:B:241:ALA:HB3	1:B:242:TYR:CE2	2.43	0.53
1:A:397:THR:HA	1:A:400:LEU:HD12	1.91	0.53
1:C:321:ASN:H	1:C:323:ILE:CD1	2.22	0.53
1:D:121:PRO:HA	1:D:146:ASN:HA	1.91	0.53
1:E:47:HIS:CE1	1:E:49:TYR:N	2.77	0.53
1:F:36:HIS:CE1	1:F:463:PHE:CE1	2.97	0.53
1:A:322:GLY:C	1:A:323:ILE:HD12	2.34	0.53
1:A:343:SER:HA	1:A:364:TYR:O	2.09	0.53
1:A:442:TYR:HA	1:A:445:LEU:HD13	1.91	0.53
1:D:36:HIS:CD2	1:D:463:PHE:CG	2.96	0.53
1:D:218:SER:H	1:D:219:GLU:HG2	1.72	0.53
1:D:341:ASN:HD21	1:D:367:HIS:HB2	1.73	0.53
1:A:47:HIS:CE1	1:A:50:PHE:CD1	2.97	0.53
1:A:69:GLN:HB3	1:A:200:MET:SD	2.49	0.53
1:D:150:ASP:HA	1:D:151:TYR:CZ	2.44	0.53
1:D:469:PHE:C	1:D:469:PHE:CD2	2.85	0.53
1:E:413:ALA:HB3	1:E:414:SER:C	2.33	0.53
1:B:350:SER:HA	1:C:182:GLN:CD	2.34	0.52
1:C:325:TRP:C	1:C:326:HIS:CG	2.87	0.52
1:D:100:TRP:HA	1:D:379:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ALA:HA	1:D:165:ILE:HD12	1.90	0.52
1:D:73:PHE:CD2	1:D:448:TRP:HB3	2.44	0.52
1:D:79:ASP:HA	1:D:327:ASN:HD21	1.74	0.52
1:D:97:ARG:HG2	1:D:384:LEU:HD11	1.91	0.52
1:A:121:PRO:HA	1:A:146:ASN:HA	1.90	0.52
1:B:421:PHE:CG	1:B:422:VAL:N	2.75	0.52
1:C:78:PRO:HD3	1:C:456:PHE:CE1	2.44	0.52
1:E:37:ALA:HA	1:E:455:ARG:O	2.09	0.52
1:E:74:ARG:H	1:E:447:PHE:HB3	1.73	0.52
1:F:373:LEU:C	1:F:375:PHE:CZ	2.87	0.52
1:B:26:GLU:HB2	1:B:27:TYR:CE1	2.44	0.52
1:B:169:TRP:CZ2	1:B:190:LEU:HD13	2.45	0.52
1:A:166:GLY:HA2	1:A:232:PRO:HA	1.91	0.52
1:B:33:ILE:O	1:B:378:GLN:HA	2.10	0.52
1:E:440:ASP:CG	1:E:442:TYR:CE2	2.88	0.52
1:F:393:HIS:C	1:F:393:HIS:CD2	2.86	0.52
1:F:472:GLN:CD	1:F:472:GLN:C	2.78	0.52
1:E:70:TYR:CZ	1:E:201:VAL:HA	2.44	0.52
1:E:344:VAL:O	1:E:363:GLU:HA	2.10	0.52
1:E:391:TYR:CE1	1:E:395:MET:HE1	2.44	0.52
1:F:43:LEU:HD13	1:F:43:LEU:C	2.35	0.52
1:F:360:SER:HB2	1:F:361:PHE:CE2	2.43	0.52
1:A:99:VAL:HG12	1:A:382:ILE:HD11	1.90	0.52
1:B:423:GLN:HE21	1:B:423:GLN:HA	1.75	0.52
1:C:43:LEU:HD11	1:C:368:VAL:CG1	2.40	0.52
1:E:356:TYR:C	1:E:356:TYR:CD2	2.88	0.52
1:F:100:TRP:HA	1:F:100:TRP:CE3	2.45	0.52
1:A:47:HIS:HE1	1:A:49:TYR:HB2	1.72	0.52
1:A:149:VAL:HG22	1:A:150:ASP:H	1.75	0.52
1:B:35:TYR:O	1:B:376:ILE:HA	2.10	0.52
1:E:169:TRP:CZ2	1:E:190:LEU:HB2	2.45	0.52
1:E:393:HIS:CG	1:E:408:THR:HG21	2.45	0.52
1:E:420:ARG:O	1:E:421:PHE:CD1	2.63	0.52
1:E:424:SER:HA	1:E:425:ALA:CB	2.40	0.52
1:F:391:TYR:C	1:F:391:TYR:CD1	2.87	0.52
1:A:157:CYS:SG	1:A:158:ILE:N	2.83	0.52
1:A:448:TRP:CE2	1:F:419:TYR:CZ	2.98	0.52
1:B:150:ASP:HA	1:B:151:TYR:CZ	2.45	0.52
1:B:240:ASP:CG	1:B:243:GLY:H	2.18	0.52
1:E:33:ILE:O	1:E:378:GLN:HG3	2.10	0.52
1:E:210:PHE:C	1:E:212:LEU:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:HA	1:A:371:PHE:CE1	2.45	0.52
1:B:80:PRO:HB2	1:B:379:LEU:HD21	1.91	0.52
1:B:231:TYR:CD1	1:B:232:PRO:HD2	2.45	0.52
1:C:66:SER:HA	1:C:367:HIS:CG	2.45	0.52
1:D:78:PRO:HA	1:D:453:LYS:HG2	1.92	0.52
1:E:467:ARG:HA	1:E:470:LEU:HD12	1.91	0.52
1:F:26:GLU:N	1:F:26:GLU:CD	2.68	0.52
1:B:386:THR:HA	1:B:389:MET:SD	2.50	0.51
1:C:309:LYS:O	1:C:311:TYR:CZ	2.63	0.51
1:C:469:PHE:HA	1:C:472:GLN:OE1	2.09	0.51
1:D:35:TYR:CD1	1:D:456:PHE:CD2	2.99	0.51
1:D:363:GLU:N	1:E:268:GLY:H	2.09	0.51
1:F:103:VAL:HG22	1:F:376:ILE:O	2.10	0.51
1:E:27:TYR:CD1	1:E:27:TYR:N	2.74	0.51
1:E:160:GLY:HA3	1:E:245:SER:O	2.10	0.51
1:E:347:SER:HA	1:E:361:PHE:HA	1.93	0.51
1:C:30:ARG:HA	1:C:380:CYS:SG	2.51	0.51
1:E:25:ASP:HA	1:E:28:VAL:HB	1.93	0.51
1:F:169:TRP:CZ2	1:F:190:LEU:HB2	2.45	0.51
1:F:190:LEU:HD12	1:F:191:ILE:N	2.26	0.51
1:F:314:HIS:N	1:F:314:HIS:CD2	2.74	0.51
1:A:275:LEU:HA	1:E:226:GLN:HE21	1.75	0.51
1:B:176:LYS:HG2	1:B:178:THR:HG23	1.91	0.51
1:B:392:ILE:HG21	1:B:400:LEU:HD21	1.91	0.51
1:F:36:HIS:CG	1:F:463:PHE:CG	2.98	0.51
1:F:243:GLY:HA3	1:F:318:GLY:HA3	1.92	0.51
1:C:173:THR:H	1:C:189:GLU:CD	2.19	0.51
1:D:278:LYS:HB2	1:D:284:ALA:HA	1.91	0.51
1:A:232:PRO:O	1:A:234:TYR:CE2	2.64	0.51
1:A:395:MET:SD	1:A:395:MET:C	2.94	0.51
1:B:462:GLN:N	1:B:462:GLN:CD	2.69	0.51
1:C:34:PHE:CE1	1:C:378:GLN:HB2	2.45	0.51
1:D:120:HIS:CD2	1:D:222:LEU:HD21	2.46	0.51
1:F:409:PRO:HB2	1:F:411:PRO:HD3	1.93	0.51
1:A:74:ARG:HH22	1:A:440:ASP:CG	2.18	0.51
1:A:100:TRP:HA	1:A:379:LEU:HD12	1.92	0.51
1:A:196:GLU:H	1:A:199:ASP:CG	2.19	0.51
1:C:27:TYR:N	1:C:27:TYR:CD1	2.79	0.51
1:C:48:PRO:HB2	1:C:49:TYR:CZ	2.46	0.51
1:C:309:LYS:O	1:C:311:TYR:CE1	2.63	0.51
1:D:120:HIS:CD2	1:D:120:HIS:C	2.87	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:PHE:CD2	1:D:227:SER:O	2.64	0.51
1:E:80:PRO:HD3	1:E:327:ASN:HD21	1.76	0.51
1:C:421:PHE:C	1:C:423:GLN:H	2.19	0.51
1:A:375:PHE:HB3	1:A:377:PHE:CE2	2.46	0.51
1:D:169:TRP:CZ2	1:D:190:LEU:HB2	2.46	0.51
1:F:35:TYR:CE2	1:F:458:ALA:HA	2.46	0.51
1:A:38:GLY:HA2	1:A:373:LEU:O	2.10	0.50
1:B:120:HIS:CD2	1:B:122:LEU:N	2.79	0.50
1:C:310:PRO:HB2	1:C:312:TRP:CE2	2.46	0.50
1:E:91:TYR:CD2	1:E:96:GLN:HB2	2.46	0.50
1:E:209:ASP:HB3	1:E:212:LEU:HD22	1.93	0.50
1:C:97:ARG:HB2	1:C:403:TRP:CZ3	2.47	0.50
1:D:195:ILE:HD13	1:D:230:LYS:HD3	1.94	0.50
1:D:384:LEU:HD13	1:D:405:PHE:CD2	2.46	0.50
1:F:244:ASP:HB3	1:F:320:ASN:HB3	1.92	0.50
1:A:97:ARG:HB3	1:A:403:TRP:CZ2	2.46	0.50
1:D:235:LEU:H	1:D:235:LEU:CD1	2.20	0.50
1:E:200:MET:SD	1:E:229:CYS:HB2	2.52	0.50
1:F:123:TYR:O	1:F:144:ARG:HA	2.12	0.50
1:F:307:PHE:CE1	1:F:307:PHE:HA	2.40	0.50
1:B:70:TYR:CE2	1:B:201:VAL:HA	2.46	0.50
1:E:168:HIS:HA	1:E:207:ALA:HB1	1.94	0.50
1:F:35:TYR:CE1	1:F:456:PHE:CE2	2.99	0.50
1:A:70:TYR:CE1	1:A:201:VAL:HG12	2.45	0.50
1:A:169:TRP:CH2	1:A:190:LEU:HB2	2.46	0.50
1:B:165:ILE:HA	1:B:194:PRO:HA	1.94	0.50
1:B:190:LEU:HD12	1:B:191:ILE:H	1.76	0.50
1:B:442:TYR:HA	1:B:445:LEU:HD12	1.92	0.50
1:D:120:HIS:CE1	1:D:122:LEU:C	2.90	0.50
1:D:467:ARG:O	1:D:471:LEU:HG	2.11	0.50
1:E:32:SER:C	1:E:34:PHE:CE2	2.90	0.50
1:A:141:LYS:H	1:A:141:LYS:HD3	1.77	0.50
1:A:448:TRP:CD2	1:F:419:TYR:CZ	3.00	0.50
1:D:391:TYR:CE2	1:D:392:ILE:HD13	2.46	0.50
1:E:139:ASP:CG	1:E:141:LYS:HZ1	2.19	0.50
1:E:259:HIS:H	1:E:294:SER:HB3	1.76	0.50
1:F:68:TYR:C	1:F:201:VAL:HG13	2.37	0.50
1:F:232:PRO:HB2	1:F:234:TYR:CE1	2.47	0.50
1:F:262:ASN:HA	1:F:290:LEU:O	2.12	0.50
1:A:73:PHE:HB3	1:A:450:VAL:HG21	1.94	0.50
1:A:74:ARG:HB2	1:A:447:PHE:CG	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG13	1:A:375:PHE:CE1	2.47	0.50
1:A:448:TRP:CE2	1:F:419:TYR:CE2	3.00	0.50
1:B:35:TYR:HB2	1:B:377:PHE:HB2	1.94	0.50
1:C:209:ASP:O	1:C:213:LEU:HD13	2.12	0.50
1:D:78:PRO:CA	1:D:453:LYS:HG2	2.42	0.50
1:D:91:TYR:CZ	1:D:98:LEU:HG	2.46	0.50
1:D:305:GLN:CD	1:D:307:PHE:H	2.20	0.50
1:D:392:ILE:HG21	1:D:400:LEU:HD21	1.94	0.50
1:F:439:GLN:HA	1:F:443:ASP:OD2	2.10	0.50
1:A:377:PHE:CD2	1:A:377:PHE:N	2.79	0.50
1:A:430:GLN:NE2	1:A:432:ASP:H	2.10	0.50
1:B:33:ILE:O	1:B:34:PHE:CD1	2.65	0.50
1:B:36:HIS:CG	1:B:463:PHE:CD2	3.00	0.50
1:C:101:ALA:HA	1:C:324:CYS:HG	1.76	0.50
1:C:105:VAL:O	1:C:311:TYR:CD2	2.65	0.50
1:D:461:ASP:HA	1:D:467:ARG:HG2	1.94	0.50
1:F:209:ASP:CG	1:F:212:LEU:HG	2.37	0.50
1:A:96:GLN:HA	1:A:383:THR:HA	1.93	0.50
1:C:152:LYS:HA	1:C:297:GLY:HA2	1.93	0.50
1:C:214:GLN:CD	1:C:219:GLU:H	2.20	0.50
1:C:231:TYR:CD1	1:C:232:PRO:HD2	2.47	0.50
1:D:409:PRO:HB2	1:D:410:PRO:HA	1.94	0.50
1:E:42:LEU:O	1:E:370:GLU:HA	2.12	0.50
1:F:102:CYS:HA	1:F:377:PHE:CD1	2.46	0.50
1:F:107:ILE:H	1:F:107:ILE:CD1	2.21	0.50
1:F:241:ALA:HB3	1:F:242:TYR:CD2	2.47	0.50
1:A:38:GLY:H	1:A:455:ARG:CB	2.23	0.49
1:A:71:ARG:O	1:A:332:THR:HA	2.12	0.49
1:B:19:ALA:H	1:F:407:VAL:N	2.10	0.49
1:D:36:HIS:CD2	1:D:463:PHE:CD1	3.00	0.49
1:E:73:PHE:CE2	1:E:448:TRP:HB2	2.47	0.49
1:F:11:VAL:HG13	1:F:12:TYR:CE2	2.47	0.49
1:A:42:LEU:H	1:A:371:PHE:H	1.59	0.49
1:B:38:GLY:H	1:B:455:ARG:HB3	1.76	0.49
1:C:73:PHE:CD2	1:C:448:TRP:HB3	2.47	0.49
1:E:342:LEU:O	1:E:365:ALA:HA	2.12	0.49
1:A:243:GLY:HA3	1:A:319:LEU:H	1.77	0.49
1:B:464:PRO:HA	1:B:467:ARG:HD2	1.94	0.49
1:A:256:PHE:CZ	1:A:296:SER:HB3	2.47	0.49
1:A:448:TRP:CZ3	1:F:419:TYR:CE1	3.00	0.49
1:B:97:ARG:CB	1:B:403:TRP:CE2	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:GLY:HA2	1:E:232:PRO:HA	1.94	0.49
1:F:385:THR:O	1:F:389:MET:HG3	2.11	0.49
1:A:22:VAL:HG11	1:A:391:TYR:CE2	2.48	0.49
1:A:78:PRO:CD	1:A:456:PHE:CZ	2.95	0.49
1:A:180:VAL:HG22	1:A:181:VAL:H	1.77	0.49
1:D:373:LEU:C	1:D:375:PHE:CZ	2.90	0.49
1:A:393:HIS:CD2	1:A:394:ASN:ND2	2.81	0.49
1:B:42:LEU:C	1:B:43:LEU:HG	2.37	0.49
1:B:400:LEU:HB3	1:B:405:PHE:CG	2.48	0.49
1:C:262:ASN:HA	1:C:290:LEU:O	2.11	0.49
1:D:35:TYR:CE1	1:D:457:SER:C	2.91	0.49
1:E:69:GLN:N	1:E:201:VAL:HG13	2.26	0.49
1:F:372:ASP:C	1:F:373:LEU:HD23	2.37	0.49
1:A:84:GLY:HA3	1:F:83:PHE:CE2	2.48	0.49
1:B:168:HIS:O	1:B:190:LEU:HD12	2.12	0.49
1:C:388:VAL:O	1:C:392:ILE:HG12	2.13	0.49
1:D:248:PHE:CG	1:D:249:CYS:N	2.81	0.49
1:A:78:PRO:HD3	1:A:456:PHE:CE1	2.46	0.49
1:A:440:ASP:OD1	1:A:442:TYR:CD2	2.66	0.49
1:B:168:HIS:CE1	1:B:191:ILE:HB	2.48	0.49
1:C:158:ILE:HG23	1:C:248:PHE:O	2.13	0.49
1:E:33:ILE:O	1:E:378:GLN:HA	2.13	0.49
1:B:169:TRP:CZ2	1:B:190:LEU:HB2	2.48	0.49
1:B:385:THR:O	1:B:388:VAL:HB	2.13	0.49
1:B:398:THR:O	1:B:402:ASP:CG	2.56	0.49
1:C:94:ASN:O	1:C:384:LEU:HD12	2.13	0.49
1:D:234:TYR:HA	1:D:237:MET:SD	2.53	0.49
1:E:36:HIS:CG	1:E:37:ALA:N	2.80	0.49
1:E:165:ILE:HA	1:E:194:PRO:HA	1.95	0.49
1:B:121:PRO:HD2	1:B:222:LEU:HD11	1.95	0.49
1:B:173:THR:H	1:F:427:VAL:HG23	1.78	0.49
1:C:345:CYS:HA	1:C:363:GLU:HG3	1.93	0.49
1:C:454:GLU:CD	1:C:454:GLU:N	2.71	0.49
1:D:165:ILE:HD12	1:D:165:ILE:N	2.28	0.49
1:D:169:TRP:CH2	1:D:189:GLU:C	2.91	0.49
1:B:252:ARG:HB3	1:B:306:LEU:HD11	1.94	0.48
1:C:33:ILE:O	1:C:378:GLN:HG2	2.13	0.48
1:D:169:TRP:HE1	1:D:190:LEU:HD22	1.77	0.48
1:E:210:PHE:CD2	1:E:227:SER:O	2.66	0.48
1:E:259:HIS:HB2	1:E:261:TRP:CH2	2.48	0.48
1:E:267:MET:HA	1:E:267:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:ASP:HA	1:F:28:VAL:HB	1.95	0.48
1:D:320:ASN:CG	1:D:323:ILE:HD12	2.39	0.48
1:D:461:ASP:CG	1:E:20:LYS:HZ2	2.21	0.48
1:F:33:ILE:O	1:F:378:GLN:HA	2.13	0.48
1:A:469:PHE:CD2	1:A:469:PHE:C	2.91	0.48
1:D:39:SER:O	1:D:372:ASP:CG	2.55	0.48
1:E:242:TYR:HA	1:E:319:LEU:HD12	1.95	0.48
1:F:79:ASP:HA	1:F:327:ASN:HD21	1.78	0.48
1:F:210:PHE:CD2	1:F:227:SER:O	2.67	0.48
1:A:80:PRO:HG3	1:A:379:LEU:HD11	1.94	0.48
1:B:41:ARG:HH22	1:C:233:ASP:CG	2.21	0.48
1:B:97:ARG:HB2	1:B:403:TRP:CH2	2.49	0.48
1:B:312:TRP:HB2	1:B:314:HIS:CE1	2.49	0.48
1:B:454:GLU:CD	1:B:454:GLU:N	2.72	0.48
1:C:75:VAL:O	1:C:328:GLN:HA	2.14	0.48
1:D:47:HIS:CE1	1:D:49:TYR:N	2.79	0.48
1:D:254:GLN:HE21	1:D:254:GLN:C	2.22	0.48
1:E:73:PHE:O	1:E:330:PHE:HA	2.13	0.48
1:B:85:LEU:HD21	1:B:87:ASP:OD2	2.13	0.48
1:C:208:MET:HG3	1:C:210:PHE:CZ	2.48	0.48
1:D:120:HIS:CE1	1:D:218:SER:HA	2.48	0.48
1:E:193:THR:HB	1:E:230:LYS:HD3	1.94	0.48
1:E:325:TRP:C	1:E:326:HIS:CD2	2.91	0.48
1:E:440:ASP:HB3	1:E:442:TYR:CZ	2.48	0.48
1:E:464:PRO:HA	1:E:467:ARG:CZ	2.42	0.48
1:F:79:ASP:CG	1:F:81:ASN:H	2.21	0.48
1:A:32:SER:C	1:A:34:PHE:CE2	2.92	0.48
1:A:232:PRO:HB2	1:A:234:TYR:CE1	2.49	0.48
1:A:279:GLY:H	1:A:284:ALA:HA	1.78	0.48
1:A:416:VAL:CG2	1:A:417:ASP:H	2.27	0.48
1:B:76:LYS:H	1:B:76:LYS:HD2	1.77	0.48
1:C:259:HIS:HB2	1:C:261:TRP:CH2	2.49	0.48
1:C:469:PHE:CD1	1:C:472:GLN:OE1	2.67	0.48
1:F:455:ARG:HH11	1:F:455:ARG:HB3	1.78	0.48
1:A:375:PHE:CB	1:A:377:PHE:CE2	2.97	0.48
1:A:420:ARG:HH11	1:F:370:GLU:HG2	1.78	0.48
1:B:438:LYS:HG2	1:B:439:GLN:H	1.78	0.48
1:C:126:LEU:HB3	1:C:262:ASN:O	2.13	0.48
1:D:48:PRO:HB2	1:D:49:TYR:CE1	2.48	0.48
1:D:168:HIS:O	1:D:190:LEU:HD12	2.13	0.48
1:E:97:ARG:HD3	1:E:97:ARG:HA	1.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:370:GLU:O	1:E:371:PHE:CD2	2.67	0.48
1:A:102:CYS:HA	1:A:377:PHE:CD1	2.48	0.48
1:A:361:PHE:N	1:A:361:PHE:CD2	2.81	0.48
1:B:96:GLN:HA	1:B:384:LEU:HG	1.96	0.48
1:B:250:LEU:HD11	1:B:306:LEU:HD13	1.96	0.48
1:D:172:GLY:HA2	1:D:189:GLU:HB2	1.95	0.48
1:F:166:GLY:HA2	1:F:232:PRO:HA	1.95	0.48
1:A:24:THR:HG23	1:A:320:ASN:HA	1.96	0.48
1:A:43:LEU:HA	1:A:369:GLU:O	2.14	0.48
1:C:248:PHE:CZ	1:C:250:LEU:HB2	2.49	0.48
1:C:469:PHE:CZ	1:C:473:LEU:HD21	2.48	0.48
1:D:256:PHE:CE1	1:D:296:SER:HB3	2.49	0.48
1:D:364:TYR:HB3	1:D:366:ARG:CZ	2.44	0.48
1:E:273:GLU:CD	1:E:273:GLU:N	2.71	0.48
1:E:391:TYR:HA	1:E:394:ASN:ND2	2.29	0.48
1:E:442:TYR:HA	1:E:445:LEU:HD12	1.96	0.48
1:E:464:PRO:O	1:E:468:LYS:HG3	2.14	0.48
1:F:27:TYR:C	1:F:27:TYR:CD2	2.92	0.48
1:A:309:LYS:O	1:A:311:TYR:CE2	2.66	0.48
1:B:73:PHE:CD2	1:B:448:TRP:HB3	2.49	0.48
1:B:130:GLU:CD	1:B:260:PHE:H	2.21	0.48
1:B:341:ASN:ND2	1:B:367:HIS:CD2	2.79	0.48
1:C:33:ILE:O	1:C:378:GLN:CG	2.61	0.48
1:C:391:TYR:CZ	1:C:395:MET:SD	3.07	0.48
1:D:379:LEU:HG	1:D:380:CYS:N	2.29	0.48
1:E:47:HIS:CE1	1:E:50:PHE:CD1	3.02	0.48
1:A:22:VAL:HG21	1:A:391:TYR:CE1	2.49	0.47
1:B:100:TRP:CZ2	1:B:456:PHE:CE2	3.01	0.47
1:B:174:ALA:HB2	1:B:187:PRO:HG3	1.96	0.47
1:C:248:PHE:C	1:C:248:PHE:CD2	2.92	0.47
1:C:350:SER:HA	1:D:182:GLN:HG2	1.94	0.47
1:F:38:GLY:HA2	1:F:375:PHE:CE2	2.48	0.47
1:F:171:LYS:HA	1:F:188:LEU:HD23	1.95	0.47
1:C:168:HIS:CE1	1:C:193:THR:OG1	2.67	0.47
1:C:169:TRP:CH2	1:C:190:LEU:HB2	2.49	0.47
1:D:26:GLU:HG2	1:D:27:TYR:CD1	2.49	0.47
1:D:346:ALA:HB1	1:E:183:GLY:O	2.15	0.47
1:E:469:PHE:CD2	1:E:469:PHE:C	2.92	0.47
1:A:262:ASN:HA	1:A:290:LEU:O	2.14	0.47
1:A:326:HIS:CE1	1:A:399:ILE:HG13	2.48	0.47
1:B:13:LEU:HD12	1:B:390:SER:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:PHE:CE2	1:C:448:TRP:HB3	2.49	0.47
1:E:167:GLU:CD	1:E:233:ASP:HB2	2.39	0.47
1:F:36:HIS:CD2	1:F:463:PHE:CG	3.03	0.47
1:F:397:THR:HA	1:F:400:LEU:HD12	1.96	0.47
1:F:464:PRO:HD3	1:F:467:ARG:HH21	1.78	0.47
1:A:96:GLN:HA	1:A:382:ILE:O	2.15	0.47
1:A:273:GLU:HB3	1:A:278:LYS:HZ1	1.79	0.47
1:B:13:LEU:O	1:B:393:HIS:CE1	2.68	0.47
1:B:340:THR:C	1:B:341:ASN:HD22	2.21	0.47
1:D:47:HIS:CD2	1:D:48:PRO:HD2	2.49	0.47
1:D:91:TYR:CE2	1:D:96:GLN:HB2	2.50	0.47
1:D:148:SER:HB3	1:E:291:TYR:CD1	2.49	0.47
1:D:369:GLU:C	1:D:369:GLU:CD	2.83	0.47
1:D:379:LEU:HG	1:D:380:CYS:H	1.80	0.47
1:D:469:PHE:CE1	1:D:472:GLN:NE2	2.82	0.47
1:D:470:LEU:HD23	1:D:473:LEU:HD11	1.96	0.47
1:B:142:ASP:CG	1:C:283:ARG:HE	2.22	0.47
1:B:179:THR:OG1	1:B:181:VAL:HG23	2.15	0.47
1:C:356:TYR:CD1	1:E:277:ILE:HD12	2.50	0.47
1:C:460:LEU:HD22	1:C:470:LEU:HG	1.96	0.47
1:F:165:ILE:HA	1:F:194:PRO:HA	1.96	0.47
1:A:208:MET:SD	1:A:208:MET:C	2.97	0.47
1:A:209:ASP:C	1:A:213:LEU:HD12	2.40	0.47
1:A:444:LYS:HB2	1:A:445:LEU:HD12	1.97	0.47
1:B:24:THR:HA	1:B:27:TYR:CZ	2.50	0.47
1:B:312:TRP:CZ3	1:B:469:PHE:HB2	2.50	0.47
1:C:169:TRP:CZ3	1:C:190:LEU:CA	2.98	0.47
1:E:26:GLU:N	1:E:26:GLU:CD	2.72	0.47
1:E:91:TYR:CE1	1:E:93:PRO:HB3	2.49	0.47
1:E:461:ASP:C	1:E:463:PHE:H	2.23	0.47
1:A:36:HIS:HD1	1:A:457:SER:HB3	1.80	0.47
1:A:80:PRO:CB	1:A:379:LEU:HD11	2.45	0.47
1:A:83:PHE:CD2	1:F:84:GLY:HA2	2.50	0.47
1:B:405:PHE:CD2	1:B:406:GLY:N	2.83	0.47
1:C:97:ARG:CG	1:C:384:LEU:HD11	2.44	0.47
1:D:70:TYR:CZ	1:D:201:VAL:HA	2.50	0.47
1:D:81:ASN:HA	1:D:98:LEU:HD12	1.96	0.47
1:E:70:TYR:C	1:E:71:ARG:HE	2.23	0.47
1:E:323:ILE:HB	1:E:325:TRP:CZ2	2.49	0.47
1:A:121:PRO:HD2	1:A:222:LEU:HD11	1.96	0.47
1:A:124:ASN:HA	1:A:144:ARG:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HD12	1:A:314:HIS:H	1.79	0.47
1:B:81:ASN:HD21	1:B:403:TRP:NE1	2.11	0.47
1:C:91:TYR:HB3	1:C:381:LYS:HE2	1.96	0.47
1:D:34:PHE:HA	1:D:377:PHE:O	2.15	0.47
1:D:162:VAL:HG21	1:D:244:ASP:HB2	1.96	0.47
1:D:334:VAL:HG12	1:D:335:ASP:N	2.30	0.47
1:E:373:LEU:HB3	1:E:375:PHE:CZ	2.50	0.47
1:E:385:THR:O	1:E:388:VAL:HB	2.15	0.47
1:E:466:GLY:O	1:E:470:LEU:HG	2.15	0.47
1:F:190:LEU:HD12	1:F:191:ILE:H	1.79	0.47
1:A:47:HIS:CD2	1:A:48:PRO:CD	2.95	0.47
1:A:170:THR:CB	1:A:191:ILE:HD11	2.45	0.47
1:A:317:GLN:HG3	1:A:318:GLY:H	1.80	0.47
1:A:459:ASP:O	1:A:463:PHE:CD2	2.68	0.47
1:B:256:PHE:CZ	1:B:296:SER:HB3	2.50	0.47
1:B:328:GLN:O	1:B:329:LEU:HD12	2.15	0.47
1:C:319:LEU:N	1:C:319:LEU:HD22	2.30	0.47
1:D:392:ILE:O	1:D:392:ILE:HG22	2.14	0.47
1:E:373:LEU:HB3	1:E:375:PHE:CE2	2.50	0.47
1:F:43:LEU:HD21	1:F:45:VAL:HG13	1.95	0.47
1:A:121:PRO:CD	1:A:222:LEU:HD11	2.45	0.46
1:C:196:GLU:CD	1:C:446:LYS:H	2.22	0.46
1:C:346:ALA:HB1	1:D:183:GLY:HA2	1.97	0.46
1:C:391:TYR:CD2	1:C:392:ILE:HD13	2.50	0.46
1:D:209:ASP:HB3	1:D:212:LEU:HB3	1.97	0.46
1:E:168:HIS:CD2	1:E:191:ILE:HD12	2.50	0.46
1:F:170:THR:HG22	1:F:171:LYS:N	2.30	0.46
1:F:256:PHE:CZ	1:F:296:SER:HB3	2.51	0.46
1:A:26:GLU:C	1:A:27:TYR:CD1	2.93	0.46
1:A:169:TRP:CZ2	1:A:190:LEU:HD22	2.50	0.46
1:A:391:TYR:CE1	1:A:395:MET:HB2	2.51	0.46
1:B:277:ILE:HG23	1:B:278:LYS:O	2.16	0.46
1:C:78:PRO:CD	1:C:456:PHE:CE1	2.99	0.46
1:C:374:GLN:O	1:C:375:PHE:CE1	2.67	0.46
1:E:169:TRP:HE1	1:E:190:LEU:HD22	1.80	0.46
1:E:175:CYS:SG	1:E:176:LYS:HD2	2.55	0.46
1:F:99:VAL:HB	1:F:382:ILE:HD11	1.96	0.46
1:F:259:HIS:C	1:F:260:PHE:CD1	2.94	0.46
