



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:48 PM UTC

PDB ID : 1RBA / pdb_00001rba
Title : SUBSTITUTION OF ASP193 TO ASN AT THE ACTIVE SITE OF RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE RESULTS IN CONFORMATIONAL CHANGES
Authors : Schneider, G.; Soderlind, E.
Deposited on : 1991-11-18
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

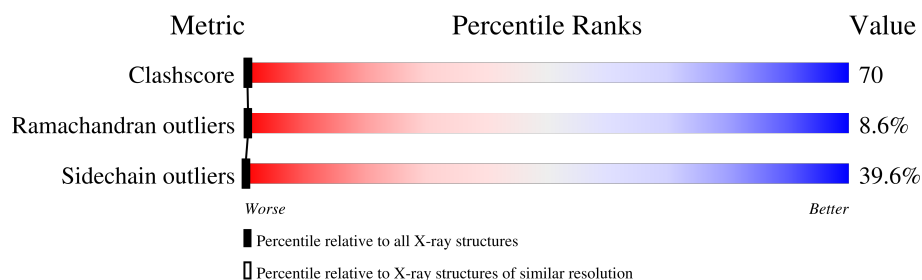
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	466	
1	B	466	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6695 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RUBISCO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3200	2029	566	590	15			
1	B	443	Total	C	N	O	S	0	0	0
			3385	2146	596	627	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASP	HIS	conflict	UNP P04718
A	193	ASN	ASP	engineered mutation	UNP P04718
B	91	ASP	HIS	conflict	UNP P04718
B	193	ASN	ASP	engineered mutation	UNP P04718

- Molecule 2 is water.

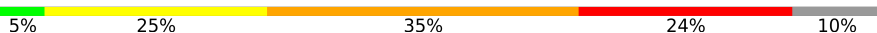
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	67	Total	O	0	0
			67	67		
2	B	43	Total	O	0	0
			43	43		

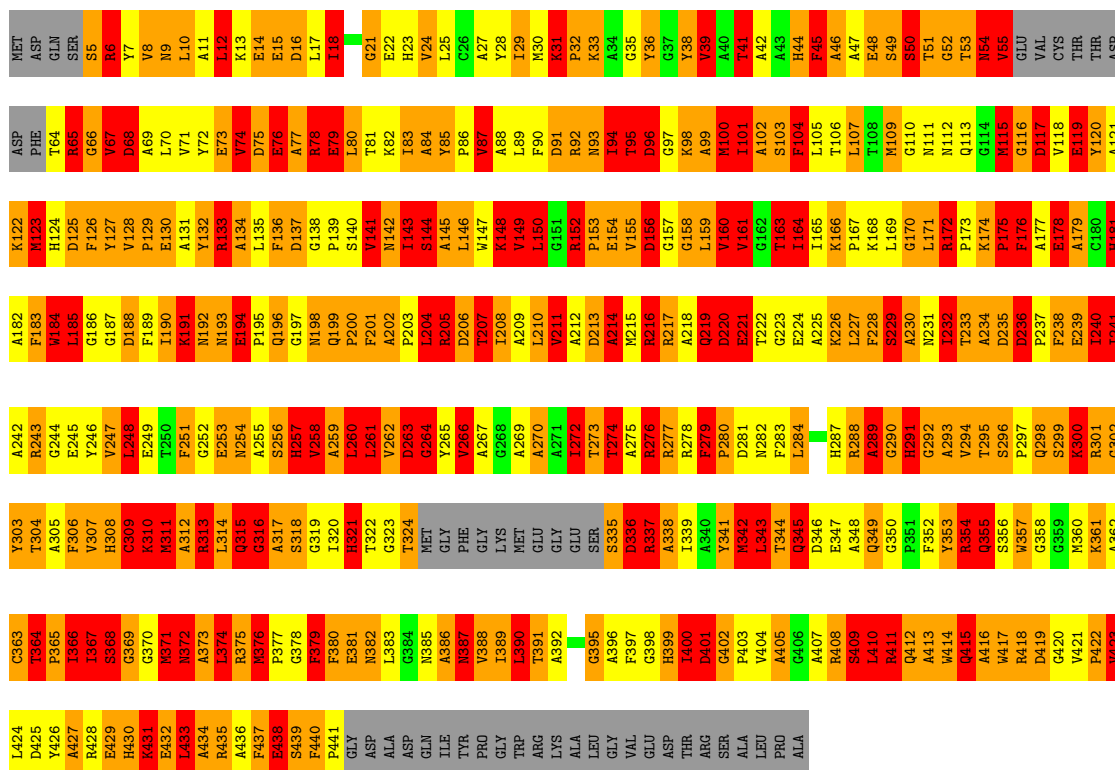
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

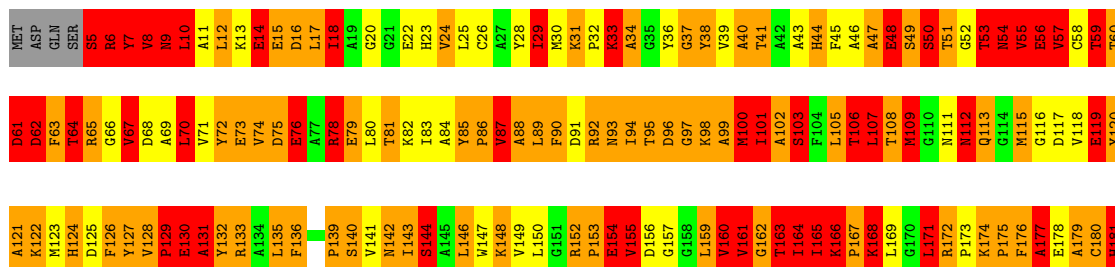
• Molecule 1: RUBISCO

Chain A: 



• Molecule 1: RUBISCO

Chain B: 



A182	A242	T304	T364	L424
F183	R243	A305	P365	D425
W184	G244	F306	I366	Y426
L185	E245	V307	S368	A427
G186	Y246	H308	G369	R428
G187	V247	C309	G370	E429
D188	L248	K310	M371	H430
F189	E249	M311	M371	A431
I190	T250	A312	N372	E432
K191	F251	R313	A373	L433
M192	G252	L314	L374	A434
M193	E253	Q315	R375	R435
E194	N254	G316	M376	A436
P195	A255	A317	P377	A437
Q196	S256	S318	G378	E438
G197	H257	G319	F379	S439
N198	V258	I320	F380	F440
Q199	A259	H321	E381	P441
P200	L260	T322	N382	G442
F201	L261	G323	L383	D443
A202	V262	T324	G384	A444
P203	D263	MET	N385	D445
L204	G264	GLY	A386	Q446
R205	Y265	PHE	N387	I447
D206	V266	GLY	Y388	Y448
T207		LYS	I389	P449
I208	A269	MET	L390	G450
A209		GLU	T391	W451
L210	T272	GLY	A392	R452
V211	T273	GLU	G393	K453
A212	T274	SER	G394	A454
D213	A275	S395	G395	L455
A214	R276	D396	A396	G456
M215	R277	A397	F397	Y457
R216	R278	A398	G398	GLU
R217	F279	H399	H399	ASP
A218	P280	A340	I400	THR
Q219	D281	Y341	D401	ARG
D220	M282	M342	G402	SER
E221	F283	L343	P403	ALA
T222	L284	T344	V404	LEU
G223	H285	Q345	A405	PRO
E224	Y286	D346	G406	ALA
A225	H287	E347	A407	
K226	R288	A348	R408	
L227	A289	Q349	S409	
F228	G290	G350	L410	
S229	H291	P351	R411	
A230	G292	F352	Q412	
M231	A293	Y353	A413	
I232	V294	R354	W414	
T233	T295	Q355	Q415	
A234	S296	S356	A416	
D235	P297	W357	W417	
D236	Q298	G358	R418	
P237	S299	G359	D419	
F238	K300	M360	G420	
E239	R301	K361	V421	
I240	G302	A362	P422	
I241	Y303	C363	Y423	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.50Å 69.30Å 103.10Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.207 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6695	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

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	2.06	56/3275 (1.7%)	4.27	800/4436 (18.0%)
1	B	2.01	59/3467 (1.7%)	4.26	871/4702 (18.5%)
All	All	2.03	115/6742 (1.7%)	4.27	1671/9138 (18.3%)

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	1	3
1	B	0	2
All	All	1	5

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	ILE	C-N	34.30	1.82	1.33
1	A	78	ARG	CA-CB	-33.88	0.98	1.53
1	A	361	LYS	CD-CE	23.53	2.23	1.52
1	B	278	ARG	CA-CB	-18.62	1.20	1.53
1	A	349	GLN	CA-CB	-18.34	1.22	1.53
1	A	164	ILE	CA-CB	16.86	1.74	1.53
1	A	176	PHE	CA-C	-14.52	1.33	1.52
1	B	41	THR	CA-CB	13.66	1.75	1.53
1	A	150	LEU	CA-CB	-12.58	1.32	1.53
1	A	164	ILE	CA-C	11.97	1.68	1.52
1	B	321	HIS	CB-CG	11.36	1.66	1.50
1	B	323	GLY	C-N	-11.19	1.17	1.33
1	A	376	MET	CA-CB	11.15	1.71	1.53
1	B	7	TYR	C-N	10.95	1.48	1.33
1	B	10	LEU	N-CA	10.28	1.59	1.46
1	B	321	HIS	CG-ND1	9.77	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	ASN	CA-C	9.58	1.64	1.53
1	B	9	ASN	N-CA	9.55	1.55	1.46
1	A	55	VAL	N-CA	-9.53	1.28	1.46
1	B	7	TYR	CA-C	9.08	1.65	1.52
1	A	176	PHE	C-N	-9.05	1.21	1.33
1	B	425	ASP	CA-C	8.87	1.64	1.52
1	A	67	VAL	CA-C	8.70	1.65	1.52
1	A	191	LYS	CD-CE	8.59	1.78	1.52
1	A	5	SER	N-CA	-8.38	1.30	1.46
1	A	336	ASP	N-CA	8.34	1.55	1.46
1	A	278	ARG	NE-CZ	8.30	1.42	1.33
1	A	387	ASN	CA-C	8.07	1.62	1.53
1	A	431	LYS	C-N	-8.03	1.23	1.33
1	B	165	ILE	CA-C	-8.03	1.43	1.52
1	A	278	ARG	CD-NE	7.72	1.57	1.46
1	B	322	THR	C-N	-7.26	1.25	1.33
1	B	8	VAL	CA-C	7.19	1.61	1.52
1	B	447	ILE	CA-CB	7.13	1.64	1.54
1	B	187	GLY	CA-C	7.03	1.58	1.51
1	B	142	ASN	CA-CB	-7.00	1.48	1.54
1	A	386	ALA	C-N	-6.84	1.23	1.33
1	B	289	ALA	C-O	6.81	1.28	1.23
1	B	191	LYS	CD-CE	6.80	1.72	1.52
1	A	387	ASN	N-CA	-6.68	1.37	1.46
1	B	120	TYR	C-N	-6.68	1.25	1.33
1	B	191	LYS	CA-CB	6.67	1.64	1.53
1	A	66	GLY	N-CA	6.57	1.54	1.45
1	A	295	THR	CA-CB	6.41	1.61	1.52
1	B	166	LYS	N-CA	-6.36	1.34	1.45
1	A	233	THR	CA-CB	6.36	1.61	1.53
1	B	167	PRO	N-CD	-6.36	1.39	1.47
1	B	141	VAL	C-N	-6.36	1.28	1.33
1	B	48	GLU	C-N	-6.31	1.24	1.33
1	A	186	GLY	N-CA	6.31	1.54	1.45
1	B	55	VAL	C-N	-6.24	1.24	1.33
1	A	304	THR	CA-C	6.20	1.60	1.52
1	B	7	TYR	CA-CB	-6.16	1.43	1.53
1	B	323	GLY	C-O	-6.14	1.16	1.23
1	B	233	THR	CA-CB	6.10	1.61	1.53
1	B	191	LYS	CG-CD	6.08	1.70	1.52
1	A	306	PHE	C-N	-6.05	1.26	1.33
1	A	150	LEU	N-CA	-6.04	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	THR	N-CA	5.92	1.53	1.46
1	A	13	LYS	N-CA	-5.91	1.38	1.46
1	B	88	ALA	CA-C	5.90	1.60	1.52
1	B	321	HIS	N-CA	5.89	1.53	1.45
1	B	444	ALA	N-CA	-5.86	1.38	1.46
1	A	165	ILE	CA-CB	5.85	1.62	1.54
1	B	321	HIS	ND1-CE1	5.79	1.38	1.32
1	A	22	GLU	C-O	-5.76	1.19	1.23
1	A	150	LEU	CA-C	-5.75	1.44	1.52
1	A	190	ILE	C-N	5.73	1.41	1.33
1	A	85	TYR	CA-CB	5.72	1.62	1.52
1	A	236	ASP	CA-CB	-5.70	1.44	1.53
1	A	264	GLY	N-CA	-5.69	1.37	1.45
1	A	65	ARG	NE-CZ	5.66	1.39	1.33
1	A	128	VAL	N-CA	5.62	1.50	1.46
1	B	10	LEU	C-N	-5.59	1.25	1.33
1	A	191	LYS	CA-CB	5.50	1.63	1.53
1	A	391	THR	C-N	-5.46	1.26	1.33
1	B	191	LYS	CB-CG	5.41	1.68	1.52
1	A	46	ALA	C-O	5.40	1.30	1.24
1	B	188	ASP	C-N	-5.40	1.26	1.33
1	A	432	GLU	CA-C	5.39	1.59	1.52
1	A	100	MET	C-O	5.36	1.30	1.23
1	B	262	VAL	N-CA	-5.34	1.40	1.46
1	B	262	VAL	CA-C	5.32	1.59	1.52
1	B	315	GLN	C-N	-5.32	1.27	1.34
1	B	7	TYR	N-CA	5.31	1.53	1.46
1	B	18	ILE	CA-CB	5.29	1.60	1.54
1	B	223	GLY	N-CA	5.28	1.53	1.45
1	B	457	VAL	C-O	5.27	1.34	1.23
1	A	149	VAL	CA-C	-5.24	1.46	1.53
1	B	5	SER	C-N	-5.23	1.26	1.33
1	B	67	VAL	CA-C	5.21	1.57	1.52
1	B	8	VAL	N-CA	5.21	1.52	1.46
1	B	230	ALA	C-N	-5.20	1.26	1.33
1	A	153	PRO	C-O	5.17	1.29	1.23
1	A	193	ASN	N-CA	5.16	1.52	1.45
1	B	292	GLY	N-CA	5.16	1.52	1.45
1	B	288	ARG	NE-CZ	5.15	1.38	1.33
1	A	277	ARG	N-CA	5.15	1.52	1.46
1	B	285	HIS	CA-CB	5.14	1.59	1.53
1	A	255	ALA	C-N	-5.13	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	PRO	CA-C	-5.12	1.47	1.52
1	B	425	ASP	CB-CG	5.12	1.64	1.52
1	A	278	ARG	CB-CG	5.10	1.67	1.52
1	A	311	MET	C-N	-5.09	1.27	1.33
1	B	75	ASP	N-CA	5.09	1.53	1.46
1	A	239	GLU	C-O	-5.08	1.18	1.24
1	B	275	ALA	N-CA	-5.07	1.40	1.46
1	B	303	TYR	N-CA	-5.07	1.39	1.46
1	A	263	ASP	N-CA	5.07	1.52	1.46
1	B	273	THR	N-CA	5.06	1.52	1.46
1	A	366	ILE	C-N	-5.03	1.27	1.33
1	B	335	SER	N-CA	5.02	1.55	1.46
1	A	245	GLU	N-CA	5.01	1.52	1.46
1	B	50	SER	C-O	5.01	1.27	1.23
1	A	202	ALA	N-CA	-5.00	1.42	1.46

