



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 03:40 PM EDT

PDB ID : 1HC1  
Title : CRYSTAL STRUCTURE OF HEXAMERIC HAEMOCYANIN FROM PAN-  
ULIRUS INTERRUPTUS REFINED AT 3.2 ANGSTROMS RESOLUTION  
Authors : Volbeda, A.; Hol, W.G.J.  
Deposited on : 1991-05-15  
Resolution : 3.20 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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

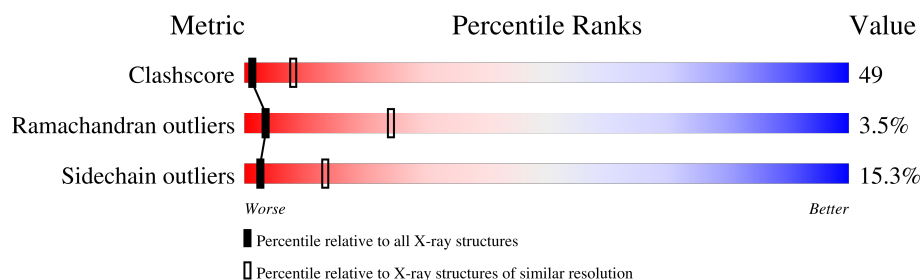
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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  $\geq 3$ , 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	657	
1	B	657	
1	C	657	
1	D	657	
1	E	657	
1	F	657	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32166 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 ARTHROPODAN HEMOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	B	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	C	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	D	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	E	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	F	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ASP	GLU	conflict	UNP P04254
A	163	PRO	GLN	conflict	UNP P04254
A	458	ASN	LYS	conflict	UNP P04254
A	514	SER	LYS	conflict	UNP P04254
B	32	ASP	GLU	conflict	UNP P04254
B	163	PRO	GLN	conflict	UNP P04254
B	458	ASN	LYS	conflict	UNP P04254
B	514	SER	LYS	conflict	UNP P04254
C	32	ASP	GLU	conflict	UNP P04254
C	163	PRO	GLN	conflict	UNP P04254
C	458	ASN	LYS	conflict	UNP P04254
C	514	SER	LYS	conflict	UNP P04254
D	32	ASP	GLU	conflict	UNP P04254
D	163	PRO	GLN	conflict	UNP P04254
D	458	ASN	LYS	conflict	UNP P04254
D	514	SER	LYS	conflict	UNP P04254
E	32	ASP	GLU	conflict	UNP P04254

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Chain	Residue	Modelled	Actual	Comment	Reference
E	163	PRO	GLN	conflict	UNP P04254
E	458	ASN	LYS	conflict	UNP P04254
E	514	SER	LYS	conflict	UNP P04254
F	32	ASP	GLU	conflict	UNP P04254
F	163	PRO	GLN	conflict	UNP P04254
F	458	ASN	LYS	conflict	UNP P04254
F	514	SER	LYS	conflict	UNP P04254

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0
2	E	2	Total Cu 2 2	0	0
2	F	2	Total Cu 2 2	0	0

- Molecule 3 is water.

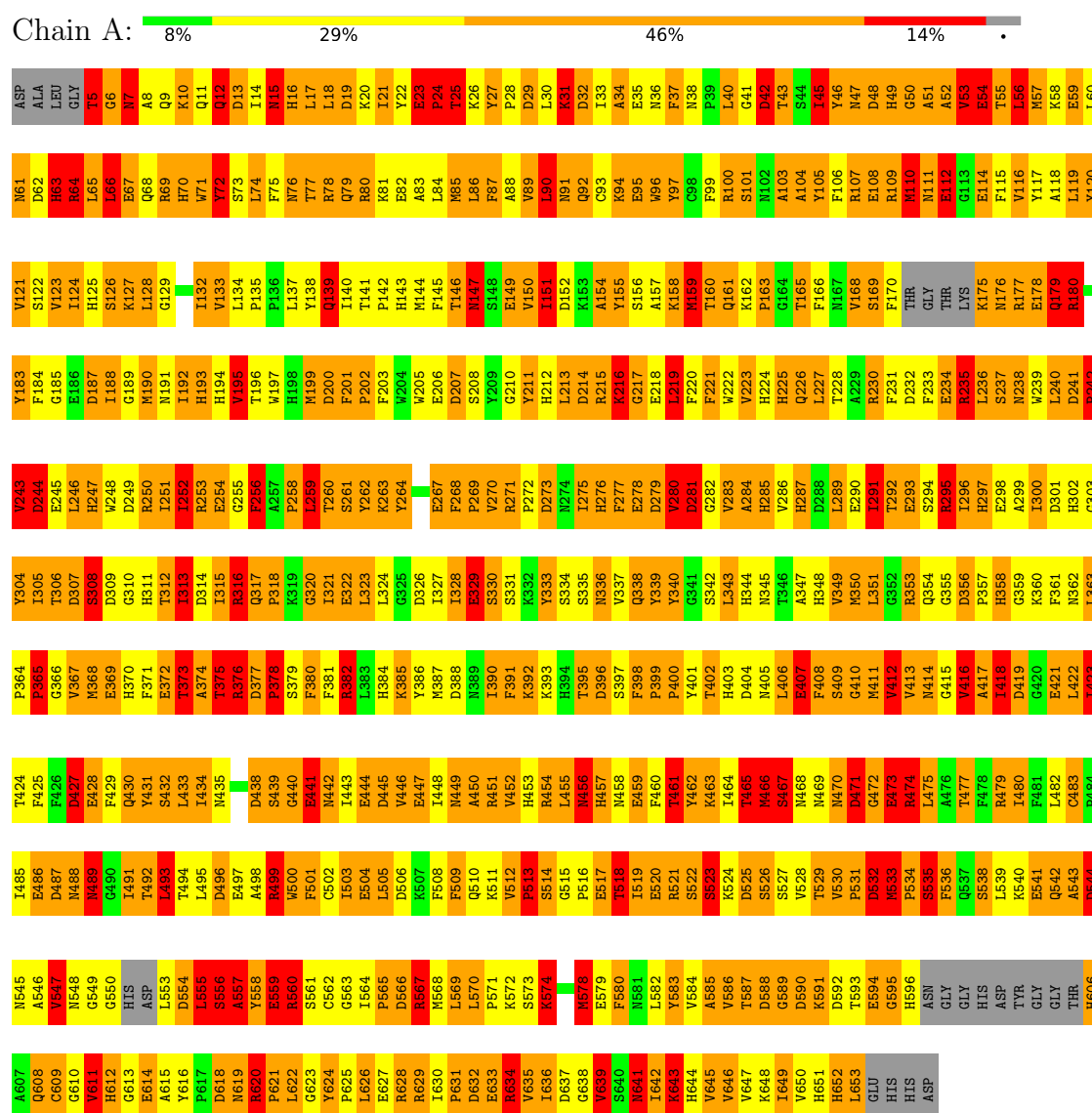
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	186	Total O 186 186	0	0
3	B	186	Total O 186 186	0	0
3	C	186	Total O 186 186	0	0
3	D	186	Total O 186 186	0	0
3	E	186	Total O 186 186	0	0
3	F	186	Total O 186 186	0	0

### 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: ARTHROPODAN HEMOCYANIN

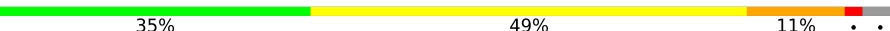


#### • Molecule 1: ARTHROPODAN HEMOCYANIN

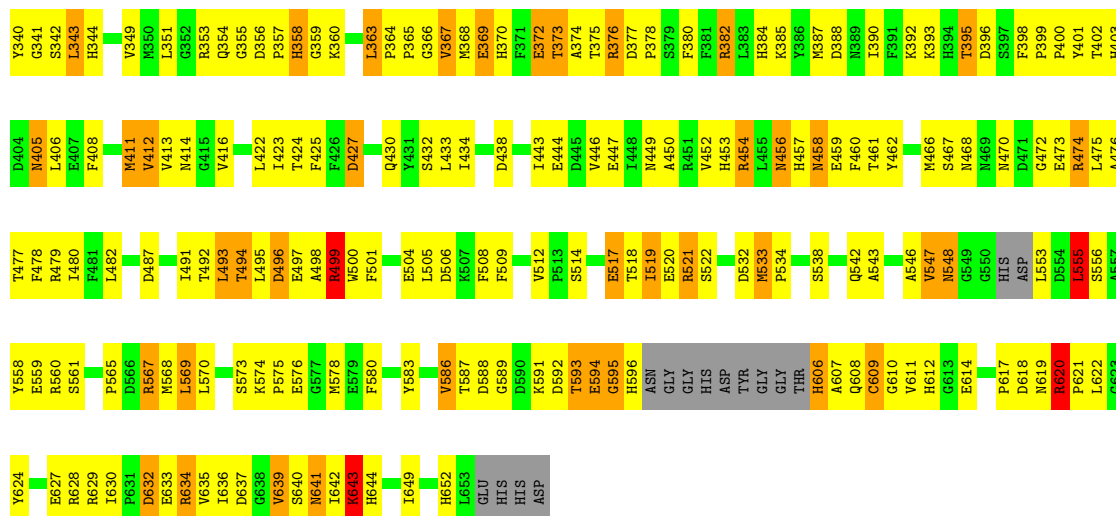


ASP	N61	V121	A182	P242	H302	N362	I422	L482	Q542	TYR
ALA	D62	S122	Y183	V243	G303	L363	I423	C483	A543	GLY
LEU	H63	V123	F184	D244	Y304	P364	T424	P484	D544	GLY
GLY	R64	I124	G185	E245	I305	P365	F425	I485	D545	THR
T5	L65	H125	E186	L246	T306	G366	F426	A486	A546	H606
G6	L66	S126	D187	H247	S308	V367	D427	D487	V547	A607
R7	E67	K127	I188	V248	R309	M368	E428	M488	B488	Q608
A8	Q68	L128	G189	D249	G310	E369	F429	G489	G549	Q609
Q9	R69	G129	M190	R250	H312	H370	F431	I491	H541	G610
K10	H70	D130	N191	I251	T312	F371	Y432	T492	ASP	H611
Q11	Y71	G131	I192	L252	T313	T372	A433	L493	L553	G613
Q12	Y72	I132	H193	R253	D314	A374	I434	T494	D554	E614
D13	S73	V133	H194	E254	L315	T375	M435	L495	L555	A615
I14	L74	L134	V195	G255	R316	R376	A436	D496	S556	V616
N15	F75	P135	T196	F256	R317	D377	V437	E497	A557	P617
H16	N76	F136	W197	A257	P318	P378	D438	Y498	Y558	D618
L17	T77	L137	H199	L259	K319	S379	S439	R499	R559	G619
L18	R78	Y138	Q200	T260	G320	F380	G440	W500	R560	R620
D19	Q79	Q139	D201	S261	I321	F381	M441	F501	S561	P621
K20	R80	T140	F202	Y262	E322	R382	M442	G502	C562	L622
I21	R81	T141	P203	F263	L323	L383	I443	E503	G563	G623
E22	E82	P142	W204	H264	H324	H384	E444	E504	G564	Y624
E23	A83	H143	W205	G265	G325	K385	D445	L505	P565	P625
P24	L84	M144	W206	G266	G326	Y386	V446	D506	D566	L626
T25	R85	F145	E207	G267	I327	M387	E447	K507	R567	E627
K26	L86	T146	D207	E267	I328	R388	M448	F508	M568	R628
Y27	F87	M147	S208	F268	E329	N389	M449	F509	L569	R629
P28	A88	Y138	Y209	P269	S330	R390	A450	Q510	L570	I630
L30	V89	E149	G210	E170	S331	F391	K511	K511	L571	P631
L30	N90	V150	Y211	R271	S332	K392	V452	V512	K572	D632
K31	N91	I151	H212	P272	Y333	K393	H453	P513	S573	E633
D32	Q92	D152	L213	D273	Y334	H394	R454	K514	K574	R634
I33	C93	D153	R215	I275	S335	T395	L455	G515	P575	V635
E35	E95	S156	K216	I276	S336	D396	M456	P516	E576	I636
N36	F37	A157	G217	F277	V337	S397	H457	E517	G577	D637
L37	Y97	K158	E218	E278	Q338	F398	M458	T518	M578	G638
N38	C98	M159	L219	D279	Y339	P399	E459	I519	E579	V639
P39	F99	F160	F220	V280	G340	P400	F460	E520	F580	S640
L40	R100	Q161	F221	D281	S342	Y401	T461	R521	M581	I642
G41	D42	P163	W222	G282	L343	H403	K463	S522	L582	I643
E43	N102	P163	V223	G283	L344	H404	K464	S523	Y583	R643
T43	D43	G164	H224	A284	H344	D405	T465	K524	V584	H644
S44	A104	T165	H225	H285	N345	M406	T466	D525	A585	V645
L45	Y105	F166	Q226	V286	T346	L406	M466	S526	V586	I649
Y46	F106	M167	L227	H287	A347	E407	S467	S527	T587	V650
N47	R107	V168	T228	D288	H348	F408	M468	V528	D588	H650
D48	E108	S169	A229	L289	V349	M469	S409	T529	G589	H651
H49	R109	R230	R230	E290	M350	G410	M470	V530	D590	H652
G50	M110	F170	F231	I291	L351	M411	D471	P531	K591	L653
A51	N111	THR	D232	T292	G352	V412	G472	D532	D582	GLU
A52	E112	THR	F233	E293	R353	V413	E473	M533	T593	HIS
V53	G113	LYS	E234	R294	M354	M414	R474	P534	E594	HIS
E54	E114	K175	R235	R295	G355	G415	L475	S535	G595	ASP
T55	R115	L236	L236	I296	D356	V416	A476	F536	H596	
L56	V116	R177	G237	H297	P357	A417	T477	Q637	ASN	
N57	Y117	E178	N238	E298	H358	I418	F478	S538	GLY	
K58	A118	Q179	D239	A299	G359	D419	R479	L539	GLY	
L119	L119	R180	L240	I300	K360	G420	I480	K540	GLY	
L60	Y120	V181	D241	D301	F361	E421	F481	E541	ASP	

• Molecule 1: ARTHROPODAN HEMOCYANIN

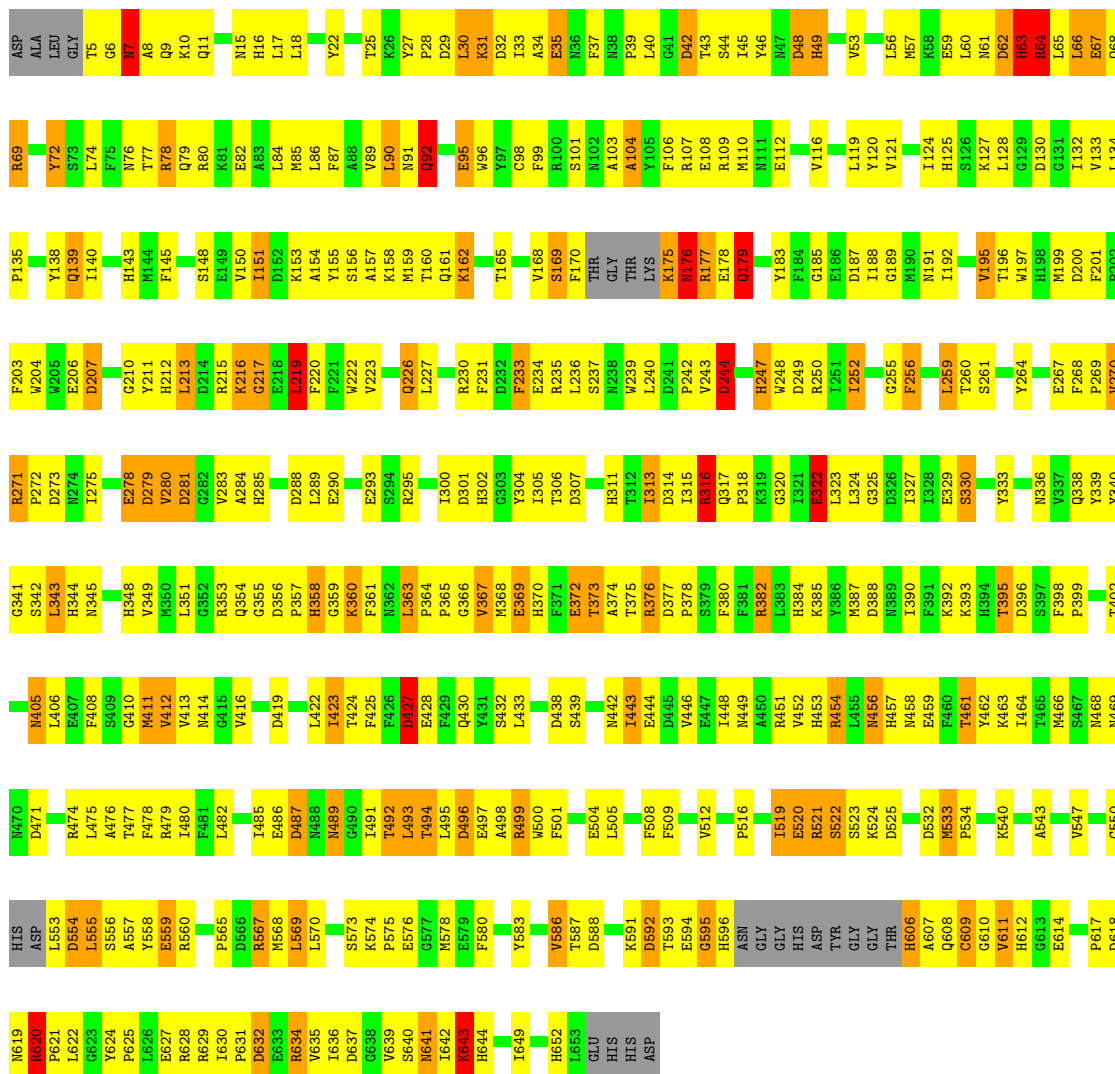
Chain C:  35% 49% 11%

ASP	L66	V133	W204	P272	
ALA	E67	L134	W205	D273	
LEU	Q68	P135	E206	I274	
GLY	R69		D207	I275	
T5	H70	Y138	G210	E278	
G6	W71	Q139	Y211	D279	
R7	Y72	I140	H212	W280	
A8	S73	T141	P142	D281	
Q9	F75	H143	D214	G282	
K10	N76	H143	R215	V283	
Q11	Y77	T146	K216	A284	
			G217	H285	
N15	R78	V150	E218	D288	
H16	Q79	I151	D219	L289	
L17	R80	D152	F220	E290	
L18	K81	K153	F221		
D19	E82	A154	W222		
K20	A83	Y155	V223		
I21	L84	S156			
Y22	M85	A157	Q226		
E23	L86	K158	L227		
P24	F87	M159			
T25	A88	T160	F231		
K26	V89	Q161	D232		
Y27	L90		F233		
P28	N91	T165	D234		
	Q92		R235		
E95		V168	H302		
		S169	G303		
F99		F170	Y304		
L100		THR	K305		
S101		GLY	T306		
I102		THR	D307		
N103		LYS			
F37		K175	H311		
N38		N176	I313		
P39		Y105	I315		
L40		F106	D314		
G41		R107			
D42		Q179	R316		
E108			Q317		
M109			P318		
S44			G319		
I45			G320		
Y46			I321		
M46			E322		
D47			L323		
H49			L324		
			G325		
V53			D326		
			I327		
L56			I328		
M57			E329		
K58			S330		
H125					
S126			Y264		
K127					
L128			E267		
N61			F268		
D62			P269		
H63			V270		
R64			D271		
L65					

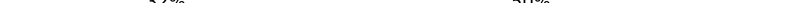


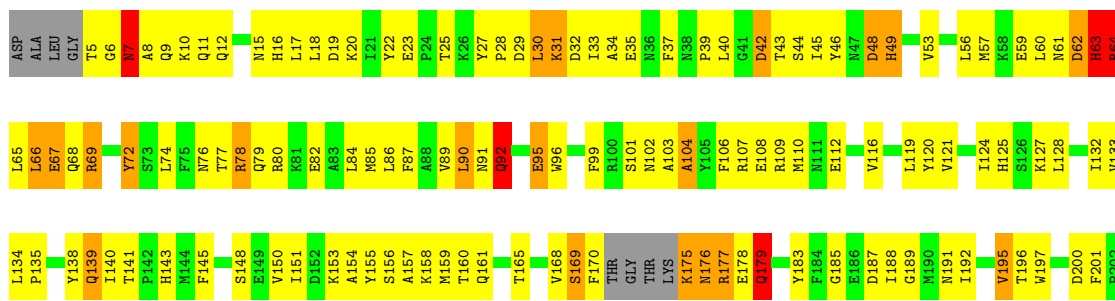
- Molecule 1: ARTHROPODAN HEMOCYANIN

Chain E:  34% 47% 13% . .



- Molecule 1: ARTHROPODAN HEMOCYANIN

Chain F:  32% 50% 13% 5%





G610	G611	G612	G613	G614	P617	D618	M619	R620	P621	L622	G623	Y624	P625	L626	E627	R628	R629	L630	P631	D632	E633	R634	V635	L636	D637	G638	V639	S640	M641	L642	K643	H644	V650	H651	H652	L653	GLU	HIS	ASP																	
N548	G549	G550	HIS	ASP	L553	D554	L555	S556	A557	Y558	E559	R560	S561	G562	G563	F564	P565	D566	R567	M568	L569	L570	S573	K574	P575	E576	G577	V578	M579	F580	N581	L582	Y583	V584	A585	V586	T587	D588	K591	D592	T593	E594	G595	H596	ASN	GLY	GLY	HIS	ASP							
N470	D471	G472	E473	R474	L475	A476	T477	F478	R479	I480	F481	N482	L486	E486	D487	M488	M489	G490	I491	T492	L493	T494	L495	D496	E497	A498	R499	V500	F501	E504	L505	F508	F509	V512	P513	S514	E517	T518	I519	E520	R521	S522	D532	M533	P534	S535	F536	A543	D544	M545	A546	Y547				
N402	N405	L406	E407	F408	S409	G410	M411	V412	V413	N414	G415	V416	L422	I423	M423	T424	F425	F426	D427	E428	F429	Q430	L435	Y431	S432	L433	I434	D438	S439	N442	I443	A444	D445	V446	E447	I448	N449	A450	R451	V452	H453	R454	L455	N456	H457	M458	E459	F460	T461	Y462	K463	M466	S467	N468	N469	
Q338	Y339	Y340	G341	S342	L343	H344	N345	H348	V349	D281	M350	G352	R353	Q354	G355	D356	P357	H358	G359	K360	L363	P364	P365	G366	V367	M368	E369	H370	F371	E372	T373	A374	T375	R376	D377	P378	S379	F380	F381	R382	L383	H384	K385	Y386	M387	D388	M389	I390	F391	K392	K393	H394	T395	D396	S397	P399
V270	R271	P272	D273	N274	L275	E278	D279	V280	D281	G282	V283	A284	H285	D288	G289	L289	E290	E293	S294	R295	I296	H297	I300	D301	H302	G303	Y304	I305	I306	D307	H311	T312	I313	D314	I315	R316	Q317	P318	K319	G320	I321	E322	L323	L324	G325	F256	L259	T260	S261	Y264	E267	F268	P269			

## 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, $\alpha$ , $\beta$ , $\gamma$	119.80Å 193.10Å 122.20Å 90.00° 118.10° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.201 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:  
CU

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	1.41	11/5316 (0.2%)	4.13	1053/7205 (14.6%)
1	B	1.40	14/5316 (0.3%)	3.74	1016/7205 (14.1%)
1	C	0.75	0/5316	1.64	87/7205 (1.2%)
1	D	0.77	1/5316 (0.0%)	1.66	94/7205 (1.3%)
1	E	0.76	2/5316 (0.0%)	1.64	87/7205 (1.2%)
1	F	0.75	0/5316	1.65	94/7205 (1.3%)
All	All	1.02	28/31896 (0.1%)	2.64	2431/43230 (5.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	550	GLY	C-O	7.84	1.36	1.23
1	B	208	SER	CB-OG	7.79	1.52	1.42
1	A	441	GLU	CB-CG	7.42	1.66	1.52
1	A	526	SER	CB-OG	6.86	1.51	1.42
1	B	267	GLU	CD-OE2	-6.23	1.18	1.25
1	A	217	GLY	N-CA	6.11	1.55	1.46
1	A	69	ARG	CZ-NH2	6.11	1.41	1.33
1	B	112	GLU	CG-CD	-6.07	1.42	1.51
1	A	409	SER	CB-OG	6.02	1.50	1.42
1	E	540	LYS	CE-NZ	5.90	1.63	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	409	SER	CB-OG	5.74	1.49	1.42
1	B	126	SER	CB-OG	5.71	1.49	1.42
1	B	218	GLU	CD-OE2	5.65	1.31	1.25
1	B	215	ARG	NE-CZ	5.62	1.40	1.33
1	B	382	ARG	CZ-NH1	5.57	1.40	1.33
1	B	352	GLY	C-O	5.54	1.32	1.23
1	A	504	GLU	CD-OE1	5.45	1.31	1.25
1	A	353	ARG	CZ-NH2	5.43	1.40	1.33
1	A	486	GLU	CD-OE1	-5.38	1.19	1.25
1	A	216	LYS	C-O	5.34	1.33	1.23
1	B	215	ARG	CZ-NH2	5.33	1.40	1.33
1	B	217	GLY	N-CA	5.31	1.54	1.46
1	B	322	GLU	CD-OE1	5.26	1.31	1.25
1	B	561	SER	CA-CB	5.20	1.60	1.52
1	B	583	TYR	CE1-CZ	5.18	1.45	1.38
1	A	282	GLY	C-O	5.17	1.31	1.23
1	B	112	GLU	CB-CG	-5.16	1.42	1.52
1	A	499	ARG	CZ-NH2	5.10	1.39	1.33