1:F:259:HIS:HB2	1:F:261:TRP:CH2	2.51	0.46
1:F:310:PRO:HG2	1:F:312:TRP:CZ2	2.50	0.46
1:A:404:ASN:C	1:A:405:PHE:CG	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:MET:SD	1:B:210:PHE:CD2	3.08	0.46
1:C:47:HIS:HE1	1:C:50:PHE:CE2	2.32	0.46
1:C:373:LEU:HB3	1:C:375:PHE:CE2	2.51	0.46
1:F:36:HIS:CG	1:F:37:ALA:N	2.83	0.46
1:F:374:GLN:OE1	1:F:463:PHE:HB3	2.16	0.46
1:A:36:HIS:CD2	1:A:463:PHE:CG	3.02	0.46
1:B:421:PHE:CE2	1:B:422:VAL:HB	2.51	0.46
1:D:70:TYR:CE2	1:D:201:VAL:HA	2.50	0.46
1:D:104:GLY:HA2	1:D:311:TYR:O	2.15	0.46
1:D:240:ASP:CG	1:D:241:ALA:N	2.73	0.46
1:E:30:ARG:HD3	1:E:378:GLN:OE1	2.16	0.46
1:E:78:PRO:N	1:E:453:LYS:HG2	2.30	0.46
1:A:100:TRP:CE2	1:A:379:LEU:HD13	2.51	0.46
1:B:202:ASP:CG	1:B:204:GLY:H	2.24	0.46
1:C:208:MET:HG3	1:C:210:PHE:CE1	2.50	0.46
1:C:424:SER:H	1:C:428:THR:HG21	1.79	0.46
1:E:34:PHE:HA	1:E:377:PHE:O	2.15	0.46
1:A:61:ASP:O	1:F:423:GLN:HB3	2.15	0.46
1:A:335:ASP:CG	1:A:337:THR:H	2.24	0.46
1:B:47:HIS:CG	1:B:48:PRO:HD2	2.50	0.46
1:C:73:PHE:HB3	1:C:450:VAL:HG21	1.96	0.46
1:C:123:TYR:CE2	1:C:263:ARG:NH1	2.84	0.46
1:C:313:LEU:C	1:C:314:HIS:CG	2.93	0.46
1:D:26:GLU:CD	1:D:26:GLU:N	2.72	0.46
1:D:57:ASN:C	1:D:59:ARG:HA	2.41	0.46
1:D:97:ARG:HB3	1:D:403:TRP:CZ2	2.49	0.46
1:D:169:TRP:H	1:D:208:MET:HA	1.80	0.46
1:D:389:MET:HA	1:D:392:ILE:HG12	1.98	0.46
1:F:153:GLN:OE1	1:F:253:GLU:HA	2.15	0.46
1:A:47:HIS:CE1	1:A:49:TYR:C	2.93	0.46
1:B:70:TYR:CD1	1:B:201:VAL:HG12	2.51	0.46
1:B:74:ARG:HB2	1:B:447:PHE:CG	2.51	0.46
1:C:312:TRP:CH2	1:C:469:PHE:HA	2.50	0.46
1:D:32:SER:C	1:D:34:PHE:CE2	2.94	0.46
1:E:55:GLY:O	1:E:57:ASN:HA	2.14	0.46
1:E:248:PHE:CG	1:E:249:CYS:N	2.84	0.46
1:F:419:TYR:CE1	1:F:420:ARG:CZ	2.99	0.46
1:F:422:VAL:HG11	1:F:428:THR:HA	1.96	0.46
1:A:130:GLU:CD	1:A:260:PHE:H	2.24	0.46
1:A:451:ASP:CG	1:A:452:LEU:N	2.74	0.46
1:B:19:ALA:H	1:F:407:VAL:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ARG:HH21	1:C:370:GLU:HG3	1.81	0.46
1:D:48:PRO:HA	1:D:65:VAL:O	2.16	0.46
1:E:323:ILE:HG21	1:E:325:TRP:CZ3	2.51	0.46
1:F:385:THR:O	1:F:388:VAL:HG12	2.15	0.46
1:A:33:ILE:O	1:A:34:PHE:CD1	2.69	0.46
1:A:309:LYS:HB2	1:A:311:TYR:CE1	2.50	0.46
1:A:346:ALA:HB1	1:B:183:GLY:HA2	1.96	0.46
1:B:91:TYR:CE2	1:B:97:ARG:HA	2.50	0.46
1:B:451:ASP:CG	1:B:453:LYS:H	2.24	0.46
1:C:77:LEU:HD12	1:C:327:ASN:HA	1.97	0.46
1:C:462:GLN:C	1:C:467:ARG:HH21	2.23	0.46
1:D:27:TYR:CD1	1:D:27:TYR:N	2.83	0.46
1:D:172:GLY:H	1:D:188:LEU:HA	1.81	0.46
1:E:343:SER:HA	1:E:364:TYR:O	2.15	0.46
1:F:42:LEU:O	1:F:370:GLU:HA	2.16	0.46
1:F:120:HIS:CE1	1:F:122:LEU:HB2	2.51	0.46
1:F:404:ASN:HB3	1:F:405:PHE:CD2	2.51	0.46
1:A:107:ILE:HB	1:A:307:PHE:CE1	2.51	0.46
1:A:172:GLY:HA3	1:A:189:GLU:HB2	1.98	0.46
1:B:12:TYR:CE2	1:B:13:LEU:HD21	2.51	0.46
1:B:47:HIS:CD2	1:B:48:PRO:HD2	2.51	0.46
1:B:391:TYR:CE1	1:F:408:THR:HG23	2.50	0.46
1:B:448:TRP:CD1	1:B:448:TRP:C	2.94	0.46
1:C:33:ILE:O	1:C:378:GLN:HA	2.15	0.46
1:C:153:GLN:HB3	1:C:254:GLN:HG2	1.98	0.46
1:C:196:GLU:OE2	1:C:445:LEU:HA	2.15	0.46
1:D:375:PHE:HB2	1:D:377:PHE:CE2	2.51	0.46
1:D:460:LEU:HA	1:D:466:GLY:HA3	1.98	0.46
1:E:91:TYR:CD2	1:E:98:LEU:HD21	2.51	0.46
1:E:388:VAL:O	1:E:391:TYR:HB3	2.15	0.46
1:A:393:HIS:HA	1:A:400:LEU:HD12	1.98	0.45
1:B:157:CYS:SG	1:B:158:ILE:N	2.89	0.45
1:B:387:GLU:CD	1:B:387:GLU:N	2.68	0.45
1:D:24:THR:HA	1:D:27:TYR:CZ	2.52	0.45
1:D:126:LEU:HB3	1:D:262:ASN:O	2.16	0.45
1:D:209:ASP:C	1:D:209:ASP:OD1	2.59	0.45
1:F:75:VAL:HG13	1:F:450:VAL:HB	1.98	0.45
1:A:252:ARG:HH22	1:A:254:GLN:HB3	1.82	0.45
1:B:448:TRP:CE2	1:B:449:PRO:HD2	2.50	0.45
1:C:30:ARG:HH12	1:C:378:GLN:CD	2.24	0.45
1:C:36:HIS:CG	1:C:37:ALA:N	2.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:TYR:H	1:C:69:GLN:HG2	1.81	0.45
1:C:441:PRO:C	1:C:443:ASP:H	2.24	0.45
1:D:150:ASP:CG	1:D:151:TYR:H	2.24	0.45
1:D:153:GLN:HB3	1:D:254:GLN:HB3	1.98	0.45
1:D:393:HIS:CG	1:D:394:ASN:N	2.84	0.45
1:F:102:CYS:HA	1:F:377:PHE:CG	2.51	0.45
1:A:47:HIS:HE1	1:A:50:PHE:CG	2.35	0.45
1:A:73:PHE:CD1	1:A:73:PHE:N	2.82	0.45
1:A:77:LEU:HG	1:A:327:ASN:HB3	1.99	0.45
1:A:172:GLY:H	1:A:188:LEU:HA	1.81	0.45
1:B:426:ALA:HA	1:B:427:VAL:HG13	1.97	0.45
1:C:210:PHE:CD2	1:C:227:SER:O	2.69	0.45
1:E:98:LEU:HB3	1:E:379:LEU:HD21	1.98	0.45
1:E:109:ARG:HD3	1:E:110:GLY:N	2.32	0.45
1:E:167:GLU:HG2	1:E:231:TYR:O	2.16	0.45
1:A:71:ARG:C	1:A:73:PHE:CE1	2.94	0.45
1:A:240:ASP:CG	1:A:244:ASP:H	2.25	0.45
1:B:78:PRO:HB2	1:B:100:TRP:HE1	1.81	0.45
1:C:43:LEU:HD11	1:C:368:VAL:HG12	1.99	0.45
1:C:80:PRO:HD3	1:C:100:TRP:HE1	1.81	0.45
1:D:24:THR:HG21	1:D:320:ASN:HA	1.99	0.45
1:D:170:THR:HG22	1:D:191:ILE:CG2	2.46	0.45
1:A:330:PHE:N	1:A:330:PHE:CD2	2.81	0.45
1:A:398:THR:HA	1:A:401:GLU:OE1	2.17	0.45
1:B:43:LEU:HA	1:B:369:GLU:O	2.17	0.45
1:B:117:LEU:HD21	1:C:260:PHE:CE1	2.52	0.45
1:B:356:TYR:CE2	1:C:142:ASP:HB3	2.52	0.45
1:D:107:ILE:HB	1:D:308:ASN:H	1.82	0.45
1:E:128:ASP:CG	1:E:129:THR:H	2.25	0.45
1:A:43:LEU:O	1:F:419:TYR:HB2	2.15	0.45
1:B:273:GLU:HA	1:B:276:TYR:CE1	2.51	0.45
1:C:273:GLU:C	1:C:275:LEU:H	2.25	0.45
1:C:362:LYS:HD2	1:D:268:GLY:HA2	1.98	0.45
1:C:391:TYR:O	1:C:395:MET:HB3	2.16	0.45
1:D:71:ARG:C	1:D:73:PHE:CE1	2.95	0.45
1:D:208:MET:HG2	1:D:210:PHE:CE1	2.51	0.45
1:E:35:TYR:O	1:E:376:ILE:HA	2.17	0.45
1:E:70:TYR:N	1:E:199:ASP:O	2.50	0.45
1:E:80:PRO:HG2	1:E:98:LEU:HB2	1.98	0.45
1:E:438:LYS:HG2	1:E:439:GLN:H	1.81	0.45
1:F:35:TYR:CD1	1:F:456:PHE:CD1	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:HIS:CE1	1:F:37:ALA:C	2.95	0.45
1:A:68:TYR:O	1:A:201:VAL:HG22	2.17	0.45
1:A:347:SER:HA	1:A:361:PHE:CD1	2.51	0.45
1:B:77:LEU:CD1	1:B:100:TRP:CD1	3.00	0.45
1:C:74:ARG:HH22	1:C:440:ASP:CG	2.24	0.45
1:C:392:ILE:CG2	1:C:400:LEU:HD21	2.46	0.45
1:D:397:THR:HA	1:D:400:LEU:HD12	1.97	0.45
1:E:33:ILE:O	1:E:34:PHE:CD1	2.69	0.45
1:E:36:HIS:CG	1:E:463:PHE:CG	3.05	0.45
1:E:76:LYS:C	1:E:77:LEU:HG	2.42	0.45
1:E:96:GLN:HA	1:E:382:ILE:O	2.16	0.45
1:E:176:LYS:C	1:E:178:THR:H	2.24	0.45
1:E:402:ASP:HB2	1:E:403:TRP:CE3	2.52	0.45
1:F:196:GLU:CD	1:F:446:LYS:H	2.25	0.45
1:F:325:TRP:C	1:F:326:HIS:CG	2.92	0.45
1:F:436:PRO:HA	1:F:439:GLN:OE1	2.16	0.45
1:A:27:TYR:CD1	1:A:27:TYR:N	2.85	0.45
1:A:35:TYR:CE1	1:A:457:SER:N	2.84	0.45
1:A:78:PRO:HD3	1:A:456:PHE:CZ	2.52	0.45
1:A:87:ASP:CG	1:A:89:THR:HG23	2.41	0.45
1:A:256:PHE:CE1	1:A:296:SER:HB3	2.51	0.45
1:A:325:TRP:HB2	1:A:326:HIS:CE1	2.52	0.45
1:A:460:LEU:HD12	1:A:470:LEU:HD21	1.99	0.45
1:B:196:GLU:H	1:B:199:ASP:CG	2.25	0.45
1:C:242:TYR:OH	1:C:395:MET:HA	2.17	0.45
1:D:326:HIS:CE1	1:D:399:ILE:CG1	2.99	0.45
1:E:114:GLY:H	1:E:338:ARG:HA	1.82	0.45
1:E:130:GLU:C	1:E:132:SER:H	2.25	0.45
1:E:168:HIS:CB	1:E:207:ALA:HA	2.47	0.45
1:F:47:HIS:HE1	1:F:49:TYR:HB2	1.79	0.45
1:A:356:TYR:C	1:A:356:TYR:CD2	2.95	0.45
1:A:367:HIS:CE1	1:A:368:VAL:O	2.69	0.45
1:A:464:PRO:O	1:A:468:LYS:HG3	2.15	0.45
1:B:24:THR:O	1:B:28:VAL:HG23	2.17	0.45
1:B:172:GLY:HA2	1:B:189:GLU:HB2	1.99	0.45
1:C:36:HIS:CE1	1:C:37:ALA:C	2.95	0.45
1:D:33:ILE:O	1:D:378:GLN:HA	2.17	0.45
1:D:100:TRP:CZ2	1:D:379:LEU:HD13	2.51	0.45
1:E:171:LYS:N	1:E:212:LEU:HD23	2.29	0.45
1:E:181:VAL:HB	1:E:184:ASP:CG	2.42	0.45
1:E:391:TYR:O	1:E:395:MET:SD	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:LEU:HA	1:F:369:GLU:O	2.17	0.45
1:F:70:TYR:CG	1:F:201:VAL:HG12	2.51	0.45
1:A:454:GLU:N	1:A:454:GLU:CD	2.74	0.45
1:C:43:LEU:HG	1:C:369:GLU:O	2.17	0.45
1:C:73:PHE:CD1	1:C:73:PHE:N	2.85	0.45
1:D:356:TYR:CE1	1:D:361:PHE:CE2	3.05	0.45
1:D:442:TYR:HB3	1:D:445:LEU:HD12	1.99	0.45
1:E:139:ASP:C	1:E:141:LYS:H	2.25	0.45
1:E:447:PHE:CD2	1:E:447:PHE:N	2.84	0.45
1:A:121:PRO:HA	1:A:146:ASN:CA	2.46	0.44
1:B:175:CYS:HB2	1:F:428:THR:HG21	1.98	0.44
1:B:396:ASN:CG	1:B:398:THR:H	2.24	0.44
1:B:420:ARG:NH2	1:B:427:VAL:H	2.16	0.44
1:D:272:PRO:HB2	1:D:275:LEU:HD13	1.99	0.44
1:D:329:LEU:HD12	1:D:329:LEU:HA	1.88	0.44
1:E:47:HIS:CE1	1:E:50:PHE:CZ	3.05	0.44
1:E:97:ARG:HG3	1:E:403:TRP:CD2	2.52	0.44
1:F:200:MET:HB3	1:F:229:CYS:SG	2.58	0.44
1:F:208:MET:SD	1:F:208:MET:C	3.00	0.44
1:F:422:VAL:CG1	1:F:428:THR:HA	2.47	0.44
1:A:23:SER:O	1:A:27:TYR:CE1	2.70	0.44
1:A:416:VAL:HB	1:F:41:ARG:HD2	2.00	0.44
1:B:47:HIS:CE1	1:B:49:TYR:N	2.84	0.44
1:B:172:GLY:CA	1:B:189:GLU:HB2	2.47	0.44
1:B:222:LEU:HD23	1:B:225:CYS:HB2	2.00	0.44
1:B:241:ALA:C	1:B:242:TYR:CG	2.94	0.44
1:C:47:HIS:CD2	1:C:48:PRO:N	2.86	0.44
1:C:121:PRO:HA	1:C:146:ASN:HA	1.99	0.44
1:C:167:GLU:HG3	1:C:231:TYR:O	2.17	0.44
1:C:419:TYR:HA	1:C:421:PHE:HB3	1.99	0.44
1:E:172:GLY:N	1:E:187:PRO:O	2.50	0.44
1:E:234:TYR:H	1:E:251:ARG:NH2	2.15	0.44
1:E:388:VAL:HG12	1:E:392:ILE:HD12	1.99	0.44
1:F:51:LYS:CE	1:F:61:ASP:HB2	2.48	0.44
1:A:69:GLN:HA	1:A:199:ASP:O	2.17	0.44
1:A:100:TRP:CD2	1:A:379:LEU:HD12	2.53	0.44
1:A:109:ARG:C	1:A:109:ARG:CD	2.90	0.44
1:B:460:LEU:HA	1:B:463:PHE:HD2	1.83	0.44
1:C:43:LEU:HD12	1:C:369:GLU:C	2.43	0.44
1:C:73:PHE:CE2	1:C:448:TRP:CB	3.00	0.44
1:C:91:TYR:CE2	1:C:98:LEU:HG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:VAL:HB	1:C:382:ILE:HD11	1.99	0.44
1:C:125:LYS:HE2	1:C:261:TRP:CD1	2.52	0.44
1:C:176:LYS:HB2	1:C:177:PRO:HD2	1.98	0.44
1:C:392:ILE:O	1:C:392:ILE:HG22	2.17	0.44
1:E:51:LYS:HG3	1:E:62:VAL:O	2.16	0.44
1:E:409:PRO:HB2	1:E:410:PRO:HD3	1.99	0.44
1:A:99:VAL:HG22	1:A:100:TRP:N	2.33	0.44
1:A:209:ASP:CG	1:A:212:LEU:HB3	2.43	0.44
1:B:124:ASN:HB3	1:B:219:GLU:CD	2.43	0.44
1:B:464:PRO:O	1:B:468:LYS:HG3	2.18	0.44
1:C:70:TYR:CD1	1:C:201:VAL:HG12	2.53	0.44
1:D:97:ARG:HG3	1:D:403:TRP:CE3	2.53	0.44
1:D:167:GLU:H	1:D:231:TYR:H	1.65	0.44
1:D:209:ASP:OD1	1:D:211:LYS:HD2	2.18	0.44
1:D:387:GLU:N	1:D:387:GLU:CD	2.75	0.44
1:E:71:ARG:C	1:E:73:PHE:CZ	2.95	0.44
1:E:79:ASP:O	1:E:83:PHE:CD1	2.70	0.44
1:F:28:VAL:HG13	1:F:380:CYS:SG	2.57	0.44
1:F:130:GLU:CD	1:F:260:PHE:H	2.26	0.44
1:F:252:ARG:C	1:F:252:ARG:HE	2.24	0.44
1:F:396:ASN:OD1	1:F:398:THR:HG23	2.17	0.44
1:A:41:ARG:O	1:F:417:ASP:HB2	2.16	0.44
1:A:154:THR:H	1:A:336:THR:CG2	2.31	0.44
1:A:378:GLN:CD	1:A:380:CYS:SG	3.01	0.44
1:B:65:VAL:O	1:B:367:HIS:CD2	2.70	0.44
1:B:76:LYS:HD2	1:B:76:LYS:N	2.33	0.44
1:B:81:ASN:HD21	1:B:403:TRP:HE1	1.66	0.44
1:B:379:LEU:HD13	1:B:380:CYS:N	2.32	0.44
1:C:45:VAL:HA	1:C:367:HIS:O	2.18	0.44
1:D:120:HIS:CD2	1:D:121:PRO:N	2.85	0.44
1:D:260:PHE:N	1:D:260:PHE:CD1	2.85	0.44
1:A:43:LEU:HB3	1:F:418:THR:HA	1.98	0.44
1:A:385:THR:O	1:A:389:MET:N	2.50	0.44
1:B:48:PRO:HA	1:B:65:VAL:O	2.18	0.44
1:B:71:ARG:C	1:B:73:PHE:CE1	2.96	0.44
1:C:460:LEU:HB2	1:C:470:LEU:HD11	2.00	0.44
1:D:25:ASP:HA	1:D:28:VAL:HB	1.98	0.44
1:D:300:VAL:HG12	1:D:301:THR:N	2.33	0.44
1:E:169:TRP:HB2	1:E:207:ALA:O	2.16	0.44
1:E:259:HIS:H	1:E:294:SER:CB	2.30	0.44
1:E:379:LEU:HG	1:E:380:CYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:THR:HB	1:F:381:LYS:HB2	1.99	0.44
1:F:82:LYS:HA	1:F:82:LYS:HZ2	1.83	0.44
1:F:156:LEU:HD12	1:F:157:CYS:CA	2.47	0.44
1:F:167:GLU:N	1:F:231:TYR:O	2.50	0.44
1:F:391:TYR:O	1:F:395:MET:N	2.50	0.44
1:A:133:HIS:CE1	1:A:134:VAL:HG12	2.52	0.44
1:B:20:LYS:HG2	1:B:21:VAL:H	1.82	0.44
1:B:69:GLN:O	1:B:71:ARG:HD2	2.18	0.44
1:B:70:TYR:CZ	1:B:201:VAL:HA	2.53	0.44
1:B:120:HIS:CG	1:B:123:TYR:CE1	3.06	0.44
1:B:248:PHE:CZ	1:B:250:LEU:CB	3.01	0.44
1:B:360:SER:HB2	1:B:361:PHE:CE2	2.53	0.44
1:B:384:LEU:HG	1:B:384:LEU:H	1.55	0.44
1:B:430:GLN:NE2	1:B:430:GLN:HA	2.33	0.44
1:C:26:GLU:HB2	1:C:27:TYR:CD1	2.52	0.44
1:C:37:ALA:HA	1:C:455:ARG:O	2.17	0.44
1:C:97:ARG:HD2	1:C:403:TRP:CD1	2.52	0.44
1:C:419:TYR:HA	1:C:421:PHE:CB	2.48	0.44
1:D:30:ARG:HA	1:D:380:CYS:SG	2.58	0.44
1:D:259:HIS:O	1:D:294:SER:N	2.51	0.44
1:D:308:ASN:C	1:D:309:LYS:HG3	2.42	0.44
1:D:326:HIS:CE1	1:D:399:ILE:HG13	2.52	0.44
1:D:346:ALA:HB3	1:D:364:TYR:HE1	1.81	0.44
1:D:356:TYR:CE2	1:D:358:PRO:HA	2.52	0.44
1:D:442:TYR:C	1:D:445:LEU:H	2.26	0.44
1:D:451:ASP:OD2	1:D:453:LYS:HG3	2.18	0.44
1:E:120:HIS:CD2	1:E:122:LEU:H	2.35	0.44
1:E:276:TYR:CD2	1:E:276:TYR:C	2.96	0.44
1:F:323:ILE:HB	1:F:325:TRP:CZ2	2.52	0.44
1:C:101:ALA:HA	1:C:324:CYS:SG	2.58	0.44
1:C:463:PHE:O	1:C:464:PRO:C	2.58	0.44
1:D:91:TYR:CE2	1:D:98:LEU:HD21	2.53	0.44
1:D:121:PRO:HD2	1:D:222:LEU:HD11	2.00	0.44
1:D:263:ARG:H	1:D:290:LEU:HG	1.82	0.44
1:D:441:PRO:HD2	1:D:442:TYR:CE2	2.53	0.44
1:D:463:PHE:O	1:D:464:PRO:C	2.60	0.44
1:F:120:HIS:HA	1:F:222:LEU:HG	1.98	0.44
1:B:70:TYR:CE1	1:B:201:VAL:HG12	2.53	0.44
1:B:97:ARG:NH1	1:B:97:ARG:HG2	2.33	0.44
1:D:77:LEU:HG	1:D:327:ASN:O	2.17	0.44
1:D:83:PHE:CE1	1:D:85:LEU:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:PRO:HB3	1:E:83:PHE:CZ	2.53	0.44
1:C:51:LYS:HA	1:C:63:PRO:C	2.43	0.43
1:C:278:LYS:H	1:C:278:LYS:NZ	2.15	0.43
1:C:422:VAL:HG22	1:C:431:LYS:HE2	2.00	0.43
1:E:124:ASN:HA	1:E:144:ARG:HB3	1.99	0.43
1:F:128:ASP:HA	1:F:261:TRP:HA	1.99	0.43
1:A:46:GLY:N	1:A:65:VAL:HB	2.32	0.43
1:A:47:HIS:CE1	1:A:50:PHE:CG	3.07	0.43
1:A:231:TYR:CD1	1:A:232:PRO:HD2	2.53	0.43
1:A:425:ALA:HB3	1:F:60:GLN:H	1.82	0.43
1:C:91:TYR:CD2	1:C:93:PRO:HA	2.53	0.43
1:C:97:ARG:HG2	1:C:97:ARG:HH11	1.82	0.43
1:D:20:LYS:HE2	1:D:20:LYS:C	2.43	0.43
1:D:312:TRP:CE2	1:D:472:GLN:HG3	2.53	0.43
1:E:214:GLN:C	1:E:217:LYS:HZ3	2.25	0.43
1:F:68:TYR:CD2	1:F:68:TYR:N	2.86	0.43
1:F:71:ARG:HE	1:F:71:ARG:HA	1.83	0.43
1:F:102:CYS:HB2	1:F:377:PHE:CZ	2.53	0.43
1:F:161:CYS:HA	1:F:329:LEU:HA	2.00	0.43
1:A:70:TYR:HB2	1:A:199:ASP:HB2	2.00	0.43
1:A:80:PRO:CG	1:A:379:LEU:HD11	2.48	0.43
1:A:469:PHE:O	1:A:472:GLN:HB3	2.18	0.43
1:B:46:GLY:HA3	1:B:63:PRO:HG2	2.01	0.43
1:C:68:TYR:C	1:C:201:VAL:HG13	2.43	0.43
1:C:110:GLY:H	1:C:370:GLU:CD	2.26	0.43
1:C:119:GLY:O	1:C:222:LEU:HG	2.18	0.43
1:C:259:HIS:HB2	1:C:261:TRP:CZ2	2.53	0.43
1:D:160:GLY:HA2	1:D:247:PHE:CE1	2.53	0.43
1:D:448:TRP:CE2	1:D:449:PRO:HD2	2.53	0.43
1:E:119:GLY:O	1:E:120:HIS:HB2	2.18	0.43
1:F:305:GLN:OE1	1:F:307:PHE:CD2	2.72	0.43
1:A:382:ILE:HD12	1:A:382:ILE:N	2.34	0.43
1:B:27:TYR:CD1	1:B:27:TYR:N	2.84	0.43
1:D:345:CYS:SG	1:D:361:PHE:HB3	2.58	0.43
1:D:447:PHE:CD2	1:D:447:PHE:N	2.85	0.43
1:E:312:TRP:CZ3	1:E:469:PHE:HB2	2.53	0.43
1:A:234:TYR:CD2	1:A:234:TYR:N	2.82	0.43
1:A:448:TRP:CH2	1:F:419:TYR:CE1	3.07	0.43
1:C:155:GLN:HA	1:C:335:ASP:HA	1.99	0.43
1:D:267:MET:SD	1:D:288:SER:HA	2.59	0.43
1:E:155:GLN:HE22	1:E:305:GLN:NE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:341:ASN:HD21	1:F:367:HIS:CD2	2.36	0.43
1:A:83:PHE:CD2	1:A:83:PHE:C	2.97	0.43
1:A:124:ASN:HA	1:A:144:ARG:CB	2.48	0.43
1:A:356:TYR:CZ	1:A:361:PHE:CD2	3.07	0.43
1:C:113:LEU:HD22	1:C:337:THR:HB	2.01	0.43
1:C:272:PRO:HG2	1:C:275:LEU:HD23	2.01	0.43
1:D:162:VAL:HG21	1:D:244:ASP:CB	2.49	0.43
1:D:373:LEU:HB2	1:D:375:PHE:CZ	2.53	0.43
1:D:385:THR:C	1:D:389:MET:SD	3.01	0.43
1:D:401:GLU:C	1:D:404:ASN:H	2.27	0.43
1:D:460:LEU:CB	1:D:470:LEU:HD11	2.48	0.43
1:F:36:HIS:NE2	1:F:463:PHE:CD1	2.86	0.43
1:F:392:ILE:HG22	1:F:400:LEU:HD11	2.00	0.43
1:A:112:PRO:HB3	1:B:231:TYR:CE1	2.53	0.43
1:B:73:PHE:CE2	1:B:448:TRP:CB	3.01	0.43
1:B:341:ASN:HD21	1:B:367:HIS:CE1	2.36	0.43
1:B:389:MET:O	1:B:393:HIS:HB3	2.19	0.43
1:B:441:PRO:HD2	1:B:442:TYR:CD1	2.54	0.43
1:C:47:HIS:CE1	1:C:49:TYR:N	2.83	0.43
1:C:452:LEU:O	1:C:456:PHE:CD1	2.71	0.43
1:C:466:GLY:O	1:C:469:PHE:HB3	2.18	0.43
1:F:347:SER:HA	1:F:361:PHE:CD1	2.53	0.43
1:A:47:HIS:CE1	1:A:49:TYR:CB	3.01	0.43
1:A:262:ASN:HA	1:A:291:TYR:HA	2.01	0.43
1:C:74:ARG:HB2	1:C:447:PHE:CG	2.53	0.43
1:C:256:PHE:CZ	1:C:296:SER:HB3	2.54	0.43
1:D:111:GLN:HB3	1:D:112:PRO:HD2	2.01	0.43
1:D:167:GLU:OE2	1:D:190:LEU:HG	2.18	0.43
1:D:375:PHE:HB2	1:D:377:PHE:CZ	2.54	0.43
1:E:36:HIS:HB3	1:E:457:SER:HB2	2.00	0.43
1:E:45:VAL:HG22	1:E:368:VAL:HA	2.01	0.43
1:E:162:VAL:HB	1:E:245:SER:HB3	2.00	0.43
1:F:186:PRO:HG2	1:F:188:LEU:HD21	2.00	0.43
1:F:438:LYS:O	1:F:442:TYR:CD2	2.72	0.43
1:F:469:PHE:CZ	1:F:473:LEU:HD21	2.54	0.43
1:A:144:ARG:CZ	1:E:356:TYR:HB2	2.48	0.43
1:A:164:ALA:O	1:A:195:ILE:N	2.51	0.43
1:C:47:HIS:O	1:C:64:LYS:HG3	2.19	0.43
1:C:167:GLU:C	1:C:168:HIS:CE1	2.97	0.43
1:D:47:HIS:NE2	1:D:49:TYR:CD2	2.84	0.43
1:D:312:TRP:HB2	1:D:314:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:MET:SD	1:D:395:MET:N	2.92	0.43
1:E:210:PHE:CD2	1:E:210:PHE:N	2.86	0.43
1:E:324:CYS:SG	1:E:324:CYS:O	2.77	0.43
1:A:96:GLN:H	1:A:96:GLN:HG2	1.54	0.43
1:A:180:VAL:HG22	1:A:181:VAL:N	2.33	0.43
1:A:220:VAL:HB	1:A:224:ILE:HD11	2.01	0.43
1:A:392:ILE:C	1:A:395:MET:H	2.27	0.43
1:C:199:ASP:OD1	1:C:446:LYS:NZ	2.50	0.43
1:D:78:PRO:N	1:D:453:LYS:HG2	2.34	0.43
1:D:157:CYS:SG	1:D:158:ILE:N	2.91	0.43
1:D:440:ASP:HB2	1:D:443:ASP:CG	2.44	0.43
1:D:444:LYS:HG3	1:D:445:LEU:HG	2.00	0.43
1:E:48:PRO:HD3	1:E:341:ASN:OD1	2.19	0.43
1:E:121:PRO:C	1:E:123:TYR:H	2.27	0.43
1:E:324:CYS:SG	1:E:327:ASN:HA	2.59	0.43