All (1671) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ASP	CA-CB-CG	32.93	145.53	112.60
1	A	401	ASP	CA-CB-CG	31.16	143.76	112.60
1	B	354	ARG	CD-NE-CZ	29.86	166.20	124.40
1	B	441	PRO	CA-C-N	29.73	179.67	121.41
1	B	441	PRO	C-N-CA	29.73	179.67	121.41
1	A	254	ASN	CA-CB-CG	29.25	141.85	112.60
1	B	142	ASN	CA-CB-CG	28.34	140.94	112.60
1	A	435	ARG	CD-NE-CZ	27.76	163.27	124.40
1	A	189	PHE	CA-CB-CG	27.39	141.19	113.80
1	B	263	ASP	CA-CB-CG	27.35	139.95	112.60
1	A	91	ASP	CA-CB-CG	26.95	139.55	112.60
1	B	92	ARG	CD-NE-CZ	26.88	162.03	124.40
1	A	75	ASP	CA-CB-CG	26.84	139.44	112.60
1	B	188	ASP	CA-CB-CG	26.83	139.43	112.60
1	B	93	ASN	CA-CB-CG	25.39	137.99	112.60
1	B	284	LEU	CA-C-N	24.00	159.10	121.66
1	B	284	LEU	C-N-CA	24.00	159.10	121.66
1	B	302	GLY	CA-C-N	23.86	162.41	122.33
1	B	302	GLY	C-N-CA	23.86	162.41	122.33
1	A	321	HIS	CA-CB-CG	23.81	137.61	113.80
1	B	192	ASN	CA-CB-CG	23.80	136.40	112.60
1	A	263	ASP	CA-C-N	22.19	164.90	121.41
1	A	263	ASP	C-N-CA	22.19	164.90	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	PHE	CA-CB-CG	21.12	134.92	113.80
1	A	206	ASP	CA-CB-CG	20.36	132.96	112.60
1	A	385	ASN	CA-CB-CG	19.98	132.58	112.60
1	A	68	ASP	CA-CB-CG	19.64	132.24	112.60
1	B	346	ASP	CA-CB-CG	19.44	132.04	112.60
1	B	221	GLU	CA-CB-CG	19.38	152.86	114.10
1	B	7	TYR	CA-C-N	19.22	156.57	121.97
1	B	7	TYR	C-N-CA	19.22	156.57	121.97
1	B	231	ASN	OD1-CG-ND2	18.37	140.97	122.60
1	B	360	MET	CA-C-N	18.24	146.54	120.82
1	B	360	MET	C-N-CA	18.24	146.54	120.82
1	B	253	GLU	CA-CB-CG	18.10	150.30	114.10
1	A	137	ASP	CA-CB-CG	17.75	130.35	112.60
1	B	321	HIS	CA-CB-CG	17.72	131.52	113.80
1	B	278	ARG	CB-CA-C	17.31	142.95	109.72
1	A	194	GLU	O-C-N	-17.18	101.56	121.32
1	B	195	PRO	CA-C-N	17.05	148.15	121.56
1	B	195	PRO	C-N-CA	17.05	148.15	121.56
1	A	154	GLU	CA-C-N	16.93	152.44	121.97
1	A	154	GLU	C-N-CA	16.93	152.44	121.97
1	A	216	ARG	CD-NE-CZ	16.80	147.91	124.40
1	A	161	VAL	O-C-N	16.60	140.24	122.98
1	B	16	ASP	CA-CB-CG	16.57	129.17	112.60
1	A	315	GLN	CA-C-O	16.23	140.15	119.05
1	A	403	PRO	CA-C-N	16.14	151.03	121.97
1	A	403	PRO	C-N-CA	16.14	151.03	121.97
1	A	53	THR	CA-C-N	15.94	151.98	121.54
1	A	53	THR	C-N-CA	15.94	151.98	121.54
1	A	429	GLU	CB-CG-CD	15.79	139.44	112.60
1	A	54	ASN	CA-CB-CG	15.76	128.36	112.60
1	B	283	PHE	CA-CB-CG	15.72	129.52	113.80
1	A	395	GLY	CA-C-N	15.65	149.39	122.79
1	A	395	GLY	C-N-CA	15.65	149.39	122.79
1	A	313	ARG	NE-CZ-NH2	15.64	133.28	119.20
1	A	361	LYS	CA-C-O	15.59	138.34	121.19
1	B	126	PHE	CA-CB-CG	15.49	129.29	113.80
1	A	349	GLN	CB-CG-CD	15.48	138.92	112.60
1	A	336	ASP	CA-C-O	15.11	137.31	119.78
1	B	284	LEU	CA-C-O	15.11	139.60	120.57
1	B	243	ARG	CA-CB-CG	14.99	144.07	114.10
1	A	276	ARG	CD-NE-CZ	14.85	145.19	124.40
1	A	126	PHE	CA-CB-CG	14.79	128.59	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	GLN	CB-CG-CD	14.72	137.63	112.60
1	A	213	ASP	CA-CB-CG	14.70	127.30	112.60
1	A	240	ILE	CA-C-N	14.69	139.06	120.56
1	A	240	ILE	C-N-CA	14.69	139.06	120.56
1	A	187	GLY	CA-C-N	14.64	149.50	121.54
1	A	187	GLY	C-N-CA	14.64	149.50	121.54
1	B	93	ASN	OD1-CG-ND2	-14.59	108.01	122.60
1	B	430	HIS	CA-CB-CG	-14.59	99.21	113.80
1	B	57	VAL	CB-CA-C	14.53	135.12	111.29
1	B	216	ARG	N-CA-C	-14.49	95.17	110.97
1	B	429	GLU	CA-CB-CG	14.44	142.98	114.10
1	B	220	ASP	CA-C-N	14.39	140.20	120.63
1	B	220	ASP	C-N-CA	14.39	140.20	120.63
1	B	249	GLU	CA-C-N	14.33	142.09	120.31
1	B	249	GLU	C-N-CA	14.33	142.09	120.31
1	B	15	GLU	CA-CB-CG	14.32	142.74	114.10
1	B	130	GLU	CB-CG-CD	14.24	136.81	112.60
1	A	428	ARG	N-CA-C	14.23	126.79	111.28
1	A	142	ASN	CA-CB-CG	14.19	126.79	112.60
1	B	133	ARG	NE-CZ-NH2	-14.18	106.44	119.20
1	A	306	PHE	CA-C-N	14.16	140.53	120.42
1	A	306	PHE	C-N-CA	14.16	140.53	120.42
1	A	364	THR	N-CA-C	14.16	127.81	109.83
1	B	443	ASP	CA-C-N	14.14	148.37	122.06
1	B	443	ASP	C-N-CA	14.14	148.37	122.06
1	A	105	LEU	CA-C-N	14.09	140.57	120.28
1	A	105	LEU	C-N-CA	14.09	140.57	120.28
1	B	429	GLU	CB-CG-CD	13.80	136.07	112.60
1	B	18	ILE	CB-CG1-CD1	13.77	142.71	113.80
1	A	156	ASP	CA-CB-CG	13.75	126.35	112.60
1	A	336	ASP	CA-C-N	13.56	147.43	121.54
1	A	336	ASP	C-N-CA	13.56	147.43	121.54
1	B	442	GLY	CA-C-N	13.55	147.41	121.54
1	B	442	GLY	C-N-CA	13.55	147.41	121.54
1	B	14	GLU	CB-CG-CD	13.53	135.60	112.60
1	A	408	ARG	CA-C-O	13.49	133.41	118.97
1	A	9	ASN	CA-CB-CG	-13.43	99.17	112.60
1	B	177	ALA	CA-C-N	13.27	139.75	120.38
1	B	177	ALA	C-N-CA	13.27	139.75	120.38
1	A	232	ILE	CA-C-O	-13.25	106.89	120.14
1	A	176	PHE	CA-CB-CG	-13.24	100.56	113.80
1	A	12	LEU	CA-C-N	13.19	146.73	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	LEU	C-N-CA	13.19	146.73	121.54
1	A	301	ARG	CA-C-N	13.19	133.07	121.86
1	A	301	ARG	C-N-CA	13.19	133.07	121.86
1	A	367	ILE	CA-C-O	13.18	134.23	120.39
1	B	181	HIS	CA-CB-CG	13.18	126.98	113.80
1	A	152	ARG	O-C-N	13.17	132.74	121.54
1	A	296	SER	O-C-N	13.17	130.14	121.71
1	B	368	SER	CA-C-O	13.12	134.66	121.14
1	B	360	MET	CA-C-O	13.11	135.78	120.70
1	B	211	VAL	N-CA-C	-13.09	96.73	111.00
1	B	260	LEU	CA-C-N	13.08	140.08	121.24
1	B	260	LEU	C-N-CA	13.08	140.08	121.24
1	B	17	LEU	CA-C-N	13.00	137.20	120.56
1	B	17	LEU	C-N-CA	13.00	137.20	120.56
1	A	133	ARG	CD-NE-CZ	12.99	142.59	124.40
1	A	352	PHE	CA-CB-CG	12.95	126.75	113.80
1	B	221	GLU	CB-CG-CD	12.94	134.59	112.60
1	A	188	ASP	CA-C-O	-12.92	102.03	120.51
1	A	298	GLN	CG-CD-OE1	12.92	146.65	120.80
1	A	163	THR	O-C-N	12.86	137.18	123.42
1	B	102	ALA	CA-C-O	-12.84	105.83	120.20
1	A	201	PHE	CA-CB-CG	12.79	126.59	113.80
1	A	366	ILE	N-CA-C	-12.76	90.20	108.58
1	A	156	ASP	N-CA-CB	12.76	132.05	110.49
1	A	373	ALA	CA-C-N	12.75	147.00	122.53
1	A	373	ALA	C-N-CA	12.75	147.00	122.53
1	A	361	LYS	CA-C-N	12.74	139.59	121.24
1	A	361	LYS	C-N-CA	12.74	139.59	121.24
1	B	64	THR	CB-CA-C	-12.74	95.06	111.50
1	B	262	VAL	CA-C-N	12.71	140.86	122.05
1	B	262	VAL	C-N-CA	12.71	140.86	122.05
1	A	263	ASP	CB-CA-C	12.60	131.06	111.91
1	A	408	ARG	CA-C-N	12.59	142.11	120.58
1	A	408	ARG	C-N-CA	12.59	142.11	120.58
1	A	145	ALA	CB-CA-C	12.55	127.59	111.40
1	B	357	TRP	CA-C-O	12.48	132.62	118.90
1	A	67	VAL	N-CA-CB	-12.47	95.14	112.35
1	B	7	TYR	CA-CB-CG	-12.46	91.47	113.90
1	B	70	LEU	CA-C-O	-12.43	107.53	120.71
1	B	201	PHE	CA-CB-CG	12.41	126.21	113.80
1	A	125	ASP	CA-C-O	-12.37	107.97	121.33
1	A	183	PHE	N-CA-C	-12.37	98.14	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	GLY	CA-C-N	12.34	136.54	121.85
1	A	66	GLY	C-N-CA	12.34	136.54	121.85
1	A	400	ILE	CA-C-O	-12.34	107.35	121.05
1	B	346	ASP	N-CA-CB	12.34	130.73	110.37
1	A	347	GLU	N-CA-CB	12.32	133.57	110.90
1	B	165	ILE	O-C-N	12.28	136.67	123.04
1	B	190	ILE	CB-CA-C	12.24	128.74	110.63
1	A	431	LYS	N-CA-C	12.22	125.76	111.71
1	A	437	PHE	N-CA-C	-12.18	97.69	110.97
1	A	290	GLY	N-CA-C	-12.17	100.56	113.58
1	A	354	ARG	CA-C-O	-12.17	106.94	120.32
1	B	188	ASP	N-CA-C	12.15	131.01	114.12
1	B	243	ARG	CB-CG-CD	12.15	139.25	111.30
1	B	136	PHE	CA-C-N	12.14	140.50	121.19
1	B	136	PHE	C-N-CA	12.14	140.50	121.19
1	A	311	MET	N-CA-C	-12.13	98.14	111.36
1	B	384	GLY	CA-C-N	12.13	141.85	122.81
1	B	384	GLY	C-N-CA	12.13	141.85	122.81
1	B	322	THR	CA-C-N	12.12	137.77	120.56
1	B	322	THR	C-N-CA	12.12	137.77	120.56
1	B	322	THR	O-C-N	12.12	138.70	122.59
1	A	176	PHE	N-CA-C	-12.11	85.00	110.80
1	A	311	MET	CA-C-N	12.10	136.96	120.38
1	A	311	MET	C-N-CA	12.10	136.96	120.38
1	B	303	TYR	N-CA-CB	12.09	131.12	110.81
1	A	243	ARG	CD-NE-CZ	12.02	141.22	124.40
1	A	366	ILE	N-CA-CB	11.98	123.78	110.72
1	B	389	ILE	CA-C-O	-11.98	107.78	120.48
1	A	298	GLN	OE1-CD-NE2	-11.97	110.63	122.60
1	A	361	LYS	N-CA-C	11.89	127.47	110.23
1	A	185	LEU	CA-C-O	-11.86	108.17	120.98
1	A	255	ALA	CA-C-N	11.83	140.81	122.24
1	A	255	ALA	C-N-CA	11.83	140.81	122.24
1	B	146	LEU	N-CA-C	-11.73	97.08	111.40
1	B	436	ALA	N-CA-C	-11.72	98.19	110.97
1	A	387	ASN	CB-CA-C	11.70	131.22	111.68
1	A	78	ARG	CA-C-N	11.69	138.94	122.46
1	A	78	ARG	C-N-CA	11.69	138.94	122.46
1	B	54	ASN	CA-C-N	11.64	142.91	121.97
1	B	54	ASN	C-N-CA	11.64	142.91	121.97
1	B	354	ARG	CA-C-O	-11.62	108.89	121.56
1	B	216	ARG	CA-C-N	11.61	138.23	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	ARG	C-N-CA	11.61	138.23	120.82
1	B	186	GLY	CA-C-N	11.53	137.93	121.56
1	B	186	GLY	C-N-CA	11.53	137.93	121.56
1	B	457	VAL	CB-CA-C	-11.52	89.50	111.40
1	B	260	LEU	N-CA-CB	-11.51	89.52	110.82
1	B	425	ASP	CB-CA-C	11.50	129.62	109.15
1	B	399	HIS	O-C-N	11.48	136.98	122.97
1	B	219	GLN	CA-CB-CG	11.45	137.01	114.10
1	B	279	PHE	CA-CB-CG	11.45	125.25	113.80
1	A	6	ARG	CD-NE-CZ	11.45	140.43	124.40
1	A	201	PHE	CA-C-N	11.41	132.32	122.28
1	A	201	PHE	C-N-CA	11.41	132.32	122.28
1	B	313	ARG	NE-CZ-NH1	11.39	132.89	121.50
1	A	304	THR	N-CA-CB	11.38	127.65	110.70
1	A	243	ARG	NE-CZ-NH1	11.35	132.85	121.50
1	B	371	MET	O-C-N	11.35	138.10	123.01
1	A	337	ARG	CA-C-O	11.35	136.74	120.51
1	B	10	LEU	O-C-N	-11.31	107.54	122.59
1	B	136	PHE	CA-C-O	11.28	133.90	121.16
1	B	262	VAL	CA-C-O	11.24	133.12	120.76
1	B	93	ASN	CB-CG-OD1	11.23	143.26	120.80
1	B	111	ASN	CB-CA-C	11.19	129.37	110.79
1	B	160	VAL	CB-CA-C	11.16	126.01	110.84
1	B	206	ASP	N-CA-C	-11.13	99.20	113.12
1	B	193	ASN	CA-CB-CG	11.10	123.70	112.60
1	B	346	ASP	O-C-N	11.10	136.26	123.05
1	B	260	LEU	CB-CA-C	11.08	128.62	111.77
1	A	172	ARG	NE-CZ-NH1	11.04	132.54	121.50
1	B	163	THR	O-C-N	11.03	133.34	123.41
1	A	251	PHE	CA-C-O	11.02	133.56	119.12
1	B	162	GLY	CA-C-O	11.02	132.30	121.72
1	B	243	ARG	CG-CD-NE	11.02	136.25	112.00
1	B	369	GLY	N-CA-C	10.96	131.03	110.86
1	B	399	HIS	N-CA-CB	10.95	127.11	109.69
1	A	10	LEU	N-CA-C	-10.94	95.08	110.50
1	B	183	PHE	N-CA-C	-10.93	99.98	113.97
1	B	277	ARG	NE-CZ-NH1	10.93	132.43	121.50
1	A	349	GLN	N-CA-CB	10.90	128.91	110.49
1	A	48	GLU	CB-CG-CD	10.90	131.13	112.60
1	B	141	VAL	N-CA-CB	10.88	129.17	111.23
1	A	223	GLY	CA-C-O	10.82	130.65	118.96
1	B	5	SER	O-C-N	10.81	140.29	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	PHE	CA-CB-CG	10.79	124.59	113.80
1	A	239	GLU	CA-C-N	10.76	134.48	120.60
1	A	239	GLU	C-N-CA	10.76	134.48	120.60
1	A	70	LEU	O-C-N	10.76	135.78	123.19
1	A	207	THR	N-CA-CB	10.75	128.66	110.49
1	A	317	ALA	N-CA-C	-10.68	93.35	110.32
1	B	192	ASN	N-CA-C	-10.65	93.37	110.20
1	B	321	HIS	O-C-N	10.64	134.98	123.06
1	B	302	GLY	O-C-N	-10.60	108.92	122.70
1	B	171	LEU	O-C-N	10.60	135.15	122.75
1	A	368	SER	CA-C-O	10.59	134.58	121.66
1	A	337	ARG	CA-C-N	10.59	141.76	121.54
1	A	337	ARG	C-N-CA	10.59	141.76	121.54
1	B	216	ARG	CB-CG-CD	10.55	135.57	111.30
1	B	238	PHE	CA-C-O	-10.54	108.18	120.10
1	A	70	LEU	CA-C-O	-10.52	109.12	120.80
1	B	230	ALA	CA-C-N	10.50	138.04	121.66
1	B	230	ALA	C-N-CA	10.50	138.04	121.66
1	B	183	PHE	N-CA-CB	10.49	125.26	110.67
1	A	317	ALA	CA-C-O	-10.49	108.77	121.36
1	A	142	ASN	OD1-CG-ND2	-10.48	112.12	122.60
1	A	196	GLN	OE1-CD-NE2	-10.46	112.14	122.60
1	A	230	ALA	CA-C-O	10.43	131.62	120.36
1	B	345	GLN	CB-CG-CD	10.41	130.30	112.60
1	A	235	ASP	CB-CA-C	10.38	127.74	111.02
1	B	188	ASP	CB-CA-C	-10.38	91.95	109.38
1	A	301	ARG	N-CA-C	10.31	126.12	110.14
1	A	245	GLU	CA-C-N	10.28	134.42	120.54
1	A	245	GLU	C-N-CA	10.28	134.42	120.54
1	B	225	ALA	N-CA-C	10.28	123.61	110.65
1	B	282	ASN	CA-C-O	-10.28	109.08	121.11
1	B	66	GLY	CA-C-N	10.27	133.56	122.77
1	B	66	GLY	C-N-CA	10.27	133.56	122.77
1	A	8	VAL	CA-C-O	10.24	131.21	120.36
1	A	238	PHE	N-CA-C	-10.21	101.32	113.88
1	A	94	ILE	N-CA-C	-10.20	100.62	110.42
1	A	152	ARG	CA-C-O	-10.16	111.87	120.71
1	A	181	HIS	CA-CB-CG	10.15	123.95	113.80
1	A	355	GLN	CG-CD-NE2	10.15	131.62	116.40
1	A	164	ILE	CB-CA-C	10.13	125.27	111.19
1	B	43	ALA	CA-C-O	10.11	131.10	119.27
1	B	224	GLU	CB-CG-CD	10.08	129.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	MET	N-CA-C	-10.07	101.13	113.41
1	A	296	SER	N-CA-C	-10.04	92.89	108.55
1	A	48	GLU	CA-C-O	10.04	131.80	119.95
1	A	189	PHE	CA-C-N	-10.03	107.64	122.68
1	A	189	PHE	C-N-CA	-10.03	107.64	122.68
1	A	411	ARG	NE-CZ-NH2	-10.02	110.18	119.20
1	B	97	GLY	CA-C-O	10.02	130.58	119.06
1	A	385	ASN	OD1-CG-ND2	-10.01	112.59	122.60
1	A	313	ARG	NE-CZ-NH1	-10.01	111.49	121.50
1	A	343	LEU	CB-CA-C	9.97	125.18	109.03
1	B	69	ALA	CA-C-O	-9.96	108.93	120.49
1	B	243	ARG	N-CA-CB	9.96	124.46	109.91
1	A	75	ASP	N-CA-CB	9.92	126.83	111.06
1	A	176	PHE	CA-C-N	9.91	140.46	121.54
1	A	176	PHE	C-N-CA	9.91	140.46	121.54
1	B	185	LEU	CA-C-O	-9.88	110.52	120.70
1	B	446	GLN	CA-C-N	9.87	136.35	120.55
1	B	446	GLN	C-N-CA	9.87	136.35	120.55
1	A	298	GLN	O-C-N	9.87	135.06	122.23
1	B	346	ASP	CA-C-O	-9.86	110.28	120.54
1	A	119	GLU	CA-CB-CG	9.86	133.82	114.10
1	A	270	ALA	O-C-N	9.86	133.76	122.22
1	A	148	LYS	N-CA-CB	-9.86	93.83	110.49
1	A	178	GLU	O-C-N	9.86	133.44	122.11
1	A	283	PHE	N-CA-C	9.85	124.39	108.63
1	A	221	GLU	N-CA-CB	9.84	126.71	111.06
1	A	419	ASP	CA-CB-CG	9.82	122.42	112.60
1	A	382	ASN	CA-CB-CG	9.82	122.42	112.60
1	B	288	ARG	CA-C-O	-9.82	109.41	120.70
1	B	219	GLN	CA-C-N	9.81	141.37	122.53
1	B	219	GLN	C-N-CA	9.81	141.37	122.53
1	A	314	LEU	CA-CB-CG	9.79	150.57	116.30
1	B	216	ARG	NH1-CZ-NH2	-9.78	106.59	119.30
1	B	238	PHE	CA-CB-CG	-9.78	104.02	113.80
1	A	400	ILE	N-CA-C	9.78	119.72	110.53
1	B	290	GLY	CA-C-N	9.76	140.22	122.06
1	B	290	GLY	C-N-CA	9.76	140.22	122.06
1	A	143	ILE	CA-C-O	-9.74	107.14	119.70
1	B	193	ASN	OD1-CG-ND2	-9.73	112.87	122.60
1	A	251	PHE	CA-CB-CG	9.73	123.53	113.80
1	B	146	LEU	CB-CA-C	9.72	127.12	110.79
1	A	263	ASP	CA-CB-CG	9.70	122.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	PRO	N-CA-C	-9.69	99.31	113.75
1	A	429	GLU	CA-CB-CG	9.68	133.46	114.10
1	B	81	THR	N-CA-C	9.68	124.46	108.49
1	B	288	ARG	N-CA-C	-9.65	95.58	109.96
1	B	303	TYR	N-CA-C	-9.65	91.61	108.69
1	A	9	ASN	N-CA-CB	9.64	127.47	110.79
1	A	109	MET	N-CA-CB	9.63	130.12	111.53
1	A	103	SER	CA-C-N	9.63	139.94	121.54
1	A	103	SER	C-N-CA	9.63	139.94	121.54
1	A	419	ASP	CB-CA-C	9.63	129.82	110.17
1	B	10	LEU	CA-C-N	9.63	139.24	121.52
1	B	10	LEU	C-N-CA	9.63	139.24	121.52
1	B	18	ILE	N-CA-C	-9.62	101.49	110.53
1	A	93	ASN	CA-C-O	9.61	131.64	120.49
1	A	361	LYS	O-C-N	-9.61	111.05	122.87
1	B	133	ARG	CA-C-O	9.60	130.94	120.10
1	B	80	LEU	N-CA-C	9.59	125.48	109.76
1	A	117	ASP	O-C-N	9.57	135.32	122.59
1	B	348	ALA	CA-C-N	9.56	135.17	121.02
1	B	348	ALA	C-N-CA	9.56	135.17	121.02
1	B	199	GLN	N-CA-CB	9.56	124.06	110.11
1	B	7	TYR	N-CA-C	9.55	131.15	110.80
1	A	411	ARG	CD-NE-CZ	9.54	137.75	124.40
1	B	387	ASN	CA-CB-CG	9.50	122.10	112.60
1	A	294	VAL	CA-C-O	9.49	129.22	120.30
1	A	199	GLN	N-CA-CB	9.49	123.97	110.11
1	B	278	ARG	CA-CB-CG	9.48	133.06	114.10
1	A	17	LEU	CA-C-N	9.47	139.02	121.97
1	A	17	LEU	C-N-CA	9.47	139.02	121.97
1	A	263	ASP	O-C-N	-9.46	110.12	122.61
1	A	133	ARG	N-CA-CB	9.45	124.01	110.12
1	A	283	PHE	CA-CB-CG	9.44	123.24	113.80
1	A	427	ALA	CA-C-N	9.43	132.91	120.28
1	A	427	ALA	C-N-CA	9.43	132.91	120.28
1	B	235	ASP	CA-CB-CG	9.41	122.01	112.60
1	A	258	VAL	N-CA-CB	9.40	124.38	111.41
1	A	185	LEU	N-CA-C	-9.39	92.08	108.23
1	A	302	GLY	O-C-N	9.38	129.18	123.08
1	B	313	ARG	N-CA-C	-9.38	100.61	112.90
1	B	220	ASP	CA-CB-CG	9.37	121.97	112.60
1	B	67	VAL	N-CA-C	-9.37	104.25	112.12
1	B	199	GLN	N-CA-C	-9.35	97.18	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	ASP	CA-C-O	9.35	133.88	120.51
1	B	281	ASP	CA-CB-CG	9.33	121.93	112.60
1	B	203	PRO	CA-C-O	9.33	133.24	121.86
1	A	314	LEU	N-CA-C	-9.31	101.13	111.28
1	A	337	ARG	CD-NE-CZ	9.31	137.44	124.40
1	A	403	PRO	CA-C-O	9.30	137.53	120.60
1	B	447	ILE	N-CA-C	9.29	121.13	111.00
1	B	7	TYR	O-C-N	-9.29	110.24	122.59
1	B	293	ALA	CA-C-N	9.27	138.66	121.97
1	B	293	ALA	C-N-CA	9.27	138.66	121.97
1	B	241	ILE	CA-CB-CG2	9.27	126.26	110.50
1	A	115	MET	CA-C-O	9.24	133.73	120.51
1	A	354	ARG	O-C-N	9.24	134.17	123.27
1	B	159	LEU	N-CA-C	9.24	123.82	109.96
1	B	285	HIS	CA-CB-CG	-9.24	104.56	113.80
1	B	364	THR	N-CA-C	9.24	121.71	110.07
1	B	222	THR	N-CA-CB	9.23	124.60	110.39
1	B	172	ARG	CD-NE-CZ	9.20	137.28	124.40
1	B	285	HIS	CA-C-O	-9.19	109.68	120.62
1	A	28	TYR	CA-CB-CG	9.16	130.39	113.90
1	B	243	ARG	NH1-CZ-NH2	-9.16	107.39	119.30
1	A	344	THR	CA-C-N	9.15	139.01	121.54
1	A	344	THR	C-N-CA	9.15	139.01	121.54
1	A	420	GLY	CA-C-N	9.15	139.05	122.13
1	A	420	GLY	C-N-CA	9.15	139.05	122.13
1	B	47	ALA	N-CA-C	-9.15	100.70	112.23
1	B	206	ASP	O-C-N	9.14	135.55	122.20
1	B	190	ILE	CB-CG1-CD1	9.14	132.99	113.80
1	B	379	PHE	CA-C-O	9.14	130.24	120.55
1	A	94	ILE	CB-CA-C	9.12	123.65	111.97
1	A	298	GLN	CG-CD-NE2	-9.12	102.72	116.40
1	B	273	THR	CB-CA-C	9.12	127.23	109.72
1	B	92	ARG	NH1-CZ-NH2	-9.12	107.45	119.30
1	B	67	VAL	CA-C-N	9.11	135.74	121.26
1	B	67	VAL	C-N-CA	9.11	135.74	121.26
1	A	122	LYS	CA-C-O	-9.10	110.47	120.38
1	B	217	ARG	CD-NE-CZ	9.09	137.13	124.40
1	B	171	LEU	CA-C-O	-9.08	111.88	121.87
1	B	440	PHE	CA-C-N	9.07	131.18	119.84
1	B	440	PHE	C-N-CA	9.07	131.18	119.84
1	B	179	ALA	CA-C-N	9.06	135.86	120.72
1	B	179	ALA	C-N-CA	9.06	135.86	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	ARG	N-CA-CB	-9.06	96.23	110.46
1	A	232	ILE	N-CA-C	-9.04	103.87	111.91
1	B	316	GLY	CA-C-O	-9.04	111.70	119.56
1	A	270	ALA	CA-C-O	-9.03	109.89	120.10
1	B	111	ASN	N-CA-C	-9.01	101.46	111.28
1	A	22	GLU	CA-C-N	9.00	135.50	122.44
1	A	22	GLU	C-N-CA	9.00	135.50	122.44
1	A	85	TYR	CB-CA-C	-9.00	95.67	109.08
1	A	172	ARG	CD-NE-CZ	8.99	136.99	124.40
1	A	314	LEU	N-CA-CB	8.99	123.34	110.12
1	A	85	TYR	N-CA-C	8.98	120.94	109.72
1	B	249	GLU	CA-C-O	8.96	132.67	120.13
1	B	154	GLU	CA-C-N	8.95	138.07	121.97
1	B	154	GLU	C-N-CA	8.95	138.07	121.97