All (2431) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ARG	NE-CZ-NH2	89.27	164.93	120.30
1	A	207	ASP	CB-CG-OD1	43.98	157.88	118.30
1	B	271	ARG	NE-CZ-NH1	43.24	141.92	120.30
1	A	273	ASP	CB-CG-OD1	40.24	154.52	118.30
1	B	273	ASP	CB-CG-OD1	39.23	153.61	118.30
1	A	62	ASP	CB-CG-OD2	38.49	152.94	118.30
1	A	64	ARG	CD-NE-CZ	38.42	177.39	123.60
1	A	235	ARG	NE-CZ-NH1	-33.73	103.44	120.30
1	B	80	ARG	NE-CZ-NH2	-33.39	103.61	120.30
1	A	567	ARG	NE-CZ-NH1	33.03	136.82	120.30
1	B	353	ARG	NE-CZ-NH1	-31.62	104.49	120.30
1	A	64	ARG	NH1-CZ-NH2	-30.42	85.94	119.40
1	A	215	ARG	NE-CZ-NH2	26.71	133.65	120.30
1	A	180	ARG	NE-CZ-NH2	-26.50	107.05	120.30
1	B	215	ARG	NE-CZ-NH1	26.24	133.42	120.30
1	B	316	ARG	CD-NE-CZ	26.06	160.08	123.60
1	A	80	ARG	NE-CZ-NH2	-26.00	107.30	120.30
1	A	474	ARG	NE-CZ-NH1	24.74	132.67	120.30
1	A	632	ASP	CB-CG-OD2	24.70	140.53	118.30
1	B	295	ARG	NE-CZ-NH2	23.88	132.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	560	ARG	NE-CZ-NH1	-23.67	108.46	120.30
1	A	207	ASP	CB-CG-OD2	-23.38	97.26	118.30
1	A	64	ARG	NE-CZ-NH1	-23.30	108.65	120.30
1	A	629	ARG	NE-CZ-NH2	23.30	131.95	120.30
1	B	314	ASP	CB-CG-OD2	23.05	139.04	118.30
1	A	567	ARG	CD-NE-CZ	22.27	154.78	123.60
1	A	206	GLU	OE1-CD-OE2	-22.06	96.83	123.30
1	A	253	ARG	NE-CZ-NH1	22.02	131.31	120.30
1	B	496	ASP	CB-CG-OD2	21.61	137.75	118.30
1	B	521	ARG	NE-CZ-NH2	-21.61	109.49	120.30
1	A	326	ASP	CB-CG-OD1	20.93	137.13	118.30
1	A	29	ASP	CB-CG-OD2	-20.55	99.81	118.30
1	B	235	ARG	NE-CZ-NH1	20.07	130.34	120.30
1	B	479	ARG	NE-CZ-NH2	19.92	130.26	120.30
1	B	560	ARG	NE-CZ-NH1	19.69	130.15	120.30
1	A	316	ARG	CD-NE-CZ	19.63	151.08	123.60
1	A	521	ARG	NE-CZ-NH2	-19.51	110.54	120.30
1	A	628	ARG	NE-CZ-NH2	-19.22	110.69	120.30
1	B	353	ARG	NH1-CZ-NH2	19.14	140.45	119.40
1	A	278	GLU	OE1-CD-OE2	-19.10	100.38	123.30
1	A	177	ARG	NE-CZ-NH2	18.96	129.78	120.30
1	A	235	ARG	NH1-CZ-NH2	18.80	140.09	119.40
1	A	279	ASP	CB-CG-OD1	18.75	135.18	118.30
1	A	230	ARG	NE-CZ-NH1	-18.18	111.21	120.30
1	A	35	GLU	OE1-CD-OE2	-17.67	102.09	123.30
1	A	594	GLU	OE1-CD-OE2	17.67	144.50	123.30
1	A	624	TYR	CB-CG-CD1	17.51	131.51	121.00
1	A	333	TYR	CB-CG-CD1	17.43	131.46	121.00
1	A	643	LYS	CA-CB-CG	17.38	151.64	113.40
1	A	25	THR	O-C-N	17.27	150.33	122.70
1	A	620	ARG	NE-CZ-NH2	17.26	128.93	120.30
1	B	100	ARG	NE-CZ-NH1	17.24	128.92	120.30
1	B	567	ARG	NE-CZ-NH2	-17.19	111.70	120.30
1	A	65	LEU	O-C-N	-16.95	95.59	122.70
1	B	17	LEU	O-C-N	16.87	149.69	122.70
1	A	19	ASP	CB-CG-OD2	16.69	133.32	118.30
1	A	567	ARG	NE-CZ-NH2	-16.66	111.97	120.30
1	A	454	ARG	NE-CZ-NH2	16.64	128.62	120.30
1	A	560	ARG	NH1-CZ-NH2	16.46	137.50	119.40
1	A	271	ARG	NE-CZ-NH1	16.09	128.35	120.30
1	B	438	ASP	CB-CG-OD2	-16.09	103.82	118.30
1	A	215	ARG	NE-CZ-NH1	-16.04	112.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	TYR	CB-CG-CD1	16.04	130.62	121.00
1	B	382	ARG	NE-CZ-NH1	15.86	128.23	120.30
1	A	520	GLU	OE1-CD-OE2	15.84	142.31	123.30
1	B	462	TYR	CB-CG-CD2	15.81	130.49	121.00
1	B	376	ARG	NE-CZ-NH2	-15.76	112.42	120.30
1	A	62	ASP	CB-CG-OD1	-15.71	104.16	118.30
1	A	486	GLU	O-C-N	-15.68	97.61	122.70
1	A	632	ASP	CB-CG-OD1	-15.67	104.19	118.30
1	B	560	ARG	CD-NE-CZ	15.53	145.35	123.60
1	C	316	ARG	CD-NE-CZ	15.47	145.26	123.60
1	B	48	ASP	CA-CB-CG	15.47	147.43	113.40
1	B	244	ASP	CB-CG-OD1	15.38	132.14	118.30
1	E	316	ARG	CD-NE-CZ	15.35	145.09	123.60
1	A	250	ARG	NE-CZ-NH2	-15.30	112.65	120.30
1	A	206	GLU	CG-CD-OE2	15.28	148.87	118.30
1	D	316	ARG	CD-NE-CZ	15.28	144.99	123.60
1	F	316	ARG	CD-NE-CZ	15.27	144.98	123.60
1	B	207	ASP	CB-CG-OD1	15.23	132.01	118.30
1	A	309	ASP	CB-CG-OD2	-15.19	104.63	118.30
1	B	454	ARG	NE-CZ-NH1	15.18	127.89	120.30
1	B	69	ARG	NE-CZ-NH1	15.18	127.89	120.30
1	B	271	ARG	NH1-CZ-NH2	-15.04	102.85	119.40
1	A	624	TYR	CG-CD2-CE2	15.02	133.32	121.30
1	F	206	GLU	OE1-CD-OE2	-14.84	105.49	123.30
1	B	462	TYR	CB-CG-CD1	-14.81	112.11	121.00
1	A	560	ARG	CD-NE-CZ	-14.74	102.96	123.60
1	A	544	ASP	CB-CG-OD1	-14.65	105.12	118.30
1	A	152	ASP	O-C-N	14.63	146.10	122.70
1	A	241	ASP	CB-CG-OD1	-14.61	105.15	118.30
1	A	27	TYR	CB-CG-CD1	14.58	129.75	121.00
1	A	107	ARG	NE-CZ-NH2	14.53	127.56	120.30
1	B	16	HIS	O-C-N	14.50	145.91	122.70
1	A	54	GLU	OE1-CD-OE2	14.45	140.63	123.30
1	A	308	SER	O-C-N	14.36	145.67	122.70
1	B	19	ASP	CB-CG-OD2	14.30	131.17	118.30
1	B	560	ARG	C-N-CA	14.21	157.22	121.70
1	B	307	ASP	CB-CG-OD2	14.20	131.08	118.30
1	B	624	TYR	CB-CG-CD1	14.12	129.47	121.00
1	A	295	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	A	438	ASP	CB-CG-OD2	-13.98	105.72	118.30
1	B	474	ARG	NE-CZ-NH1	-13.98	113.31	120.30
1	A	273	ASP	OD1-CG-OD2	-13.95	96.79	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	TYR	CB-CG-CD2	-13.92	112.65	121.00
1	B	273	ASP	CB-CG-OD2	-13.91	105.78	118.30
1	A	496	ASP	CB-CG-OD2	13.90	130.81	118.30
1	A	401	TYR	CB-CG-CD2	13.85	129.31	121.00
1	A	474	ARG	NE-CZ-NH2	-13.83	113.38	120.30
1	B	49	HIS	C-N-CA	13.83	151.34	122.30
1	A	438	ASP	CB-CG-OD1	13.81	130.73	118.30
1	A	245	GLU	OE1-CD-OE2	-13.80	106.74	123.30
1	A	578	MET	CA-CB-CG	13.80	136.76	113.30
1	A	624	TYR	CZ-CE2-CD2	-13.79	107.39	119.80
1	A	618	ASP	CB-CG-OD1	13.73	130.66	118.30
1	A	107	ARG	NE-CZ-NH1	13.68	127.14	120.30
1	A	422	LEU	CB-CA-C	13.67	136.17	110.20
1	A	190	MET	O-C-N	13.57	144.41	122.70
1	F	206	GLU	CG-CD-OE2	13.54	145.38	118.30
1	B	304	TYR	CB-CG-CD1	-13.47	112.92	121.00
1	B	107	ARG	NE-CZ-NH2	13.45	127.03	120.30
1	B	307	ASP	CB-CG-OD1	-13.44	106.21	118.30
1	B	177	ARG	NE-CZ-NH1	13.37	126.98	120.30
1	B	63	HIS	N-CA-CB	13.35	134.63	110.60
1	A	180	ARG	O-C-N	13.30	143.98	122.70
1	A	66	LEU	CA-CB-CG	13.21	145.68	115.30
1	A	462	TYR	CB-CG-CD1	13.18	128.91	121.00
1	B	295	ARG	NE-CZ-NH1	-13.15	113.72	120.30
1	B	63	HIS	O-C-N	13.00	143.50	122.70
1	B	17	LEU	CA-C-O	-12.99	92.81	120.10
1	B	206	GLU	OE1-CD-OE2	-12.96	107.75	123.30
1	A	624	TYR	CB-CG-CD2	-12.95	113.23	121.00
1	B	138	TYR	CG-CD2-CE2	12.95	131.66	121.30
1	B	417	ALA	N-CA-CB	-12.95	91.98	110.10
1	A	428	GLU	OE1-CD-OE2	12.94	138.83	123.30
1	A	560	ARG	NE-CZ-NH2	-12.94	113.83	120.30
1	B	215	ARG	NH1-CZ-NH2	-12.93	105.18	119.40
1	A	107	ARG	NH1-CZ-NH2	-12.85	105.27	119.40
1	A	471	ASP	C-N-CA	12.81	149.20	122.30
1	A	407	GLU	OE1-CD-OE2	-12.64	108.13	123.30
1	E	206	GLU	OE1-CD-OE2	-12.64	108.14	123.30
1	B	19	ASP	CB-CG-OD1	-12.63	106.94	118.30
1	B	454	ARG	NE-CZ-NH2	-12.61	114.00	120.30
1	A	404	ASP	CB-CG-OD2	-12.55	107.01	118.30
1	A	284	ALA	N-CA-CB	12.48	127.57	110.10
1	B	244	ASP	CB-CG-OD2	-12.36	107.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	TYR	CB-CG-CD1	-12.32	113.61	121.00
1	B	434	ILE	O-C-N	12.22	142.25	122.70
1	B	242	PRO	O-C-N	-12.18	103.21	122.70
1	A	637	ASP	CB-CG-OD2	-12.18	107.34	118.30
1	C	555	LEU	CA-CB-CG	12.15	143.24	115.30
1	E	206	GLU	CG-CD-OE2	12.14	142.58	118.30
1	B	469	ASN	O-C-N	12.14	142.12	122.70
1	B	35	GLU	OE1-CD-OE2	-12.13	108.74	123.30
1	B	521	ARG	NH1-CZ-NH2	12.04	132.64	119.40
1	A	25	THR	N-CA-CB	12.03	133.16	110.30
1	A	80	ARG	NE-CZ-NH1	12.03	126.31	120.30
1	B	445	ASP	CB-CG-OD2	12.03	129.12	118.30
1	A	152	ASP	CB-CG-OD2	-11.97	107.53	118.30
1	B	273	ASP	OD1-CG-OD2	-11.95	100.59	123.30
1	A	177	ARG	NH1-CZ-NH2	-11.93	106.28	119.40
1	B	421	GLU	OE1-CD-OE2	11.89	137.57	123.30
1	A	293	GLU	CG-CD-OE2	11.88	142.06	118.30
1	B	474	ARG	NE-CZ-NH2	11.83	126.22	120.30
1	B	105	TYR	CB-CG-CD1	11.79	128.08	121.00
1	B	120	TYR	CB-CG-CD2	-11.72	113.97	121.00
1	B	232	ASP	CB-CG-OD2	11.72	128.85	118.30
1	A	356	ASP	CB-CG-OD2	-11.71	107.76	118.30
1	B	616	TYR	CB-CG-CD2	11.70	128.02	121.00
1	B	299	ALA	CB-CA-C	11.68	127.62	110.10
1	B	353	ARG	NE-CZ-NH2	-11.68	114.46	120.30
1	A	232	ASP	CB-CG-OD1	11.63	128.77	118.30
1	A	231	PHE	CB-CG-CD2	-11.59	112.69	120.80
1	B	200	ASP	CB-CG-OD2	11.58	128.72	118.30
1	A	231	PHE	O-C-N	11.51	141.12	122.70
1	A	147	ASN	CB-CG-OD1	-11.50	98.60	121.60
1	A	322	GLU	CA-CB-CG	11.48	138.65	113.40
1	A	369	GLU	CA-CB-CG	11.40	138.48	113.40
1	A	94	LYS	CB-CA-C	11.37	133.13	110.40
1	B	451	ARG	NE-CZ-NH1	-11.35	114.62	120.30
1	B	529	THR	O-C-N	-11.31	104.60	122.70
1	D	35	GLU	OE1-CD-OE2	-11.30	109.74	123.30
1	A	353	ARG	NE-CZ-NH1	11.30	125.95	120.30
1	C	206	GLU	OE1-CD-OE2	-11.29	109.76	123.30
1	B	350	MET	CG-SD-CE	-11.27	82.17	100.20
1	B	460	PHE	O-C-N	11.23	140.67	122.70
1	B	78	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	B	499	ARG	CD-NE-CZ	11.21	139.29	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	206	GLU	OE1-CD-OE2	-11.18	109.89	123.30
1	B	80	ARG	NH1-CZ-NH2	11.17	131.69	119.40
1	B	342	SER	O-C-N	-11.16	104.83	122.70
1	B	180	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	A	369	GLU	OE1-CD-OE2	-11.11	109.97	123.30
1	A	615	ALA	N-CA-CB	-11.09	94.58	110.10
1	B	627	GLU	CG-CD-OE1	-11.09	96.12	118.30
1	A	303	GLY	O-C-N	11.08	140.44	122.70
1	A	128	LEU	O-C-N	11.06	142.00	123.20
1	B	229	ALA	N-CA-CB	11.01	125.52	110.10
1	B	272	PRO	O-C-N	11.01	140.31	122.70
1	B	333	TYR	CB-CG-CD2	-10.99	114.40	121.00
1	A	441	GLU	CG-CD-OE2	-10.99	96.32	118.30
1	A	250	ARG	NH1-CZ-NH2	10.98	131.47	119.40
1	A	94	LYS	CD-CE-NZ	10.97	136.94	111.70
1	A	491	ILE	CA-C-N	10.97	141.33	117.20
1	B	289	LEU	CB-CA-C	10.96	131.03	110.20
1	A	244	ASP	CB-CG-OD1	10.96	128.16	118.30
1	B	432	SER	O-C-N	-10.95	105.18	122.70
1	A	629	ARG	NH1-CZ-NH2	-10.95	107.36	119.40
1	A	89	VAL	CB-CA-C	10.94	132.19	111.40
1	B	554	ASP	CB-CG-OD2	10.94	128.15	118.30
1	A	62	ASP	OD1-CG-OD2	-10.93	102.53	123.30
1	B	62	ASP	O-C-N	10.93	140.19	122.70
1	A	59	GLU	O-C-N	10.92	140.17	122.70
1	A	117	TYR	CG-CD1-CE1	10.90	130.02	121.30
1	B	69	ARG	CB-CG-CD	10.89	139.91	111.60
1	B	356	ASP	CB-CG-OD2	10.88	128.10	118.30
1	A	406	LEU	N-CA-CB	-10.88	88.64	110.40
1	B	434	ILE	CA-C-O	-10.87	97.27	120.10
1	A	435	ASN	OD1-CG-ND2	10.86	146.89	121.90
1	B	627	GLU	OE1-CD-OE2	10.86	136.33	123.30
1	A	17	LEU	O-C-N	10.85	140.06	122.70
1	A	360	LYS	CA-CB-CG	10.84	137.25	113.40
1	B	130	ASP	CB-CG-OD1	-10.83	108.55	118.30
1	B	454	ARG	CA-CB-CG	10.82	137.19	113.40
1	A	583	TYR	CB-CG-CD1	10.81	127.48	121.00
1	B	293	GLU	OE1-CD-OE2	10.80	136.27	123.30
1	A	376	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	A	120	TYR	CB-CG-CD1	10.76	127.45	121.00
1	B	431	TYR	CZ-CE2-CD2	-10.75	110.12	119.80
1	A	138	TYR	CB-CG-CD2	10.74	127.44	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	GLU	OE1-CD-OE2	10.73	136.18	123.30
1	A	479	ARG	NE-CZ-NH1	-10.71	114.95	120.30
1	B	316	ARG	CG-CD-NE	10.69	134.26	111.80
1	A	273	ASP	CB-CG-OD2	-10.69	108.68	118.30
1	A	109	ARG	NE-CZ-NH2	-10.67	114.97	120.30
1	B	260	THR	CA-CB-OG1	-10.66	86.61	109.00
1	B	17	LEU	CB-CG-CD2	-10.64	92.92	111.00
1	A	427	ASP	CB-CG-OD1	-10.62	108.74	118.30
1	B	387	MET	CA-CB-CG	10.61	131.33	113.30
1	B	106	PHE	O-C-N	10.59	139.65	122.70
1	A	376	ARG	CB-CG-CD	10.58	139.11	111.60
1	A	387	MET	CA-CB-CG	10.56	131.25	113.30
1	B	6	GLY	N-CA-C	-10.56	86.70	113.10
1	B	30	LEU	CB-CA-C	10.54	130.23	110.20
1	B	408	PHE	CA-CB-CG	10.53	139.18	113.90
1	A	326	ASP	CB-CG-OD2	-10.52	108.83	118.30
1	A	445	ASP	CB-CG-OD2	10.51	127.76	118.30
1	C	7	ASN	CA-CB-CG	10.51	136.52	113.40
1	D	7	ASN	CA-CB-CG	10.51	136.51	113.40
1	A	230	ARG	NH1-CZ-NH2	10.50	130.95	119.40
1	B	369	GLU	CA-CB-CG	10.49	136.49	113.40
1	B	11	GLN	CA-CB-CG	-10.46	90.40	113.40
1	A	356	ASP	OD1-CG-OD2	10.45	143.16	123.30
1	B	359	GLY	CA-C-O	10.45	139.41	120.60
1	B	231	PHE	CD1-CE1-CZ	10.45	132.64	120.10
1	A	462	TYR	CB-CG-CD2	-10.43	114.75	121.00
1	B	570	LEU	CA-CB-CG	10.41	139.24	115.30
1	B	287	HIS	O-C-N	10.40	139.34	122.70
1	B	190	MET	CA-CB-CG	-10.39	95.63	113.30
1	B	298	GLU	CA-CB-CG	10.39	136.25	113.40
1	A	120	TYR	CB-CG-CD2	-10.35	114.79	121.00
1	F	7	ASN	CA-CB-CG	10.34	136.15	113.40
1	A	214	ASP	CB-CG-OD1	10.32	127.59	118.30
1	A	264	TYR	CB-CG-CD1	-10.32	114.81	121.00
1	B	73	SER	N-CA-CB	10.31	125.97	110.50
1	B	271	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	183	TYR	O-C-N	10.27	139.14	122.70
1	A	53	VAL	CG1-CB-CG2	10.27	127.32	110.90
1	A	356	ASP	CB-CG-OD1	-10.26	109.07	118.30
1	A	458	ASN	CA-CB-CG	10.26	135.96	113.40
1	A	278	GLU	CG-CD-OE2	10.25	138.79	118.30
1	A	441	GLU	CA-CB-CG	-10.22	90.92	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	LEU	N-CA-CB	-10.21	89.97	110.40
1	A	463	LYS	N-CA-CB	10.20	128.96	110.60
1	B	165	THR	CA-CB-CG2	10.20	126.68	112.40
1	B	100	ARG	NH1-CZ-NH2	-10.19	108.19	119.40
1	A	454	ARG	NE-CZ-NH1	-10.17	115.21	120.30
1	A	632	ASP	O-C-N	10.16	138.96	122.70
1	A	491	ILE	CA-C-O	-10.15	98.79	120.10
1	A	440	GLY	CA-C-O	-10.14	102.34	120.60
1	B	432	SER	CA-C-O	10.14	141.39	120.10
1	B	206	GLU	CG-CD-OE1	10.13	138.56	118.30
1	A	308	SER	CA-C-O	-10.12	98.85	120.10
1	E	7	ASN	CA-CB-CG	10.11	135.65	113.40
1	B	309	ASP	CB-CG-OD1	10.11	127.40	118.30
1	B	78	ARG	CD-NE-CZ	10.10	137.73	123.60
1	B	25	THR	O-C-N	10.08	138.82	122.70
1	A	212	HIS	O-C-N	10.07	138.82	122.70
1	A	177	ARG	CA-C-O	10.06	141.23	120.10
1	B	162	LYS	CB-CA-C	10.05	130.51	110.40
1	A	19	ASP	CB-CG-OD1	-10.05	109.26	118.30
1	A	588	ASP	CB-CG-OD2	-10.04	109.26	118.30
1	B	554	ASP	CA-CB-CG	10.04	135.48	113.40
1	B	332	LYS	O-C-N	10.03	138.74	122.70
1	A	535	SER	CB-CA-C	-10.01	91.08	110.10
1	B	203	PHE	CB-CG-CD2	-10.01	113.80	120.80
1	B	253	ARG	CA-CB-CG	9.98	135.35	113.40
1	A	407	GLU	CA-C-O	9.96	141.03	120.10
1	D	322	GLU	CA-CB-CG	9.92	135.23	113.40
1	B	469	ASN	OD1-CG-ND2	9.92	144.72	121.90
1	B	496	ASP	N-CA-CB	9.92	128.46	110.60
1	D	206	GLU	CG-CD-OE1	9.92	138.14	118.30
1	A	128	LEU	CB-CG-CD2	-9.92	94.14	111.00
1	A	375	THR	OG1-CB-CG2	9.91	132.79	110.00
1	B	116	VAL	CA-CB-CG2	9.91	125.76	110.90
1	A	479	ARG	CD-NE-CZ	-9.90	109.73	123.60
1	A	489	ASN	N-CA-C	-9.89	84.30	111.00
1	A	211	TYR	CG-CD2-CE2	9.87	129.20	121.30
1	B	25	THR	OG1-CB-CG2	9.85	132.65	110.00
1	B	259	LEU	CB-CA-C	9.84	128.90	110.20
1	B	273	ASP	CB-CA-C	9.80	130.01	110.40
1	A	65	LEU	CA-C-N	9.80	138.76	117.20
1	B	25	THR	CA-CB-OG1	-9.79	88.44	109.00
1	A	489	ASN	CA-C-O	9.78	140.63	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	LYS	O-C-N	9.77	138.34	122.70
1	A	487	ASP	O-C-N	9.77	138.32	122.70
1	B	472	GLY	C-N-CA	9.77	146.12	121.70
1	A	228	THR	CA-CB-OG1	-9.76	88.51	109.00
1	B	607	ALA	CB-CA-C	9.75	124.72	110.10
1	A	24	PRO	N-CD-CG	-9.74	88.58	103.20
1	A	439	SER	C-N-CA	-9.74	101.84	122.30
1	B	502	CYS	CA-CB-SG	9.74	131.53	114.00
1	A	207	ASP	OD1-CG-OD2	-9.73	104.81	123.30
1	B	164	GLY	N-CA-C	9.72	137.41	113.10
1	B	427	ASP	CB-CG-OD2	9.71	127.04	118.30
1	C	206	GLU	CG-CD-OE1	9.71	137.72	118.30
1	A	534	PRO	CA-C-O	-9.70	96.91	120.20
1	B	499	ARG	NE-CZ-NH2	9.69	125.15	120.30
1	B	109	ARG	NE-CZ-NH1	-9.68	115.46	120.30
1	B	485	ILE	CA-C-N	9.68	138.49	117.20
1	B	201	PHE	CB-CG-CD2	-9.67	114.03	120.80
1	A	73	SER	N-CA-CB	9.67	125.01	110.50
1	A	32	ASP	CB-CG-OD2	-9.66	109.60	118.30
1	A	83	ALA	N-CA-CB	9.66	123.63	110.10
1	B	462	TYR	O-C-N	9.65	138.15	122.70
1	A	417	ALA	CB-CA-C	-9.64	95.64	110.10
1	B	29	ASP	CB-CG-OD1	-9.64	109.63	118.30
1	A	557	ALA	N-CA-CB	9.63	123.58	110.10
1	B	138	TYR	CD1-CE1-CZ	9.61	128.45	119.80
1	B	35	GLU	CG-CD-OE1	9.60	137.50	118.30
1	B	163	PRO	O-C-N	9.59	139.50	123.20
1	B	183	TYR	CA-C-O	-9.59	99.97	120.10
1	C	322	GLU	CA-CB-CG	9.58	134.47	113.40
1	A	385	LYS	N-CA-CB	9.57	127.83	110.60
1	A	496	ASP	N-CA-CB	9.56	127.80	110.60
1	B	339	TYR	CB-CG-CD2	9.56	126.73	121.00
1	A	353	ARG	CD-NE-CZ	9.55	136.97	123.60
1	F	322	GLU	CA-CB-CG	9.55	134.41	113.40
1	B	48	ASP	CB-CG-OD1	9.55	126.89	118.30
1	A	63	HIS	N-CA-CB	9.54	127.78	110.60
1	B	75	PHE	CA-C-O	-9.54	100.06	120.10
1	E	322	GLU	CA-CB-CG	9.52	134.35	113.40
1	A	529	THR	C-N-CA	9.52	145.50	121.70
1	B	407	GLU	CG-CD-OE2	9.51	137.31	118.30
1	A	279	ASP	CB-CG-OD2	-9.49	109.76	118.30
1	B	74	LEU	O-C-N	9.49	137.88	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	ILE	O-C-N	9.47	137.86	122.70
1	B	51	ALA	CB-CA-C	9.47	124.31	110.10
1	B	184	PHE	CZ-CE2-CD2	-9.47	108.73	120.10
1	B	75	PHE	O-C-N	9.47	137.85	122.70
1	B	246	LEU	CA-C-O	-9.46	100.24	120.10
1	A	519	ILE	CA-C-O	9.45	139.95	120.10
1	A	534	PRO	O-C-N	9.45	137.82	122.70
1	B	403	HIS	N-CA-CB	9.44	127.59	110.60
1	A	234	GLU	O-C-N	9.44	137.80	122.70
1	B	587	THR	C-N-CA	9.44	145.29	121.70
1	A	152	ASP	N-CA-CB	9.42	127.56	110.60
1	A	293	GLU	OE1-CD-OE2	-9.41	112.01	123.30
1	A	139	GLN	CA-C-O	-9.40	100.36	120.10
1	C	548	ASN	CA-CB-CG	9.39	134.06	113.40
1	B	307	ASP	O-C-N	9.39	137.72	122.70
1	B	53	VAL	CA-C-O	9.37	139.78	120.10
1	B	314	ASP	OD1-CG-OD2	-9.37	105.49	123.30
1	B	439	SER	CA-C-O	-9.37	100.43	120.10
1	A	461	THR	O-C-N	-9.36	107.73	122.70
1	A	250	ARG	NE-CZ-NH1	-9.35	115.62	120.30
1	B	525	ASP	CB-CG-OD1	9.35	126.72	118.30
1	A	226	GLN	CB-CA-C	9.35	129.10	110.40
1	B	624	TYR	CB-CG-CD2	-9.35	115.39	121.00
1	A	422	LEU	CB-CG-CD1	9.34	126.88	111.00
1	A	328	ILE	O-C-N	-9.34	107.76	122.70
1	A	628	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	B	485	ILE	O-C-N	-9.32	107.78	122.70
1	B	554	ASP	CA-C-N	-9.32	96.69	117.20
1	A	147	ASN	CA-CB-CG	-9.31	92.92	113.40
1	B	215	ARG	CB-CG-CD	9.31	135.80	111.60
1	B	13	ASP	CB-CG-OD1	-9.30	109.93	118.30
1	A	264	TYR	CB-CG-CD2	9.30	126.58	121.00
1	A	260	THR	CA-CB-CG2	9.29	125.41	112.40
1	A	499	ARG	NE-CZ-NH1	-9.29	115.65	120.30
1	B	241	ASP	CB-CG-OD2	-9.27	109.96	118.30
1	B	518	THR	O-C-N	9.26	137.51	122.70
1	A	486	GLU	C-N-CA	9.25	144.81	121.70
1	B	439	SER	O-C-N	9.21	138.86	123.20
1	A	80	ARG	O-C-N	9.21	137.44	122.70
1	A	370	HIS	CA-CB-CG	9.21	129.26	113.60
1	A	83	ALA	CB-CA-C	-9.19	96.31	110.10
1	B	418	ILE	N-CA-CB	9.18	131.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	LEU	CB-CG-CD2	-9.17	95.41	111.00
1	A	260	THR	CA-CB-OG1	-9.16	89.77	109.00
1	B	218	GLU	N-CA-CB	9.15	127.06	110.60
1	A	441	GLU	OE1-CD-OE2	9.14	134.28	123.30
1	B	226	GLN	CB-CA-C	9.14	128.69	110.40
1	B	201	PHE	CD1-CG-CD2	9.14	130.18	118.30
1	A	245	GLU	O-C-N	-9.13	108.08	122.70
1	B	539	LEU	O-C-N	9.13	137.30	122.70
1	A	253	ARG	NH1-CZ-NH2	-9.10	109.39	119.40
1	A	277	PHE	CB-CG-CD2	9.10	127.17	120.80
1	B	296	ILE	O-C-N	9.09	137.24	122.70
1	B	423	ILE	CB-CA-C	9.08	129.76	111.60
1	B	53	VAL	O-C-N	-9.08	108.17	122.70
1	A	262	TYR	CG-CD1-CE1	9.07	128.56	121.30
1	E	643	LYS	CA-CB-CG	9.07	133.36	113.40
1	A	179	GLN	N-CA-C	-9.06	86.54	111.00
1	D	525	ASP	CB-CG-OD2	9.06	126.45	118.30
1	B	105	TYR	CB-CG-CD2	-9.05	115.57	121.00
1	A	308	SER	N-CA-CB	9.05	124.08	110.50
1	B	319	LYS	O-C-N	9.05	138.59	123.20
1	B	372	GLU	CG-CD-OE1	-9.05	100.20	118.30
1	A	25	THR	OG1-CB-CG2	9.04	130.80	110.00
1	B	439	SER	N-CA-C	-9.04	86.58	111.00
1	A	486	GLU	CA-C-O	9.04	139.09	120.10
1	B	554	ASP	C-N-CA	9.02	144.25	121.70
1	A	262	TYR	CB-CG-CD1	9.01	126.40	121.00
1	B	99	PHE	CA-CB-CG	8.99	135.47	113.90
1	A	100	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	A	456	ASN	CA-C-O	8.98	138.95	120.10
1	A	65	LEU	N-CA-CB	-8.95	92.49	110.40
1	A	313	ILE	CA-CB-CG2	8.95	128.79	110.90
1	B	277	PHE	CB-CA-C	-8.94	92.52	110.40
1	B	304	TYR	CB-CG-CD2	8.93	126.36	121.00
1	A	32	ASP	CB-CG-OD1	8.93	126.33	118.30
1	A	149	GLU	CG-CD-OE2	-8.93	100.45	118.30
1	A	361	PHE	O-C-N	8.92	136.97	122.70
1	A	38	ASN	CB-CG-OD1	8.91	139.42	121.60
1	A	546	ALA	O-C-N	8.91	136.96	122.70
1	B	306	THR	OG1-CB-CG2	8.91	130.48	110.00
1	D	643	LYS	CA-CB-CG	8.89	132.97	113.40
1	B	489	ASN	N-CA-C	-8.89	86.99	111.00
1	C	643	LYS	CA-CB-CG	8.88	132.94	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ASP	CB-CG-OD1	8.88	126.29	118.30
1	B	399	PRO	O-C-N	8.88	137.96	121.10
1	A	329	GLU	O-C-N	8.87	136.89	122.70
1	A	407	GLU	O-C-N	-8.87	108.51	122.70
1	A	435	ASN	CB-CG-OD1	-8.87	103.87	121.60
1	B	143	HIS	O-C-N	8.87	136.88	122.70
1	B	178	GLU	O-C-N	8.86	136.88	122.70
1	A	521	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	632	ASP	CA-CB-CG	8.86	132.88	113.40
1	A	312	THR	O-C-N	8.85	136.86	122.70
1	B	461	THR	CA-CB-OG1	-8.83	90.45	109.00
1	A	35	GLU	CG-CD-OE2	8.82	135.95	118.30
1	A	179	GLN	CB-CA-C	8.82	128.04	110.40
1	A	583	TYR	CB-CG-CD2	-8.81	115.72	121.00
1	A	614	GLU	OE1-CD-OE2	8.81	133.87	123.30
1	B	442	ASN	CA-CB-CG	-8.80	94.04	113.40
1	B	181	VAL	CB-CA-C	8.79	128.10	111.40
1	B	319	LYS	N-CA-CB	8.79	126.42	110.60
1	B	583	TYR	CB-CG-CD2	-8.79	115.73	121.00
1	A	291	ILE	CA-C-N	8.79	136.53	117.20
1	B	29	ASP	CB-CG-OD2	8.78	126.21	118.30
1	B	309	ASP	CB-CG-OD2	-8.78	110.40	118.30
1	A	23	GLU	OE1-CD-OE2	8.77	133.83	123.30
1	A	152	ASP	CB-CG-OD1	8.77	126.19	118.30
1	B	184	PHE	CB-CG-CD1	8.76	126.93	120.80
1	A	340	TYR	CD1-CE1-CZ	-8.76	111.92	119.80
1	B	342	SER	CA-C-O	8.75	138.47	120.10
1	B	479	ARG	NE-CZ-NH1	-8.75	115.93	120.30
1	A	309	ASP	C-N-CA	-8.72	103.98	122.30
1	B	500	TRP	CB-CG-CD2	-8.72	115.26	126.60
1	A	67	GLU	CA-CB-CG	8.71	132.57	113.40
1	A	157	ALA	N-CA-CB	8.70	122.28	110.10
1	A	302	HIS	N-CA-CB	8.70	126.25	110.60
1	B	474	ARG	CG-CD-NE	8.69	130.06	111.80
1	B	65	LEU	O-C-N	-8.69	108.79	122.70
1	A	474	ARG	CD-NE-CZ	8.69	135.76	123.60
1	B	625	PRO	N-CA-CB	-8.69	92.88	103.30
1	B	407	GLU	CA-CB-CG	8.68	132.50	113.40
1	A	86	LEU	O-C-N	8.67	136.58	122.70
1	A	295	ARG	NH1-CZ-NH2	8.65	128.92	119.40
1	A	388	ASP	CB-CG-OD1	-8.65	110.51	118.30
1	B	486	GLU	CG-CD-OE1	8.63	135.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	THR	CA-C-O	8.62	138.21	120.10
1	A	175	LYS	O-C-N	8.62	136.50	122.70
1	B	242	PRO	N-CA-CB	-8.62	92.96	103.30
1	B	643	LYS	CA-CB-CG	8.61	132.34	113.40
1	F	643	LYS	CA-CB-CG	8.60	132.31	113.40
1	B	456	ASN	CB-CG-OD1	-8.59	104.41	121.60
1	B	487	ASP	CB-CG-OD1	8.59	126.03	118.30
1	B	359	GLY	O-C-N	-8.58	108.97	122.70
1	A	72	TYR	CG-CD1-CE1	-8.58	114.44	121.30
1	A	8	ALA	CB-CA-C	-8.58	97.23	110.10
1	A	496	ASP	N-CA-C	-8.57	87.86	111.00
1	B	504	GLU	O-C-N	8.56	136.40	122.70
1	A	316	ARG	CG-CD-NE	8.56	129.78	111.80
1	B	582	LEU	CB-CA-C	8.56	126.46	110.20
1	A	543	ALA	C-N-CA	8.56	143.09	121.70
1	B	560	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	A	152	ASP	CA-C-O	-8.53	102.18	120.10
1	B	218	GLU	OE1-CD-OE2	8.53	133.54	123.30
1	B	226	GLN	OE1-CD-NE2	8.52	141.50	121.90
1	A	331	SER	O-C-N	8.51	136.32	122.70
1	C	555	LEU	CB-CA-C	8.50	126.35	110.20
1	A	412	VAL	N-CA-CB	-8.49	92.82	111.50
1	A	180	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	A	99	PHE	CA-CB-CG	8.48	134.25	113.90
1	A	162	LYS	N-CA-C	-8.47	88.13	111.00
1	A	169	SER	N-CA-CB	-8.47	97.79	110.50
1	A	501	PHE	N-CA-CB	-8.46	95.37	110.60
1	A	525	ASP	CB-CG-OD2	-8.46	110.69	118.30
1	B	295	ARG	CB-CG-CD	8.46	133.59	111.60
1	B	78	ARG	NH1-CZ-NH2	-8.45	110.11	119.40
1	A	216	LYS	N-CA-CB	8.44	125.79	110.60
1	A	442	ASN	N-CA-CB	8.44	125.78	110.60
1	A	494	THR	N-CA-C	8.43	133.77	111.00
1	A	387	MET	N-CA-CB	8.43	125.77	110.60
1	A	304	TYR	CB-CG-CD2	8.42	126.05	121.00
1	B	311	HIS	O-C-N	8.42	136.17	122.70
1	B	412	VAL	O-C-N	8.41	136.16	122.70
1	A	26	LYS	CD-CE-NZ	8.41	131.04	111.70
1	B	416	VAL	CA-CB-CG1	8.39	123.49	110.90
1	A	53	VAL	CA-CB-CG2	-8.39	98.31	110.90
1	B	583	TYR	O-C-N	8.39	136.12	122.70
1	A	117	TYR	CD1-CE1-CZ	-8.38	112.26	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	TYR	CG-CD2-CE2	8.37	128.00	121.30
1	A	149	GLU	CA-CB-CG	8.37	131.81	113.40
1	B	149	GLU	N-CA-CB	-8.37	95.53	110.60
1	B	308	SER	CA-CB-OG	8.36	133.77	111.20
1	B	61	ASN	OD1-CG-ND2	8.35	141.11	121.90
1	A	376	ARG	NH1-CZ-NH2	8.35	128.58	119.40
1	B	77	THR	N-CA-CB	8.35	126.16	110.30
1	B	386	TYR	O-C-N	-8.34	109.35	122.70
1	A	470	ASN	CA-C-O	8.34	137.61	120.10
1	A	585	ALA	CB-CA-C	8.33	122.60	110.10
1	B	67	GLU	OE1-CD-OE2	8.31	133.28	123.30
1	A	235	ARG	O-C-N	8.31	136.00	122.70
1	A	375	THR	CA-CB-OG1	-8.31	91.55	109.00
1	A	73	SER	O-C-N	8.31	135.99	122.70
1	B	187	ASP	CB-CG-OD1	-8.29	110.84	118.30
1	B	138	TYR	CB-CG-CD1	8.29	125.97	121.00
1	B	338	GLN	O-C-N	8.29	135.96	122.70
1	B	46	TYR	CB-CG-CD2	8.28	125.97	121.00
1	B	346	THR	CA-CB-CG2	-8.27	100.82	112.40
1	B	114	GLU	OE1-CD-OE2	-8.27	113.38	123.30
1	B	30	LEU	CA-CB-CG	-8.26	96.30	115.30
1	A	251	ILE	CA-CB-CG1	-8.26	95.31	111.00
1	A	322	GLU	OE1-CD-OE2	-8.26	113.39	123.30
1	B	240	LEU	CB-CG-CD2	-8.26	96.97	111.00
1	A	227	LEU	N-CA-CB	8.24	126.89	110.40
1	A	34	ALA	O-C-N	8.22	135.86	122.70
1	A	380	PHE	CG-CD1-CE1	8.22	129.84	120.80
1	B	401	TYR	CB-CG-CD2	8.22	125.93	121.00
1	A	489	ASN	CA-C-N	-8.21	99.77	116.20
1	A	235	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	A	584	VAL	CG1-CB-CG2	8.21	124.04	110.90
1	A	469	ASN	CB-CA-C	8.20	126.80	110.40
1	B	313	ILE	CA-CB-CG2	8.20	127.31	110.90
1	B	458	ASN	N-CA-CB	-8.20	95.84	110.60
1	A	254	GLU	CG-CD-OE1	-8.20	101.90	118.30
1	A	52	ALA	O-C-N	8.20	135.81	122.70
1	B	503	ILE	CA-CB-CG1	8.20	126.57	111.00
1	A	47	ASN	CA-CB-CG	8.19	131.42	113.40
1	A	212	HIS	CA-C-O	-8.19	102.91	120.10
1	A	47	ASN	N-CA-CB	8.18	125.33	110.60
1	A	169	SER	N-CA-C	8.18	133.10	111.00
1	A	407	GLU	C-N-CA	8.18	142.15	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	432	SER	N-CA-CB	-8.18	98.23	110.50
1	B	408	PHE	N-CA-CB	8.18	125.31	110.60
1	A	180	ARG	NH1-CZ-NH2	8.17	128.39	119.40
1	A	228	THR	CA-CB-CG2	8.17	123.84	112.40
1	A	449	ASN	O-C-N	8.17	135.77	122.70
1	A	317	GLN	CG-CD-OE1	8.17	137.93	121.60
1	D	35	GLU	CG-CD-OE2	8.16	134.62	118.30
1	B	231	PHE	CE1-CZ-CE2	-8.16	105.32	120.00
1	C	67	GLU	CA-CB-CG	8.16	131.35	113.40
1	A	201	PHE	CB-CG-CD1	-8.15	115.09	120.80
1	B	497	GLU	N-CA-CB	8.15	125.28	110.60
1	A	275	ILE	CB-CA-C	-8.15	95.31	111.60
1	B	51	ALA	N-CA-CB	-8.14	98.70	110.10
1	B	177	ARG	CA-C-O	8.14	137.21	120.10
1	A	78	ARG	CD-NE-CZ	8.14	134.99	123.60
1	B	88	ALA	CA-C-O	-8.13	103.02	120.10
1	A	431	TYR	CB-CG-CD2	8.13	125.88	121.00
1	A	241	ASP	CB-CG-OD2	8.13	125.62	118.30
1	B	100	ARG	CB-CG-CD	8.12	132.72	111.60
1	B	132	ILE	O-C-N	8.12	135.70	122.70
1	B	344	HIS	ND1-CG-CD2	8.12	120.17	108.80
1	A	149	GLU	CG-CD-OE1	8.12	134.53	118.30
1	A	219	LEU	CB-CA-C	8.11	125.62	110.20
1	B	165	THR	CA-CB-OG1	-8.11	91.96	109.00
1	B	391	PHE	CB-CG-CD2	8.11	126.48	120.80
1	B	520	GLU	CB-CG-CD	8.11	136.09	114.20
1	A	254	GLU	CG-CD-OE2	8.11	134.51	118.30
1	E	67	GLU	CA-CB-CG	8.08	131.17	113.40
1	A	505	LEU	O-C-N	-8.08	109.78	122.70
1	B	469	ASN	CB-CG-ND2	-8.07	97.32	116.70
1	A	410	GLY	CA-C-O	-8.07	106.08	120.60
1	A	487	ASP	CB-CG-OD1	8.06	125.56	118.30
1	F	67	GLU	CA-CB-CG	8.06	131.14	113.40
1	B	585	ALA	O-C-N	8.05	135.59	122.70
1	B	384	HIS	O-C-N	8.05	135.58	122.70
1	B	554	ASP	CA-C-O	8.05	137.00	120.10
1	A	234	GLU	N-CA-CB	8.05	125.08	110.60
1	A	608	GLN	O-C-N	8.04	135.57	122.70
1	B	504	GLU	OE1-CD-OE2	8.04	132.95	123.30
1	A	268	PHE	CB-CG-CD2	-8.04	115.17	120.80
1	A	554	ASP	N-CA-CB	8.04	125.08	110.60
1	A	9	GLN	O-C-N	8.04	135.56	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	HIS	CA-CB-CG	-8.03	99.94	113.60
1	B	407	GLU	CG-CD-OE1	-8.02	102.27	118.30
1	B	166	PHE	CA-C-O	8.02	136.94	120.10
1	B	70	HIS	CA-C-O	-8.02	103.27	120.10
1	B	231	PHE	CB-CG-CD1	8.01	126.41	120.80
1	D	67	GLU	CA-CB-CG	8.01	131.03	113.40
1	A	374	ALA	CB-CA-C	8.01	122.12	110.10
1	A	373	THR	CA-CB-OG1	-8.01	92.19	109.00
1	A	213	LEU	C-N-CA	8.00	141.71	121.70
1	A	279	ASP	CB-CA-C	8.00	126.40	110.40
1	A	457	HIS	O-C-N	8.00	135.50	122.70
1	F	92	GLN	CA-CB-CG	8.00	130.99	113.40
1	A	309	ASP	CA-CB-CG	-7.99	95.82	113.40
1	A	432	SER	CA-C-O	7.99	136.87	120.10
1	A	479	ARG	NH1-CZ-NH2	7.97	128.17	119.40
1	C	92	GLN	CA-CB-CG	7.97	130.93	113.40
1	B	187	ASP	O-C-N	-7.96	109.96	122.70
1	B	561	SER	N-CA-C	7.96	132.50	111.00
1	B	614	GLU	N-CA-CB	-7.96	96.27	110.60
1	A	277	PHE	N-CA-CB	7.96	124.92	110.60
1	B	488	ASN	N-CA-CB	7.96	124.92	110.60
1	B	330	SER	CA-C-O	-7.96	103.39	120.10
1	A	211	TYR	N-CA-CB	-7.95	96.29	110.60
1	B	528	VAL	CA-C-O	-7.95	103.40	120.10
1	B	427	ASP	N-CA-CB	-7.95	96.30	110.60
1	A	376	ARG	NE-CZ-NH1	-7.94	116.33	120.30
1	C	169	SER	N-CA-C	7.94	132.44	111.00
1	B	162	LYS	N-CA-CB	-7.94	96.31	110.60
1	B	529	THR	CA-C-O	7.94	136.78	120.10
1	A	279	ASP	CA-CB-CG	7.93	130.85	113.40
1	B	253	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	A	407	GLU	CG-CD-OE2	7.93	134.16	118.30
1	D	494	THR	N-CA-C	7.93	132.40	111.00
1	B	304	TYR	CG-CD1-CE1	-7.92	114.96	121.30
1	F	494	THR	N-CA-C	7.92	132.38	111.00
1	F	547	VAL	N-CA-C	-7.92	89.62	111.00
1	D	169	SER	N-CA-C	7.92	132.37	111.00
1	A	217	GLY	N-CA-C	-7.91	93.32	113.10
1	A	337	VAL	CA-CB-CG2	7.91	122.77	110.90
1	E	169	SER	N-CA-C	7.91	132.36	111.00
1	A	628	ARG	CB-CA-C	7.91	126.22	110.40
1	B	86	LEU	CB-CA-C	7.91	125.22	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	PHE	CA-C-O	-7.90	103.51	120.10
1	F	169	SER	N-CA-C	7.89	132.32	111.00
1	B	235	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	B	317	GLN	CB-CG-CD	7.88	132.10	111.60
1	B	178	GLU	CB-CA-C	-7.88	94.63	110.40
1	A	32	ASP	O-C-N	7.88	135.31	122.70
1	A	160	THR	CA-CB-CG2	-7.88	101.37	112.40
1	A	216	LYS	CA-CB-CG	7.88	130.73	113.40
1	A	299	ALA	CB-CA-C	7.88	121.92	110.10
1	A	259	LEU	CB-CG-CD1	7.87	124.37	111.00
1	A	406	LEU	CA-CB-CG	-7.86	97.22	115.30
1	B	108	GLU	CG-CD-OE1	7.86	134.01	118.30
1	B	298	GLU	CG-CD-OE2	7.85	134.01	118.30
1	A	566	ASP	CB-CG-OD2	-7.85	111.24	118.30
1	B	496	ASP	OD1-CG-OD2	-7.84	108.40	123.30
1	B	232	ASP	OD1-CG-OD2	-7.84	108.41	123.30
1	A	635	VAL	O-C-N	7.83	135.23	122.70
1	B	522	SER	N-CA-C	7.83	132.14	111.00
1	A	358	HIS	CB-CA-C	7.83	126.05	110.40
1	B	581	ASN	N-CA-CB	-7.83	96.52	110.60
1	A	374	ALA	O-C-N	-7.82	110.18	122.70
1	A	505	LEU	CB-CA-C	7.82	125.06	110.20
1	B	201	PHE	CB-CG-CD1	-7.82	115.33	120.80
1	A	161	GLN	CA-CB-CG	-7.82	96.20	113.40
1	D	92	GLN	CA-CB-CG	7.82	130.60	113.40
1	B	145	PHE	CA-CB-CG	7.82	132.66	113.90
1	C	494	THR	N-CA-C	7.81	132.09	111.00
1	B	80	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	B	555	LEU	O-C-N	7.80	135.18	122.70
1	A	444	GLU	CA-CB-CG	7.79	130.53	113.40
1	A	380	PHE	CD1-CE1-CZ	-7.78	110.76	120.10
1	A	594	GLU	CG-CD-OE1	-7.78	102.73	118.30
1	B	393	LYS	N-CA-CB	7.78	124.60	110.60
1	B	46	TYR	CA-C-N	7.78	134.31	117.20
1	A	520	GLU	CG-CD-OE1	-7.77	102.76	118.30
1	B	175	LYS	CA-CB-CG	7.76	130.48	113.40
1	B	65	LEU	CB-CA-C	7.76	124.94	110.20
1	A	211	TYR	CB-CA-C	7.75	125.89	110.40
1	A	429	PHE	CB-CG-CD1	-7.75	115.38	120.80
1	B	401	TYR	CA-CB-CG	7.74	128.10	113.40
1	B	32	ASP	O-C-N	7.72	135.06	122.70
1	B	217	GLY	O-C-N	7.72	135.06	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	ASN	CA-C-O	-7.72	103.89	120.10
1	B	390	ILE	N-CA-CB	7.71	128.54	110.80
1	B	11	GLN	CG-CD-OE1	-7.70	106.20	121.60
1	A	190	MET	N-CA-CB	7.68	124.43	110.60
1	A	584	VAL	CA-CB-CG1	-7.68	99.37	110.90
1	A	622	LEU	CB-CG-CD2	-7.68	97.94	111.00
1	A	67	GLU	OE1-CD-OE2	-7.67	114.09	123.30
1	B	279	ASP	CB-CG-OD1	7.66	125.20	118.30
1	B	330	SER	N-CA-CB	7.66	122.00	110.50
1	A	559	GLU	OE1-CD-OE2	7.66	132.49	123.30
1	A	25	THR	CB-CA-C	-7.65	90.95	111.60
1	A	634	ARG	CB-CG-CD	7.65	131.49	111.60
1	B	197	TRP	CE3-CZ3-CH2	-7.64	112.80	121.20
1	B	364	PRO	CA-C-O	-7.64	101.87	120.20
1	B	491	ILE	CB-CA-C	7.64	126.88	111.60
1	B	7	ASN	N-CA-CB	7.63	124.34	110.60
1	B	289	LEU	CA-CB-CG	7.63	132.85	115.30
1	B	618	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	299	ALA	N-CA-C	-7.62	90.43	111.00
1	A	240	LEU	O-C-N	-7.61	110.53	122.70
1	B	263	LYS	N-CA-CB	7.61	124.29	110.60
1	B	416	VAL	C-N-CA	7.61	140.71	121.70
1	B	13	ASP	O-C-N	-7.60	110.53	122.70
1	E	494	THR	N-CA-C	7.60	131.53	111.00
1	A	16	HIS	N-CA-CB	7.59	124.27	110.60
1	A	158	LYS	CD-CE-NZ	-7.59	94.25	111.70
1	A	285	HIS	O-C-N	-7.59	110.56	122.70
1	B	264	TYR	CB-CG-CD1	-7.58	116.45	121.00
1	B	88	ALA	O-C-N	7.57	134.82	122.70
1	B	229	ALA	CB-CA-C	-7.57	98.74	110.10
1	A	178	GLU	OE1-CD-OE2	-7.55	114.23	123.30
1	B	353	ARG	CD-NE-CZ	-7.55	113.03	123.60
1	A	213	LEU	CB-CA-C	7.55	124.54	110.20
1	A	629	ARG	CA-CB-CG	7.55	130.00	113.40
1	A	620	ARG	NH1-CZ-NH2	-7.54	111.10	119.40
1	A	555	LEU	CA-C-O	-7.54	104.27	120.10
1	B	276	HIS	CA-CB-CG	-7.54	100.78	113.60
1	E	92	GLN	CA-CB-CG	7.54	129.99	113.40
1	A	159	MET	CA-CB-CG	7.54	126.11	113.30
1	B	281	ASP	CB-CG-OD1	-7.53	111.52	118.30
1	B	592	ASP	O-C-N	7.53	134.75	122.70
1	A	513	PRO	CB-CA-C	7.53	130.82	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	LEU	N-CA-CB	-7.53	95.34	110.40
1	A	415	GLY	O-C-N	7.53	134.74	122.70
1	B	149	GLU	OE1-CD-OE2	7.52	132.32	123.30
1	A	121	VAL	CA-CB-CG2	-7.52	99.63	110.90
1	B	578	MET	O-C-N	7.51	134.72	122.70
1	A	460	PHE	CA-CB-CG	7.51	131.93	113.90
1	B	375	THR	CA-CB-CG2	7.50	122.91	112.40
1	A	8	ALA	C-N-CA	7.50	140.45	121.70
1	B	314	ASP	CA-C-O	-7.50	104.35	120.10
1	B	496	ASP	N-CA-C	-7.50	90.76	111.00
1	B	306	THR	CA-CB-CG2	-7.50	101.91	112.40
1	B	463	LYS	N-CA-CB	7.50	124.09	110.60
1	A	406	LEU	O-C-N	-7.50	110.71	122.70
1	A	7	ASN	N-CA-CB	7.49	124.08	110.60
1	B	379	SER	O-C-N	-7.48	110.73	122.70
1	B	498	ALA	O-C-N	-7.48	110.72	122.70
1	A	210	GLY	N-CA-C	7.48	131.81	113.10
1	B	200	ASP	CB-CG-OD1	-7.48	111.57	118.30
1	B	155	TYR	CG-CD1-CE1	7.47	127.28	121.30
1	B	231	PHE	CZ-CE2-CD2	7.46	129.06	120.10
1	D	458	ASN	CA-CB-CG	7.46	129.81	113.40
1	A	567	ARG	NH1-CZ-NH2	-7.46	111.20	119.40
1	B	67	GLU	CB-CA-C	-7.45	95.49	110.40
1	B	45	ILE	O-C-N	7.45	134.62	122.70
1	B	197	TRP	N-CA-CB	7.44	124.00	110.60
1	A	556	SER	N-CA-CB	7.44	121.66	110.50
1	B	534	PRO	CB-CA-C	-7.44	93.40	112.00
1	A	160	THR	OG1-CB-CG2	7.43	127.10	110.00
1	A	292	THR	CA-CB-CG2	7.43	122.80	112.40
1	A	534	PRO	N-CD-CG	-7.42	92.06	103.20
1	B	77	THR	CA-C-O	-7.42	104.52	120.10
1	B	112	GLU	CB-CA-C	-7.41	95.59	110.40
1	B	147	ASN	CB-CA-C	-7.40	95.60	110.40
1	A	76	ASN	OD1-CG-ND2	7.39	138.91	121.90
1	A	183	TYR	CD1-CE1-CZ	-7.39	113.15	119.80
1	A	302	HIS	CB-CA-C	-7.39	95.63	110.40
1	A	278	GLU	CA-C-N	-7.38	100.96	117.20
1	A	458	ASN	CB-CG-OD1	7.38	136.36	121.60
1	B	230	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	347	ALA	N-CA-CB	7.37	120.42	110.10
1	B	36	ASN	N-CA-CB	-7.37	97.33	110.60
1	B	92	GLN	CB-CG-CD	-7.37	92.44	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	HIS	CA-C-O	-7.37	104.63	120.10
1	A	231	PHE	CA-C-O	-7.37	104.63	120.10
1	A	249	ASP	CB-CG-OD1	-7.37	111.67	118.30
1	E	207	ASP	CB-CG-OD1	7.37	124.93	118.30
1	B	376	ARG	N-CA-CB	7.36	123.85	110.60
1	B	322	GLU	N-CA-CB	7.36	123.84	110.60
1	A	563	GLY	N-CA-C	7.35	131.47	113.10
1	A	151	ILE	O-C-N	7.35	134.46	122.70
1	A	322	GLU	CB-CA-C	7.34	125.08	110.40
1	B	419	ASP	CB-CG-OD1	-7.34	111.69	118.30
1	A	15	ASN	CB-CG-OD1	-7.33	106.93	121.60
1	A	80	ARG	N-CA-CB	7.33	123.79	110.60
1	A	145	PHE	C-N-CA	7.33	140.02	121.70
1	A	48	ASP	CA-CB-CG	7.32	129.51	113.40
1	A	101	SER	CB-CA-C	7.32	124.01	110.10
1	B	463	LYS	CB-CG-CD	7.32	130.64	111.60
1	A	61	ASN	CA-CB-CG	-7.32	97.29	113.40
1	B	399	PRO	CA-C-O	-7.32	102.63	120.20
1	B	192	ILE	CA-CB-CG1	-7.32	97.09	111.00
1	A	339	TYR	CD1-CE1-CZ	7.31	126.38	119.80
1	B	108	GLU	OE1-CD-OE2	-7.31	114.53	123.30
1	B	521	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	A	444	GLU	OE1-CD-OE2	-7.30	114.55	123.30
1	B	259	LEU	O-C-N	-7.29	111.03	122.70
1	A	501	PHE	O-C-N	-7.29	111.03	122.70
1	D	419	ASP	CB-CA-C	7.29	124.98	110.40
1	A	441	GLU	CB-CG-CD	-7.29	94.53	114.20
1	A	283	VAL	CB-CA-C	7.29	125.24	111.40
1	B	149	GLU	CG-CD-OE2	-7.28	103.74	118.30
1	A	489	ASN	CB-CA-C	7.28	124.96	110.40
1	B	214	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	B	616	TYR	CB-CG-CD1	-7.27	116.64	121.00
1	B	489	ASN	C-N-CA	-7.27	107.03	122.30
1	C	387	MET	CA-CB-CG	7.27	125.66	113.30
1	B	205	TRP	CG-CD1-NE1	7.26	117.36	110.10