1:F:69:GLN:HA	1:F:199:ASP:O	2.18	0.43
1:A:76:LYS:HB3	1:A:451:ASP:HA	2.01	0.42
1:A:79:ASP:CG	1:A:81:ASN:O	2.62	0.42
1:A:204:GLY:C	1:A:205:TYR:CD1	2.96	0.42
1:A:360:SER:HG	1:A:361:PHE:HE2	1.66	0.42
1:B:73:PHE:CD1	1:B:73:PHE:N	2.84	0.42
1:B:154:THR:H	1:B:336:THR:CG2	2.32	0.42
1:C:169:TRP:CZ3	1:C:190:LEU:HB2	2.54	0.42
1:C:464:PRO:O	1:C:468:LYS:HG3	2.19	0.42
1:F:34:PHE:HA	1:F:377:PHE:O	2.19	0.42
1:F:73:PHE:CD1	1:F:73:PHE:N	2.84	0.42
1:F:161:CYS:HG	1:F:325:TRP:HD1	1.66	0.42
1:F:356:TYR:C	1:F:356:TYR:CD2	2.97	0.42
1:A:234:TYR:O	1:A:238:SER:N	2.51	0.42
1:B:47:HIS:CE1	1:B:50:PHE:CD1	3.07	0.42
1:B:299:VAL:HG23	1:C:256:PHE:HB3	1.99	0.42
1:B:300:VAL:HB	1:C:255:VAL:HG13	2.02	0.42
1:B:356:TYR:CD1	1:D:277:ILE:HD12	2.54	0.42
1:B:369:GLU:OE2	1:B:371:PHE:CE2	2.73	0.42
1:C:36:HIS:CE1	1:C:463:PHE:CE1	3.06	0.42
1:C:47:HIS:HB3	1:C:50:PHE:O	2.20	0.42
1:C:120:HIS:CD2	1:C:120:HIS:C	2.96	0.42
1:C:392:ILE:O	1:C:396:ASN:N	2.51	0.42
1:C:441:PRO:HG2	1:C:442:TYR:CE2	2.55	0.42
1:D:157:CYS:SG	1:D:331:LEU:HD11	2.59	0.42
1:D:271:LEU:HD11	1:D:276:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:ASP:HA	1:E:151:TYR:CZ	2.54	0.42
1:F:111:GLN:HB3	1:F:112:PRO:HD2	2.02	0.42
1:A:34:PHE:HA	1:A:377:PHE:O	2.19	0.42
1:A:47:HIS:CE1	1:A:50:PHE:CE1	3.07	0.42
1:B:32:SER:O	1:B:34:PHE:CD2	2.72	0.42
1:B:68:TYR:CD2	1:B:68:TYR:N	2.87	0.42
1:B:467:ARG:O	1:B:471:LEU:HG	2.19	0.42
1:C:76:LYS:HA	1:C:327:ASN:O	2.20	0.42
1:C:460:LEU:CB	1:C:470:LEU:HD11	2.50	0.42
1:D:91:TYR:CE1	1:D:93:PRO:HB3	2.54	0.42
1:D:448:TRP:HA	1:D:449:PRO:HD2	1.85	0.42
1:E:440:ASP:CB	1:E:442:TYR:H	2.32	0.42
1:F:79:ASP:HA	1:F:327:ASN:ND2	2.34	0.42
1:F:399:ILE:CD1	1:F:399:ILE:H	2.28	0.42
1:A:149:VAL:HG22	1:A:150:ASP:N	2.34	0.42
1:A:183:GLY:HA2	1:E:346:ALA:HB1	2.01	0.42
1:A:319:LEU:HD22	1:A:319:LEU:N	2.35	0.42
1:A:328:GLN:HB3	1:A:330:PHE:CE2	2.53	0.42
1:A:460:LEU:H	1:A:460:LEU:HG	1.47	0.42
1:B:97:ARG:HG3	1:B:403:TRP:CD2	2.55	0.42
1:B:167:GLU:HA	1:B:192:ASN:HA	2.01	0.42
1:B:312:TRP:CH2	1:B:469:PHE:HA	2.54	0.42
1:C:91:TYR:CE1	1:C:93:PRO:HB3	2.54	0.42
1:E:46:GLY:O	1:E:367:HIS:N	2.52	0.42
1:E:105:VAL:HG22	1:E:375:PHE:CD1	2.54	0.42
1:E:385:THR:N	1:E:389:MET:SD	2.92	0.42
1:F:102:CYS:SG	1:F:376:ILE:O	2.77	0.42
1:A:233:ASP:C	1:A:237:MET:HE2	2.45	0.42
1:A:441:PRO:C	1:A:443:ASP:H	2.28	0.42
1:B:158:ILE:HG12	1:B:249:CYS:HA	2.00	0.42
1:C:36:HIS:HA	1:C:375:PHE:O	2.20	0.42
1:D:43:LEU:HD11	1:D:368:VAL:CG2	2.50	0.42
1:D:197:ASP:HB2	1:D:447:PHE:HA	2.02	0.42
1:E:109:ARG:HD3	1:E:109:ARG:C	2.43	0.42
1:E:391:TYR:CD1	1:E:395:MET:HE1	2.55	0.42
1:E:398:THR:HA	1:E:401:GLU:HB3	2.01	0.42
1:F:54:LYS:HG3	1:F:61:ASP:HA	2.02	0.42
1:F:68:TYR:HB3	1:F:201:VAL:HG22	2.02	0.42
1:F:107:ILE:HD12	1:F:107:ILE:N	2.31	0.42
1:A:33:ILE:N	1:A:33:ILE:HD13	2.35	0.42
1:A:76:LYS:HA	1:A:327:ASN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLY:N	1:A:372:ASP:O	2.52	0.42
1:A:370:GLU:O	1:A:371:PHE:CD2	2.73	0.42
1:A:400:LEU:O	1:A:404:ASN:N	2.53	0.42
1:B:97:ARG:CB	1:B:403:TRP:CD2	3.02	0.42
1:B:97:ARG:HB2	1:B:403:TRP:CZ3	2.54	0.42
1:B:421:PHE:CZ	1:B:422:VAL:HG12	2.55	0.42
1:B:467:ARG:HA	1:B:470:LEU:HD12	2.00	0.42
1:C:74:ARG:HD2	1:C:447:PHE:CD2	2.54	0.42
1:D:346:ALA:HA	1:E:215:ASP:CG	2.45	0.42
1:E:68:TYR:CD2	1:E:68:TYR:N	2.88	0.42
1:E:169:TRP:NE1	1:E:190:LEU:HD13	2.34	0.42
1:E:231:TYR:CE1	1:E:232:PRO:HD2	2.54	0.42
1:E:464:PRO:HA	1:E:467:ARG:NE	2.35	0.42
1:F:460:LEU:HB2	1:F:470:LEU:HD11	2.02	0.42
1:A:75:VAL:HA	1:A:450:VAL:HB	2.02	0.42
1:A:312:TRP:CH2	1:A:469:PHE:HA	2.53	0.42
1:B:36:HIS:CG	1:B:37:ALA:N	2.85	0.42
1:B:76:LYS:HG3	1:B:328:GLN:NE2	2.34	0.42
1:C:23:SER:O	1:C:27:TYR:CE1	2.73	0.42
1:C:48:PRO:HB3	1:C:341:ASN:HD21	1.84	0.42
1:D:335:ASP:CG	1:D:336:THR:N	2.78	0.42
1:E:25:ASP:N	1:E:26:GLU:OE1	2.52	0.42
1:E:48:PRO:HD3	1:E:341:ASN:CG	2.45	0.42
1:E:70:TYR:CE2	1:E:201:VAL:HA	2.54	0.42
1:F:156:LEU:HD12	1:F:156:LEU:C	2.45	0.42
1:F:462:GLN:HB2	1:F:463:PHE:CE2	2.55	0.42
1:A:56:GLY:O	1:A:60:GLN:HB2	2.19	0.42
1:B:153:GLN:HE22	1:B:299:VAL:C	2.28	0.42
1:C:47:HIS:CD2	1:C:48:PRO:CD	3.02	0.42
1:C:100:TRP:CE3	1:C:456:PHE:CE2	3.07	0.42
1:D:155:GLN:HB2	1:D:252:ARG:HB3	2.01	0.42
1:D:373:LEU:HB2	1:D:375:PHE:CE1	2.55	0.42
1:E:43:LEU:HD12	1:E:369:GLU:O	2.20	0.42
1:E:68:TYR:CA	1:E:201:VAL:HG22	2.49	0.42
1:E:248:PHE:CZ	1:E:249:CYS:O	2.73	0.42
1:E:453:LYS:H	1:E:453:LYS:HG3	1.69	0.42
1:E:461:ASP:HA	1:E:467:ARG:HG3	2.01	0.42
1:F:96:GLN:HA	1:F:382:ILE:O	2.20	0.42
1:F:404:ASN:HB3	1:F:405:PHE:CG	2.55	0.42
1:A:448:TRP:CD1	1:A:448:TRP:C	2.98	0.42
1:B:364:TYR:CE2	1:C:185:CYS:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:TYR:CE1	1:C:457:SER:C	2.98	0.42
1:C:43:LEU:HD11	1:C:368:VAL:HG13	2.02	0.42
1:C:168:HIS:HD1	1:C:230:LYS:HA	1.84	0.42
1:C:248:PHE:CE2	1:C:250:LEU:HB2	2.54	0.42
1:C:271:LEU:HA	1:C:272:PRO:HD2	1.94	0.42
1:D:186:PRO:HA	1:D:187:PRO:HD3	1.87	0.42
1:D:454:GLU:CD	1:D:455:ARG:NH1	2.78	0.42
1:E:438:LYS:CG	1:E:439:GLN:H	2.33	0.42
1:E:441:PRO:O	1:E:444:LYS:HG2	2.18	0.42
1:A:158:ILE:HB	1:A:332:THR:HB	2.02	0.42
1:B:205:TYR:CE2	1:B:295:PRO:HG3	2.55	0.42
1:D:301:THR:HA	1:E:254:GLN:HA	2.01	0.42
1:E:157:CYS:SG	1:E:248:PHE:CE2	3.13	0.42
1:E:168:HIS:CE1	1:E:193:THR:HB	2.55	0.42
1:E:197:ASP:CB	1:E:447:PHE:HA	2.47	0.42
1:E:210:PHE:HB2	1:E:211:LYS:HD3	2.01	0.42
1:E:374:GLN:OE1	1:E:463:PHE:HB3	2.19	0.42
1:F:100:TRP:CE3	1:F:377:PHE:HB3	2.55	0.42
1:F:216:ASN:HB2	1:F:218:SER:HB2	2.02	0.42
1:A:320:ASN:HD21	1:A:323:ILE:H	1.68	0.41
1:A:420:ARG:HB3	1:F:43:LEU:HD12	2.01	0.41
1:C:128:ASP:HA	1:C:261:TRP:CD1	2.55	0.41
1:C:391:TYR:CE1	1:C:395:MET:SD	3.13	0.41
1:D:24:THR:O	1:D:27:TYR:CG	2.73	0.41
1:D:459:ASP:O	1:D:463:PHE:CD2	2.74	0.41
1:E:71:ARG:O	1:E:332:THR:HA	2.20	0.41
1:E:216:ASN:CG	1:E:219:GLU:HG2	2.45	0.41
1:E:248:PHE:CE2	1:E:250:LEU:HB2	2.55	0.41
1:E:452:LEU:C	1:E:454:GLU:H	2.28	0.41
1:A:22:VAL:H	1:A:22:VAL:HG23	1.46	0.41
1:A:347:SER:HB3	1:A:361:PHE:HE1	1.84	0.41
1:C:38:GLY:HA3	1:C:374:GLN:HA	2.02	0.41
1:C:121:PRO:HA	1:C:146:ASN:CG	2.45	0.41
1:C:392:ILE:HA	1:C:395:MET:SD	2.60	0.41
1:E:45:VAL:C	1:E:65:VAL:HG21	2.44	0.41
1:E:79:ASP:OD2	1:E:81:ASN:HB2	2.21	0.41
1:E:96:GLN:HG2	1:E:383:THR:HA	2.01	0.41
1:E:196:GLU:OE1	1:E:446:LYS:N	2.53	0.41
1:F:35:TYR:CZ	1:F:458:ALA:HA	2.54	0.41
1:A:37:ALA:HA	1:A:455:ARG:C	2.46	0.41
1:A:160:GLY:HA3	1:A:246:MET:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLY:HA3	1:A:245:SER:O	2.20	0.41
1:B:31:THR:H	1:B:378:GLN:CD	2.28	0.41
1:B:49:TYR:HA	1:B:223:ASP:OD2	2.20	0.41
1:B:84:GLY:O	1:B:86:PRO:HD3	2.21	0.41
1:B:125:LYS:HA	1:B:263:ARG:CZ	2.51	0.41
1:B:276:TYR:CD1	1:B:276:TYR:N	2.89	0.41
1:C:105:VAL:HG13	1:C:375:PHE:CD1	2.55	0.41
1:C:124:ASN:HA	1:C:144:ARG:HA	2.03	0.41
1:C:153:GLN:HE21	1:C:336:THR:C	2.28	0.41
1:C:259:HIS:CB	1:C:261:TRP:CZ2	3.03	0.41
1:D:48:PRO:HB2	1:D:49:TYR:CZ	2.54	0.41
1:E:68:TYR:C	1:E:201:VAL:HG13	2.46	0.41
1:F:47:HIS:CD2	1:F:365:ALA:O	2.73	0.41
1:F:121:PRO:HA	1:F:146:ASN:CA	2.51	0.41
1:F:177:PRO:C	1:F:179:THR:H	2.28	0.41
1:F:261:TRP:CD2	1:F:261:TRP:N	2.88	0.41
1:F:386:THR:HA	1:F:389:MET:CE	2.49	0.41
1:F:388:VAL:O	1:F:392:ILE:HG12	2.20	0.41
1:A:329:LEU:HD23	1:A:330:PHE:H	1.86	0.41
1:A:461:ASP:OD1	1:A:462:GLN:HG2	2.20	0.41
1:B:309:LYS:O	1:B:311:TYR:CE2	2.73	0.41
1:B:389:MET:HA	1:B:392:ILE:HD12	2.01	0.41
1:C:40:SER:H	1:C:455:ARG:HH12	1.67	0.41
1:C:79:ASP:CG	1:C:82:LYS:H	2.28	0.41
1:C:105:VAL:HG13	1:C:375:PHE:HE1	1.83	0.41
1:D:28:VAL:HA	1:D:382:ILE:HG12	2.01	0.41
1:D:422:VAL:HG23	1:D:423:GLN:OE1	2.21	0.41
1:E:156:LEU:O	1:E:333:VAL:HG23	2.20	0.41
1:E:241:ALA:C	1:E:242:TYR:CD2	2.98	0.41
1:E:360:SER:HB2	1:E:361:PHE:CE2	2.56	0.41
1:E:408:THR:N	1:E:409:PRO:HD2	2.35	0.41
1:F:392:ILE:HA	1:F:395:MET:CB	2.51	0.41
1:F:441:PRO:HG2	1:F:442:TYR:CD1	2.55	0.41
1:A:325:TRP:C	1:A:326:HIS:CG	2.98	0.41
1:A:447:PHE:CD2	1:A:447:PHE:N	2.86	0.41
1:C:444:LYS:C	1:C:445:LEU:HD23	2.45	0.41
1:D:241:ALA:C	1:D:242:TYR:CG	2.99	0.41
1:D:388:VAL:O	1:D:392:ILE:N	2.53	0.41
1:E:81:ASN:HA	1:E:98:LEU:HD12	2.02	0.41
1:E:109:ARG:HG3	1:E:307:PHE:CD2	2.56	0.41
1:E:204:GLY:O	1:E:205:TYR:CD1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:440:ASP:HB3	1:E:442:TYR:H	1.86	0.41
1:F:77:LEU:HG	1:F:327:ASN:O	2.20	0.41
1:F:169:TRP:CE3	1:F:170:THR:N	2.89	0.41
1:A:97:ARG:O	1:A:382:ILE:HD12	2.20	0.41
1:A:266:THR:O	1:E:363:GLU:HG2	2.21	0.41
1:B:37:ALA:O	1:B:375:PHE:N	2.54	0.41
1:B:102:CYS:HA	1:B:377:PHE:CD1	2.55	0.41
1:B:210:PHE:CD2	1:B:227:SER:O	2.73	0.41
1:C:172:GLY:HA2	1:C:189:GLU:CD	2.45	0.41
1:C:256:PHE:N	1:C:256:PHE:CD1	2.89	0.41
1:C:347:SER:HB3	1:C:361:PHE:CE1	2.56	0.41
1:D:93:PRO:C	1:D:95:SER:H	2.28	0.41
1:D:100:TRP:CZ3	1:D:377:PHE:CB	3.03	0.41
1:D:166:GLY:H	1:D:193:THR:C	2.28	0.41
1:E:91:TYR:CE2	1:E:93:PRO:HA	2.54	0.41
1:E:170:THR:CG2	1:E:189:GLU:HB2	2.50	0.41
1:E:462:GLN:HB2	1:E:463:PHE:CZ	2.56	0.41
1:F:211:LYS:HD3	1:F:211:LYS:H	1.85	0.41
1:F:419:TYR:HB3	1:F:420:ARG:H	1.73	0.41
1:A:141:LYS:HB2	1:E:357:THR:HA	2.03	0.41
1:A:168:HIS:HB2	1:A:207:ALA:C	2.46	0.41
1:B:51:LYS:HE2	1:B:53:PRO:HA	2.02	0.41
1:B:91:TYR:CG	1:B:92:ASP:N	2.87	0.41
1:B:261:TRP:CD2	1:B:261:TRP:N	2.88	0.41
1:B:396:ASN:HD21	1:B:398:THR:CB	2.32	0.41
1:C:232:PRO:HB2	1:C:234:TYR:CE1	2.56	0.41
1:C:325:TRP:HB2	1:C:326:HIS:NE2	2.35	0.41
1:D:118:SER:O	1:D:148:SER:HA	2.20	0.41
1:D:312:TRP:CH2	1:D:469:PHE:HA	2.55	0.41
1:E:24:THR:C	1:E:26:GLU:H	2.23	0.41
1:E:243:GLY:HA3	1:E:318:GLY:HA3	2.02	0.41
1:F:36:HIS:CG	1:F:463:PHE:CD1	3.09	0.41
1:F:67:ALA:C	1:F:69:GLN:HG3	2.46	0.41
1:F:188:LEU:C	1:F:189:GLU:HG3	2.45	0.41
1:A:120:HIS:HE1	1:A:218:SER:C	2.29	0.41
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.93	0.41
1:D:222:LEU:HD23	1:D:222:LEU:HA	1.91	0.41
1:D:275:LEU:N	1:D:275:LEU:CD1	2.83	0.41
1:D:459:ASP:O	1:D:463:PHE:CE2	2.74	0.41
1:E:68:TYR:HA	1:E:201:VAL:HG22	2.03	0.41
1:E:122:LEU:HD13	1:E:144:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:ILE:HA	1:E:395:MET:CE	2.51	0.41
1:E:419:TYR:HA	1:E:421:PHE:CE1	2.55	0.41
1:F:18:VAL:HG13	1:F:19:ALA:H	1.86	0.41
1:F:120:HIS:O	1:F:123:TYR:HB2	2.20	0.41
1:F:160:GLY:HA3	1:F:246:MET:HA	2.03	0.41
1:F:168:HIS:HB2	1:F:207:ALA:C	2.45	0.41
1:F:361:PHE:CD2	1:F:361:PHE:N	2.88	0.41
1:A:40:SER:H	1:A:455:ARG:NH1	2.18	0.41
1:A:152:LYS:HA	1:A:297:GLY:HA2	2.02	0.41
1:B:18:VAL:HG13	1:F:404:ASN:CG	2.46	0.41
1:B:35:TYR:CB	1:B:377:PHE:H	2.32	0.41
1:B:91:TYR:CD2	1:B:96:GLN:O	2.73	0.41
1:B:107:ILE:HB	1:B:307:PHE:CD2	2.55	0.41
1:B:390:SER:HA	1:B:393:HIS:HB3	2.02	0.41
1:C:57:ASN:CG	1:C:59:ARG:HA	2.46	0.41
1:C:70:TYR:CG	1:C:201:VAL:HG12	2.56	0.41
1:C:77:LEU:HD13	1:C:100:TRP:CD1	2.56	0.41
1:C:224:ILE:O	1:C:225:CYS:C	2.64	0.41
1:C:396:ASN:OD1	1:C:398:THR:HG23	2.19	0.41
1:D:123:TYR:O	1:D:144:ARG:HA	2.20	0.41
1:D:392:ILE:HA	1:D:395:MET:SD	2.61	0.41
1:E:46:GLY:N	1:E:65:VAL:HB	2.36	0.41
1:E:60:GLN:N	1:E:60:GLN:CD	2.79	0.41
1:E:267:MET:H	1:E:267:MET:HG2	1.65	0.41
1:E:319:LEU:H	1:E:319:LEU:HG	1.58	0.41
1:E:396:ASN:O	1:E:399:ILE:HD12	2.21	0.41
1:F:77:LEU:CA	1:F:453:LYS:HG2	2.50	0.41
1:F:122:LEU:O	1:F:144:ARG:HB2	2.20	0.41
1:F:233:ASP:O	1:F:237:MET:SD	2.78	0.41
1:F:313:LEU:C	1:F:314:HIS:CD2	2.99	0.41
1:F:393:HIS:HA	1:F:400:LEU:HD12	2.02	0.41
1:A:148:SER:HB3	1:B:291:TYR:CD1	2.56	0.41
1:A:231:TYR:CE1	1:E:112:PRO:HB3	2.56	0.41
1:A:233:ASP:OD1	1:A:235:LEU:HG	2.21	0.41
1:A:273:GLU:O	1:A:276:TYR:CD1	2.74	0.41
1:A:443:ASP:C	1:A:445:LEU:H	2.27	0.41
1:B:312:TRP:HB2	1:B:314:HIS:NE2	2.36	0.41
1:C:325:TRP:HB2	1:C:326:HIS:CE1	2.55	0.41
1:C:361:PHE:HB3	1:C:363:GLU:OE1	2.21	0.41
1:D:121:PRO:HA	1:D:146:ASN:CG	2.46	0.41
1:D:150:ASP:CG	1:D:151:TYR:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:PRO:HD2	1:E:140:THR:C	2.46	0.41
1:D:398:THR:O	1:D:402:ASP:N	2.51	0.41
1:E:23:SER:O	1:E:26:GLU:HB2	2.20	0.41
1:E:36:HIS:HA	1:E:375:PHE:O	2.20	0.41
1:E:97:ARG:CB	1:E:382:ILE:HD12	2.49	0.41
1:E:451:ASP:OD1	1:E:453:LYS:HG3	2.20	0.41
1:F:248:PHE:CD2	1:F:248:PHE:C	2.98	0.41
1:A:45:VAL:HA	1:A:367:HIS:O	2.21	0.40
1:A:84:GLY:HA3	1:F:83:PHE:CZ	2.57	0.40
1:A:469:PHE:HA	1:A:472:GLN:HB3	2.03	0.40
1:B:13:LEU:HB2	1:B:393:HIS:ND1	2.36	0.40
1:B:65:VAL:HG12	1:B:367:HIS:CG	2.56	0.40
1:B:93:PRO:O	1:B:97:ARG:NH1	2.52	0.40
1:B:155:GLN:OE1	1:B:306:LEU:HG	2.21	0.40
1:B:266:THR:C	1:B:267:MET:HE2	2.46	0.40
1:B:374:GLN:CD	1:B:465:LEU:HB3	2.46	0.40
1:C:202:ASP:HA	1:C:206:GLY:HA3	2.03	0.40
1:C:208:MET:CB	1:C:213:LEU:HD21	2.51	0.40
1:D:43:LEU:HD11	1:D:368:VAL:HG22	2.03	0.40
1:D:138:VAL:HG13	1:D:141:LYS:HG2	2.04	0.40
1:D:231:TYR:CG	1:D:232:PRO:CD	3.05	0.40
1:D:289:TYR:HA	1:D:291:TYR:CZ	2.56	0.40
1:E:33:ILE:C	1:E:34:PHE:CG	3.00	0.40
1:E:48:PRO:HG2	1:E:49:TYR:CD2	2.56	0.40
1:E:169:TRP:CB	1:E:208:MET:HA	2.50	0.40
1:E:234:TYR:CE1	1:E:249:CYS:SG	3.13	0.40
1:E:423:GLN:H	1:E:423:GLN:CD	2.29	0.40
1:F:126:LEU:HD22	1:F:264:SER:OG	2.21	0.40
1:F:152:LYS:HA	1:F:297:GLY:CA	2.50	0.40
1:F:365:ALA:O	1:F:366:ARG:NE	2.54	0.40
1:F:398:THR:HA	1:F:401:GLU:HB3	2.03	0.40
1:A:183:GLY:CA	1:E:347:SER:O	2.69	0.40
1:B:30:ARG:HD3	1:B:378:GLN:HE22	1.86	0.40
1:B:181:VAL:HG12	1:B:182:GLN:N	2.35	0.40
1:B:209:ASP:OD1	1:B:210:PHE:N	2.54	0.40
1:C:97:ARG:HB3	1:C:403:TRP:CE2	2.56	0.40
1:C:162:VAL:HG12	1:C:163:PRO:N	2.36	0.40
1:C:311:TYR:HB2	1:C:313:LEU:HD21	2.03	0.40
1:C:347:SER:HA	1:C:361:PHE:CD1	2.56	0.40
1:C:430:GLN:C	1:C:430:GLN:CD	2.89	0.40
1:D:35:TYR:CE1	1:D:456:PHE:CD2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:HIS:CD2	1:D:48:PRO:CD	3.05	0.40
1:D:69:GLN:CA	1:D:201:VAL:HG13	2.51	0.40
1:D:391:TYR:O	1:D:394:ASN:ND2	2.54	0.40
1:D:460:LEU:O	1:D:463:PHE:O	2.39	0.40
1:E:47:HIS:CG	1:E:48:PRO:CD	3.01	0.40
1:E:126:LEU:HB3	1:E:263:ARG:C	2.46	0.40
1:E:155:GLN:HE22	1:E:305:GLN:CD	2.30	0.40
1:F:59:ARG:HB3	1:F:61:ASP:CG	2.47	0.40
1:F:220:VAL:CG2	1:F:225:CYS:HA	2.50	0.40
1:F:389:MET:O	1:F:393:HIS:N	2.53	0.40
1:F:451:ASP:CG	1:F:453:LYS:HG3	2.46	0.40
1:A:69:GLN:N	1:A:201:VAL:HG13	2.36	0.40
1:A:161:CYS:SG	1:A:244:ASP:C	3.04	0.40
1:B:77:LEU:HD12	1:B:100:TRP:CD1	2.56	0.40
1:B:333:VAL:HG22	1:B:334:VAL:N	2.37	0.40
1:B:429:CYS:O	1:B:430:GLN:HB2	2.21	0.40
1:C:91:TYR:CE2	1:C:97:ARG:HA	2.56	0.40
1:C:197:ASP:HB2	1:C:447:PHE:HA	2.03	0.40
1:C:289:TYR:HA	1:C:291:TYR:CE2	2.56	0.40
1:D:81:ASN:ND2	1:D:403:TRP:HE1	2.19	0.40
1:D:120:HIS:ND1	1:D:123:TYR:HA	2.36	0.40
1:D:241:ALA:C	1:D:242:TYR:CD2	2.99	0.40
1:D:399:ILE:HG13	1:D:399:ILE:H	1.60	0.40
1:E:71:ARG:C	1:E:73:PHE:CE1	3.00	0.40
1:F:169:TRP:CH2	1:F:189:GLU:C	3.00	0.40
1:F:204:GLY:O	1:F:205:TYR:CG	2.74	0.40
1:F:231:TYR:HA	1:F:232:PRO:HD3	1.85	0.40
1:A:307:PHE:CD1	1:A:308:ASN:N	2.89	0.40
1:A:434:ALA:HA	1:A:435:PRO:HD3	1.89	0.40
1:B:111:GLN:HB3	1:B:112:PRO:HD2	2.04	0.40
1:B:444:LYS:HD3	1:B:444:LYS:N	2.36	0.40
1:C:77:LEU:O	1:C:327:ASN:HB3	2.21	0.40
1:C:142:ASP:CG	1:C:144:ARG:HE	2.30	0.40
1:C:274:SER:C	1:C:275:LEU:HD22	2.46	0.40
1:C:374:GLN:N	1:C:375:PHE:CZ	2.90	0.40
1:C:401:GLU:C	1:C:404:ASN:H	2.30	0.40
1:D:21:VAL:HG22	1:D:22:VAL:N	2.36	0.40
1:D:102:CYS:SG	1:D:376:ILE:O	2.80	0.40
1:D:109:ARG:HA	1:D:371:PHE:CD1	2.57	0.40
1:D:169:TRP:N	1:D:207:ALA:O	2.53	0.40
1:D:271:LEU:HD11	1:D:276:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:PHE:CE1	1:D:426:ALA:HB1	2.57	0.40
1:E:167:GLU:CG	1:E:231:TYR:O	2.69	0.40
1:E:220:VAL:HB	1:E:221:PRO:CD	2.52	0.40
1:F:91:TYR:CD1	1:F:93:PRO:HD3	2.57	0.40
1:F:106:GLU:OE2	1:F:308:ASN:C	2.64	0.40
1:F:187:PRO:C	1:F:188:LEU:HG	2.46	0.40
1:F:341:ASN:HD21	1:F:367:HIS:CG	2.39	0.40
1:A:47:HIS:CE1	1:A:49:TYR:N	2.88	0.40
1:A:102:CYS:SG	1:A:375:PHE:HB3	2.61	0.40
1:A:120:HIS:CE1	1:A:218:SER:C	3.00	0.40
1:A:235:LEU:HA	1:A:238:SER:OG	2.22	0.40
1:B:124:ASN:HD21	1:B:265:GLY:N	2.19	0.40
1:B:144:ARG:H	1:C:283:ARG:NH2	2.20	0.40
1:B:312:TRP:CH2	1:B:469:PHE:CA	3.05	0.40
1:B:460:LEU:HD12	1:B:470:LEU:HD11	2.03	0.40
1:D:170:THR:HG22	1:D:191:ILE:HG21	2.04	0.40
1:D:325:TRP:CD2	1:D:325:TRP:N	2.85	0.40
1:D:460:LEU:HD13	1:D:470:LEU:HD21	2.04	0.40
1:E:51:LYS:NZ	1:E:63:PRO:HA	2.36	0.40
1:E:323:ILE:HG21	1:E:325:TRP:CH2	2.56	0.40
1:F:23:SER:HB3	1:F:26:GLU:OE1	2.22	0.40
1:F:28:VAL:O	1:F:28:VAL:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 EM 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	454/500 (91%)	359 (79%)	59 (13%)	36 (8%)	1	9
1	B	462/500 (92%)	356 (77%)	65 (14%)	41 (9%)	0	8
1	C	455/500 (91%)	363 (80%)	57 (12%)	35 (8%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	452/500 (90%)	370 (82%)	53 (12%)	29 (6%)	1	12
1	E	452/500 (90%)	351 (78%)	70 (16%)	31 (7%)	1	11
1	F	462/500 (92%)	367 (79%)	62 (13%)	33 (7%)	1	10
All	All	2737/3000 (91%)	2166 (79%)	366 (13%)	205 (8%)	1	10