1	B	425	ASP	N-CA-CB	-8.94	97.58	110.81
1	A	427	ALA	N-CA-C	-8.93	101.52	111.07
1	A	225	ALA	CA-C-O	8.92	131.17	120.92
1	A	371	MET	CB-CA-C	8.91	124.89	109.65
1	B	135	LEU	N-CA-C	-8.91	101.94	113.17
1	B	421	VAL	CA-C-O	-8.90	113.99	119.51
1	A	387	ASN	N-CA-CB	-8.89	95.77	110.53
1	A	90	PHE	CA-CB-CG	8.84	122.64	113.80
1	A	310	LYS	N-CA-CB	8.82	125.39	110.49
1	A	414	TRP	CA-C-N	8.80	138.35	121.54
1	A	414	TRP	C-N-CA	8.80	138.35	121.54
1	B	184	TRP	CA-C-N	8.80	132.41	120.44
1	B	184	TRP	C-N-CA	8.80	132.41	120.44
1	A	364	THR	CA-C-O	8.78	129.73	120.25
1	B	254	ASN	N-CA-C	8.75	125.29	111.81
1	A	160	VAL	N-CA-C	-8.75	94.98	107.75
1	A	243	ARG	NH1-CZ-NH2	-8.74	107.94	119.30
1	A	239	GLU	CA-C-O	8.73	129.69	120.70
1	B	216	ARG	NE-CZ-NH2	8.73	127.05	119.20
1	A	223	GLY	CA-C-N	8.71	136.49	122.81
1	A	223	GLY	C-N-CA	8.71	136.49	122.81
1	A	205	ARG	CD-NE-CZ	8.71	136.60	124.40
1	B	217	ARG	CA-C-N	8.70	135.46	120.58
1	B	217	ARG	C-N-CA	8.70	135.46	120.58
1	B	86	PRO	O-C-N	-8.70	111.94	122.99
1	B	433	LEU	N-CA-C	8.70	122.99	112.38
1	A	32	PRO	N-CA-C	8.65	124.63	111.14
1	A	198	ASN	CA-CB-CG	-8.65	103.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	LEU	N-CA-C	-8.63	99.62	112.04
1	B	372	ASN	CA-CB-CG	8.62	121.22	112.60
1	A	239	GLU	CG-CD-OE1	-8.61	98.59	118.40
1	B	441	PRO	CA-N-CD	-8.61	99.94	112.00
1	A	403	PRO	O-C-N	-8.61	111.02	122.64
1	A	54	ASN	N-CA-CB	-8.60	95.95	110.49
1	B	178	GLU	N-CA-C	8.60	122.76	111.75
1	A	100	MET	CA-CB-CG	8.60	131.29	114.10
1	A	33	LYS	N-CA-C	-8.58	98.68	110.35
1	A	78	ARG	N-CA-CB	8.58	123.67	110.46
1	A	99	ALA	CA-C-O	-8.58	108.24	120.51
1	B	449	PRO	CA-C-O	-8.58	111.56	121.34
1	A	209	ALA	N-CA-C	-8.57	102.02	111.36
1	B	204	LEU	O-C-N	8.57	132.57	122.20
1	A	233	THR	N-CA-C	8.56	122.35	109.25
1	B	207	THR	CA-CB-OG1	-8.56	96.76	109.60
1	B	276	ARG	CD-NE-CZ	-8.55	112.42	124.40
1	A	308	HIS	CA-CB-CG	8.55	122.35	113.80
1	B	101	ILE	CA-C-N	8.55	132.86	120.38
1	B	101	ILE	C-N-CA	8.55	132.86	120.38
1	A	234	ALA	CA-C-N	-8.54	109.09	122.67
1	A	234	ALA	C-N-CA	-8.54	109.09	122.67
1	B	178	GLU	CA-C-O	8.54	129.76	120.20
1	B	346	ASP	N-CA-C	-8.52	93.63	108.20
1	B	192	ASN	CB-CA-C	8.51	123.92	109.53
1	B	216	ARG	CB-CA-C	8.51	124.07	110.96
1	A	404	VAL	O-C-N	8.51	133.21	122.57
1	B	397	PHE	N-CA-CB	8.50	123.46	110.28
1	B	389	ILE	O-C-N	8.50	132.10	123.18
1	B	438	GLU	CA-CB-CG	8.49	131.08	114.10
1	B	90	PHE	CA-CB-CG	8.48	122.28	113.80
1	B	236	ASP	N-CA-CB	-8.48	98.18	110.14
1	A	97	GLY	O-C-N	8.48	132.37	122.45
1	B	130	GLU	CA-C-O	8.47	132.96	120.42
1	B	243	ARG	CA-C-N	8.46	130.71	120.14
1	B	243	ARG	C-N-CA	8.46	130.71	120.14
1	B	11	ALA	CA-C-N	8.45	132.73	120.82
1	B	11	ALA	C-N-CA	8.45	132.73	120.82
1	A	164	ILE	O-C-N	-8.45	111.82	122.88
1	B	421	VAL	CB-CA-C	8.44	118.32	110.13
1	A	6	ARG	N-CA-CB	8.44	124.90	110.98
1	B	276	ARG	NE-CZ-NH2	8.43	126.79	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ASP	N-CA-C	8.43	128.75	110.80
1	A	133	ARG	NH1-CZ-NH2	8.42	130.25	119.30
1	A	51	THR	CA-CB-CG2	8.42	124.81	110.50
1	A	76	GLU	CA-C-N	8.41	131.88	120.44
1	A	76	GLU	C-N-CA	8.41	131.88	120.44
1	A	395	GLY	CA-C-O	8.40	135.19	120.57
1	B	95	THR	N-CA-C	-8.40	90.44	107.41
1	B	205	ARG	NE-CZ-NH2	-8.39	111.65	119.20
1	A	144	SER	CA-C-O	8.38	129.08	119.27
1	A	371	MET	N-CA-C	-8.38	97.88	110.28
1	B	106	THR	CA-C-N	8.38	134.91	120.58
1	B	106	THR	C-N-CA	8.38	134.91	120.58
1	B	119	GLU	CA-C-O	8.38	129.30	119.67
1	B	412	GLN	CA-CB-CG	8.37	130.84	114.10
1	A	432	GLU	N-CA-CB	-8.36	97.95	110.07
1	B	192	ASN	N-CA-CB	8.34	122.66	110.06
1	B	119	GLU	CA-CB-CG	8.34	130.78	114.10
1	B	447	ILE	CB-CA-C	-8.33	101.08	112.24
1	B	124	HIS	CA-C-O	-8.32	109.83	119.24
1	A	164	ILE	N-CA-CB	-8.32	101.18	111.67
1	B	92	ARG	NE-CZ-NH1	8.32	129.82	121.50
1	A	39	VAL	CA-C-O	-8.30	110.40	120.78
1	A	344	THR	CA-CB-OG1	-8.30	97.15	109.60
1	A	17	LEU	CA-C-O	8.29	129.44	120.24
1	A	401	ASP	CB-CG-OD1	8.29	137.47	118.40
1	B	202	ALA	N-CA-CB	-8.29	99.51	111.20
1	A	131	ALA	CA-C-N	8.29	137.37	121.54
1	A	131	ALA	C-N-CA	8.29	137.37	121.54
1	A	276	ARG	NE-CZ-NH1	8.25	129.75	121.50
1	B	198	ASN	N-CA-C	8.25	122.86	111.55
1	B	440	PHE	CB-CA-C	8.25	119.64	110.15
1	A	300	LYS	N-CA-C	-8.25	102.67	112.89
1	B	133	ARG	CA-C-N	8.24	136.74	122.56
1	B	133	ARG	C-N-CA	8.24	136.74	122.56
1	A	105	LEU	CA-C-O	-8.23	110.50	119.97
1	A	116	GLY	N-CA-C	-8.22	93.69	113.18
1	B	441	PRO	N-CA-CB	-8.22	94.62	103.25
1	A	254	ASN	CA-C-O	8.20	128.94	119.35
1	A	272	ILE	O-C-N	8.18	129.92	121.91
1	B	315	GLN	N-CA-C	8.18	122.83	113.02
1	A	335	SER	O-C-N	-8.17	109.93	123.00
1	B	68	ASP	CB-CA-C	-8.14	98.75	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	SER	N-CA-C	-8.13	101.09	111.02
1	B	442	GLY	CA-C-O	8.13	134.72	120.57
1	A	129	PRO	O-C-N	-8.13	113.34	123.10
1	B	181	HIS	CA-C-N	8.13	133.61	120.60
1	B	181	HIS	C-N-CA	8.13	133.61	120.60
1	A	221	GLU	CB-CA-C	-8.13	97.02	109.29
1	B	348	ALA	N-CA-C	8.12	120.73	108.46
1	B	180	CYS	CA-CB-SG	8.12	133.07	114.40
1	A	179	ALA	CA-C-O	-8.11	108.72	119.11
1	A	361	LYS	N-CA-CB	-8.11	97.58	109.83
1	A	157	GLY	N-CA-C	-8.10	93.98	113.18
1	B	226	LYS	CA-CB-CG	8.09	130.27	114.10
1	A	70	LEU	N-CA-C	8.08	123.01	109.76
1	B	205	ARG	NH1-CZ-NH2	8.08	129.80	119.30
1	A	88	ALA	N-CA-C	-8.06	100.49	110.65
1	B	133	ARG	N-CA-C	8.06	120.98	111.71
1	B	244	GLY	N-CA-C	8.03	123.76	113.24
1	B	40	ALA	CB-CA-C	8.02	123.47	110.88
1	B	415	GLN	CB-CG-CD	-8.02	98.97	112.60
1	B	254	ASN	OD1-CG-ND2	-8.01	114.59	122.60
1	B	446	GLN	CB-CG-CD	8.01	126.21	112.60
1	B	203	PRO	O-C-N	-8.01	113.04	123.13
1	B	36	TYR	CA-CB-CG	7.99	128.29	113.90
1	B	445	ASP	CA-CB-CG	7.99	120.59	112.60
1	A	181	HIS	O-C-N	7.99	133.40	122.46
1	B	342	MET	CB-CA-C	7.99	126.67	110.38
1	A	45	PHE	CB-CA-C	7.98	127.17	110.32
1	B	157	GLY	N-CA-C	-7.98	94.27	113.18
1	B	95	THR	N-CA-CB	7.97	125.38	110.56
1	B	231	ASN	CB-CG-ND2	-7.97	104.45	116.40
1	A	296	SER	CA-CB-OG	7.95	127.01	111.10
1	A	260	LEU	CA-C-O	-7.95	111.53	120.43
1	A	29	ILE	CA-C-N	7.94	136.14	122.64
1	A	29	ILE	C-N-CA	7.94	136.14	122.64
1	B	57	VAL	O-C-N	7.94	132.50	122.57
1	A	50	SER	N-CA-C	7.93	127.69	110.80
1	B	421	VAL	N-CA-CB	-7.92	103.98	112.37
1	A	14	GLU	N-CA-C	7.91	120.90	111.33
1	B	215	MET	CA-C-O	-7.91	110.47	119.41
1	B	354	ARG	N-CA-C	-7.91	99.35	110.50
1	A	410	LEU	CB-CA-C	7.89	125.00	110.56
1	B	357	TRP	CB-CA-C	7.88	122.62	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	MET	CA-CB-CG	-7.88	98.34	114.10
1	B	310	LYS	CA-CB-CG	7.87	129.83	114.10
1	B	284	LEU	O-C-N	-7.86	111.01	122.96
1	A	160	VAL	CB-CA-C	7.86	121.93	110.77
1	A	372	ASN	CA-CB-CG	7.86	120.46	112.60
1	B	430	HIS	CA-C-N	7.86	131.15	120.54
1	B	430	HIS	C-N-CA	7.86	131.15	120.54
1	A	183	PHE	N-CA-CB	7.86	121.59	110.67
1	B	273	THR	OG1-CB-CG2	-7.85	93.59	109.30
1	B	340	ALA	N-CA-CB	-7.85	97.23	110.49
1	A	231	ASN	CA-C-O	7.84	131.72	120.51
1	A	379	PHE	N-CA-C	-7.84	99.56	111.56
1	A	423	VAL	N-CA-CB	-7.84	98.30	111.23
1	A	101	ILE	CA-CB-CG2	7.83	123.81	110.50
1	A	291	HIS	CA-CB-CG	7.83	121.63	113.80
1	B	44	HIS	CA-CB-CG	-7.82	105.98	113.80
1	B	443	ASP	CA-CB-CG	7.81	120.41	112.60
1	A	272	ILE	N-CA-CB	7.79	119.67	110.55
1	B	194	GLU	CG-CD-OE2	7.78	136.29	118.40
1	B	292	GLY	N-CA-C	-7.78	94.74	113.18
1	A	208	ILE	CB-CG1-CD1	7.78	130.14	113.80
1	A	220	ASP	CA-CB-CG	7.78	120.38	112.60
1	B	341	TYR	CA-C-O	7.78	131.63	120.51
1	B	16	ASP	N-CA-C	-7.77	100.85	112.04
1	B	273	THR	CA-CB-CG2	7.77	123.71	110.50
1	B	62	ASP	O-C-N	7.77	132.79	123.24
1	B	66	GLY	CA-C-O	7.76	134.08	120.57
1	A	17	LEU	N-CA-C	-7.76	102.15	111.69
1	B	157	GLY	O-C-N	7.75	132.78	122.70
1	B	64	THR	N-CA-CB	7.75	121.87	110.25
1	A	161	VAL	CA-CB-CG1	-7.74	97.24	110.40
1	B	82	LYS	N-CA-C	7.74	120.96	109.59
1	B	426	TYR	N-CA-C	-7.72	102.81	111.07
1	A	419	ASP	N-CA-C	-7.72	103.75	113.01
1	B	120	TYR	CA-C-N	7.72	134.76	121.64
1	B	120	TYR	C-N-CA	7.72	134.76	121.64
1	A	48	GLU	CA-C-N	7.70	134.75	122.11
1	A	48	GLU	C-N-CA	7.70	134.75	122.11
1	A	387	ASN	OD1-CG-ND2	-7.70	114.90	122.60
1	A	172	ARG	NE-CZ-NH2	-7.69	112.28	119.20
1	B	362	ALA	CA-C-O	7.69	131.51	120.51
1	A	263	ASP	CA-C-O	7.67	132.72	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	GLY	CA-C-O	-7.67	113.89	120.64
1	A	426	TYR	N-CA-C	-7.67	103.51	113.17
1	A	93	ASN	CB-CA-C	7.66	122.85	110.29
1	A	135	LEU	CA-CB-CG	7.66	143.10	116.30
1	A	304	THR	N-CA-C	-7.65	98.90	110.14
1	A	217	ARG	NE-CZ-NH2	7.65	126.08	119.20
1	B	193	ASN	O-C-N	-7.65	114.32	122.96
1	A	176	PHE	CA-C-O	-7.64	109.58	120.51
1	A	264	GLY	N-CA-C	7.64	131.30	113.18
1	B	217	ARG	CB-CG-CD	7.64	128.88	111.30
1	A	251	PHE	O-C-N	-7.64	111.08	122.39
1	A	260	LEU	N-CA-CB	-7.64	97.33	110.17
1	B	50	SER	O-C-N	7.64	127.61	122.03
1	A	135	LEU	CB-CA-C	7.63	123.83	110.85
1	A	265	TYR	N-CA-C	-7.60	101.88	112.45
1	A	316	GLY	O-C-N	7.60	132.58	122.70
1	B	402	GLY	O-C-N	7.60	129.37	121.77
1	B	418	ARG	CD-NE-CZ	7.60	135.04	124.40
1	B	57	VAL	CA-CB-CG1	7.60	123.32	110.40
1	A	93	ASN	O-C-N	-7.60	113.67	123.02
1	B	384	GLY	N-CA-C	7.59	124.11	115.08
1	A	278	ARG	NE-CZ-NH2	7.59	126.03	119.20
1	B	379	PHE	CA-CB-CG	-7.58	106.22	113.80
1	B	188	ASP	CA-C-N	7.57	133.61	122.86
1	B	188	ASP	C-N-CA	7.57	133.61	122.86
1	B	434	ALA	CA-C-O	7.57	128.19	119.18
1	A	435	ARG	CA-C-O	-7.55	109.58	119.10
1	A	295	THR	CA-C-O	-7.55	111.13	122.38
1	B	264	GLY	CA-C-O	-7.55	107.23	119.31
1	A	222	THR	CB-CA-C	7.55	123.79	111.26
1	B	339	ILE	CA-C-O	7.54	130.21	120.78
1	B	221	GLU	CA-C-N	7.53	132.18	121.71
1	B	221	GLU	C-N-CA	7.53	132.18	121.71
1	A	262	VAL	N-CA-CB	7.53	121.39	111.90
1	A	54	ASN	O-C-N	7.52	132.59	122.59
1	A	422	PRO	O-C-N	7.52	132.79	122.64
1	A	229	SER	N-CA-CB	7.51	121.60	109.95
1	A	336	ASP	O-C-N	-7.51	111.97	122.26
1	A	428	ARG	N-CA-CB	-7.51	99.08	110.12
1	A	346	ASP	CA-C-N	7.51	134.80	123.24
1	A	346	ASP	C-N-CA	7.51	134.80	123.24
1	B	320	ILE	N-CA-CB	-7.50	98.85	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	ARG	CD-NE-CZ	7.49	134.89	124.40
1	B	43	ALA	N-CA-C	-7.49	103.94	113.23
1	B	204	LEU	CA-C-O	-7.47	112.28	121.02
1	A	96	ASP	CA-CB-CG	7.46	120.06	112.60
1	B	386	ALA	CA-C-N	7.46	135.04	122.65
1	B	386	ALA	C-N-CA	7.46	135.04	122.65
1	A	294	VAL	CA-CB-CG1	7.46	123.09	110.40
1	A	254	ASN	OD1-CG-ND2	-7.46	115.14	122.60
1	A	222	THR	O-C-N	-7.46	113.22	121.95
1	A	411	ARG	O-C-N	7.44	131.21	122.20
1	B	143	ILE	O-C-N	-7.44	111.63	121.82
1	A	109	MET	CA-CB-CG	7.44	128.97	114.10
1	A	391	THR	CA-C-O	7.43	131.14	120.51
1	A	145	ALA	CA-C-O	7.43	134.46	121.38
1	B	346	ASP	OD1-CG-OD2	7.43	140.73	122.90
1	A	75	ASP	CA-C-O	-7.42	109.15	118.43
1	A	145	ALA	CA-C-N	7.42	135.72	121.54
1	A	145	ALA	C-N-CA	7.42	135.72	121.54
1	A	357	TRP	CA-C-O	7.42	127.30	119.14
1	B	68	ASP	CA-CB-CG	7.40	120.00	112.60
1	A	399	HIS	CA-C-N	7.39	130.02	120.56
1	A	399	HIS	C-N-CA	7.39	130.02	120.56
1	B	43	ALA	CA-C-N	7.39	132.85	120.88
1	B	43	ALA	C-N-CA	7.39	132.85	120.88
1	A	161	VAL	CA-C-O	-7.39	112.02	121.40
1	B	61	ASP	O-C-N	7.38	131.01	122.67
1	B	142	ASN	CA-C-O	7.38	125.51	120.19
1	A	409	SER	N-CA-CB	-7.38	99.21	110.20
1	A	276	ARG	CG-CD-NE	7.37	128.22	112.00
1	B	185	LEU	CB-CA-C	7.37	122.55	110.90
1	A	132	TYR	CA-C-O	-7.36	109.98	120.51
1	A	245	GLU	CB-CG-CD	7.36	125.12	112.60
1	B	265	TYR	CA-C-N	7.36	132.98	121.35
1	B	265	TYR	C-N-CA	7.36	132.98	121.35
1	B	130	GLU	N-CA-C	-7.35	101.59	111.96
1	B	141	VAL	CA-C-N	7.35	132.79	120.81
1	B	141	VAL	C-N-CA	7.35	132.79	120.81
1	A	154	GLU	CB-CG-CD	7.33	125.07	112.60
1	B	427	ALA	CA-C-N	7.33	134.60	121.92
1	B	427	ALA	C-N-CA	7.33	134.60	121.92
1	B	397	PHE	N-CA-C	-7.33	103.32	111.82
1	B	202	ALA	CA-C-N	7.32	127.90	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ALA	C-N-CA	7.32	127.90	120.14
1	A	109	MET	N-CA-C	-7.32	99.60	110.06
1	B	243	ARG	N-CA-C	-7.32	102.99	110.97
1	B	28	TYR	N-CA-C	7.31	121.40	109.85
1	B	211	VAL	N-CA-CB	7.31	122.76	110.56
1	B	143	ILE	CA-C-N	7.29	130.93	120.79
1	B	143	ILE	C-N-CA	7.29	130.93	120.79
1	A	174	LYS	N-CA-C	-7.29	102.71	112.55
1	A	194	GLU	CA-C-N	7.29	128.95	119.84
1	A	194	GLU	C-N-CA	7.29	128.95	119.84
1	A	433	LEU	CA-C-O	-7.28	110.10	120.51
1	A	368	SER	N-CA-CB	-7.28	99.21	110.56
1	A	153	PRO	CB-CA-C	7.27	120.25	111.46
1	B	190	ILE	CA-C-N	-7.27	110.29	122.64
1	B	190	ILE	C-N-CA	-7.27	110.29	122.64
1	B	132	TYR	N-CA-C	7.26	122.55	112.45
1	B	389	ILE	N-CA-C	-7.25	98.02	108.17
1	B	149	VAL	CA-C-O	-7.25	112.74	120.64
1	A	131	ALA	CA-C-O	7.24	128.19	119.43
1	B	425	ASP	N-CA-C	-7.24	105.06	114.04
1	B	112	ASN	OD1-CG-ND2	7.24	129.84	122.60
1	B	16	ASP	CB-CG-OD1	7.23	135.03	118.40
1	B	363	CYS	N-CA-C	-7.23	96.55	108.76
1	B	86	PRO	CA-C-N	-7.22	109.00	120.55
1	B	86	PRO	C-N-CA	-7.22	109.00	120.55
1	B	29	ILE	N-CA-CB	7.21	120.76	111.67
1	A	401	ASP	OD1-CG-OD2	-7.21	105.60	122.90
1	A	355	GLN	OE1-CD-NE2	-7.19	115.41	122.60
1	B	31	LYS	CA-C-O	-7.19	112.65	119.55
1	B	53	THR	CA-C-N	7.18	135.26	121.54
1	B	53	THR	C-N-CA	7.18	135.26	121.54
1	B	17	LEU	CA-C-O	7.17	128.17	119.49
1	B	229	SER	CA-C-N	7.17	132.31	122.77
1	B	229	SER	C-N-CA	7.17	132.31	122.77
1	A	93	ASN	CB-CG-ND2	7.17	127.16	116.40
1	B	431	LYS	CB-CA-C	-7.17	99.34	110.81
1	B	39	VAL	CA-C-N	-7.17	111.12	120.44
1	B	39	VAL	C-N-CA	-7.17	111.12	120.44
1	A	229	SER	CB-CA-C	-7.17	98.16	109.84
1	B	102	ALA	O-C-N	7.16	130.37	122.20
1	A	297	PRO	CA-C-N	7.16	132.83	120.58
1	A	297	PRO	C-N-CA	7.16	132.83	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	ASN	N-CA-C	7.16	119.03	108.14
1	B	102	ALA	N-CA-CB	7.16	121.45	110.14
1	B	395	GLY	CA-C-N	7.16	135.21	121.54
1	B	395	GLY	C-N-CA	7.16	135.21	121.54
1	A	232	ILE	O-C-N	7.15	129.35	122.05
1	A	293	ALA	N-CA-CB	-7.15	99.29	110.30
1	B	310	LYS	N-CA-C	-7.15	102.90	111.69
1	B	354	ARG	O-C-N	7.15	131.29	122.86
1	B	90	PHE	CA-C-O	7.13	128.60	120.54
1	B	156	ASP	O-C-N	7.13	131.14	122.58
1	B	443	ASP	N-CA-C	-7.13	95.62	110.80
1	A	412	GLN	CB-CG-CD	-7.12	100.49	112.60
1	A	355	GLN	CA-C-N	7.12	133.03	122.99
1	A	355	GLN	C-N-CA	7.12	133.03	122.99
1	A	186	GLY	CA-C-O	-7.12	108.18	120.57
1	B	417	TRP	N-CA-C	7.12	119.65	111.11
1	B	154	GLU	CG-CD-OE2	7.11	134.76	118.40
1	A	309	CYS	CA-C-N	7.11	135.12	121.54
1	A	309	CYS	C-N-CA	7.11	135.12	121.54
1	B	373	ALA	CA-C-O	-7.11	111.80	119.97
1	A	408	ARG	NE-CZ-NH2	-7.10	112.81	119.20
1	B	94	ILE	N-CA-C	7.09	117.70	110.82
1	A	391	THR	N-CA-C	-7.09	95.70	110.80
1	A	428	ARG	NE-CZ-NH2	-7.09	112.82	119.20
1	B	439	SER	N-CA-C	-7.09	104.50	113.43
1	A	171	LEU	CB-CA-C	7.08	121.44	109.75
1	B	241	ILE	CA-C-O	7.08	128.29	120.71
1	A	315	GLN	O-C-N	-7.07	112.70	122.46
1	A	269	ALA	CA-C-N	7.07	130.46	120.28
1	A	269	ALA	C-N-CA	7.07	130.46	120.28
1	A	303	TYR	N-CA-C	-7.07	99.52	109.69
1	A	8	VAL	N-CA-CB	7.06	121.83	111.52
1	A	49	SER	O-C-N	7.06	131.02	122.48
1	A	156	ASP	CB-CA-C	-7.06	96.37	110.42
1	B	180	CYS	N-CA-CB	-7.06	98.68	110.39
1	B	371	MET	CA-C-N	-7.06	110.05	123.32
1	B	371	MET	C-N-CA	-7.06	110.05	123.32
1	B	303	TYR	CB-CG-CD1	7.05	131.38	120.80
1	B	251	PHE	CA-CB-CG	7.05	120.85	113.80
1	A	304	THR	CA-CB-CG2	7.05	122.48	110.50
1	B	418	ARG	CA-C-O	-7.05	113.04	120.58
1	B	313	ARG	NH1-CZ-NH2	-7.04	110.14	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	GLU	CA-C-N	7.04	130.66	120.38
1	A	14	GLU	C-N-CA	7.04	130.66	120.38
1	A	120	TYR	N-CA-CB	-7.04	100.86	111.56
1	B	301	ARG	CB-CG-CD	7.03	127.48	111.30
1	B	310	LYS	CB-CA-C	7.03	123.57	110.70
1	B	149	VAL	N-CA-C	7.03	120.87	111.17
1	B	349	GLN	CA-C-O	7.02	128.77	120.70
1	B	418	ARG	N-CA-C	-7.01	97.12	108.41
1	A	343	LEU	N-CA-C	-7.01	105.26	113.88
1	A	95	THR	CA-C-N	7.01	134.93	121.54
1	A	95	THR	C-N-CA	7.01	134.93	121.54
1	A	150	LEU	N-CA-C	-7.01	104.20	112.89
1	A	274	THR	CB-CA-C	6.99	121.94	110.90
1	B	140	SER	N-CA-CB	6.98	120.67	110.26
1	A	216	ARG	CA-C-O	-6.97	112.39	120.20
1	A	6	ARG	CA-CB-CG	6.97	128.04	114.10
1	A	412	GLN	CA-C-N	6.97	129.50	120.44
1	A	412	GLN	C-N-CA	6.97	129.50	120.44
1	B	23	HIS	N-CA-C	6.97	125.64	110.80
1	B	294	VAL	O-C-N	-6.96	113.88	122.57
1	B	206	ASP	CA-CB-CG	6.95	119.55	112.60
1	B	41	THR	N-CA-C	6.95	119.74	111.33
1	B	272	ILE	CA-CB-CG2	6.95	122.31	110.50
1	A	33	LYS	CA-C-N	6.94	131.66	121.31
1	A	33	LYS	C-N-CA	6.94	131.66	121.31
1	A	204	LEU	CA-C-O	-6.94	113.13	120.63
1	B	431	LYS	N-CA-C	6.94	119.44	111.11
1	A	277	ARG	CB-CA-C	6.94	122.58	110.64
1	A	54	ASN	CA-C-N	6.94	134.19	121.70
1	A	54	ASN	C-N-CA	6.94	134.19	121.70
1	B	189	PHE	CA-C-O	-6.94	112.84	120.33
1	B	262	VAL	N-CA-CB	6.94	122.83	111.45
1	A	207	THR	O-C-N	6.94	131.81	122.59
1	A	357	TRP	N-CA-C	-6.94	104.97	113.50
1	B	408	ARG	N-CA-C	-6.93	104.56	113.16
1	A	265	TYR	N-CA-CB	6.92	120.57	110.26
1	B	139	PRO	CA-C-O	-6.92	113.78	121.32
1	B	99	ALA	N-CA-C	-6.92	101.40	110.53
1	A	128	VAL	CB-CA-C	6.92	118.97	110.95
1	B	349	GLN	CB-CG-CD	6.91	124.35	112.60
1	B	47	ALA	N-CA-CB	6.91	120.94	110.30
1	A	142	ASN	CA-C-O	6.91	130.39	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	PRO	N-CD-CG	-6.91	95.51	103.80
1	A	254	ASN	O-C-N	-6.91	113.71	122.34
1	A	94	ILE	CA-CB-CG1	6.91	122.14	110.40
1	A	278	ARG	N-CA-C	-6.91	104.85	113.55
1	B	248	LEU	CA-CB-CG	6.90	140.47	116.30
1	A	51	THR	CA-CB-OG1	-6.90	99.25	109.60
1	B	127	TYR	CA-C-N	6.90	134.89	122.13
1	B	127	TYR	C-N-CA	6.90	134.89	122.13
1	B	393	GLY	N-CA-C	-6.90	96.82	113.18
1	B	256	SER	N-CA-C	-6.89	105.02	113.50
1	A	288	ARG	NE-CZ-NH2	6.89	125.40	119.20
1	A	251	PHE	CA-C-N	6.88	134.91	121.41
1	A	251	PHE	C-N-CA	6.88	134.91	121.41
1	B	299	SER	N-CA-C	-6.88	97.68	108.90
1	B	84	ALA	CA-C-N	6.88	130.82	121.74
1	B	84	ALA	C-N-CA	6.88	130.82	121.74
1	A	374	LEU	N-CA-C	6.87	121.71	113.12
1	B	40	ALA	CA-C-N	6.87	129.79	120.38
1	B	40	ALA	C-N-CA	6.87	129.79	120.38