1	B	179	GLN	CA-C-N	-7.26	101.23	117.20
1	B	299	ALA	N-CA-CB	-7.26	99.94	110.10
1	A	234	GLU	CA-C-O	-7.25	104.88	120.10
1	A	74	LEU	O-C-N	7.25	134.29	122.70
1	A	513	PRO	N-CA-CB	-7.25	94.60	103.30
1	A	386	TYR	CA-C-O	-7.25	104.89	120.10
1	A	339	TYR	CG-CD1-CE1	-7.24	115.51	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	ASN	CA-C-O	-7.24	104.89	120.10
1	B	613	GLY	O-C-N	7.24	134.29	122.70
1	A	25	THR	CA-C-O	-7.24	104.91	120.10
1	F	279	ASP	CB-CG-OD1	7.24	124.81	118.30
1	B	116	VAL	CG1-CB-CG2	-7.23	99.33	110.90
1	A	557	ALA	CB-CA-C	-7.22	99.27	110.10
1	A	653	LEU	CB-CA-C	7.22	123.92	110.20
1	B	62	ASP	CB-CG-OD1	7.22	124.80	118.30
1	B	429	PHE	N-CA-CB	-7.22	97.61	110.60
1	A	542	GLN	CG-CD-OE1	-7.22	107.17	121.60
1	A	518	THR	CA-CB-CG2	7.21	122.50	112.40
1	B	169	SER	N-CA-CB	-7.21	99.68	110.50
1	B	579	GLU	O-C-N	-7.21	111.16	122.70
1	B	313	ILE	CA-C-O	7.21	135.24	120.10
1	B	548	ASN	CB-CG-OD1	7.20	136.01	121.60
1	F	207	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	459	GLU	OE1-CD-OE2	7.19	131.93	123.30
1	A	80	ARG	CA-C-O	-7.19	105.00	120.10
1	A	111	ASN	CB-CG-OD1	-7.18	107.23	121.60
1	A	177	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	401	TYR	CB-CG-CD1	-7.17	116.69	121.00
1	B	6	GLY	CA-C-N	-7.17	101.42	117.20
1	F	387	MET	CA-CB-CG	7.17	125.50	113.30
1	B	382	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	401	TYR	CG-CD1-CE1	7.17	127.03	121.30
1	A	396	ASP	CA-C-N	7.16	132.96	117.20
1	A	183	TYR	CA-C-O	-7.16	105.06	120.10
1	A	608	GLN	CG-CD-OE1	-7.16	107.28	121.60
1	B	559	GLU	N-CA-CB	7.15	123.48	110.60
1	B	372	GLU	CG-CD-OE2	7.15	132.59	118.30
1	A	79	GLN	CB-CA-C	7.15	124.69	110.40
1	B	202	PRO	O-C-N	7.14	134.13	122.70
1	B	481	PHE	CB-CG-CD2	-7.14	115.80	120.80
1	B	391	PHE	CG-CD2-CE2	7.14	128.66	120.80
1	A	129	GLY	CA-C-O	-7.13	107.77	120.60
1	B	69	ARG	NH1-CZ-NH2	-7.13	111.56	119.40
1	B	138	TYR	CA-CB-CG	7.13	126.94	113.40
1	A	7	ASN	OD1-CG-ND2	7.12	138.29	121.90
1	A	59	GLU	N-CA-CB	7.12	123.42	110.60
1	B	455	LEU	CA-CB-CG	7.12	131.68	115.30
1	C	207	ASP	CB-CG-OD1	7.12	124.71	118.30
1	B	542	GLN	CA-CB-CG	7.12	129.06	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	HIS	CA-CB-CG	-7.11	101.51	113.60
1	A	463	LYS	N-CA-C	-7.10	91.84	111.00
1	A	372	GLU	CG-CD-OE2	-7.09	104.13	118.30
1	A	92	GLN	CB-CG-CD	-7.08	93.18	111.60
1	B	438	ASP	CB-CG-OD1	7.08	124.68	118.30
1	E	279	ASP	CB-CG-OD1	7.08	124.67	118.30
1	A	32	ASP	N-CA-CB	7.07	123.33	110.60
1	A	27	TYR	CG-CD1-CE1	7.07	126.95	121.30
1	A	548	ASN	CA-CB-CG	7.07	128.95	113.40
1	D	521	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	512	VAL	CA-CB-CG1	-7.06	100.31	110.90
1	A	479	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	328	ILE	O-C-N	-7.06	111.41	122.70
1	B	404	ASP	CB-CG-OD1	-7.05	111.95	118.30
1	D	387	MET	CA-CB-CG	7.05	125.28	113.30
1	B	509	PHE	CZ-CE2-CD2	-7.05	111.64	120.10
1	A	168	VAL	C-N-CA	7.04	139.31	121.70
1	B	406	LEU	O-C-N	-7.04	111.44	122.70
1	A	57	MET	CG-SD-CE	7.04	111.46	100.20
1	B	288	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	B	306	THR	CA-C-O	-7.03	105.33	120.10
1	A	231	PHE	CZ-CE2-CD2	-7.03	111.67	120.10
1	A	303	GLY	CA-C-O	-7.03	107.95	120.60
1	A	331	SER	CA-C-O	-7.03	105.34	120.10
1	A	509	PHE	CG-CD2-CE2	7.03	128.53	120.80
1	B	216	LYS	N-CA-CB	7.03	123.25	110.60
1	B	319	LYS	CB-CA-C	-7.03	96.35	110.40
1	B	554	ASP	CB-CA-C	7.02	124.45	110.40
1	A	62	ASP	CA-C-O	7.02	134.84	120.10
1	A	309	ASP	OD1-CG-OD2	7.02	136.63	123.30
1	B	518	THR	N-CA-CB	7.00	123.60	110.30
1	A	460	PHE	CB-CG-CD1	7.00	125.70	120.80
1	B	179	GLN	CB-CA-C	7.00	124.39	110.40
1	E	99	PHE	CA-CB-CG	7.00	130.70	113.90
1	A	558	TYR	N-CA-CB	-7.00	98.01	110.60
1	B	376	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	10	LYS	CD-CE-NZ	6.99	127.78	111.70
1	D	279	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	267	GLU	CG-CD-OE1	-6.98	104.34	118.30
1	B	78	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	A	137	LEU	O-C-N	6.97	133.85	122.70
1	A	343	LEU	CD1-CG-CD2	-6.97	89.59	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	TYR	CB-CG-CD2	6.97	125.18	121.00
1	A	387	MET	CB-CA-C	-6.96	96.47	110.40
1	B	196	THR	O-C-N	6.96	133.84	122.70
1	B	344	HIS	CG-CD2-NE2	-6.96	95.97	109.20
1	B	85	MET	N-CA-CB	6.96	123.13	110.60
1	A	373	THR	N-CA-CB	-6.96	97.08	110.30
1	B	91	ASN	CA-C-O	-6.96	105.49	120.10
1	B	214	ASP	O-C-N	-6.95	111.58	122.70
1	A	487	ASP	CA-C-O	-6.95	105.50	120.10
1	A	70	HIS	O-C-N	6.95	133.81	122.70
1	A	419	ASP	N-CA-CB	-6.95	98.10	110.60
1	B	170	PHE	CA-C-O	-6.94	105.52	120.10
1	B	505	LEU	O-C-N	-6.94	111.60	122.70
1	B	476	ALA	CA-C-O	6.94	134.67	120.10
1	D	219	LEU	CB-CA-C	6.94	123.38	110.20
1	F	99	PHE	CA-CB-CG	6.93	130.54	113.90
1	B	241	ASP	CB-CG-OD1	6.93	124.54	118.30
1	B	265	GLY	O-C-N	-6.93	111.42	123.20
1	B	386	TYR	CG-CD1-CE1	6.93	126.85	121.30
1	E	387	MET	CA-CB-CG	6.93	125.08	113.30
1	D	513	PRO	N-CA-C	6.93	130.12	112.10
1	B	233	PHE	N-CA-CB	6.93	123.07	110.60
1	A	350	MET	CA-CB-CG	-6.92	101.53	113.30
1	B	92	GLN	CG-CD-OE1	-6.92	107.75	121.60
1	B	528	VAL	O-C-N	6.92	133.77	122.70
1	E	360	LYS	CA-CB-CG	6.92	128.61	113.40
1	A	620	ARG	CA-CB-CG	6.91	128.61	113.40
1	C	99	PHE	CA-CB-CG	6.91	130.49	113.90
1	B	494	THR	CA-CB-CG2	-6.91	102.72	112.40
1	B	49	HIS	N-CA-CB	6.91	123.03	110.60
1	B	75	PHE	CZ-CE2-CD2	6.91	128.39	120.10
1	A	307	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	B	139	GLN	CA-CB-CG	6.90	128.57	113.40
1	B	203	PHE	O-C-N	-6.89	111.67	122.70
1	B	250	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	32	ASP	CA-C-O	-6.89	105.63	120.10
1	A	190	MET	CA-C-N	-6.89	102.03	117.20
1	A	588	ASP	CB-CG-OD1	6.89	124.50	118.30
1	B	567	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	129	GLY	CA-C-N	6.89	132.36	117.20
1	A	460	PHE	CB-CA-C	-6.89	96.62	110.40
1	B	404	ASP	CB-CG-OD2	6.89	124.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ALA	N-CA-CB	6.89	119.74	110.10
1	B	5	THR	CB-CA-C	-6.88	93.01	111.60
1	A	320	GLY	O-C-N	6.88	133.71	122.70
1	B	278	GLU	CA-CB-CG	-6.88	98.27	113.40
1	B	620	ARG	CD-NE-CZ	-6.87	113.98	123.60
1	B	217	GLY	N-CA-C	-6.87	95.92	113.10
1	A	567	ARG	CG-CD-NE	6.87	126.22	111.80
1	B	57	MET	O-C-N	6.86	133.68	122.70
1	A	590	ASP	CB-CG-OD2	6.86	124.47	118.30
1	B	443	ILE	CB-CA-C	6.86	125.31	111.60
1	B	12	GLN	CB-CA-C	6.86	124.11	110.40
1	E	219	LEU	CB-CA-C	6.86	123.23	110.20
1	A	505	LEU	N-CA-CB	-6.85	96.69	110.40
1	B	446	VAL	CB-CA-C	-6.85	98.38	111.40
1	A	377	ASP	CB-CG-OD2	6.85	124.46	118.30
1	B	336	ASN	CB-CG-OD1	6.85	135.29	121.60
1	B	478	PHE	CB-CG-CD2	-6.85	116.01	120.80
1	A	562	CYS	CB-CA-C	-6.84	96.71	110.40
1	A	49	HIS	N-CA-CB	6.84	122.92	110.60
1	A	323	LEU	CB-CG-CD1	6.84	122.63	111.00
1	B	477	THR	CA-CB-OG1	-6.84	94.63	109.00
1	B	376	ARG	CB-CA-C	-6.84	96.72	110.40
1	A	147	ASN	CB-CA-C	-6.83	96.73	110.40
1	B	443	ILE	CA-CB-CG2	6.83	124.57	110.90
1	D	99	PHE	CA-CB-CG	6.83	130.30	113.90
1	F	179	GLN	N-CA-C	-6.83	92.55	111.00
1	A	646	VAL	CA-CB-CG1	6.83	121.14	110.90
1	A	13	ASP	CB-CG-OD1	-6.83	112.16	118.30
1	B	469	ASN	CA-CB-CG	-6.83	98.38	113.40
1	A	29	ASP	OD1-CG-OD2	6.82	136.26	123.30
1	C	219	LEU	CB-CA-C	6.82	123.16	110.20
1	B	275	ILE	CB-CA-C	-6.82	97.96	111.60
1	B	339	TYR	CZ-CE2-CD2	6.82	125.94	119.80
1	B	543	ALA	C-N-CA	6.82	138.75	121.70
1	B	500	TRP	CB-CG-CD1	6.82	135.86	127.00
1	B	555	LEU	CA-CB-CG	6.82	130.98	115.30
1	A	65	LEU	CB-CA-C	6.81	123.14	110.20
1	F	423	ILE	CB-CA-C	6.81	125.22	111.60
1	B	252	ILE	N-CA-C	-6.81	92.62	111.00
1	C	179	GLN	N-CA-C	-6.81	92.62	111.00
1	B	496	ASP	O-C-N	6.80	133.59	122.70
1	C	279	ASP	CB-CG-OD1	6.80	124.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	MET	CA-CB-CG	-6.80	101.74	113.30
1	B	473	GLU	N-CA-C	-6.80	92.64	111.00
1	B	169	SER	N-CA-C	6.79	129.34	111.00
1	B	93	CYS	CA-CB-SG	-6.79	101.78	114.00
1	B	205	TRP	CD1-NE1-CE2	-6.79	102.89	109.00
1	A	227	LEU	CB-CG-CD1	-6.79	99.46	111.00
1	B	242	PRO	CA-C-N	6.79	132.13	117.20
1	B	93	CYS	O-C-N	6.78	133.56	122.70
1	A	261	SER	O-C-N	6.78	133.55	122.70
1	B	473	GLU	N-CA-CB	6.78	122.80	110.60
1	E	179	GLN	N-CA-C	-6.77	92.71	111.00
1	B	554	ASP	OD1-CG-OD2	-6.77	110.44	123.30
1	A	144	MET	O-C-N	6.77	133.53	122.70
1	A	404	ASP	CB-CG-OD1	6.77	124.39	118.30
1	B	237	SER	N-CA-CB	-6.77	100.35	110.50
1	B	84	LEU	CB-CA-C	6.76	123.05	110.20
1	A	295	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	B	417	ALA	N-CA-C	6.76	129.26	111.00
1	A	435	ASN	O-C-N	6.76	133.51	122.70
1	B	132	ILE	CA-C-O	-6.76	105.91	120.10
1	B	544	ASP	CA-CB-CG	6.76	128.27	113.40
1	A	281	ASP	CB-CG-OD1	-6.76	112.22	118.30
1	A	458	ASN	CA-C-O	-6.76	105.91	120.10
1	B	417	ALA	CB-CA-C	-6.75	99.97	110.10
1	B	398	PHE	CB-CG-CD1	-6.75	116.08	120.80
1	A	349	VAL	CA-C-O	6.75	134.27	120.10
1	A	72	TYR	CB-CG-CD2	-6.74	116.95	121.00
1	A	455	LEU	CB-CG-CD2	-6.74	99.54	111.00
1	D	179	GLN	N-CA-C	-6.74	92.80	111.00
1	B	125	HIS	CA-CB-CG	-6.74	102.14	113.60
1	B	422	LEU	CB-CA-C	6.74	123.00	110.20
1	A	231	PHE	N-CA-CB	6.73	122.71	110.60
1	A	245	GLU	CG-CD-OE2	6.73	131.76	118.30
1	B	449	ASN	CA-CB-CG	6.73	128.20	113.40
1	B	452	VAL	CA-CB-CG1	6.73	120.99	110.90
1	A	144	MET	CG-SD-CE	6.72	110.96	100.20
1	A	536	PHE	CB-CG-CD1	6.72	125.51	120.80
1	E	169	SER	N-CA-CB	-6.72	100.42	110.50
1	F	219	LEU	CB-CA-C	6.72	122.97	110.20
1	A	509	PHE	CZ-CE2-CD2	-6.72	112.04	120.10
1	B	287	HIS	CA-C-N	-6.72	102.42	117.20
1	A	24	PRO	O-C-N	6.71	133.44	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	GLU	O-C-N	6.71	133.44	122.70
1	A	68	GLN	O-C-N	6.71	133.43	122.70
1	A	423	ILE	CB-CA-C	6.70	125.00	111.60
1	B	43	THR	N-CA-CB	-6.70	97.57	110.30
1	A	317	GLN	CA-C-O	6.70	134.17	120.10
1	A	624	TYR	CD1-CE1-CZ	6.70	125.83	119.80
1	A	624	TYR	CG-CD1-CE1	-6.69	115.94	121.30
1	A	183	TYR	N-CA-CB	6.69	122.65	110.60
1	B	561	SER	N-CA-CB	-6.69	100.46	110.50
1	D	496	ASP	N-CA-CB	6.69	122.64	110.60
1	B	416	VAL	CG1-CB-CG2	-6.69	100.20	110.90
1	D	216	LYS	N-CA-CB	6.69	122.64	110.60
1	B	98	CYS	CB-CA-C	6.69	123.78	110.40
1	C	360	LYS	CA-CB-CG	6.69	128.11	113.40
1	B	228	THR	CA-C-O	-6.69	106.06	120.10
1	B	420	GLY	CA-C-O	-6.68	108.57	120.60
1	B	183	TYR	C-N-CA	6.68	138.40	121.70
1	A	277	PHE	CB-CA-C	-6.68	97.05	110.40
1	E	444	GLU	CA-CB-CG	6.68	128.09	113.40
1	A	30	LEU	CB-CA-C	6.67	122.88	110.20
1	C	216	LYS	N-CA-CB	6.67	122.61	110.60
1	A	67	GLU	CB-CA-C	-6.67	97.06	110.40
1	B	533	MET	CA-CB-CG	6.67	124.64	113.30
1	A	652	HIS	O-C-N	6.66	133.36	122.70
1	A	522	SER	N-CA-C	6.66	128.99	111.00
1	B	364	PRO	O-C-N	6.66	133.75	121.10
1	B	358	HIS	CB-CA-C	6.66	123.71	110.40
1	E	620	ARG	CA-CB-CG	6.66	128.04	113.40
1	B	25	THR	CB-CA-C	-6.65	93.63	111.60
1	B	184	PHE	CG-CD2-CE2	6.65	128.12	120.80
1	A	633	GLU	CA-C-O	6.65	134.06	120.10
1	B	117	TYR	CA-C-O	-6.65	106.13	120.10
1	B	177	ARG	NH1-CZ-NH2	-6.65	112.08	119.40
1	A	308	SER	CA-CB-OG	-6.65	93.25	111.20
1	A	155	TYR	CZ-CE2-CD2	-6.64	113.82	119.80
1	B	395	THR	CA-CB-OG1	-6.64	95.05	109.00
1	B	105	TYR	CG-CD2-CE2	6.64	126.61	121.30
1	B	228	THR	CA-C-N	6.64	131.80	117.20
1	B	624	TYR	CG-CD2-CE2	6.64	126.61	121.30
1	A	515	GLY	N-CA-C	-6.63	96.51	113.10
1	B	100	ARG	CD-NE-CZ	-6.63	114.31	123.60
1	A	357	PRO	N-CD-CG	-6.63	93.25	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ASP	CA-CB-CG	6.62	127.97	113.40
1	A	633	GLU	CA-C-N	-6.62	102.64	117.20
1	B	329	GLU	OE1-CD-OE2	6.62	131.24	123.30
1	B	315	ILE	O-C-N	-6.62	112.11	122.70
1	E	216	LYS	N-CA-CB	6.62	122.51	110.60
1	A	340	TYR	CB-CG-CD1	-6.61	117.03	121.00
1	B	414	ASN	CB-CG-OD1	-6.61	108.38	121.60
1	B	43	THR	N-CA-C	-6.61	93.15	111.00
1	B	306	THR	CA-CB-OG1	-6.61	95.12	109.00
1	B	469	ASN	CA-C-O	-6.61	106.22	120.10
1	F	32	ASP	CA-CB-CG	6.61	127.94	113.40
1	B	473	GLU	CA-CB-CG	6.60	127.92	113.40
1	A	326	ASP	CA-CB-CG	6.60	127.92	113.40
1	B	190	MET	CG-SD-CE	-6.60	89.64	100.20
1	B	433	LEU	CB-CG-CD2	-6.60	99.78	111.00
1	B	206	GLU	N-CA-CB	6.60	122.47	110.60
1	B	486	GLU	CG-CD-OE2	-6.59	105.11	118.30
1	A	491	ILE	CB-CA-C	6.59	124.77	111.60
1	A	611	VAL	CG1-CB-CG2	-6.58	100.37	110.90
1	A	36	ASN	O-C-N	6.58	133.23	122.70
1	E	279	ASP	N-CA-CB	-6.58	98.76	110.60
1	B	401	TYR	CD1-CG-CD2	-6.58	110.66	117.90
1	C	32	ASP	CA-CB-CG	6.58	127.87	113.40
1	A	111	ASN	CA-C-O	-6.58	106.29	120.10
1	D	207	ASP	CB-CG-OD1	6.57	124.22	118.30
1	A	377	ASP	CB-CG-OD1	-6.57	112.39	118.30
1	A	31	LYS	CB-CA-C	-6.57	97.27	110.40
1	B	46	TYR	CA-C-O	-6.57	106.31	120.10
1	B	190	MET	C-N-CA	-6.56	105.30	121.70
1	A	297	HIS	CB-CA-C	-6.56	97.28	110.40
1	B	198	HIS	CB-CA-C	-6.56	97.28	110.40
1	B	576	GLU	OE1-CD-OE2	6.56	131.17	123.30
1	B	580	PHE	CB-CG-CD1	-6.56	116.21	120.80
1	B	312	THR	CA-CB-OG1	-6.56	95.23	109.00
1	B	585	ALA	N-CA-CB	6.55	119.27	110.10
1	A	177	ARG	O-C-N	-6.55	112.23	122.70
1	A	470	ASN	O-C-N	-6.55	112.22	122.70
1	B	611	VAL	CA-CB-CG1	6.55	120.72	110.90
1	D	489	ASN	CB-CA-C	6.54	123.49	110.40
1	B	182	ALA	O-C-N	6.54	133.17	122.70
1	B	621	PRO	CB-CA-C	6.54	128.36	112.00
1	A	336	ASN	CB-CG-OD1	6.54	134.68	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	TYR	O-C-N	6.54	133.16	122.70
1	A	391	PHE	N-CA-CB	6.53	122.36	110.60
1	B	411	MET	N-CA-CB	-6.53	98.84	110.60
1	A	413	VAL	CG1-CB-CG2	6.53	121.35	110.90
1	B	97	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	B	120	TYR	CB-CG-CD1	6.53	124.92	121.00
1	B	594	GLU	CA-CB-CG	6.53	127.77	113.40
1	D	322	GLU	N-CA-CB	6.53	122.35	110.60
1	A	208	SER	CA-C-O	-6.53	106.40	120.10
1	A	247	HIS	CB-CA-C	-6.53	97.35	110.40
1	A	353	ARG	O-C-N	-6.52	112.26	122.70
1	F	216	LYS	N-CA-CB	6.52	122.34	110.60
1	A	502	CYS	CA-CB-SG	6.52	125.74	114.00
1	B	147	ASN	OD1-CG-ND2	6.52	136.90	121.90
1	B	562	CYS	N-CA-C	6.52	128.60	111.00
1	A	114	GLU	OE1-CD-OE2	-6.52	115.48	123.30
1	B	412	VAL	CA-CB-CG1	6.52	120.67	110.90
1	A	46	TYR	O-C-N	6.51	133.12	122.70
1	A	560	ARG	CA-CB-CG	6.51	127.73	113.40
1	A	613	GLY	O-C-N	6.51	133.12	122.70
1	A	360	LYS	N-CA-CB	6.50	122.30	110.60
1	F	360	LYS	CA-CB-CG	6.50	127.70	113.40
1	B	451	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	A	632	ASP	N-CA-CB	6.50	122.30	110.60
1	B	270	VAL	CA-C-O	-6.50	106.45	120.10
1	E	496	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	207	ASP	OD1-CG-OD2	-6.50	110.96	123.30
1	C	496	ASP	N-CA-CB	6.49	122.29	110.60
1	B	24	PRO	N-CD-CG	-6.49	93.46	103.20
1	B	265	GLY	CA-C-N	6.49	129.19	116.20
1	B	413	VAL	CB-CA-C	6.49	123.73	111.40
1	B	559	GLU	CA-CB-CG	6.49	127.68	113.40
1	A	215	ARG	CB-CA-C	6.49	123.37	110.40
1	C	63	HIS	N-CA-CB	6.49	122.27	110.60
1	B	31	LYS	N-CA-CB	6.48	122.27	110.60
1	A	456	ASN	CA-C-N	-6.48	102.94	117.20
1	C	620	ARG	CA-CB-CG	6.48	127.65	113.40
1	F	620	ARG	CA-CB-CG	6.48	127.65	113.40
1	B	203	PHE	CA-C-N	6.47	131.44	117.20
1	D	360	LYS	CA-CB-CG	6.47	127.64	113.40
1	A	471	ASP	CA-CB-CG	6.47	127.64	113.40
1	F	279	ASP	N-CA-CB	-6.47	98.95	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	HIS	CA-CB-CG	6.47	124.60	113.60
1	B	387	MET	N-CA-CB	6.47	122.25	110.60
1	A	280	VAL	CA-CB-CG2	-6.47	101.20	110.90
1	A	280	VAL	CA-CB-CG1	6.46	120.59	110.90
1	B	460	PHE	CZ-CE2-CD2	-6.46	112.35	120.10
1	A	203	PHE	CB-CG-CD2	-6.46	116.28	120.80
1	A	467	SER	CB-CA-C	-6.46	97.83	110.10
1	A	10	LYS	CB-CG-CD	6.46	128.38	111.60
1	A	277	PHE	CB-CG-CD1	-6.46	116.28	120.80
1	B	220	PHE	CZ-CE2-CD2	6.46	127.85	120.10
1	F	63	HIS	N-CA-CB	6.46	122.22	110.60
1	E	496	ASP	N-CA-CB	6.45	122.21	110.60
1	A	91	ASN	C-N-CA	-6.45	105.57	121.70
1	A	396	ASP	CA-C-O	-6.45	106.56	120.10
1	A	611	VAL	CA-CB-CG2	6.45	120.57	110.90
1	A	410	GLY	N-CA-C	-6.44	96.99	113.10
1	F	322	GLU	N-CA-CB	6.44	122.19	110.60
1	B	12	GLN	OE1-CD-NE2	-6.44	107.10	121.90
1	E	520	GLU	CA-CB-CG	6.44	127.56	113.40
1	B	95	GLU	CG-CD-OE2	-6.43	105.43	118.30
1	B	105	TYR	CZ-CE2-CD2	-6.43	114.01	119.80
1	B	132	ILE	CB-CA-C	-6.43	98.73	111.60
1	B	290	GLU	CG-CD-OE2	-6.43	105.44	118.30
1	A	625	PRO	N-CD-CG	-6.43	93.56	103.20
1	B	233	PHE	CB-CG-CD2	-6.43	116.30	120.80
1	B	260	THR	OG1-CB-CG2	6.43	124.78	110.00
1	A	653	LEU	N-CA-CB	-6.42	97.56	110.40
1	A	303	GLY	N-CA-C	-6.42	97.05	113.10
1	B	620	ARG	CA-CB-CG	6.42	127.52	113.40
1	A	126	SER	N-CA-CB	6.42	120.12	110.50
1	A	388	ASP	OD1-CG-OD2	6.42	135.49	123.30
1	B	503	ILE	CG1-CB-CG2	-6.41	97.29	111.40
1	A	139	GLN	CA-CB-CG	6.41	127.50	113.40
1	A	247	HIS	CA-CB-CG	-6.41	102.71	113.60
1	A	380	PHE	CB-CA-C	6.41	123.22	110.40
1	A	501	PHE	CA-C-O	6.41	133.56	120.10
1	B	186	GLU	O-C-N	-6.41	112.45	122.70
1	F	458	ASN	CA-CB-CG	6.41	127.49	113.40
1	A	267	GLU	CG-CD-OE2	6.40	131.11	118.30
1	B	233	PHE	CG-CD1-CE1	-6.40	113.75	120.80
1	C	169	SER	N-CA-CB	-6.40	100.89	110.50
1	F	496	ASP	N-CA-CB	6.40	122.13	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LEU	CB-CG-CD2	-6.40	100.12	111.00
1	B	267	GLU	OE1-CD-OE2	6.40	130.98	123.30
1	A	32	ASP	CB-CA-C	6.40	123.20	110.40
1	B	487	ASP	N-CA-C	6.39	128.27	111.00
1	A	211	TYR	CD1-CE1-CZ	6.39	125.55	119.80
1	B	466	MET	CB-CA-C	-6.39	97.62	110.40
1	B	474	ARG	CD-NE-CZ	-6.39	114.65	123.60
1	C	322	GLU	N-CA-CB	6.39	122.11	110.60
1	C	521	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	427	ASP	CB-CG-OD2	6.38	124.05	118.30
1	B	5	THR	N-CA-CB	6.38	122.43	110.30
1	B	86	LEU	O-C-N	6.38	132.91	122.70
1	B	606	HIS	CB-CA-C	-6.38	97.63	110.40
1	A	180	ARG	CA-C-O	-6.38	106.70	120.10
1	B	233	PHE	CD1-CE1-CZ	6.38	127.76	120.10
1	B	503	ILE	O-C-N	-6.38	112.49	122.70
1	A	300	ILE	C-N-CA	-6.38	105.75	121.70
1	A	298	GLU	N-CA-CB	-6.38	99.12	110.60
1	B	458	ASN	CA-CB-CG	6.38	127.43	113.40
1	E	521	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	441	GLU	CB-CA-C	-6.37	97.65	110.40
1	C	244	ASP	CB-CG-OD1	6.37	124.04	118.30
1	A	417	ALA	N-CA-C	6.37	128.20	111.00
1	B	594	GLU	CG-CD-OE1	-6.37	105.56	118.30
1	E	30	LEU	CB-CA-C	6.37	122.30	110.20
1	A	496	ASP	O-C-N	6.37	132.89	122.70
1	A	625	PRO	O-C-N	-6.37	112.52	122.70
1	F	169	SER	N-CA-CB	-6.36	100.95	110.50
1	E	322	GLU	N-CA-CB	6.36	122.05	110.60
1	F	244	ASP	CB-CG-OD1	6.36	124.03	118.30
1	B	190	MET	CB-CG-SD	-6.36	93.32	112.40
1	B	533	MET	N-CA-CB	6.36	122.04	110.60
1	A	78	ARG	CA-CB-CG	-6.36	99.42	113.40
1	A	440	GLY	O-C-N	6.36	132.87	122.70
1	B	553	LEU	C-N-CA	-6.35	105.81	121.70
1	E	370	HIS	CA-CB-CG	6.35	124.40	113.60
1	B	237	SER	CA-CB-OG	-6.35	94.05	111.20
1	E	279	ASP	CB-CA-C	6.35	123.11	110.40
1	D	620	ARG	CA-CB-CG	6.35	127.37	113.40
1	A	486	GLU	OE1-CD-OE2	6.35	130.92	123.30
1	A	452	VAL	CA-CB-CG2	-6.34	101.38	110.90
1	A	305	ILE	CA-CB-CG1	6.34	123.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	GLY	N-CA-C	-6.33	97.27	113.10
1	A	460	PHE	CD1-CG-CD2	-6.33	110.07	118.30
1	B	494	THR	N-CA-C	6.33	128.10	111.00
1	A	75	PHE	CB-CG-CD1	-6.32	116.38	120.80
1	A	80	ARG	NH1-CZ-NH2	6.32	126.35	119.40
1	A	205	TRP	O-C-N	-6.32	112.59	122.70
1	A	368	MET	CG-SD-CE	-6.32	90.09	100.20
1	B	274	ASN	CB-CG-OD1	-6.32	108.96	121.60
1	B	395	THR	O-C-N	6.32	132.81	122.70
1	D	63	HIS	CA-CB-CG	6.32	124.34	113.60
1	A	99	PHE	CB-CG-CD1	-6.32	116.38	120.80
1	C	138	TYR	CA-CB-CG	6.31	125.39	113.40
1	B	9	GLN	CA-C-N	-6.31	103.32	117.20
1	A	583	TYR	CZ-CE2-CD2	6.31	125.48	119.80
1	B	370	HIS	CA-C-O	-6.31	106.85	120.10
1	B	509	PHE	CB-CG-CD2	-6.31	116.38	120.80
1	A	416	VAL	CB-CA-C	6.31	123.39	111.40
1	B	272	PRO	N-CA-C	-6.31	95.70	112.10
1	B	488	ASN	CA-C-N	-6.31	103.32	117.20
1	A	293	GLU	CG-CD-OE1	-6.30	105.69	118.30
1	B	558	TYR	CB-CG-CD1	6.30	124.78	121.00
1	D	63	HIS	N-CA-CB	6.30	121.95	110.60
1	B	152	ASP	CB-CG-OD1	6.30	123.97	118.30
1	C	370	HIS	CA-CB-CG	6.30	124.31	113.60
1	A	557	ALA	CA-C-N	-6.30	103.34	117.20
1	E	489	ASN	CB-CA-C	6.29	122.99	110.40
1	B	270	VAL	O-C-N	6.29	132.77	122.70
1	C	63	HIS	CA-CB-CG	6.29	124.30	113.60
1	F	547	VAL	CB-CA-C	6.29	123.36	111.40
1	A	247	HIS	CA-C-O	-6.29	106.89	120.10
1	B	227	LEU	O-C-N	6.29	132.77	122.70
1	B	80	ARG	N-CA-CB	6.29	121.92	110.60
1	B	101	SER	CB-CA-C	6.29	122.05	110.10
1	A	645	VAL	N-CA-CB	-6.29	97.67	111.50
1	B	46	TYR	CG-CD2-CE2	6.29	126.33	121.30
1	B	219	LEU	CB-CA-C	6.29	122.14	110.20
1	B	583	TYR	CB-CG-CD1	6.29	124.77	121.00
1	B	456	ASN	CA-CB-CG	-6.28	99.58	113.40
1	F	279	ASP	CB-CA-C	6.28	122.96	110.40
1	B	82	GLU	CG-CD-OE2	6.28	130.86	118.30
1	C	279	ASP	N-CA-CB	-6.28	99.30	110.60
1	C	458	ASN	CA-CB-CG	6.28	127.21	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	496	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	475	LEU	CB-CG-CD1	-6.27	100.33	111.00
1	B	166	PHE	CD1-CE1-CZ	-6.27	112.57	120.10
1	A	450	ALA	CB-CA-C	6.27	119.51	110.10
1	A	546	ALA	C-N-CA	-6.27	106.03	121.70
1	E	63	HIS	CA-CB-CG	6.27	124.26	113.60
1	F	67	GLU	CB-CA-C	-6.27	97.86	110.40
1	A	67	GLU	CB-CG-CD	-6.27	97.28	114.20
1	A	416	VAL	C-N-CA	6.26	137.36	121.70
1	B	261	SER	O-C-N	6.26	132.72	122.70
1	A	246	LEU	CA-C-O	-6.26	106.95	120.10
1	B	24	PRO	O-C-N	6.26	132.71	122.70
1	D	474	ARG	CB-CG-CD	6.25	127.86	111.60
1	A	582	LEU	O-C-N	6.25	132.71	122.70
1	A	273	ASP	CB-CA-C	6.25	122.90	110.40
1	B	140	ILE	C-N-CA	6.25	137.32	121.70
1	B	201	PHE	CG-CD1-CE1	-6.25	113.92	120.80
1	B	99	PHE	O-C-N	6.25	132.70	122.70
1	A	413	VAL	CA-CB-CG1	-6.25	101.53	110.90
1	B	16	HIS	CA-C-N	-6.25	103.46	117.20
1	B	329	GLU	CA-C-N	-6.25	103.46	117.20
1	D	67	GLU	CB-CA-C	-6.25	97.91	110.40
1	F	370	HIS	CA-CB-CG	6.24	124.21	113.60
1	E	32	ASP	CA-CB-CG	6.24	127.13	113.40
1	B	362	ASN	CB-CA-C	6.24	122.87	110.40
1	A	472	GLY	N-CA-C	6.24	128.69	113.10
1	B	226	GLN	CG-CD-NE2	-6.24	101.73	116.70
1	B	485	ILE	N-CA-CB	6.24	125.14	110.80
1	A	438	ASP	CB-CA-C	6.23	122.87	110.40
1	A	317	GLN	O-C-N	-6.23	109.26	121.10
1	B	411	MET	O-C-N	-6.23	112.73	122.70
1	A	591	LYS	CA-CB-CG	6.23	127.11	113.40
1	A	43	THR	CA-CB-OG1	-6.23	95.92	109.00
1	A	361	PHE	CA-C-O	-6.23	107.02	120.10
1	E	63	HIS	N-CA-CB	6.23	121.81	110.60
1	D	138	TYR	CA-CB-CG	6.22	125.23	113.40
1	D	279	ASP	N-CA-CB	-6.22	99.40	110.60
1	A	226	GLN	O-C-N	-6.22	112.75	122.70
1	A	429	PHE	N-CA-CB	-6.22	99.41	110.60
1	A	637	ASP	CA-CB-CG	6.21	127.07	113.40
1	B	74	LEU	CA-C-O	-6.21	107.05	120.10
1	A	161	GLN	OE1-CD-NE2	6.21	136.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	TRP	CB-CG-CD1	6.21	135.08	127.00
1	B	497	GLU	O-C-N	6.21	132.64	122.70
1	C	95	GLU	CA-CB-CG	6.21	127.06	113.40
1	A	199	MET	CG-SD-CE	-6.21	90.27	100.20
1	A	430	GLN	N-CA-CB	-6.21	99.42	110.60
1	B	606	HIS	CA-C-O	6.21	133.13	120.10
1	E	67	GLU	CB-CA-C	-6.21	97.99	110.40
1	C	496	ASP	CB-CG-OD2	6.21	123.88	118.30
1	B	263	LYS	CA-CB-CG	6.20	127.04	113.40
1	B	89	VAL	CB-CA-C	6.20	123.17	111.40
1	A	503	ILE	CB-CG1-CD1	-6.20	96.55	113.90
1	A	146	THR	CA-CB-CG2	6.19	121.07	112.40
1	B	97	TYR	CB-CG-CD1	6.19	124.72	121.00
1	B	549	GLY	O-C-N	-6.19	112.67	123.20
1	A	493	LEU	CB-CA-C	6.19	121.97	110.20
1	E	179	GLN	CA-C-N	-6.19	103.58	117.20
1	B	175	LYS	N-CA-CB	6.19	121.74	110.60
1	B	180	ARG	O-C-N	6.19	132.60	122.70
1	A	571	PRO	CA-C-O	6.19	135.05	120.20
1	B	86	LEU	CA-C-O	-6.19	107.11	120.10
1	B	582	LEU	CB-CG-CD2	-6.19	100.48	111.00
1	B	197	TRP	O-C-N	6.18	132.59	122.70
1	B	203	PHE	CB-CG-CD1	6.18	125.13	120.80
1	B	437	VAL	CG1-CB-CG2	-6.18	101.01	110.90
1	B	134	LEU	CA-CB-CG	6.18	129.52	115.30
1	B	251	ILE	CA-CB-CG1	-6.18	99.26	111.00
1	A	100	ARG	CA-C-N	-6.17	103.62	117.20
1	A	322	GLU	CB-CG-CD	6.17	130.87	114.20
1	A	376	ARG	C-N-CA	6.17	137.13	121.70
1	B	16	HIS	CA-CB-CG	-6.17	103.11	113.60
1	A	9	GLN	CG-CD-OE1	6.17	133.94	121.60
1	B	7	ASN	CA-CB-CG	6.17	126.97	113.40
1	B	556	SER	C-N-CA	6.17	137.11	121.70
1	A	201	PHE	CD1-CG-CD2	6.16	126.31	118.30
1	F	521	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	67	GLU	CB-CA-C	-6.16	98.08	110.40
1	B	332	LYS	CB-CG-CD	-6.16	95.59	111.60
1	B	501	PHE	N-CA-CB	-6.16	99.52	110.60
1	A	52	ALA	CA-C-O	-6.15	107.18	120.10
1	B	573	SER	CA-CB-OG	-6.15	94.58	111.20
1	A	128	LEU	N-CA-CB	-6.15	98.10	110.40
1	A	187	ASP	CB-CG-OD1	-6.15	112.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	PHE	CE1-CZ-CE2	-6.15	108.93	120.00
1	B	183	TYR	N-CA-CB	6.15	121.67	110.60
1	D	32	ASP	CA-CB-CG	6.15	126.93	113.40
1	A	162	LYS	CD-CE-NZ	6.15	125.84	111.70
1	B	253	ARG	NH1-CZ-NH2	6.15	126.16	119.40
1	D	521	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	647	VAL	CG1-CB-CG2	-6.14	101.07	110.90
1	A	107	ARG	CB-CG-CD	6.14	127.57	111.60
1	B	588	ASP	CB-CG-OD1	-6.14	112.77	118.30
1	D	169	SER	N-CA-CB	-6.14	101.29	110.50
1	A	29	ASP	CB-CG-OD1	6.14	123.82	118.30
1	A	87	PHE	O-C-N	-6.14	112.88	122.70
1	B	401	TYR	CG-CD2-CE2	6.13	126.21	121.30
1	F	63	HIS	CA-CB-CG	6.13	124.03	113.60
1	A	147	ASN	OD1-CG-ND2	6.13	136.00	121.90
1	A	158	LYS	CA-C-N	6.13	130.68	117.20
1	B	143	HIS	CA-C-O	-6.12	107.24	120.10
1	A	548	ASN	CB-CA-C	6.12	122.65	110.40
1	B	439	SER	N-CA-CB	-6.12	101.31	110.50
1	A	69	ARG	CB-CG-CD	6.12	127.52	111.60
1	B	489	ASN	O-C-N	6.12	133.60	123.20
1	A	138	TYR	CA-CB-CG	6.12	125.03	113.40
1	A	233	PHE	CB-CA-C	-6.12	98.16	110.40
1	A	534	PRO	CB-CA-C	-6.12	96.71	112.00
1	A	61	ASN	CB-CG-OD1	-6.11	109.37	121.60
1	B	215	ARG	CA-CB-CG	6.11	126.85	113.40
1	B	393	LYS	CB-CA-C	-6.11	98.18	110.40
1	B	612	HIS	CA-CB-CG	6.11	123.99	113.60
1	A	232	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	B	412	VAL	CA-C-O	-6.11	107.28	120.10
1	B	155	TYR	CD1-CG-CD2	-6.11	111.19	117.90
1	D	271	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	37	PHE	O-C-N	6.10	132.46	122.70
1	F	179	GLN	CA-C-N	-6.10	103.78	117.20
1	A	284	ALA	CA-C-N	-6.10	103.78	117.20
1	B	216	LYS	CB-CA-C	-6.09	98.22	110.40
1	B	357	PRO	C-N-CA	-6.09	106.47	121.70
1	A	545	ASN	OD1-CG-ND2	6.09	135.91	121.90
1	B	126	SER	CA-C-O	6.09	132.88	120.10
1	A	449	ASN	CA-C-O	-6.08	107.32	120.10
1	A	629	ARG	CD-NE-CZ	-6.08	115.08	123.60
1	B	548	ASN	CB-CG-ND2	-6.08	102.10	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	637	ASP	CB-CG-OD1	6.08	123.78	118.30
1	A	514	SER	C-N-CA	-6.08	109.53	122.30
1	A	628	ARG	N-CA-CB	-6.08	99.65	110.60
1	B	98	CYS	CA-CB-SG	-6.08	103.06	114.00
1	A	259	LEU	CB-CA-C	6.08	121.75	110.20
1	B	31	LYS	CA-C-O	-6.08	107.33	120.10
1	B	414	ASN	N-CA-CB	6.08	121.54	110.60
1	A	142	PRO	N-CA-CB	6.08	110.59	103.30
1	B	26	LYS	CA-CB-CG	-6.08	100.03	113.40
1	A	146	THR	CA-C-O	6.07	132.86	120.10
1	A	372	GLU	OE1-CD-OE2	6.07	130.59	123.30
1	A	25	THR	CA-CB-CG2	-6.07	103.90	112.40
1	B	7	ASN	N-CA-C	-6.07	94.61	111.00
1	B	376	ARG	CA-CB-CG	6.07	126.75	113.40
1	A	110	MET	O-C-N	-6.07	112.99	122.70
1	A	402	THR	CA-CB-OG1	-6.07	96.26	109.00
1	D	62	ASP	CB-CG-OD2	6.06	123.76	118.30
1	A	608	GLN	N-CA-CB	6.06	121.51	110.60
1	B	90	LEU	O-C-N	-6.06	113.00	122.70
1	D	370	HIS	CA-CB-CG	6.06	123.90	113.60
1	A	584	VAL	C-N-CA	-6.06	106.55	121.70
1	E	271	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	278	GLU	OE1-CD-OE2	6.05	130.56	123.30
1	B	611	VAL	N-CA-CB	-6.05	98.20	111.50
1	A	108	GLU	CB-CG-CD	6.04	130.52	114.20
1	A	365	PRO	CA-C-N	6.04	128.29	116.20
1	B	274	ASN	N-CA-CB	6.04	121.48	110.60
1	B	445	ASP	C-N-CA	6.04	136.81	121.70
1	B	209	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	B	12	GLN	CG-CD-OE1	6.04	133.67	121.60
1	B	84	LEU	C-N-CA	-6.03	106.62	121.70
1	B	474	ARG	N-CA-CB	-6.03	99.74	110.60
1	B	596	HIS	CA-C-O	-6.03	107.44	120.10
1	D	513	PRO	CA-C-N	6.03	130.46	117.20
1	B	295	ARG	CD-NE-CZ	-6.03	115.16	123.60
1	D	64	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	B	128	LEU	CB-CA-C	-6.02	98.76	110.20
1	A	112	GLU	CG-CD-OE2	-6.02	106.26	118.30
1	B	155	TYR	CB-CG-CD2	6.02	124.61	121.00
1	B	328	ILE	CA-CB-CG1	-6.02	99.56	111.00
1	A	635	VAL	CA-C-O	-6.02	107.46	120.10
1	B	243	VAL	CB-CA-C	-6.02	99.97	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	LYS	CA-C-O	-6.02	107.46	120.10
1	E	62	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	253	ARG	CA-CB-CG	6.01	126.63	113.40
1	A	271	ARG	O-C-N	6.01	132.53	121.10
1	E	138	TYR	CA-CB-CG	6.01	124.83	113.40
1	B	468	ASN	OD1-CG-ND2	6.01	135.73	121.90
1	A	376	ARG	CD-NE-CZ	-6.01	115.19	123.60
1	A	399	PRO	O-C-N	6.01	132.51	121.10
1	B	220	PHE	CB-CG-CD1	6.01	125.00	120.80
1	E	31	LYS	CA-CB-CG	6.01	126.61	113.40
1	B	278	GLU	CA-C-O	6.00	132.71	120.10
1	F	489	ASN	CB-CA-C	6.00	122.41	110.40
1	A	124	ILE	O-C-N	-6.00	113.10	122.70
1	A	139	GLN	OE1-CD-NE2	6.00	135.70	121.90
1	B	139	GLN	CB-CA-C	6.00	122.40	110.40
1	C	62	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	234	GLU	OE1-CD-OE2	-5.99	116.11	123.30
1	B	121	VAL	CA-CB-CG2	-5.99	101.91	110.90
1	A	22	TYR	O-C-N	-5.99	113.11	122.70
1	A	107	ARG	CA-CB-CG	5.99	126.57	113.40
1	F	138	TYR	CA-CB-CG	5.99	124.78	113.40
1	B	494	THR	CA-CB-OG1	5.99	121.57	109.00
1	A	585	ALA	O-C-N	5.99	132.28	122.70
1	B	441	GLU	C-N-CA	5.99	136.66	121.70
1	A	465	THR	CA-C-O	-5.98	107.53	120.10
1	A	213	LEU	CA-C-O	-5.98	107.53	120.10
1	A	412	VAL	CA-C-N	5.98	130.36	117.20
1	A	356	ASP	N-CA-CB	-5.98	99.84	110.60
1	A	471	ASP	CA-C-O	5.98	132.66	120.10
1	A	41	GLY	O-C-N	5.98	132.26	122.70
1	A	473	GLU	CG-CD-OE2	5.98	130.25	118.30
1	B	191	ASN	OD1-CG-ND2	5.97	135.64	121.90
1	B	272	PRO	CA-N-CD	-5.97	103.14	111.50
1	D	279	ASP	CB-CA-C	5.97	122.34	110.40
1	A	382	ARG	CA-CB-CG	-5.97	100.27	113.40
1	A	414	ASN	N-CA-CB	5.97	121.35	110.60
1	A	555	LEU	CA-C-N	5.97	130.33	117.20
1	C	179	GLN	CA-C-N	-5.97	104.07	117.20
1	A	184	PHE	CD1-CE1-CZ	-5.96	112.94	120.10
1	B	6	GLY	O-C-N	5.96	132.24	122.70
1	F	561	SER	N-CA-C	5.96	127.10	111.00
1	A	294	SER	O-C-N	5.96	132.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	ASN	CB-CG-OD1	5.96	133.53	121.60
1	B	518	THR	CA-C-O	-5.96	107.58	120.10
1	E	244	ASP	CB-CG-OD1	5.96	123.67	118.30
1	F	517	GLU	N-CA-CB	5.96	121.33	110.60
1	B	61	ASN	CA-CB-CG	-5.96	100.29	113.40
1	A	188	ILE	CA-CB-CG2	5.96	122.81	110.90
1	A	194	HIS	CA-C-N	5.96	130.30	117.20
1	B	23	GLU	CA-CB-CG	5.96	126.50	113.40
1	D	244	ASP	CB-CG-OD1	5.96	123.66	118.30
1	D	179	GLN	CA-C-N	-5.96	104.10	117.20
1	A	333	TYR	CD1-CE1-CZ	5.95	125.16	119.80
1	A	560	ARG	CB-CA-C	5.95	122.30	110.40
1	B	529	THR	CA-CB-OG1	-5.95	96.51	109.00
1	F	80	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	465	THR	CA-C-O	-5.95	107.61	120.10
1	A	251	ILE	CA-CB-CG2	5.94	122.78	110.90
1	B	482	LEU	O-C-N	5.94	132.21	122.70
1	A	116	VAL	CA-CB-CG2	-5.94	101.99	110.90
1	A	639	VAL	N-CA-C	-5.94	94.96	111.00
1	A	25	THR	CA-C-N	-5.94	104.13	117.20
1	B	177	ARG	CB-CG-CD	-5.94	96.16	111.60
1	A	367	VAL	CA-CB-CG1	5.94	119.80	110.90
1	A	12	GLN	O-C-N	-5.93	113.21	122.70
1	A	264	TYR	CB-CA-C	5.93	122.26	110.40
1	A	221	PHE	O-C-N	5.93	132.19	122.70
1	A	287	HIS	CA-C-N	-5.93	104.16	117.20
1	B	217	GLY	CA-C-O	-5.93	109.93	120.60
1	B	274	ASN	CB-CG-ND2	5.93	130.92	116.70
1	B	311	HIS	CA-C-O	-5.93	107.65	120.10
1	A	264	TYR	CZ-CE2-CD2	-5.92	114.47	119.80
1	A	295	ARG	CB-CG-CD	5.92	126.99	111.60
1	A	353	ARG	CA-C-O	5.92	132.53	120.10
1	B	213	LEU	CB-CG-CD1	5.92	121.07	111.00
1	D	559	GLU	CA-CB-CG	5.92	126.42	113.40
1	B	245	GLU	CG-CD-OE2	5.92	130.13	118.30
1	A	512	VAL	CA-C-O	5.91	132.52	120.10
1	A	298	GLU	OE1-CD-OE2	5.91	130.39	123.30
1	A	211	TYR	CB-CG-CD2	5.91	124.55	121.00
1	A	234	GLU	CG-CD-OE2	5.91	130.12	118.30
1	A	474	ARG	NH1-CZ-NH2	-5.91	112.90	119.40
1	B	170	PHE	CB-CG-CD1	-5.91	116.67	120.80
1	B	179	GLN	N-CA-C	-5.91	95.06	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	GLN	OE1-CD-NE2	-5.90	108.32	121.90
1	B	65	LEU	CA-C-N	5.90	130.19	117.20
1	B	537	GLN	CB-CG-CD	-5.90	96.25	111.60
1	B	296	ILE	CA-C-N	-5.90	104.21	117.20
1	B	238	ASN	CB-CA-C	5.90	122.20	110.40
1	B	426	PHE	O-C-N	-5.90	113.26	122.70
1	B	110	MET	CA-CB-CG	5.90	123.33	113.30
1	A	632	ASP	CA-C-N	-5.89	104.23	117.20
1	B	305	ILE	O-C-N	5.89	132.13	122.70
1	B	10	LYS	CG-CD-CE	5.89	129.58	111.90
1	C	279	ASP	CB-CA-C	5.89	122.18	110.40
1	A	291	ILE	CB-CG1-CD1	-5.89	97.41	113.90
1	A	112	GLU	OE1-CD-OE2	5.88	130.36	123.30
1	A	243	VAL	CB-CA-C	-5.88	100.22	111.40
1	B	264	TYR	CB-CG-CD2	5.88	124.53	121.00
1	B	458	ASN	CA-C-N	5.88	130.15	117.20
1	B	279	ASP	N-CA-CB	-5.88	100.01	110.60
1	B	360	LYS	N-CA-CB	5.88	121.19	110.60
1	B	536	PHE	CG-CD1-CE1	5.88	127.27	120.80
1	A	522	SER	N-CA-CB	-5.88	101.68	110.50
1	B	106	PHE	CD1-CE1-CZ	-5.88	113.05	120.10
1	A	155	TYR	CB-CG-CD1	5.88	124.53	121.00
1	E	35	GLU	CG-CD-OE1	5.88	130.05	118.30
1	A	139	GLN	N-CA-CB	5.87	121.17	110.60
1	A	501	PHE	CZ-CE2-CD2	-5.87	113.05	120.10
1	A	522	SER	CA-C-O	5.87	132.43	120.10
1	F	637	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	63	HIS	O-C-N	5.87	132.09	122.70
1	A	460	PHE	CA-C-N	5.87	130.11	117.20
1	A	496	ASP	OD1-CG-OD2	-5.87	112.15	123.30
1	A	59	GLU	CA-C-O	-5.86	107.79	120.10
1	A	201	PHE	CZ-CE2-CD2	-5.86	113.06	120.10
1	A	88	ALA	CB-CA-C	5.86	118.89	110.10
1	A	434	ILE	CA-CB-CG2	5.86	122.62	110.90
1	D	216	LYS	CA-CB-CG	5.86	126.29	113.40
1	F	522	SER	N-CA-C	5.86	126.82	111.00
1	A	419	ASP	CA-CB-CG	5.86	126.28	113.40
1	A	76	ASN	CA-CB-CG	-5.85	100.53	113.40
1	B	40	LEU	CB-CA-C	-5.85	99.08	110.20
1	B	408	PHE	CA-C-N	-5.85	104.33	117.20
1	F	226	GLN	CB-CA-C	5.85	122.11	110.40
1	B	48	ASP	OD1-CG-OD2	-5.85	112.18	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	ARG	CB-CG-CD	5.85	126.81	111.60
1	A	532	ASP	CA-CB-CG	5.85	126.27	113.40
1	B	587	THR	CA-CB-OG1	-5.85	96.72	109.00
1	B	587	THR	CA-CB-CG2	5.84	120.58	112.40
1	B	180	ARG	NH1-CZ-NH2	5.84	125.83	119.40
1	A	203	PHE	CB-CG-CD1	5.84	124.89	120.80
1	B	248	TRP	CZ3-CH2-CZ2	-5.84	114.59	121.60
1	A	406	LEU	CB-CA-C	5.84	121.29	110.20
1	B	288	ASP	CA-C-N	-5.83	104.36	117.20
1	A	175	LYS	N-CA-C	-5.83	95.27	111.00
1	A	223	VAL	CA-CB-CG2	-5.83	102.16	110.90
1	A	448	ILE	CG1-CB-CG2	5.83	124.22	111.40
1	B	435	ASN	CB-CG-OD1	-5.83	109.95	121.60
1	B	606	HIS	N-CA-C	5.83	126.73	111.00
1	D	488	ASN	N-CA-CB	5.82	121.08	110.60
1	A	566	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	159	MET	N-CA-CB	5.82	121.08	110.60
1	A	97	TYR	CB-CG-CD1	5.82	124.49	121.00
1	A	150	VAL	CA-CB-CG2	-5.82	102.17	110.90
1	B	461	THR	CA-CB-CG2	5.82	120.55	112.40
1	D	226	GLN	CB-CA-C	5.82	122.03	110.40
1	A	43	THR	OG1-CB-CG2	5.82	123.38	110.00
1	A	231	PHE	CB-CG-CD1	5.82	124.87	120.80
1	D	462	TYR	N-CA-CB	5.82	121.07	110.60
1	A	361	PHE	N-CA-CB	-5.81	100.14	110.60
1	B	120	TYR	CZ-CE2-CD2	-5.81	114.57	119.80
1	F	30	LEU	CB-CA-C	5.81	121.24	110.20
1	A	547	VAL	C-N-CA	-5.81	107.17	121.70
1	A	112	GLU	CB-CA-C	-5.81	98.78	110.40
1	A	514	SER	CA-C-N	5.81	127.82	116.20
1	B	210	GLY	O-C-N	-5.81	113.41	122.70
1	A	499	ARG	NH1-CZ-NH2	5.80	125.78	119.40
1	B	619	ASN	CB-CG-OD1	-5.80	109.99	121.60
1	A	87	PHE	CA-C-O	5.80	132.29	120.10
1	A	31	LYS	CA-C-N	-5.80	104.44	117.20
1	A	264	TYR	CG-CD2-CE2	5.80	125.94	121.30
1	B	415	GLY	O-C-N	5.80	131.98	122.70
1	F	216	LYS	CA-CB-CG	5.80	126.15	113.40
1	A	646	VAL	C-N-CA	5.79	136.18	121.70
1	B	618	ASP	OD1-CG-OD2	5.79	134.30	123.30
1	B	539	LEU	CA-C-O	-5.79	107.95	120.10
1	B	296	ILE	N-CA-CB	5.79	124.11	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	62	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	329	GLU	C-N-CA	5.78	136.16	121.70
1	B	546	ALA	N-CA-CB	5.78	118.20	110.10
1	C	30	LEU	CB-CA-C	5.78	121.19	110.20
1	A	642	ILE	CA-C-O	-5.78	107.96	120.10
1	A	117	TYR	CB-CG-CD1	5.78	124.47	121.00
1	A	417	ALA	N-CA-CB	-5.78	102.01	110.10
1	B	69	ARG	CA-CB-CG	-5.78	100.69	113.40
1	B	378	PRO	O-C-N	5.78	131.94	122.70
1	A	175	LYS	CA-C-O	-5.77	107.97	120.10
1	A	503	ILE	CA-CB-CG1	5.77	121.97	111.00
1	A	104	ALA	N-CA-C	-5.77	95.42	111.00
1	A	263	LYS	N-CA-C	-5.77	95.42	111.00
1	A	646	VAL	CG1-CB-CG2	-5.77	101.67	110.90