All (205) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	50	PHE
1	A	67	ALA
1	A	86	PRO
1	A	404	ASN
1	A	405	PHE
1	A	410	PRO
1	A	411	PRO
1	A	417	ASP
1	A	423	GLN
1	A	436	PRO
1	A	437	VAL
1	B	86	PRO
1	B	91	TYR
1	B	298	SER
1	B	339	SER
1	B	411	PRO
1	B	418	THR
1	B	419	TYR
1	B	436	PRO
1	B	441	PRO
1	C	67	ALA
1	C	207	ALA
1	C	225	CYS
1	C	227	SER
1	C	278	LYS
1	C	307	PHE
1	C	411	PRO
1	C	418	THR
1	C	421	PHE
1	C	424	SER
1	C	436	PRO
1	D	140	THR

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Mol	Chain	Res	Type
1	D	192	ASN
1	D	227	SER
1	D	298	SER
1	D	339	SER
1	D	386	THR
1	D	411	PRO
1	D	453	LYS
1	E	115	VAL
1	E	142	ASP
1	E	144	ARG
1	E	293	PRO
1	E	298	SER
1	E	339	SER
1	E	386	THR
1	E	399	ILE
1	E	421	PHE
1	E	422	VAL
1	E	425	ALA
1	E	440	ASP
1	E	441	PRO
1	F	18	VAL
1	F	57	ASN
1	F	88	ASN
1	F	210	PHE
1	F	244	ASP
1	F	299	VAL
1	F	414	SER
1	F	417	ASP
1	F	425	ALA
1	A	27	TYR
1	A	66	SER
1	A	129	THR
1	A	181	VAL
1	A	240	ASP
1	A	274	SER
1	A	308	ASN
1	A	421	PHE
1	A	439	GLN
1	A	454	GLU
1	B	11	VAL
1	B	19	ALA
1	B	67	ALA