1	A	312	ALA	N-CA-CB	-6.86	99.76	110.06
1	A	122	LYS	CB-CG-CD	6.86	127.08	111.30
1	B	353	TYR	N-CA-C	6.86	120.07	108.90
1	B	179	ALA	N-CA-C	-6.85	103.74	111.07
1	A	135	LEU	O-C-N	-6.84	114.35	122.15
1	A	86	PRO	CB-CA-C	6.84	119.95	111.12
1	A	163	THR	CA-C-N	6.84	132.41	123.11
1	A	163	THR	C-N-CA	6.84	132.41	123.11
1	A	5	SER	N-CA-CB	-6.84	98.88	110.50
1	A	116	GLY	O-C-N	6.84	131.59	122.70
1	A	253	GLU	CA-CB-CG	6.82	127.74	114.10
1	B	136	PHE	O-C-N	-6.82	114.57	123.16
1	B	29	ILE	CA-C-O	6.82	128.63	120.66
1	B	119	GLU	CB-CA-C	6.81	119.90	109.34
1	B	189	PHE	CA-C-N	-6.81	114.22	123.14
1	B	189	PHE	C-N-CA	-6.81	114.22	123.14
1	A	433	LEU	O-C-N	-6.81	113.53	122.59
1	B	240	ILE	CA-CB-CG2	6.81	122.07	110.50
1	B	152	ARG	CA-C-O	6.80	128.21	120.04
1	B	455	LEU	O-C-N	6.80	131.64	122.59
1	B	56	GLU	N-CA-C	-6.80	98.98	109.52
1	A	181	HIS	CA-C-O	-6.80	111.31	119.27
1	B	225	ALA	CA-C-N	6.78	132.13	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ALA	C-N-CA	6.78	132.13	121.56
1	A	430	HIS	N-CA-C	6.77	119.86	108.02
1	B	98	LYS	O-C-N	6.77	130.52	122.94
1	A	293	ALA	CA-C-N	6.76	129.22	122.66
1	A	293	ALA	C-N-CA	6.76	129.22	122.66
1	B	314	LEU	CA-C-N	6.76	134.19	122.56
1	B	314	LEU	C-N-CA	6.76	134.19	122.56
1	B	91	ASP	CB-CA-C	6.75	121.89	109.46
1	A	131	ALA	CB-CA-C	6.75	122.39	110.37
1	B	143	ILE	CA-C-O	6.75	127.54	120.25
1	B	54	ASN	CA-C-O	6.75	130.16	120.51
1	B	161	VAL	N-CA-CB	6.75	127.73	111.81
1	B	258	VAL	CB-CA-C	6.75	120.49	110.98
1	B	394	GLY	N-CA-C	6.74	129.16	113.18
1	A	295	THR	CB-CA-C	-6.74	102.38	111.88
1	B	142	ASN	CB-CA-C	-6.73	104.71	114.87
1	B	371	MET	N-CA-C	-6.73	99.93	109.96
1	A	185	LEU	CB-CA-C	6.72	122.41	111.05
1	A	231	ASN	CB-CG-OD1	-6.72	107.36	120.80
1	A	276	ARG	NE-CZ-NH2	-6.71	113.16	119.20
1	A	84	ALA	CA-C-N	6.70	144.04	121.27
1	A	84	ALA	C-N-CA	6.70	144.04	121.27
1	A	303	TYR	N-CA-CB	6.69	120.98	110.87
1	A	298	GLN	CA-CB-CG	6.69	127.48	114.10
1	B	416	ALA	CA-C-N	6.69	129.57	120.54
1	B	416	ALA	C-N-CA	6.69	129.57	120.54
1	B	208	ILE	N-CA-C	-6.69	103.71	111.00
1	B	251	PHE	N-CA-C	-6.68	104.14	112.90
1	A	314	LEU	CB-CA-C	6.68	121.88	110.79
1	A	183	PHE	CB-CA-C	6.68	120.29	109.07
1	A	270	ALA	N-CA-CB	6.67	120.49	110.22
1	A	411	ARG	CA-C-N	6.66	131.26	120.60
1	A	411	ARG	C-N-CA	6.66	131.26	120.60
1	A	374	LEU	N-CA-CB	-6.65	100.24	110.42
1	A	247	VAL	CA-C-O	-6.65	113.06	120.25
1	B	241	ILE	CA-C-N	6.65	129.49	120.44
1	B	241	ILE	C-N-CA	6.65	129.49	120.44
1	A	348	ALA	CA-C-N	6.65	134.24	121.54
1	A	348	ALA	C-N-CA	6.65	134.24	121.54
1	A	133	ARG	CA-C-O	-6.65	113.50	120.55
1	B	78	ARG	CA-C-N	6.65	131.85	122.08
1	B	78	ARG	C-N-CA	6.65	131.85	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	VAL	O-C-N	6.65	130.88	122.57
1	B	388	VAL	CA-C-O	-6.64	112.47	120.78
1	A	93	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	A	343	LEU	CA-CB-CG	6.64	139.54	116.30
1	A	342	MET	CB-CG-SD	-6.64	92.79	112.70
1	B	47	ALA	O-C-N	6.63	131.22	122.33
1	A	232	ILE	CA-C-N	6.63	131.34	121.72
1	A	232	ILE	C-N-CA	6.63	131.34	121.72
1	B	260	LEU	O-C-N	-6.63	112.33	122.93
1	B	309	CYS	N-CA-CB	-6.63	99.60	110.40
1	A	41	THR	CA-C-N	6.62	129.82	120.28
1	A	41	THR	C-N-CA	6.62	129.82	120.28
1	A	73	GLU	CB-CG-CD	-6.62	101.34	112.60
1	A	284	LEU	CA-C-O	-6.62	113.41	121.02
1	A	321	HIS	CA-C-O	6.61	127.65	120.58
1	A	298	GLN	N-CA-CB	6.61	120.05	110.20
1	A	245	GLU	CG-CD-OE1	6.60	133.59	118.40
1	A	405	ALA	CA-C-N	6.60	132.10	120.74
1	A	405	ALA	C-N-CA	6.60	132.10	120.74
1	A	396	ALA	N-CA-CB	-6.60	98.86	110.34
1	A	211	VAL	N-CA-C	-6.58	103.82	111.00
1	B	155	VAL	N-CA-CB	6.58	122.09	111.23
1	B	223	GLY	N-CA-C	-6.58	97.58	113.18
1	A	174	LYS	CA-C-N	6.58	128.06	119.84
1	A	174	LYS	C-N-CA	6.58	128.06	119.84
1	B	309	CYS	CA-C-N	6.58	131.82	120.58
1	B	309	CYS	C-N-CA	6.58	131.82	120.58
1	A	400	ILE	O-C-N	6.57	128.73	121.90
1	B	87	VAL	CA-CB-CG2	6.57	121.57	110.40
1	B	255	ALA	N-CA-C	6.56	119.92	112.97
1	B	94	ILE	CB-CA-C	-6.55	103.45	112.04
1	A	389	ILE	O-C-N	-6.55	116.15	123.03
1	B	126	PHE	CA-C-O	6.55	128.41	121.33
1	B	287	HIS	CB-CA-C	6.55	122.23	111.23
1	B	34	ALA	N-CA-CB	6.54	121.55	110.49
1	A	155	VAL	CA-C-N	6.53	134.01	121.54
1	A	155	VAL	C-N-CA	6.53	134.01	121.54
1	B	204	LEU	N-CA-CB	6.53	120.82	109.72
1	A	79	GLU	CA-C-O	-6.53	114.39	122.03
1	B	23	HIS	N-CA-CB	-6.53	99.46	110.49
1	A	6	ARG	NE-CZ-NH2	6.52	125.07	119.20
1	B	438	GLU	CG-CD-OE1	-6.52	103.40	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	GLU	O-C-N	-6.52	113.65	122.19
1	B	275	ALA	N-CA-C	-6.51	104.11	111.14
1	A	175	PRO	CB-CA-C	-6.51	100.81	111.56
1	A	227	LEU	CA-C-O	-6.51	113.34	120.24
1	A	45	PHE	N-CA-CB	-6.51	99.25	110.32
1	B	414	TRP	CA-C-N	6.51	128.90	120.44
1	B	414	TRP	C-N-CA	6.51	128.90	120.44
1	A	412	GLN	CA-C-O	-6.50	111.62	119.49
1	A	90	PHE	N-CA-C	6.50	119.30	108.96
1	A	128	VAL	CA-C-O	6.50	122.76	119.12
1	B	221	GLU	O-C-N	6.50	129.05	122.03
1	A	208	ILE	CA-C-O	6.49	125.43	119.20
1	A	430	HIS	CA-CB-CG	-6.48	107.32	113.80
1	A	208	ILE	N-CA-C	-6.48	103.86	113.39
1	B	313	ARG	N-CA-CB	6.48	120.05	110.33
1	A	117	ASP	CB-CA-C	-6.48	97.53	110.42
1	A	353	TYR	O-C-N	6.47	131.57	123.15
1	A	74	VAL	CA-C-O	6.47	127.86	121.19
1	A	145	ALA	O-C-N	-6.47	111.86	121.89
1	B	91	ASP	N-CA-CB	-6.47	100.45	110.29
1	B	203	PRO	N-CA-C	6.47	122.48	111.68
1	B	301	ARG	CD-NE-CZ	-6.47	115.34	124.40
1	A	429	GLU	CG-CD-OE1	6.47	133.28	118.40
1	A	95	THR	CA-CB-OG1	6.46	119.29	109.60
1	A	296	SER	CA-C-O	-6.46	114.56	120.50
1	A	343	LEU	N-CA-CB	-6.46	102.00	110.59
1	B	111	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	269	ALA	CA-C-O	6.45	127.59	119.78
1	A	175	PRO	N-CA-C	6.45	125.75	112.47
1	B	236	ASP	CB-CA-C	6.45	118.74	109.26
1	B	246	TYR	N-CA-C	-6.45	104.17	111.07
1	B	274	THR	CA-C-N	6.45	129.21	120.44
1	B	274	THR	C-N-CA	6.45	129.21	120.44
1	B	83	ILE	CA-C-N	6.45	130.99	122.42
1	B	83	ILE	C-N-CA	6.45	130.99	122.42
1	B	310	LYS	CA-C-O	6.44	127.39	120.24
1	B	194	GLU	CB-CG-CD	6.44	123.55	112.60
1	B	448	TYR	CA-C-O	6.44	125.51	119.59
1	A	357	TRP	CB-CA-C	6.43	121.00	109.29
1	B	298	GLN	O-C-N	6.43	130.38	121.83
1	A	337	ARG	O-C-N	-6.43	114.04	122.59
1	B	288	ARG	N-CA-CB	6.43	119.66	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	GLU	N-CA-C	-6.42	104.20	111.14
1	A	313	ARG	N-CA-C	-6.42	105.60	113.50
1	B	20	GLY	CA-C-N	6.42	133.99	121.41
1	B	20	GLY	C-N-CA	6.42	133.99	121.41
1	B	310	LYS	CB-CG-CD	6.42	126.05	111.30
1	A	16	ASP	CA-CB-CG	-6.41	106.19	112.60
1	B	95	THR	CA-C-O	-6.41	113.23	121.11
1	B	366	ILE	CB-CA-C	6.41	121.79	111.29
1	A	125	ASP	CA-C-N	6.40	133.21	121.94
1	A	125	ASP	C-N-CA	6.40	133.21	121.94
1	B	14	GLU	CA-CB-CG	6.40	126.90	114.10
1	B	435	ARG	CA-CB-CG	-6.40	101.30	114.10
1	A	212	ALA	CA-C-N	6.39	129.17	120.54
1	A	212	ALA	C-N-CA	6.39	129.17	120.54
1	B	395	GLY	N-CA-C	-6.39	107.64	114.67
1	A	413	ALA	CA-C-O	6.39	127.53	120.82
1	A	266	VAL	CA-C-N	6.39	132.25	122.23
1	A	266	VAL	C-N-CA	6.39	132.25	122.23
1	B	85	TYR	CB-CA-C	-6.39	102.73	110.08
1	A	255	ALA	N-CA-CB	-6.38	97.41	110.67
1	A	315	GLN	N-CA-CB	-6.37	99.24	110.39
1	B	408	ARG	NE-CZ-NH2	-6.37	113.47	119.20
1	A	236	ASP	N-CA-C	-6.37	95.73	109.81
1	A	205	ARG	NE-CZ-NH1	-6.37	115.13	121.50
1	A	23	HIS	CA-C-N	6.36	131.27	122.93
1	A	23	HIS	C-N-CA	6.36	131.27	122.93
1	A	254	ASN	CA-C-N	6.36	143.97	122.20
1	A	254	ASN	C-N-CA	6.36	143.97	122.20
1	A	303	TYR	CA-C-O	-6.36	113.90	121.60
1	B	411	ARG	CB-CA-C	-6.36	100.80	110.92
1	B	224	GLU	CA-C-O	-6.36	114.43	121.23
1	B	259	ALA	CB-CA-C	6.35	121.98	109.66
1	A	418	ARG	CD-NE-CZ	-6.34	115.52	124.40
1	A	312	ALA	N-CA-C	6.34	119.00	111.33
1	B	409	SER	CA-C-N	6.34	131.15	120.88
1	B	409	SER	C-N-CA	6.34	131.15	120.88
1	A	360	MET	O-C-N	6.33	130.43	123.27
1	A	15	GLU	O-C-N	6.33	129.42	122.20
1	A	65	ARG	CD-NE-CZ	6.33	133.26	124.40
1	B	76	GLU	O-C-N	6.33	131.01	122.59
1	A	10	LEU	CB-CA-C	6.33	121.18	109.54
1	B	321	HIS	CB-CG-ND1	6.33	132.19	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ALA	CA-C-N	6.32	129.27	120.29
1	A	134	ALA	C-N-CA	6.32	129.27	120.29
1	B	371	MET	CA-C-O	-6.32	113.43	120.70
1	B	294	VAL	CA-C-N	6.32	129.38	120.28
1	B	294	VAL	C-N-CA	6.32	129.38	120.28
1	A	202	ALA	CA-C-O	6.31	127.63	121.32
1	B	184	TRP	N-CA-CB	6.30	120.86	110.39
1	B	309	CYS	CA-C-O	6.30	127.12	119.31
1	B	408	ARG	CA-C-N	6.30	132.44	122.11
1	B	408	ARG	C-N-CA	6.30	132.44	122.11
1	B	275	ALA	CA-C-O	-6.30	114.22	120.70
1	B	176	PHE	N-CA-CB	6.29	121.12	110.49
1	A	336	ASP	N-CA-CB	-6.29	101.05	111.49
1	A	98	LYS	CA-C-N	6.29	133.55	121.54
1	A	98	LYS	C-N-CA	6.29	133.55	121.54
1	B	38	TYR	CA-CB-CG	-6.28	102.59	113.90
1	B	347	GLU	N-CA-CB	6.28	121.10	110.49
1	A	429	GLU	N-CA-C	-6.27	104.52	111.36
1	A	413	ALA	CA-C-N	6.27	129.50	120.79
1	A	413	ALA	C-N-CA	6.27	129.50	120.79
1	B	17	LEU	N-CA-C	6.26	120.02	112.38
1	A	14	GLU	O-C-N	-6.26	115.49	122.12
1	B	121	ALA	N-CA-C	-6.25	98.06	108.32
1	B	243	ARG	NE-CZ-NH2	6.25	124.82	119.20
1	A	365	PRO	CB-CA-C	6.24	119.02	111.46
1	A	300	LYS	CB-CG-CD	6.24	125.65	111.30
1	A	428	ARG	O-C-N	-6.24	115.51	122.12
1	B	20	GLY	N-CA-C	-6.24	98.39	113.18
1	B	105	LEU	O-C-N	6.24	131.22	122.36
1	A	396	ALA	N-CA-C	6.24	121.23	112.93
1	B	411	ARG	NE-CZ-NH2	-6.24	113.58	119.20
1	B	195	PRO	CA-C-O	6.24	128.51	119.34
1	B	243	ARG	NE-CZ-NH1	6.23	127.73	121.50
1	A	278	ARG	N-CA-CB	6.23	119.43	110.40
1	A	387	ASN	CA-CB-CG	6.23	118.83	112.60
1	B	195	PRO	O-C-N	-6.23	113.86	122.27
1	B	263	ASP	N-CA-C	-6.23	100.28	109.62
1	B	350	GLY	N-CA-C	-6.22	99.65	112.34
1	A	125	ASP	CA-CB-CG	-6.22	106.38	112.60
1	B	111	ASN	CB-CG-ND2	6.22	125.73	116.40
1	B	291	HIS	CA-CB-CG	-6.22	107.58	113.80
1	B	420	GLY	O-C-N	-6.22	114.61	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	VAL	CA-CB-CG2	6.22	120.97	110.40
1	A	256	SER	N-CA-C	-6.22	106.29	114.31
1	B	418	ARG	CA-CB-CG	6.22	126.53	114.10
1	B	439	SER	CA-CB-OG	6.22	123.53	111.10
1	A	38	TYR	N-CA-CB	6.21	120.99	110.49
1	A	98	LYS	CA-CB-CG	6.21	126.52	114.10
1	A	176	PHE	CB-CA-C	6.21	122.78	110.42
1	A	245	GLU	N-CA-C	-6.21	103.44	111.02
1	B	224	GLU	N-CA-C	-6.21	99.29	108.79
1	B	260	LEU	CA-CB-CG	6.21	138.02	116.30
1	B	445	ASP	CB-CA-C	6.20	122.76	110.42
1	B	269	ALA	N-CA-C	6.20	118.04	111.28
1	A	161	VAL	CA-C-N	-6.19	111.71	121.37
1	A	161	VAL	C-N-CA	-6.19	111.71	121.37
1	A	183	PHE	O-C-N	-6.19	114.99	122.48
1	B	350	GLY	CA-C-O	-6.19	112.67	121.52
1	A	390	LEU	N-CA-C	-6.18	99.74	109.50
1	B	64	THR	O-C-N	6.18	131.10	122.08
1	B	13	LYS	O-C-N	6.18	130.32	123.16
1	A	337	ARG	CB-CG-CD	6.17	125.50	111.30
1	B	192	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	A	198	ASN	CA-C-N	6.17	130.06	120.68
1	A	198	ASN	C-N-CA	6.17	130.06	120.68
1	A	231	ASN	OD1-CG-ND2	6.17	128.76	122.60
1	B	120	TYR	CB-CG-CD1	6.16	130.04	120.80
1	A	343	LEU	CA-C-O	-6.16	112.28	119.24
1	A	115	MET	CA-C-N	6.16	133.48	121.41
1	A	115	MET	C-N-CA	6.16	133.48	121.41
1	B	226	LYS	CA-C-N	6.16	131.82	122.65
1	B	226	LYS	C-N-CA	6.16	131.82	122.65
1	A	83	ILE	CA-C-N	6.15	131.70	122.47
1	A	83	ILE	C-N-CA	6.15	131.70	122.47
1	A	253	GLU	CA-C-N	6.15	132.69	122.54
1	A	253	GLU	C-N-CA	6.15	132.69	122.54
1	A	365	PRO	N-CA-CB	6.15	108.77	103.36
1	B	109	MET	CG-SD-CE	6.15	114.42	100.90
1	B	133	ARG	NE-CZ-NH1	6.15	127.65	121.50
1	A	437	PHE	CA-CB-CG	6.15	119.95	113.80
1	B	33	LYS	N-CA-CB	6.14	119.80	109.78
1	B	112	ASN	CB-CG-ND2	-6.14	107.18	116.40
1	B	175	PRO	CB-CA-C	6.14	123.33	112.64
1	A	207	THR	CA-CB-OG1	6.14	118.81	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	320	ILE	CA-CB-CG1	6.14	120.84	110.40
1	B	265	TYR	N-CA-C	-6.14	103.92	112.45
1	A	373	ALA	N-CA-C	6.13	123.87	110.80
1	B	79	GLU	CA-CB-CG	6.13	126.37	114.10
1	B	339	ILE	O-C-N	-6.13	114.90	122.57
1	B	15	GLU	CG-CD-OE2	-6.13	104.30	118.40
1	B	189	PHE	CB-CA-C	-6.13	101.36	110.62
1	A	221	GLU	N-CA-C	-6.13	105.33	114.64
1	B	24	VAL	N-CA-CB	6.13	117.21	110.53
1	B	215	MET	O-C-N	6.12	131.05	122.36
1	B	382	ASN	O-C-N	-6.11	114.24	122.43
1	B	238	PHE	O-C-N	6.11	129.37	122.22
1	A	408	ARG	O-C-N	-6.11	115.09	122.48
1	B	226	LYS	N-CA-C	6.10	119.33	110.42
1	A	221	GLU	CA-C-O	6.09	126.04	118.43
1	A	248	LEU	N-CA-C	-6.09	104.56	112.23
1	B	150	LEU	CA-C-N	6.09	133.34	121.41
1	B	150	LEU	C-N-CA	6.09	133.34	121.41
1	A	134	ALA	CB-CA-C	-6.08	98.67	110.46
1	B	261	LEU	N-CA-CB	6.08	119.07	109.71
1	A	117	ASP	CA-C-O	-6.08	111.82	120.51
1	B	439	SER	O-C-N	6.08	130.24	122.10
1	B	28	TYR	CB-CA-C	-6.07	97.88	109.66
1	B	404	VAL	CA-C-N	6.07	133.35	122.06
1	B	404	VAL	C-N-CA	6.07	133.35	122.06
1	B	157	GLY	CA-C-O	-6.07	110.01	120.57
1	A	202	ALA	CA-C-N	6.07	126.98	120.13
1	A	202	ALA	C-N-CA	6.07	126.98	120.13
1	A	338	ALA	N-CA-C	-6.06	97.89	110.80
1	B	366	ILE	CA-CB-CG1	6.06	120.70	110.40
1	B	261	LEU	CB-CA-C	-6.05	101.18	110.26
1	A	17	LEU	CB-CA-C	6.05	121.77	110.70
1	A	355	GLN	O-C-N	-6.04	116.15	123.10
1	A	90	PHE	CB-CA-C	6.04	120.31	110.22
1	B	235	ASP	N-CA-C	-6.04	103.45	111.24
1	A	87	VAL	CA-CB-CG1	6.03	120.66	110.40
1	A	429	GLU	O-C-N	6.03	129.03	122.15
1	B	9	ASN	N-CA-C	6.03	122.70	112.99
1	B	168	LYS	CA-CB-CG	6.03	126.16	114.10
1	A	261	LEU	CA-CB-CG	6.03	137.40	116.30
1	B	31	LYS	O-C-N	6.03	128.52	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	ARG	NE-CZ-NH1	6.03	127.53	121.50
1	B	261	LEU	CA-C-O	-6.03	113.59	120.58
1	B	33	LYS	CA-C-O	-6.00	114.20	120.92
1	A	12	LEU	CB-CA-C	6.00	121.03	111.73
1	B	279	PHE	O-C-N	6.00	128.22	121.32
1	A	206	ASP	CA-C-O	-6.00	111.94	120.51
1	B	435	ARG	CD-NE-CZ	6.00	132.79	124.40
1	A	76	GLU	N-CA-C	5.99	123.56	110.80
1	A	221	GLU	CA-CB-CG	5.99	126.08	114.10
1	B	353	TYR	N-CA-CB	-5.99	100.62	110.68
1	B	388	VAL	CA-CB-CG2	5.99	120.58	110.40
1	B	277	ARG	NH1-CZ-NH2	-5.98	111.52	119.30
1	A	78	ARG	CA-C-O	5.98	128.44	119.23
1	A	31	LYS	O-C-N	5.98	128.19	121.32
1	A	78	ARG	CA-CB-CG	5.98	126.06	114.10
1	B	139	PRO	N-CA-C	-5.98	101.52	111.26
1	A	432	GLU	CB-CA-C	5.97	120.34	110.90
1	B	130	GLU	CA-C-N	5.97	132.95	121.54
1	B	130	GLU	C-N-CA	5.97	132.95	121.54
1	B	115	MET	CB-CG-SD	-5.97	94.78	112.70
1	B	171	LEU	N-CA-CB	5.97	118.80	110.26
1	B	213	ASP	CB-CA-C	5.97	123.29	110.21
1	A	18	ILE	CA-CB-CG2	5.96	120.64	110.50
1	A	304	THR	CA-CB-OG1	-5.96	100.66	109.60
1	B	199	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	A	249	GLU	CA-C-N	5.96	128.86	120.28
1	A	249	GLU	C-N-CA	5.96	128.86	120.28
1	B	365	PRO	O-C-N	-5.96	116.71	123.03
1	B	401	ASP	CA-C-N	5.95	131.22	121.87
1	B	401	ASP	C-N-CA	5.95	131.22	121.87
1	B	366	ILE	CA-C-O	5.95	128.22	120.78
1	B	288	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	A	92	ARG	N-CA-C	5.94	116.94	108.74
1	B	430	HIS	N-CA-C	5.94	118.91	108.75
1	A	318	SER	O-C-N	5.94	129.95	122.23
1	A	438	GLU	CB-CG-CD	5.94	122.70	112.60
1	B	193	ASN	CB-CA-C	5.94	120.39	109.46
1	B	372	ASN	CB-CA-C	5.94	123.22	111.22
1	A	133	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	B	413	ALA	O-C-N	5.94	128.26	122.09
1	B	251	PHE	CB-CA-C	5.93	121.59	109.67
1	B	26	CYS	CA-C-O	-5.93	114.46	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	VAL	CA-C-O	5.93	128.93	121.40
1	A	11	ALA	O-C-N	5.93	128.22	121.88
1	A	274	THR	CA-CB-OG1	5.93	118.49	109.60
1	B	164	ILE	CB-CA-C	-5.93	101.37	110.50
1	B	224	GLU	CG-CD-OE1	5.92	132.03	118.40
1	A	369	GLY	N-CA-C	5.92	122.57	111.80
1	B	123	MET	CA-C-O	-5.91	113.96	120.69
1	B	355	GLN	CA-C-N	5.91	131.49	122.93
1	B	355	GLN	C-N-CA	5.91	131.49	122.93
1	A	404	VAL	CA-C-O	-5.90	113.40	120.78
1	A	220	ASP	CB-CA-C	-5.90	101.92	111.06
1	A	50	SER	N-CA-CB	-5.90	100.52	110.49
1	A	231	ASN	CA-CB-CG	-5.89	106.71	112.60
1	B	350	GLY	O-C-N	5.89	127.67	121.77
1	B	11	ALA	N-CA-C	-5.89	105.18	112.90
1	A	229	SER	CA-CB-OG	5.89	122.88	111.10
1	A	238	PHE	O-C-N	5.89	130.25	122.36
1	A	64	THR	CA-C-N	5.88	131.48	122.24
1	A	64	THR	C-N-CA	5.88	131.48	122.24
1	B	385	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	374	LEU	CA-C-N	-5.88	113.43	122.60
1	A	374	LEU	C-N-CA	-5.88	113.43	122.60
1	A	104	PHE	CA-C-O	5.88	128.92	120.51
1	A	158	GLY	N-CA-C	5.88	127.11	113.18
1	B	222	THR	N-CA-C	-5.88	99.16	110.56
1	A	245	GLU	O-C-N	-5.87	115.80	122.08
1	A	36	TYR	N-CA-C	5.87	118.51	110.24
1	B	399	HIS	CB-CA-C	-5.87	100.25	109.70
1	B	401	ASP	CA-C-O	5.87	127.46	120.53
1	B	308	HIS	N-CA-C	5.85	117.46	111.14
1	B	13	LYS	CA-C-O	-5.84	114.20	120.92
1	B	112	ASN	CA-C-O	5.83	128.85	120.51
1	A	258	VAL	CA-C-O	5.83	126.51	120.39
1	A	16	ASP	CB-CA-C	5.83	121.38	109.55
1	A	362	ALA	CA-C-O	5.83	127.34	120.58
1	A	152	ARG	N-CA-C	-5.83	101.44	108.14
1	B	342	MET	N-CA-C	-5.83	104.89	112.23
1	B	387	ASN	N-CA-CB	-5.82	102.52	110.56
1	A	281	ASP	CA-C-N	5.82	131.95	122.81
1	A	281	ASP	C-N-CA	5.82	131.95	122.81
1	B	258	VAL	CA-CB-CG2	5.82	120.29	110.40
1	B	275	ALA	O-C-N	5.82	128.37	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	THR	CB-CA-C	5.82	122.00	110.42
1	B	124	HIS	CA-CB-CG	-5.82	107.98	113.80
1	A	220	ASP	N-CA-C	-5.81	106.00	112.57
1	B	294	VAL	N-CA-CB	-5.81	101.65	111.23
1	B	232	ILE	CA-C-N	5.80	130.13	122.30
1	B	232	ILE	C-N-CA	5.80	130.13	122.30
1	B	324	THR	CA-CB-CG2	5.79	120.35	110.50
1	A	77	ALA	N-CA-C	-5.79	104.88	111.14
1	A	135	LEU	N-CA-C	-5.79	105.05	111.36
1	A	361	LYS	CG-CD-CE	-5.79	97.98	111.30
1	B	205	ARG	CB-CA-C	-5.79	99.64	110.36
1	A	68	ASP	CB-CG-OD1	5.79	131.72	118.40
1	B	100	MET	CA-C-N	5.79	128.40	120.46
1	B	100	MET	C-N-CA	5.79	128.40	120.46
1	B	17	LEU	N-CA-CB	-5.79	100.48	110.32
1	B	278	ARG	CB-CG-CD	5.79	124.61	111.30
1	B	400	ILE	CA-C-N	5.79	133.03	122.50
1	B	400	ILE	C-N-CA	5.79	133.03	122.50
1	A	29	ILE	N-CA-CB	-5.78	101.69	111.23
1	A	149	VAL	O-C-N	5.78	128.23	122.04