1	B	60	LEU	CA-C-N	-5.77	104.51	117.20
1	B	364	PRO	N-CA-CB	-5.77	96.25	102.60
1	C	64	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	C	522	SER	N-CA-C	5.77	126.58	111.00
1	A	78	ARG	N-CA-CB	5.77	120.98	110.60
1	C	80	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	40	LEU	N-CA-CB	-5.77	98.87	110.40
1	A	109	ARG	NH1-CZ-NH2	5.76	125.74	119.40
1	B	271	ARG	CB-CA-C	5.76	121.93	110.40
1	A	58	LYS	O-C-N	5.76	131.92	122.70
1	A	386	TYR	CA-C-N	5.76	129.87	117.20
1	B	413	VAL	O-C-N	5.76	131.92	122.70
1	B	201	PHE	O-C-N	5.76	132.04	121.10
1	B	316	ARG	O-C-N	5.76	131.91	122.70
1	A	362	ASN	CA-C-O	5.75	132.19	120.10
1	A	92	GLN	CA-CB-CG	5.75	126.06	113.40
1	B	7	ASN	O-C-N	5.75	131.90	122.70
1	B	424	THR	CA-CB-CG2	5.75	120.45	112.40
1	A	179	GLN	CA-C-N	-5.75	104.55	117.20
1	A	318	PRO	CA-C-N	5.75	129.85	117.20
1	A	514	SER	CB-CA-C	5.75	121.03	110.10
1	B	231	PHE	O-C-N	5.75	131.90	122.70
1	C	216	LYS	CA-CB-CG	5.75	126.06	113.40
1	E	162	LYS	N-CA-C	-5.75	95.47	111.00
1	A	47	ASN	CB-CG-OD1	5.75	133.10	121.60
1	B	556	SER	CA-CB-OG	5.75	126.72	111.20
1	A	281	ASP	N-CA-CB	5.75	120.95	110.60
1	B	357	PRO	N-CD-CG	-5.75	94.58	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	226	GLN	CB-CA-C	5.75	121.89	110.40
1	A	75	PHE	CG-CD2-CE2	-5.74	114.48	120.80
1	A	202	PRO	O-C-N	5.74	131.89	122.70
1	A	560	ARG	N-CA-CB	-5.74	100.27	110.60
1	A	263	LYS	C-N-CA	-5.74	107.35	121.70
1	A	350	MET	CG-SD-CE	-5.74	91.02	100.20
1	A	195	VAL	N-CA-CB	5.74	124.12	111.50
1	A	396	ASP	CB-CG-OD1	5.74	123.46	118.30
1	B	333	TYR	CG-CD2-CE2	5.74	125.89	121.30
1	B	644	HIS	CA-CB-CG	5.74	123.35	113.60
1	A	94	LYS	N-CA-CB	-5.74	100.28	110.60
1	C	556	SER	N-CA-C	-5.73	95.52	111.00
1	E	644	HIS	CA-CB-CG	5.73	123.35	113.60
1	A	392	LYS	CD-CE-NZ	5.73	124.88	111.70
1	A	427	ASP	CA-CB-CG	-5.73	100.79	113.40
1	B	39	PRO	O-C-N	5.73	131.87	122.70
1	B	443	ILE	CA-C-O	-5.73	108.07	120.10
1	A	25	THR	CA-CB-OG1	-5.73	96.97	109.00
1	B	497	GLU	OE1-CD-OE2	-5.73	116.43	123.30
1	B	87	PHE	O-C-N	-5.72	113.54	122.70
1	B	459	GLU	N-CA-CB	5.72	120.90	110.60
1	A	105	TYR	CA-CB-CG	-5.72	102.53	113.40
1	B	594	GLU	CG-CD-OE2	5.72	129.75	118.30
1	B	530	VAL	N-CA-CB	-5.72	98.92	111.50
1	E	216	LYS	CA-CB-CG	5.72	125.98	113.40
1	B	507	LYS	O-C-N	5.71	131.84	122.70
1	A	637	ASP	OD1-CG-OD2	5.71	134.15	123.30
1	B	63	HIS	CA-C-O	-5.71	108.11	120.10
1	B	184	PHE	CB-CG-CD2	-5.71	116.80	120.80
1	B	389	ASN	CA-C-O	-5.71	108.11	120.10
1	B	150	VAL	CA-CB-CG2	-5.71	102.34	110.90
1	B	235	ARG	NH1-CZ-NH2	-5.71	113.12	119.40
1	B	220	PHE	O-C-N	-5.71	113.57	122.70
1	E	226	GLN	CB-CA-C	5.71	121.81	110.40
1	A	158	LYS	CB-CA-C	5.70	121.80	110.40
1	A	201	PHE	CE1-CZ-CE2	5.70	130.26	120.00
1	A	254	GLU	CB-CA-C	-5.70	99.00	110.40
1	E	80	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	E	487	ASP	N-CA-C	5.70	126.39	111.00
1	A	192	ILE	CB-CA-C	5.70	122.99	111.60
1	E	217	GLY	N-CA-C	-5.70	98.86	113.10
1	B	66	LEU	CB-CG-CD2	5.69	120.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ILE	CA-C-O	-5.69	108.15	120.10
1	B	165	THR	C-N-CA	5.69	135.93	121.70
1	B	50	GLY	CA-C-O	5.69	130.84	120.60
1	B	511	LYS	O-C-N	5.69	131.81	122.70
1	B	247	HIS	N-CA-CB	5.69	120.84	110.60
1	A	444	GLU	CG-CD-OE1	5.69	129.67	118.30
1	A	438	ASP	CA-C-O	5.69	132.04	120.10
1	B	526	SER	CA-CB-OG	-5.68	95.85	111.20
1	D	487	ASP	N-CA-C	5.68	126.35	111.00
1	A	69	ARG	O-C-N	5.68	131.79	122.70
1	B	504	GLU	CG-CD-OE1	-5.68	106.94	118.30
1	A	281	ASP	O-C-N	5.68	132.85	123.20
1	F	252	ILE	N-CA-C	-5.68	95.67	111.00
1	F	217	GLY	N-CA-C	-5.68	98.91	113.10
1	B	250	ARG	N-CA-CB	-5.68	100.38	110.60
1	D	217	GLY	N-CA-C	-5.68	98.91	113.10
1	B	448	ILE	CB-CG1-CD1	-5.67	98.01	113.90
1	B	42	ASP	CA-CB-CG	5.67	125.87	113.40
1	B	253	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	B	296	ILE	CB-CA-C	-5.67	100.26	111.60
1	A	526	SER	CA-CB-OG	-5.67	95.90	111.20
1	B	388	ASP	O-C-N	5.67	131.76	122.70
1	E	213	LEU	CB-CA-C	5.66	120.96	110.20
1	B	133	VAL	O-C-N	-5.66	113.64	122.70
1	B	272	PRO	N-CA-CB	5.66	110.09	103.30
1	A	177	ARG	CB-CG-CD	-5.66	96.89	111.60
1	A	386	TYR	CG-CD2-CE2	5.66	125.82	121.30
1	B	334	SER	O-C-N	5.66	131.75	122.70
1	C	217	GLY	N-CA-C	-5.66	98.96	113.10
1	D	496	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	422	LEU	CA-C-N	-5.65	104.77	117.20
1	B	508	PHE	O-C-N	5.65	131.75	122.70
1	D	139	GLN	CA-CB-CG	5.65	125.83	113.40
1	E	558	TYR	N-CA-C	5.65	126.26	111.00
1	B	583	TYR	CA-C-O	-5.65	108.23	120.10
1	E	423	ILE	CB-CA-C	5.65	122.90	111.60
1	A	594	GLU	CB-CG-CD	-5.65	98.95	114.20
1	D	419	ASP	N-CA-C	-5.65	95.75	111.00
1	D	443	ILE	N-CA-C	-5.65	95.75	111.00
1	A	296	ILE	CB-CG1-CD1	-5.65	98.09	113.90
1	D	637	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	423	ILE	CA-C-O	-5.64	108.25	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ASN	CA-C-O	-5.64	108.25	120.10
1	A	78	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	371	PHE	CA-C-O	-5.64	108.25	120.10
1	A	501	PHE	CB-CG-CD2	-5.64	116.85	120.80
1	A	570	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	583	TYR	CG-CD1-CE1	5.64	125.81	121.30
1	B	121	VAL	CA-CB-CG1	5.64	119.36	110.90
1	B	66	LEU	O-C-N	-5.64	113.68	122.70
1	B	224	HIS	C-N-CA	-5.63	107.61	121.70
1	F	644	HIS	CA-CB-CG	5.63	123.18	113.60
1	A	289	LEU	CB-CG-CD2	-5.63	101.43	111.00
1	B	361	PHE	CZ-CE2-CD2	-5.63	113.35	120.10
1	A	84	LEU	CB-CG-CD2	-5.63	101.44	111.00
1	B	66	LEU	CA-CB-CG	5.63	128.24	115.30
1	B	133	VAL	CG1-CB-CG2	-5.62	101.90	110.90
1	B	462	TYR	N-CA-CB	5.62	120.72	110.60
1	C	444	GLU	CA-CB-CG	5.62	125.77	113.40
1	A	17	LEU	CA-C-O	-5.62	108.30	120.10
1	C	139	GLN	CA-CB-CG	5.62	125.77	113.40
1	A	128	LEU	CA-C-O	-5.62	108.30	120.10
1	E	316	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	54	GLU	CB-CG-CD	-5.62	99.04	114.20
1	A	56	LEU	O-C-N	5.62	131.69	122.70
1	A	250	ARG	CG-CD-NE	-5.62	100.01	111.80
1	A	390	ILE	N-CA-CB	5.62	123.72	110.80
1	A	422	LEU	CA-C-N	5.62	129.55	117.20
1	A	528	VAL	O-C-N	5.61	131.68	122.70
1	A	409	SER	N-CA-CB	-5.61	102.08	110.50
1	A	543	ALA	CA-C-O	5.61	131.88	120.10
1	A	400	PRO	O-C-N	5.61	131.67	122.70
1	A	236	LEU	CA-C-N	-5.61	104.86	117.20
1	B	422	LEU	C-N-CA	-5.61	107.68	121.70
1	A	357	PRO	N-CA-CB	-5.61	96.43	102.60
1	B	506	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	E	78	ARG	N-CA-CB	5.61	120.69	110.60
1	F	64	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	A	69	ARG	N-CA-CB	-5.60	100.51	110.60
1	A	519	ILE	CA-C-N	-5.60	104.88	117.20
1	B	495	LEU	N-CA-CB	5.60	121.60	110.40
1	B	467	SER	C-N-CA	5.60	135.70	121.70
1	A	382	ARG	CB-CA-C	5.60	121.60	110.40
1	A	119	LEU	O-C-N	-5.60	113.74	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	HIS	CA-C-N	5.60	129.51	117.20
1	B	46	TYR	CD1-CG-CD2	-5.60	111.74	117.90
1	B	418	ILE	O-C-N	5.59	131.65	122.70
1	A	385	LYS	CA-C-O	-5.59	108.35	120.10
1	D	213	LEU	CB-CA-C	5.59	120.82	110.20
1	A	137	LEU	CA-C-O	-5.59	108.36	120.10
1	A	549	GLY	CA-C-O	5.59	130.66	120.60
1	A	29	ASP	O-C-N	5.59	131.64	122.70
1	A	542	GLN	OE1-CD-NE2	5.59	134.75	121.90
1	A	585	ALA	N-CA-C	-5.58	95.92	111.00
1	B	199	MET	N-CA-C	-5.58	95.93	111.00
1	C	35	GLU	CG-CD-OE1	5.58	129.47	118.30
1	A	75	PHE	CZ-CE2-CD2	5.58	126.80	120.10
1	A	194	HIS	CB-CA-C	5.58	121.56	110.40
1	A	242	PRO	N-CA-CB	-5.58	96.46	102.60
1	A	574	LYS	CB-CG-CD	5.58	126.11	111.60
1	D	7	ASN	CB-CA-C	5.58	121.56	110.40
1	B	390	ILE	CA-CB-CG1	5.58	121.60	111.00
1	A	16	HIS	O-C-N	5.58	131.62	122.70
1	A	27	TYR	CD1-CG-CD2	-5.57	111.77	117.90
1	A	87	PHE	CB-CG-CD1	5.57	124.70	120.80
1	A	305	ILE	CA-C-N	5.57	129.46	117.20
1	B	31	LYS	C-N-CA	-5.57	107.77	121.70
1	B	268	PHE	O-C-N	5.57	131.69	121.10
1	B	133	VAL	CA-C-N	5.57	129.45	117.20
1	A	21	ILE	CA-C-O	-5.57	108.41	120.10
1	A	163	PRO	CA-CB-CG	-5.57	93.42	104.00
1	A	301	ASP	CB-CA-C	5.57	121.53	110.40
1	B	107	ARG	CG-CD-NE	-5.57	100.11	111.80
1	A	433	LEU	CB-CG-CD1	-5.56	101.54	111.00
1	B	620	ARG	CG-CD-NE	-5.56	100.11	111.80
1	B	46	TYR	CG-CD1-CE1	5.56	125.75	121.30
1	B	68	GLN	O-C-N	5.56	131.60	122.70
1	B	176	ASN	CB-CA-C	5.56	121.53	110.40
1	B	637	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	421	GLU	C-N-CA	-5.56	107.80	121.70
1	A	63	HIS	CB-CA-C	-5.56	99.28	110.40
1	B	40	LEU	N-CA-C	5.56	126.01	111.00
1	B	167	ASN	CA-C-O	5.56	131.78	120.10
1	B	368	MET	N-CA-CB	-5.56	100.59	110.60
1	A	41	GLY	N-CA-C	-5.56	99.20	113.10
1	A	381	PHE	CZ-CE2-CD2	-5.56	113.43	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	SER	CA-C-N	-5.56	104.97	117.20
1	F	95	GLU	CA-CB-CG	5.56	125.63	113.40
1	A	42	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	B	418	ILE	CA-C-N	-5.56	104.98	117.20
1	A	187	ASP	OD1-CG-OD2	5.55	133.85	123.30
1	D	80	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	270	VAL	CG1-CB-CG2	5.55	119.78	110.90
1	F	369	GLU	CA-CB-CG	5.55	125.61	113.40
1	B	379	SER	CA-C-O	5.55	131.75	120.10
1	B	389	ASN	CA-C-N	5.55	129.40	117.20
1	C	78	ARG	N-CA-CB	5.55	120.58	110.60
1	A	7	ASN	CB-CG-OD1	-5.54	110.52	121.60
1	A	372	GLU	CB-CG-CD	5.54	129.16	114.20
1	B	301	ASP	O-C-N	5.54	131.56	122.70
1	B	470	ASN	CA-C-O	5.54	131.73	120.10
1	D	632	ASP	CA-CB-CG	5.54	125.58	113.40
1	E	7	ASN	CB-CA-C	5.54	121.48	110.40
1	B	91	ASN	C-N-CA	-5.54	107.86	121.70
1	F	316	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	235	ARG	CB-CG-CD	-5.53	97.21	111.60
1	B	595	GLY	C-N-CA	-5.53	107.86	121.70
1	C	7	ASN	CB-CA-C	5.53	121.47	110.40
1	D	556	SER	N-CA-C	-5.53	96.06	111.00
1	A	108	GLU	OE1-CD-OE2	-5.53	116.66	123.30
1	B	147	ASN	CB-CG-OD1	-5.53	110.54	121.60
1	F	7	ASN	CB-CA-C	5.53	121.46	110.40
1	B	381	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	A	270	VAL	O-C-N	-5.53	113.86	122.70
1	A	638	GLY	C-N-CA	5.53	135.52	121.70
1	E	369	GLU	CA-CB-CG	5.53	125.56	113.40
1	A	187	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	B	142	PRO	O-C-N	-5.53	113.86	122.70
1	B	373	THR	N-CA-CB	-5.53	99.80	110.30
1	A	631	PRO	CA-C-O	-5.52	106.95	120.20
1	A	442	ASN	O-C-N	5.52	131.53	122.70
1	A	570	LEU	O-C-N	5.52	131.59	121.10
1	B	388	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	E	333	TYR	CB-CG-CD1	5.52	124.31	121.00
1	C	561	SER	N-CA-C	5.51	125.89	111.00
1	A	225	HIS	O-C-N	-5.51	113.88	122.70
1	A	543	ALA	O-C-N	-5.51	113.88	122.70
1	F	35	GLU	CG-CD-OE1	5.51	129.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ILE	CG1-CB-CG2	5.51	123.52	111.40
1	B	532	ASP	N-CA-CB	5.51	120.52	110.60
1	B	574	LYS	O-C-N	-5.51	110.63	121.10
1	D	78	ARG	N-CA-CB	5.50	120.51	110.60
1	A	12	GLN	CB-CA-C	5.50	121.41	110.40
1	B	279	ASP	CA-CB-CG	5.50	125.51	113.40
1	E	35	GLU	OE1-CD-OE2	-5.50	116.69	123.30
1	A	158	LYS	CG-CD-CE	-5.50	95.39	111.90
1	B	468	ASN	N-CA-CB	-5.50	100.70	110.60
1	A	329	GLU	CG-CD-OE1	5.50	129.30	118.30
1	A	439	SER	CA-CB-OG	-5.50	96.35	111.20
1	A	514	SER	CA-CB-OG	5.50	126.05	111.20
1	B	139	GLN	O-C-N	-5.50	113.90	122.70
1	A	371	PHE	CB-CG-CD2	5.50	124.65	120.80
1	A	533	MET	N-CA-CB	5.50	120.49	110.60
1	B	147	ASN	CA-CB-CG	-5.50	101.31	113.40
1	B	332	LYS	CA-CB-CG	-5.50	101.31	113.40
1	B	351	LEU	CB-CG-CD2	-5.50	101.66	111.00
1	A	50	GLY	O-C-N	5.50	131.49	122.70
1	F	78	ARG	N-CA-CB	5.49	120.49	110.60
1	A	143	HIS	N-CA-CB	-5.49	100.71	110.60
1	A	422	LEU	N-CA-CB	-5.49	99.42	110.40
1	B	67	GLU	CG-CD-OE2	-5.49	107.32	118.30
1	F	444	GLU	CA-CB-CG	5.49	125.48	113.40
1	A	146	THR	CA-C-N	-5.49	105.12	117.20
1	B	447	GLU	O-C-N	5.49	131.48	122.70
1	B	580	PHE	CZ-CE2-CD2	-5.49	113.51	120.10
1	B	588	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	479	ARG	CA-CB-CG	-5.49	101.33	113.40
1	C	213	LEU	CB-CA-C	5.49	120.62	110.20
1	B	414	ASN	CA-C-N	5.49	127.17	116.20
1	A	7	ASN	CB-CA-C	5.48	121.37	110.40
1	A	501	PHE	C-N-CA	5.48	135.41	121.70
1	B	442	ASN	C-N-CA	5.48	135.41	121.70
1	B	458	ASN	CA-C-O	-5.48	108.59	120.10
1	B	584	VAL	CB-CA-C	5.48	121.81	111.40
1	A	191	ASN	CB-CA-C	5.48	121.36	110.40
1	B	326	ASP	CA-CB-CG	5.48	125.45	113.40
1	C	637	ASP	CB-CG-OD1	5.48	123.23	118.30
1	F	213	LEU	CB-CA-C	5.48	120.61	110.20
1	B	290	GLU	CG-CD-OE1	5.48	129.25	118.30
1	C	333	TYR	CB-CG-CD1	5.48	124.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	GLU	N-CA-CB	-5.47	100.74	110.60
1	A	246	LEU	CA-C-N	5.47	129.24	117.20
1	B	431	TYR	CG-CD1-CE1	-5.47	116.92	121.30
1	A	367	VAL	O-C-N	-5.47	113.95	122.70
1	B	225	HIS	CB-CA-C	5.47	121.34	110.40
1	B	410	GLY	CA-C-O	-5.47	110.75	120.60
1	A	408	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	A	299	ALA	CA-C-O	-5.46	108.62	120.10
1	A	632	ASP	CB-CA-C	5.46	121.33	110.40
1	A	390	ILE	N-CA-C	-5.46	96.25	111.00
1	C	23	GLU	CA-CB-CG	5.46	125.42	113.40
1	F	253	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	158	LYS	N-CA-CB	-5.46	100.77	110.60
1	A	618	ASP	OD1-CG-OD2	-5.46	112.92	123.30
1	B	492	THR	O-C-N	-5.46	113.96	122.70
1	B	431	TYR	CE1-CZ-CE2	5.46	128.53	119.80
1	F	472	GLY	N-CA-C	5.46	126.75	113.10
1	A	422	LEU	C-N-CA	-5.46	108.06	121.70
1	B	286	VAL	CA-C-N	-5.45	105.20	117.20
1	B	292	THR	CB-CA-C	5.45	126.32	111.60
1	D	444	GLU	CA-CB-CG	5.45	125.40	113.40
1	C	179	GLN	CB-CA-C	5.45	121.30	110.40
1	A	62	ASP	CA-C-N	-5.45	105.22	117.20
1	A	78	ARG	CA-C-N	-5.45	105.22	117.20
1	A	491	ILE	CB-CG1-CD1	-5.45	98.65	113.90
1	B	321	ILE	C-N-CA	-5.45	108.09	121.70
1	A	69	ARG	CA-CB-CG	-5.44	101.43	113.40
1	A	289	LEU	CA-C-N	-5.44	105.23	117.20
1	B	102	ASN	CA-CB-CG	-5.44	101.42	113.40
1	B	408	PHE	CA-C-O	5.44	131.53	120.10
1	A	235	ARG	CA-C-N	-5.44	105.23	117.20
1	A	438	ASP	CA-C-N	-5.44	105.23	117.20
1	B	422	LEU	N-CA-C	-5.44	96.31	111.00
1	A	431	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	B	39	PRO	CB-CA-C	5.44	125.59	112.00
1	B	192	ILE	CA-C-O	-5.44	108.68	120.10
1	B	421	GLU	CB-CA-C	-5.44	99.53	110.40
1	A	510	GLN	CB-CA-C	-5.43	99.53	110.40
1	B	33	ILE	CG1-CB-CG2	-5.43	99.44	111.40
1	A	237	SER	C-N-CA	-5.43	108.12	121.70
1	B	99	PHE	CA-C-O	-5.43	108.69	120.10
1	B	141	THR	CA-C-O	-5.43	108.69	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	614	GLU	O-C-N	-5.43	114.01	122.70
1	B	213	LEU	CB-CA-C	5.43	120.52	110.20
1	B	36	ASN	CB-CA-C	5.43	121.26	110.40
1	B	549	GLY	N-CA-C	5.43	126.67	113.10
1	C	632	ASP	CA-CB-CG	5.43	125.34	113.40
1	A	439	SER	CB-CA-C	-5.42	99.79	110.10
1	B	242	PRO	N-CD-CG	-5.42	95.06	103.20
1	A	373	THR	N-CA-C	5.42	125.64	111.00
1	C	499	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	154	ALA	CA-C-N	5.42	129.13	117.20
1	A	451	ARG	CD-NE-CZ	-5.42	116.01	123.60
1	B	248	TRP	CE3-CZ3-CH2	5.42	127.16	121.20
1	A	649	ILE	O-C-N	5.42	131.37	122.70
1	B	246	LEU	CA-C-N	5.42	129.12	117.20
1	A	193	HIS	CB-CA-C	-5.42	99.56	110.40
1	A	208	SER	O-C-N	5.42	131.37	122.70
1	A	504	GLU	CG-CD-OE1	-5.42	107.47	118.30
1	A	544	ASP	OD1-CG-OD2	5.42	133.59	123.30
1	B	155	TYR	CA-CB-CG	5.42	123.69	113.40
1	B	190	MET	O-C-N	5.42	131.37	122.70
1	E	499	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	132	ILE	N-CA-C	5.41	125.62	111.00
1	A	218	GLU	OE1-CD-OE2	5.41	129.79	123.30
1	A	49	HIS	O-C-N	5.41	132.39	123.20
1	F	49	HIS	C-N-CA	5.41	133.66	122.30
1	A	139	GLN	CA-C-N	5.41	129.09	117.20
1	B	614	GLU	OE1-CD-OE2	5.41	129.79	123.30
1	A	123	VAL	CB-CA-C	5.40	121.67	111.40
1	A	127	LYS	N-CA-CB	-5.40	100.88	110.60
1	C	271	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	441	GLU	CG-CD-OE1	5.40	129.10	118.30
1	B	218	GLU	CB-CA-C	-5.40	99.60	110.40
1	F	273	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	256	PHE	CB-CG-CD2	-5.40	117.02	120.80
1	B	402	THR	O-C-N	5.40	131.34	122.70
1	B	470	ASN	CA-CB-CG	5.40	125.27	113.40
1	B	55	THR	CA-C-O	-5.40	108.77	120.10
1	A	47	ASN	CA-C-O	-5.39	108.77	120.10
1	A	309	ASP	O-C-N	5.39	132.37	123.20
1	B	32	ASP	CB-CG-OD1	-5.39	113.44	118.30
1	A	55	THR	CA-CB-OG1	-5.39	97.67	109.00
1	A	238	ASN	O-C-N	5.39	131.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ILE	CA-C-O	-5.39	108.78	120.10
1	D	316	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	E	252	ILE	N-CA-C	-5.39	96.44	111.00
1	B	121	VAL	CA-C-O	5.39	131.42	120.10
1	B	548	ASN	N-CA-CB	5.39	120.30	110.60
1	B	562	CYS	CB-CA-C	-5.39	99.62	110.40
1	F	632	ASP	CA-CB-CG	5.39	125.25	113.40
1	B	64	ARG	CD-NE-CZ	-5.38	116.06	123.60
1	B	349	VAL	CG1-CB-CG2	5.38	119.52	110.90
1	A	570	LEU	CA-C-O	-5.38	108.80	120.10
1	B	58	LYS	CD-CE-NZ	-5.38	99.33	111.70
1	F	32	ASP	CB-CA-C	5.38	121.15	110.40
1	B	231	PHE	CA-C-O	-5.38	108.81	120.10
1	C	32	ASP	CB-CA-C	5.37	121.15	110.40
1	A	363	LEU	N-CA-C	-5.37	96.50	111.00
1	C	49	HIS	C-N-CA	5.37	133.57	122.30
1	A	271	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	152	ASP	CA-C-O	-5.37	108.83	120.10
1	C	358	HIS	CA-CB-CG	-5.37	104.48	113.60
1	F	463	LYS	CB-CA-C	5.37	121.13	110.40
1	A	474	ARG	O-C-N	5.36	131.28	122.70
1	B	138	TYR	CD1-CG-CD2	-5.36	112.00	117.90
1	B	555	LEU	N-CA-C	-5.36	96.52	111.00
1	D	358	HIS	CA-CB-CG	-5.36	104.48	113.60
1	B	61	ASN	CB-CG-OD1	-5.36	110.88	121.60
1	B	391	PHE	CZ-CE2-CD2	-5.36	113.67	120.10
1	A	40	LEU	O-C-N	-5.36	114.09	123.20
1	A	580	PHE	CB-CA-C	5.36	121.11	110.40
1	B	357	PRO	CA-C-N	-5.36	105.42	117.20
1	B	208	SER	O-C-N	5.35	131.26	122.70
1	B	348	HIS	O-C-N	-5.35	114.14	122.70
1	B	431	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	A	385	LYS	O-C-N	5.35	131.26	122.70
1	D	162	LYS	N-CA-C	-5.35	96.56	111.00
1	A	512	VAL	CB-CA-C	5.35	121.56	111.40
1	A	302	HIS	C-N-CA	-5.34	111.08	122.30
1	B	431	TYR	CB-CA-C	5.34	121.09	110.40
1	A	338	GLN	O-C-N	5.34	131.25	122.70
1	C	644	HIS	CA-CB-CG	5.34	122.68	113.60
1	A	621	PRO	CA-C-O	-5.34	107.38	120.20
1	B	21	ILE	O-C-N	5.34	131.24	122.70
1	B	62	ASP	CA-C-N	-5.34	105.45	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	MET	N-CA-CB	5.34	120.21	110.60
1	B	452	VAL	CA-C-O	5.34	131.31	120.10
1	D	216	LYS	N-CA-C	-5.34	96.58	111.00
1	E	139	GLN	CA-CB-CG	5.34	125.15	113.40
1	F	139	GLN	CA-CB-CG	5.34	125.15	113.40
1	A	51	ALA	C-N-CA	-5.34	108.36	121.70
1	C	273	ASP	CB-CG-OD2	5.34	123.10	118.30
1	D	132	ILE	N-CA-C	5.34	125.41	111.00
1	E	358	HIS	CA-CB-CG	-5.34	104.53	113.60
1	E	637	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	374	ALA	CA-C-N	5.33	128.93	117.20
1	C	216	LYS	N-CA-C	-5.33	96.61	111.00
1	F	216	LYS	N-CA-C	-5.33	96.62	111.00
1	F	333	TYR	CB-CG-CD1	5.33	124.20	121.00
1	A	163	PRO	O-C-N	5.33	132.25	123.20
1	B	370	HIS	O-C-N	5.33	131.22	122.70
1	A	384	HIS	N-CA-CB	5.32	120.18	110.60
1	B	155	TYR	CB-CG-CD1	5.32	124.19	121.00
1	E	632	ASP	CA-CB-CG	5.32	125.11	113.40
1	A	349	VAL	CA-CB-CG1	-5.32	102.92	110.90
1	A	505	LEU	CB-CG-CD2	5.32	120.05	111.00
1	B	390	ILE	N-CA-C	-5.32	96.64	111.00
1	B	507	LYS	N-CA-CB	5.32	120.17	110.60
1	B	579	GLU	CG-CD-OE1	5.32	128.93	118.30
1	A	408	PHE	CA-C-N	-5.31	105.52	117.20
1	B	11	GLN	OE1-CD-NE2	5.31	134.11	121.90
1	E	64	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	A	201	PHE	CD1-CE1-CZ	-5.31	113.73	120.10
1	B	460	PHE	C-N-CA	-5.31	108.43	121.70
1	A	138	TYR	CB-CG-CD1	-5.31	117.82	121.00
1	A	321	ILE	O-C-N	5.30	131.19	122.70
1	B	418	ILE	CG1-CB-CG2	-5.30	99.73	111.40
1	A	644	HIS	CA-CB-CG	5.30	122.61	113.60
1	B	363	LEU	N-CA-C	-5.30	96.69	111.00
1	B	365	PRO	CA-N-CD	-5.30	104.08	111.50
1	B	481	PHE	CB-CG-CD1	5.30	124.51	120.80
1	B	342	SER	N-CA-CB	-5.30	102.55	110.50
1	F	271	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	530	VAL	CA-CB-CG1	5.30	118.85	110.90
1	F	521	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	418	ILE	C-N-CA	5.30	134.94	121.70
1	E	522	SER	N-CA-C	5.29	125.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ARG	O-C-N	5.29	131.17	122.70
1	A	388	ASP	CA-C-O	-5.29	108.98	120.10
1	B	161	GLN	CG-CD-OE1	-5.29	111.01	121.60
1	B	405	ASN	C-N-CA	5.29	134.94	121.70
1	F	31	LYS	CA-CB-CG	5.29	125.05	113.40
1	A	55	THR	CA-CB-CG2	-5.29	104.99	112.40
1	B	165	THR	O-C-N	-5.29	114.24	122.70
1	B	168	VAL	C-N-CA	5.29	134.92	121.70
1	C	35	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	C	253	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	447	GLU	CA-C-O	5.29	131.20	120.10
1	E	49	HIS	C-N-CA	5.29	133.40	122.30
1	A	365	PRO	CA-N-CD	-5.29	104.10	111.50
1	C	132	ILE	N-CA-C	5.29	125.27	111.00
1	B	183	TYR	CE1-CZ-OH	-5.28	105.84	120.10
1	B	262	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	D	179	GLN	CB-CA-C	5.28	120.96	110.40
1	D	247	HIS	N-CA-CB	5.28	120.11	110.60
1	A	100	ARG	NH1-CZ-NH2	5.28	125.21	119.40
1	A	245	GLU	CA-CB-CG	5.28	125.01	113.40
1	B	134	LEU	CB-CA-C	5.28	120.23	110.20
1	A	190	MET	C-N-CA	-5.28	108.51	121.70
1	A	316	ARG	CB-CG-CD	5.28	125.32	111.60
1	B	385	LYS	CB-CA-C	5.28	120.95	110.40
1	B	504	GLU	N-CA-CB	5.28	120.09	110.60
1	A	351	LEU	CB-CG-CD2	-5.27	102.03	111.00
1	B	330	SER	O-C-N	5.27	131.14	122.70
1	B	248	TRP	CB-CG-CD2	5.27	133.45	126.60
1	C	369	GLU	CA-CB-CG	5.27	125.00	113.40
1	A	421	GLU	N-CA-CB	5.27	120.08	110.60
1	A	509	PHE	C-N-CA	5.27	134.87	121.70
1	B	257	ALA	N-CA-C	-5.27	96.78	111.00
1	B	634	ARG	CG-CD-NE	5.27	122.86	111.80
1	B	345	ASN	CB-CG-ND2	-5.26	104.06	116.70
1	A	93	CYS	N-CA-CB	-5.26	101.13	110.60
1	A	143	HIS	C-N-CA	5.26	134.85	121.70
1	A	269	PRO	C-N-CA	5.26	134.85	121.70
1	B	308	SER	CB-CA-C	-5.26	100.11	110.10
1	A	96	TRP	CA-C-O	-5.26	109.06	120.10
1	A	243	VAL	CA-C-O	5.26	131.14	120.10
1	A	378	PRO	C-N-CA	-5.25	108.56	121.70
1	E	216	LYS	N-CA-C	-5.25	96.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	PHE	CD1-CG-CD2	5.25	125.13	118.30
1	B	584	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	B	487	ASP	CA-C-O	-5.25	109.07	120.10
1	B	632	ASP	CA-CB-CG	5.25	124.95	113.40
1	F	358	HIS	CA-CB-CG	-5.25	104.67	113.60
1	B	27	TYR	CG-CD2-CE2	5.25	125.50	121.30
1	B	452	VAL	C-N-CA	5.25	134.82	121.70
1	F	23	GLU	CA-CB-CG	5.25	124.95	113.40
1	A	369	GLU	CG-CD-OE2	5.25	128.79	118.30
1	A	111	ASN	OD1-CG-ND2	5.25	133.96	121.90
1	B	344	HIS	CG-ND1-CE1	-5.24	98.88	105.70
1	D	407	GLU	N-CA-C	5.24	125.15	111.00
1	A	56	LEU	CB-CA-C	5.24	120.16	110.20
1	A	154	ALA	CB-CA-C	5.24	117.96	110.10
1	A	287	HIS	CG-CD2-NE2	-5.24	99.24	109.20
1	A	119	LEU	CB-CG-CD2	-5.23	102.10	111.00
1	A	565	PRO	O-C-N	5.23	131.07	122.70
1	A	555	LEU	N-CA-CB	-5.23	99.95	110.40
1	B	373	THR	N-CA-C	5.23	125.11	111.00
1	B	161	GLN	OE1-CD-NE2	5.23	133.92	121.90
1	B	179	GLN	CA-C-O	5.23	131.07	120.10
1	A	558	TYR	CA-C-N	5.22	128.69	117.20
1	A	619	ASN	CA-C-O	-5.22	109.13	120.10
1	F	499	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	78	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	151	ILE	CA-C-N	-5.22	105.71	117.20
1	B	160	THR	CA-CB-CG2	-5.22	105.09	112.40
1	B	380	PHE	CA-C-O	5.22	131.07	120.10
1	A	639	VAL	O-C-N	5.22	131.05	122.70
1	B	16	HIS	N-CA-CB	5.22	120.00	110.60
1	A	491	ILE	CA-CB-CG1	-5.22	101.08	111.00
1	B	18	LEU	CB-CA-C	-5.22	100.28	110.20
1	B	72	TYR	CB-CA-C	5.22	120.84	110.40
1	B	151	ILE	O-C-N	5.22	131.05	122.70
1	A	563	GLY	C-N-CA	-5.22	108.66	121.70
1	A	194	HIS	O-C-N	-5.22	114.35	122.70
1	D	369	GLU	CA-CB-CG	5.22	124.88	113.40
1	B	213	LEU	C-N-CA	5.21	134.74	121.70
1	A	71	TRP	CH2-CZ2-CE2	-5.21	112.19	117.40
1	A	145	PHE	CA-CB-CG	5.21	126.41	113.90
1	B	92	GLN	CA-CB-CG	5.21	124.87	113.40
1	A	5	THR	N-CA-CB	-5.21	100.40	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	TYR	CA-C-N	-5.21	105.74	117.20
1	A	473	GLU	CA-CB-CG	5.21	124.86	113.40
1	F	487	ASP	N-CA-C	5.21	125.06	111.00
1	B	251	ILE	CG1-CB-CG2	5.20	122.85	111.40
1	A	312	THR	N-CA-C	-5.20	96.96	111.00
1	B	592	ASP	CB-CA-C	5.20	120.80	110.40
1	B	362	ASN	O-C-N	-5.20	114.38	122.70
1	E	132	ILE	N-CA-C	5.20	125.04	111.00
1	B	214	ASP	N-CA-C	5.20	125.03	111.00
1	B	357	PRO	O-C-N	5.20	131.02	122.70
1	D	69	ARG	CB-CG-CD	5.20	125.11	111.60
1	A	276	HIS	CA-CB-CG	-5.20	104.77	113.60
1	B	90	LEU	CA-C-O	5.20	131.01	120.10
1	A	43	THR	O-C-N	5.19	131.01	122.70
1	B	251	ILE	CA-C-O	-5.19	109.19	120.10
1	A	546	ALA	CA-C-N	-5.19	105.78	117.20
1	A	571	PRO	O-C-N	-5.19	114.39	122.70
1	A	103	ALA	N-CA-CB	-5.19	102.83	110.10
1	B	117	TYR	N-CA-CB	5.19	119.94	110.60
1	E	540	LYS	CD-CE-NZ	-5.19	99.76	111.70
1	B	91	ASN	CA-C-N	5.19	128.62	117.20
1	B	377	ASP	N-CA-CB	-5.19	101.26	110.60
1	B	409	SER	C-N-CA	-5.19	111.40	122.30
1	B	309	ASP	CA-C-O	-5.19	109.21	120.10
1	A	391	PHE	CB-CG-CD2	5.18	124.43	120.80
1	B	191	ASN	O-C-N	5.18	131.00	122.70
1	B	554	ASP	N-CA-CB	5.18	119.93	110.60
1	B	247	HIS	CB-CA-C	-5.18	100.04	110.40
1	A	277	PHE	CG-CD2-CE2	5.18	126.50	120.80
1	A	285	HIS	N-CA-CB	-5.18	101.28	110.60
1	B	217	GLY	C-N-CA	-5.18	108.75	121.70
1	B	305	ILE	CB-CG1-CD1	-5.18	99.40	113.90
1	A	126	SER	CA-C-N	-5.18	105.81	117.20
1	B	307	ASP	CA-C-O	-5.18	109.23	120.10
1	D	376	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	64	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	414	ASN	C-N-CA	-5.17	111.43	122.30
1	B	216	LYS	CA-CB-CG	5.17	124.78	113.40
1	B	251	ILE	O-C-N	5.17	130.98	122.70
1	B	292	THR	CA-CB-OG1	-5.17	98.14	109.00
1	E	95	GLU	CA-CB-CG	5.17	124.78	113.40
1	E	247	HIS	N-CA-CB	5.17	119.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	641	ASN	CA-CB-CG	-5.17	102.03	113.40
1	B	539	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	E	443	ILE	N-CA-C	-5.17	97.04	111.00
1	B	578	MET	N-CA-CB	5.17	119.90	110.60
1	A	76	ASN	CB-CG-OD1	-5.16	111.27	121.60
1	B	35	GLU	CA-C-O	5.16	130.94	120.10
1	B	70	HIS	O-C-N	5.16	130.96	122.70
1	B	271	ARG	CG-CD-NE	5.16	122.64	111.80
1	A	396	ASP	N-CA-CB	-5.16	101.31	110.60
1	B	379	SER	CB-CA-C	5.16	119.91	110.10
1	F	35	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	B	473	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	C	247	HIS	N-CA-CB	5.16	119.89	110.60
1	B	197	TRP	CZ3-CH2-CZ2	5.16	127.79	121.60
1	A	72	TYR	CZ-CE2-CD2	-5.16	115.16	119.80
1	B	148	SER	N-CA-CB	5.16	118.23	110.50
1	B	461	THR	N-CA-CB	5.16	120.09	110.30
1	A	73	SER	CA-C-O	-5.15	109.28	120.10
1	B	42	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	448	ILE	CA-C-N	5.15	128.54	117.20
1	B	474	ARG	CA-CB-CG	5.15	124.74	113.40
1	A	242	PRO	CA-C-N	5.15	128.53	117.20
1	F	247	HIS	N-CA-CB	5.15	119.88	110.60
1	A	410	GLY	CA-C-N	5.15	128.53	117.20
1	A	463	LYS	CB-CG-CD	5.15	124.99	111.60
1	B	258	PRO	CA-C-O	5.15	132.56	120.20
1	A	301	ASP	O-C-N	-5.15	114.47	122.70
1	B	401	TYR	O-C-N	5.15	130.94	122.70
1	C	69	ARG	CB-CG-CD	5.15	124.98	111.60
1	F	132	ILE	N-CA-C	5.15	124.90	111.00
1	B	264	TYR	CA-C-O	-5.14	109.30	120.10
1	F	69	ARG	CB-CG-CD	5.14	124.98	111.60
1	B	594	GLU	CB-CG-CD	-5.14	100.31	114.20
1	D	470	ASN	CB-CA-C	5.14	120.69	110.40
1	D	499	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	184	PHE	CB-CA-C	-5.14	100.12	110.40
1	B	13	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	398	PHE	N-CA-CB	5.14	119.85	110.60
1	A	530	VAL	CG1-CB-CG2	-5.14	102.68	110.90
1	C	521	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	162	LYS	O-C-N	5.14	130.86	121.10
1	A	295	ARG	CB-CA-C	5.14	120.68	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	PHE	CZ-CE2-CD2	-5.14	113.94	120.10
1	B	574	LYS	CB-CA-C	5.13	120.67	110.40
1	A	18	LEU	N-CA-CB	-5.13	100.13	110.40
1	A	139	GLN	CG-CD-OE1	-5.13	111.33	121.60
1	A	270	VAL	CA-C-O	5.13	130.88	120.10
1	A	398	PHE	O-C-N	5.13	130.85	121.10
1	B	191	ASN	N-CA-CB	5.13	119.84	110.60
1	D	363	LEU	N-CA-C	-5.13	97.14	111.00
1	D	644	HIS	CA-CB-CG	5.13	122.32	113.60
1	D	544	ASP	CB-CG-OD1	5.13	122.92	118.30
1	E	278	GLU	CA-C-N	-5.13	105.91	117.20
1	B	522	SER	N-CA-CB	-5.13	102.81	110.50
1	F	179	GLN	CB-CA-C	5.13	120.65	110.40
1	A	237	SER	CB-CA-C	5.12	119.83	110.10
1	A	323	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	B	340	TYR	CZ-CE2-CD2	5.12	124.41	119.80
1	B	354	GLN	O-C-N	5.12	131.90	123.20
1	C	443	ILE	N-CA-C	-5.12	97.18	111.00
1	A	528	VAL	CG1-CB-CG2	5.12	119.08	110.90
1	C	363	LEU	N-CA-C	-5.12	97.19	111.00
1	E	179	GLN	CB-CA-C	5.12	120.63	110.40
1	A	21	ILE	CA-C-N	5.11	128.45	117.20
1	A	144	MET	N-CA-CB	5.11	119.81	110.60
1	A	166	PHE	CA-C-O	5.11	130.84	120.10
1	A	431	TYR	CZ-CE2-CD2	5.11	124.40	119.80
1	B	78	ARG	N-CA-CB	5.11	119.81	110.60
1	B	408	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	B	137	LEU	O-C-N	5.11	130.88	122.70
1	A	103	ALA	O-C-N	-5.11	114.52	122.70
1	A	460	PHE	N-CA-CB	-5.11	101.40	110.60
1	A	542	GLN	CB-CG-CD	-5.11	98.31	111.60
1	E	496	ASP	N-CA-C	-5.11	97.20	111.00
1	F	48	ASP	CB-CG-OD1	5.11	122.90	118.30
1	F	278	GLU	CA-C-N	-5.11	105.96	117.20
1	B	63	HIS	CB-CA-C	-5.11	100.19	110.40
1	B	117	TYR	O-C-N	5.11	130.87	122.70
1	B	147	ASN	O-C-N	5.11	130.87	122.70
1	B	298	GLU	CG-CD-OE1	-5.10	108.09	118.30
1	A	159	MET	O-C-N	-5.10	114.54	122.70
1	D	43	THR	N-CA-C	-5.10	97.22	111.00
1	E	179	GLN	CA-C-O	5.10	130.82	120.10
1	E	210	GLY	N-CA-C	5.10	125.85	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	210	GLY	N-CA-C	5.10	125.85	113.10
1	A	483	CYS	O-C-N	5.10	130.79	121.10
1	A	531	PRO	O-C-N	5.10	130.86	122.70
1	B	326	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	D	487	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	626	LEU	O-C-N	5.10	130.86	122.70
1	D	419	ASP	CA-C-N	-5.10	106.00	116.20
1	F	443	ILE	N-CA-C	-5.10	97.24	111.00
1	B	464	ILE	N-CA-CB	-5.10	99.08	110.80
1	E	363	LEU	N-CA-C	-5.10	97.24	111.00
1	B	216	LYS	N-CA-C	-5.09	97.24	111.00
1	B	264	TYR	N-CA-C	-5.09	97.25	111.00
1	B	479	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
1	B	532	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	C	316	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	639	VAL	N-CA-C	-5.09	97.25	111.00
1	A	133	VAL	CA-C-N	5.09	128.40	117.20
1	B	144	MET	O-C-N	-5.09	114.56	122.70
1	A	95	GLU	CG-CD-OE2	-5.09	108.13	118.30
1	A	253	ARG	CA-C-O	-5.09	109.42	120.10
1	B	108	GLU	CA-CB-CG	5.09	124.59	113.40
1	B	294	SER	CA-CB-OG	-5.09	97.47	111.20
1	A	236	LEU	CA-CB-CG	5.08	127.00	115.30
1	B	375	THR	O-C-N	5.08	130.84	122.70
1	B	624	TYR	CD1-CE1-CZ	5.08	124.38	119.80
1	A	54	GLU	CG-CD-OE2	-5.08	108.13	118.30
1	A	243	VAL	CA-CB-CG1	5.08	118.52	110.90
1	E	177	ARG	N-CA-C	5.08	124.72	111.00
1	A	238	ASN	CB-CA-C	5.08	120.56	110.40
1	B	25	THR	CA-C-N	-5.08	106.03	117.20
1	B	313	ILE	O-C-N	-5.08	114.57	122.70
1	B	67	GLU	CB-CG-CD	-5.08	100.49	114.20
1	A	84	LEU	CB-CA-C	5.08	119.85	110.20
1	A	309	ASP	N-CA-CB	5.08	119.74	110.60
1	A	460	PHE	CD1-CE1-CZ	5.08	126.19	120.10
1	A	304	TYR	CG-CD1-CE1	-5.08	117.24	121.30
1	B	560	ARG	NH1-CZ-NH2	-5.08	113.82	119.40
1	C	401	TYR	CA-CB-CG	5.08	123.04	113.40
1	B	386	TYR	CD1-CE1-CZ	-5.07	115.23	119.80
1	D	401	TYR	CA-CB-CG	5.07	123.04	113.40
1	A	91	ASN	CA-C-O	-5.07	109.45	120.10
1	B	501	PHE	C-N-CA	5.07	134.38	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	566	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	260	THR	O-C-N	-5.07	114.59	122.70
1	C	48	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	542	GLN	O-C-N	5.07	130.81	122.70
1	B	227	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	F	639	VAL	N-CA-C	-5.07	97.31	111.00
1	B	304	TYR	OH-CZ-CE2	5.07	133.78	120.10
1	F	496	ASP	N-CA-C	-5.07	97.32	111.00
1	A	434	ILE	CA-C-O	-5.07	109.46	120.10
1	B	532	ASP	C-N-CA	-5.06	109.04	121.70
1	F	363	LEU	N-CA-C	-5.06	97.33	111.00
1	B	322	GLU	O-C-N	5.06	130.80	122.70
1	A	416	VAL	CA-C-N	-5.06	106.07	117.20
1	B	104	ALA	N-CA-C	-5.06	97.33	111.00
1	A	252	ILE	N-CA-C	-5.06	97.34	111.00
1	B	507	LYS	CA-C-O	-5.06	109.47	120.10
1	E	32	ASP	CB-CA-C	5.06	120.52	110.40
1	E	279	ASP	CA-CB-CG	5.06	124.53	113.40
1	A	42	ASP	N-CA-C	-5.06	97.34	111.00
1	A	386	TYR	CG-CD1-CE1	-5.06	117.25	121.30
1	B	421	GLU	CG-CD-OE2	-5.06	108.19	118.30
1	B	518	THR	N-CA-C	-5.06	97.34	111.00
1	D	177	ARG	N-CA-C	5.06	124.65	111.00
1	A	621	PRO	CA-C-N	5.05	128.32	117.20
1	B	197	TRP	CA-C-O	-5.05	109.48	120.10
1	B	272	PRO	CA-C-O	-5.05	108.07	120.20
1	D	23	GLU	CA-CB-CG	5.05	124.52	113.40
1	D	47	ASN	CA-CB-CG	5.05	124.52	113.40
1	F	177	ARG	N-CA-C	5.05	124.65	111.00
1	E	555	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	363	LEU	CB-CA-C	5.05	119.80	110.20
1	A	432	SER	CA-C-N	-5.05	106.08	117.20
1	A	557	ALA	N-CA-C	-5.05	97.36	111.00
1	C	558	TYR	N-CA-CB	-5.05	101.51	110.60
1	A	421	GLU	CG-CD-OE2	5.05	128.39	118.30
1	B	278	GLU	CB-CG-CD	-5.05	100.58	114.20
1	C	299	ALA	CB-CA-C	5.05	117.67	110.10
1	A	132	ILE	CB-CA-C	-5.04	101.51	111.60
1	C	517	GLU	N-CA-CB	5.04	119.68	110.60
1	B	244	ASP	C-N-CA	5.04	134.31	121.70
1	B	304	TYR	CE1-CZ-OH	-5.04	106.48	120.10
1	B	339	TYR	CB-CG-CD1	-5.04	117.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	GLU	CA-CB-CG	5.04	124.49	113.40
1	A	149	GLU	C-N-CA	-5.04	109.10	121.70
1	B	209	TYR	CZ-CE2-CD2	-5.04	115.26	119.80
1	B	421	GLU	O-C-N	5.04	130.77	122.70
1	F	279	ASP	CA-CB-CG	5.04	124.49	113.40
1	C	210	GLY	N-CA-C	5.04	125.70	113.10
1	B	540	LYS	CB-CG-CD	5.04	124.70	111.60
1	C	639	VAL	N-CA-C	-5.04	97.39	111.00
1	A	200	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	B	545	ASN	CA-CB-CG	5.04	124.48	113.40
1	B	57	MET	CA-C-N	-5.03	106.13	117.20
1	A	327	ILE	CA-C-N	5.03	128.27	117.20
1	C	496	ASP	N-CA-C	-5.03	97.42	111.00
1	F	179	GLN	CA-C-O	5.03	130.66	120.10
1	A	90	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	B	447	GLU	CA-C-O	-5.03	109.54	120.10
1	F	218	GLU	CA-CB-CG	5.03	124.46	113.40
1	A	86	LEU	CA-CB-CG	-5.03	103.74	115.30
1	A	362	ASN	CB-CA-C	5.03	120.45	110.40
1	B	110	MET	N-CA-C	-5.03	97.43	111.00
1	B	198	HIS	CG-CD2-NE2	-5.03	99.65	109.20
1	B	518	THR	CA-CB-CG2	-5.03	105.37	112.40
1	C	278	GLU	CA-C-N	-5.03	106.14	117.20
1	D	210	GLY	N-CA-C	5.03	125.66	113.10
1	F	442	ASN	CB-CA-C	5.03	120.45	110.40
1	B	492	THR	CA-CB-OG1	-5.02	98.45	109.00
1	A	224	HIS	CA-C-O	5.02	130.65	120.10
1	A	516	PRO	CA-C-O	5.02	132.25	120.20
1	B	9	GLN	CG-CD-OE1	5.02	131.65	121.60
1	B	49	HIS	CA-CB-CG	-5.02	105.06	113.60
1	E	69	ARG	CB-CG-CD	5.02	124.66	111.60
1	B	578	MET	C-N-CA	-5.02	109.15	121.70
1	E	442	ASN	CB-CA-C	5.02	120.44	110.40
1	A	538	SER	CA-C-N	5.02	128.24	117.20
1	A	559	GLU	CG-CD-OE2	-5.02	108.26	118.30
1	A	103	ALA	CA-C-N	5.02	128.24	117.20
1	A	159	MET	N-CA-CB	5.02	119.63	110.60
1	A	541	GLU	CG-CD-OE1	-5.02	108.26	118.30
1	D	639	VAL	N-CA-C	-5.02	97.45	111.00
1	D	333	TYR	CB-CG-CD1	5.02	124.01	121.00
1	A	17	LEU	CA-CB-CG	5.01	126.83	115.30
1	A	466	MET	CA-CB-CG	-5.01	104.78	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	550	GLY	CA-C-O	-5.01	111.58	120.60
1	B	31	LYS	CA-C-N	5.01	128.23	117.20
1	A	480	ILE	CA-CB-CG2	5.01	120.92	110.90
1	B	365	PRO	CB-CG-CD	-5.01	86.96	106.50
1	D	496	ASP	N-CA-C	-5.01	97.47	111.00
1	A	279	ASP	N-CA-CB	-5.01	101.58	110.60
1	A	588	ASP	N-CA-CB	-5.01	101.58	110.60
1	A	108	GLU	CG-CD-OE1	5.01	128.31	118.30
1	A	263	LYS	CA-CB-CG	5.01	124.42	113.40
1	B	107	ARG	CD-NE-CZ	-5.01	116.59	123.60
1	B	500	TRP	CB-CA-C	5.01	120.41	110.40
1	B	555	LEU	CB-CG-CD2	5.01	119.51	111.00
1	B	462	TYR	CA-C-O	-5.00	109.59	120.10
1	A	632	ASP	N-CA-C	-5.00	97.49	111.00
1	D	73	SER	N-CA-CB	5.00	118.00	110.50
1	E	48	ASP	CB-CG-OD1	5.00	122.80	118.30
1	A	155	TYR	CA-CB-CG	5.00	122.90	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	521	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	5173	0	4880	687	0
1	B	5173	0	4883	651	1
1	C	5173	0	4888	416	3
1	D	5173	0	4888	472	1
1	E	5173	0	4888	428	0
1	F	5173	0	4888	416	1
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	186	0	0	39	0
3	B	186	0	0	15	0
3	C	186	0	0	11	0
3	D	186	0	0	11	0
3	E	186	0	0	10	0
3	F	186	0	0	9	0
All	All	32166	0	29315	2986	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 49.