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Mol	Chain	Res	Type
1	B	90	VAL
1	B	111	GLN
1	B	205	TYR
1	B	286	PRO
1	B	415	LEU
1	B	421	PHE
1	B	424	SER
1	B	427	VAL
1	B	433	THR
1	B	440	ASP
1	C	19	ALA
1	C	22	VAL
1	C	115	VAL
1	C	136	SER
1	C	138	VAL
1	C	339	SER
1	C	416	VAL
1	C	422	VAL
1	C	426	ALA
1	C	437	VAL
1	C	459	ASP
1	D	137	ALA
1	D	175	CYS
1	D	194	PRO
1	D	225	CYS
1	D	409	PRO
1	D	415	LEU
1	D	420	ARG
1	E	111	GLN
1	E	129	THR
1	E	186	PRO
1	E	213	LEU
1	E	404	ASN
1	F	11	VAL
1	F	125	LYS
1	F	152	LYS
1	F	205	TYR
1	F	227	SER
1	F	228	ILE
1	F	240	ASP
1	F	317	GLN
1	F	339	SER

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Mol	Chain	Res	Type
1	F	420	ARG
1	F	435	PRO
1	F	453	LYS
1	A	131	ASN
1	A	407	VAL
1	B	48	PRO
1	B	140	THR
1	B	152	LYS
1	B	175	CYS
1	B	184	ASP
1	B	264	SER
1	B	275	LEU
1	B	288	SER
1	B	308	ASN
1	B	337	THR
1	B	416	VAL
1	B	430	GLN
1	C	91	TYR
1	C	245	SER
1	C	413	ALA
1	C	438	LYS
1	D	32	SER
1	D	89	THR
1	D	111	GLN
1	D	246	MET
1	D	359	THR
1	D	413	ALA
1	D	414	SER
1	D	435	PRO
1	E	87	ASP
1	E	353	PRO
1	E	396	ASN
1	F	132	SER
1	F	142	ASP
1	F	410	PRO
1	F	413	ALA
1	F	421	PHE
1	A	24	THR
1	A	163	PRO
1	A	298	SER
1	A	384	LEU
1	A	416	VAL