1	B	408	ARG	CB-CA-C	5.78	120.42	110.01
1	B	57	VAL	N-CA-CB	-5.78	101.69	111.23
1	A	144	SER	N-CA-CB	5.78	119.45	110.44
1	A	266	VAL	N-CA-C	5.77	119.44	112.80
1	A	296	SER	N-CA-CB	5.77	121.57	111.18
1	A	421	VAL	N-CA-CB	5.77	119.29	111.21
1	B	124	HIS	O-C-N	5.77	130.10	122.36
1	B	107	LEU	O-C-N	5.76	129.72	122.23
1	B	144	SER	CA-C-O	-5.75	114.75	121.07
1	A	100	MET	CA-C-O	-5.75	114.39	121.06
1	B	237	PRO	CA-C-N	5.75	128.56	120.28
1	B	237	PRO	C-N-CA	5.75	128.56	120.28
1	A	253	GLU	CB-CG-CD	5.74	122.36	112.60
1	B	62	ASP	N-CA-C	-5.74	100.44	109.50
1	B	368	SER	CA-CB-OG	5.73	122.56	111.10
1	B	428	ARG	N-CA-CB	5.72	118.95	110.53
1	B	100	MET	CA-C-O	-5.72	112.49	120.21
1	B	218	ALA	CA-C-O	5.72	126.59	120.24
1	B	362	ALA	CA-C-N	5.72	131.55	122.74
1	B	362	ALA	C-N-CA	5.72	131.55	122.74
1	A	260	LEU	CA-CB-CG	5.71	136.29	116.30
1	B	273	THR	CA-CB-OG1	-5.70	101.05	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ARG	CA-C-N	5.70	124.90	118.97
1	A	172	ARG	C-N-CA	5.70	124.90	118.97
1	B	168	LYS	N-CA-CB	5.70	118.23	109.91
1	B	93	ASN	CA-C-N	5.69	128.88	120.74
1	B	93	ASN	C-N-CA	5.69	128.88	120.74
1	B	304	THR	CA-CB-OG1	-5.69	101.06	109.60
1	A	120	TYR	CA-CB-CG	5.69	124.14	113.90
1	B	124	HIS	N-CA-CB	5.69	118.15	110.59
1	A	129	PRO	CB-CA-C	5.68	118.77	111.21
1	B	364	THR	CA-C-O	5.68	124.97	120.19
1	B	423	VAL	N-CA-C	5.68	121.16	109.34
1	A	121	ALA	CA-C-O	-5.67	113.34	119.98
1	A	199	GLN	OE1-CD-NE2	5.67	128.27	122.60
1	A	117	ASP	CB-CG-OD1	-5.67	105.35	118.40
1	B	119	GLU	N-CA-CB	-5.67	102.17	110.40
1	B	142	ASN	N-CA-C	-5.67	101.97	108.49
1	A	400	ILE	CB-CA-C	-5.67	104.60	112.02
1	B	263	ASP	CB-CA-C	5.67	120.62	112.12
1	A	197	GLY	CA-C-O	5.66	130.43	120.57
1	A	379	PHE	O-C-N	5.66	128.83	122.32
1	B	206	ASP	CB-CA-C	5.66	118.89	109.56
1	A	75	ASP	N-CA-C	-5.66	106.04	114.64
1	A	15	GLU	CB-CA-C	-5.65	99.49	110.46
1	B	23	HIS	CA-C-N	5.65	129.46	121.66
1	B	23	HIS	C-N-CA	5.65	129.46	121.66
1	B	143	ILE	CA-CB-CG2	5.65	120.10	110.50
1	B	152	ARG	CB-CA-C	5.65	117.35	108.88
1	B	286	TYR	N-CA-CB	-5.65	101.60	110.69
1	A	133	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	B	24	VAL	O-C-N	-5.64	116.55	122.81
1	B	194	GLU	CA-CB-CG	5.64	125.39	114.10
1	B	432	GLU	CB-CG-CD	5.64	122.19	112.60
1	B	132	TYR	N-CA-CB	-5.64	101.86	110.26
1	A	257	HIS	CA-CB-CG	5.63	119.44	113.80
1	B	340	ALA	CA-C-N	5.63	132.30	121.54
1	B	340	ALA	C-N-CA	5.63	132.30	121.54
1	A	376	MET	O-C-N	-5.62	114.85	121.32
1	A	6	ARG	NH1-CZ-NH2	-5.62	111.99	119.30
1	B	216	ARG	CA-C-O	-5.62	115.10	121.00
1	A	213	ASP	CB-CA-C	5.62	119.80	110.81
1	A	321	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	A	440	PHE	CA-CB-CG	5.62	119.42	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	ALA	N-CA-CB	-5.61	101.84	111.21
1	A	226	LYS	CA-CB-CG	5.60	125.31	114.10
1	A	243	ARG	CA-C-O	-5.60	113.53	119.97
1	B	179	ALA	CB-CA-C	5.60	119.67	110.88
1	B	131	ALA	O-C-N	5.60	130.03	122.59
1	A	29	ILE	CB-CA-C	5.59	120.46	111.29
1	A	299	SER	CA-CB-OG	5.59	122.29	111.10
1	B	266	VAL	O-C-N	-5.59	115.63	122.12
1	A	204	LEU	CB-CA-C	5.58	120.16	110.68
1	B	31	LYS	CB-CG-CD	5.58	124.12	111.30
1	B	385	ASN	CA-C-O	-5.57	114.81	121.11
1	B	79	GLU	CA-C-O	-5.57	114.12	121.08
1	A	123	MET	CA-C-O	-5.57	114.41	120.81
1	B	179	ALA	CA-C-O	5.57	126.67	120.82
1	B	146	LEU	CD1-CG-CD2	-5.56	98.56	110.80
1	A	70	LEU	CB-CA-C	-5.56	100.14	109.48
1	A	174	LYS	CA-C-O	-5.56	113.80	119.08
1	B	195	PRO	N-CA-C	5.56	120.85	113.57
1	B	357	TRP	CA-C-N	5.56	132.30	121.41
1	B	357	TRP	C-N-CA	5.56	132.30	121.41
1	B	343	LEU	CA-CB-CG	5.55	135.74	116.30
1	B	435	ARG	O-C-N	5.55	129.70	122.42
1	B	276	ARG	NH1-CZ-NH2	-5.55	112.08	119.30
1	B	111	ASN	CA-CB-CG	5.55	118.15	112.60
1	A	73	GLU	CA-C-N	5.55	130.22	122.23
1	A	73	GLU	C-N-CA	5.55	130.22	122.23
1	B	49	SER	N-CA-C	-5.54	106.21	114.64
1	A	51	THR	N-CA-C	5.54	120.75	112.94
1	B	428	ARG	CB-CG-CD	5.54	124.04	111.30
1	B	244	GLY	O-C-N	5.54	128.11	122.24
1	B	280	PRO	CA-C-O	-5.54	112.00	120.03
1	A	380	PHE	CB-CA-C	5.53	120.02	110.84
1	B	33	LYS	CG-CD-CE	5.53	124.02	111.30
1	A	178	GLU	CA-C-O	-5.53	114.73	120.92
1	A	349	GLN	CA-CB-CG	5.52	125.15	114.10
1	B	408	ARG	NH1-CZ-NH2	5.52	126.48	119.30
1	B	309	CYS	O-C-N	-5.52	114.84	122.46
1	B	58	CYS	CB-CA-C	5.52	118.30	110.24
1	B	85	TYR	CA-C-N	5.52	125.52	119.89
1	B	85	TYR	C-N-CA	5.52	125.52	119.89
1	B	197	GLY	O-C-N	5.52	129.87	122.70
1	B	320	ILE	CB-CG1-CD1	5.52	125.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	GLN	N-CA-C	-5.51	104.92	111.69
1	B	112	ASN	CA-C-N	5.51	132.06	121.54
1	B	112	ASN	C-N-CA	5.51	132.06	121.54
1	B	273	THR	N-CA-C	-5.51	106.56	113.28
1	A	236	ASP	CB-CA-C	5.50	121.01	110.17
1	A	321	HIS	N-CA-CB	5.50	118.96	110.21
1	B	155	VAL	CA-C-N	5.50	129.99	122.34
1	B	155	VAL	C-N-CA	5.50	129.99	122.34
1	A	45	PHE	CA-C-N	5.50	129.98	120.58
1	A	45	PHE	C-N-CA	5.50	129.98	120.58
1	A	31	LYS	CA-C-O	-5.50	112.63	120.16
1	A	13	LYS	N-CA-C	5.50	122.51	110.80
1	A	337	ARG	N-CA-CB	5.49	119.77	110.49
1	B	261	LEU	O-C-N	5.49	129.88	122.96
1	B	311	MET	N-CA-CB	-5.49	101.76	110.22
1	A	306	PHE	CA-C-O	5.49	126.42	119.78
1	B	318	SER	CA-C-O	5.49	126.02	119.60
1	B	93	ASN	CB-CA-C	5.49	119.41	109.37
1	A	129	PRO	CA-C-N	5.48	132.01	121.54
1	A	129	PRO	C-N-CA	5.48	132.01	121.54
1	A	265	TYR	CB-CG-CD2	5.48	129.03	120.80
1	B	105	LEU	N-CA-CB	5.48	118.47	110.47
1	B	368	SER	N-CA-C	5.48	115.36	108.45
1	A	157	GLY	CA-C-N	5.47	132.14	121.41
1	A	157	GLY	C-N-CA	5.47	132.14	121.41
1	A	219	GLN	N-CA-CB	5.47	119.62	110.32
1	A	222	THR	CA-CB-OG1	5.47	117.81	109.60
1	A	366	ILE	CA-CB-CG1	5.47	119.70	110.40
1	A	413	ALA	N-CA-C	-5.47	105.22	111.07
1	B	360	MET	O-C-N	-5.47	115.73	123.01
1	B	438	GLU	N-CA-C	-5.47	105.92	112.59
1	A	405	ALA	CB-CA-C	-5.47	99.23	110.38
1	A	301	ARG	CA-CB-CG	-5.46	103.18	114.10
1	B	361	LYS	CG-CD-CE	5.46	123.86	111.30
1	A	210	LEU	CA-C-O	-5.46	112.66	119.38
1	B	61	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	264	GLY	O-C-N	5.46	129.79	122.70
1	A	347	GLU	CA-CB-CG	5.45	125.01	114.10
1	B	117	ASP	CA-C-O	5.45	125.81	119.32
1	B	390	LEU	CA-C-N	5.45	129.67	122.42
1	B	390	LEU	C-N-CA	5.45	129.67	122.42
1	A	199	GLN	CB-CG-CD	-5.45	103.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	VAL	CA-CB-CG2	5.45	119.66	110.40
1	B	228	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	73	GLU	CA-CB-CG	5.44	124.98	114.10
1	B	294	VAL	N-CA-C	5.44	120.65	109.34
1	A	32	PRO	CB-CA-C	-5.44	104.44	111.46
1	B	68	ASP	CA-C-O	-5.44	114.93	120.80
1	B	225	ALA	N-CA-CB	-5.44	104.10	110.35
1	B	37	GLY	O-C-N	-5.44	115.63	122.70
1	B	156	ASP	N-CA-CB	5.44	120.17	111.91
1	B	436	ALA	CA-C-N	5.44	128.32	120.38
1	B	436	ALA	C-N-CA	5.44	128.32	120.38
1	A	293	ALA	CB-CA-C	5.43	121.47	110.38
1	A	347	GLU	CB-CG-CD	5.43	121.84	112.60
1	B	400	ILE	N-CA-C	-5.43	106.19	112.98
1	A	385	ASN	O-C-N	-5.43	117.86	123.29
1	B	142	ASN	CA-C-N	5.43	129.63	120.29
1	B	142	ASN	C-N-CA	5.43	129.63	120.29
1	A	170	GLY	O-C-N	5.43	129.76	122.70
1	B	387	ASN	CB-CG-ND2	5.43	124.54	116.40
1	A	241	ILE	N-CA-CB	-5.43	104.20	110.55
1	B	413	ALA	CA-C-O	-5.42	115.09	120.90
1	B	338	ALA	N-CA-C	-5.42	105.02	111.69
1	A	196	GLN	CB-CG-CD	5.42	121.82	112.60
1	A	289	ALA	N-CA-CB	5.42	119.65	110.49
1	B	241	ILE	O-C-N	-5.42	114.69	121.84
1	B	239	GLU	CA-CB-CG	5.42	124.93	114.10
1	B	282	ASN	N-CA-C	-5.42	100.94	109.50
1	B	213	ASP	CA-C-N	5.41	132.18	122.38
1	B	213	ASP	C-N-CA	5.41	132.18	122.38
1	A	278	ARG	NH1-CZ-NH2	-5.41	112.26	119.30
1	B	53	THR	O-C-N	5.41	129.78	122.59
1	B	387	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	A	245	GLU	CG-CD-OE2	-5.40	105.98	118.40
1	B	433	LEU	O-C-N	-5.40	115.37	122.39
1	B	95	THR	O-C-N	5.40	129.32	122.84
1	A	437	PHE	N-CA-CB	5.39	117.78	109.91
1	B	63	PHE	CA-CB-CG	-5.39	108.41	113.80
1	A	233	THR	CA-CB-OG1	-5.39	101.52	109.60
1	A	341	TYR	CB-CA-C	5.39	120.42	110.88
1	B	221	GLU	N-CA-CB	5.39	117.79	109.98
1	B	184	TRP	N-CA-C	-5.39	105.97	112.54
1	B	260	LEU	CA-C-O	5.39	131.09	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	436	ALA	CA-C-O	5.39	126.66	121.00
1	A	120	TYR	CA-C-O	-5.38	115.18	121.10
1	A	226	LYS	CB-CA-C	5.38	119.40	109.71
1	A	223	GLY	N-CA-C	-5.38	107.79	115.64
1	A	295	THR	O-C-N	5.38	130.10	122.68
1	B	304	THR	CB-CA-C	5.38	119.36	109.46
1	A	99	ALA	O-C-N	5.37	129.74	122.59
1	B	208	ILE	CA-C-N	5.37	127.47	120.28
1	B	208	ILE	C-N-CA	5.37	127.47	120.28
1	A	371	MET	CA-CB-CG	5.37	124.83	114.10
1	B	124	HIS	CA-C-N	5.37	130.97	121.80
1	B	124	HIS	C-N-CA	5.37	130.97	121.80
1	B	217	ARG	N-CA-C	5.36	120.22	111.37
1	B	202	ALA	O-C-N	5.36	126.20	121.32
1	B	354	ARG	CB-CG-CD	-5.35	98.98	111.30
1	A	44	HIS	CA-CB-CG	-5.35	108.45	113.80
1	B	409	SER	N-CA-C	-5.35	107.12	113.97
1	A	9	ASN	O-C-N	5.34	132.84	121.35
1	A	306	PHE	N-CA-C	-5.34	106.44	113.12
1	B	99	ALA	CB-CA-C	5.34	120.62	109.68
1	A	84	ALA	O-C-N	5.34	129.97	123.14
1	B	74	VAL	O-C-N	-5.33	116.92	123.00
1	B	161	VAL	CB-CA-C	-5.33	102.36	110.95
1	B	241	ILE	N-CA-CB	5.33	119.47	110.56
1	B	257	HIS	CA-C-O	5.33	125.53	119.18
1	B	112	ASN	N-CA-CB	-5.33	101.48	110.49
1	B	288	ARG	CD-NE-CZ	-5.33	116.94	124.40
1	A	196	GLN	CA-C-N	5.33	131.86	121.41
1	A	196	GLN	C-N-CA	5.33	131.86	121.41
1	B	296	SER	CB-CA-C	5.33	118.20	109.46
1	A	10	LEU	CA-C-O	-5.33	115.75	121.56
1	B	213	ASP	O-C-N	-5.33	115.35	122.43
1	A	303	TYR	CA-CB-CG	5.32	123.48	113.90
1	A	427	ALA	O-C-N	-5.32	116.59	122.07
1	A	267	ALA	CA-C-N	5.32	129.67	121.42
1	A	267	ALA	C-N-CA	5.32	129.67	121.42
1	A	279	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	277	ARG	CA-CB-CG	5.32	124.73	114.10
1	A	321	HIS	CB-CG-ND1	5.31	130.67	122.70
1	A	402	GLY	CA-C-N	5.31	126.48	119.84
1	A	402	GLY	C-N-CA	5.31	126.48	119.84
1	A	428	ARG	CA-C-O	5.31	126.18	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	TYR	O-C-N	-5.31	116.60	122.07
1	A	159	LEU	N-CA-C	5.31	118.17	110.42
1	A	65	ARG	NH1-CZ-NH2	-5.30	112.40	119.30
1	B	72	TYR	CB-CA-C	5.30	120.32	109.55
1	A	103	SER	CA-C-O	5.30	127.52	121.58
1	A	236	ASP	N-CA-CB	5.30	119.80	110.37
1	B	372	ASN	OD1-CG-ND2	5.30	127.90	122.60
1	A	31	LYS	CA-C-N	5.30	125.22	119.76
1	A	31	LYS	C-N-CA	5.30	125.22	119.76
1	B	8	VAL	CB-CA-C	-5.30	102.60	111.29
1	B	108	THR	OG1-CB-CG2	-5.29	98.71	109.30
1	B	228	PHE	CA-C-N	5.29	131.38	123.23
1	B	228	PHE	C-N-CA	5.29	131.38	123.23
1	A	153	PRO	N-CA-C	-5.29	102.81	110.80
1	B	192	ASN	CB-CG-OD1	5.29	131.38	120.80
1	A	28	TYR	O-C-N	5.29	129.56	123.17
1	B	60	THR	N-CA-C	-5.29	106.86	113.15
1	B	274	THR	N-CA-CB	5.28	117.95	110.13
1	B	221	GLU	CB-CA-C	-5.28	102.77	110.95
1	B	352	PHE	CA-C-O	5.28	126.54	119.47
1	A	342	MET	CG-SD-CE	-5.27	89.30	100.90
1	B	264	GLY	N-CA-C	5.27	122.22	115.32
1	A	141	VAL	N-CA-CB	-5.27	102.81	111.45
1	A	217	ARG	NH1-CZ-NH2	-5.26	112.45	119.30
1	A	269	ALA	CB-CA-C	5.26	118.24	109.56
1	B	120	TYR	N-CA-C	-5.26	100.74	108.79
1	B	282	ASN	O-C-N	5.26	129.71	123.24
1	B	321	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	A	9	ASN	N-CA-C	-5.26	99.30	109.24
1	A	184	TRP	N-CA-CB	5.25	118.39	110.30
1	B	103	SER	N-CA-CB	5.25	118.46	110.42
1	A	391	THR	CA-C-N	5.25	129.75	120.87
1	A	391	THR	C-N-CA	5.25	129.75	120.87
1	B	107	LEU	CA-C-O	-5.25	114.41	120.24
1	B	440	PHE	CA-CB-CG	-5.25	108.55	113.80
1	B	285	HIS	CB-CA-C	-5.25	102.69	110.67
1	A	35	GLY	CA-C-N	5.24	128.29	120.90
1	A	35	GLY	C-N-CA	5.24	128.29	120.90
1	A	240	ILE	CA-C-O	5.24	126.72	121.27
1	A	338	ALA	CA-C-N	5.23	129.29	120.29
1	A	338	ALA	C-N-CA	5.23	129.29	120.29
1	B	194	GLU	N-CA-C	5.23	121.38	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	444	ALA	N-CA-C	-5.23	106.89	113.28
1	B	217	ARG	O-C-N	-5.23	116.09	122.11
1	B	411	ARG	N-CA-CB	5.23	117.78	109.82
1	B	256	SER	CA-C-N	5.23	131.79	122.06
1	B	256	SER	C-N-CA	5.23	131.79	122.06
1	A	300	LYS	CB-CA-C	5.23	120.92	109.99
1	A	155	VAL	N-CA-CB	5.22	119.85	111.23
1	B	262	VAL	N-CA-C	-5.22	100.72	108.45
1	B	62	ASP	CA-C-N	5.22	131.52	121.54
1	B	62	ASP	C-N-CA	5.22	131.52	121.54
1	B	357	TRP	CA-CB-CG	5.22	123.52	113.60
1	B	198	ASN	CA-CB-CG	-5.22	107.38	112.60
1	B	51	THR	CA-CB-CG2	5.22	119.37	110.50
1	A	295	THR	N-CA-C	5.21	117.93	110.68
1	B	402	GLY	CA-C-N	5.21	126.35	119.84
1	B	402	GLY	C-N-CA	5.21	126.35	119.84
1	B	448	TYR	CA-CB-CG	-5.21	104.52	113.90
1	B	448	TYR	CB-CA-C	5.21	115.95	110.17
1	B	141	VAL	CA-CB-CG2	5.21	119.26	110.40
1	A	226	LYS	CG-CD-CE	5.21	123.28	111.30
1	B	93	ASN	CB-CG-ND2	-5.21	108.59	116.40
1	A	214	ALA	CA-C-N	5.20	131.47	121.54
1	A	214	ALA	C-N-CA	5.20	131.47	121.54
1	A	360	MET	N-CA-C	-5.19	100.78	109.24
1	A	395	GLY	N-CA-C	-5.19	100.87	113.18
1	B	55	VAL	CA-C-N	5.19	130.74	122.59
1	B	55	VAL	C-N-CA	5.19	130.74	122.59
1	B	236	ASP	N-CA-C	5.19	116.37	109.93
1	A	399	HIS	O-C-N	5.18	130.05	123.11
1	B	269	ALA	O-C-N	-5.18	116.63	122.12
1	B	367	ILE	CA-C-N	5.18	131.11	122.20
1	B	367	ILE	C-N-CA	5.18	131.11	122.20
1	B	189	PHE	CA-CB-CG	-5.17	108.63	113.80
1	B	16	ASP	OD1-CG-OD2	-5.17	110.49	122.90
1	A	53	THR	O-C-N	-5.17	115.72	122.59
1	A	228	PHE	CA-CB-CG	-5.17	108.63	113.80
1	B	359	GLY	O-C-N	5.17	129.42	122.70
1	B	102	ALA	N-CA-C	-5.16	105.14	111.75
1	A	196	GLN	CA-CB-CG	5.16	124.42	114.10
1	B	264	GLY	O-C-N	5.16	129.96	122.68
1	A	6	ARG	N-CA-C	-5.16	105.67	112.94
1	A	32	PRO	CA-C-O	5.16	127.22	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ARG	CA-C-N	-5.15	113.37	120.28
1	A	313	ARG	C-N-CA	-5.15	113.37	120.28
1	B	22	GLU	CB-CG-CD	5.15	121.35	112.60
1	B	191	LYS	CA-C-N	-5.15	114.06	121.42
1	B	191	LYS	C-N-CA	-5.15	114.06	121.42
1	A	24	VAL	CA-C-N	5.15	129.25	122.30
1	A	24	VAL	C-N-CA	5.15	129.25	122.30
1	A	211	VAL	N-CA-CB	5.14	119.14	110.56
1	B	129	PRO	CA-C-N	5.14	130.38	122.42
1	B	129	PRO	C-N-CA	5.14	130.38	122.42
1	A	136	PHE	N-CA-C	5.13	116.95	110.33
1	B	84	ALA	O-C-N	-5.13	116.77	122.93
1	B	411	ARG	N-CA-C	-5.13	104.76	111.02
1	B	452	ARG	O-C-N	5.13	128.22	122.22
1	A	355	GLN	CA-CB-CG	-5.12	103.86	114.10
1	B	302	GLY	CA-C-O	5.12	129.47	120.57
1	B	457	VAL	CA-C-O	-5.12	112.10	120.80
1	A	10	LEU	N-CA-CB	-5.11	102.81	110.17
1	A	65	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	A	76	GLU	CG-CD-OE1	-5.11	106.66	118.40
1	B	304	THR	CA-C-N	5.11	131.30	121.54
1	B	304	THR	C-N-CA	5.11	131.30	121.54
1	B	51	THR	N-CA-CB	-5.11	102.44	110.30
1	B	160	VAL	O-C-N	-5.10	117.37	123.03
1	A	212	ALA	N-CA-C	-5.10	103.01	111.37
1	A	401	ASP	N-CA-C	-5.10	107.01	113.18
1	A	22	GLU	CA-C-O	5.09	125.31	118.38
1	A	245	GLU	CA-CB-CG	5.09	124.29	114.10
1	A	422	PRO	CA-N-CD	-5.09	104.87	112.00
1	A	78	ARG	O-C-N	-5.09	114.23	122.42
1	B	346	ASP	CB-CG-OD1	-5.09	106.69	118.40
1	A	104	PHE	N-CA-CB	5.09	119.08	110.49
1	B	153	PRO	CA-C-O	-5.08	111.35	120.60
1	A	100	MET	N-CA-CB	-5.08	102.08	111.53
1	B	412	GLN	CB-CA-C	-5.08	102.40	110.84
1	A	208	ILE	CB-CA-C	5.08	118.47	110.95
1	B	309	CYS	N-CA-C	5.08	119.18	112.89
1	B	392	ALA	N-CA-C	5.07	117.67	109.40
1	A	273	THR	CA-C-O	-5.06	114.15	119.97
1	A	246	TYR	CA-CB-CG	-5.06	104.79	113.90
1	B	22	GLU	O-C-N	5.06	129.32	122.59
1	A	347	GLU	O-C-N	5.06	130.55	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	PHE	CB-CA-C	5.06	120.49	110.42
1	B	245	GLU	N-CA-CB	5.06	117.62	110.13
1	A	196	GLN	CG-CD-OE1	5.06	130.91	120.80
1	B	43	ALA	O-C-N	-5.06	115.53	122.46
1	B	375	ARG	CB-CA-C	5.06	118.72	110.17
1	B	240	ILE	CB-CA-C	5.05	118.78	111.65
1	B	321	HIS	CA-C-N	5.05	131.19	121.54
1	B	321	HIS	C-N-CA	5.05	131.19	121.54
1	B	284	LEU	N-CA-CB	5.05	119.02	110.69
1	A	119	GLU	CB-CA-C	-5.05	102.93	110.90
1	A	127	TYR	CA-C-O	5.04	125.70	120.40
1	B	183	PHE	O-C-N	5.04	128.58	122.48
1	B	240	ILE	N-CA-C	-5.04	105.24	112.35
1	A	21	GLY	N-CA-C	5.04	123.58	114.46
1	A	186	GLY	N-CA-C	-5.04	101.23	113.18
1	A	256	SER	CA-C-O	5.04	124.36	118.77
1	B	209	ALA	CA-C-O	-5.04	115.21	120.55
1	B	376	MET	CA-C-N	5.04	125.31	119.47
1	B	376	MET	C-N-CA	5.04	125.31	119.47
1	B	351	PRO	N-CA-CB	-5.04	97.96	103.25
1	A	96	ASP	CA-C-O	5.03	127.71	120.51
1	B	285	HIS	O-C-N	5.03	129.56	122.77
1	A	385	ASN	N-CA-CB	-5.03	103.12	111.57
1	A	104	PHE	N-CA-C	-5.03	100.09	110.80
1	B	106	THR	CA-C-O	5.03	125.56	119.38
1	B	349	GLN	N-CA-C	5.03	117.45	109.96
1	A	39	VAL	N-CA-CB	5.03	119.52	111.23
1	B	90	PHE	O-C-N	-5.03	117.49	123.22
1	B	441	PRO	CA-C-O	5.03	129.75	120.60
1	A	191	LYS	CD-CE-NZ	5.02	127.98	111.90
1	A	200	PRO	N-CA-C	5.02	122.81	112.47
1	A	313	ARG	N-CA-CB	5.02	117.91	110.53
1	A	407	ALA	N-CA-C	-5.02	105.54	113.02
1	A	352	PHE	N-CA-C	5.02	120.34	114.62
1	B	50	SER	CA-C-O	5.02	123.91	119.34
1	B	288	ARG	O-C-N	5.02	129.69	123.01
1	B	303	TYR	CB-CG-CD2	-5.02	113.27	120.80
1	B	404	VAL	CA-CB-CG1	5.02	118.93	110.40
1	A	259	ALA	N-CA-CB	-5.02	102.69	110.57
1	B	78	ARG	CA-C-O	5.02	127.69	120.51
1	B	291	HIS	N-CA-C	5.02	119.40	113.28
1	A	319	GLY	CA-C-O	-5.01	111.84	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	GLU	O-C-N	5.01	127.23	122.07
1	B	94	ILE	N-CA-CB	5.01	117.74	110.52
1	B	452	ARG	CB-CA-C	-5.01	101.36	110.63
1	A	365	PRO	N-CA-C	-5.01	103.23	110.80
1	B	266	VAL	CA-C-O	5.01	125.27	119.36
1	A	439	SER	N-CA-CB	5.01	118.23	109.72
1	A	248	LEU	N-CA-CB	5.01	118.01	110.30
1	B	91	ASP	O-C-N	-5.01	117.30	122.96
1	A	76	GLU	O-C-N	-5.00	115.94	122.59
1	B	88	ALA	N-CA-CB	-5.00	102.04	110.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	349	GLN	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	GLU	Mainchain
1	A	354	ARG	Sidechain
1	A	433	LEU	Mainchain
1	B	288	ARG	Sidechain
1	B	301	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	3200	0	3110	485	2
1	B	3385	0	3278	478	2
2	A	67	0	0	3	0
2	B	43	0	0	1	0
All	All	6695	0	6388	903	3