All (2986) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLN:OE1	1:B:443:ILE:HD13	1.28	1.29
1:A:422:LEU:CD2	1:A:570:LEU:HD21	1.66	1.23
1:A:316:ARG:HD3	3:A:829:HOH:O	1.41	1.19
1:A:165:THR:CG2	1:A:449:ASN:HB2	1.73	1.17
1:B:456:ASN:HD22	1:B:457:HIS:N	1.42	1.17
1:A:456:ASN:HD22	1:A:457:HIS:N	1.43	1.16
1:A:411:MET:HG3	3:A:834:HOH:O	0.96	1.13
1:A:513:PRO:CG	1:A:517:GLU:HG3	1.79	1.13
1:A:56:LEU:HD11	1:A:110:MET:HE3	1.27	1.12
1:A:135:PRO:HB2	1:A:140:ILE:HD11	1.24	1.11
1:A:422:LEU:HD22	1:A:570:LEU:HD21	1.18	1.10
1:B:95:GLU:HA	1:B:128:LEU:HD21	1.32	1.10
1:A:313:ILE:HD11	1:A:323:LEU:HD13	1.33	1.10
1:A:412:VAL:O	1:A:412:VAL:HG22	1.47	1.09
1:C:368:MET:HE1	1:C:380:PHE:HA	1.29	1.09
1:A:533:MET:HB3	1:A:534:PRO:HD2	1.33	1.07
1:D:165:THR:HG22	1:D:449:ASN:HB2	1.33	1.06
1:C:165:THR:HG22	1:C:449:ASN:HB2	1.36	1.05
1:A:253:ARG:NH1	3:A:701:HOH:O	1.90	1.05
1:A:313:ILE:CD1	1:A:323:LEU:HD13	1.87	1.04
1:A:634:ARG:NH1	1:A:634:ARG:HG2	1.53	1.04
1:A:412:VAL:HG13	1:A:467:SER:O	1.55	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ARG:HH11	1:A:634:ARG:CG	1.71	1.04
1:B:456:ASN:ND2	1:B:457:HIS:H	1.54	1.04
1:B:168:VAL:HG21	1:B:452:VAL:HG12	1.39	1.04
1:C:175:LYS:HB2	1:D:491:ILE:HG12	1.40	1.03
1:A:456:ASN:ND2	1:A:457:HIS:H	1.56	1.03
1:A:416:VAL:HG22	1:A:645:VAL:HG11	1.41	1.02
1:A:513:PRO:HG3	1:A:517:GLU:CG	1.91	1.01
1:D:634:ARG:HH21	1:F:64:ARG:HD2	1.22	1.01
1:D:150:VAL:HG21	1:D:168:VAL:HG12	1.40	1.01
1:A:373:THR:O	1:A:376:ARG:HB2	1.59	1.01
1:D:456:ASN:HD22	1:D:457:HIS:N	1.59	1.00
1:B:417:ALA:HB3	1:B:463:LYS:O	1.58	1.00
1:B:185:GLY:O	1:B:375:THR:HG22	1.61	1.00
1:B:120:TYR:CD2	1:B:134:LEU:HD13	1.95	0.99
1:B:611:VAL:HG12	1:B:612:HIS:HD2	1.25	0.99
1:E:239:TRP:CH2	1:E:574:LYS:HD3	1.97	0.99
1:E:368:MET:HE1	1:E:380:PHE:HA	1.39	0.99
1:F:423:ILE:HD11	1:F:652:HIS:NE2	1.77	0.99
1:C:472:GLY:HA2	1:C:514:SER:HB2	1.45	0.99
1:C:456:ASN:HD22	1:C:457:HIS:N	1.60	0.99
1:F:456:ASN:HD22	1:F:457:HIS:N	1.59	0.99
1:B:606:HIS:HD2	1:B:608:GLN:HG2	1.27	0.99
1:B:416:VAL:HG22	1:B:645:VAL:HG11	1.45	0.99
1:F:56:LEU:HD11	1:F:110:MET:HE3	1.45	0.99
1:D:421:GLU:HG2	1:D:422:LEU:H	1.28	0.98
1:E:456:ASN:HD22	1:E:457:HIS:N	1.60	0.98
1:D:46:TYR:CZ	1:D:53:VAL:HG21	1.98	0.98
1:E:423:ILE:HD11	1:E:652:HIS:NE2	1.78	0.98
1:C:150:VAL:HG21	1:C:168:VAL:HG12	1.44	0.98
1:F:165:THR:HG22	1:F:449:ASN:HB2	1.45	0.98
1:B:423:ILE:HD11	1:B:652:HIS:NE2	1.79	0.97
1:D:272:PRO:HG2	1:E:272:PRO:HG2	1.41	0.97
1:E:606:HIS:HD2	1:E:608:GLN:HG2	1.29	0.97
1:A:423:ILE:HD11	1:A:652:HIS:CE1	1.98	0.97
1:A:165:THR:HG22	1:A:449:ASN:HB2	1.43	0.96
1:F:368:MET:HE1	1:F:380:PHE:HA	1.45	0.96
1:A:89:VAL:O	1:A:92:GLN:N	1.98	0.96
1:C:56:LEU:HD11	1:C:110:MET:HE3	1.45	0.96
1:A:120:TYR:CD2	1:A:134:LEU:HD13	1.99	0.96
1:A:423:ILE:HD11	1:A:652:HIS:NE2	1.79	0.96
1:D:56:LEU:HD11	1:D:110:MET:HE3	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:PRO:HB2	1:B:140:ILE:HD11	1.46	0.96
1:E:165:THR:HG22	1:E:449:ASN:HB2	1.45	0.96
1:A:135:PRO:CB	1:A:140:ILE:HD11	1.96	0.95
1:A:513:PRO:HG3	1:A:517:GLU:HG3	0.96	0.95
1:B:283:VAL:HG11	1:B:349:VAL:HB	1.44	0.95
1:A:477:THR:HG23	1:A:509:PHE:CD1	2.02	0.95
1:F:150:VAL:HG21	1:F:168:VAL:HG12	1.47	0.95
1:A:634:ARG:HG2	1:A:634:ARG:HH11	0.78	0.95
1:E:5:THR:HG22	1:E:6:GLY:H	1.30	0.95
1:A:31:LYS:O	1:A:34:ALA:HB3	1.67	0.95
1:A:48:ASP:HB3	1:A:92:GLN:NE2	1.81	0.94
1:C:423:ILE:HD11	1:C:652:HIS:NE2	1.81	0.94
1:D:368:MET:HE1	1:D:380:PHE:HA	1.49	0.94
1:C:606:HIS:HD2	1:C:608:GLN:HG2	1.32	0.94
1:F:493:LEU:HD13	1:F:498:ALA:HB2	1.49	0.94
1:D:95:GLU:HG2	1:D:96:TRP:H	1.30	0.94
1:B:65:LEU:HD12	1:B:82:GLU:HG2	1.49	0.94
1:F:239:TRP:CH2	1:F:574:LYS:HD3	2.01	0.94
1:B:76:ASN:HD22	1:B:79:GLN:H	1.15	0.94
1:D:413:VAL:HA	1:D:466:MET:HB3	1.48	0.94
1:A:560:ARG:NH2	1:A:606:HIS:N	2.14	0.94
1:B:143:HIS:CE1	1:B:151:ILE:HG21	2.03	0.94
1:C:8:ALA:HB1	1:C:546:ALA:HB3	1.50	0.94
1:C:239:TRP:CH2	1:C:574:LYS:HD3	2.03	0.94
1:C:493:LEU:HD13	1:C:498:ALA:HB2	1.50	0.94
1:E:456:ASN:ND2	1:E:457:HIS:H	1.65	0.94
1:A:411:MET:HE3	1:A:512:VAL:HB	1.47	0.94
1:D:239:TRP:CH2	1:D:574:LYS:HD3	2.03	0.94
1:E:56:LEU:HD11	1:E:110:MET:HE3	1.48	0.93
1:E:150:VAL:HG21	1:E:168:VAL:HG12	1.49	0.93
1:A:21:ILE:HG13	1:A:21:ILE:O	1.65	0.93
1:C:272:PRO:HG2	1:F:272:PRO:HG2	1.51	0.93
1:F:317:GLN:HB2	1:F:318:PRO:HD2	1.50	0.93
1:F:606:HIS:HD2	1:F:608:GLN:HG2	1.31	0.93
1:B:48:ASP:HB3	1:B:92:GLN:NE2	1.83	0.93
1:D:423:ILE:HD11	1:D:652:HIS:NE2	1.84	0.92
1:A:161:GLN:OE1	1:B:443:ILE:CD1	2.17	0.92
1:B:89:VAL:O	1:B:92:GLN:N	2.03	0.92
1:D:493:LEU:HD13	1:D:498:ALA:HB2	1.51	0.92
1:F:456:ASN:ND2	1:F:457:HIS:H	1.66	0.92
1:D:317:GLN:HB2	1:D:318:PRO:HD2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:GLU:HA	1:F:128:LEU:HD21	1.50	0.92
1:B:18:LEU:HD21	1:B:119:LEU:HD23	1.49	0.92
1:B:548:ASN:H	1:B:548:ASN:ND2	1.67	0.92
1:A:470:ASN:ND2	1:A:474:ARG:HD3	1.83	0.92
1:B:76:ASN:ND2	1:B:79:GLN:HG3	1.86	0.92
1:C:317:GLN:HB2	1:C:318:PRO:HD2	1.50	0.91
1:C:456:ASN:ND2	1:C:457:HIS:H	1.66	0.91
1:B:121:VAL:HG23	1:B:199:MET:HG2	1.52	0.91
1:E:317:GLN:HB2	1:E:318:PRO:HD2	1.50	0.91
1:D:456:ASN:ND2	1:D:457:HIS:H	1.66	0.91
1:A:248:TRP:CH2	1:A:289:LEU:HD13	2.06	0.91
1:A:422:LEU:HD22	1:A:570:LEU:CD2	2.00	0.91
1:D:606:HIS:HD2	1:D:608:GLN:HG2	1.34	0.91
1:E:408:PHE:N	1:E:641:ASN:OD1	2.04	0.90
1:F:168:VAL:HG21	1:F:452:VAL:HG12	1.54	0.90
1:A:50:GLY:O	1:A:53:VAL:HG23	1.72	0.90
1:A:412:VAL:O	1:A:412:VAL:CG2	2.18	0.90
1:A:543:ALA:O	1:A:547:VAL:HG22	1.70	0.90
1:B:487:ASP:CB	1:B:491:ILE:H	1.84	0.90
1:E:493:LEU:HD13	1:E:498:ALA:HB2	1.55	0.89
1:A:165:THR:CB	1:A:449:ASN:HB2	2.01	0.89
1:B:60:LEU:HD11	1:B:109:ARG:HG3	1.54	0.89
1:B:74:LEU:HG	1:B:74:LEU:O	1.69	0.89
1:F:313:ILE:HD11	1:F:323:LEU:HD13	1.54	0.89
1:B:589:GLY:O	1:B:593:THR:OG1	1.89	0.89
1:A:462:TYR:O	1:A:520:GLU:HA	1.72	0.89
1:A:305:ILE:HG13	1:A:315:ILE:HG21	1.54	0.89
1:B:611:VAL:HG12	1:B:612:HIS:CD2	2.07	0.89
1:C:414:ASN:HD22	1:C:466:MET:HA	1.38	0.89
1:C:168:VAL:HG21	1:C:452:VAL:HG12	1.53	0.88
1:D:95:GLU:HG2	1:D:96:TRP:N	1.86	0.88
1:E:168:VAL:HG21	1:E:452:VAL:HG12	1.53	0.88
1:C:313:ILE:HD11	1:C:323:LEU:HD13	1.54	0.88
1:B:239:TRP:CH2	1:B:574:LYS:HD3	2.08	0.88
1:E:48:ASP:HB3	1:E:92:GLN:NE2	1.88	0.88
1:F:543:ALA:HA	1:F:553:LEU:HD11	1.54	0.88
1:A:411:MET:CE	1:A:512:VAL:HB	2.03	0.88
1:A:468:ASN:OD1	1:A:470:ASN:HB2	1.73	0.88
1:B:48:ASP:HB3	1:B:92:GLN:HE21	1.39	0.88
1:E:411:MET:HG3	3:E:834:HOH:O	1.74	0.88
1:B:487:ASP:HB2	1:B:491:ILE:H	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HG21	1:A:168:VAL:HG12	1.53	0.87
1:B:416:VAL:HG22	1:B:645:VAL:CG1	2.02	0.87
1:D:508:PHE:CE2	1:D:521:ARG:HD2	2.09	0.87
1:A:11:GLN:O	1:A:15:ASN:ND2	2.08	0.87
1:A:639:VAL:HG23	1:A:641:ASN:ND2	1.89	0.87
1:D:543:ALA:O	1:D:547:VAL:HG23	1.74	0.86
1:F:8:ALA:HA	1:F:553:LEU:HD12	1.58	0.86
1:D:313:ILE:HD11	1:D:323:LEU:HD13	1.56	0.86
1:E:543:ALA:O	1:E:547:VAL:HG23	1.75	0.86
1:B:255:GLY:HA2	1:B:271:ARG:NH1	1.90	0.86
1:E:95:GLU:HA	1:E:128:LEU:HD21	1.58	0.86
1:A:408:PHE:CB	1:A:641:ASN:OD1	2.24	0.86
1:C:150:VAL:HG12	1:C:433:LEU:HD11	1.56	0.86
1:B:5:THR:HG22	1:B:10:LYS:HD3	1.57	0.85
1:A:440:GLY:C	1:A:441:GLU:CG	2.38	0.85
1:B:329:GLU:HA	1:B:344:HIS:HB3	1.56	0.85
1:B:634:ARG:HG2	1:B:634:ARG:HH11	1.41	0.85
1:A:493:LEU:HD13	1:A:498:ALA:HB2	1.58	0.85
1:B:29:ASP:O	1:B:33:ILE:HG13	1.77	0.85
1:E:553:LEU:HD22	1:E:555:LEU:HG	1.59	0.85
1:B:493:LEU:HB3	1:B:497:GLU:HB2	1.59	0.85
1:D:185:GLY:O	1:D:375:THR:HG22	1.77	0.85
1:A:417:ALA:HB3	1:A:463:LYS:O	1.77	0.85
1:F:422:LEU:HD22	1:F:570:LEU:HD21	1.58	0.85
1:E:634:ARG:HG2	1:E:634:ARG:HH11	1.42	0.84
1:E:606:HIS:CD2	1:E:608:GLN:HG2	2.12	0.84
1:F:414:ASN:HD22	1:F:466:MET:HA	1.42	0.84
1:C:576:GLU:OE1	1:D:576:GLU:OE1	1.95	0.84
1:D:150:VAL:HG12	1:D:433:LEU:HD11	1.56	0.84
1:A:125:HIS:HB3	1:A:211:TYR:OH	1.78	0.84
1:D:413:VAL:HA	1:D:466:MET:CB	2.07	0.84
1:F:606:HIS:CD2	1:F:608:GLN:HG2	2.13	0.84
1:A:594:GLU:O	1:A:594:GLU:HG2	1.76	0.84
1:B:487:ASP:HB2	1:B:491:ILE:N	1.92	0.84
1:E:313:ILE:HD11	1:E:323:LEU:HD13	1.60	0.84
1:A:368:MET:HE1	1:A:380:PHE:HA	1.59	0.83
1:A:591:LYS:HA	1:A:594:GLU:HB2	1.59	0.83
1:B:66:LEU:HD22	1:B:67:GLU:O	1.79	0.83
1:E:185:GLY:O	1:E:375:THR:HG22	1.78	0.83
1:B:101:SER:O	1:B:104:ALA:HB3	1.77	0.83
1:B:39:PRO:HB3	1:B:102:ASN:HD21	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:LEU:HB3	1:B:571:PRO:HD2	1.59	0.83
1:F:560:ARG:NH1	1:F:606:HIS:N	2.27	0.83
1:A:255:GLY:HA2	1:A:271:ARG:NH1	1.92	0.83
1:F:185:GLY:O	1:F:375:THR:HG22	1.78	0.83
1:A:200:ASP:O	1:A:202:PRO:HD3	1.78	0.83
1:B:570:LEU:HB3	1:B:571:PRO:CD	2.08	0.83
1:B:20:LYS:N	1:B:435:ASN:HD21	1.76	0.83
1:C:185:GLY:O	1:C:375:THR:HG22	1.77	0.83
1:A:418:ILE:HD11	1:A:462:TYR:CE1	2.14	0.83
1:A:86:LEU:HD23	1:A:90:LEU:HD22	1.59	0.83
1:A:74:LEU:O	1:A:74:LEU:HG	1.77	0.82
1:B:59:GLU:OE1	1:B:64:ARG:HD3	1.79	0.82
1:D:133:VAL:HG22	1:D:558:TYR:O	1.77	0.82
1:F:634:ARG:HG2	1:F:634:ARG:HH11	1.43	0.82
1:B:522:SER:O	1:B:523:SER:C	2.14	0.82
1:B:555:LEU:HD23	1:B:556:SER:H	1.44	0.82
1:B:606:HIS:CD2	1:B:608:GLN:HG2	2.14	0.82
1:C:634:ARG:HH11	1:C:634:ARG:HG2	1.43	0.82
1:B:535:SER:OG	1:B:536:PHE:N	2.12	0.82
1:D:168:VAL:HG21	1:D:452:VAL:HG12	1.58	0.82
1:F:269:PRO:HB3	1:F:363:LEU:HD23	1.61	0.82
1:C:380:PHE:CE1	1:C:384:HIS:CE1	2.68	0.82
1:A:533:MET:CE	1:A:533:MET:H	1.91	0.82
1:C:7:ASN:C	1:C:9:GLN:H	1.81	0.82
1:E:7:ASN:C	1:E:9:GLN:H	1.79	0.82
1:C:422:LEU:HD22	1:C:570:LEU:HD21	1.60	0.82
1:C:606:HIS:CD2	1:C:608:GLN:HG2	2.14	0.82
1:D:634:ARG:HG2	1:D:634:ARG:HH11	1.44	0.82
1:B:183:TYR:OH	1:B:234:GLU:OE1	1.98	0.81
1:E:560:ARG:NH1	1:E:606:HIS:N	2.28	0.81
1:A:414:ASN:HD22	1:A:466:MET:HA	1.46	0.81
1:A:533:MET:HB3	1:A:534:PRO:CD	2.10	0.81
1:B:477:THR:HG23	1:B:509:PHE:CD1	2.16	0.81
1:D:606:HIS:CD2	1:D:608:GLN:HG2	2.15	0.81
1:A:185:GLY:O	1:A:375:THR:HG22	1.81	0.81
1:B:178:GLU:HG3	1:B:178:GLU:O	1.78	0.81
1:B:486:GLU:HA	1:B:492:THR:HA	1.61	0.81
1:C:560:ARG:HG2	1:C:609:CYS:HB3	1.61	0.81
1:E:411:MET:CE	1:E:468:ASN:HD22	1.94	0.81
1:B:522:SER:O	1:B:524:LYS:N	2.13	0.81
1:F:7:ASN:C	1:F:9:GLN:H	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:ASP:OD1	1:B:588:ASP:O	1.97	0.81
1:C:175:LYS:HB2	1:D:491:ILE:CG1	2.11	0.81
1:A:411:MET:HE3	1:A:512:VAL:CB	2.10	0.81
1:A:479:ARG:NH2	1:A:618:ASP:OD2	2.14	0.81
1:A:508:PHE:CE2	1:A:521:ARG:CD	2.63	0.81
1:C:8:ALA:CB	1:C:546:ALA:HB3	2.11	0.81
1:C:175:LYS:CB	1:D:491:ILE:HG12	2.10	0.81
1:D:7:ASN:C	1:D:9:GLN:H	1.80	0.81
1:A:606:HIS:HD2	1:A:608:GLN:HG2	1.44	0.80
1:E:18:LEU:HD21	1:E:119:LEU:HD23	1.64	0.80
1:E:419:ASP:HB2	1:E:463:LYS:HD2	1.62	0.80
1:F:18:LEU:HD21	1:F:119:LEU:HD23	1.63	0.80
1:A:243:VAL:HG23	1:A:385:LYS:HD3	1.63	0.80
1:E:414:ASN:HD22	1:E:466:MET:HA	1.47	0.80
1:A:422:LEU:HD23	1:A:570:LEU:HD21	1.60	0.80
1:B:368:MET:CE	1:B:380:PHE:HA	2.11	0.80
1:A:72:TYR:HA	1:A:79:GLN:OE1	1.81	0.80
1:B:606:HIS:HB3	1:B:608:GLN:H	1.47	0.80
1:C:18:LEU:HD21	1:C:119:LEU:HD23	1.64	0.80
1:B:175:LYS:O	1:B:176:ASN:HB2	1.80	0.80
1:E:43:THR:HG23	1:E:49:HIS:C	2.02	0.80
1:E:150:VAL:HG12	1:E:433:LEU:HD11	1.64	0.80
1:E:486:GLU:HA	1:E:492:THR:HA	1.64	0.80
1:A:440:GLY:C	1:A:441:GLU:HG2	1.69	0.79
1:A:553:LEU:HD22	1:A:555:LEU:HG	1.63	0.79
1:D:456:ASN:HD22	1:D:457:HIS:H	0.81	0.79
1:F:150:VAL:HG12	1:F:433:LEU:HD11	1.63	0.79
1:A:190:MET:HG2	1:A:568:MET:HE2	1.63	0.79
1:D:18:LEU:HD21	1:D:119:LEU:HD23	1.63	0.79
1:E:269:PRO:HB3	1:E:363:LEU:HD23	1.64	0.79
1:F:43:THR:HG23	1:F:49:HIS:C	2.03	0.79
1:A:201:PHE:HB3	1:A:216:LYS:CD	2.13	0.79
1:B:248:TRP:CH2	1:B:289:LEU:HD13	2.18	0.79
1:A:252:ILE:HG13	1:A:275:ILE:HG22	1.63	0.79
1:A:300:ILE:CD1	1:A:390:ILE:HG22	2.13	0.79
1:A:256:PHE:C	1:A:256:PHE:CD1	2.54	0.79
1:C:456:ASN:HD22	1:C:457:HIS:H	0.81	0.79
1:D:40:LEU:HD12	1:D:53:VAL:HG12	1.65	0.79
1:A:237:SER:HA	1:A:574:LYS:HE3	1.65	0.78
1:A:439:SER:O	1:B:160:THR:HG22	1.83	0.78
1:A:56:LEU:HD11	1:A:110:MET:CE	2.11	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD12	1:A:110:MET:SD	2.23	0.78
1:A:220:PHE:CE2	1:A:329:GLU:HB2	2.19	0.78
1:C:43:THR:HG23	1:C:49:HIS:C	2.03	0.78
1:B:56:LEU:HD21	1:B:110:MET:CE	2.13	0.78
1:B:158:LYS:HG2	1:B:437:VAL:CG2	2.14	0.78
1:B:413:VAL:HG12	1:B:643:LYS:CG	2.13	0.78
1:A:69:ARG:HG2	1:A:264:TYR:CE2	2.19	0.77
1:A:120:TYR:O	1:A:124:ILE:HG13	1.84	0.77
1:A:178:GLU:OE1	3:A:705:HOH:O	2.01	0.77
1:C:487:ASP:HB2	1:C:491:ILE:O	1.83	0.77
1:B:313:ILE:C	1:B:313:ILE:HD12	2.04	0.77
1:B:591:LYS:HB2	1:B:591:LYS:NZ	2.00	0.77
1:D:411:MET:HE2	3:D:834:HOH:O	1.82	0.77
1:B:330:SER:HB2	1:B:342:SER:OG	1.84	0.77
1:A:76:ASN:HB3	1:A:79:GLN:HB2	1.66	0.77
1:B:26:LYS:HE2	1:B:440:GLY:O	1.83	0.77
1:A:554:ASP:O	1:A:555:LEU:C	2.20	0.77
1:E:423:ILE:HD11	1:E:652:HIS:CE1	2.19	0.77
1:F:411:MET:HG3	3:F:834:HOH:O	1.83	0.77
1:A:418:ILE:HD11	1:A:462:TYR:CD1	2.18	0.77
1:C:411:MET:HG3	3:C:834:HOH:O	1.85	0.77
1:A:323:LEU:HD11	3:A:849:HOH:O	1.84	0.77
1:B:356:ASP:OD2	1:B:359:GLY:HA2	1.84	0.77
1:C:408:PHE:N	1:C:641:ASN:OD1	2.17	0.77
1:A:86:LEU:CD2	1:A:90:LEU:HD22	2.15	0.77
1:A:165:THR:HB	1:A:449:ASN:CB	2.14	0.77
1:A:434:ILE:HD11	1:A:447:GLU:HA	1.67	0.77
1:B:591:LYS:HB2	1:B:591:LYS:HZ2	1.50	0.77
1:F:408:PHE:N	1:F:641:ASN:OD1	2.18	0.77
1:B:61:ASN:C	1:B:63:HIS:H	1.84	0.77
1:B:78:ARG:NH1	1:B:82:GLU:OE2	2.16	0.77
1:A:168:VAL:HG21	1:A:452:VAL:HG12	1.65	0.76
1:A:508:PHE:CE2	1:A:521:ARG:HD3	2.20	0.76
1:B:468:ASN:ND2	1:B:512:VAL:O	2.17	0.76
1:D:330:SER:OG	1:D:341:GLY:O	2.03	0.76
1:B:548:ASN:H	1:B:548:ASN:HD22	1.31	0.76
1:D:272:PRO:CG	1:E:272:PRO:HG2	2.15	0.76
1:A:252:ILE:HG13	1:A:275:ILE:CG2	2.15	0.76
1:B:305:ILE:HD12	1:B:315:ILE:HG21	1.66	0.76
1:E:60:LEU:HD21	1:E:109:ARG:HD2	1.66	0.76
1:D:423:ILE:HD11	1:D:652:HIS:CE1	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:PHE:CE2	1:B:101:SER:HB3	2.21	0.76
1:F:423:ILE:HD11	1:F:652:HIS:CE1	2.20	0.76
1:D:60:LEU:HD21	1:D:109:ARG:HD2	1.68	0.76
1:D:634:ARG:HH21	1:F:64:ARG:CD	1.98	0.76
1:B:316:ARG:HG3	1:B:398:PHE:HE1	1.51	0.75
1:B:565:PRO:HB2	1:B:568:MET:HG2	1.66	0.75
1:A:165:THR:HB	1:A:449:ASN:HB2	1.69	0.75
1:A:220:PHE:CZ	1:A:329:GLU:HB2	2.21	0.75
1:B:74:LEU:O	1:B:74:LEU:CG	2.32	0.75
1:B:150:VAL:HG12	1:B:433:LEU:HD11	1.67	0.75
1:B:489:ASN:HB3	1:B:491:ILE:HD11	1.66	0.75
1:D:59:GLU:OE1	1:D:64:ARG:HD3	1.87	0.75
1:A:300:ILE:HD11	1:A:390:ILE:HG22	1.68	0.75
1:B:29:ASP:OD1	1:B:29:ASP:N	2.18	0.75
1:B:423:ILE:HD11	1:B:652:HIS:CE1	2.20	0.75
1:D:634:ARG:HE	1:F:64:ARG:NE	1.83	0.75
1:B:11:GLN:HG2	1:B:132:ILE:HG23	1.67	0.75
1:B:425:PHE:N	1:B:456:ASN:O	2.18	0.75
1:C:165:THR:HA	1:C:449:ASN:O	1.87	0.75
1:B:356:ASP:CG	1:B:359:GLY:HA2	2.06	0.75
1:A:606:HIS:CD2	1:A:608:GLN:HG2	2.21	0.75
1:C:60:LEU:HD21	1:C:109:ARG:HD2	1.68	0.75
1:C:11:GLN:HG3	1:C:15:ASN:HD21	1.52	0.74
1:D:5:THR:HG22	1:D:6:GLY:H	1.52	0.74
1:D:448:ILE:C	1:D:449:ASN:HD22	1.89	0.74
1:C:248:TRP:CH2	1:C:289:LEU:HD13	2.21	0.74
1:D:487:ASP:HB3	1:D:491:ILE:H	1.50	0.74
1:E:185:GLY:HA2	1:E:375:THR:CG2	2.17	0.74
1:A:11:GLN:HG3	1:A:15:ASN:HD21	1.52	0.74
1:D:40:LEU:CD1	1:D:53:VAL:HG12	2.17	0.74
1:B:243:VAL:HG23	1:B:385:LYS:HD2	1.68	0.74
1:D:11:GLN:HG3	1:D:15:ASN:HD21	1.51	0.74
1:D:411:MET:HE1	1:D:512:VAL:HB	1.70	0.74
1:A:317:GLN:HB2	1:A:318:PRO:HD2	1.67	0.74
1:B:244:ASP:O	1:B:382:ARG:HG3	1.87	0.74
1:E:120:TYR:O	1:E:124:ILE:HG13	1.88	0.74
1:A:17:LEU:HD21	1:A:103:ALA:O	1.88	0.74
1:B:446:VAL:O	1:B:446:VAL:HG13	1.86	0.74
1:D:248:TRP:CH2	1:D:289:LEU:HD13	2.22	0.74
1:D:422:LEU:HD22	1:D:570:LEU:HD21	1.68	0.74
1:E:59:GLU:OE1	1:E:64:ARG:HD3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:MET:CB	1:A:534:PRO:HD2	2.02	0.74
1:B:148:SER:HB2	1:B:259:LEU:O	1.87	0.74
1:D:185:GLY:HA2	1:D:375:THR:CG2	2.18	0.74
1:A:133:VAL:CG2	1:A:555:LEU:HD13	2.18	0.73
1:B:62:ASP:HB2	1:B:64:ARG:HG2	1.70	0.73
1:C:508:PHE:CE2	1:C:521:ARG:HD2	2.23	0.73
1:A:139:GLN:NE2	1:A:432:SER:H	1.86	0.73
1:E:48:ASP:HB3	1:E:92:GLN:HE21	1.48	0.73
1:F:329:GLU:HA	1:F:344:HIS:HB3	1.70	0.73
1:A:557:ALA:HB3	1:A:558:TYR:CD2	2.22	0.73
1:B:72:TYR:HA	1:B:79:GLN:OE1	1.88	0.73
1:C:48:ASP:HB3	1:C:92:GLN:NE2	2.03	0.73
1:F:512:VAL:HG11	3:F:834:HOH:O	1.87	0.73
1:A:48:ASP:HB3	1:A:92:GLN:HE21	1.51	0.73
1:B:411:MET:HE3	1:B:512:VAL:HB	1.71	0.73
1:C:247:HIS:HB2	1:C:250:ARG:HG2	1.69	0.73
1:D:177:ARG:HG2	1:E:360:LYS:HB3	1.68	0.73
1:E:130:ASP:O	1:E:559:GLU:OE1	2.06	0.73
1:F:330:SER:OG	1:F:341:GLY:O	2.06	0.73
1:F:547:VAL:HG23	1:F:548:ASN:ND2	2.02	0.73
1:A:56:LEU:CD1	1:A:110:MET:HE3	2.15	0.73
1:C:59:GLU:OE1	1:C:64:ARG:HD3	1.87	0.73
1:C:185:GLY:HA2	1:C:375:THR:CG2	2.17	0.73
1:E:248:TRP:CH2	1:E:289:LEU:HD13	2.23	0.73
1:B:76:ASN:HD22	1:B:79:GLN:HG3	1.52	0.73
1:B:239:TRP:CZ3	1:B:574:LYS:NZ	2.56	0.73
1:B:416:VAL:CG2	1:B:645:VAL:HG11	2.18	0.73
1:D:69:ARG:HG2	1:D:264:TYR:CE2	2.24	0.73
1:E:247:HIS:HB2	1:E:250:ARG:HG2	1.69	0.73
1:F:59:GLU:OE1	1:F:64:ARG:HD3	1.87	0.73
1:D:197:TRP:NE1	1:D:223:VAL:HG21	2.04	0.73
1:F:48:ASP:HB3	1:F:92:GLN:NE2	2.03	0.73
1:F:248:TRP:CH2	1:F:289:LEU:HD13	2.23	0.73
1:A:7:ASN:HA	1:A:10:LYS:HB2	1.71	0.73
1:B:61:ASN:C	1:B:63:HIS:N	2.42	0.73
1:F:46:TYR:CE2	1:F:53:VAL:HG21	2.24	0.73
1:B:196:THR:HG21	1:B:561:SER:HB2	1.70	0.73
1:C:478:PHE:CZ	1:C:519:ILE:HD12	2.23	0.73
1:A:226:GLN:O	1:A:227:LEU:C	2.23	0.72
1:B:65:LEU:CD1	1:B:82:GLU:HG2	2.19	0.72
1:B:413:VAL:HG23	1:B:466:MET:HE3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:ARG:HD3	1:C:609:CYS:O	1.89	0.72
1:E:329:GLU:HA	1:E:344:HIS:HB3	1.69	0.72
1:E:456:ASN:HD22	1:E:457:HIS:H	0.80	0.72
1:C:491:ILE:HG12	1:D:175:LYS:HB2	1.71	0.72
1:D:120:TYR:O	1:D:124:ILE:HG13	1.89	0.72
1:F:60:LEU:HD21	1:F:109:ARG:HD2	1.69	0.72
1:A:533:MET:H	1:A:533:MET:HE2	1.54	0.72
1:B:456:ASN:ND2	1:B:457:HIS:N	2.25	0.72
1:D:48:ASP:N	1:D:92:GLN:HE21	1.87	0.72
1:F:120:TYR:O	1:F:124:ILE:HG13	1.89	0.72
1:B:262:TYR:CE1	1:B:268:PHE:CE1	2.76	0.72
1:C:69:ARG:HG2	1:C:264:TYR:CE2	2.25	0.72
1:C:120:TYR:O	1:C:124:ILE:HG13	1.89	0.72
1:F:247:HIS:HB2	1:F:250:ARG:HG2	1.69	0.72
1:D:486:GLU:HA	1:D:492:THR:HA	1.72	0.72
1:F:185:GLY:HA2	1:F:375:THR:CG2	2.18	0.72
1:A:354:GLN:HA	1:A:354:GLN:NE2	2.04	0.72
1:A:456:ASN:HD22	1:A:457:HIS:H	0.77	0.72
1:B:185:GLY:HA2	1:B:375:THR:HG23	1.72	0.72
1:B:493:LEU:HD13	1:B:498:ALA:HB2	1.69	0.72
1:B:406:LEU:HB2	1:B:639:VAL:HG11	1.71	0.72
1:C:5:THR:HG22	1:C:6:GLY:H	1.55	0.72
1:C:423:ILE:HD11	1:C:652:HIS:CE1	2.24	0.72
1:A:135:PRO:HB2	1:A:140:ILE:CD1	2.12	0.72
1:B:466:MET:O	1:B:466:MET:CG	2.36	0.72
1:E:11:GLN:HG3	1:E:15:ASN:HD21	1.54	0.72
1:B:353:ARG:NE	1:B:369:GLU:OE2	2.21	0.72
1:A:42:ASP:O	1:A:45:ILE:HD11	1.90	0.72
1:B:69:ARG:N	1:B:112:GLU:OE2	2.22	0.72
1:E:162:LYS:O	1:E:446:VAL:HG21	1.90	0.72
1:E:367:VAL:O	1:E:373:THR:HG22	1.90	0.72
1:F:11:GLN:HG3	1:F:15:ASN:HD21	1.55	0.72
1:D:247:HIS:HB2	1:D:250:ARG:HG2	1.71	0.71
1:A:125:HIS:CB	1:A:211:TYR:OH	2.37	0.71
1:A:427:ASP:HB3	1:A:567:ARG:HH12	1.54	0.71
1:A:441:GLU:H	1:A:443:ILE:HG22	1.54	0.71
1:B:132:ILE:HG22	1:B:133:VAL:N	2.05	0.71
1:B:466:MET:O	1:B:466:MET:HG3	1.89	0.71
1:D:634:ARG:NH2	1:F:64:ARG:HD2	2.02	0.71
1:B:313:ILE:HD11	1:B:323:LEU:HD13	1.72	0.71
1:B:592:ASP:O	1:B:619:ASN:ND2	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:SER:OG	1:C:341:GLY:O	2.09	0.71
1:A:169:SER:O	1:A:170:PHE:HB2	1.90	0.71
1:A:283:VAL:HG11	1:A:349:VAL:HB	1.72	0.71
1:D:421:GLU:CG	1:D:422:LEU:H	2.01	0.71
1:E:508:PHE:CE2	1:E:521:ARG:HD2	2.26	0.71
1:A:440:GLY:O	1:A:441:GLU:OE1	2.08	0.71
1:F:5:THR:HG22	1:F:6:GLY:H	1.54	0.71
1:A:260:THR:HG22	1:A:268:PHE:CE1	2.26	0.71
1:A:470:ASN:HD22	1:A:474:ARG:HD3	1.55	0.71
1:B:147:ASN:HD22	1:B:149:GLU:HB3	1.53	0.71
1:C:46:TYR:CE2	1:C:53:VAL:HG21	2.26	0.71
1:E:373:THR:O	1:E:376:ARG:HB2	1.91	0.71
1:F:508:PHE:CE2	1:F:521:ARG:HD2	2.25	0.71
1:A:411:MET:HE3	1:A:512:VAL:CG1	2.21	0.71
1:C:95:GLU:HA	1:C:128:LEU:HD21	1.72	0.71
1:F:69:ARG:HG2	1:F:264:TYR:CE2	2.26	0.71
1:A:374:ALA:C	1:A:376:ARG:H	1.94	0.71
1:C:237:SER:HA	1:C:574:LYS:HE3	1.73	0.71
1:A:408:PHE:HB3	1:A:641:ASN:OD1	1.91	0.71
1:C:197:TRP:NE1	1:C:223:VAL:HG21	2.06	0.71
1:B:72:TYR:HD2	1:B:79:GLN:HB3	1.56	0.70
1:E:313:ILE:C	1:E:313:ILE:HD12	2.11	0.70
1:F:367:VAL:O	1:F:373:THR:HG22	1.91	0.70
1:B:301:ASP:OD2	1:B:393:LYS:NZ	2.24	0.70
1:B:412:VAL:HB	1:B:640:SER:HB2	1.73	0.70
1:C:634:ARG:HH21	1:E:64:ARG:HD2	1.54	0.70
1:D:203:PHE:HB3	1:D:329:GLU:OE2	1.91	0.70
1:A:641:ASN:HD22	1:A:641:ASN:C	1.93	0.70
1:B:19:ASP:O	1:B:20:LYS:C	2.29	0.70
1:D:373:THR:O	1:D:376:ARG:HB2	1.91	0.70
1:E:560:ARG:HH12	1:E:606:HIS:N	1.89	0.70
1:A:201:PHE:HB3	1:A:216:LYS:HD3	1.73	0.70
1:B:193:HIS:ND1	1:B:562:CYS:O	2.24	0.70
1:C:491:ILE:CD1	1:D:175:LYS:HB2	2.22	0.70
1:F:197:TRP:NE1	1:F:223:VAL:HG21	2.07	0.70
1:A:374:ALA:O	1:A:376:ARG:N	2.25	0.70
1:D:53:VAL:HG22	1:D:89:VAL:HG13	1.73	0.70
1:A:493:LEU:HB2	1:A:497:GLU:HB2	1.73	0.70
1:A:620:ARG:HG3	1:A:624:TYR:CG	2.26	0.70
1:B:592:ASP:C	1:B:594:GLU:H	1.95	0.70
1:C:367:VAL:O	1:C:373:THR:HG22	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:TYR:CD2	1:E:134:LEU:HD13	2.27	0.70
1:B:220:PHE:O	1:B:221:PHE:C	2.27	0.70
1:B:482:LEU:HB2	1:B:505:LEU:HD22	1.73	0.70
1:C:165:THR:HG22	1:C:449:ASN:CB	2.19	0.70
1:A:411:MET:CE	1:A:512:VAL:CG1	2.70	0.70
1:B:398:PHE:HB3	1:B:399:PRO:HD2	1.74	0.70
1:D:161:GLN:OE1	1:E:443:ILE:HD13	1.92	0.70
1:A:40:LEU:HD21	1:A:54:GLU:HG3	1.73	0.69
1:A:466:MET:HG3	1:A:466:MET:O	1.91	0.69
1:B:8:ALA:HA	1:B:553:LEU:HD12	1.73	0.69
1:B:248:TRP:CZ2	1:B:289:LEU:HD13	2.27	0.69
1:B:278:GLU:H	1:B:354:GLN:HE22	1.38	0.69
1:F:517:GLU:HG2	1:F:518:THR:H	1.55	0.69
1:A:112:GLU:O	1:A:116:VAL:HG23	1.92	0.69
1:B:461:THR:OG1	1:B:521:ARG:O	2.07	0.69
1:D:183:TYR:OH	1:D:234:GLU:OE1	2.10	0.69
1:B:193:HIS:O	1:B:197:TRP:N	2.18	0.69
1:D:313:ILE:C	1:D:313:ILE:HD12	2.13	0.69
1:A:183:TYR:OH	1:A:234:GLU:OE1	2.11	0.69
1:A:554:ASP:O	1:A:556:SER:N	2.26	0.69
1:E:197:TRP:NE1	1:E:223:VAL:HG21	2.07	0.69
1:F:243:VAL:O	1:F:385:LYS:HD3	1.92	0.69
1:F:373:THR:O	1:F:376:ARG:HB2	1.93	0.69
1:A:50:GLY:C	1:A:53:VAL:HG23	2.12	0.69
1:B:425:PHE:CE1	1:B:456:ASN:HB3	2.27	0.69
1:B:475:LEU:HB3	1:B:589:GLY:HA3	1.74	0.69
1:D:130:ASP:O	1:D:559:GLU:OE1	2.10	0.69
1:D:329:GLU:HA	1:D:344:HIS:HB3	1.74	0.69
1:E:69:ARG:HG2	1:E:264:TYR:CE2	2.27	0.69
1:F:120:TYR:CD2	1:F:134:LEU:HD13	2.27	0.69
1:A:47:ASN:ND2	1:A:94:LYS:HG2	2.07	0.69
1:A:641:ASN:ND2	1:A:641:ASN:N	2.36	0.69
1:C:272:PRO:CG	1:F:272:PRO:HG2	2.22	0.69
1:E:48:ASP:CB	1:E:92:GLN:HE21	2.05	0.69
1:A:447:GLU:HG3	3:A:726:HOH:O	1.93	0.69
1:B:8:ALA:HB1	1:B:546:ALA:HB3	1.74	0.69
1:B:66:LEU:HD13	1:B:111:ASN:ND2	2.07	0.69
1:B:218:GLU:HG2	1:B:321:ILE:CG2	2.21	0.69
1:C:533:MET:H	1:C:533:MET:CE	2.06	0.69
1:D:177:ARG:CG	1:E:360:LYS:HB3	2.23	0.69
1:A:238:ASN:OD1	3:A:695:HOH:O	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:SER:HA	1:B:574:LYS:HE3	1.73	0.69
1:D:367:VAL:O	1:D:373:THR:HG22	1.92	0.69
1:D:454:ARG:HG3	1:D:567:ARG:NH1	2.08	0.69
1:A:158:LYS:HD3	1:A:446:VAL:HG11	1.74	0.68
1:B:5:THR:HG22	1:B:10:LYS:CD	2.23	0.68
1:B:255:GLY:H	1:B:273:ASP:HB3	1.58	0.68
1:B:20:LYS:N	1:B:435:ASN:ND2	2.41	0.68
1:B:89:VAL:O	1:B:91:ASN:N	2.27	0.68
1:D:260:THR:HG22	1:D:268:PHE:CE1	2.29	0.68
1:C:255:GLY:HA2	1:C:271:ARG:NH1	2.07	0.68
1:D:95:GLU:CG	1:D:96:TRP:H	2.06	0.68
1:E:533:MET:H	1:E:533:MET:CE	2.06	0.68