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Mol	Chain	Res	Type
1	A	431	LYS
1	B	404	ASN
1	B	423	GLN
1	C	90	VAL
1	C	131	ASN
1	C	134	VAL
1	C	274	SER
1	C	286	PRO
1	D	125	LYS
1	D	130	GLU
1	D	139	ASP
1	D	440	ASP
1	E	152	LYS
1	E	206	GLY
1	E	432	ASP
1	F	14	PRO
1	A	422	VAL
1	B	281	ASP
1	B	409	PRO
1	B	417	ASP
1	C	208	MET
1	E	48	PRO
1	E	174	ALA
1	E	428	THR
1	F	134	VAL
1	F	352	ILE
1	F	429	CYS
1	A	85	LEU
1	A	111	GLN
1	A	125	LYS
1	A	453	LYS
1	B	176	LYS
1	C	221	PRO
1	E	143	THR
1	E	134	VAL
1	E	90	VAL
1	E	204	GLY
1	F	111	GLN
1	A	206	GLY
1	B	14	PRO
1	C	80	PRO
1	D	85	LEU

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Mol	Chain	Res	Type
1	D	437	VAL
1	F	48	PRO
1	F	409	PRO
1	C	410	PRO

5.3.2 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 EM 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	406/444 (91%)	336 (83%)	70 (17%)	2	10
1	B	414/444 (93%)	350 (84%)	64 (16%)	2	12
1	C	407/444 (92%)	339 (83%)	68 (17%)	2	10
1	D	405/444 (91%)	323 (80%)	82 (20%)	1	7
1	E	405/444 (91%)	320 (79%)	85 (21%)	1	6
1	F	414/444 (93%)	328 (79%)	86 (21%)	1	6
All	All	2451/2664 (92%)	1996 (81%)	455 (19%)	3	8

All (455) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	22	VAL
1	A	24	THR
1	A	25	ASP
1	A	26	GLU
1	A	33	ILE
1	A	35	TYR
1	A	45	VAL
1	A	47	HIS
1	A	52	VAL
1	A	60	GLN
1	A	61	ASP
1	A	66	SER
1	A	77	LEU

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Mol	Chain	Res	Type
1	A	88	ASN
1	A	96	GLN
1	A	109	ARG
1	A	123	TYR
1	A	124	ASN
1	A	126	LEU
1	A	141	LYS
1	A	145	ASP
1	A	149	VAL
1	A	156	LEU
1	A	162	VAL
1	A	173	THR
1	A	189	GLU
1	A	193	THR
1	A	208	MET
1	A	211	LYS
1	A	221	PRO
1	A	226	GLN
1	A	234	TYR
1	A	235	LEU
1	A	242	TYR
1	A	247	PHE
1	A	251	ARG
1	A	252	ARG
1	A	260	PHE
1	A	283	ARG
1	A	307	PHE
1	A	317	GLN
1	A	319	LEU
1	A	325	TRP
1	A	328	GLN
1	A	345	CYS
1	A	359	THR
1	A	360	SER
1	A	369	GLU
1	A	382	ILE
1	A	384	LEU
1	A	386	THR
1	A	387	GLU
1	A	391	TYR
1	A	393	HIS
1	A	398	THR

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Mol	Chain	Res	Type
1	A	403	TRP
1	A	404	ASN
1	A	405	PHE
1	A	410	PRO
1	A	418	THR
1	A	423	GLN
1	A	430	GLN
1	A	433	THR
1	A	436	PRO
1	A	440	ASP
1	A	442	TYR
1	A	457	SER
1	A	461	ASP
1	A	462	GLN
1	B	24	THR
1	B	27	TYR
1	B	44	THR
1	B	60	GLN
1	B	62	VAL
1	B	66	SER
1	B	69	GLN
1	B	72	VAL
1	B	76	LYS
1	B	77	LEU
1	B	88	ASN
1	B	91	TYR
1	B	92	ASP
1	B	99	VAL
1	B	107	ILE
1	B	109	ARG
1	B	122	LEU
1	B	123	TYR
1	B	127	ASP
1	B	128	ASP
1	B	134	VAL
1	B	140	THR
1	B	144	ARG
1	B	150	ASP
1	B	151	TYR
1	B	162	VAL
1	B	165	ILE
1	B	168	HIS

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Mol	Chain	Res	Type
1	B	176	LYS
1	B	181	VAL
1	B	193	THR
1	B	208	MET
1	B	213	LEU
1	B	220	VAL
1	B	242	TYR
1	B	244	ASP
1	B	248	PHE
1	B	260	PHE
1	B	277	ILE
1	B	281	ASP
1	B	289	TYR
1	B	302	SER
1	B	304	SER
1	B	305	GLN
1	B	329	LEU
1	B	340	THR
1	B	366	ARG
1	B	378	GLN
1	B	379	LEU
1	B	383	THR
1	B	387	GLU
1	B	388	VAL
1	B	393	HIS
1	B	397	THR
1	B	423	GLN
1	B	427	VAL
1	B	430	GLN
1	B	436	PRO
1	B	439	GLN
1	B	444	LYS
1	B	450	VAL
1	B	454	GLU
1	B	457	SER
1	B	472	GLN
1	C	25	ASP
1	C	27	TYR
1	C	30	ARG
1	C	50	PHE
1	C	51	LYS
1	C	59	ARG

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Mol	Chain	Res	Type
1	C	60	GLN
1	C	66	SER
1	C	69	GLN
1	C	72	VAL
1	C	77	LEU
1	C	91	TYR
1	C	96	GLN
1	C	109	ARG
1	C	126	LEU
1	C	138	VAL
1	C	140	THR
1	C	141	LYS
1	C	145	ASP
1	C	151	TYR
1	C	154	THR
1	C	163	PRO
1	C	167	GLU
1	C	168	HIS
1	C	177	PRO
1	C	187	PRO
1	C	196	GLU
1	C	205	TYR
1	C	211	LYS
1	C	213	LEU
1	C	223	ASP
1	C	224	ILE
1	C	226	GLN
1	C	234	TYR
1	C	244	ASP
1	C	246	MET
1	C	251	ARG
1	C	252	ARG
1	C	260	PHE
1	C	267	MET
1	C	278	LYS
1	C	283	ARG
1	C	289	TYR
1	C	290	LEU
1	C	300	VAL
1	C	326	HIS
1	C	329	LEU
1	C	334	VAL

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Mol	Chain	Res	Type
1	C	339	SER
1	C	340	THR
1	C	366	ARG
1	C	379	LEU
1	C	387	GLU
1	C	391	TYR
1	C	394	ASN
1	C	397	THR
1	C	401	GLU
1	C	409	PRO
1	C	422	VAL
1	C	423	GLN
1	C	427	VAL
1	C	428	THR
1	C	429	CYS
1	C	454	GLU
1	C	457	SER
1	C	460	LEU
1	C	464	PRO
1	C	472	GLN
1	D	20	LYS
1	D	26	GLU
1	D	27	TYR
1	D	35	TYR
1	D	36	HIS
1	D	41	ARG
1	D	42	LEU
1	D	45	VAL
1	D	60	GLN
1	D	69	GLN
1	D	71	ARG
1	D	85	LEU
1	D	89	THR
1	D	99	VAL
1	D	105	VAL
1	D	109	ARG
1	D	117	LEU
1	D	121	PRO
1	D	125	LYS
1	D	129	THR
1	D	132	SER
1	D	138	VAL

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Mol	Chain	Res	Type
1	D	142	ASP
1	D	145	ASP
1	D	151	TYR
1	D	179	THR
1	D	181	VAL
1	D	185	CYS
1	D	190	LEU
1	D	191	ILE
1	D	193	THR
1	D	208	MET
1	D	211	LYS
1	D	216	ASN
1	D	223	ASP
1	D	224	ILE
1	D	226	GLN
1	D	234	TYR
1	D	235	LEU
1	D	242	TYR
1	D	244	ASP
1	D	247	PHE
1	D	249	CYS
1	D	254	GLN
1	D	260	PHE
1	D	289	TYR
1	D	292	SER
1	D	294	SER
1	D	300	VAL
1	D	302	SER
1	D	305	GLN
1	D	307	PHE
1	D	324	CYS
1	D	325	TRP
1	D	332	THR
1	D	336	THR
1	D	339	SER
1	D	340	THR
1	D	341	ASN
1	D	343	SER
1	D	345	CYS
1	D	357	THR
1	D	359	THR
1	D	360	SER

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Mol	Chain	Res	Type
1	D	363	GLU
1	D	364	TYR
1	D	366	ARG
1	D	369	GLU
1	D	370	GLU
1	D	373	LEU
1	D	386	THR
1	D	387	GLU
1	D	401	GLU
1	D	409	PRO
1	D	415	LEU
1	D	421	PHE
1	D	429	CYS
1	D	431	LYS
1	D	437	VAL
1	D	456	PHE
1	D	464	PRO
1	D	472	GLN
1	E	27	TYR
1	E	33	ILE
1	E	57	ASN
1	E	59	ARG
1	E	60	GLN
1	E	71	ARG
1	E	72	VAL
1	E	81	ASN
1	E	82	LYS
1	E	88	ASN
1	E	91	TYR
1	E	109	ARG
1	E	111	GLN
1	E	115	VAL
1	E	124	ASN
1	E	126	LEU
1	E	127	ASP
1	E	129	THR
1	E	140	THR
1	E	150	ASP
1	E	151	TYR
1	E	155	GLN
1	E	157	CYS
1	E	159	ILE