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 70.

All (903) 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:B:41:THR:CB	1:B:41:THR:CA	1.75	1.61
1:A:164:ILE:CA	1:A:164:ILE:CB	1.74	1.60
1:A:335:SER:HB3	1:A:338:ALA:CB	1.21	1.56
1:A:191:LYS:CD	1:A:191:LYS:CE	1.78	1.56
1:B:190:ILE:C	1:B:191:LYS:N	1.82	1.37
1:A:335:SER:CB	1:A:338:ALA:HB2	1.59	1.32
1:A:335:SER:CB	1:A:338:ALA:CB	2.16	1.22
1:B:166:LYS:HD3	1:B:167:PRO:HA	1.21	1.17
1:B:346:ASP:HB3	1:B:357:TRP:HB2	1.25	1.17
1:A:361:LYS:CD	1:A:361:LYS:CE	2.23	1.16
1:A:109:MET:HE2	1:A:303:TYR:HB3	1.25	1.15
1:B:457:VAL:O	1:B:457:VAL:HG13	1.30	1.10
1:B:32:PRO:HB3	1:B:41:THR:HG21	1.34	1.10
1:A:170:GLY:C	1:B:64:THR:HG22	1.79	1.07
1:A:309:CYS:HB3	1:A:320:ILE:HD13	1.34	1.07
1:A:439:SER:C	1:A:440:PHE:N	2.16	1.04
1:A:156:ASP:HB3	1:A:387:ASN:ND2	1.72	1.03
1:B:323:GLY:O	1:B:324:THR:HB	1.25	1.03
1:A:156:ASP:HB3	1:A:387:ASN:HD22	1.18	1.03
1:A:335:SER:HB3	1:A:338:ALA:HB1	1.40	1.02
1:A:439:SER:C	1:A:440:PHE:CA	2.33	1.00
1:B:56:GLU:O	1:B:57:VAL:CB	2.09	0.99
1:B:187:GLY:HA2	1:B:411:ARG:HH22	1.28	0.99
1:A:376:MET:SD	1:A:380:PHE:CZ	2.56	0.99
1:B:323:GLY:O	1:B:324:THR:CB	2.10	0.98
1:B:346:ASP:CB	1:B:357:TRP:HB2	1.92	0.98
1:B:14:GLU:HB2	1:B:72:TYR:HE1	1.27	0.97
1:A:169:LEU:O	1:B:51:THR:HG23	1.65	0.96
1:B:371:MET:HE2	1:B:376:MET:HA	1.48	0.95
1:A:439:SER:C	1:A:440:PHE:HA	1.91	0.95
1:B:56:GLU:O	1:B:57:VAL:HB	1.16	0.95
1:B:38:TYR:HE2	1:B:74:VAL:HG13	1.31	0.94
1:B:59:THR:CG2	1:B:64:THR:HG23	1.98	0.94
1:A:14:GLU:HG2	1:A:18:ILE:HD12	1.50	0.94
1:B:7:TYR:OH	1:B:51:THR:HB	1.68	0.93
1:A:170:GLY:CA	1:B:64:THR:HG22	1.98	0.93
1:A:355:GLN:HE21	1:A:356:SER:N	1.65	0.93
1:B:128:VAL:HG23	1:B:355:GLN:HE22	1.32	0.93
1:A:324:THR:HG21	1:A:336:ASP:HB3	1.52	0.92
1:B:12:LEU:HD12	1:B:17:LEU:HD11	1.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASN:ND2	1:A:375:ARG:HE	1.67	0.91
1:A:229:SER:HA	1:A:259:ALA:HB3	1.53	0.90
1:A:390:LEU:HD23	1:A:392:ALA:HB2	1.51	0.90
1:A:164:ILE:HG12	1:A:392:ALA:O	1.72	0.89
1:A:166:LYS:HE3	1:B:54:ASN:HB2	1.54	0.89
1:A:355:GLN:NE2	1:A:356:SER:H	1.69	0.89
1:A:116:GLY:O	1:A:117:ASP:HB2	1.70	0.89
1:A:433:LEU:HD12	1:A:436:ALA:HB3	1.56	0.88
1:A:371:MET:HE1	1:A:379:PHE:HD2	1.39	0.87
1:B:38:TYR:CE2	1:B:74:VAL:HG13	2.08	0.87
1:A:379:PHE:HE1	1:A:383:LEU:HD22	1.38	0.87
1:B:45:PHE:HA	1:B:115:MET:HE1	1.56	0.87
1:B:457:VAL:O	1:B:457:VAL:CG1	2.01	0.86
1:B:38:TYR:CE2	1:B:74:VAL:CG1	2.58	0.86
1:B:456:GLY:O	1:B:457:VAL:HB	1.73	0.85
1:A:170:GLY:HA3	1:B:64:THR:HG22	1.58	0.85
1:B:192:ASN:HD21	1:B:231:ASN:H	1.19	0.85
1:B:59:THR:HG21	1:B:64:THR:HG23	1.59	0.84
1:B:377:PRO:HG3	1:B:423:VAL:HG21	1.59	0.84
1:B:52:GLY:C	1:B:54:ASN:H	1.85	0.84
1:B:421:VAL:HG12	1:B:426:TYR:HB2	1.60	0.84
1:B:261:LEU:HA	1:B:285:HIS:HB3	1.59	0.83
1:B:367:ILE:HD12	1:B:390:LEU:HD12	1.60	0.83
1:A:173:PRO:HA	1:A:207:THR:HG23	1.59	0.83
1:B:312:ALA:HA	1:B:315:GLN:HG2	1.62	0.82
1:A:171:LEU:CD2	1:A:176:PHE:HB2	2.09	0.82
1:B:163:THR:HB	1:B:183:PHE:CD1	2.15	0.82
1:B:452:ARG:HB2	1:B:453:LYS:HD2	1.59	0.82
1:A:142:ASN:ND2	1:A:361:LYS:CE	2.42	0.82
1:B:87:VAL:HG11	1:B:132:TYR:HB2	1.62	0.82
1:B:454:ALA:O	1:B:455:LEU:HB2	1.80	0.82
1:A:126:PHE:CZ	1:A:310:LYS:HD3	2.14	0.81
1:A:8:VAL:HG21	1:A:39:VAL:HG13	1.61	0.81
1:B:301:ARG:NH1	1:B:301:ARG:HB2	1.96	0.81
1:A:113:GLN:O	1:B:292:GLY:HA3	1.79	0.81
1:A:160:VAL:HG12	1:A:389:ILE:HG23	1.63	0.81
1:A:365:PRO:HD2	1:A:388:VAL:HG12	1.62	0.81
1:A:142:ASN:ND2	1:A:361:LYS:HE2	1.97	0.80
1:A:232:ILE:HG12	1:A:260:LEU:HD22	1.61	0.80
1:A:355:GLN:HE21	1:A:356:SER:H	0.85	0.80
1:B:38:TYR:CD2	1:B:74:VAL:HG11	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:SER:HB3	1:B:301:ARG:NH2	1.97	0.80
1:A:427:ALA:O	1:A:434:ALA:HB2	1.83	0.79
1:B:255:ALA:HA	1:B:258:VAL:HG22	1.62	0.79
1:A:324:THR:CG2	1:A:336:ASP:HB3	2.13	0.79
1:B:418:ARG:O	1:B:419:ASP:HB2	1.83	0.79
1:A:295:THR:CG2	1:A:305:ALA:HB2	2.13	0.79
1:B:169:LEU:HD11	1:B:195:PRO:HB2	1.65	0.79
1:A:208:ILE:HA	1:A:211:VAL:HG12	1.63	0.79
1:A:374:LEU:HD11	1:A:437:PHE:HA	1.64	0.78
1:B:14:GLU:HB2	1:B:72:TYR:CE1	2.17	0.78
1:A:172:ARG:HB2	1:A:175:PRO:HG2	1.64	0.78
1:B:194:GLU:HG2	1:B:287:HIS:HE1	1.46	0.78
1:A:92:ARG:HG3	1:A:93:ASN:H	1.47	0.78
1:B:59:THR:HG22	1:B:64:THR:HG23	1.66	0.78
1:A:164:ILE:CB	1:A:164:ILE:N	2.47	0.77
1:A:75:ASP:OD1	1:A:78:ARG:HB2	1.84	0.77
1:B:298:GLN:HA	1:B:298:GLN:NE2	1.98	0.77
1:B:309:CYS:HB3	1:B:343:LEU:HD11	1.66	0.77
1:B:371:MET:CE	1:B:376:MET:HA	2.15	0.77
1:B:187:GLY:HA2	1:B:411:ARG:NH2	2.00	0.76
1:B:294:VAL:HG13	1:B:302:GLY:HA2	1.65	0.76
1:A:170:GLY:C	1:B:64:THR:CG2	2.58	0.76
1:B:161:VAL:HG13	1:B:390:LEU:HD23	1.67	0.75
1:A:100:MET:HE1	1:B:233:THR:O	1.86	0.75
1:B:89:LEU:HD12	1:B:89:LEU:H	1.52	0.75
1:A:284:LEU:HD12	1:A:317:ALA:HA	1.69	0.75
1:B:177:ALA:O	1:B:180:CYS:HB3	1.86	0.75
1:A:6:ARG:NH2	1:A:53:THR:OG1	2.19	0.75
1:A:433:LEU:O	1:A:434:ALA:C	2.29	0.75
1:A:400:ILE:HD12	1:A:435:ARG:HB3	1.69	0.75
1:B:148:LYS:HG3	1:B:154:GLU:HG2	1.69	0.75
1:A:192:ASN:ND2	1:A:196:GLN:HB2	2.02	0.74
1:A:216:ARG:HH21	1:A:254:ASN:ND2	1.84	0.74
1:A:53:THR:N	1:B:166:LYS:HD2	2.02	0.74
1:A:390:LEU:CD2	1:A:392:ALA:HB2	2.17	0.74
1:A:142:ASN:HD21	1:A:361:LYS:HE2	1.51	0.74
1:A:266:VAL:HG21	1:B:106:THR:HG23	1.69	0.74
1:A:335:SER:HB3	1:A:338:ALA:HB2	0.75	0.74
1:B:414:TRP:O	1:B:417:TRP:HB3	1.87	0.74
1:A:237:PRO:O	1:A:241:ILE:HD12	1.88	0.73
1:A:163:THR:HB	1:A:183:PHE:CE1	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLY:O	1:B:294:VAL:N	2.21	0.73
1:A:372:ASN:CG	1:A:375:ARG:HE	1.96	0.73
1:B:38:TYR:CD2	1:B:74:VAL:CG1	2.72	0.73
1:B:366:ILE:HB	1:B:389:ILE:HB	1.71	0.73
1:A:7:TYR:CE1	1:A:68:ASP:HB3	2.24	0.73
1:A:9:ASN:HB3	1:A:12:LEU:HD22	1.69	0.73
1:A:93:ASN:ND2	1:B:239:GLU:HG2	2.03	0.73
1:B:10:LEU:HD23	1:B:73:GLU:HA	1.71	0.73
1:B:232:ILE:HG12	1:B:240:ILE:HD12	1.70	0.73
1:A:24:VAL:HG23	1:A:87:VAL:HG23	1.71	0.72
1:A:379:PHE:CE1	1:A:383:LEU:HD22	2.24	0.72
1:B:8:VAL:HG22	1:B:71:VAL:HB	1.70	0.72
1:B:128:VAL:HG23	1:B:355:GLN:NE2	2.04	0.72
1:B:38:TYR:HD2	1:B:74:VAL:HG11	1.52	0.72
1:A:54:ASN:O	1:A:55:VAL:HB	1.88	0.72
1:A:270:ALA:HA	1:B:235:ASP:O	1.89	0.72
1:B:346:ASP:HB3	1:B:357:TRP:CB	2.13	0.72
1:A:290:GLY:O	1:A:291:HIS:C	2.32	0.72
1:A:378:GLY:O	1:A:382:ASN:HB2	1.90	0.72
1:B:71:VAL:HG11	1:B:74:VAL:CG2	2.20	0.72
1:A:94:ILE:HG23	1:B:239:GLU:OE2	1.90	0.71
1:A:163:THR:HB	1:A:183:PHE:CZ	2.24	0.71
1:A:171:LEU:HD21	1:A:176:PHE:HB2	1.72	0.71
1:B:59:THR:CG2	1:B:64:THR:CG2	2.67	0.71
1:B:215:MET:SD	1:B:251:PHE:HE2	2.13	0.71
1:B:164:ILE:HG13	1:B:164:ILE:O	1.90	0.71
1:B:130:GLU:CG	1:B:131:ALA:H	2.02	0.71
1:A:172:ARG:O	1:A:175:PRO:HB2	1.90	0.71
1:A:166:LYS:HZ1	1:B:52:GLY:HA3	1.57	0.70
1:A:192:ASN:HD21	1:A:196:GLN:CB	2.03	0.70
1:B:172:ARG:HB3	1:B:173:PRO:HD2	1.72	0.70
1:A:106:THR:HG22	1:A:107:LEU:HD12	1.72	0.70
1:B:173:PRO:HD3	1:B:202:ALA:HA	1.72	0.70
1:A:372:ASN:OD1	1:A:375:ARG:HG2	1.91	0.70
1:A:195:PRO:O	1:A:199:GLN:NE2	2.24	0.70
1:B:163:THR:HB	1:B:183:PHE:CE1	2.26	0.70
1:A:65:ARG:C	1:A:67:VAL:H	1.98	0.70
1:B:24:VAL:HG13	1:B:127:TYR:O	1.92	0.70
1:A:303:TYR:HB2	1:A:307:VAL:HG11	1.74	0.70
1:B:6:ARG:HB3	1:B:7:TYR:CD2	2.27	0.69
1:B:166:LYS:CD	1:B:167:PRO:HA	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ARG:NH2	1:B:254:ASN:HB2	2.07	0.69
1:B:422:PRO:O	1:B:424:LEU:N	2.26	0.69
1:A:294:VAL:HG22	1:A:302:GLY:HA3	1.74	0.69
1:B:234:ALA:HB3	1:B:240:ILE:HG22	1.75	0.69
1:A:31:LYS:O	1:A:119:GLU:HB2	1.93	0.69
1:A:198:ASN:HA	1:A:204:LEU:H	1.57	0.69
1:B:159:LEU:HD11	1:B:390:LEU:HB3	1.74	0.69
1:A:6:ARG:NH2	1:A:51:THR:HG22	2.08	0.69
1:A:171:LEU:HD12	1:B:59:THR:OG1	1.93	0.69
1:A:185:LEU:HD12	1:A:221:GLU:HG2	1.75	0.68
1:B:95:THR:O	1:B:96:ASP:HB2	1.92	0.68
1:B:418:ARG:HG2	1:B:418:ARG:HH11	1.57	0.68
1:B:424:LEU:HD21	1:B:448:TYR:HB3	1.75	0.68
1:A:53:THR:H	1:B:166:LYS:HD2	1.59	0.68
1:A:142:ASN:ND2	1:A:361:LYS:NZ	2.42	0.68
1:A:401:ASP:HB3	1:A:405:ALA:HB2	1.75	0.68
1:B:103:SER:O	1:B:107:LEU:HB2	1.94	0.68
1:B:312:ALA:O	1:B:317:ALA:HB3	1.94	0.68
1:A:184:TRP:CH2	1:A:228:PHE:HB2	2.29	0.68
1:A:433:LEU:HD12	1:A:433:LEU:O	1.92	0.68
1:A:243:ARG:O	1:A:247:VAL:HG23	1.93	0.67
1:A:166:LYS:NZ	1:B:52:GLY:HA3	2.09	0.67
1:A:372:ASN:ND2	1:A:375:ARG:NE	2.41	0.67
1:A:91:ASP:OD1	1:B:243:ARG:NH2	2.26	0.67
1:B:172:ARG:CB	1:B:173:PRO:HD2	2.24	0.67
1:A:173:PRO:CA	1:A:207:THR:HG23	2.23	0.67
1:A:440:PHE:O	1:A:440:PHE:CD1	2.47	0.67
1:B:51:THR:HG21	1:B:64:THR:O	1.95	0.67
1:A:164:ILE:CA	1:A:164:ILE:CG2	2.71	0.67
1:A:294:VAL:CG2	1:A:302:GLY:HA3	2.24	0.67
1:A:372:ASN:HA	1:A:395:GLY:HA2	1.75	0.67
1:B:78:ARG:HG3	1:B:78:ARG:O	1.95	0.67
1:A:339:ILE:O	1:A:343:LEU:HB3	1.94	0.66
1:A:274:THR:HB	1:B:237:PRO:CG	2.25	0.66
1:A:172:ARG:HH22	1:B:62:ASP:CB	2.08	0.66
1:B:183:PHE:HD1	1:B:190:ILE:HD11	1.59	0.66
1:A:263:ASP:O	1:A:266:VAL:HG23	1.96	0.66
1:B:8:VAL:CG1	1:B:9:ASN:N	2.59	0.66
1:A:377:PRO:HA	1:A:380:PHE:HB2	1.78	0.66
1:A:8:VAL:HG21	1:A:39:VAL:CG1	2.26	0.66
1:A:46:ALA:HB1	1:A:69:ALA:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLY:O	1:B:64:THR:HG22	1.95	0.66
1:A:288:ARG:O	1:A:289:ALA:CB	2.42	0.66
1:B:32:PRO:HB3	1:B:41:THR:CG2	2.19	0.66
1:A:110:GLY:O	1:A:113:GLN:HB2	1.95	0.66
1:A:128:VAL:CG2	1:A:132:TYR:HD2	2.07	0.66
1:B:194:GLU:HG2	1:B:287:HIS:CE1	2.29	0.66
1:A:228:PHE:CE2	1:A:230:ALA:HB2	2.31	0.66
1:A:238:PHE:CE2	1:B:278:ARG:HD3	2.31	0.66
1:A:433:LEU:CD1	1:A:436:ALA:HB3	2.24	0.66
1:B:408:ARG:HG2	1:B:432:GLU:HG2	1.78	0.66
1:B:379:PHE:O	1:B:383:LEU:HB3	1.95	0.66
1:A:33:LYS:O	1:A:36:TYR:HB2	1.94	0.65
1:B:452:ARG:HB2	1:B:453:LYS:CD	2.26	0.65
1:A:169:LEU:HD11	1:A:195:PRO:HB2	1.78	0.65
1:A:8:VAL:HG22	1:A:71:VAL:HB	1.77	0.65
1:A:24:VAL:HG23	1:A:87:VAL:CG2	2.25	0.65
1:A:435:ARG:HA	1:A:438:GLU:HB3	1.78	0.65
1:B:128:VAL:HG12	1:B:132:TYR:CD2	2.32	0.65
1:A:109:MET:HE3	1:A:123:MET:SD	2.37	0.65
1:B:322:THR:CG2	1:B:323:GLY:N	2.58	0.65
1:A:270:ALA:O	1:A:274:THR:HG22	1.96	0.65
1:A:293:ALA:HB2	1:B:113:GLN:HG2	1.78	0.65
1:B:425:ASP:HA	1:B:428:ARG:HB2	1.79	0.65
1:A:371:MET:SD	1:A:376:MET:HG3	2.37	0.64
1:B:130:GLU:HG2	1:B:131:ALA:H	1.60	0.64
1:A:232:ILE:CG1	1:A:260:LEU:HD22	2.26	0.64
1:B:374:LEU:O	1:B:448:TYR:HE2	1.80	0.64
1:A:21:GLY:HA2	1:A:129:PRO:HB2	1.79	0.64
1:A:274:THR:HB	1:B:237:PRO:HG3	1.79	0.64
1:B:255:ALA:HA	1:B:258:VAL:CG2	2.27	0.64
1:A:75:ASP:HB3	1:A:80:LEU:HD23	1.80	0.64
1:A:139:PRO:HG2	1:A:361:LYS:HB3	1.79	0.64
1:A:364:THR:HG22	1:A:388:VAL:HA	1.80	0.64
1:B:217:ARG:O	1:B:221:GLU:HG2	1.97	0.64
1:B:254:ASN:HB3	1:B:257:HIS:CD2	2.32	0.64
1:A:32:PRO:HG3	1:A:41:THR:HG21	1.78	0.64
1:B:59:THR:HG22	1:B:64:THR:CG2	2.28	0.64
1:B:261:LEU:HG	1:B:285:HIS:CD2	2.33	0.64
1:B:442:GLY:HA2	1:B:445:ASP:N	2.12	0.64
1:B:215:MET:O	1:B:219:GLN:HG2	1.98	0.64
1:A:92:ARG:CD	1:A:99:ALA:HA	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:HD11	1:B:17:LEU:HD21	1.80	0.64
1:A:262:VAL:HG12	1:A:264:GLY:HA2	1.80	0.63
1:B:190:ILE:C	1:B:191:LYS:CA	2.70	0.63
1:B:427:ALA:O	1:B:434:ALA:HB2	1.98	0.63
1:B:86:PRO:O	1:B:89:LEU:HD12	1.98	0.63
1:A:414:TRP:O	1:A:417:TRP:HB3	1.98	0.63
1:B:418:ARG:O	1:B:419:ASP:CB	2.46	0.63
1:A:192:ASN:HD21	1:A:196:GLN:HB2	1.63	0.63
1:A:273:THR:HG21	1:B:236:ASP:HB2	1.81	0.63
1:A:372:ASN:HD22	1:A:440:PHE:HE1	1.46	0.63
1:B:59:THR:HG21	1:B:64:THR:CG2	2.29	0.63
1:B:71:VAL:HG11	1:B:74:VAL:HG23	1.79	0.63
1:B:421:VAL:CG1	1:B:426:TYR:HB2	2.27	0.63
1:A:303:TYR:HB2	1:A:307:VAL:CG1	2.29	0.63
1:B:6:ARG:CD	1:B:7:TYR:H	2.11	0.63
1:B:8:VAL:HG13	1:B:9:ASN:N	2.14	0.63
1:B:166:LYS:HD3	1:B:167:PRO:CA	2.14	0.63
1:A:9:ASN:O	1:A:12:LEU:HB3	1.98	0.62
1:A:30:MET:HE3	1:A:81:THR:OG1	1.99	0.62
1:B:301:ARG:HB2	1:B:301:ARG:HH11	1.64	0.62
1:A:76:GLU:O	1:A:79:GLU:HG3	1.98	0.62
1:A:429:GLU:HB3	1:A:430:HIS:ND1	2.14	0.62
1:B:139:PRO:HD3	1:B:313:ARG:O	1.97	0.62
1:A:173:PRO:HA	1:A:207:THR:CG2	2.29	0.62
1:A:14:GLU:O	1:A:18:ILE:HB	1.99	0.62
1:A:122:LYS:NZ	1:A:296:SER:O	2.32	0.62
1:B:355:GLN:HG3	1:B:356:SER:N	2.14	0.62
1:B:357:TRP:O	1:B:359:GLY:N	2.32	0.62
1:A:122:LYS:HB2	1:A:300:LYS:O	2.00	0.62
1:A:171:LEU:HD21	1:A:176:PHE:CA	2.30	0.62
1:A:199:GLN:HB3	1:A:200:PRO:HD2	1.81	0.62
1:B:371:MET:HB3	1:B:390:LEU:HD11	1.80	0.62
1:B:41:THR:CB	1:B:41:THR:N	2.61	0.62
1:B:192:ASN:ND2	1:B:231:ASN:HB2	2.15	0.62
1:B:454:ALA:O	1:B:455:LEU:CB	2.48	0.62
1:A:192:ASN:ND2	1:A:196:GLN:CB	2.63	0.62
1:A:415:GLN:O	1:A:419:ASP:HB2	2.00	0.62
1:A:398:GLY:O	1:A:440:PHE:HD2	1.81	0.62
1:B:396:ALA:HA	1:B:406:GLY:HA3	1.82	0.62
1:B:294:VAL:HG13	1:B:302:GLY:CA	2.30	0.61
1:B:371:MET:HE2	1:B:376:MET:HE3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ILE:O	1:B:240:ILE:HB	1.99	0.61
1:B:233:THR:OG1	1:B:262:VAL:HA	1.99	0.61
1:A:145:ALA:HA	1:A:148:LYS:HD3	1.82	0.61
1:B:218:ALA:HA	1:B:221:GLU:HG2	1.81	0.61
1:A:148:LYS:HB3	1:A:154:GLU:HG2	1.81	0.61
1:A:171:LEU:HD21	1:A:176:PHE:CB	2.30	0.61
1:B:59:THR:HG23	1:B:60:THR:H	1.66	0.61
1:A:141:VAL:HG22	1:A:145:ALA:CB	2.30	0.61
1:B:176:PHE:O	1:B:177:ALA:C	2.44	0.61
1:B:443:ASP:O	1:B:447:ILE:HD12	2.00	0.61
1:A:295:THR:HG22	1:A:305:ALA:HB2	1.82	0.61
1:B:211:VAL:O	1:B:212:ALA:C	2.43	0.61
1:B:216:ARG:O	1:B:220:ASP:HB2	2.01	0.61
1:A:226:LYS:O	1:A:257:HIS:HB3	2.00	0.61
1:B:99:ALA:HB2	1:B:135:LEU:HB2	1.83	0.61
1:B:457:VAL:O	1:B:457:VAL:HG22	2.01	0.61
1:A:172:ARG:HH22	1:B:62:ASP:CG	2.07	0.61
1:B:102:ALA:O	1:B:106:THR:OG1	2.19	0.61
1:A:216:ARG:HH21	1:A:254:ASN:HD21	1.48	0.61
1:B:160:VAL:HG22	1:B:389:ILE:HG23	1.83	0.61
1:A:139:PRO:HD3	1:A:313:ARG:O	2.00	0.61
1:A:295:THR:HG21	1:A:305:ALA:HB2	1.82	0.61
1:A:427:ALA:HB2	1:A:437:PHE:CE1	2.34	0.61
1:B:412:GLN:HB3	1:B:426:TYR:HE2	1.66	0.61
1:A:276:ARG:O	1:A:280:PRO:HB3	2.01	0.60
1:B:204:LEU:HG	1:B:208:ILE:HD13	1.83	0.60
1:A:198:ASN:HB2	1:A:204:LEU:HD23	1.84	0.60
1:A:244:GLY:HA3	1:A:279:PHE:CZ	2.36	0.60
1:A:292:GLY:O	1:B:301:ARG:NH2	2.33	0.60
1:A:230:ALA:O	1:A:232:ILE:HG23	2.02	0.60
1:B:438:GLU:HG3	1:B:451:TRP:HH2	1.67	0.60
1:A:171:LEU:HD21	1:A:176:PHE:N	2.16	0.60
1:A:398:GLY:O	1:A:440:PHE:CD2	2.55	0.60
1:A:440:PHE:O	1:A:440:PHE:HD1	1.84	0.60
1:A:429:GLU:HB3	1:A:430:HIS:CE1	2.36	0.60
1:A:229:SER:HB3	1:A:261:LEU:HD23	1.82	0.59
1:A:21:GLY:HA2	1:A:129:PRO:CB	2.32	0.59
1:A:418:ARG:NH1	1:A:419:ASP:OD1	2.35	0.59
1:A:372:ASN:HA	1:A:395:GLY:CA	2.32	0.59
1:B:119:GLU:HG3	1:B:120:TYR:CD2	2.37	0.59
1:B:407:ALA:HA	1:B:410:LEU:HB2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:GLN:OE1	1:B:432:GLU:HB2	2.02	0.59
1:B:215:MET:SD	1:B:251:PHE:CE2	2.95	0.59
1:A:310:LYS:O	1:A:310:LYS:HG2	2.02	0.59
1:A:164:ILE:HG21	1:A:391:THR:O	2.03	0.59
1:A:183:PHE:CD1	1:A:183:PHE:O	2.56	0.59
1:A:126:PHE:CE2	1:A:310:LYS:HD3	2.38	0.59
1:A:170:GLY:O	1:B:64:THR:CG2	2.50	0.58
1:A:273:THR:O	1:A:277:ARG:HG2	2.03	0.58
1:A:310:LYS:NZ	1:A:342:MET:HE1	2.18	0.58
1:A:401:ASP:HB2	1:A:435:ARG:HH21	1.68	0.58
1:B:321:HIS:HA	1:B:366:ILE:O	2.03	0.58
1:B:25:LEU:HD22	1:B:72:TYR:CE2	2.38	0.58
1:B:32:PRO:CB	1:B:41:THR:HG21	2.22	0.58
1:B:86:PRO:O	1:B:89:LEU:CD1	2.51	0.58
1:B:128:VAL:HG12	1:B:132:TYR:HD2	1.68	0.58
1:B:254:ASN:HB3	1:B:257:HIS:HD2	1.66	0.58
1:A:364:THR:CG2	1:A:388:VAL:HA	2.33	0.58
1:A:173:PRO:CB	1:A:207:THR:HG23	2.33	0.58
1:A:215:MET:CE	1:A:251:PHE:HE2	2.16	0.58
1:A:276:ARG:HD3	1:A:316:GLY:O	2.04	0.58
1:A:45:PHE:HD1	1:A:83:ILE:HD11	1.68	0.58
1:A:335:SER:CA	1:A:338:ALA:HB2	2.30	0.58
1:B:248:LEU:HD12	1:B:258:VAL:HG23	1.86	0.58
1:A:156:ASP:CB	1:A:387:ASN:HD22	2.05	0.58
1:A:234:ALA:HB3	1:A:240:ILE:HG12	1.86	0.58
1:B:85:TYR:CZ	1:B:108:THR:HG22	2.38	0.58
1:B:128:VAL:HB	1:B:133:ARG:HB2	1.84	0.58
1:A:143:ILE:HG12	1:A:143:ILE:O	2.04	0.58
1:A:184:TRP:O	1:A:226:LYS:HE2	2.04	0.58
1:A:234:ALA:O	1:A:240:ILE:HD11	2.05	0.57
1:A:213:ASP:O	1:A:214:ALA:C	2.47	0.57
1:B:261:LEU:HG	1:B:285:HIS:HD2	1.68	0.57
1:A:205:ARG:NH1	1:B:94:ILE:HB	2.19	0.57
1:B:71:VAL:CG1	1:B:74:VAL:HG23	2.35	0.57
1:A:103:SER:HA	1:A:106:THR:HB	1.85	0.57
1:B:179:ALA:O	1:B:182:ALA:HB3	2.04	0.57
1:B:215:MET:HE2	1:B:226:LYS:O	2.05	0.57
1:B:219:GLN:OE1	1:B:254:ASN:ND2	2.38	0.57
1:A:50:SER:OG	1:A:89:LEU:HD21	2.05	0.57
1:A:307:VAL:O	1:A:311:MET:HB2	2.04	0.57
1:B:59:THR:C	1:B:61:ASP:H	2.09	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HD3	1:A:99:ALA:HA	1.86	0.57
1:A:423:VAL:HG12	1:A:437:PHE:CZ	2.39	0.57
1:A:39:VAL:O	1:A:42:ALA:HB3	2.05	0.57
1:A:288:ARG:O	1:A:289:ALA:HB3	2.03	0.57
1:B:367:ILE:HD12	1:B:390:LEU:CD1	2.31	0.57
1:A:53:THR:H	1:B:166:LYS:CD	2.18	0.57
1:B:41:THR:CA	1:B:41:THR:CG2	2.77	0.57
1:B:292:GLY:O	1:B:293:ALA:C	2.48	0.57
1:B:364:THR:HG22	1:B:366:ILE:HG22	1.87	0.56
1:A:39:VAL:HA	1:A:42:ALA:HB3	1.87	0.56
1:B:161:VAL:HG23	1:B:411:ARG:CZ	2.35	0.56
1:A:372:ASN:HB2	1:A:440:PHE:CZ	2.41	0.56
1:B:120:TYR:HA	1:B:301:ARG:CD	2.36	0.56
1:B:165:ILE:HD13	1:B:179:ALA:HB1	1.87	0.56
1:B:194:GLU:O	1:B:263:ASP:OD2	2.23	0.56
1:B:365:PRO:HB2	1:B:388:VAL:HG12	1.87	0.56
1:A:38:TYR:O	1:A:39:VAL:C	2.49	0.56
1:A:144:SER:O	1:A:148:LYS:HG2	2.05	0.56
1:A:260:LEU:HD13	1:A:275:ALA:HB1	1.87	0.56
1:A:32:PRO:HG3	1:A:41:THR:CG2	2.36	0.56
1:A:75:ASP:O	1:A:77:ALA:N	2.39	0.56
1:A:211:VAL:HG22	1:A:251:PHE:CZ	2.41	0.56
1:A:39:VAL:HG23	1:A:74:VAL:HG21	1.88	0.56
1:A:109:MET:O	1:B:290:GLY:HA3	2.05	0.56
1:A:140:SER:OG	1:A:276:ARG:NH1	2.38	0.56
1:A:184:TRP:HH2	1:A:228:PHE:HB2	1.68	0.56
1:A:139:PRO:HG2	1:A:361:LYS:CB	2.36	0.56
1:B:120:TYR:HA	1:B:301:ARG:HG3	1.88	0.56
1:B:427:ALA:HB2	1:B:433:LEU:HG	1.88	0.56
1:A:95:THR:OG1	1:B:239:GLU:OE1	2.18	0.55
1:A:215:MET:HE3	1:A:251:PHE:HE2	1.72	0.55
1:A:277:ARG:HD2	1:B:236:ASP:CG	2.31	0.55
1:A:364:THR:O	1:A:366:ILE:HD13	2.06	0.55
1:B:32:PRO:O	1:B:33:LYS:C	2.49	0.55
1:B:231:ASN:HD22	1:B:261:LEU:HB3	1.71	0.55
1:A:92:ARG:HD2	1:A:99:ALA:HA	1.88	0.55
1:A:423:VAL:HG12	1:A:437:PHE:HZ	1.71	0.55
1:A:338:ALA:O	1:A:342:MET:HB2	2.06	0.55
1:B:14:GLU:CB	1:B:72:TYR:HE1	2.10	0.55
1:A:349:GLN:HA	1:A:354:ARG:HA	1.88	0.55
1:A:296:SER:CB	1:B:301:ARG:NH2	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ILE:HG21	1:A:435:ARG:HH12	1.72	0.55
1:B:376:MET:N	1:B:377:PRO:HD2	2.21	0.55
1:A:337:ARG:O	1:A:337:ARG:HD3	2.06	0.55
1:A:33:LYS:HA	1:A:119:GLU:OE2	2.07	0.55
1:A:184:TRP:CD1	1:A:190:ILE:HD13	2.42	0.55
1:A:248:LEU:HD22	1:A:282:ASN:ND2	2.22	0.55
1:A:374:LEU:HD11	1:A:437:PHE:CA	2.34	0.55
1:A:439:SER:HG	1:A:440:PHE:N	2.05	0.55
1:B:269:ALA:O	1:B:273:THR:OG1	2.25	0.55
1:A:192:ASN:HD21	1:A:196:GLN:HB3	1.72	0.55
1:A:411:ARG:O	1:A:414:TRP:HB3	2.07	0.55
1:B:81:THR:HG22	1:B:81:THR:O	2.07	0.55
1:A:113:GLN:HE22	1:A:301:ARG:HD2	1.72	0.54
1:A:159:LEU:HD21	1:A:376:MET:HE1	1.89	0.54
1:A:173:PRO:HB3	1:A:207:THR:HG23	1.88	0.54
1:B:130:GLU:O	1:B:131:ALA:C	2.50	0.54
1:B:162:GLY:O	1:B:183:PHE:CE1	2.60	0.54
1:A:31:LYS:HG3	1:A:79:GLU:OE2	2.08	0.54
1:A:185:LEU:CD1	1:A:221:GLU:HG2	2.37	0.54
1:A:408:ARG:O	1:A:412:GLN:CD	2.50	0.54
1:B:425:ASP:O	1:B:428:ARG:HB2	2.07	0.54
1:A:69:ALA:HA	1:A:85:TYR:HA	1.88	0.54
1:B:183:PHE:CD1	1:B:190:ILE:HD11	2.41	0.54
1:A:184:TRP:NE1	1:A:190:ILE:HD13	2.22	0.54
1:A:119:GLU:HB3	1:A:120:TYR:CD2	2.43	0.54
1:A:199:GLN:CB	1:A:200:PRO:HD2	2.37	0.54
1:B:98:LYS:HB3	1:B:135:LEU:O	2.08	0.54
1:A:405:ALA:O	1:A:409:SER:HB2	2.08	0.54
1:A:416:ALA:O	1:A:417:TRP:C	2.51	0.54
1:B:128:VAL:O	1:B:129:PRO:O	2.25	0.54
1:A:122:LYS:HD2	1:A:303:TYR:O	2.08	0.54
1:A:263:ASP:HA	1:A:287:HIS:HB3	1.90	0.54
1:A:216:ARG:NH2	1:A:254:ASN:ND2	2.56	0.53
1:A:239:GLU:O	1:A:242:ALA:HB3	2.07	0.53
1:A:301:ARG:HG3	1:A:301:ARG:HH11	1.73	0.53
1:A:310:LYS:NZ	1:A:355:GLN:HG3	2.23	0.53
1:A:376:MET:SD	1:A:380:PHE:HZ	2.26	0.53
1:A:439:SER:O	1:A:440:PHE:HA	2.06	0.53
1:B:186:GLY:O	1:B:407:ALA:HB3	2.08	0.53
1:B:310:LYS:NZ	1:B:355:GLN:NE2	2.56	0.53
1:B:322:THR:HG23	1:B:323:GLY:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:MET:HE2	1:A:118:VAL:HG23	1.91	0.53