1:E:533:MET:H	1:E:533:MET:HE3	1.58	0.68
1:A:16:HIS:CD2	1:A:27:TYR:CE2	2.82	0.68
1:A:422:LEU:HB3	1:A:649:ILE:HG12	1.74	0.68
1:B:374:ALA:C	1:B:376:ARG:N	2.45	0.68
1:C:243:VAL:O	1:C:385:LYS:HD3	1.94	0.68
1:A:165:THR:HA	1:A:449:ASN:O	1.94	0.68
1:A:620:ARG:NE	3:A:839:HOH:O	2.26	0.68
1:B:368:MET:HE1	1:B:380:PHE:HA	1.75	0.68
1:B:533:MET:CE	1:B:533:MET:H	2.07	0.68
1:B:573:SER:HA	1:B:578:MET:HE3	1.74	0.68
1:C:120:TYR:CD2	1:C:134:LEU:HD13	2.29	0.68
1:B:135:PRO:CB	1:B:140:ILE:HD11	2.23	0.68
1:A:255:GLY:HA2	1:A:271:ARG:HH12	1.59	0.68
1:A:300:ILE:HG12	1:A:324:LEU:HD11	1.75	0.68
1:B:120:TYR:O	1:B:124:ILE:HG13	1.93	0.68
1:B:195:VAL:HG22	1:B:196:THR:N	2.07	0.68
1:A:425:PHE:N	1:A:456:ASN:O	2.22	0.68
1:A:477:THR:HG23	1:A:509:PHE:CE1	2.29	0.68
1:E:46:TYR:CE2	1:E:53:VAL:HG21	2.29	0.68
1:D:413:VAL:HG23	1:D:466:MET:SD	2.34	0.67
1:E:7:ASN:C	1:E:9:GLN:N	2.48	0.67
1:B:247:HIS:HB2	1:B:250:ARG:HG2	1.76	0.67
1:B:260:THR:HG22	1:B:268:PHE:CE2	2.28	0.67
1:B:412:VAL:O	1:B:412:VAL:CG2	2.42	0.67
1:C:203:PHE:HB3	1:C:329:GLU:OE2	1.94	0.67
1:B:255:GLY:HA2	1:B:271:ARG:HH12	1.59	0.67
1:B:470:ASN:HD22	1:B:474:ARG:HG3	1.59	0.67
1:B:487:ASP:HB3	1:B:491:ILE:H	1.59	0.67
1:F:12:GLN:NE2	1:F:544:ASP:OD1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HD11	1:B:110:MET:HE3	1.75	0.67
1:C:353:ARG:O	1:C:356:ASP:N	2.23	0.67
1:C:491:ILE:CG1	1:D:175:LYS:HB2	2.24	0.67
1:D:243:VAL:O	1:D:385:LYS:HD3	1.94	0.67
1:A:522:SER:O	1:A:525:ASP:N	2.27	0.67
1:B:158:LYS:HG2	1:B:437:VAL:HG21	1.75	0.67
1:B:207:ASP:OD2	1:B:212:HIS:HB2	1.95	0.67
1:C:305:ILE:HG13	1:C:315:ILE:HG21	1.77	0.67
1:A:522:SER:O	1:A:523:SER:C	2.33	0.67
1:C:37:PHE:CE2	1:C:101:SER:HB3	2.30	0.67
1:D:353:ARG:O	1:D:356:ASP:N	2.20	0.67
1:D:533:MET:CE	1:D:533:MET:H	2.07	0.67
1:E:412:VAL:HB	1:E:640:SER:HB2	1.75	0.67
1:F:456:ASN:HD22	1:F:457:HIS:H	0.80	0.67
1:A:368:MET:CE	1:A:380:PHE:CD2	2.78	0.67
1:B:487:ASP:HB3	1:B:490:GLY:H	1.60	0.67
1:C:329:GLU:HA	1:C:344:HIS:HB3	1.75	0.67
1:E:256:PHE:CD1	1:E:256:PHE:C	2.66	0.67
1:F:533:MET:CE	1:F:533:MET:H	2.07	0.67
1:C:454:ARG:HG3	1:C:567:ARG:NH1	2.10	0.67
1:A:185:GLY:O	1:A:375:THR:CG2	2.43	0.67
1:A:272:PRO:HG2	1:B:272:PRO:HG2	1.76	0.67
1:B:5:THR:CG2	1:B:10:LYS:HE3	2.25	0.67
1:B:488:ASN:N	1:B:490:GLY:H	1.93	0.67
1:F:72:TYR:CD2	1:F:79:GLN:HB3	2.29	0.67
1:A:468:ASN:HD22	1:A:514:SER:HA	1.59	0.66
1:B:95:GLU:HA	1:B:128:LEU:CD2	2.18	0.66
1:C:183:TYR:OH	1:C:234:GLU:OE1	2.10	0.66
1:C:313:ILE:C	1:C:313:ILE:HD12	2.15	0.66
1:F:37:PHE:CE2	1:F:101:SER:HB3	2.30	0.66
1:A:471:ASP:OD1	1:A:474:ARG:NH1	2.27	0.66
1:B:402:THR:O	1:B:405:ASN:HB2	1.94	0.66
1:C:313:ILE:CD1	1:C:323:LEU:HD13	2.24	0.66
1:E:243:VAL:O	1:E:385:LYS:HD3	1.94	0.66
1:E:411:MET:HE1	1:E:468:ASN:HD22	1.60	0.66
1:A:573:SER:OG	1:A:574:LYS:N	2.29	0.66
1:B:495:LEU:HD23	1:B:630:ILE:HG21	1.75	0.66
1:B:573:SER:HA	1:B:578:MET:CE	2.25	0.66
1:E:183:TYR:OH	1:E:234:GLU:OE1	2.11	0.66
1:F:72:TYR:HA	1:F:79:GLN:OE1	1.96	0.66
1:A:244:ASP:CG	1:A:382:ARG:HD3	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:SER:HA	1:D:574:LYS:HE3	1.77	0.66
1:A:491:ILE:CG1	1:F:175:LYS:HB2	2.26	0.66
1:F:256:PHE:CD1	1:F:256:PHE:C	2.68	0.66
1:B:386:TYR:O	1:B:387:MET:C	2.30	0.66
1:C:269:PRO:HB3	1:C:363:LEU:HD23	1.76	0.66
1:A:491:ILE:HD11	1:F:175:LYS:HB2	1.78	0.66
1:B:86:LEU:HD22	1:B:90:LEU:HD22	1.78	0.66
1:B:256:PHE:CD1	1:B:256:PHE:C	2.69	0.66
1:C:373:THR:O	1:C:376:ARG:HB2	1.96	0.66
1:B:374:ALA:C	1:B:376:ARG:H	1.98	0.66
1:D:120:TYR:CD2	1:D:134:LEU:HD13	2.31	0.66
1:A:239:TRP:CH2	1:A:574:LYS:HD3	2.30	0.66
1:A:307:ASP:OD2	1:A:311:HIS:HB2	1.94	0.66
1:A:427:ASP:CB	1:A:567:ARG:HH12	2.09	0.66
1:B:60:LEU:HD21	1:B:109:ARG:HD2	1.77	0.66
1:E:37:PHE:CE2	1:E:101:SER:HB3	2.31	0.66
1:F:313:ILE:CD1	1:F:323:LEU:HD13	2.25	0.66
1:A:639:VAL:HG23	1:A:641:ASN:HD21	1.60	0.66
1:D:368:MET:CE	1:D:380:PHE:HA	2.22	0.66
1:D:408:PHE:CD1	1:D:588:ASP:HB2	2.30	0.66
1:A:423:ILE:HD11	1:A:652:HIS:CD2	2.30	0.65
1:A:641:ASN:ND2	1:A:641:ASN:H	1.94	0.65
1:B:165:THR:HG22	1:B:449:ASN:HB2	1.78	0.65
1:B:293:GLU:O	1:B:297:HIS:HB2	1.96	0.65
1:B:547:VAL:C	1:B:549:GLY:H	1.99	0.65
1:E:86:LEU:HD12	1:E:110:MET:SD	2.36	0.65
1:F:305:ILE:HG13	1:F:315:ILE:HG21	1.77	0.65
1:A:60:LEU:HD21	1:A:109:ARG:HD2	1.78	0.65
1:A:89:VAL:O	1:A:91:ASN:N	2.29	0.65
1:A:585:ALA:HB1	1:A:642:ILE:HG12	1.78	0.65
1:B:76:ASN:ND2	1:B:79:GLN:H	1.91	0.65
1:E:11:GLN:HE22	1:E:133:VAL:H	1.44	0.65
1:F:368:MET:CE	1:F:380:PHE:HA	2.24	0.65
1:A:313:ILE:HD13	1:A:323:LEU:HD13	1.78	0.65
1:B:46:TYR:OH	1:B:53:VAL:HG11	1.96	0.65
1:B:56:LEU:HD21	1:B:110:MET:HE1	1.78	0.65
1:B:89:VAL:O	1:B:90:LEU:C	2.35	0.65
1:B:239:TRP:CH2	1:B:574:LYS:CD	2.78	0.65
1:C:65:LEU:HD12	1:C:82:GLU:HG2	1.78	0.65
1:D:65:LEU:HD12	1:D:82:GLU:HG2	1.77	0.65
1:D:313:ILE:CD1	1:D:323:LEU:HD13	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:VAL:HG22	1:A:645:VAL:CG1	2.23	0.65
1:B:313:ILE:HD11	1:B:323:LEU:CD1	2.27	0.65
1:C:256:PHE:CD1	1:C:256:PHE:C	2.70	0.65
1:D:86:LEU:HD12	1:D:110:MET:SD	2.37	0.65
1:D:573:SER:HA	1:D:578:MET:HE3	1.78	0.65
1:F:237:SER:HA	1:F:574:LYS:HE3	1.78	0.65
1:C:260:THR:HG22	1:C:268:PHE:CE1	2.31	0.65
1:D:269:PRO:HB3	1:D:363:LEU:HD23	1.78	0.65
1:F:553:LEU:CD2	1:F:555:LEU:HD13	2.27	0.65
1:A:133:VAL:HG21	1:A:555:LEU:HD13	1.79	0.65
1:A:200:ASP:C	1:A:202:PRO:HD3	2.17	0.65
1:A:375:THR:HB	3:A:747:HOH:O	1.95	0.65
1:B:187:ASP:OD1	1:B:189:GLY:N	2.28	0.65
1:C:462:TYR:O	1:C:520:GLU:HA	1.96	0.65
1:E:65:LEU:HD12	1:E:82:GLU:HG2	1.79	0.65
1:A:356:ASP:CG	1:A:359:GLY:HA2	2.17	0.65
1:B:392:LYS:O	1:B:396:ASP:HB2	1.97	0.65
1:E:330:SER:OG	1:E:341:GLY:O	2.12	0.65
1:F:65:LEU:HD12	1:F:82:GLU:HG2	1.78	0.65
1:F:313:ILE:C	1:F:313:ILE:HD12	2.16	0.65
1:A:493:LEU:HA	1:A:497:GLU:OE1	1.97	0.65
1:B:480:ILE:HG12	1:B:584:VAL:HG22	1.79	0.65
1:C:7:ASN:C	1:C:9:GLN:N	2.50	0.65
1:F:17:LEU:HD21	1:F:103:ALA:O	1.97	0.65
1:F:165:THR:CG2	1:F:449:ASN:HB2	2.22	0.65
1:F:168:VAL:CG2	1:F:452:VAL:HG12	2.26	0.65
1:F:513:PRO:HG3	1:F:517:GLU:OE2	1.97	0.65
1:A:269:PRO:HB3	1:A:363:LEU:HD23	1.79	0.65
1:A:353:ARG:O	1:A:355:GLY:N	2.30	0.65
1:A:412:VAL:CG1	1:A:467:SER:O	2.39	0.65
1:A:570:LEU:HB2	3:A:858:HOH:O	1.96	0.65
1:B:86:LEU:CD2	1:B:90:LEU:HD22	2.27	0.65
1:B:368:MET:HE3	1:B:380:PHE:HA	1.79	0.65
1:D:434:ILE:HD11	1:D:447:GLU:HA	1.79	0.65
1:D:513:PRO:O	1:D:514:SER:HB3	1.96	0.65
1:F:29:ASP:O	1:F:33:ILE:HG13	1.96	0.65
1:F:195:VAL:HG11	1:F:372:GLU:HB3	1.78	0.65
1:A:408:PHE:N	1:A:641:ASN:OD1	2.29	0.64
1:B:68:GLN:HB3	1:B:69:ARG:NH1	2.12	0.64
1:B:408:PHE:N	1:B:641:ASN:OD1	2.29	0.64
1:B:412:VAL:O	1:B:412:VAL:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:PHE:C	1:D:256:PHE:CD1	2.70	0.64
1:D:513:PRO:O	1:D:514:SER:CB	2.45	0.64
1:F:592:ASP:C	1:F:594:GLU:H	2.00	0.64
1:A:168:VAL:CG2	1:A:452:VAL:HG12	2.26	0.64
1:C:491:ILE:HG12	1:D:175:LYS:CB	2.27	0.64
1:A:464:ILE:HG22	1:A:464:ILE:O	1.96	0.64
1:B:575:PRO:HD2	1:B:576:GLU:HG3	1.78	0.64
1:E:168:VAL:CG2	1:E:452:VAL:HG12	2.25	0.64
1:B:197:TRP:NE1	1:B:223:VAL:HG21	2.12	0.64
1:C:560:ARG:HG2	1:C:609:CYS:CB	2.27	0.64
1:D:17:LEU:HD21	1:D:103:ALA:O	1.96	0.64
1:D:95:GLU:HA	1:D:128:LEU:HD21	1.80	0.64
1:D:478:PHE:CZ	1:D:519:ILE:HD12	2.32	0.64
1:F:330:SER:HB2	1:F:342:SER:OG	1.98	0.64
1:B:163:PRO:HG3	1:B:446:VAL:HG23	1.79	0.64
1:C:17:LEU:HD21	1:C:103:ALA:O	1.97	0.64
1:C:86:LEU:HD12	1:C:110:MET:SD	2.37	0.64
1:E:169:SER:O	1:E:170:PHE:HB2	1.98	0.64
1:E:305:ILE:HG13	1:E:315:ILE:HG21	1.79	0.64
1:A:639:VAL:CG2	1:A:641:ASN:HD21	2.11	0.64
1:C:560:ARG:CG	1:C:609:CYS:HB3	2.28	0.64
1:D:7:ASN:C	1:D:9:GLN:N	2.50	0.64
1:E:5:THR:HG22	1:E:6:GLY:N	2.10	0.64
1:E:17:LEU:HD21	1:E:103:ALA:O	1.98	0.64
1:E:408:PHE:HB3	1:E:641:ASN:OD1	1.97	0.64
1:E:425:PHE:CE1	1:E:456:ASN:HB3	2.33	0.64
1:A:111:ASN:C	1:A:111:ASN:OD1	2.36	0.64
1:C:29:ASP:O	1:C:33:ILE:HG13	1.97	0.64
1:C:86:LEU:CD2	1:C:90:LEU:HD22	2.28	0.64
1:C:380:PHE:HE1	1:C:384:HIS:CE1	2.15	0.64
1:D:53:VAL:CG2	1:D:89:VAL:HG13	2.27	0.64
1:D:165:THR:CG2	1:D:449:ASN:HB2	2.17	0.64
1:D:191:ASN:O	1:D:195:VAL:HG13	1.98	0.64
1:E:269:PRO:HB3	1:E:363:LEU:CD2	2.28	0.64
1:E:313:ILE:CD1	1:E:323:LEU:HD13	2.27	0.64
1:A:258:PRO:O	1:A:259:LEU:C	2.33	0.64
1:A:455:LEU:HG	1:A:456:ASN:H	1.62	0.64
1:A:633:GLU:O	1:A:635:VAL:N	2.31	0.64
1:A:639:VAL:CG2	1:A:641:ASN:ND2	2.61	0.64
1:C:191:ASN:O	1:C:195:VAL:HG13	1.97	0.64
1:C:244:ASP:O	1:C:382:ARG:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:LEU:HD12	1:F:110:MET:SD	2.38	0.64
1:A:269:PRO:O	3:A:708:HOH:O	2.15	0.64
1:C:135:PRO:HB2	1:C:140:ILE:HD11	1.80	0.64
1:C:491:ILE:HD11	1:D:175:LYS:HB2	1.80	0.64
1:D:244:ASP:O	1:D:382:ARG:HG3	1.98	0.64
1:D:592:ASP:C	1:D:594:GLU:H	2.01	0.64
1:E:195:VAL:HG11	1:E:372:GLU:HB3	1.80	0.64
1:F:252:ILE:HB	1:F:275:ILE:HG22	1.79	0.64
1:F:255:GLY:HA2	1:F:271:ARG:NH1	2.13	0.64
1:A:85:MET:HE1	3:A:808:HOH:O	1.98	0.64
1:A:256:PHE:C	1:A:256:PHE:HD1	1.99	0.64
1:B:56:LEU:HD21	1:B:110:MET:HE3	1.79	0.64
1:E:468:ASN:HD21	1:E:474:ARG:HG2	1.61	0.64
1:F:68:GLN:HB3	1:F:69:ARG:NH1	2.13	0.64
1:F:269:PRO:HB3	1:F:363:LEU:CD2	2.26	0.64
1:F:454:ARG:HG3	1:F:567:ARG:NH1	2.13	0.64
1:F:575:PRO:HD2	1:F:576:GLU:HG3	1.80	0.64
1:F:244:ASP:O	1:F:382:ARG:HG3	1.98	0.63
1:A:456:ASN:ND2	1:A:457:HIS:N	2.28	0.63
1:B:7:ASN:C	1:B:9:GLN:H	2.02	0.63
1:B:82:GLU:O	1:B:85:MET:N	2.27	0.63
1:B:220:PHE:CZ	1:B:329:GLU:HB2	2.34	0.63
1:B:477:THR:HB	1:B:479:ARG:NH1	2.14	0.63
1:D:533:MET:H	1:D:533:MET:HE3	1.63	0.63
1:E:68:GLN:HB3	1:E:69:ARG:NH1	2.13	0.63
1:F:61:ASN:C	1:F:63:HIS:H	2.01	0.63
1:A:278:GLU:H	1:A:354:GLN:HE22	1.46	0.63
1:B:72:TYR:CD2	1:B:79:GLN:HB3	2.33	0.63
1:B:316:ARG:HG3	1:B:398:PHE:CE1	2.33	0.63
1:B:423:ILE:HD11	1:B:652:HIS:CD2	2.33	0.63
1:C:533:MET:H	1:C:533:MET:HE3	1.64	0.63
1:D:40:LEU:HD13	1:D:57:MET:HG3	1.80	0.63
1:D:207:ASP:OD2	1:D:212:HIS:HB2	1.99	0.63
1:F:8:ALA:HB1	1:F:546:ALA:HB3	1.80	0.63
1:F:86:LEU:CD2	1:F:90:LEU:HD22	2.29	0.63
1:F:165:THR:HA	1:F:449:ASN:O	1.97	0.63
1:F:425:PHE:CE1	1:F:456:ASN:HB3	2.33	0.63
1:B:56:LEU:HD11	1:B:65:LEU:HD21	1.80	0.63
1:B:620:ARG:HG3	1:B:624:TYR:CG	2.33	0.63
1:D:300:ILE:HG12	1:D:324:LEU:HD11	1.80	0.63
1:D:353:ARG:C	1:D:355:GLY:H	2.01	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASP:OD2	1:A:358:HIS:HB3	1.99	0.63
1:B:300:ILE:HD11	1:B:390:ILE:HG22	1.79	0.63
1:B:456:ASN:HD22	1:B:457:HIS:H	0.69	0.63
1:D:634:ARG:HE	1:F:64:ARG:CZ	2.11	0.63
1:F:169:SER:O	1:F:170:PHE:HB2	1.99	0.63
1:A:85:MET:HB3	3:A:826:HOH:O	1.98	0.63
1:A:248:TRP:CZ2	1:A:289:LEU:HD13	2.34	0.63
1:A:261:SER:OG	1:A:267:GLU:HG2	1.98	0.63
1:C:414:ASN:ND2	1:C:466:MET:HA	2.11	0.63
1:A:329:GLU:HA	1:A:344:HIS:HB3	1.80	0.63
1:A:418:ILE:CD1	1:A:462:TYR:CD1	2.81	0.63
1:A:504:GLU:OE1	3:A:791:HOH:O	2.15	0.63
1:C:68:GLN:HB3	1:C:69:ARG:NH1	2.13	0.63
1:E:61:ASN:C	1:E:63:HIS:H	2.02	0.63
1:A:368:MET:HE3	1:A:380:PHE:HD2	1.64	0.63
1:A:533:MET:HG3	3:A:781:HOH:O	1.97	0.63
1:B:166:PHE:O	1:B:451:ARG:N	2.28	0.63
1:B:588:ASP:OD1	1:B:588:ASP:C	2.36	0.63
1:C:592:ASP:C	1:C:594:GLU:H	2.01	0.63
1:B:211:TYR:CE2	1:B:612:HIS:HA	2.34	0.63
1:C:300:ILE:HG12	1:C:324:LEU:HD11	1.80	0.63
1:E:255:GLY:HA2	1:E:271:ARG:NH1	2.13	0.63
1:E:411:MET:HE1	1:E:474:ARG:HB2	1.81	0.63
1:A:374:ALA:C	1:A:376:ARG:N	2.51	0.62
1:A:506:ASP:OD2	1:A:521:ARG:NE	2.25	0.62
1:C:72:TYR:HA	1:C:79:GLN:OE1	1.99	0.62
1:C:425:PHE:CE1	1:C:456:ASN:HB3	2.34	0.62
1:D:68:GLN:HB3	1:D:69:ARG:NH1	2.14	0.62
1:E:423:ILE:CD1	1:E:652:HIS:CE1	2.82	0.62
1:A:155:TYR:CG	1:B:159:MET:CE	2.82	0.62
1:E:620:ARG:HG3	1:E:624:TYR:CG	2.33	0.62
1:A:248:TRP:CZ3	1:A:289:LEU:HD13	2.34	0.62
1:A:533:MET:H	1:A:533:MET:HE3	1.64	0.62
1:B:188:ILE:O	1:B:192:ILE:HG12	1.99	0.62
1:A:19:ASP:O	1:A:20:LYS:C	2.37	0.62
1:A:630:ILE:HD13	1:A:636:ILE:HG12	1.79	0.62
1:D:425:PHE:CE1	1:D:456:ASN:HB3	2.34	0.62
1:F:300:ILE:HG12	1:F:324:LEU:HD11	1.80	0.62
1:A:97:TYR:O	1:A:101:SER:HB2	2.00	0.62
1:A:353:ARG:C	1:A:355:GLY:N	2.50	0.62
1:A:611:VAL:HG12	1:A:612:HIS:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:GLN:HE22	1:F:316:ARG:HH21	1.45	0.62
1:C:620:ARG:HG3	1:C:624:TYR:CG	2.34	0.62
1:E:244:ASP:O	1:E:382:ARG:HG3	1.99	0.62
1:C:195:VAL:HG11	1:C:372:GLU:HB3	1.82	0.62
1:D:419:ASP:HB3	1:D:463:LYS:HD2	1.82	0.62
1:E:203:PHE:HB3	1:E:329:GLU:OE2	1.99	0.62
1:F:207:ASP:OD2	1:F:212:HIS:HB2	2.00	0.62
1:F:423:ILE:CD1	1:F:652:HIS:CE1	2.83	0.62
1:D:255:GLY:HA2	1:D:271:ARG:NH1	2.14	0.62
1:D:316:ARG:HH21	1:F:338:GLN:HE22	1.47	0.62
1:E:454:ARG:HG3	1:E:567:ARG:NH1	2.14	0.62
1:F:533:MET:HB3	1:F:534:PRO:HD2	1.82	0.62
1:A:530:VAL:HG21	1:A:561:SER:HB3	1.81	0.62
1:A:633:GLU:C	1:A:635:VAL:N	2.52	0.62
1:B:69:ARG:NH1	1:B:69:ARG:HG3	2.15	0.62
1:C:353:ARG:C	1:C:355:GLY:H	2.03	0.62
1:D:61:ASN:C	1:D:63:HIS:H	2.02	0.62
1:F:7:ASN:C	1:F:9:GLN:N	2.50	0.62
1:F:620:ARG:HG3	1:F:624:TYR:CG	2.34	0.62
1:A:95:GLU:HG3	1:A:96:TRP:N	2.15	0.62
1:A:262:TYR:CE1	1:A:268:PHE:CE2	2.87	0.62
1:B:252:ILE:HD11	1:B:277:PHE:CD1	2.34	0.62
1:D:403:HIS:NE2	1:D:407:GLU:OE1	2.33	0.62
1:E:487:ASP:HB3	1:E:491:ILE:H	1.65	0.62
1:A:40:LEU:HD11	1:A:54:GLU:HA	1.82	0.62
1:A:592:ASP:O	1:A:619:ASN:ND2	2.33	0.62
1:B:141:THR:OG1	1:B:141:THR:O	2.07	0.62
1:B:256:PHE:CE2	1:B:377:ASP:HA	2.35	0.62
1:B:289:LEU:O	1:B:290:GLU:C	2.38	0.62
1:B:461:THR:OG1	1:B:462:TYR:N	2.33	0.62
1:E:368:MET:CE	1:E:380:PHE:HA	2.24	0.62
1:F:183:TYR:OH	1:F:234:GLU:OE1	2.11	0.62
1:A:177:ARG:HD3	1:A:179:GLN:HG3	1.82	0.61
1:A:292:THR:OG1	3:A:787:HOH:O	2.15	0.61
1:A:392:LYS:O	1:A:396:ASP:HB2	2.00	0.61
1:A:411:MET:HE3	1:A:512:VAL:HG11	1.81	0.61
1:A:560:ARG:HH21	1:A:606:HIS:N	1.97	0.61
1:B:37:PHE:CZ	1:B:101:SER:HB3	2.35	0.61
1:B:43:THR:HG23	1:B:49:HIS:O	2.00	0.61
1:C:61:ASN:C	1:C:63:HIS:H	2.01	0.61
1:C:576:GLU:CD	1:D:576:GLU:OE1	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:ASP:OD2	1:E:212:HIS:HB2	2.00	0.61
1:B:307:ASP:C	1:B:307:ASP:OD1	2.37	0.61
1:C:207:ASP:OD2	1:C:212:HIS:HB2	2.00	0.61
1:E:611:VAL:HG12	1:E:612:HIS:HD2	1.64	0.61
1:F:367:VAL:HA	1:F:373:THR:CG2	2.31	0.61
1:A:411:MET:CE	1:A:512:VAL:CB	2.76	0.61
1:A:634:ARG:HH21	1:C:64:ARG:HD2	1.65	0.61
1:B:300:ILE:HG12	1:B:324:LEU:HD11	1.81	0.61
1:D:330:SER:HB2	1:D:342:SER:OG	1.99	0.61
1:D:392:LYS:O	1:D:396:ASP:HB2	1.99	0.61
1:E:300:ILE:HG12	1:E:324:LEU:HD11	1.80	0.61
1:A:177:ARG:NH1	1:A:179:GLN:HG3	2.15	0.61
1:A:180:ARG:HG3	1:A:180:ARG:O	1.99	0.61
1:A:353:ARG:O	1:A:354:GLN:C	2.36	0.61
1:B:168:VAL:CG2	1:B:452:VAL:HG12	2.25	0.61
1:B:416:VAL:CG2	1:B:645:VAL:CG1	2.75	0.61
1:B:610:GLY:HA2	1:B:614:GLU:HB2	1.82	0.61
1:E:462:TYR:O	1:E:520:GLU:HA	2.01	0.61
1:E:611:VAL:HG12	1:E:612:HIS:CD2	2.36	0.61
1:B:220:PHE:CE2	1:B:329:GLU:HB2	2.35	0.61
1:B:548:ASN:HD22	1:B:548:ASN:N	1.89	0.61
1:D:8:ALA:HA	1:D:553:LEU:HD12	1.82	0.61
1:B:177:ARG:NH1	1:B:179:GLN:HG3	2.14	0.61
1:B:317:GLN:HB2	1:B:318:PRO:HD2	1.83	0.61
1:D:168:VAL:CG2	1:D:452:VAL:HG12	2.30	0.61
1:D:353:ARG:C	1:D:355:GLY:N	2.53	0.61
1:F:412:VAL:HB	1:F:640:SER:HB2	1.82	0.61
1:F:533:MET:H	1:F:533:MET:HE3	1.65	0.61
1:E:533:MET:HB3	1:E:534:PRO:HD2	1.83	0.61
1:A:60:LEU:HD22	1:A:106:PHE:HE1	1.66	0.61
1:B:593:THR:C	1:B:595:GLY:H	2.04	0.61
1:D:155:TYR:O	1:D:159:MET:HG3	2.01	0.61
1:F:46:TYR:CZ	1:F:53:VAL:HG21	2.36	0.61
1:B:9:GLN:O	1:B:10:LYS:C	2.39	0.61
1:C:69:ARG:NH1	1:C:69:ARG:HG3	2.14	0.61
1:C:168:VAL:CG2	1:C:452:VAL:HG12	2.26	0.61
1:E:252:ILE:HB	1:E:275:ILE:HG22	1.81	0.61
1:A:7:ASN:O	1:A:11:GLN:N	2.31	0.61
1:A:59:GLU:OE1	1:A:64:ARG:HD3	2.01	0.61
1:A:408:PHE:CE2	1:A:411:MET:HG2	2.36	0.61
1:A:423:ILE:CD1	1:A:652:HIS:CE1	2.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:VAL:HG13	1:A:446:VAL:O	2.01	0.61
1:A:620:ARG:CZ	3:A:839:HOH:O	2.49	0.61
1:D:159:MET:HE2	1:E:155:TYR:HB3	1.83	0.61
1:D:195:VAL:HG11	1:D:372:GLU:HB3	1.83	0.61
1:E:69:ARG:NH1	1:E:69:ARG:HG3	2.16	0.61
1:F:547:VAL:HG23	1:F:548:ASN:H	1.65	0.61
1:A:456:ASN:ND2	1:A:457:HIS:O	2.34	0.60
1:A:512:VAL:HG13	1:A:513:PRO:HD2	1.81	0.60
1:B:143:HIS:CE1	1:B:151:ILE:CG2	2.79	0.60
1:C:412:VAL:HB	1:C:640:SER:HB2	1.82	0.60
1:E:86:LEU:CD2	1:E:90:LEU:HD22	2.31	0.60
1:E:158:LYS:HD3	1:E:446:VAL:CG1	2.31	0.60
1:F:468:ASN:HB3	1:F:514:SER:HA	1.84	0.60
1:C:367:VAL:HA	1:C:373:THR:CG2	2.31	0.60
1:C:533:MET:HB3	1:C:534:PRO:HD2	1.83	0.60
1:C:578:MET:HE3	1:C:580:PHE:HZ	1.64	0.60
1:D:367:VAL:HA	1:D:373:THR:CG2	2.30	0.60
1:E:330:SER:HB2	1:E:342:SER:OG	2.01	0.60
1:A:477:THR:HG23	1:A:509:PHE:HD1	1.66	0.60
1:B:190:MET:O	1:B:191:ASN:C	2.37	0.60
1:B:413:VAL:HG12	1:B:643:LYS:HG3	1.82	0.60
1:C:399:PRO:O	1:C:628:ARG:HD3	2.01	0.60
1:C:575:PRO:HD2	1:C:576:GLU:HG3	1.82	0.60
1:D:135:PRO:HB2	1:D:140:ILE:HD11	1.82	0.60
1:D:354:GLN:HA	1:D:354:GLN:NE2	2.16	0.60
1:D:533:MET:HB3	1:D:534:PRO:HD2	1.84	0.60
1:E:237:SER:HA	1:E:574:LYS:HE3	1.81	0.60
1:E:293:GLU:HG3	3:E:861:HOH:O	2.01	0.60
1:E:406:LEU:HB2	1:E:639:VAL:HG11	1.83	0.60
1:A:508:PHE:CE2	1:A:521:ARG:HD2	2.35	0.60
1:B:175:LYS:O	1:B:176:ASN:CB	2.49	0.60
1:B:222:TRP:CD1	1:B:622:LEU:HD23	2.36	0.60
1:C:46:TYR:CZ	1:C:53:VAL:HG21	2.36	0.60
1:D:69:ARG:NH1	1:D:69:ARG:HG3	2.16	0.60
1:D:177:ARG:HD3	1:D:179:GLN:HG3	1.83	0.60
1:F:591:LYS:NZ	1:F:591:LYS:HB2	2.16	0.60
1:B:413:VAL:HG12	1:B:643:LYS:HG2	1.82	0.60
1:C:293:GLU:HG3	3:C:861:HOH:O	2.01	0.60
1:D:48:ASP:OD2	1:D:92:GLN:HG3	2.01	0.60
1:D:72:TYR:HA	1:D:79:GLN:OE1	2.02	0.60
1:D:508:PHE:CE2	1:D:521:ARG:CD	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:LEU:O	1:B:554:ASP:HB2	2.02	0.60
1:C:48:ASP:HB3	1:C:92:GLN:HE21	1.65	0.60
1:F:69:ARG:NH1	1:F:69:ARG:HG3	2.16	0.60
1:F:392:LYS:O	1:F:396:ASP:HB2	2.01	0.60
1:F:399:PRO:O	1:F:628:ARG:HD3	2.01	0.60
1:A:256:PHE:HD1	1:A:256:PHE:O	1.84	0.60
1:B:593:THR:O	1:B:595:GLY:N	2.34	0.60
1:C:158:LYS:HD3	1:C:446:VAL:CG1	2.32	0.60
1:C:353:ARG:NE	1:C:369:GLU:OE2	2.35	0.60
1:E:367:VAL:HA	1:E:373:THR:CG2	2.30	0.60
1:F:553:LEU:HD22	1:F:555:LEU:HD13	1.83	0.60
1:F:560:ARG:HH12	1:F:606:HIS:N	2.00	0.60
1:A:281:ASP:OD2	1:A:358:HIS:HA	2.02	0.60
1:A:594:GLU:O	1:A:594:GLU:CG	2.46	0.60
1:E:392:LYS:O	1:E:396:ASP:HB2	2.02	0.60
1:E:399:PRO:O	1:E:628:ARG:HD3	2.02	0.60
1:F:408:PHE:HB3	1:F:641:ASN:OD1	2.02	0.60
1:F:479:ARG:NH1	1:F:587:THR:OG1	2.35	0.60
1:A:155:TYR:HB3	1:B:159:MET:HE2	1.82	0.60
1:C:408:PHE:HB3	1:C:641:ASN:OD1	2.01	0.60
1:D:64:ARG:O	1:D:78:ARG:NH1	2.35	0.60
1:D:316:ARG:HH21	1:F:338:GLN:NE2	1.99	0.60
1:D:366:GLY:H	1:D:369:GLU:HG3	1.67	0.60
1:E:8:ALA:HA	1:E:553:LEU:HD12	1.83	0.60
1:E:191:ASN:O	1:E:195:VAL:HG13	2.02	0.60
1:F:611:VAL:HG12	1:F:612:HIS:HD2	1.67	0.60
1:A:260:THR:C	1:A:268:PHE:HD1	2.05	0.60
1:B:143:HIS:HE1	1:B:151:ILE:HG21	1.62	0.60
1:B:487:ASP:HB3	1:B:490:GLY:N	2.17	0.60
1:E:160:THR:O	1:E:161:GLN:HB2	2.02	0.60
1:E:366:GLY:H	1:E:369:GLU:HG3	1.67	0.60
1:F:366:GLY:H	1:F:369:GLU:HG3	1.66	0.60
1:A:43:THR:HG22	1:A:43:THR:O	2.02	0.59
1:A:425:PHE:CE1	1:A:456:ASN:HB3	2.37	0.59
1:B:60:LEU:CD1	1:B:109:ARG:HG3	2.30	0.59
1:C:18:LEU:CD2	1:C:119:LEU:HD23	2.32	0.59
1:C:392:LYS:O	1:C:396:ASP:HB2	2.02	0.59
1:C:591:LYS:HB2	1:C:591:LYS:NZ	2.17	0.59
1:D:18:LEU:CD2	1:D:119:LEU:HD23	2.32	0.59
1:D:305:ILE:HG13	1:D:315:ILE:HG21	1.83	0.59
1:E:72:TYR:HA	1:E:79:GLN:OE1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:GLN:HE22	1:F:133:VAL:H	1.50	0.59
1:F:293:GLU:HG3	3:F:861:HOH:O	2.01	0.59
1:A:349:VAL:HG21	3:A:756:HOH:O	2.01	0.59
1:B:146:THR:HG21	1:B:433:LEU:HD21	1.84	0.59
1:B:218:GLU:HG2	1:B:321:ILE:HG23	1.84	0.59
1:D:620:ARG:HG3	1:D:624:TYR:CG	2.37	0.59
1:D:632:ASP:OD1	1:D:635:VAL:HG23	2.02	0.59
1:A:29:ASP:O	1:A:33:ILE:HG13	2.03	0.59
1:C:423:ILE:CD1	1:C:652:HIS:CE1	2.85	0.59
1:D:317:GLN:HB2	1:D:318:PRO:CD	2.30	0.59
1:E:18:LEU:CD2	1:E:119:LEU:HD23	2.32	0.59
1:E:479:ARG:NH1	1:E:587:THR:OG1	2.35	0.59
1:E:543:ALA:HA	1:E:553:LEU:HD11	1.83	0.59
1:F:135:PRO:HB2	1:F:140:ILE:HD11	1.83	0.59
1:C:165:THR:CG2	1:C:449:ASN:HB2	2.22	0.59
1:D:261:SER:OG	1:D:267:GLU:HG2	2.02	0.59
1:E:64:ARG:O	1:E:78:ARG:NH1	2.35	0.59
1:E:414:ASN:ND2	1:E:466:MET:HA	2.17	0.59
1:A:57:MET:O	1:A:60:LEU:HB3	2.03	0.59
1:A:178:GLU:HG3	1:A:178:GLU:O	2.02	0.59
1:A:641:ASN:HD22	1:A:641:ASN:N	2.00	0.59
1:B:487:ASP:CB	1:B:491:ILE:HG13	2.32	0.59
1:B:555:LEU:O	1:B:557:ALA:N	2.36	0.59
1:C:22:TYR:C	1:C:69:ARG:HH21	2.05	0.59
1:C:169:SER:O	1:C:170:PHE:HB2	2.02	0.59
1:D:69:ARG:N	1:D:112:GLU:OE2	2.32	0.59
1:D:89:VAL:O	1:D:92:GLN:N	2.35	0.59
1:F:191:ASN:O	1:F:195:VAL:HG13	2.01	0.59
1:A:106:PHE:O	1:A:107:ARG:C	2.40	0.59
1:B:177:ARG:HH11	1:B:179:GLN:HG3	1.67	0.59
1:C:155:TYR:O	1:C:159:MET:HG3	2.02	0.59
1:C:330:SER:HB2	1:C:342:SER:OG	2.02	0.59
1:D:423:ILE:CD1	1:D:652:HIS:CE1	2.85	0.59
1:D:493:LEU:HA	1:D:497:GLU:OE1	2.03	0.59
1:E:592:ASP:C	1:E:594:GLU:H	2.05	0.59
1:F:89:VAL:O	1:F:92:GLN:N	2.35	0.59
1:B:185:GLY:O	1:B:375:THR:CG2	2.44	0.59
1:B:418:ILE:HD11	1:B:462:TYR:CE1	2.37	0.59
1:B:533:MET:H	1:B:533:MET:HE3	1.66	0.59
1:D:8:ALA:HB2	1:D:553:LEU:HB2	1.83	0.59
1:D:72:TYR:CD2	1:D:79:GLN:HB3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:ARG:CD	1:E:360:LYS:HB3	2.33	0.59
1:D:482:LEU:HB2	1:D:505:LEU:HD22	1.84	0.59
1:F:25:THR:HG23	1:F:107:ARG:CZ	2.33	0.59
1:F:48:ASP:HB3	1:F:92:GLN:HE21	1.65	0.59
1:B:305:ILE:CD1	1:B:315:ILE:HG21	2.31	0.59
1:B:380:PHE:CE1	1:B:384:HIS:CE1	2.91	0.59
1:C:89:VAL:O	1:C:92:GLN:N	2.35	0.59
1:F:410:GLY:HA3	1:F:470:ASN:ND2	2.17	0.59
1:A:21:ILE:O	1:A:21:ILE:CG1	2.45	0.59
1:A:67:GLU:O	1:A:111:ASN:HB2	2.02	0.59
1:A:454:ARG:HG3	1:A:567:ARG:NH1	2.18	0.59
1:B:25:THR:HG23	1:B:107:ARG:CZ	2.32	0.59
1:B:43:THR:HG23	1:B:49:HIS:C	2.24	0.59
1:B:107:ARG:HD3	1:B:108:GLU:OE1	2.03	0.59
1:B:632:ASP:OD1	1:B:635:VAL:HG23	2.03	0.59
1:C:255:GLY:HA2	1:C:271:ARG:HH12	1.68	0.59
1:C:366:GLY:H	1:C:369:GLU:HG3	1.68	0.59
1:D:508:PHE:CD2	1:D:521:ARG:HD2	2.37	0.59
1:E:482:LEU:HB2	1:E:505:LEU:HD22	1.85	0.59
1:A:155:TYR:CD1	1:B:159:MET:HE1	2.38	0.59
1:A:160:THR:C	1:A:161:GLN:HG3	2.23	0.59
1:D:169:SER:O	1:D:170:PHE:HB2	2.02	0.59
1:D:222:TRP:CZ2	1:D:226:GLN:NE2	2.71	0.59
1:D:399:PRO:O	1:D:628:ARG:HD3	2.01	0.59
1:E:69:ARG:N	1:E:112:GLU:OE2	2.32	0.59
1:F:281:ASP:OD2	1:F:358:HIS:HA	2.03	0.59
1:A:159:MET:HE2	1:B:155:TYR:HB3	1.85	0.58
1:B:148:SER:CB	1:B:259:LEU:O	2.51	0.58
1:C:160:THR:O	1:C:161:GLN:HB2	2.03	0.58
1:E:135:PRO:HB2	1:E:140:ILE:HD11	1.84	0.58
1:C:479:ARG:NH1	1:C:587:THR:OG1	2.36	0.58
1:D:11:GLN:HE22	1:D:133:VAL:H	1.48	0.58
1:D:46:TYR:CE1	1:D:53:VAL:HG21	2.37	0.58
1:D:86:LEU:CD2	1:D:90:LEU:HD22	2.33	0.58
1:D:177:ARG:NH1	1:E:361:PHE:HE1	2.01	0.58
1:D:555:LEU:O	1:D:557:ALA:N	2.36	0.58
1:D:611:VAL:HG12	1:D:612:HIS:HD2	1.67	0.58
1:F:203:PHE:HB3	1:F:329:GLU:OE2	2.03	0.58
1:F:632:ASP:OD1	1:F:635:VAL:HG23	2.03	0.58
1:A:592:ASP:C	1:A:594:GLU:H	2.06	0.58
1:C:368:MET:CE	1:C:380:PHE:HD1	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:LEU:HG	1:F:74:LEU:O	2.03	0.58
1:F:86:LEU:HD22	1:F:90:LEU:HD22	1.86	0.58
1:F:482:LEU:HB2	1:F:505:LEU:HD22	1.85	0.58
1:A:18:LEU:HD21	1:A:119:LEU:HD23	1.85	0.58
1:A:158:LYS:HD3	1:A:446:VAL:CG1	2.32	0.58
1:A:414:ASN:HD21	1:A:467:SER:H	1.51	0.58
1:A:495:LEU:HD13	1:A:583:TYR:CZ	2.38	0.58
1:B:60:LEU:HD22	1:B:106:PHE:HE1	1.68	0.58
1:B:522:SER:C	1:B:524:LYS:N	2.54	0.58
1:C:8:ALA:HA	1:C:553:LEU:HD12	1.86	0.58
1:E:281:ASP:OD2	1:E:358:HIS:HA	2.03	0.58
1:A:51:ALA:O	1:A:52:ALA:C	2.37	0.58