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Mol	Chain	Res	Type
1	E	165	ILE
1	E	167	GLU
1	E	176	LYS
1	E	185	CYS
1	E	189	GLU
1	E	190	LEU
1	E	191	ILE
1	E	212	LEU
1	E	216	ASN
1	E	219	GLU
1	E	220	VAL
1	E	223	ASP
1	E	242	TYR
1	E	252	ARG
1	E	255	VAL
1	E	266	THR
1	E	267	MET
1	E	273	GLU
1	E	277	ILE
1	E	281	ASP
1	E	282	ILE
1	E	285	ASN
1	E	289	TYR
1	E	292	SER
1	E	300	VAL
1	E	307	PHE
1	E	315	LYS
1	E	317	GLN
1	E	326	HIS
1	E	329	LEU
1	E	332	THR
1	E	334	VAL
1	E	339	SER
1	E	340	THR
1	E	345	CYS
1	E	362	LYS
1	E	363	GLU
1	E	387	GLU
1	E	393	HIS
1	E	395	MET
1	E	396	ASN
1	E	400	LEU

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Mol	Chain	Res	Type
1	E	401	GLU
1	E	403	TRP
1	E	404	ASN
1	E	407	VAL
1	E	408	THR
1	E	410	PRO
1	E	412	THR
1	E	415	LEU
1	E	428	THR
1	E	430	GLN
1	E	432	ASP
1	E	437	VAL
1	E	444	LYS
1	E	446	LYS
1	E	450	VAL
1	E	453	LYS
1	E	459	ASP
1	E	464	PRO
1	E	472	GLN
1	F	11	VAL
1	F	15	PRO
1	F	26	GLU
1	F	30	ARG
1	F	33	ILE
1	F	35	TYR
1	F	36	HIS
1	F	43	LEU
1	F	45	VAL
1	F	51	LYS
1	F	69	GLN
1	F	72	VAL
1	F	75	VAL
1	F	82	LYS
1	F	85	LEU
1	F	87	ASP
1	F	90	VAL
1	F	126	LEU
1	F	128	ASP
1	F	132	SER
1	F	150	ASP
1	F	151	TYR
1	F	156	LEU

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Mol	Chain	Res	Type
1	F	159	ILE
1	F	165	ILE
1	F	167	GLU
1	F	169	TRP
1	F	192	ASN
1	F	195	ILE
1	F	201	VAL
1	F	208	MET
1	F	211	LYS
1	F	221	PRO
1	F	237	MET
1	F	244	ASP
1	F	247	PHE
1	F	250	LEU
1	F	251	ARG
1	F	252	ARG
1	F	278	LYS
1	F	281	ASP
1	F	289	TYR
1	F	290	LEU
1	F	295	PRO
1	F	304	SER
1	F	312	TRP
1	F	317	GLN
1	F	324	CYS
1	F	328	GLN
1	F	333	VAL
1	F	339	SER
1	F	345	CYS
1	F	352	ILE
1	F	355	VAL
1	F	363	GLU
1	F	367	HIS
1	F	371	PHE
1	F	373	LEU
1	F	383	THR
1	F	387	GLU
1	F	388	VAL
1	F	391	TYR
1	F	393	HIS
1	F	396	ASN
1	F	399	ILE

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Mol	Chain	Res	Type
1	F	401	GLU
1	F	410	PRO
1	F	412	THR
1	F	416	VAL
1	F	419	TYR
1	F	422	VAL
1	F	427	VAL
1	F	430	GLN
1	F	431	LYS
1	F	436	PRO
1	F	439	GLN
1	F	444	LYS
1	F	450	VAL
1	F	451	ASP
1	F	453	LYS
1	F	454	GLU
1	F	455	ARG
1	F	461	ASP
1	F	464	PRO
1	F	465	LEU
1	F	472	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	88	ASN
1	A	120	HIS
1	A	153	GLN
1	A	314	HIS
1	A	326	HIS
1	A	394	ASN
1	A	462	GLN
1	B	131	ASN
1	B	341	ASN
1	B	367	HIS
1	B	423	GLN
1	C	47	HIS
1	C	153	GLN
1	C	270	GLN
1	C	317	GLN
1	C	321	ASN

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Mol	Chain	Res	Type
1	C	326	HIS
1	C	394	ASN
1	C	423	GLN
1	C	472	GLN
1	D	120	HIS
1	D	131	ASN
1	D	168	HIS
1	D	216	ASN
1	D	236	GLN
1	D	254	GLN
1	D	314	HIS
1	D	326	HIS
1	D	327	ASN
1	D	462	GLN
1	D	472	GLN
1	E	133	HIS
1	E	168	HIS
1	E	182	GLN
1	E	226	GLN
1	E	326	HIS
1	E	354	ASN
1	E	430	GLN
1	F	120	HIS
1	F	133	HIS
1	F	168	HIS
1	F	192	ASN
1	F	236	GLN
1	F	393	HIS
1	F	472	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

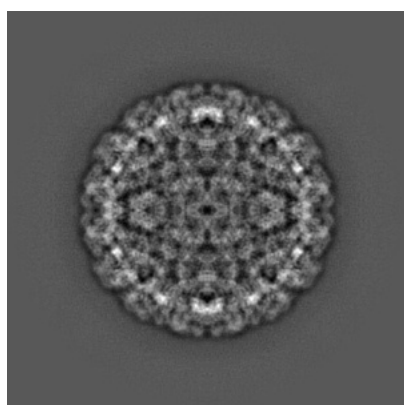
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8147. These allow visual inspection of the internal detail of the map and identification of artifacts.

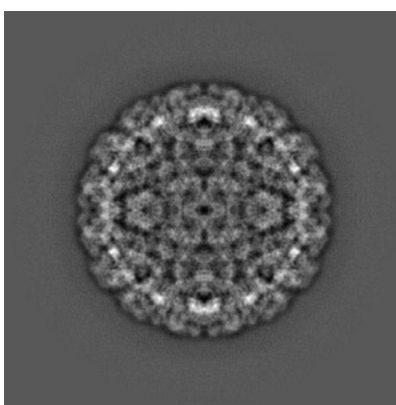
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

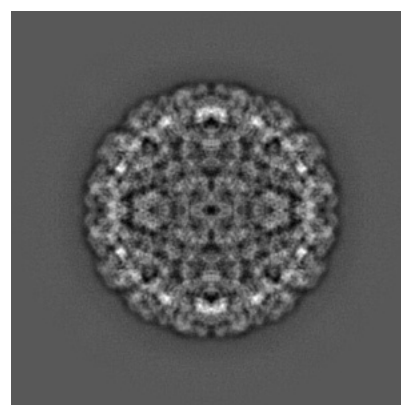
6.1.1 Primary map



X



Y

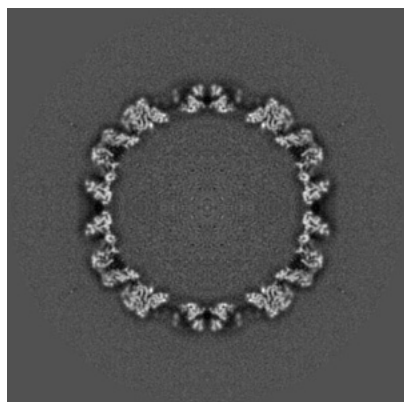


Z

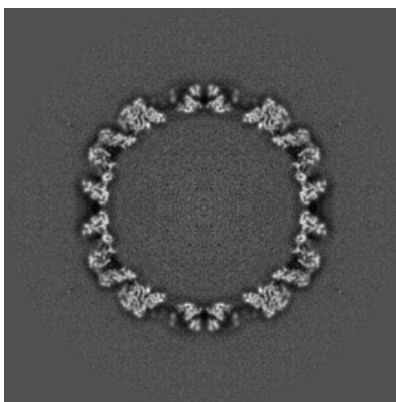
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

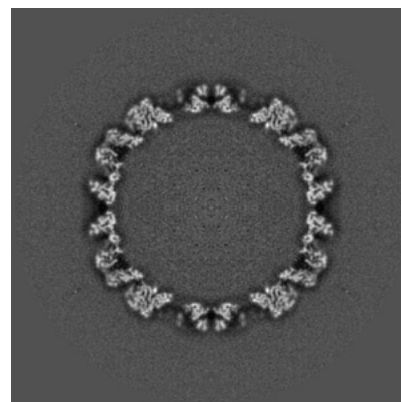
6.2.1 Primary map



X Index: 410



Y Index: 410

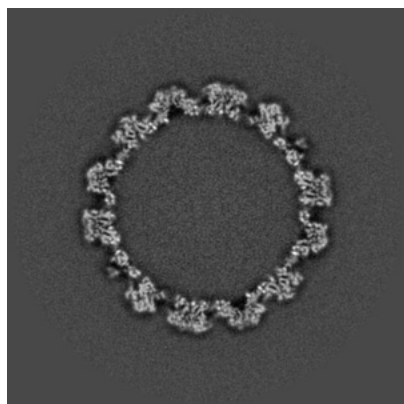


Z Index: 410

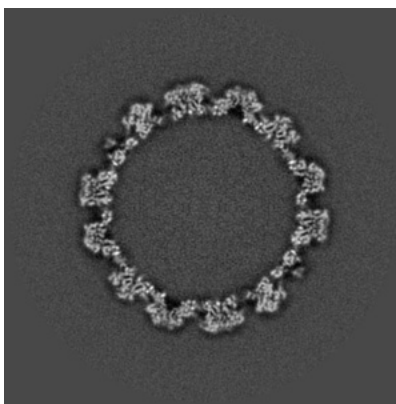
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

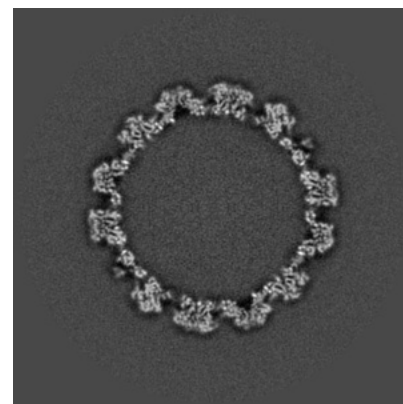
6.3.1 Primary map



X Index: 356



Y Index: 464

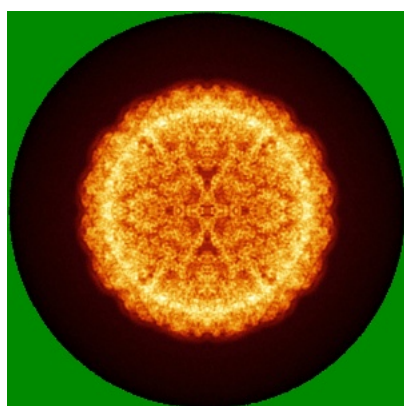


Z Index: 356

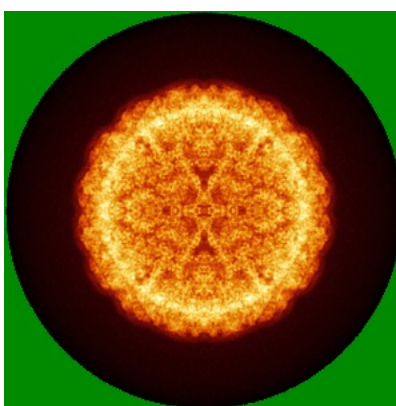
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

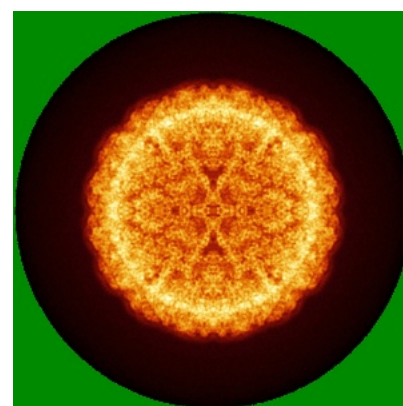
6.4.1 Primary map



X



Y

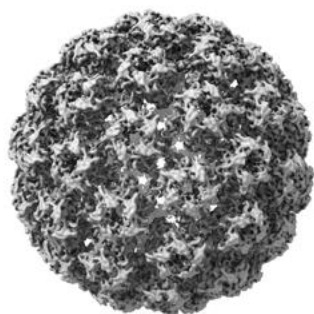


Z

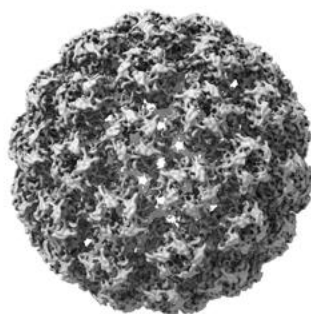
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

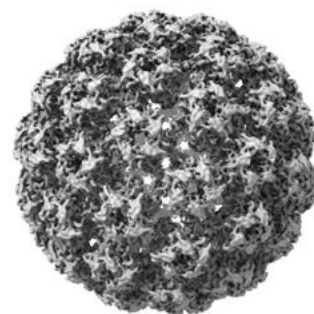
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

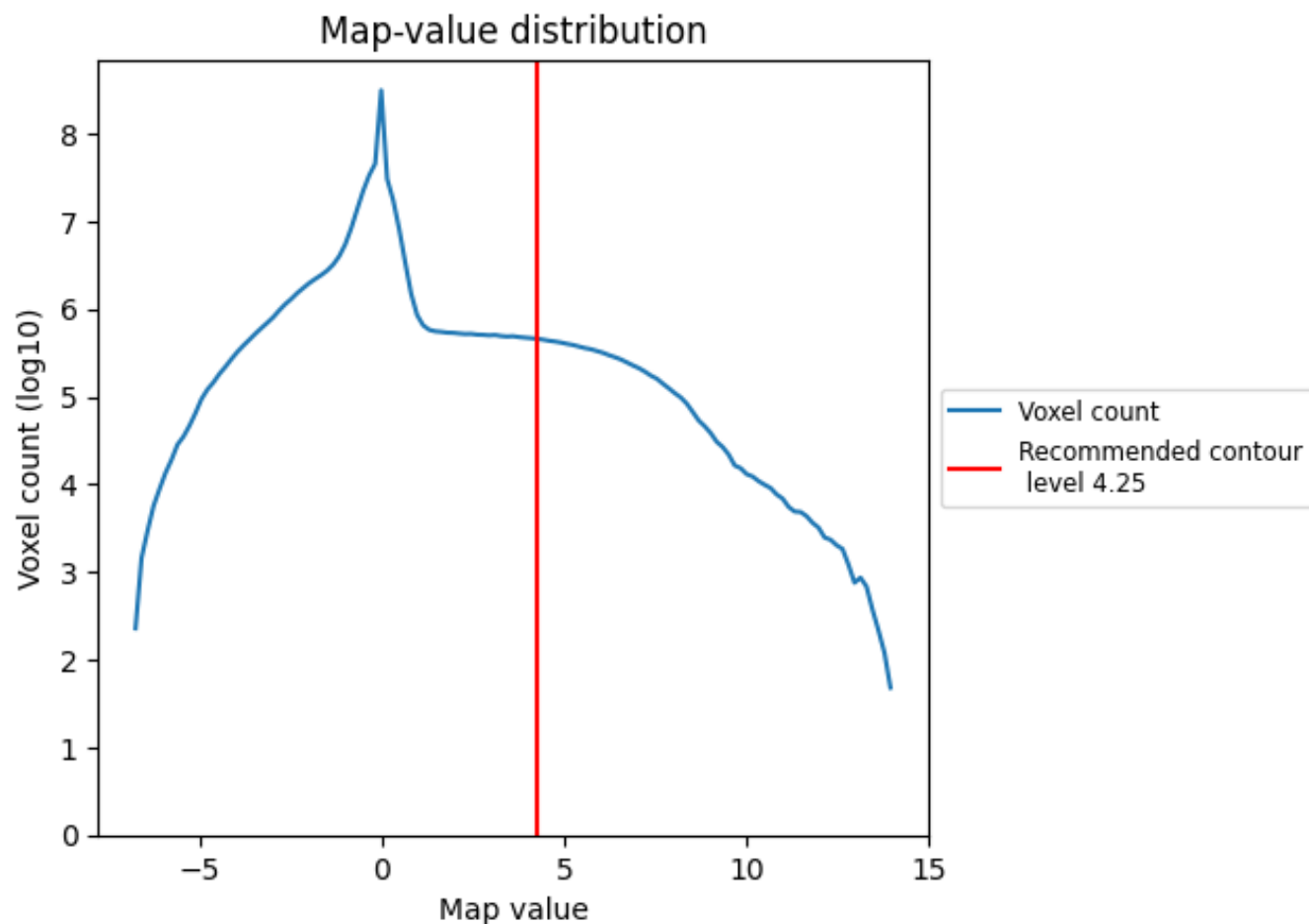
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