1:B:436:ALA:O	1:B:439:SER:HB2	2.09	0.53
1:B:122:LYS:HZ2	1:B:302:GLY:HA3	1.74	0.53
1:B:128:VAL:HG21	1:B:314:LEU:HD11	1.91	0.53
1:A:272:ILE:HG13	1:A:284:LEU:HD11	1.90	0.53
1:B:248:LEU:HD12	1:B:258:VAL:CG2	2.38	0.53
1:A:168:LYS:HD2	1:A:194:GLU:OE2	2.08	0.53
1:A:211:VAL:O	1:A:214:ALA:HB3	2.08	0.53
1:B:93:ASN:HB2	1:B:96:ASP:HB3	1.90	0.53
1:B:122:LYS:HZ2	1:B:302:GLY:CA	2.22	0.53
1:B:320:ILE:N	1:B:366:ILE:HD13	2.24	0.53
1:B:444:ALA:O	1:B:451:TRP:HD1	1.91	0.53
1:A:21:GLY:CA	1:A:129:PRO:HB2	2.39	0.53
1:A:205:ARG:CZ	1:B:94:ILE:HD12	2.38	0.53
1:B:7:TYR:CD2	1:B:7:TYR:N	2.76	0.53
1:B:415:GLN:O	1:B:416:ALA:C	2.51	0.52
1:A:122:LYS:HE3	1:A:304:THR:HG22	1.90	0.52
1:A:145:ALA:O	1:A:146:LEU:HD23	2.10	0.52
1:A:386:ALA:N	1:A:387:ASN:OD1	2.39	0.52
1:B:128:VAL:C	1:B:129:PRO:O	2.53	0.52
1:B:128:VAL:CG2	1:B:355:GLN:HE22	2.13	0.52
1:B:442:GLY:HA3	1:B:445:ASP:HB2	1.91	0.52
1:A:401:ASP:HB3	1:A:405:ALA:CB	2.40	0.52
1:A:427:ALA:HB1	1:A:434:ALA:HA	1.90	0.52
1:B:409:SER:HA	1:B:412:GLN:CG	2.40	0.52
1:A:145:ALA:HA	1:A:148:LYS:CD	2.39	0.52
1:A:148:LYS:HG3	1:A:149:VAL:N	2.24	0.52
1:A:164:ILE:CA	1:A:164:ILE:HB	2.17	0.52
1:B:139:PRO:HA	1:B:316:GLY:O	2.09	0.52
1:B:143:ILE:O	1:B:144:SER:C	2.53	0.52
1:A:211:VAL:HG22	1:A:251:PHE:HZ	1.75	0.52
1:A:378:GLY:O	1:A:382:ASN:CB	2.58	0.52
1:B:139:PRO:HG3	1:B:317:ALA:O	2.09	0.52
1:B:194:GLU:HB3	1:B:287:HIS:ND1	2.23	0.52
1:A:30:MET:CE	1:A:42:ALA:HA	2.39	0.52
1:A:128:VAL:HG13	1:A:133:ARG:HB3	1.92	0.52
1:A:166:LYS:HA	1:A:167:PRO:C	2.34	0.52
1:B:147:TRP:HE3	1:B:154:GLU:HA	1.75	0.52
1:B:231:ASN:HA	1:B:261:LEU:O	2.10	0.52
1:A:172:ARG:HH22	1:B:62:ASP:HB3	1.75	0.51
1:A:361:LYS:CE	1:A:361:LYS:CG	2.87	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:PRO:HD3	1:B:202:ALA:CA	2.40	0.51
1:B:335:SER:HB2	1:B:351:PRO:CG	2.40	0.51
1:B:335:SER:HB2	1:B:351:PRO:HG3	1.93	0.51
1:A:301:ARG:HG3	1:A:301:ARG:NH1	2.25	0.51
1:B:65:ARG:HG3	1:B:65:ARG:O	2.09	0.51
1:B:349:GLN:OE1	1:B:350:GLY:O	2.29	0.51
1:B:407:ALA:HA	1:B:410:LEU:HD22	1.92	0.51
1:A:49:SER:O	1:A:107:LEU:HB3	2.10	0.51
1:A:104:PHE:CD1	1:A:104:PHE:C	2.89	0.51
1:B:6:ARG:HD2	1:B:7:TYR:H	1.75	0.51
1:B:9:ASN:HB2	1:B:70:LEU:HB2	1.92	0.51
1:B:449:PRO:O	1:B:450:GLY:C	2.53	0.51
1:A:14:GLU:HG2	1:A:18:ILE:CD1	2.32	0.51
1:A:168:LYS:N	1:B:51:THR:O	2.35	0.51
1:A:372:ASN:HD21	1:A:375:ARG:NE	2.06	0.51
1:B:192:ASN:HD21	1:B:231:ASN:HB2	1.76	0.51
1:B:308:HIS:O	1:B:311:MET:HB3	2.10	0.51
1:B:324:THR:HA	1:B:379:PHE:HE2	1.75	0.51
1:B:126:PHE:CE1	1:B:310:LYS:HG3	2.46	0.51
1:B:232:ILE:HG12	1:B:240:ILE:CD1	2.39	0.51
1:B:276:ARG:HD2	1:B:316:GLY:HA3	1.92	0.51
1:A:71:VAL:HA	1:A:82:LYS:O	2.11	0.51
1:A:243:ARG:NH1	1:B:100:MET:HE1	2.25	0.51
1:B:37:GLY:O	1:B:38:TYR:C	2.51	0.51
1:B:139:PRO:O	1:B:361:LYS:HD2	2.11	0.51
1:A:128:VAL:CG2	1:A:132:TYR:CD2	2.92	0.51
1:A:167:PRO:HD2	1:B:59:THR:HB	1.93	0.51
1:B:49:SER:HB3	1:B:85:TYR:CE1	2.46	0.51
1:B:184:TRP:CD1	1:B:226:LYS:HG3	2.46	0.51
1:B:252:GLY:O	1:B:253:GLU:C	2.52	0.51
1:A:159:LEU:HD13	1:A:380:PHE:CZ	2.46	0.50
1:A:184:TRP:CZ2	1:A:228:PHE:HB2	2.46	0.50
1:A:110:GLY:O	1:B:290:GLY:HA2	2.12	0.50
1:A:335:SER:O	1:A:338:ALA:HB3	2.11	0.50
1:A:410:LEU:O	1:A:413:ALA:HB3	2.11	0.50
1:B:241:ILE:HG13	1:B:242:ALA:N	2.26	0.50
1:B:307:VAL:O	1:B:311:MET:HB2	2.11	0.50
1:B:418:ARG:HG2	1:B:418:ARG:NH1	2.20	0.50
1:A:376:MET:O	1:A:379:PHE:N	2.35	0.50
1:A:435:ARG:O	1:A:439:SER:N	2.43	0.50
1:B:207:THR:O	1:B:211:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:VAL:HG23	1:B:408:ARG:NH2	2.26	0.50
1:A:310:LYS:HG3	1:A:357:TRP:CH2	2.47	0.50
1:A:367:ILE:HG22	1:A:390:LEU:HD12	1.94	0.50
1:B:46:ALA:O	1:B:50:SER:OG	2.21	0.50
1:B:49:SER:HB3	1:B:85:TYR:HE1	1.76	0.50
1:B:403:PRO:O	1:B:406:GLY:N	2.42	0.50
1:A:27:ALA:HB2	1:A:353:TYR:OH	2.11	0.50
1:A:141:VAL:HG22	1:A:145:ALA:HB1	1.94	0.50
1:A:372:ASN:ND2	1:A:440:PHE:CE1	2.80	0.50
1:A:15:GLU:O	1:A:18:ILE:HG22	2.12	0.49
1:A:161:VAL:HG12	1:A:390:LEU:HB3	1.93	0.49
1:A:308:HIS:O	1:A:312:ALA:HB2	2.11	0.49
1:B:14:GLU:CB	1:B:72:TYR:CE1	2.90	0.49
1:B:247:VAL:O	1:B:251:PHE:HB2	2.12	0.49
1:B:54:ASN:O	1:B:55:VAL:HG23	2.12	0.49
1:B:93:ASN:ND2	1:B:96:ASP:OD2	2.37	0.49
1:B:393:GLY:HA2	1:B:397:PHE:CD1	2.47	0.49
1:B:208:ILE:HG22	1:B:250:THR:HG21	1.95	0.49
1:A:309:CYS:HB3	1:A:320:ILE:HG21	1.94	0.49
1:A:422:PRO:O	1:A:425:ASP:HB2	2.13	0.49
1:B:252:GLY:O	1:B:254:ASN:N	2.45	0.49
1:B:436:ALA:O	1:B:439:SER:N	2.42	0.49
1:A:116:GLY:O	1:A:117:ASP:CB	2.54	0.49
1:B:163:THR:HG22	1:B:190:ILE:HG13	1.93	0.49
1:A:128:VAL:HG22	1:A:132:TYR:HD2	1.75	0.49
1:A:372:ASN:ND2	1:A:375:ARG:HH21	2.10	0.49
1:B:400:ILE:HD13	1:B:438:GLU:O	2.13	0.49
1:B:433:LEU:HG	1:B:433:LEU:O	2.12	0.49
1:A:94:ILE:HD13	1:B:243:ARG:HA	1.94	0.49
1:B:126:PHE:CZ	1:B:310:LYS:HG3	2.47	0.49
1:B:409:SER:HA	1:B:412:GLN:HG3	1.94	0.49
1:A:139:PRO:HD3	1:A:316:GLY:HA2	1.95	0.49
1:A:142:ASN:CG	1:A:361:LYS:NZ	2.70	0.49
1:A:323:GLY:HA3	1:A:368:SER:OG	2.13	0.49
1:A:341:TYR:O	1:A:345:GLN:HG3	2.13	0.49
1:B:266:VAL:HG13	1:B:289:ALA:HB3	1.94	0.49
1:A:169:LEU:HD21	1:A:195:PRO:HG2	1.94	0.48
1:B:194:GLU:HB3	1:B:287:HIS:CE1	2.48	0.48
1:B:241:ILE:HA	1:B:279:PHE:CZ	2.48	0.48
1:B:379:PHE:CE1	1:B:383:LEU:HD22	2.47	0.48
1:A:6:ARG:NH2	1:A:51:THR:CG2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:HG2	1:A:134:ALA:N	2.24	0.48
1:B:8:VAL:HG13	1:B:9:ASN:H	1.78	0.48
1:B:168:LYS:HZ1	1:B:194:GLU:CD	2.21	0.48
1:B:216:ARG:HG3	1:B:216:ARG:HH11	1.77	0.48
1:A:112:ASN:HA	1:A:115:MET:HG3	1.95	0.48
1:A:30:MET:HE1	1:A:42:ALA:HA	1.96	0.48
1:A:379:PHE:O	1:A:380:PHE:C	2.56	0.48
1:B:44:HIS:ND1	1:B:44:HIS:C	2.69	0.48
1:B:398:GLY:HA3	1:B:440:PHE:HZ	1.78	0.48
1:A:168:LYS:NZ	1:B:48:GLU:HG3	2.28	0.48
1:B:29:ILE:HB	1:B:124:HIS:CD2	2.49	0.48
1:B:239:GLU:OE2	1:B:243:ARG:HD2	2.13	0.48
1:A:238:PHE:HE2	1:B:278:ARG:HD3	1.78	0.48
1:A:371:MET:O	1:A:395:GLY:HA3	2.13	0.48
1:B:89:LEU:HD12	1:B:89:LEU:N	2.21	0.48
1:B:338:ALA:O	1:B:341:TYR:HB2	2.14	0.48
1:A:128:VAL:HG12	1:A:355:GLN:OE1	2.13	0.48
1:A:182:ALA:HA	1:A:185:LEU:HD22	1.94	0.48
1:A:301:ARG:HH21	1:B:296:SER:CB	2.26	0.48
1:A:335:SER:C	1:A:338:ALA:HB3	2.38	0.48
1:A:369:GLY:O	1:A:371:MET:N	2.43	0.48
1:B:6:ARG:HG3	1:B:53:THR:HG21	1.96	0.48
1:B:29:ILE:O	1:B:122:LYS:N	2.46	0.48
1:B:364:THR:O	1:B:366:ILE:HG23	2.14	0.48
1:A:303:TYR:CE1	1:A:308:HIS:HB2	2.48	0.47
1:B:30:MET:HG2	1:B:118:VAL:HG13	1.95	0.47
1:B:146:LEU:O	1:B:147:TRP:C	2.57	0.47
1:A:159:LEU:HD13	1:A:380:PHE:HZ	1.79	0.47
1:A:167:PRO:CD	1:B:59:THR:HB	2.44	0.47
1:A:237:PRO:HA	1:A:240:ILE:HB	1.97	0.47
1:A:324:THR:C	2:A:518:HOH:O	2.56	0.47
1:B:140:SER:O	1:B:361:LYS:HE3	2.14	0.47
1:B:404:VAL:CG2	1:B:408:ARG:HH21	2.26	0.47
1:A:45:PHE:CD1	1:A:83:ILE:HD11	2.48	0.47
1:A:109:MET:HE2	1:A:303:TYR:CB	2.19	0.47
1:A:141:VAL:HG22	1:A:145:ALA:HB3	1.95	0.47
1:A:163:THR:CB	1:A:183:PHE:CZ	2.96	0.47
1:A:410:LEU:O	1:A:411:ARG:C	2.57	0.47
1:B:174:LYS:O	1:B:175:PRO:C	2.56	0.47
1:B:283:PHE:HE1	1:B:285:HIS:ND1	2.12	0.47
1:B:298:GLN:HA	1:B:298:GLN:HE21	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:PHE:HB2	1:B:335:SER:O	2.13	0.47
1:A:44:HIS:CE1	1:A:115:MET:HE3	2.50	0.47
1:A:208:ILE:CG2	1:A:247:VAL:HG13	2.44	0.47
1:A:106:THR:O	1:A:110:GLY:HA3	2.14	0.47
1:A:273:THR:CG2	1:B:236:ASP:HB2	2.43	0.47
1:B:199:GLN:HB3	1:B:200:PRO:CD	2.44	0.47
1:B:205:ARG:HB3	1:B:246:TYR:CZ	2.49	0.47
1:B:241:ILE:O	1:B:245:GLU:N	2.47	0.47
1:B:29:ILE:O	1:B:121:ALA:HA	2.15	0.47
1:B:41:THR:CA	1:B:41:THR:HB	2.19	0.47
1:A:238:PHE:HA	1:A:241:ILE:HB	1.96	0.47
1:A:295:THR:HG23	1:A:305:ALA:N	2.29	0.47
1:A:365:PRO:CD	1:A:388:VAL:HG12	2.41	0.47
1:B:120:TYR:HB2	1:B:300:LYS:O	2.15	0.47
1:B:189:PHE:O	1:B:190:ILE:HD12	2.15	0.47
1:B:244:GLY:O	1:B:248:LEU:HD22	2.14	0.47
1:A:92:ARG:HG3	1:A:93:ASN:N	2.23	0.47
1:A:101:ILE:O	1:A:102:ALA:C	2.57	0.47
1:A:313:ARG:HB3	1:A:363:CYS:HB3	1.97	0.47
1:A:376:MET:SD	1:A:380:PHE:CE2	3.08	0.47
1:B:371:MET:HE1	1:B:379:PHE:HB2	1.97	0.47
1:A:72:TYR:CE1	1:A:84:ALA:HB2	2.49	0.47
1:A:310:LYS:HG3	1:A:357:TRP:HH2	1.80	0.47
1:B:192:ASN:ND2	1:B:231:ASN:H	1.98	0.47
1:B:366:ILE:HG21	1:B:389:ILE:HD12	1.95	0.47
1:A:194:GLU:HG2	1:A:287:HIS:HE1	1.80	0.47
1:A:349:GLN:HG2	1:A:350:GLY:N	2.30	0.47
1:A:44:HIS:ND1	1:A:115:MET:HE3	2.30	0.46
1:A:167:PRO:CG	1:B:59:THR:HB	2.44	0.46
1:A:342:MET:SD	1:A:357:TRP:HZ2	2.38	0.46
1:B:161:VAL:HG11	1:B:410:LEU:HD23	1.97	0.46
1:B:264:GLY:HA3	1:B:272:ILE:HD11	1.96	0.46
1:B:431:LYS:O	1:B:432:GLU:C	2.57	0.46
1:A:181:HIS:O	1:A:185:LEU:HB3	2.14	0.46
1:B:48:GLU:HB2	1:B:115:MET:HE2	1.96	0.46
1:B:211:VAL:CG2	1:B:212:ALA:N	2.78	0.46
1:B:393:GLY:HA2	1:B:397:PHE:CE1	2.50	0.46
1:A:181:HIS:HA	1:A:184:TRP:HB2	1.97	0.46
1:A:204:LEU:HD21	1:A:243:ARG:HG2	1.98	0.46
1:B:109:MET:HE3	1:B:303:TYR:CD2	2.50	0.46
1:B:184:TRP:CZ2	1:B:215:MET:HE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:CA	1:A:164:ILE:CG1	2.83	0.46
1:A:379:PHE:CD1	1:A:379:PHE:C	2.93	0.46
1:B:357:TRP:O	1:B:360:MET:N	2.48	0.46
1:B:78:ARG:O	1:B:78:ARG:CG	2.62	0.46
1:B:165:ILE:CD1	1:B:171:LEU:HD11	2.46	0.46
1:A:119:GLU:O	1:A:301:ARG:NH1	2.49	0.46
1:A:125:ASP:OD2	1:A:353:TYR:HD2	1.99	0.46
1:A:208:ILE:HG21	1:A:247:VAL:HG13	1.97	0.46
1:A:262:VAL:HG11	1:A:272:ILE:HD12	1.98	0.46
1:B:55:VAL:HG22	2:B:495:HOH:O	2.14	0.46
1:B:147:TRP:O	1:B:148:LYS:C	2.58	0.46
1:B:209:ALA:HB2	1:B:246:TYR:OH	2.16	0.46
1:A:194:GLU:O	1:A:263:ASP:OD2	2.33	0.46
1:A:306:PHE:HZ	1:A:342:MET:HE3	1.80	0.46
1:B:184:TRP:CG	1:B:226:LYS:HG3	2.51	0.46
1:A:172:ARG:CB	1:A:175:PRO:HG2	2.40	0.46
1:B:30:MET:SD	1:B:30:MET:C	2.99	0.46
1:B:204:LEU:O	1:B:208:ILE:HB	2.16	0.46
1:B:323:GLY:N	1:B:367:ILE:HG22	2.31	0.46
1:B:426:TYR:O	1:B:430:HIS:NE2	2.48	0.46
1:A:39:VAL:CG2	1:A:74:VAL:HG21	2.45	0.46
1:A:322:THR:HB	1:A:365:PRO:HB3	1.97	0.46
1:B:258:VAL:O	1:B:282:ASN:OD1	2.34	0.46
1:B:380:PHE:CE2	1:B:414:TRP:HB2	2.51	0.46
1:A:100:MET:HE2	1:B:234:ALA:HA	1.98	0.46
1:A:164:ILE:CB	1:A:164:ILE:HA	2.18	0.46
1:A:177:ALA:O	1:A:178:GLU:C	2.59	0.46
1:A:183:PHE:HD1	1:A:190:ILE:HD11	1.80	0.46
1:B:148:LYS:HG3	1:B:154:GLU:CG	2.43	0.46
1:A:150:LEU:HD11	1:A:227:LEU:CD1	2.46	0.45
1:A:184:TRP:O	1:A:226:LYS:NZ	2.48	0.45
1:B:239:GLU:OE2	1:B:243:ARG:NE	2.45	0.45
1:B:399:HIS:HB2	1:B:406:GLY:HA2	1.98	0.45
1:B:31:LYS:O	1:B:119:GLU:HB3	2.16	0.45
1:B:401:ASP:OD2	1:B:435:ARG:HD3	2.16	0.45
1:A:170:GLY:HA2	1:B:67:VAL:HG11	1.97	0.45
1:A:218:ALA:O	1:A:221:GLU:N	2.49	0.45
1:B:37:GLY:O	1:B:40:ALA:N	2.49	0.45
1:B:93:ASN:O	1:B:97:GLY:HA2	2.16	0.45
1:B:163:THR:HG23	1:B:164:ILE:N	2.31	0.45
1:B:291:HIS:O	1:B:292:GLY:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:PHE:HE2	1:B:414:TRP:HB2	1.81	0.45
1:A:164:ILE:N	1:A:164:ILE:CG2	2.80	0.45
1:B:15:GLU:HA	1:B:18:ILE:HB	1.99	0.45
1:A:232:ILE:CD1	1:A:260:LEU:HD22	2.46	0.45
1:B:304:THR:O	1:B:307:VAL:N	2.50	0.45
1:A:291:HIS:O	1:A:293:ALA:N	2.49	0.45
1:B:453:LYS:HD2	1:B:453:LYS:N	2.32	0.45
1:A:95:THR:HB	1:A:96:ASP:H	1.61	0.45
1:A:147:TRP:CH2	1:A:156:ASP:HA	2.52	0.45
1:A:371:MET:HE1	1:A:379:PHE:CD2	2.32	0.45
1:A:371:MET:CE	1:A:379:PHE:HD2	2.21	0.45
1:B:47:ALA:O	1:B:52:GLY:HA2	2.17	0.45
1:B:403:PRO:O	1:B:404:VAL:C	2.60	0.45
1:B:444:ALA:O	1:B:451:TRP:CD1	2.70	0.45
1:A:150:LEU:HD11	1:A:227:LEU:HD11	1.99	0.45
1:A:228:PHE:O	1:A:258:VAL:HG12	2.16	0.45
1:B:143:ILE:HG22	1:B:364:THR:OG1	2.15	0.45
1:B:232:ILE:HD13	1:B:262:VAL:CG1	2.46	0.45
1:B:44:HIS:O	1:B:47:ALA:N	2.35	0.45
1:B:217:ARG:O	1:B:221:GLU:CG	2.63	0.45
1:B:223:GLY:O	1:B:224:GLU:HG3	2.17	0.45
1:B:349:GLN:HA	1:B:354:ARG:HA	1.97	0.45
1:B:365:PRO:HG2	1:B:388:VAL:HG12	1.98	0.45
1:A:291:HIS:O	1:A:294:VAL:HG12	2.17	0.45
1:A:412:GLN:HA	1:A:415:GLN:HB2	1.98	0.45
1:B:183:PHE:HD2	1:B:403:PRO:HB3	1.81	0.45
1:A:127:TYR:HB2	1:A:353:TYR:HB3	1.99	0.44
1:B:101:ILE:HG23	1:B:105:LEU:CD1	2.47	0.44
1:B:216:ARG:HH22	1:B:254:ASN:HB2	1.82	0.44
1:A:383:LEU:O	1:A:383:LEU:HG	2.17	0.44
1:A:402:GLY:O	1:A:405:ALA:N	2.50	0.44
1:A:219:GLN:HB3	1:A:224:GLU:O	2.16	0.44
1:A:291:HIS:NE2	2:A:486:HOH:O	2.36	0.44
1:A:94:ILE:HD13	1:A:94:ILE:HG21	1.75	0.44
1:A:106:THR:HG21	1:B:195:PRO:HA	2.00	0.44
1:A:292:GLY:HA2	1:A:295:THR:O	2.18	0.44
1:B:75:ASP:OD2	1:B:78:ARG:NH1	2.50	0.44
1:B:251:PHE:O	1:B:252:GLY:C	2.61	0.44
1:B:346:ASP:HA	1:B:357:TRP:HB2	1.98	0.44
1:B:374:LEU:O	1:B:448:TYR:CE2	2.66	0.44
1:A:146:LEU:HD22	1:A:227:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:CYS:HA	1:A:312:ALA:CB	2.47	0.44
1:B:6:ARG:HB3	1:B:7:TYR:CE2	2.53	0.44
1:B:130:GLU:HG2	1:B:130:GLU:H	1.18	0.44
1:B:416:ALA:HB2	1:B:426:TYR:CD2	2.52	0.44
1:A:159:LEU:HD22	1:A:380:PHE:CZ	2.53	0.44
1:A:229:SER:CB	1:A:261:LEU:HD23	2.45	0.44
1:B:172:ARG:CB	1:B:173:PRO:CD	2.93	0.44
1:B:203:PRO:O	1:B:204:LEU:C	2.59	0.44
1:B:365:PRO:HG2	1:B:388:VAL:CG1	2.48	0.44
1:A:101:ILE:HG12	1:A:136:PHE:CE1	2.52	0.44
1:A:440:PHE:HA	1:A:441:PRO:HD3	1.88	0.44
1:B:142:ASN:HB2	1:B:144:SER:H	1.82	0.44
1:A:89:LEU:O	1:B:199:GLN:NE2	2.41	0.44
1:A:184:TRP:CD1	1:A:226:LYS:HB3	2.52	0.44
1:A:303:TYR:CD1	1:A:308:HIS:HB2	2.53	0.44
1:A:335:SER:C	1:A:338:ALA:CB	2.91	0.44
1:A:364:THR:HA	1:A:365:PRO:HD3	1.82	0.44
1:B:239:GLU:O	1:B:243:ARG:HD2	2.17	0.44
1:A:184:TRP:CE2	1:A:226:LYS:HB3	2.53	0.44
1:A:400:ILE:HG13	1:A:439:SER:HB3	1.99	0.44
1:B:165:ILE:HD11	1:B:171:LEU:HD11	1.99	0.44
1:B:262:VAL:O	1:B:287:HIS:N	2.46	0.44
1:A:147:TRP:CZ3	1:A:156:ASP:HA	2.53	0.43
1:A:174:LYS:N	1:A:175:PRO:HD2	2.33	0.43
1:A:241:ILE:HG22	1:A:242:ALA:N	2.33	0.43
1:B:75:ASP:HB3	1:B:78:ARG:HB3	2.00	0.43
1:B:166:LYS:HA	1:B:167:PRO:HA	1.58	0.43
1:B:285:HIS:CE1	1:B:366:ILE:HD12	2.53	0.43
1:B:337:ARG:O	1:B:337:ARG:HG2	2.18	0.43
1:B:376:MET:O	1:B:379:PHE:HB3	2.18	0.43
1:A:103:SER:HA	1:A:106:THR:CB	2.47	0.43
1:A:156:ASP:CB	1:A:387:ASN:ND2	2.63	0.43
1:A:227:LEU:HD23	1:A:257:HIS:HA	1.99	0.43
1:A:371:MET:HE3	1:A:371:MET:HB2	1.75	0.43
1:A:400:ILE:CG2	1:A:435:ARG:HH12	2.30	0.43
1:B:109:MET:HE3	1:B:303:TYR:HD2	1.83	0.43
1:B:241:ILE:O	1:B:245:GLU:HB2	2.18	0.43
1:A:119:GLU:O	1:A:120:TYR:HB3	2.18	0.43
1:A:125:ASP:HB3	1:A:353:TYR:CE2	2.53	0.43
1:A:194:GLU:HG2	1:A:287:HIS:CE1	2.53	0.43
1:A:440:PHE:CD1	1:A:440:PHE:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ARG:HA	1:B:202:ALA:HB2	2.00	0.43
1:B:421:VAL:HA	1:B:422:PRO:HD3	1.91	0.43
1:A:208:ILE:HA	1:A:211:VAL:CG1	2.43	0.43
1:B:310:LYS:HZ2	1:B:355:GLN:NE2	2.16	0.43
1:B:376:MET:SD	1:B:380:PHE:CE2	3.11	0.43
1:A:233:THR:OG1	1:A:262:VAL:HA	2.18	0.43
1:A:272:ILE:HG21	1:A:315:GLN:NE2	2.33	0.43
1:B:101:ILE:HG12	1:B:136:PHE:CE1	2.54	0.43
1:B:147:TRP:CE3	1:B:154:GLU:HA	2.53	0.43
1:B:404:VAL:HG23	1:B:408:ARG:HH21	1.83	0.43
1:B:440:PHE:O	1:B:441:PRO:C	2.61	0.43
1:A:184:TRP:O	1:A:226:LYS:CE	2.66	0.43
1:B:7:TYR:HH	1:B:51:THR:HB	1.76	0.43
1:B:121:ALA:O	1:B:301:ARG:HA	2.19	0.43
1:B:313:ARG:HD3	1:B:357:TRP:CZ3	2.54	0.43
1:A:6:ARG:HH21	1:A:51:THR:HG22	1.82	0.43
1:A:127:TYR:O	1:A:129:PRO:HD3	2.18	0.43
1:A:176:PHE:O	1:A:179:ALA:N	2.52	0.43
1:A:387:ASN:OD1	1:A:387:ASN:N	2.52	0.43
1:A:399:HIS:ND1	1:A:400:ILE:N	2.67	0.43
1:B:448:TYR:HA	1:B:449:PRO:HD2	1.69	0.43
1:A:173:PRO:HG3	1:A:202:ALA:HA	1.99	0.43
1:A:216:ARG:O	1:A:220:ASP:OD1	2.37	0.43
1:A:244:GLY:HA3	1:A:279:PHE:CE2	2.54	0.43
1:B:386:ALA:HB2	1:B:417:TRP:CZ3	2.54	0.43
1:B:408:ARG:O	1:B:412:GLN:HG2	2.18	0.43
1:B:422:PRO:O	1:B:423:VAL:C	2.59	0.43
1:A:93:ASN:HA	1:B:239:GLU:CD	2.44	0.42
1:A:109:MET:HB3	1:A:113:GLN:HG3	2.01	0.42
1:A:272:ILE:HG21	1:A:315:GLN:CG	2.48	0.42
1:A:320:ILE:HG12	1:A:321:HIS:H	1.85	0.42
1:A:324:THR:HG21	1:A:336:ASP:CB	2.37	0.42
1:B:118:VAL:HG12	1:B:119:GLU:N	2.34	0.42
1:B:323:GLY:H	1:B:367:ILE:HG22	1.83	0.42
1:B:440:PHE:HA	1:B:441:PRO:HD2	1.65	0.42
1:A:7:TYR:CE2	1:A:47:ALA:HB2	2.54	0.42
1:A:152:ARG:HB3	1:A:153:PRO:HD2	2.02	0.42
1:A:376:MET:HE2	1:A:390:LEU:HD22	2.02	0.42
1:A:320:ILE:O	1:A:366:ILE:HG12	2.19	0.42
1:B:24:VAL:HG21	1:B:90:PHE:CE2	2.54	0.42
1:B:126:PHE:CE1	1:B:307:VAL:HG13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ARG:HH11	1:B:288:ARG:HD3	1.60	0.42
1:B:181:HIS:HA	1:B:184:TRP:HE3	1.85	0.42
1:B:452:ARG:O	1:B:456:GLY:O	2.36	0.42
1:B:5:SER:O	1:B:6:ARG:HB2	2.20	0.42
1:B:14:GLU:HG3	1:B:72:TYR:OH	2.20	0.42
1:B:366:ILE:CG2	1:B:389:ILE:HD12	2.49	0.42
1:A:52:GLY:HA3	1:B:166:LYS:NZ	2.35	0.42
1:A:313:ARG:CB	1:A:363:CYS:HB3	2.49	0.42
1:B:127:TYR:HE1	1:B:355:GLN:HA	1.85	0.42
1:B:306:PHE:HA	1:B:339:ILE:CD1	2.50	0.42
1:B:336:ASP:HA	1:B:339:ILE:HG13	2.01	0.42
1:A:98:LYS:C	1:A:99:ALA:O	2.60	0.42
1:B:71:VAL:CG1	1:B:74:VAL:CG2	2.94	0.42
1:A:73:GLU:HB3	1:A:82:LYS:HD3	2.02	0.42
1:A:122:LYS:HB3	1:A:124:HIS:HE1	1.85	0.42
1:A:128:VAL:HG13	1:A:133:ARG:CB	2.49	0.42
1:A:408:ARG:O	1:A:412:GLN:NE2	2.53	0.42
1:B:152:ARG:HA	1:B:153:PRO:HD2	1.82	0.42
1:B:161:VAL:HG23	1:B:411:ARG:NH2	2.34	0.42
1:B:365:PRO:CB	1:B:388:VAL:HG12	2.50	0.42
1:B:393:GLY:O	1:B:397:PHE:HD1	2.03	0.42
1:B:409:SER:HA	1:B:412:GLN:HG2	2.02	0.42
1:A:248:LEU:HD23	1:A:258:VAL:HG21	2.00	0.41
1:A:296:SER:CB	1:B:301:ARG:HH21	2.33	0.41
1:B:9:ASN:O	1:B:12:LEU:HB2	2.20	0.41
1:B:94:ILE:HG13	1:B:95:THR:N	2.34	0.41
1:B:96:ASP:OD2	1:B:98:LYS:HB2	2.20	0.41
1:B:298:GLN:OE1	1:B:300:LYS:HD2	2.20	0.41
1:A:12:LEU:HD23	1:A:12:LEU:O	2.20	0.41
1:B:90:PHE:CD1	1:B:107:LEU:HD13	2.55	0.41
1:B:160:VAL:HG23	1:B:189:PHE:HB2	2.02	0.41
1:B:172:ARG:C	1:B:175:PRO:HD2	2.46	0.41
1:B:193:ASN:O	1:B:196:GLN:HB2	2.20	0.41
1:A:400:ILE:HB	1:A:435:ARG:CZ	2.50	0.41
1:B:216:ARG:NH1	1:B:216:ARG:CG	2.82	0.41
1:B:338:ALA:O	1:B:339:ILE:C	2.63	0.41
1:B:444:ALA:HA	1:B:448:TYR:HB2	2.02	0.41
1:A:181:HIS:ND1	1:A:181:HIS:C	2.79	0.41
1:A:199:GLN:HB3	1:A:200:PRO:CD	2.48	0.41
1:A:263:ASP:CG	1:B:106:THR:HG21	2.46	0.41
1:B:306:PHE:CE1	1:B:342:MET:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:CG	1:A:93:ASN:N	2.83	0.41
1:A:371:MET:CG	1:A:376:MET:HG3	2.51	0.41
1:A:401:ASP:CB	1:A:405:ALA:HB2	2.44	0.41
1:B:70:LEU:HD12	1:B:70:LEU:H	1.85	0.41
1:A:215:MET:CE	1:A:251:PHE:CE2	3.01	0.41
1:A:335:SER:CB	1:A:338:ALA:HB1	2.20	0.41
1:A:106:THR:CG2	1:A:107:LEU:HD12	2.46	0.41
1:A:113:GLN:NE2	1:A:113:GLN:HA	2.34	0.41
1:B:33:LYS:HE2	1:B:116:GLY:O	2.20	0.41
1:B:109:MET:HE2	1:B:109:MET:HB2	1.89	0.41
1:A:274:THR:HB	1:B:237:PRO:CD	2.51	0.41
1:A:295:THR:CG2	1:A:305:ALA:CB	2.94	0.41
1:A:318:SER:O	1:A:363:CYS:HA	2.21	0.41
1:B:355:GLN:HG3	1:B:356:SER:H	1.83	0.41
1:B:443:ASP:O	1:B:447:ILE:HB	2.20	0.41
1:A:100:MET:CE	1:B:234:ALA:HA	2.51	0.41
1:A:236:ASP:OD2	1:B:277:ARG:NH1	2.54	0.41
1:A:237:PRO:O	1:A:241:ILE:CD1	2.63	0.41
1:A:439:SER:C	1:A:440:PHE:CB	2.91	0.41
2:A:502:HOH:O	1:B:235:ASP:HB2	2.21	0.41
1:B:41:THR:O	1:B:44:HIS:HB3	2.20	0.41
1:B:78:ARG:HH11	1:B:78:ARG:CB	2.34	0.41
1:B:403:PRO:HB2	1:B:404:VAL:H	1.51	0.41
1:A:127:TYR:HB2	1:A:353:TYR:CB	2.52	0.40
1:A:299:SER:HB2	1:B:301:ARG:HH22	1.87	0.40
1:B:45:PHE:HA	1:B:115:MET:CE	2.39	0.40
1:B:48:GLU:CB	1:B:115:MET:HE2	2.51	0.40
1:B:199:GLN:HB3	1:B:200:PRO:HD2	2.02	0.40
1:A:51:THR:O	1:A:53:THR:N	2.54	0.40
1:A:203:PRO:O	1:A:204:LEU:C	2.63	0.40
1:A:381:GLU:OE1	1:A:381:GLU:HA	2.21	0.40
1:B:67:VAL:O	1:B:89:LEU:HG	2.21	0.40
1:B:186:GLY:HA3	1:B:404:VAL:O	2.21	0.40
1:B:212:ALA:O	1:B:216:ARG:NH1	2.54	0.40
1:B:243:ARG:O	1:B:247:VAL:HG23	2.21	0.40
1:B:146:LEU:HD23	1:B:227:LEU:HD13	2.03	0.40
1:B:400:ILE:HD13	1:B:439:SER:HA	2.03	0.40
1:A:30:MET:O	1:A:79:GLU:O	2.39	0.40
1:A:181:HIS:CD2	1:A:217:ARG:NH1	2.89	0.40
1:A:175:PRO:O	1:A:176:PHE:O	2.39	0.40
1:A:309:CYS:CB	1:A:320:ILE:HG21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ASP:HB2	1:B:351:PRO:HB2	2.03	0.40
1:B:301:ARG:NH1	1:B:301:ARG:CB	2.77	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASP:OD1	1:B:60:THR:O[2_646]	1.73	0.47
1:A:358:GLY:O	1:A:431:LYS:CB[2_646]	1.97	0.23
1:B:172:ARG:NH1	1:B:419:ASP:OD1[2_745]	2.17	0.03