1:A:610:GLY:O	1:A:612:HIS:N	2.36	0.58
1:B:533:MET:HB3	1:B:534:PRO:CD	2.34	0.58
1:F:56:LEU:HD11	1:F:110:MET:CE	2.28	0.58
1:A:491:ILE:CD1	1:F:175:LYS:HB2	2.34	0.58
1:B:57:MET:O	1:B:61:ASN:ND2	2.37	0.58
1:C:11:GLN:HG3	1:C:15:ASN:ND2	2.19	0.58
1:C:632:ASP:OD1	1:C:635:VAL:HG23	2.03	0.58
1:D:52:ALA:O	1:D:89:VAL:HG22	2.03	0.58
1:D:53:VAL:HG22	1:D:89:VAL:CG1	2.32	0.58
1:A:86:LEU:CD2	1:A:90:LEU:CD2	2.81	0.58
1:A:465:THR:O	1:A:466:MET:HB3	2.03	0.58
1:A:499:ARG:NE	1:A:628:ARG:O	2.36	0.58
1:B:158:LYS:HG2	1:B:437:VAL:HG23	1.82	0.58
1:C:611:VAL:HG12	1:C:612:HIS:CD2	2.39	0.58
1:D:421:GLU:HG2	1:D:422:LEU:N	2.10	0.58
1:E:243:VAL:HG23	1:E:385:LYS:HD2	1.86	0.58
1:F:18:LEU:CD2	1:F:119:LEU:HD23	2.31	0.58
1:F:243:VAL:HG23	1:F:385:LYS:HD2	1.86	0.58
1:E:201:PHE:HB3	1:E:216:LYS:CD	2.34	0.58
1:F:64:ARG:O	1:F:78:ARG:NH1	2.37	0.58
1:A:485:ILE:HG22	1:A:486:GLU:HG2	1.86	0.58
1:B:188:ILE:O	1:B:192:ILE:CG1	2.51	0.58
1:D:293:GLU:HG3	3:D:861:HOH:O	2.02	0.58
1:E:632:ASP:OD1	1:E:635:VAL:HG23	2.03	0.58
1:F:414:ASN:ND2	1:F:466:MET:HA	2.17	0.58
1:F:611:VAL:HG12	1:F:612:HIS:CD2	2.39	0.58
1:B:158:LYS:HD3	1:B:446:VAL:CG1	2.34	0.58
1:C:64:ARG:O	1:C:78:ARG:NH1	2.36	0.58
1:E:317:GLN:HB2	1:E:318:PRO:CD	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:ARG:HD3	1:F:179:GLN:HG3	1.86	0.58
1:A:305:ILE:HG23	1:A:340:TYR:CE2	2.39	0.57
1:D:462:TYR:HB3	1:D:464:ILE:HD12	1.85	0.57
1:D:573:SER:HA	1:D:578:MET:CE	2.34	0.57
1:E:565:PRO:HB2	1:E:568:MET:HG2	1.86	0.57
1:A:486:GLU:HA	1:A:492:THR:HA	1.85	0.57
1:A:522:SER:O	1:A:524:LYS:N	2.37	0.57
1:D:8:ALA:HB1	1:D:546:ALA:HB3	1.84	0.57
1:D:185:GLY:HA2	1:D:375:THR:HG23	1.85	0.57
1:D:565:PRO:HB2	1:D:568:MET:HG2	1.86	0.57
1:E:165:THR:CG2	1:E:449:ASN:HB2	2.27	0.57
1:E:177:ARG:HD3	1:E:179:GLN:HG3	1.86	0.57
1:E:422:LEU:HD22	1:E:570:LEU:HD21	1.85	0.57
1:E:573:SER:HA	1:E:578:MET:HE3	1.86	0.57
1:F:185:GLY:HA2	1:F:375:THR:HG23	1.86	0.57
1:A:155:TYR:CG	1:B:159:MET:HE1	2.40	0.57
1:B:474:ARG:NH1	3:B:851:HOH:O	2.36	0.57
1:B:482:LEU:HD11	1:B:580:PHE:HB2	1.85	0.57
1:B:560:ARG:HG2	1:B:609:CYS:HB3	1.86	0.57
1:D:25:THR:HG23	1:D:107:ARG:CZ	2.34	0.57
1:D:538:SER:O	1:D:542:GLN:HG3	2.03	0.57
1:E:573:SER:HA	1:E:578:MET:CE	2.34	0.57
1:A:280:VAL:O	1:A:280:VAL:HG22	2.03	0.57
1:E:185:GLY:HA2	1:E:375:THR:HG23	1.87	0.57
1:B:247:HIS:HB2	1:B:250:ARG:CG	2.34	0.57
1:B:620:ARG:HG3	1:B:624:TYR:CD2	2.39	0.57
1:C:201:PHE:HB3	1:C:216:LYS:CD	2.35	0.57
1:F:317:GLN:HB2	1:F:318:PRO:CD	2.30	0.57
1:F:477:THR:HB	1:F:479:ARG:NH1	2.20	0.57
1:A:74:LEU:O	1:A:74:LEU:CG	2.52	0.57
1:B:564:ILE:HB	1:B:565:PRO:HD2	1.87	0.57
1:B:591:LYS:NZ	1:B:591:LYS:CB	2.68	0.57
1:C:177:ARG:HD3	1:C:179:GLN:HG3	1.87	0.57
1:E:46:TYR:CZ	1:E:53:VAL:HG21	2.40	0.57
1:F:222:TRP:CZ2	1:F:226:GLN:NE2	2.73	0.57
1:F:239:TRP:HH2	1:F:574:LYS:HD3	1.66	0.57
1:F:543:ALA:HA	1:F:553:LEU:CD1	2.33	0.57
1:A:135:PRO:HB3	1:A:536:PHE:CD1	2.38	0.57
1:B:353:ARG:C	1:B:355:GLY:N	2.55	0.57
1:B:423:ILE:CD1	1:B:652:HIS:CE1	2.87	0.57
1:B:571:PRO:HB2	3:B:857:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:611:VAL:HG12	1:D:612:HIS:CD2	2.39	0.57
1:E:8:ALA:O	1:E:547:VAL:CG2	2.53	0.57
1:E:89:VAL:O	1:E:92:GLN:N	2.37	0.57
1:A:368:MET:CE	1:A:380:PHE:HD2	2.16	0.57
1:B:139:GLN:HE21	1:B:431:TYR:HB2	1.70	0.57
1:B:147:ASN:ND2	1:B:149:GLU:H	2.03	0.57
1:B:305:ILE:HD12	1:B:315:ILE:CG2	2.34	0.57
1:C:11:GLN:HE22	1:C:133:VAL:H	1.50	0.57
1:C:281:ASP:OD2	1:C:358:HIS:HA	2.04	0.57
1:C:576:GLU:HG2	3:D:687:HOH:O	2.04	0.57
1:D:520:GLU:CG	1:D:521:ARG:N	2.67	0.57
1:E:25:THR:HG23	1:E:107:ARG:CZ	2.35	0.57
1:F:565:PRO:HB2	1:F:568:MET:HG2	1.87	0.57
1:A:79:GLN:NE2	3:A:859:HOH:O	2.37	0.57
1:A:256:PHE:CE2	1:A:377:ASP:HA	2.40	0.57
1:A:368:MET:HE1	1:A:380:PHE:CD2	2.38	0.57
1:B:158:LYS:HD2	1:B:158:LYS:O	2.04	0.57
1:B:280:VAL:HG21	1:B:353:ARG:HG3	1.85	0.57
1:C:222:TRP:CZ2	1:C:226:GLN:NE2	2.73	0.57
1:A:13:ASP:OD1	1:A:100:ARG:NE	2.33	0.57
1:A:177:ARG:HH11	1:A:179:GLN:HG3	1.70	0.57
1:A:411:MET:CE	1:A:512:VAL:HG11	2.35	0.57
1:A:629:ARG:HH11	1:A:629:ARG:HG3	1.70	0.57
1:B:46:TYR:CZ	1:B:53:VAL:HG11	2.40	0.57
1:B:140:ILE:O	1:B:140:ILE:HG22	2.03	0.57
1:C:48:ASP:CB	1:C:92:GLN:HE21	2.18	0.57
1:C:611:VAL:HG12	1:C:612:HIS:HD2	1.67	0.57
1:D:591:LYS:HB2	1:D:591:LYS:NZ	2.20	0.57
1:E:512:VAL:HG11	3:E:834:HOH:O	2.03	0.57
1:F:201:PHE:HB3	1:F:216:LYS:CD	2.35	0.57
1:B:42:ASP:O	1:B:44:SER:N	2.38	0.56
1:B:69:ARG:HA	1:B:264:TYR:CD2	2.39	0.56
1:C:256:PHE:CD2	1:C:378:PRO:HD3	2.40	0.56
1:C:395:THR:HG23	1:C:627:GLU:O	2.05	0.56
1:D:395:THR:HG23	1:D:627:GLU:O	2.05	0.56
1:E:66:LEU:HD22	1:E:67:GLU:O	2.05	0.56
1:F:283:VAL:HG11	1:F:349:VAL:HB	1.87	0.56
1:C:185:GLY:HA2	1:C:375:THR:HG23	1.86	0.56
1:C:243:VAL:HG23	1:C:385:LYS:HD2	1.87	0.56
1:A:368:MET:HE3	1:A:380:PHE:CD2	2.39	0.56
1:B:197:TRP:CD1	1:B:223:VAL:HG21	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ILE:HD11	3:B:861:HOH:O	2.04	0.56
1:B:433:LEU:HB2	1:B:448:ILE:HG22	1.88	0.56
1:C:477:THR:HB	1:C:479:ARG:NH1	2.20	0.56
1:D:479:ARG:NH1	1:D:587:THR:OG1	2.38	0.56
1:E:72:TYR:CD2	1:E:79:GLN:HB3	2.40	0.56
1:E:76:ASN:HB3	1:E:79:GLN:HB2	1.88	0.56
1:E:86:LEU:HD22	1:E:90:LEU:HD22	1.87	0.56
1:E:155:TYR:O	1:E:159:MET:HG3	2.04	0.56
1:E:260:THR:HG22	1:E:268:PHE:CE1	2.40	0.56
1:F:475:LEU:HD23	1:F:476:ALA:H	1.68	0.56
1:A:533:MET:CE	1:A:533:MET:N	2.67	0.56
1:B:457:HIS:HE1	1:B:523:SER:OG	1.89	0.56
1:B:533:MET:CE	1:B:533:MET:N	2.68	0.56
1:C:354:GLN:HA	1:C:354:GLN:NE2	2.19	0.56
1:D:281:ASP:OD2	1:D:358:HIS:HA	2.05	0.56
1:D:591:LYS:HA	1:D:594:GLU:HB2	1.88	0.56
1:F:48:ASP:CB	1:F:92:GLN:HE21	2.18	0.56
1:A:190:MET:O	1:A:193:HIS:HB3	2.06	0.56
1:A:368:MET:SD	1:A:380:PHE:HB2	2.46	0.56
1:C:565:PRO:HB2	1:C:568:MET:HG2	1.87	0.56
1:D:522:SER:HB3	1:D:525:ASP:OD1	2.05	0.56
1:E:74:LEU:HG	1:E:74:LEU:O	2.04	0.56
1:A:353:ARG:O	1:A:356:ASP:N	2.34	0.56
1:A:459:GLU:OE1	1:A:524:LYS:HD2	2.05	0.56
1:A:489:ASN:HB3	1:A:491:ILE:CD1	2.35	0.56
1:B:65:LEU:HD12	1:B:82:GLU:CG	2.32	0.56
1:C:591:LYS:HA	1:C:594:GLU:HB2	1.87	0.56
1:D:74:LEU:O	1:D:74:LEU:HG	2.06	0.56
1:D:76:ASN:HB3	1:D:79:GLN:HB2	1.87	0.56
1:E:395:THR:HG23	1:E:627:GLU:O	2.06	0.56
1:A:495:LEU:HD23	1:A:630:ILE:HG21	1.87	0.56
1:C:261:SER:OG	1:C:267:GLU:HG2	2.06	0.56
1:C:482:LEU:HB2	1:C:505:LEU:HD22	1.86	0.56
1:D:31:LYS:O	1:D:35:GLU:HG3	2.06	0.56
1:D:135:PRO:HB3	1:D:536:PHE:CD1	2.41	0.56
1:D:574:LYS:HG3	1:D:578:MET:HE2	1.87	0.56
1:E:201:PHE:HB3	1:E:216:LYS:HD2	1.88	0.56
1:E:222:TRP:CZ2	1:E:226:GLN:NE2	2.73	0.56
1:F:158:LYS:HD3	1:F:446:VAL:CG1	2.36	0.56
1:F:160:THR:O	1:F:161:GLN:HB2	2.05	0.56
1:F:260:THR:HG22	1:F:268:PHE:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ASP:O	1:E:45:ILE:HG12	2.05	0.56
1:F:317:GLN:CB	1:F:318:PRO:HD2	2.28	0.56
1:F:395:THR:HG23	1:F:627:GLU:O	2.05	0.56
1:F:591:LYS:HA	1:F:594:GLU:HB2	1.88	0.56
1:A:222:TRP:CG	1:A:622:LEU:HD23	2.40	0.56
1:B:555:LEU:O	1:B:556:SER:C	2.44	0.56
1:D:477:THR:HG23	1:D:509:PHE:CD1	2.41	0.56
1:E:353:ARG:NE	1:E:369:GLU:OE2	2.39	0.56
1:A:71:TRP:CZ3	1:A:365:PRO:HG2	2.41	0.56
1:A:155:TYR:CG	1:B:159:MET:HE2	2.41	0.56
1:A:211:TYR:CE1	1:A:612:HIS:HA	2.41	0.56
1:A:421:GLU:O	1:A:423:ILE:N	2.39	0.56
1:C:69:ARG:N	1:C:112:GLU:OE2	2.32	0.56
1:C:408:PHE:CD1	1:C:588:ASP:HB2	2.41	0.56
1:C:576:GLU:OE1	1:D:576:GLU:CD	2.44	0.56
1:D:521:ARG:NH2	1:D:525:ASP:O	2.38	0.56
1:E:261:SER:OG	1:E:267:GLU:HG2	2.06	0.56
1:F:22:TYR:C	1:F:69:ARG:HH21	2.09	0.56
1:A:243:VAL:O	1:A:244:ASP:C	2.42	0.55
1:A:253:ARG:HH11	1:A:253:ARG:HG3	1.70	0.55
1:B:69:ARG:HG2	1:B:264:TYR:CE2	2.42	0.55
1:B:285:HIS:HB2	1:B:288:ASP:CG	2.26	0.55
1:B:470:ASN:ND2	1:B:474:ARG:HG3	2.21	0.55
1:C:25:THR:HG23	1:C:107:ARG:CZ	2.36	0.55
1:C:560:ARG:NH1	1:C:606:HIS:N	2.54	0.55
1:D:52:ALA:O	1:D:89:VAL:CG2	2.54	0.55
1:D:256:PHE:CD2	1:D:378:PRO:HD3	2.41	0.55
1:E:256:PHE:CD2	1:E:378:PRO:HD3	2.42	0.55
1:A:135:PRO:HG3	1:A:536:PHE:CE1	2.41	0.55
1:B:95:GLU:CA	1:B:128:LEU:HD21	2.20	0.55
1:B:235:ARG:O	1:B:240:LEU:HB2	2.06	0.55
1:B:248:TRP:CH2	1:B:289:LEU:CD1	2.87	0.55
1:C:353:ARG:C	1:C:355:GLY:N	2.56	0.55
1:E:11:GLN:HG3	1:E:15:ASN:ND2	2.20	0.55
1:E:62:ASP:HB2	1:E:64:ARG:HG2	1.88	0.55
1:F:188:ILE:O	1:F:192:ILE:HG12	2.05	0.55
1:F:354:GLN:HA	1:F:354:GLN:NE2	2.19	0.55
1:A:187:ASP:OD1	1:A:189:GLY:N	2.35	0.55
1:B:293:GLU:HG2	1:B:297:HIS:HD2	1.72	0.55
1:B:553:LEU:HD13	3:B:867:HOH:O	2.05	0.55
1:D:11:GLN:HG3	1:D:15:ASN:ND2	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:ILE:O	1:E:192:ILE:HG12	2.07	0.55
1:E:278:GLU:H	1:E:354:GLN:HE22	1.54	0.55
1:A:7:ASN:O	1:A:11:GLN:CB	2.54	0.55
1:A:66:LEU:HD13	1:A:111:ASN:ND2	2.22	0.55
1:B:485:ILE:HG13	1:B:581:ASN:ND2	2.22	0.55
1:C:72:TYR:CD2	1:C:79:GLN:HB3	2.41	0.55
1:D:575:PRO:HD2	1:D:576:GLU:HG3	1.89	0.55
1:E:591:LYS:HB2	1:E:591:LYS:NZ	2.21	0.55
1:A:269:PRO:HB3	1:A:363:LEU:CD2	2.36	0.55
1:A:411:MET:HE1	1:A:512:VAL:CG1	2.37	0.55
1:B:45:ILE:O	1:B:94:LYS:HG3	2.06	0.55
1:D:201:PHE:HB3	1:D:216:LYS:CD	2.36	0.55
1:D:466:MET:HE2	3:D:834:HOH:O	2.07	0.55
1:F:278:GLU:H	1:F:354:GLN:HE22	1.55	0.55
1:A:468:ASN:HB2	1:A:512:VAL:CG1	2.36	0.55
1:B:100:ARG:O	1:B:104:ALA:HB2	2.06	0.55
1:B:113:GLY:O	1:B:114:GLU:C	2.38	0.55
1:C:76:ASN:HB3	1:C:79:GLN:HB2	1.89	0.55
1:F:76:ASN:HB3	1:F:79:GLN:HB2	1.87	0.55
1:F:324:LEU:HD23	1:F:327:ILE:HD11	1.89	0.55
1:A:287:HIS:HA	1:A:290:GLU:HB2	1.88	0.55
1:B:178:GLU:O	1:B:178:GLU:CG	2.36	0.55
1:B:316:ARG:HD3	3:B:829:HOH:O	2.07	0.55
1:B:377:ASP:OD1	1:B:378:PRO:HD2	2.07	0.55
1:C:62:ASP:HB2	1:C:64:ARG:HG2	1.88	0.55
1:C:317:GLN:HB2	1:C:318:PRO:CD	2.30	0.55
1:C:517:GLU:HG2	1:C:518:THR:H	1.71	0.55
1:D:62:ASP:HB2	1:D:64:ARG:HG2	1.88	0.55
1:D:87:PHE:CD1	1:D:121:VAL:HG12	2.42	0.55
1:D:177:ARG:CZ	1:E:361:PHE:HE1	2.20	0.55
1:E:508:PHE:CE2	1:E:521:ARG:CD	2.89	0.55
1:F:61:ASN:C	1:F:63:HIS:N	2.60	0.55
1:B:564:ILE:HB	1:B:565:PRO:CD	2.37	0.55
1:C:8:ALA:CB	1:C:546:ALA:CB	2.85	0.55
1:C:220:PHE:CE2	1:C:329:GLU:HB2	2.42	0.55
1:C:324:LEU:HD23	1:C:327:ILE:HD11	1.89	0.55
1:A:273:ASP:OD2	1:B:360:LYS:HE3	2.06	0.55
1:A:421:GLU:O	1:A:422:LEU:C	2.45	0.55
1:B:145:PHE:CZ	1:B:192:ILE:HD11	2.42	0.55
1:B:258:PRO:HG2	1:B:259:LEU:N	2.22	0.55
1:D:89:VAL:O	1:D:91:ASN:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:MET:HE2	1:E:155:TYR:CG	2.41	0.55
1:F:62:ASP:HB2	1:F:64:ARG:HG2	1.88	0.55
1:A:48:ASP:CG	1:A:52:ALA:H	2.10	0.55
1:A:195:VAL:HG11	1:A:372:GLU:HB3	1.88	0.55
1:A:235:ARG:O	1:A:240:LEU:HB2	2.07	0.55
1:B:89:VAL:C	1:B:91:ASN:N	2.60	0.55
1:B:313:ILE:HD12	1:B:314:ASP:N	2.21	0.55
1:C:86:LEU:HD22	1:C:90:LEU:HD22	1.88	0.55
1:C:283:VAL:HG11	1:C:349:VAL:HB	1.87	0.55
1:E:239:TRP:HH2	1:E:574:LYS:HD3	1.62	0.55
1:B:5:THR:HG22	1:B:10:LYS:HE3	1.88	0.54
1:B:293:GLU:OE1	1:B:386:TYR:OH	2.15	0.54
1:B:373:THR:HG23	1:B:373:THR:O	2.06	0.54
1:B:461:THR:HG1	1:B:462:TYR:H	1.55	0.54
1:E:639:VAL:HG23	1:E:641:ASN:ND2	2.22	0.54
1:A:185:GLY:CA	1:A:375:THR:HG23	2.37	0.54
1:C:634:ARG:HE	1:E:64:ARG:NE	2.05	0.54
1:E:477:THR:HB	1:E:479:ARG:NH1	2.22	0.54
1:F:155:TYR:O	1:F:159:MET:HG3	2.07	0.54
1:F:408:PHE:CD1	1:F:588:ASP:HB2	2.41	0.54
1:A:87:PHE:CD1	1:A:121:VAL:HG12	2.42	0.54
1:A:300:ILE:HG12	1:A:324:LEU:CD1	2.37	0.54
1:A:330:SER:CB	1:A:342:SER:OG	2.55	0.54
1:B:256:PHE:CD2	1:B:378:PRO:HD3	2.42	0.54
1:C:76:ASN:HD22	1:C:79:GLN:H	1.56	0.54
1:D:76:ASN:HD22	1:D:79:GLN:H	1.55	0.54
1:F:89:VAL:O	1:F:91:ASN:N	2.41	0.54
1:F:201:PHE:HB3	1:F:216:LYS:HD2	1.89	0.54
1:F:201:PHE:HA	1:F:213:LEU:HD23	1.89	0.54
1:A:154:ALA:HB2	1:A:433:LEU:HD12	1.90	0.54
1:A:159:MET:CE	1:B:155:TYR:CG	2.91	0.54
1:A:356:ASP:OD1	1:A:359:GLY:HA2	2.06	0.54
1:A:463:LYS:HE3	1:A:520:GLU:OE2	2.08	0.54
1:B:5:THR:HG22	1:B:10:LYS:CE	2.38	0.54
1:B:18:LEU:CD2	1:B:119:LEU:HD23	2.29	0.54
1:B:260:THR:HG22	1:B:268:PHE:CD2	2.42	0.54
1:B:338:GLN:NE2	1:F:316:ARG:HH21	2.05	0.54
1:C:61:ASN:C	1:C:63:HIS:N	2.61	0.54
1:A:475:LEU:HB3	1:A:589:GLY:HA3	1.90	0.54
1:A:586:VAL:O	1:A:641:ASN:HB2	2.06	0.54
1:B:195:VAL:CG2	1:B:196:THR:N	2.67	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLY:N	1:B:465:THR:O	2.38	0.54
1:B:424:THR:HA	1:B:457:HIS:HA	1.90	0.54
1:C:87:PHE:CD1	1:C:121:VAL:HG12	2.43	0.54
1:D:384:HIS:O	1:D:388:ASP:HB2	2.07	0.54
1:D:477:THR:HB	1:D:479:ARG:NH1	2.22	0.54
1:E:5:THR:CG2	1:E:6:GLY:H	2.01	0.54
1:E:354:GLN:NE2	1:E:354:GLN:HA	2.23	0.54
1:E:402:THR:O	1:E:405:ASN:HB2	2.08	0.54
1:F:462:TYR:O	1:F:520:GLU:HA	2.07	0.54
1:A:78:ARG:C	1:A:80:ARG:N	2.59	0.54
1:A:244:ASP:O	1:A:382:ARG:HG3	2.08	0.54
1:A:353:ARG:C	1:A:355:GLY:H	2.11	0.54
1:A:367:VAL:O	1:A:373:THR:HG22	2.07	0.54
1:A:428:GLU:OE2	1:A:451:ARG:HD2	2.08	0.54
1:A:529:THR:HG23	1:A:566:ASP:HA	1.90	0.54
1:B:151:ILE:CD1	1:B:433:LEU:HD22	2.37	0.54
1:B:243:VAL:O	1:B:385:LYS:HD3	2.08	0.54
1:C:43:THR:CG2	1:C:49:HIS:C	2.75	0.54
1:D:44:SER:O	1:D:94:LYS:HD2	2.08	0.54
1:E:458:ASN:O	1:E:459:GLU:C	2.46	0.54
1:E:591:LYS:HA	1:E:594:GLU:HB2	1.88	0.54
1:F:66:LEU:HD12	1:F:79:GLN:HG2	1.90	0.54
1:F:69:ARG:N	1:F:112:GLU:OE2	2.32	0.54
1:A:40:LEU:CD2	1:A:54:GLU:HG3	2.36	0.54
1:A:433:LEU:HG	1:A:450:ALA:HB2	1.89	0.54
1:A:487:ASP:HB3	1:A:491:ILE:H	1.71	0.54
1:B:130:ASP:O	1:B:559:GLU:OE1	2.25	0.54
1:B:345:ASN:O	1:B:348:HIS:HB2	2.08	0.54
1:B:366:GLY:H	1:B:369:GLU:HG3	1.72	0.54
1:B:411:MET:HG3	3:B:834:HOH:O	2.08	0.54
1:B:515:GLY:O	1:B:516:PRO:C	2.46	0.54
1:E:53:VAL:HG22	1:E:89:VAL:HG13	1.90	0.54
1:E:89:VAL:O	1:E:91:ASN:N	2.39	0.54
1:E:201:PHE:HA	1:E:213:LEU:HD23	1.89	0.54
1:F:261:SER:OG	1:F:267:GLU:HG2	2.07	0.54
1:A:85:MET:CE	3:A:808:HOH:O	2.53	0.54
1:C:382:ARG:HD2	3:C:712:HOH:O	2.08	0.54
1:D:374:ALA:C	1:D:376:ARG:H	2.11	0.54
1:E:61:ASN:C	1:E:63:HIS:N	2.61	0.54
1:E:283:VAL:HG11	1:E:349:VAL:HB	1.89	0.54
1:A:237:SER:OG	1:A:578:MET:HE3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ASN:HB3	1:B:491:ILE:CD1	2.36	0.54
1:C:37:PHE:CE2	1:C:101:SER:CB	2.90	0.54
1:D:187:ASP:OD1	1:D:189:GLY:N	2.36	0.54
1:E:29:ASP:O	1:E:33:ILE:HG13	2.07	0.54
1:E:37:PHE:CE2	1:E:101:SER:CB	2.91	0.54
1:E:411:MET:HE3	1:E:512:VAL:HB	1.88	0.54
1:F:87:PHE:CD1	1:F:121:VAL:HG12	2.43	0.54
1:A:568:MET:O	1:A:569:LEU:C	2.44	0.54
1:B:403:HIS:CE1	1:B:407:GLU:HG2	2.43	0.54
1:B:479:ARG:HD2	1:B:587:THR:HG23	1.90	0.54
1:B:533:MET:N	1:B:533:MET:HE2	2.23	0.54
1:D:66:LEU:HD12	1:D:79:GLN:HG2	1.90	0.54
1:D:226:GLN:HE22	1:D:504:GLU:HB2	1.74	0.54
1:D:324:LEU:HD23	1:D:327:ILE:HD11	1.90	0.54
1:E:226:GLN:HE22	1:E:504:GLU:HB2	1.73	0.54
1:F:406:LEU:HB2	1:F:639:VAL:HG11	1.90	0.54
1:B:197:TRP:CE2	1:B:223:VAL:HG21	2.43	0.53
1:C:269:PRO:HB3	1:C:363:LEU:CD2	2.38	0.53
1:C:278:GLU:H	1:C:354:GLN:HE22	1.56	0.53
1:D:29:ASP:O	1:D:33:ILE:HG13	2.08	0.53
1:F:37:PHE:CE2	1:F:101:SER:CB	2.90	0.53
1:A:526:SER:OG	1:A:527:SER:N	2.40	0.53
1:B:547:VAL:C	1:B:549:GLY:N	2.62	0.53
1:C:201:PHE:HA	1:C:213:LEU:HD23	1.89	0.53
1:C:226:GLN:HE22	1:C:504:GLU:HB2	1.73	0.53
1:E:76:ASN:HD22	1:E:79:GLN:H	1.55	0.53
1:F:40:LEU:HD13	1:F:57:MET:HG3	1.90	0.53
1:F:42:ASP:O	1:F:45:ILE:HG12	2.08	0.53
1:F:76:ASN:HD22	1:F:79:GLN:H	1.57	0.53
1:F:256:PHE:CD2	1:F:378:PRO:HD3	2.43	0.53
1:A:120:TYR:CE2	1:A:134:LEU:HD13	2.43	0.53
1:A:382:ARG:HD2	3:A:712:HOH:O	2.08	0.53
1:A:540:LYS:O	1:A:544:ASP:HB2	2.07	0.53
1:A:630:ILE:HD13	1:A:636:ILE:CG1	2.39	0.53
1:B:356:ASP:OD1	1:B:359:GLY:HA2	2.08	0.53
1:B:414:ASN:ND2	1:B:467:SER:OG	2.42	0.53
1:B:538:SER:O	1:B:542:GLN:HG3	2.09	0.53
1:C:74:LEU:HG	1:C:74:LEU:O	2.06	0.53
1:C:508:PHE:CE2	1:C:521:ARG:CD	2.92	0.53
1:F:66:LEU:HD22	1:F:67:GLU:O	2.09	0.53
1:A:89:VAL:C	1:A:91:ASN:N	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ASN:ND2	1:A:467:SER:H	2.05	0.53
1:B:150:VAL:HG21	1:B:168:VAL:HG12	1.90	0.53
1:B:342:SER:O	1:B:343:LEU:C	2.45	0.53
1:C:89:VAL:O	1:C:91:ASN:N	2.41	0.53
1:C:406:LEU:HB2	1:C:639:VAL:HG11	1.89	0.53
1:D:61:ASN:C	1:D:63:HIS:N	2.61	0.53
1:D:260:THR:HG22	1:D:268:PHE:HE1	1.73	0.53
1:D:353:ARG:O	1:D:355:GLY:N	2.41	0.53
1:A:201:PHE:HA	1:A:213:LEU:HD23	1.91	0.53
1:B:48:ASP:N	1:B:92:GLN:HE21	2.06	0.53
1:B:301:ASP:CB	1:D:295:ARG:HH22	2.22	0.53
1:C:56:LEU:HD11	1:C:110:MET:CE	2.28	0.53
1:D:201:PHE:HA	1:D:213:LEU:HD23	1.88	0.53
1:E:620:ARG:HG3	1:E:624:TYR:CD2	2.44	0.53
1:A:185:GLY:HA2	1:A:375:THR:HG23	1.90	0.53
1:A:226:GLN:CD	1:A:504:GLU:H	2.11	0.53
1:A:455:LEU:HG	1:A:456:ASN:N	2.22	0.53
1:B:7:ASN:C	1:B:9:GLN:N	2.62	0.53
1:B:487:ASP:HB3	1:B:491:ILE:HG13	1.90	0.53
1:B:544:ASP:O	1:B:548:ASN:ND2	2.36	0.53
1:B:620:ARG:C	1:B:621:PRO:O	2.47	0.53
1:E:324:LEU:HD23	1:E:327:ILE:HD11	1.90	0.53
1:E:374:ALA:C	1:E:376:ARG:H	2.12	0.53
1:B:165:THR:HA	1:B:449:ASN:O	2.09	0.53
1:B:379:SER:HA	1:B:382:ARG:HB2	1.90	0.53
1:D:47:ASN:HB2	1:D:92:GLN:HB2	1.90	0.53
1:E:220:PHE:CE2	1:E:329:GLU:HB2	2.43	0.53
1:A:533:MET:HE2	1:A:533:MET:N	2.24	0.53
1:B:43:THR:CG2	1:B:49:HIS:O	2.56	0.53
1:B:573:SER:OG	1:B:574:LYS:N	2.41	0.53
1:F:639:VAL:HG23	1:F:641:ASN:ND2	2.23	0.53
1:A:185:GLY:HA2	1:A:375:THR:CG2	2.39	0.53
1:A:580:PHE:HE2	1:A:649:ILE:HB	1.73	0.53
1:B:72:TYR:CD2	1:B:114:GLU:HG2	2.44	0.53
1:B:299:ALA:O	1:B:300:ILE:C	2.42	0.53
1:D:22:TYR:C	1:D:69:ARG:HH21	2.11	0.53
1:D:201:PHE:HB3	1:D:216:LYS:HD2	1.90	0.53
1:D:367:VAL:HG23	1:D:373:THR:O	2.09	0.53
1:D:395:THR:HG21	1:D:500:TRP:CZ3	2.43	0.53
1:D:479:ARG:NH2	1:D:618:ASP:OD2	2.41	0.53
1:D:639:VAL:HG23	1:D:641:ASN:ND2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:LEU:HD12	1:E:79:GLN:HG2	1.91	0.53
1:E:317:GLN:CB	1:E:318:PRO:HD2	2.27	0.53
1:E:477:THR:HG23	1:E:509:PHE:CD1	2.44	0.53
1:F:374:ALA:C	1:F:376:ARG:H	2.11	0.53
1:F:574:LYS:HG3	1:F:578:MET:HE2	1.90	0.53
1:A:215:ARG:O	1:A:216:LYS:C	2.45	0.53
1:A:275:ILE:CG2	1:A:275:ILE:O	2.57	0.53
1:B:330:SER:HB2	1:B:342:SER:CB	2.39	0.53
1:B:353:ARG:C	1:B:355:GLY:H	2.12	0.53
1:B:593:THR:C	1:B:595:GLY:N	2.61	0.53
1:C:477:THR:HG23	1:C:509:PHE:CD1	2.44	0.53
1:E:239:TRP:CH2	1:E:574:LYS:CD	2.83	0.53
1:E:408:PHE:CD1	1:E:588:ASP:HB2	2.44	0.53
1:E:422:LEU:HB3	1:E:649:ILE:HG12	1.90	0.53
1:E:609:CYS:C	1:E:611:VAL:H	2.12	0.53
1:A:159:MET:HE1	1:B:155:TYR:CD1	2.43	0.52
1:A:345:ASN:O	1:A:348:HIS:HB2	2.09	0.52
1:A:508:PHE:CD2	1:A:521:ARG:NE	2.78	0.52
1:A:533:MET:CB	1:A:534:PRO:CD	2.70	0.52
1:B:79:GLN:NE2	3:B:859:HOH:O	2.41	0.52
1:C:639:VAL:HG23	1:C:641:ASN:ND2	2.24	0.52
1:D:188:ILE:O	1:D:192:ILE:HG12	2.09	0.52
1:D:464:ILE:HG21	1:D:478:PHE:CE1	2.43	0.52
1:D:554:ASP:CG	1:D:554:ASP:O	2.47	0.52
1:D:560:ARG:HD3	1:D:611:VAL:HB	1.90	0.52
1:E:255:GLY:HA2	1:E:271:ARG:HH12	1.74	0.52
1:F:255:GLY:HA2	1:F:271:ARG:HH12	1.73	0.52
1:A:641:ASN:ND2	1:A:641:ASN:C	2.61	0.52
1:C:188:ILE:O	1:C:192:ILE:HG12	2.09	0.52
1:F:384:HIS:O	1:F:388:ASP:HB2	2.08	0.52
1:F:411:MET:HE3	1:F:512:VAL:HB	1.92	0.52
1:A:508:PHE:CE2	3:A:864:HOH:O	2.54	0.52
1:C:201:PHE:HB3	1:C:216:LYS:HD2	1.90	0.52
1:C:307:ASP:OD2	1:C:311:HIS:HB2	2.09	0.52
1:F:43:THR:CG2	1:F:49:HIS:C	2.76	0.52
1:F:226:GLN:HE22	1:F:504:GLU:HB2	1.73	0.52
1:B:156:SER:O	1:B:157:ALA:C	2.47	0.52
1:C:395:THR:HG21	1:C:500:TRP:CZ3	2.44	0.52
1:F:307:ASP:HA	1:F:336:ASN:HB2	1.91	0.52
1:F:477:THR:HG23	1:F:509:PHE:CD1	2.44	0.52
1:A:40:LEU:HD12	1:A:57:MET:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ARG:HG3	1:A:69:ARG:NH1	2.24	0.52
1:A:618:ASP:OD1	1:A:620:ARG:HB2	2.10	0.52
1:B:56:LEU:O	1:B:59:GLU:N	2.42	0.52
1:B:96:TRP:O	1:B:97:TYR:C	2.47	0.52
1:D:491:ILE:O	1:D:492:THR:CG2	2.57	0.52
1:E:395:THR:HG21	1:E:500:TRP:CZ3	2.45	0.52
1:F:8:ALA:CA	1:F:553:LEU:HD12	2.35	0.52
1:F:395:THR:HG21	1:F:500:TRP:CZ3	2.45	0.52
1:A:45:ILE:HD12	1:A:46:TYR:CE1	2.45	0.52
1:B:508:PHE:CE2	1:B:521:ARG:HD3	2.44	0.52
1:C:42:ASP:O	1:C:45:ILE:HG12	2.09	0.52
1:E:307:ASP:HA	1:E:336:ASN:HB2	1.92	0.52
1:F:478:PHE:CZ	1:F:519:ILE:HD12	2.45	0.52
1:A:408:PHE:HB2	1:A:641:ASN:OD1	2.08	0.52
1:B:20:LYS:H	1:B:435:ASN:HD21	1.54	0.52
1:B:48:ASP:CB	1:B:92:GLN:HE21	2.14	0.52
1:B:533:MET:H	1:B:533:MET:HE2	1.75	0.52
1:C:197:TRP:CE2	1:C:223:VAL:HG21	2.45	0.52
1:C:384:HIS:O	1:C:388:ASP:HB2	2.10	0.52
1:E:575:PRO:HD2	1:E:576:GLU:HG3	1.91	0.52
1:A:574:LYS:HE3	1:A:578:MET:CE	2.39	0.52
1:F:145:PHE:CZ	1:F:372:GLU:HB2	2.45	0.52
1:F:408:PHE:CE2	1:F:411:MET:HG2	2.45	0.52
1:A:48:ASP:OD1	1:A:51:ALA:N	2.43	0.52
1:A:207:ASP:OD1	1:A:333:TYR:OH	2.13	0.52
1:A:248:TRP:CZ3	1:A:289:LEU:CD1	2.92	0.52
1:A:293:GLU:HG3	3:A:861:HOH:O	2.10	0.52
1:B:402:THR:N	1:B:405:ASN:HB2	2.25	0.52
1:B:495:LEU:CD2	1:B:630:ILE:HG21	2.38	0.52
1:B:639:VAL:HG23	1:B:641:ASN:ND2	2.25	0.52
1:D:165:THR:HA	1:D:449:ASN:O	2.10	0.52
1:A:135:PRO:CG	1:A:140:ILE:HD11	2.38	0.52
1:A:572:LYS:O	1:A:572:LYS:CG	2.56	0.52
1:B:8:ALA:CB	1:B:546:ALA:HB3	2.39	0.52
1:B:68:GLN:HB3	1:B:69:ARG:HH12	1.75	0.52
1:B:102:ASN:C	1:B:104:ALA:H	2.13	0.52
1:B:251:ILE:HG23	1:B:276:HIS:CE1	2.44	0.52
1:B:316:ARG:HH21	1:D:338:GLN:HE22	1.56	0.52
1:B:352:GLY:C	1:B:354:GLN:H	2.11	0.52
1:B:487:ASP:CB	1:B:491:ILE:N	2.60	0.52
1:C:494:THR:H	1:C:497:GLU:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:PHE:CD1	1:E:121:VAL:HG12	2.43	0.52
1:F:414:ASN:ND2	1:F:467:SER:H	2.07	0.52
1:F:620:ARG:HG3	1:F:624:TYR:CD2	2.45	0.52
1:A:150:VAL:HG12	1:A:433:LEU:HD11	1.91	0.51
1:A:632:ASP:OD1	1:A:634:ARG:HB3	2.09	0.51
1:B:207:ASP:OD2	1:B:212:HIS:CB	2.57	0.51
1:B:508:PHE:CE2	1:B:521:ARG:CD	2.93	0.51
1:B:533:MET:HB3	1:B:534:PRO:HD2	1.91	0.51
1:D:243:VAL:HG23	1:D:385:LYS:HD2	1.92	0.51
1:E:22:TYR:C	1:E:69:ARG:HH21	2.13	0.51
1:E:607:ALA:HB1	1:E:617:PRO:HD3	1.92	0.51
1:F:11:GLN:HG3	1:F:15:ASN:ND2	2.21	0.51
1:F:72:TYR:HD2	1:F:79:GLN:HB3	1.73	0.51
1:A:61:ASN:C	1:A:63:HIS:H	2.12	0.51
1:A:180:ARG:O	1:A:180:ARG:CG	2.58	0.51
1:A:455:LEU:O	1:A:567:ARG:HB2	2.10	0.51
1:B:16:HIS:CD2	1:B:27:TYR:CE2	2.99	0.51
1:C:175:LYS:HB2	1:D:491:ILE:CD1	2.39	0.51
1:C:307:ASP:HA	1:C:336:ASN:HB2	1.92	0.51
1:C:454:ARG:CZ	1:C:567:ARG:HD2	2.40	0.51
1:C:620:ARG:HG3	1:C:624:TYR:CD2	2.45	0.51
1:D:283:VAL:HG11	1:D:349:VAL:HB	1.92	0.51
1:D:382:ARG:HD2	3:D:712:HOH:O	2.10	0.51
1:E:46:TYR:HA	1:E:92:GLN:O	2.10	0.51
1:E:177:ARG:NH1	1:E:179:GLN:HG3	2.25	0.51
1:F:353:ARG:C	1:F:355:GLY:H	2.12	0.51
1:F:374:ALA:C	1:F:376:ARG:N	2.64	0.51
1:F:517:GLU:HG2	1:F:518:THR:N	2.24	0.51
1:A:225:HIS:HE1	3:A:788:HOH:O	1.91	0.51
1:B:76:ASN:O	1:B:77:THR:C	2.47	0.51
1:B:247:HIS:ND1	1:B:250:ARG:HG3	2.25	0.51
1:B:517:GLU:CG	1:B:518:THR:H	2.23	0.51
1:B:592:ASP:C	1:B:594:GLU:N	2.62	0.51
1:C:560:ARG:HG2	1:C:609:CYS:SG	2.50	0.51
1:D:278:GLU:H	1:D:354:GLN:HE22	1.58	0.51
1:D:592:ASP:O	1:D:619:ASN:ND2	2.36	0.51
1:F:409:SER:O	1:F:470:ASN:ND2	2.39	0.51
1:F:493:LEU:HA	1:F:497:GLU:OE1	2.09	0.51
1:A:165:THR:HB	1:A:449:ASN:HB3	1.91	0.51
1:B:322:GLU:O	1:B:323:LEU:C	2.49	0.51
1:D:197:TRP:CE2	1:D:223:VAL:HG21	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ASP:HA	1:D:336:ASN:HB2	1.92	0.51
1:D:462:TYR:O	1:D:520:GLU:HA	2.10	0.51
1:D:586:VAL:O	1:D:641:ASN:HB2	2.10	0.51
1:E:479:ARG:NH2	1:E:618:ASP:OD2	2.44	0.51
1:F:220:PHE:CZ	1:F:329:GLU:HB2	2.46	0.51
1:B:12:GLN:OE1	1:B:547:VAL:HG21	2.10	0.51
1:B:229:ALA:O	1:B:230:ARG:C	2.48	0.51
1:C:16:HIS:CD2	1:C:27:TYR:CE2	2.98	0.51
1:C:156:SER:O	1:C:157:ALA:C	2.49	0.51
1:C:414:ASN:ND2	1:C:467:SER:H	2.08	0.51
1:D:159:MET:CE	1:E:155:TYR:CG	2.93	0.51
1:F:382:ARG:HD2	3:F:712:HOH:O	2.10	0.51
1:F:423:ILE:HD11	1:F:652:HIS:CD2	2.44	0.51