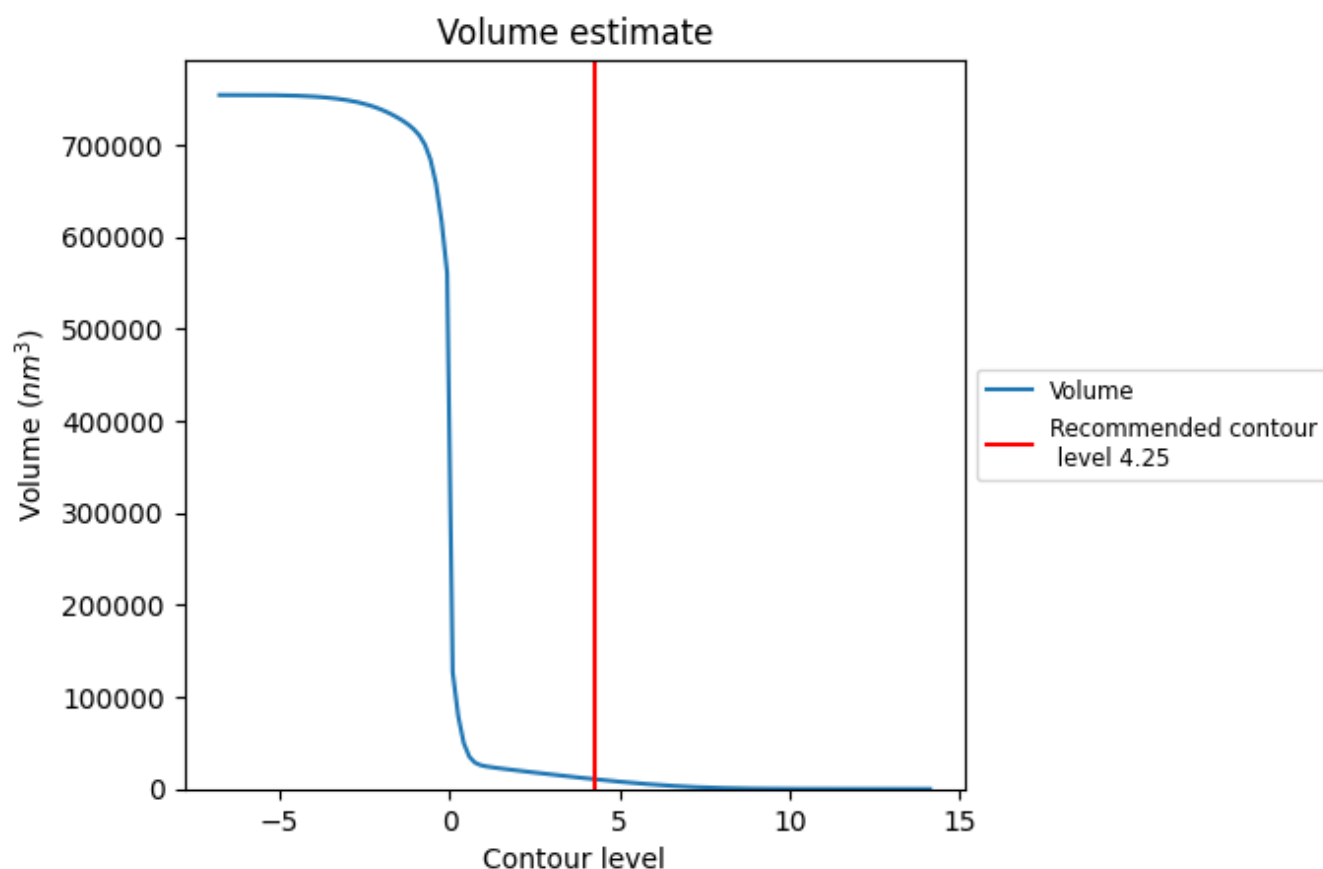
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

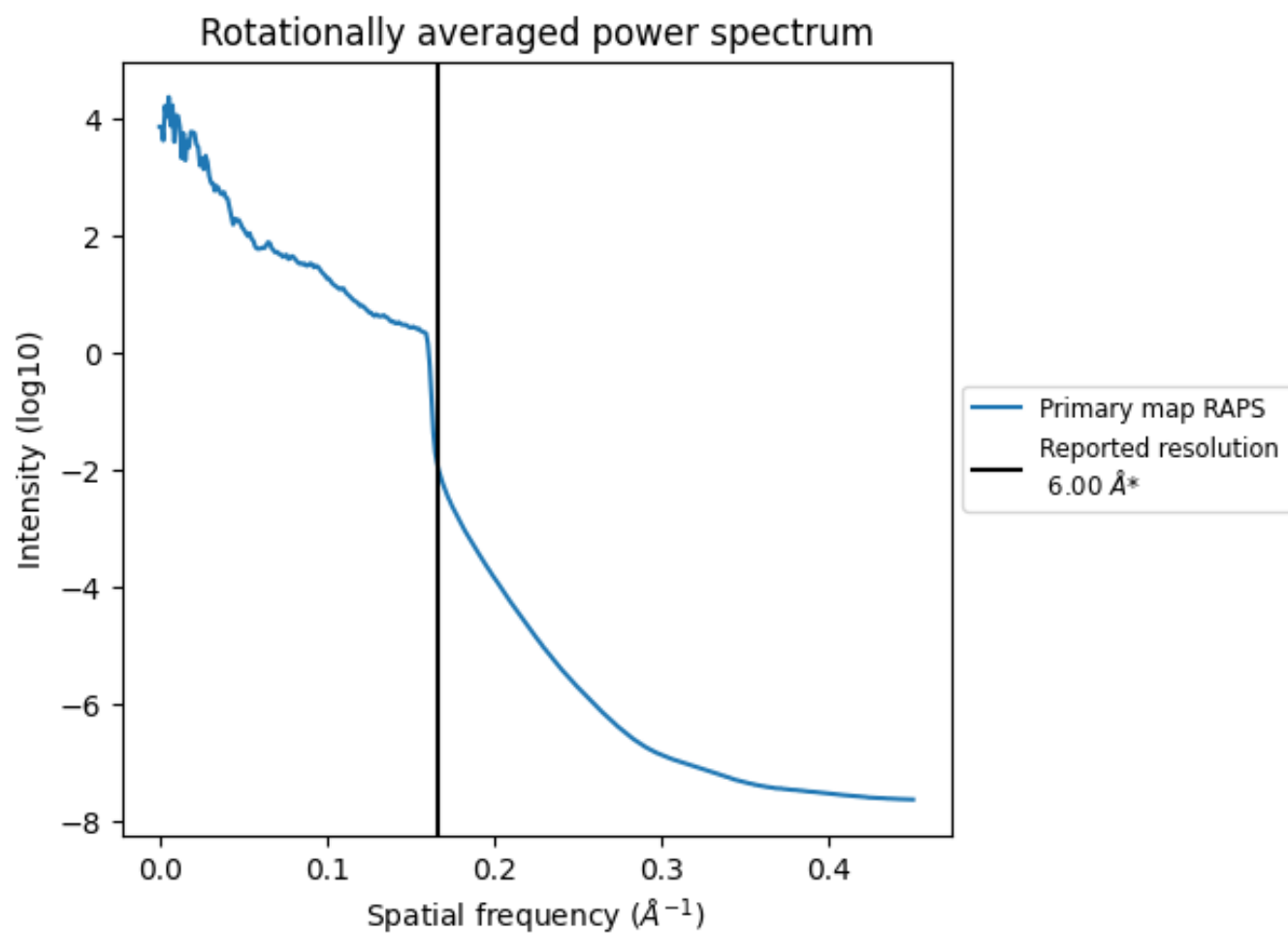
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10663 nm^3 ; this corresponds to an approximate mass of 9632 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

8 Fourier-Shell correlation

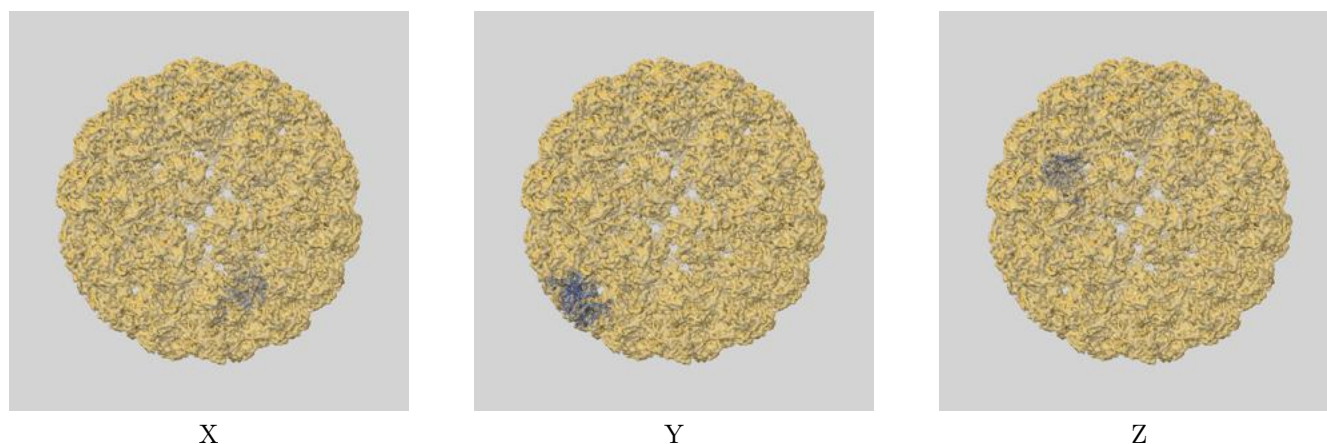
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

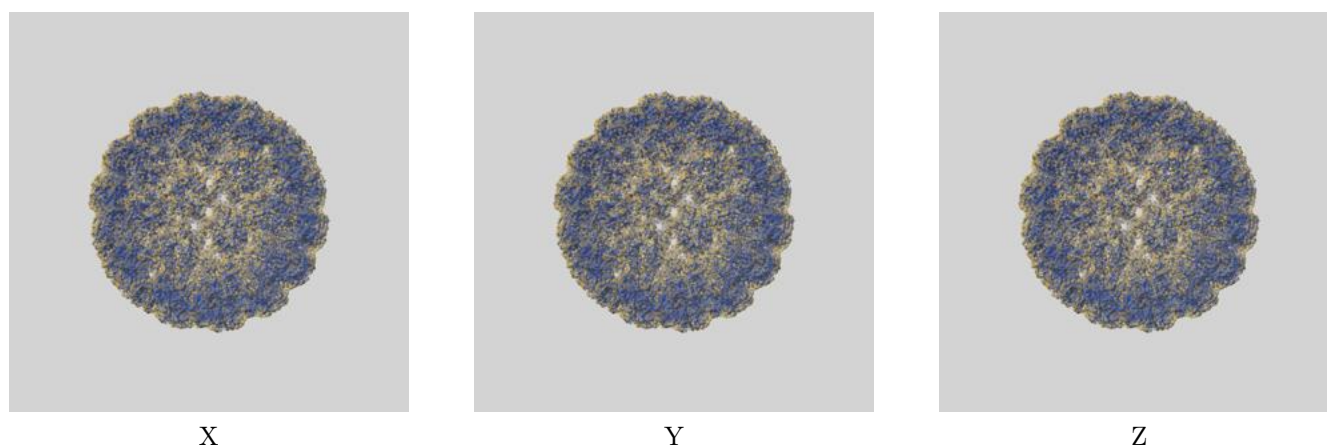
This section contains information regarding the fit between EMDB map EMD-8147 and PDB model 5JB1. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

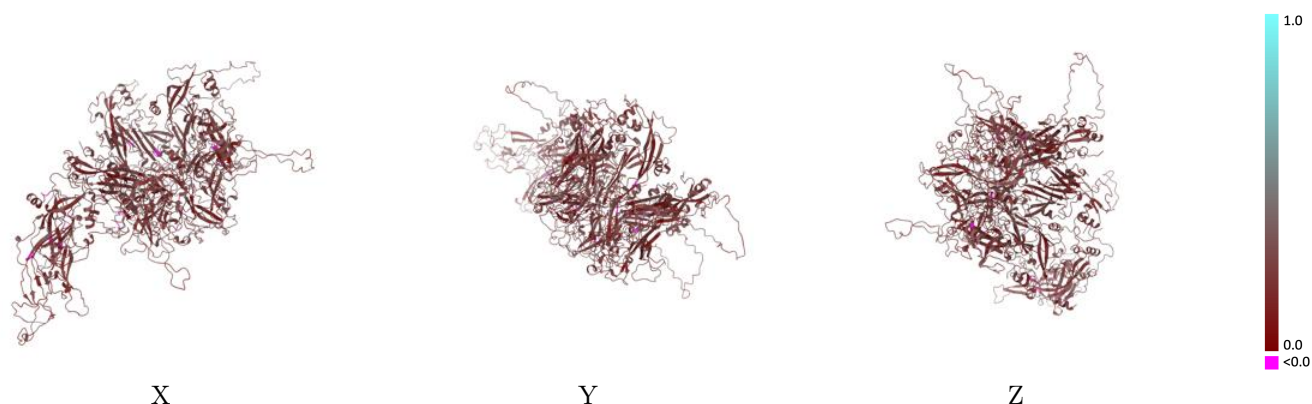


9.1.2 Map-model assembly overlay [i](#)



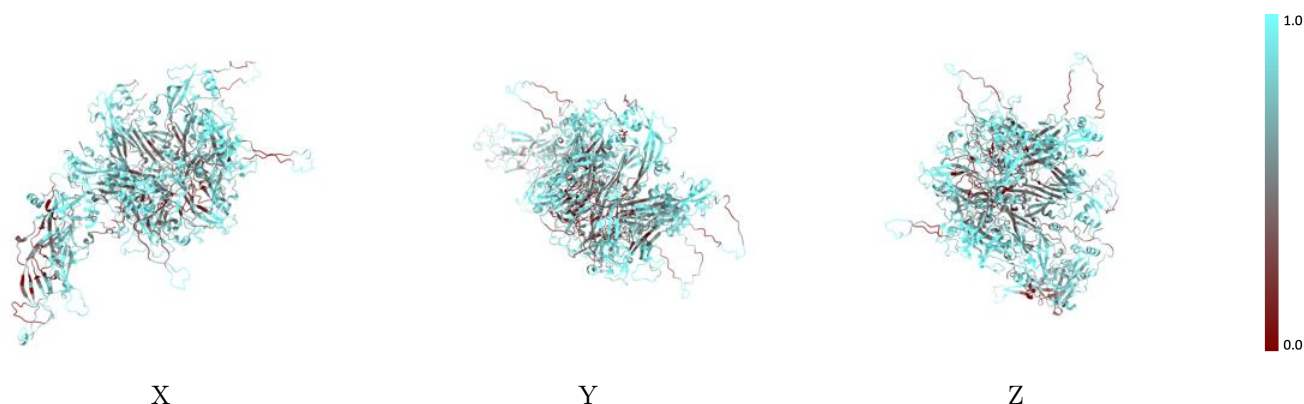
The images above show the 3D surface view of the map at the recommended contour level 4.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



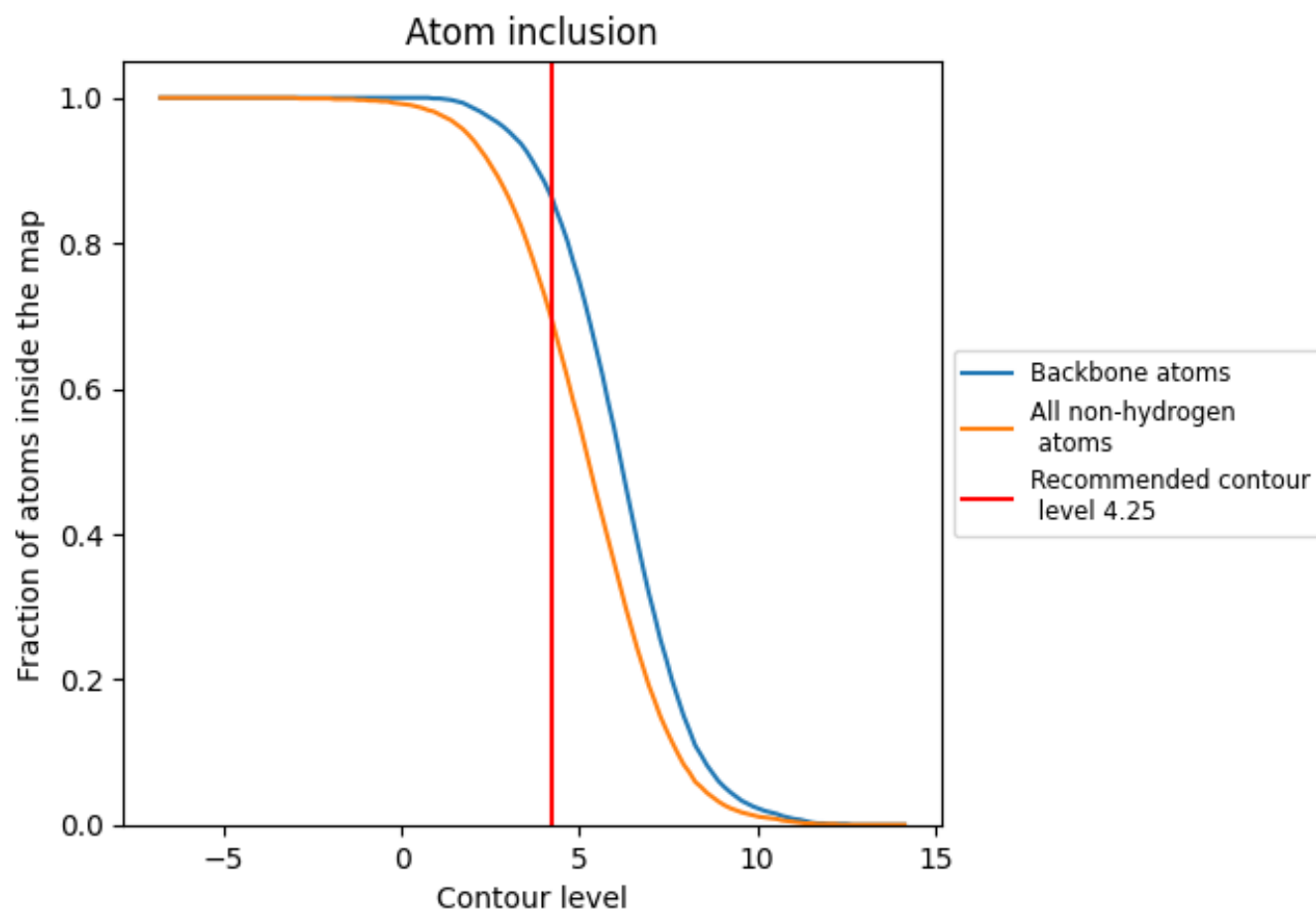
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6910	0.2550
A	0.6750	0.2530
B	0.6960	0.2540
C	0.6910	0.2550
D	0.6980	0.2580
E	0.7170	0.2570
F	0.6670	0.2560

1.0

0.0

<0.0