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 X-ray entries followed by that with respect to entries of similar resolution.

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	411/466 (88%)	303 (74%)	71 (17%)	37 (9%)	0	0
1	B	439/466 (94%)	328 (75%)	75 (17%)	36 (8%)	0	0
All	All	850/932 (91%)	631 (74%)	146 (17%)	73 (9%)	0	0

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	95	THR
1	A	130	GLU
1	A	155	VAL
1	A	188	ASP
1	A	207	THR
1	A	289	ALA
1	A	292	GLY
1	A	345	GLN

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Mol	Chain	Res	Type
1	A	370	GLY
1	A	417	TRP
1	A	423	VAL
1	B	6	ARG
1	B	7	TYR
1	B	8	VAL
1	B	10	LEU
1	B	34	ALA
1	B	55	VAL
1	B	57	VAL
1	B	59	THR
1	B	63	PHE
1	B	88	ALA
1	B	96	ASP
1	B	129	PRO
1	B	155	VAL
1	B	253	GLU
1	B	293	ALA
1	B	347	GLU
1	B	358	GLY
1	B	423	VAL
1	B	441	PRO
1	B	454	ALA
1	B	455	LEU
1	A	52	GLY
1	A	54	ASN
1	A	66	GLY
1	A	102	ALA
1	A	115	MET
1	A	117	ASP
1	A	138	GLY
1	A	158	GLY
1	A	252	GLY
1	A	264	GLY
1	A	310	LYS
1	A	373	ALA
1	A	434	ALA
1	B	54	ASN
1	B	177	ALA
1	B	302	GLY
1	B	404	VAL
1	B	419	ASP

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Mol	Chain	Res	Type
1	B	450	GLY
1	A	104	PHE
1	A	156	ASP
1	A	176	PHE
1	A	291	HIS
1	A	316	GLY
1	A	415	GLN
1	B	131	ALA
1	B	340	ALA
1	B	403	PRO
1	A	39	VAL
1	A	146	LEU
1	A	416	ALA
1	B	112	ASN
1	A	214	ALA
1	B	76	GLU
1	B	194	GLU
1	B	290	GLY
1	A	206	ASP
1	B	339	ILE
1	B	252	GLY
1	A	388	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	317/354 (90%)	188 (59%)	129 (41%)	0	0
1	B	335/354 (95%)	206 (62%)	129 (38%)	0	0
All	All	652/708 (92%)	394 (60%)	258 (40%)	0	0

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER

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Mol	Chain	Res	Type
1	A	6	ARG
1	A	10	LEU
1	A	12	LEU
1	A	16	ASP
1	A	18	ILE
1	A	25	LEU
1	A	29	ILE
1	A	31	LYS
1	A	41	THR
1	A	45	PHE
1	A	48	GLU
1	A	50	SER
1	A	54	ASN
1	A	55	VAL
1	A	65	ARG
1	A	67	VAL
1	A	68	ASP
1	A	74	VAL
1	A	78	ARG
1	A	79	GLU
1	A	80	LEU
1	A	87	VAL
1	A	94	ILE
1	A	95	THR
1	A	96	ASP
1	A	100	MET
1	A	101	ILE
1	A	107	LEU
1	A	111	ASN
1	A	117	ASP
1	A	119	GLU
1	A	123	MET
1	A	130	GLU
1	A	133	ARG
1	A	137	ASP
1	A	141	VAL
1	A	143	ILE
1	A	144	SER
1	A	148	LYS
1	A	149	VAL
1	A	150	LEU
1	A	152	ARG

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Mol	Chain	Res	Type
1	A	156	ASP
1	A	160	VAL
1	A	161	VAL
1	A	163	THR
1	A	164	ILE
1	A	166	LYS
1	A	172	ARG
1	A	175	PRO
1	A	178	GLU
1	A	181	HIS
1	A	184	TRP
1	A	185	LEU
1	A	191	LYS
1	A	192	ASN
1	A	193	ASN
1	A	194	GLU
1	A	201	PHE
1	A	204	LEU
1	A	205	ARG
1	A	207	THR
1	A	210	LEU
1	A	211	VAL
1	A	216	ARG
1	A	219	GLN
1	A	220	ASP
1	A	221	GLU
1	A	229	SER
1	A	232	ILE
1	A	235	ASP
1	A	236	ASP
1	A	240	ILE
1	A	241	ILE
1	A	248	LEU
1	A	253	GLU
1	A	256	SER
1	A	257	HIS
1	A	258	VAL
1	A	260	LEU
1	A	261	LEU
1	A	263	ASP
1	A	266	VAL
1	A	272	ILE

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Mol	Chain	Res	Type
1	A	274	THR
1	A	276	ARG
1	A	279	PHE
1	A	298	GLN
1	A	300	LYS
1	A	307	VAL
1	A	309	CYS
1	A	310	LYS
1	A	311	MET
1	A	313	ARG
1	A	314	LEU
1	A	315	GLN
1	A	321	HIS
1	A	324	THR
1	A	336	ASP
1	A	337	ARG
1	A	342	MET
1	A	343	LEU
1	A	344	THR
1	A	345	GLN
1	A	355	GLN
1	A	363	CYS
1	A	364	THR
1	A	366	ILE
1	A	367	ILE
1	A	368	SER
1	A	371	MET
1	A	372	ASN
1	A	374	LEU
1	A	375	ARG
1	A	376	MET
1	A	379	PHE
1	A	387	ASN
1	A	390	LEU
1	A	400	ILE
1	A	401	ASP
1	A	409	SER
1	A	410	LEU
1	A	411	ARG
1	A	415	GLN
1	A	424	LEU
1	A	431	LYS

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Mol	Chain	Res	Type
1	A	432	GLU
1	A	438	GLU
1	B	5	SER
1	B	6	ARG
1	B	8	VAL
1	B	9	ASN
1	B	12	LEU
1	B	14	GLU
1	B	16	ASP
1	B	18	ILE
1	B	29	ILE
1	B	33	LYS
1	B	48	GLU
1	B	50	SER
1	B	53	THR
1	B	56	GLU
1	B	57	VAL
1	B	59	THR
1	B	61	ASP
1	B	62	ASP
1	B	64	THR
1	B	65	ARG
1	B	67	VAL
1	B	70	LEU
1	B	73	GLU
1	B	76	GLU
1	B	78	ARG
1	B	79	GLU
1	B	87	VAL
1	B	89	LEU
1	B	92	ARG
1	B	100	MET
1	B	101	ILE
1	B	103	SER
1	B	106	THR
1	B	107	LEU
1	B	109	MET
1	B	112	ASN
1	B	113	GLN
1	B	119	GLU
1	B	122	LYS
1	B	128	VAL

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Mol	Chain	Res	Type
1	B	130	GLU
1	B	144	SER
1	B	148	LYS
1	B	154	GLU
1	B	155	VAL
1	B	160	VAL
1	B	161	VAL
1	B	163	THR
1	B	164	ILE
1	B	165	ILE
1	B	166	LYS
1	B	168	LYS
1	B	171	LEU
1	B	174	LYS
1	B	181	HIS
1	B	185	LEU
1	B	192	ASN
1	B	194	GLU
1	B	199	GLN
1	B	201	PHE
1	B	204	LEU
1	B	205	ARG
1	B	208	ILE
1	B	213	ASP
1	B	216	ARG
1	B	222	THR
1	B	226	LYS
1	B	227	LEU
1	B	232	ILE
1	B	240	ILE
1	B	241	ILE
1	B	248	LEU
1	B	250	THR
1	B	253	GLU
1	B	258	VAL
1	B	260	LEU
1	B	261	LEU
1	B	272	ILE
1	B	273	THR
1	B	278	ARG
1	B	281	ASP
1	B	282	ASN

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Mol	Chain	Res	Type
1	B	284	LEU
1	B	286	TYR
1	B	288	ARG
1	B	291	HIS
1	B	298	GLN
1	B	300	LYS
1	B	301	ARG
1	B	320	ILE
1	B	321	HIS
1	B	322	THR
1	B	324	THR
1	B	337	ARG
1	B	343	LEU
1	B	345	GLN
1	B	346	ASP
1	B	347	GLU
1	B	351	PRO
1	B	354	ARG
1	B	355	GLN
1	B	356	SER
1	B	366	ILE
1	B	367	ILE
1	B	372	ASN
1	B	374	LEU
1	B	375	ARG
1	B	376	MET
1	B	381	GLU
1	B	382	ASN
1	B	388	VAL
1	B	390	LEU
1	B	397	PHE
1	B	400	ILE
1	B	404	VAL
1	B	409	SER
1	B	410	LEU
1	B	411	ARG
1	B	412	GLN
1	B	418	ARG
1	B	429	GLU
1	B	431	LYS
1	B	439	SER
1	B	441	PRO

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Mol	Chain	Res	Type
1	B	443	ASP
1	B	447	ILE
1	B	453	LYS
1	B	455	LEU
1	B	457	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	93	ASN
1	A	111	ASN
1	A	113	GLN
1	A	124	HIS
1	A	142	ASN
1	A	192	ASN
1	A	193	ASN
1	A	196	GLN
1	A	254	ASN
1	A	257	HIS
1	A	282	ASN
1	A	355	GLN
1	A	385	ASN
1	A	415	GLN
1	B	23	HIS
1	B	44	HIS
1	B	54	ASN
1	B	112	ASN
1	B	113	GLN
1	B	192	ASN
1	B	231	ASN
1	B	254	ASN
1	B	282	ASN
1	B	287	HIS
1	B	349	GLN
1	B	355	GLN

5.3.3 RNA ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	439:SER	C	440:PHE	N	2.16
1	B	190:ILE	C	191:LYS	N	1.82
1	B	323:GLY	C	324:THR	N	1.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.