1:A:573:SER:N	3:A:857:HOH:O	2.42	0.51
1:B:214:ASP:OD2	1:B:615:ALA:HA	2.10	0.51
1:B:239:TRP:CZ3	1:B:574:LYS:CE	2.93	0.51
1:C:367:VAL:HG23	1:C:373:THR:O	2.10	0.51
1:E:157:ALA:CB	1:E:448:ILE:HG12	2.41	0.51
1:A:630:ILE:HD13	1:A:636:ILE:CD1	2.41	0.51
1:B:14:ILE:O	1:B:15:ASN:C	2.48	0.51
1:C:46:TYR:HA	1:C:92:GLN:O	2.11	0.51
1:D:7:ASN:O	1:D:11:GLN:N	2.37	0.51
1:F:211:TYR:CE2	1:F:612:HIS:HA	2.46	0.51
1:A:25:THR:HB	1:A:27:TYR:H	1.76	0.51
1:A:179:GLN:NE2	3:A:710:HOH:O	2.31	0.51
1:A:313:ILE:CD1	1:A:323:LEU:CD1	2.76	0.51
1:A:620:ARG:HG3	1:A:624:TYR:CD1	2.45	0.51
1:B:441:GLU:HB3	1:B:442:ASN:HD22	1.76	0.51
1:C:211:TYR:CE2	1:C:612:HIS:HA	2.46	0.51
1:D:454:ARG:CZ	1:D:567:ARG:HD2	2.41	0.51
1:E:46:TYR:CE1	1:E:98:CYS:SG	3.03	0.51
1:E:411:MET:HE1	1:E:468:ASN:ND2	2.25	0.51
1:F:220:PHE:CE2	1:F:329:GLU:HB2	2.46	0.51
1:B:293:GLU:HG3	3:B:861:HOH:O	2.10	0.51
1:C:591:LYS:HB2	1:C:591:LYS:HZ2	1.76	0.51
1:D:421:GLU:CG	1:D:422:LEU:N	2.70	0.51
1:E:165:THR:HA	1:E:449:ASN:O	2.10	0.51
1:F:353:ARG:C	1:F:355:GLY:N	2.63	0.51
1:F:491:ILE:O	1:F:492:THR:CG2	2.59	0.51
1:F:508:PHE:CE2	1:F:521:ARG:CD	2.94	0.51
1:A:289:LEU:O	1:A:293:GLU:N	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ASN:ND2	1:A:466:MET:HA	2.22	0.51
1:A:540:LYS:O	1:A:541:GLU:C	2.49	0.51
1:A:574:LYS:HG3	1:A:578:MET:HE2	1.91	0.51
1:C:133:VAL:CG2	1:C:555:LEU:HD23	2.41	0.51
1:C:374:ALA:C	1:C:376:ARG:H	2.13	0.51
1:D:86:LEU:HD22	1:D:90:LEU:HD22	1.93	0.51
1:E:211:TYR:CE2	1:E:612:HIS:HA	2.46	0.51
1:A:149:GLU:O	1:A:150:VAL:C	2.49	0.50
1:A:572:LYS:O	1:A:572:LYS:HG3	2.11	0.50
1:B:218:GLU:H	1:B:322:GLU:HB3	1.75	0.50
1:B:269:PRO:HB3	1:B:363:LEU:HD23	1.93	0.50
1:B:518:THR:O	1:B:518:THR:HG22	2.11	0.50
1:C:377:ASP:OD1	1:C:378:PRO:HD2	2.11	0.50
1:C:574:LYS:HG3	1:C:578:MET:HE2	1.92	0.50
1:D:17:LEU:CD2	1:D:103:ALA:O	2.59	0.50
1:D:177:ARG:HD2	1:E:360:LYS:HB3	1.92	0.50
1:D:259:LEU:HD11	1:E:363:LEU:HD12	1.93	0.50
1:D:374:ALA:C	1:D:376:ARG:N	2.64	0.50
1:E:220:PHE:CZ	1:E:329:GLU:HB2	2.46	0.50
1:E:408:PHE:CB	1:E:641:ASN:OD1	2.58	0.50
1:F:269:PRO:CB	1:F:363:LEU:HD23	2.39	0.50
1:F:307:ASP:OD2	1:F:311:HIS:HB2	2.10	0.50
1:F:593:THR:C	1:F:595:GLY:H	2.15	0.50
1:A:407:GLU:OE2	1:A:639:VAL:HA	2.11	0.50
1:A:410:GLY:O	1:A:412:VAL:HG12	2.10	0.50
1:B:42:ASP:O	1:B:45:ILE:HG12	2.11	0.50
1:B:57:MET:C	1:B:61:ASN:HD22	2.13	0.50
1:D:412:VAL:HB	1:D:640:SER:HB2	1.93	0.50
1:E:382:ARG:HD2	3:E:712:HOH:O	2.11	0.50
1:E:384:HIS:O	1:E:388:ASP:HB2	2.11	0.50
1:F:609:CYS:C	1:F:611:VAL:H	2.14	0.50
1:A:105:TYR:CD1	1:A:105:TYR:C	2.85	0.50
1:A:466:MET:HE1	3:A:834:HOH:O	2.12	0.50
1:A:611:VAL:HG12	1:A:612:HIS:HD2	1.77	0.50
1:B:69:ARG:HG3	1:B:69:ARG:HH11	1.75	0.50
1:B:239:TRP:HH2	1:B:574:LYS:HD3	1.68	0.50
1:B:479:ARG:HH21	1:B:618:ASP:CG	2.14	0.50
1:B:540:LYS:O	1:B:541:GLU:C	2.48	0.50
1:B:609:CYS:C	1:B:611:VAL:H	2.14	0.50
1:C:317:GLN:CB	1:C:318:PRO:HD2	2.27	0.50
1:C:374:ALA:C	1:C:376:ARG:N	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:MET:HE1	1:E:155:TYR:CD1	2.46	0.50
1:D:211:TYR:CE2	1:D:612:HIS:HA	2.46	0.50
1:D:231:PHE:HE2	1:D:243:VAL:HG11	1.77	0.50
1:D:609:CYS:C	1:D:611:VAL:H	2.15	0.50
1:E:84:LEU:HD11	1:E:204:TRP:CZ2	2.46	0.50
1:F:46:TYR:HA	1:F:92:GLN:O	2.11	0.50
1:A:286:VAL:O	1:A:289:LEU:HB2	2.12	0.50
1:A:531:PRO:O	1:A:531:PRO:HG2	2.12	0.50
1:C:423:ILE:HD11	1:C:652:HIS:CD2	2.44	0.50
1:C:586:VAL:O	1:C:641:ASN:HB2	2.12	0.50
1:D:464:ILE:HG21	1:D:478:PHE:HE1	1.74	0.50
1:F:594:GLU:O	1:F:594:GLU:HG2	2.10	0.50
1:A:190:MET:HE2	1:A:565:PRO:HD2	1.93	0.50
1:A:241:ASP:O	1:A:242:PRO:O	2.29	0.50
1:A:632:ASP:OD1	1:A:634:ARG:CB	2.60	0.50
1:B:13:ASP:CG	1:B:100:ARG:HD2	2.32	0.50
1:B:158:LYS:HD3	1:B:446:VAL:HG12	1.94	0.50
1:B:479:ARG:NH1	1:B:587:THR:OG1	2.45	0.50
1:C:479:ARG:NH2	1:C:618:ASP:OD2	2.43	0.50
1:C:575:PRO:HB2	3:D:687:HOH:O	2.10	0.50
1:C:607:ALA:HB1	1:C:617:PRO:HD3	1.92	0.50
1:D:156:SER:O	1:D:157:ALA:C	2.48	0.50
1:E:574:LYS:HG3	1:E:578:MET:HE2	1.93	0.50
1:F:53:VAL:HG22	1:F:89:VAL:HG13	1.92	0.50
1:F:466:MET:HE2	3:F:834:HOH:O	2.12	0.50
1:A:140:ILE:HG22	1:A:141:THR:HG23	1.94	0.50
1:A:395:THR:HG23	1:A:627:GLU:O	2.12	0.50
1:C:150:VAL:CG1	1:C:433:LEU:HD11	2.36	0.50
1:D:47:ASN:C	1:D:92:GLN:NE2	2.65	0.50
1:D:220:PHE:CE2	1:D:329:GLU:HB2	2.46	0.50
1:E:187:ASP:OD1	1:E:189:GLY:N	2.37	0.50
1:E:353:ARG:O	1:E:356:ASP:N	2.36	0.50
1:E:377:ASP:OD1	1:E:378:PRO:HD2	2.12	0.50
1:F:367:VAL:HG23	1:F:373:THR:O	2.11	0.50
1:A:439:SER:O	1:A:443:ILE:HG21	2.11	0.50
1:B:477:THR:HG23	1:B:509:PHE:CE1	2.46	0.50
1:B:491:ILE:O	1:B:492:THR:CG2	2.59	0.50
1:C:473:GLU:HA	1:C:512:VAL:O	2.12	0.50
1:C:609:CYS:C	1:C:611:VAL:H	2.14	0.50
1:D:68:GLN:HB3	1:D:69:ARG:HH11	1.75	0.50
1:D:255:GLY:HA2	1:D:271:ARG:HH12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:ARG:O	1:F:356:ASP:N	2.35	0.50
1:F:411:MET:CE	1:F:512:VAL:HB	2.42	0.50
1:A:491:ILE:HG12	1:F:175:LYS:HG3	1.94	0.50
1:A:557:ALA:HB3	1:A:558:TYR:CG	2.47	0.50
1:B:488:ASN:H	1:B:490:GLY:H	1.60	0.50
1:B:496:ASP:OD1	1:B:499:ARG:HD3	2.12	0.50
1:D:269:PRO:HB3	1:D:363:LEU:CD2	2.41	0.50
1:D:272:PRO:CG	1:E:272:PRO:CG	2.87	0.50
1:F:454:ARG:CZ	1:F:567:ARG:HD2	2.42	0.50
1:A:254:GLU:OE2	1:B:360:LYS:NZ	2.45	0.50
1:A:530:VAL:CG2	1:A:561:SER:HB3	2.42	0.50
1:B:33:ILE:CD1	1:B:100:ARG:HH22	2.25	0.50
1:B:169:SER:O	1:B:170:PHE:HB2	2.12	0.50
1:B:211:TYR:N	1:B:211:TYR:CD1	2.80	0.50
1:B:506:ASP:OD1	1:B:507:LYS:N	2.45	0.50
1:C:84:LEU:HD11	1:C:204:TRP:CZ2	2.47	0.50
1:C:402:THR:O	1:C:405:ASN:HB2	2.12	0.50
1:D:295:ARG:HG2	1:D:339:TYR:CZ	2.47	0.50
1:E:158:LYS:HD3	1:E:446:VAL:HG12	1.93	0.50
1:E:466:MET:HE2	3:E:834:HOH:O	2.11	0.50
1:E:591:LYS:HG3	1:E:594:GLU:OE2	2.12	0.50
1:F:592:ASP:O	1:F:619:ASN:ND2	2.36	0.50
1:A:392:LYS:NZ	1:A:396:ASP:OD2	2.44	0.49
1:A:565:PRO:HB2	1:A:568:MET:HG2	1.94	0.49
1:A:628:ARG:O	1:A:629:ARG:C	2.49	0.49
1:A:633:GLU:O	1:A:634:ARG:C	2.50	0.49
1:B:40:LEU:HD22	1:B:57:MET:HG3	1.95	0.49
1:B:575:PRO:HD2	1:B:576:GLU:CG	2.40	0.49
1:C:101:SER:O	1:C:104:ALA:HB3	2.12	0.49
1:C:177:ARG:HG2	1:F:360:LYS:HB3	1.93	0.49
1:C:187:ASP:OD1	1:C:189:GLY:N	2.36	0.49
1:C:487:ASP:HB3	1:C:491:ILE:H	1.77	0.49
1:D:239:TRP:HH2	1:D:574:LYS:HD3	1.69	0.49
1:E:231:PHE:HE2	1:E:243:VAL:HG11	1.77	0.49
1:F:377:ASP:OD1	1:F:378:PRO:HD2	2.12	0.49
1:F:411:MET:HE1	1:F:474:ARG:HB2	1.93	0.49
1:A:5:THR:O	1:A:5:THR:CG2	2.60	0.49
1:A:620:ARG:HG3	1:A:624:TYR:CD2	2.47	0.49
1:C:177:ARG:NH1	1:C:179:GLN:HG3	2.27	0.49
1:D:411:MET:HE1	1:D:468:ASN:ND2	2.27	0.49
1:E:145:PHE:CZ	1:E:372:GLU:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:ARG:C	1:E:355:GLY:N	2.65	0.49
1:F:586:VAL:O	1:F:641:ASN:HB2	2.12	0.49
1:F:591:LYS:HB2	1:F:591:LYS:HZ2	1.75	0.49
1:A:5:THR:O	1:A:6:GLY:O	2.30	0.49
1:A:188:ILE:HG12	3:A:720:HOH:O	2.11	0.49
1:A:330:SER:HB3	1:A:342:SER:OG	2.11	0.49
1:B:122:SER:O	1:B:126:SER:HB3	2.13	0.49
1:B:147:ASN:HD22	1:B:149:GLU:H	1.59	0.49
1:C:19:ASP:O	1:C:20:LYS:C	2.51	0.49
1:C:220:PHE:CZ	1:C:329:GLU:HB2	2.47	0.49
1:C:353:ARG:O	1:C:355:GLY:N	2.45	0.49
1:C:594:GLU:O	1:C:594:GLU:HG2	2.11	0.49
1:D:307:ASP:OD2	1:D:311:HIS:HB2	2.12	0.49
1:E:43:THR:CG2	1:E:49:HIS:C	2.77	0.49
1:E:353:ARG:C	1:E:355:GLY:H	2.14	0.49
1:E:592:ASP:O	1:E:619:ASN:ND2	2.40	0.49
1:E:641:ASN:ND2	1:E:641:ASN:H	2.11	0.49
1:F:485:ILE:O	1:F:492:THR:HA	2.11	0.49
1:F:592:ASP:C	1:F:594:GLU:N	2.66	0.49
1:A:308:SER:HA	1:A:336:ASN:ND2	2.28	0.49
1:A:529:THR:HG23	1:A:566:ASP:CA	2.43	0.49
1:B:149:GLU:O	1:B:152:ASP:N	2.45	0.49
1:B:641:ASN:ND2	1:B:641:ASN:H	2.10	0.49
1:C:17:LEU:CD2	1:C:103:ALA:O	2.60	0.49
1:C:560:ARG:CD	1:C:609:CYS:HB3	2.42	0.49
1:C:593:THR:C	1:C:595:GLY:H	2.15	0.49
1:D:112:GLU:O	1:D:116:VAL:HG23	2.12	0.49
1:D:392:LYS:NZ	1:D:396:ASP:OD2	2.45	0.49
1:E:295:ARG:HG2	1:E:339:TYR:CZ	2.48	0.49
1:F:607:ALA:HB1	1:F:617:PRO:HD3	1.92	0.49
1:A:165:THR:HG21	1:A:449:ASN:HB2	1.83	0.49
1:B:46:TYR:HA	1:B:92:GLN:O	2.13	0.49
1:B:252:ILE:HD11	1:B:277:PHE:CE1	2.48	0.49
1:C:68:GLN:HB3	1:C:69:ARG:HH11	1.75	0.49
1:C:231:PHE:HE2	1:C:243:VAL:HG11	1.77	0.49
1:D:56:LEU:CD1	1:D:110:MET:HE3	2.33	0.49
1:D:66:LEU:HD22	1:D:67:GLU:O	2.11	0.49
1:D:155:TYR:HB3	1:E:159:MET:HE2	1.94	0.49
1:D:235:ARG:O	1:D:240:LEU:HB2	2.12	0.49
1:D:356:ASP:CG	1:D:359:GLY:HA2	2.33	0.49
1:D:377:ASP:OD1	1:D:378:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:494:THR:H	1:E:497:GLU:HB2	1.78	0.49
1:F:177:ARG:NH1	1:F:179:GLN:HG3	2.28	0.49
1:F:487:ASP:HB3	1:F:491:ILE:H	1.77	0.49
1:A:78:ARG:O	1:A:81:LYS:N	2.45	0.49
1:A:222:TRP:CH2	1:A:623:GLY:HA2	2.48	0.49
1:A:226:GLN:O	1:A:227:LEU:O	2.31	0.49
1:D:594:GLU:O	1:D:594:GLU:HG2	2.12	0.49
1:E:7:ASN:O	1:E:9:GLN:N	2.44	0.49
1:E:39:PRO:O	1:E:53:VAL:HG11	2.13	0.49
1:E:307:ASP:OD2	1:E:311:HIS:HB2	2.12	0.49
1:E:396:ASP:O	1:E:629:ARG:NH1	2.46	0.49
1:E:408:PHE:CE2	1:E:411:MET:HG2	2.47	0.49
1:F:7:ASN:O	1:F:9:GLN:N	2.46	0.49
1:F:16:HIS:CD2	1:F:27:TYR:CE2	3.00	0.49
1:F:17:LEU:CD2	1:F:103:ALA:O	2.61	0.49
1:A:147:ASN:HB3	1:A:150:VAL:H	1.77	0.49
1:A:477:THR:OG1	1:A:592:ASP:OD2	2.29	0.49
1:A:609:CYS:C	1:A:611:VAL:H	2.16	0.49
1:C:356:ASP:CG	1:C:359:GLY:HA2	2.33	0.49
1:D:5:THR:CG2	1:D:10:LYS:HE3	2.42	0.49
1:D:84:LEU:HD11	1:D:204:TRP:CZ2	2.48	0.49
1:D:607:ALA:HB1	1:D:617:PRO:HD3	1.94	0.49
1:E:8:ALA:O	1:E:547:VAL:HG22	2.12	0.49
1:E:222:TRP:CD1	1:E:622:LEU:HD23	2.48	0.49
1:E:367:VAL:HG23	1:E:373:THR:O	2.12	0.49
1:E:411:MET:SD	1:E:468:ASN:ND2	2.85	0.49
1:E:586:VAL:O	1:E:641:ASN:HB2	2.13	0.49
1:F:56:LEU:CD1	1:F:110:MET:HE3	2.30	0.49
1:F:231:PHE:HE2	1:F:243:VAL:HG11	1.77	0.49
1:F:479:ARG:NH2	1:F:618:ASP:OD2	2.44	0.49
1:A:354:GLN:HA	1:A:354:GLN:HE21	1.77	0.49
1:B:596:HIS:ND1	1:B:596:HIS:N	2.58	0.49
1:D:177:ARG:NH1	1:D:179:GLN:HG3	2.28	0.49
1:E:374:ALA:C	1:E:376:ARG:N	2.64	0.49
1:A:521:ARG:NH2	1:A:525:ASP:O	2.46	0.49
1:B:59:GLU:HG3	1:B:85:MET:CE	2.43	0.49
1:E:39:PRO:HB2	1:E:53:VAL:HG12	1.95	0.49
1:E:101:SER:O	1:E:104:ALA:HB3	2.13	0.49
1:F:84:LEU:HD11	1:F:204:TRP:CZ2	2.47	0.49
1:F:295:ARG:HG2	1:F:339:TYR:CZ	2.47	0.49
1:B:150:VAL:CG1	1:B:433:LEU:HD11	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:PRO:HD2	1:B:275:ILE:HD12	1.94	0.49
1:B:448:ILE:HG22	1:B:448:ILE:O	2.10	0.49
1:D:101:SER:O	1:D:104:ALA:HB3	2.13	0.49
1:D:468:ASN:HB3	1:D:514:SER:HA	1.94	0.49
1:F:101:SER:O	1:F:104:ALA:HB3	2.12	0.49
1:F:356:ASP:CG	1:F:359:GLY:HA2	2.32	0.49
1:B:157:ALA:CB	1:B:448:ILE:HG12	2.43	0.48
1:B:379:SER:HB3	3:B:719:HOH:O	2.13	0.48
1:B:392:LYS:HZ3	1:B:499:ARG:HH12	1.61	0.48
1:B:517:GLU:CG	1:B:518:THR:N	2.76	0.48
1:D:620:ARG:HG3	1:D:624:TYR:CD2	2.48	0.48
1:A:86:LEU:HD23	1:A:86:LEU:O	2.13	0.48
1:A:491:ILE:HD11	1:F:175:LYS:O	2.12	0.48
1:B:303:GLY:O	1:B:315:ILE:HG12	2.11	0.48
1:B:477:THR:O	1:B:586:VAL:HA	2.13	0.48
1:C:66:LEU:HD12	1:C:79:GLN:HG2	1.95	0.48
1:D:150:VAL:CG1	1:D:433:LEU:HD11	2.36	0.48
1:D:330:SER:HB2	1:D:342:SER:CB	2.43	0.48
1:D:591:LYS:HB2	1:D:591:LYS:HZ2	1.78	0.48
1:E:156:SER:O	1:E:157:ALA:C	2.51	0.48
1:E:559:GLU:O	1:E:560:ARG:HG3	2.13	0.48
1:F:68:GLN:HB3	1:F:69:ARG:HH11	1.74	0.48
1:F:197:TRP:CE2	1:F:223:VAL:HG21	2.48	0.48
1:A:487:ASP:O	1:A:488:ASN:HB3	2.12	0.48
1:B:237:SER:OG	1:B:578:MET:HE1	2.13	0.48
1:B:454:ARG:CZ	1:B:567:ARG:HD2	2.43	0.48
1:C:40:LEU:HD13	1:C:57:MET:HG3	1.95	0.48
1:D:506:ASP:OD2	1:D:521:ARG:NE	2.46	0.48
1:E:411:MET:CE	1:E:468:ASN:ND2	2.69	0.48
1:A:214:ASP:OD2	1:A:616:TYR:N	2.43	0.48
1:A:408:PHE:CA	1:A:641:ASN:OD1	2.61	0.48
1:A:529:THR:HG21	1:A:566:ASP:OD1	2.13	0.48
1:B:214:ASP:OD2	1:B:616:TYR:N	2.40	0.48
1:C:392:LYS:NZ	1:C:396:ASP:OD2	2.46	0.48
3:C:687:HOH:O	1:D:576:GLU:HG2	2.13	0.48
1:D:158:LYS:HD3	1:D:446:VAL:CG1	2.44	0.48
1:E:17:LEU:CD2	1:E:103:ALA:O	2.62	0.48
1:E:66:LEU:CD2	1:E:67:GLU:N	2.77	0.48
1:E:68:GLN:HB3	1:E:69:ARG:HH11	1.76	0.48
1:E:423:ILE:HD11	1:E:652:HIS:CD2	2.47	0.48
1:F:475:LEU:HD23	1:F:476:ALA:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:559:GLU:O	1:F:560:ARG:HG3	2.13	0.48
1:A:120:TYR:OH	1:A:135:PRO:O	2.31	0.48
1:A:159:MET:HE2	1:B:155:TYR:CG	2.49	0.48
1:A:396:ASP:O	1:A:629:ARG:NH1	2.47	0.48
1:C:37:PHE:CZ	1:C:101:SER:HB3	2.49	0.48
1:F:343:LEU:HD11	3:F:861:HOH:O	2.13	0.48
1:F:434:ILE:HD11	1:F:447:GLU:HA	1.96	0.48
1:F:533:MET:H	1:F:533:MET:HE2	1.79	0.48
1:A:7:ASN:O	1:A:11:GLN:HB3	2.14	0.48
1:A:77:THR:HG22	1:A:80:ARG:HH12	1.78	0.48
1:A:90:LEU:HA	1:A:90:LEU:HD12	1.45	0.48
1:C:235:ARG:O	1:C:240:LEU:HB2	2.13	0.48
1:C:259:LEU:HD11	1:F:363:LEU:HD12	1.94	0.48
1:C:592:ASP:O	1:C:619:ASN:ND2	2.36	0.48
1:E:40:LEU:HD13	1:E:57:MET:HG3	1.94	0.48
1:E:424:THR:HA	1:E:457:HIS:HA	1.95	0.48
1:F:156:SER:O	1:F:157:ALA:C	2.51	0.48
1:A:48:ASP:OD2	1:A:52:ALA:N	2.46	0.48
1:A:53:VAL:C	1:A:55:THR:H	2.16	0.48
1:A:512:VAL:HA	1:A:513:PRO:HD3	1.83	0.48
1:B:201:PHE:HB3	1:B:216:LYS:CD	2.44	0.48
1:C:7:ASN:O	1:C:9:GLN:N	2.46	0.48
1:D:7:ASN:O	1:D:9:GLN:N	2.45	0.48
1:D:48:ASP:HB3	1:D:92:GLN:NE2	2.28	0.48
1:D:380:PHE:CE1	1:D:384:HIS:CE1	3.02	0.48
1:E:7:ASN:O	1:E:11:GLN:N	2.39	0.48
1:E:89:VAL:C	1:E:91:ASN:N	2.66	0.48
1:F:235:ARG:O	1:F:240:LEU:HB2	2.14	0.48
1:A:403:HIS:C	1:A:405:ASN:N	2.67	0.48
1:A:464:ILE:O	1:A:464:ILE:CG2	2.62	0.48
1:B:20:LYS:H	1:B:435:ASN:ND2	2.11	0.48
1:C:222:TRP:CD1	1:C:622:LEU:HD23	2.49	0.48
1:E:150:VAL:CG1	1:E:433:LEU:HD11	2.41	0.48
1:A:139:GLN:HE21	1:A:431:TYR:HB2	1.79	0.48
1:A:305:ILE:HG13	1:A:315:ILE:CG2	2.37	0.48
1:A:316:ARG:HG3	1:A:398:PHE:HE1	1.79	0.48
1:A:430:GLN:HA	1:A:450:ALA:O	2.14	0.48
1:B:68:GLN:HA	1:B:111:ASN:HA	1.95	0.48
1:B:280:VAL:HG22	1:B:283:VAL:HG23	1.96	0.48
1:C:7:ASN:O	1:C:11:GLN:N	2.37	0.48
1:C:434:ILE:HD11	1:C:447:GLU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:MET:H	1:C:533:MET:HE2	1.78	0.48
1:D:66:LEU:HD23	1:D:67:GLU:H	1.78	0.48
1:E:493:LEU:HA	1:E:497:GLU:OE1	2.13	0.48
1:F:392:LYS:NZ	1:F:396:ASP:OD2	2.46	0.48
1:A:78:ARG:O	1:A:79:GLN:C	2.50	0.48
1:A:411:MET:C	1:A:412:VAL:HG12	2.25	0.48
1:A:614:GLU:H	1:A:614:GLU:HG3	1.23	0.48
1:B:203:PHE:C	1:B:203:PHE:CD1	2.88	0.48
1:B:239:TRP:CH2	1:B:574:LYS:CE	2.96	0.48
1:B:278:GLU:H	1:B:354:GLN:NE2	2.10	0.48
1:B:300:ILE:CG1	1:B:324:LEU:HD11	2.42	0.48
1:B:526:SER:OG	1:B:527:SER:N	2.46	0.48
1:C:53:VAL:HG22	1:C:89:VAL:HG13	1.95	0.48
1:C:71:TRP:CZ3	1:C:365:PRO:HG2	2.49	0.48
1:C:460:PHE:HE2	1:C:462:TYR:CZ	2.32	0.48
1:D:27:TYR:HA	1:D:28:PRO:HD2	1.60	0.48
1:D:641:ASN:ND2	1:D:641:ASN:H	2.12	0.48
1:E:66:LEU:HD23	1:E:67:GLU:H	1.79	0.48
1:F:112:GLU:O	1:F:116:VAL:HG23	2.14	0.48
1:A:295:ARG:NE	1:A:339:TYR:CE1	2.82	0.47
1:A:564:ILE:HB	1:A:565:PRO:CD	2.44	0.47
1:A:593:THR:O	1:A:595:GLY:N	2.47	0.47
1:C:69:ARG:HG3	1:C:69:ARG:HH11	1.78	0.47
1:C:368:MET:HE3	1:C:380:PHE:HD1	1.79	0.47
1:C:543:ALA:HA	1:C:553:LEU:HD11	1.96	0.47
3:C:687:HOH:O	1:D:575:PRO:HB2	2.13	0.47
1:D:69:ARG:HG3	1:D:69:ARG:HH11	1.79	0.47
1:D:251:ILE:HG23	1:D:276:HIS:NE2	2.28	0.47
1:D:593:THR:C	1:D:595:GLY:H	2.17	0.47
1:F:402:THR:O	1:F:405:ASN:HB2	2.14	0.47
1:A:115:PHE:CZ	1:A:119:LEU:HD22	2.49	0.47
1:A:158:LYS:HD2	1:A:158:LYS:O	2.14	0.47
1:B:269:PRO:CB	1:B:363:LEU:HD23	2.44	0.47
1:B:300:ILE:HG12	1:B:324:LEU:CD1	2.44	0.47
1:B:367:VAL:HA	1:B:373:THR:CG2	2.44	0.47
1:D:494:THR:H	1:D:497:GLU:HB2	1.79	0.47
1:D:537:GLN:O	1:D:540:LYS:N	2.44	0.47
1:E:271:ARG:HA	1:E:272:PRO:HD3	1.67	0.47
1:E:343:LEU:HD11	3:E:861:HOH:O	2.14	0.47
1:E:356:ASP:CG	1:E:359:GLY:HA2	2.34	0.47
1:F:330:SER:HB2	1:F:342:SER:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:TRP:CH2	1:A:289:LEU:CD1	2.91	0.47
1:A:411:MET:HE2	1:A:474:ARG:HB3	1.94	0.47
1:B:78:ARG:NH1	1:B:82:GLU:CD	2.68	0.47
1:C:641:ASN:ND2	1:C:641:ASN:H	2.12	0.47
1:F:301:ASP:OD2	1:F:393:LYS:NZ	2.47	0.47
1:F:573:SER:HA	1:F:578:MET:CE	2.44	0.47
1:F:578:MET:HE3	1:F:580:PHE:HZ	1.80	0.47
1:A:201:PHE:N	1:A:201:PHE:CD1	2.82	0.47
1:A:351:LEU:HD13	1:A:379:SER:OG	2.14	0.47
1:A:366:GLY:H	1:A:369:GLU:HG3	1.79	0.47
1:A:424:THR:HA	1:A:457:HIS:HA	1.95	0.47
1:A:496:ASP:OD1	1:A:499:ARG:HD3	2.13	0.47
1:A:522:SER:C	1:A:524:LYS:N	2.64	0.47
1:B:59:GLU:HG3	1:B:85:MET:HE3	1.96	0.47
1:B:628:ARG:O	1:B:630:ILE:HG13	2.15	0.47
1:E:37:PHE:CZ	1:E:101:SER:HB3	2.48	0.47
1:E:485:ILE:O	1:E:492:THR:HA	2.15	0.47
1:F:37:PHE:CZ	1:F:101:SER:HB3	2.49	0.47
1:F:39:PRO:O	1:F:53:VAL:HG11	2.14	0.47
1:F:239:TRP:CH2	1:F:574:LYS:CD	2.87	0.47
1:A:237:SER:OG	1:A:578:MET:CE	2.61	0.47
1:A:378:PRO:C	1:A:380:PHE:H	2.16	0.47
1:A:422:LEU:HD23	1:A:422:LEU:HA	1.47	0.47
1:D:56:LEU:HD11	1:D:110:MET:CE	2.31	0.47
1:E:34:ALA:O	1:E:109:ARG:NH2	2.48	0.47
1:E:454:ARG:CZ	1:E:567:ARG:HD2	2.43	0.47
1:E:573:SER:OG	1:E:574:LYS:N	2.45	0.47
1:A:12:GLN:OE1	1:A:547:VAL:HG21	2.15	0.47
1:A:256:PHE:CD2	1:A:378:PRO:HD3	2.50	0.47
1:A:508:PHE:CZ	3:A:864:HOH:O	2.67	0.47
1:B:491:ILE:O	1:B:492:THR:HG23	2.14	0.47
1:D:48:ASP:CA	1:D:92:GLN:HE21	2.27	0.47
1:D:66:LEU:CD2	1:D:67:GLU:N	2.77	0.47
1:D:592:ASP:C	1:D:594:GLU:N	2.67	0.47
1:E:235:ARG:O	1:E:240:LEU:HB2	2.14	0.47
1:A:27:TYR:HA	1:A:28:PRO:HD2	1.66	0.47
1:A:65:LEU:HD12	1:A:65:LEU:HA	1.65	0.47
1:A:105:TYR:OH	1:A:109:ARG:NH1	2.47	0.47
1:A:151:ILE:HA	1:A:151:ILE:HD13	1.43	0.47
1:A:482:LEU:HB2	1:A:505:LEU:HD22	1.96	0.47
1:A:630:ILE:HD13	1:A:636:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ARG:NH1	1:A:634:ARG:CG	2.41	0.47
1:B:21:ILE:HG13	1:B:21:ILE:O	2.14	0.47
1:B:132:ILE:CG2	1:B:133:VAL:N	2.76	0.47
1:B:205:TRP:NE1	1:B:213:LEU:HD13	2.30	0.47
1:B:218:GLU:N	1:B:322:GLU:HB3	2.30	0.47
1:B:385:LYS:HE2	3:B:750:HOH:O	2.14	0.47
1:B:423:ILE:HA	1:B:650:VAL:O	2.15	0.47
1:C:89:VAL:C	1:C:91:ASN:N	2.67	0.47
1:C:112:GLU:O	1:C:116:VAL:HG23	2.14	0.47
1:C:130:ASP:O	1:C:559:GLU:CD	2.53	0.47
1:C:573:SER:OG	1:C:574:LYS:N	2.47	0.47
1:D:37:PHE:CZ	1:D:101:SER:HB3	2.50	0.47
1:D:56:LEU:HD11	1:D:65:LEU:HD21	1.96	0.47
1:D:255:GLY:H	1:D:273:ASP:HB3	1.79	0.47
1:D:301:ASP:OD2	1:D:393:LYS:NZ	2.48	0.47
1:D:413:VAL:HA	1:D:466:MET:HB2	1.93	0.47
1:D:491:ILE:O	1:D:492:THR:HG23	2.15	0.47
1:D:521:ARG:HB3	3:D:864:HOH:O	2.14	0.47
1:E:31:LYS:O	1:E:35:GLU:HG3	2.15	0.47
1:E:302:HIS:CE1	1:E:304:TYR:HH	2.33	0.47
1:E:521:ARG:NH2	1:E:525:ASP:O	2.48	0.47
1:F:89:VAL:C	1:F:91:ASN:N	2.67	0.47
1:A:364:PRO:HB2	1:A:365:PRO:CD	2.45	0.47
1:C:177:ARG:CG	1:F:360:LYS:HB3	2.45	0.47
1:C:301:ASP:OD2	1:C:393:LYS:NZ	2.48	0.47
1:C:543:ALA:O	1:C:547:VAL:HG12	2.15	0.47
1:C:592:ASP:C	1:C:594:GLU:N	2.66	0.47
1:E:307:ASP:C	1:E:336:ASN:HD22	2.18	0.47
1:F:307:ASP:C	1:F:336:ASN:HD22	2.17	0.47
1:A:226:GLN:OE1	1:A:504:GLU:N	2.28	0.47
1:A:487:ASP:CB	1:A:491:ILE:H	2.28	0.47
1:B:160:THR:O	1:B:161:GLN:HB2	2.15	0.47
1:B:301:ASP:CG	1:B:393:LYS:HZ2	2.18	0.47
1:B:399:PRO:O	1:B:628:ARG:HD3	2.15	0.47
1:C:323:LEU:HD11	3:C:849:HOH:O	2.15	0.47
1:C:493:LEU:HA	1:C:497:GLU:OE1	2.14	0.47
1:F:66:LEU:CD2	1:F:67:GLU:N	2.77	0.47
1:F:486:GLU:HA	1:F:492:THR:HA	1.97	0.47
1:A:34:ALA:O	1:A:109:ARG:NH2	2.48	0.47
1:A:304:TYR:CD1	1:A:304:TYR:C	2.88	0.47
1:A:368:MET:CE	1:A:380:PHE:HA	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:VAL:CG2	1:B:199:MET:HG2	2.35	0.47
1:B:219:LEU:HD12	1:B:219:LEU:HA	1.59	0.47
1:B:488:ASN:H	1:B:490:GLY:N	2.13	0.47
1:B:494:THR:O	1:B:495:LEU:C	2.52	0.47
1:C:408:PHE:CE2	1:C:411:MET:HG2	2.50	0.47
1:D:307:ASP:C	1:D:336:ASN:HD22	2.18	0.47
1:E:43:THR:HG23	1:E:49:HIS:O	2.15	0.47
1:A:338:GLN:HG2	1:A:338:GLN:O	2.15	0.46
1:B:66:LEU:N	1:B:82:GLU:OE1	2.33	0.46
1:B:521:ARG:HG2	1:B:522:SER:N	2.30	0.46
1:C:39:PRO:O	1:C:53:VAL:HG11	2.15	0.46
1:C:237:SER:HA	1:C:574:LYS:CE	2.42	0.46
1:C:280:VAL:HG21	1:C:353:ARG:HG3	1.97	0.46
1:D:8:ALA:O	1:D:547:VAL:HG22	2.14	0.46
1:D:139:GLN:NE2	1:D:432:SER:H	2.13	0.46
1:E:69:ARG:HG3	1:E:69:ARG:HH11	1.80	0.46
1:E:591:LYS:C	1:E:594:GLU:HB2	2.35	0.46
1:F:641:ASN:ND2	1:F:641:ASN:H	2.12	0.46
1:A:321:ILE:O	1:A:321:ILE:CG1	2.63	0.46
1:B:127:LYS:HD3	3:B:869:HOH:O	2.15	0.46
1:B:233:PHE:HE1	1:B:580:PHE:CE1	2.32	0.46
1:B:367:VAL:CG2	1:B:377:ASP:HB2	2.46	0.46
1:B:634:ARG:HG2	1:B:634:ARG:NH1	2.19	0.46
1:C:5:THR:CG2	1:C:6:GLY:H	2.22	0.46
1:C:34:ALA:O	1:C:109:ARG:NH2	2.48	0.46
1:C:60:LEU:HD11	1:C:109:ARG:HG3	1.97	0.46
1:C:289:LEU:O	1:C:290:GLU:C	2.53	0.46
1:D:69:ARG:HA	1:D:264:TYR:CD2	2.50	0.46
1:D:143:HIS:CE1	1:D:151:ILE:HG21	2.51	0.46
1:D:477:THR:HG23	1:D:509:PHE:CE1	2.50	0.46
1:A:418:ILE:CD1	1:A:462:TYR:HD1	2.26	0.46
1:A:479:ARG:NH1	1:A:587:THR:HG21	2.31	0.46
1:B:180:ARG:NH2	1:B:238:ASN:O	2.47	0.46
1:B:187:ASP:OD1	1:B:187:ASP:C	2.52	0.46
1:B:280:VAL:HG21	1:B:353:ARG:CG	2.45	0.46
1:B:438:ASP:HA	3:B:727:HOH:O	2.15	0.46
1:C:307:ASP:C	1:C:336:ASN:HD22	2.19	0.46
1:C:343:LEU:HD11	3:C:861:HOH:O	2.14	0.46
1:C:375:THR:HA	1:C:380:PHE:CD2	2.49	0.46
1:D:423:ILE:HD11	1:D:652:HIS:CD2	2.49	0.46
1:E:39:PRO:HB2	1:E:53:VAL:CG1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:LEU:HD11	1:F:109:ARG:HG3	1.98	0.46
1:A:40:LEU:HD21	1:A:54:GLU:CG	2.43	0.46
1:B:14:ILE:HG12	1:B:132:ILE:HD13	1.97	0.46
1:B:255:GLY:CA	1:B:271:ARG:NH1	2.71	0.46
1:B:441:GLU:O	1:B:443:ILE:HG22	2.16	0.46
1:D:5:THR:HG22	1:D:6:GLY:N	2.26	0.46
1:D:213:LEU:N	1:D:213:LEU:CD1	2.78	0.46
1:D:289:LEU:O	1:D:290:GLU:C	2.54	0.46
1:D:462:TYR:N	1:D:521:ARG:O	2.44	0.46
1:F:7:ASN:O	1:F:11:GLN:N	2.39	0.46
1:A:466:MET:CE	3:A:834:HOH:O	2.64	0.46
1:A:532:ASP:HB3	3:A:748:HOH:O	2.16	0.46
1:B:5:THR:O	1:B:5:THR:OG1	2.34	0.46
1:C:396:ASP:O	1:C:629:ARG:NH1	2.47	0.46
1:D:19:ASP:O	1:D:20:LYS:C	2.53	0.46
1:D:468:ASN:HB3	1:D:514:SER:CA	2.46	0.46
1:D:493:LEU:HB2	1:D:497:GLU:HB2	1.97	0.46
1:E:475:LEU:HD23	1:E:476:ALA:H	1.80	0.46
1:F:69:ARG:HG3	1:F:69:ARG:HH11	1.79	0.46
1:F:213:LEU:N	1:F:213:LEU:CD1	2.78	0.46
1:F:573:SER:OG	1:F:574:LYS:N	2.45	0.46
1:A:14:ILE:HD13	1:A:96:TRP:HZ2	1.81	0.46
1:A:185:GLY:CA	1:A:375:THR:CG2	2.94	0.46
1:A:238:ASN:C	1:A:240:LEU:N	2.68	0.46
1:B:522:SER:O	1:B:525:ASP:N	2.48	0.46
1:B:532:ASP:N	1:B:532:ASP:OD1	2.49	0.46
1:B:610:GLY:O	1:B:612:HIS:N	2.49	0.46
1:C:213:LEU:N	1:C:213:LEU:CD1	2.78	0.46
1:E:197:TRP:CE2	1:E:223:VAL:HG21	2.50	0.46
1:E:330:SER:HB2	1:E:342:SER:CB	2.46	0.46
1:F:56:LEU:HD11	1:F:65:LEU:HD21	1.97	0.46
1:F:143:HIS:CE1	1:F:151:ILE:HG21	2.51	0.46
1:F:477:THR:HG23	1:F:509:PHE:CE1	2.51	0.46
1:A:296:ILE:HD12	1:A:296:ILE:HG23	1.69	0.46
1:A:402:THR:O	1:A:405:ASN:HB2	2.15	0.46
1:B:499:ARG:HH21	1:B:627:GLU:C	2.19	0.46
1:C:11:GLN:O	1:C:15:ASN:ND2	2.48	0.46
1:C:195:VAL:CG2	1:C:196:THR:N	2.78	0.46
1:C:316:ARG:HH21	1:E:338:GLN:HE22	1.63	0.46
1:D:533:MET:H	1:D:533:MET:HE2	1.80	0.46
1:E:89:VAL:O	1:E:90:LEU:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:411:MET:CE	1:F:474:ARG:HB2	2.45	0.46
1:F:493:LEU:HB2	1:F:497:GLU:HB2	1.98	0.46
1:A:19:ASP:O	1:A:107:ARG:NH2	2.48	0.46
1:A:535:SER:O	1:A:539:LEU:HG	2.16	0.46
1:A:557:ALA:HB3	1:A:558:TYR:CE2	2.51	0.46
1:A:653:LEU:HD12	1:A:653:LEU:HA	1.64	0.46
1:B:102:ASN:C	1:B:104:ALA:N	2.70	0.46
1:B:183:TYR:CD1	1:B:183:TYR:C	2.88	0.46
1:B:434:ILE:CG2	1:B:434:ILE:O	2.62	0.46
1:B:641:ASN:ND2	1:B:641:ASN:N	2.63	0.46
1:C:69:ARG:HA	1:C:264:TYR:CD2	2.51	0.46
1:C:192:ILE:HD13	1:C:192:ILE:HA	1.87	0.46
1:D:448:ILE:O	1:D:449:ASN:ND2	2.38	0.46
1:A:132:ILE:HG22	1:A:133:VAL:N	2.29	0.46
1:A:441:GLU:CG	1:A:441:GLU:O	2.63	0.46
1:B:39:PRO:HB2	1:B:53:VAL:HG12	1.98	0.46
1:B:285:HIS:O	1:B:288:ASP:HB2	2.16	0.46
1:B:512:VAL:HA	1:B:513:PRO:HD2	1.54	0.46
1:B:624:TYR:CD1	1:B:625:PRO:HB3	2.51	0.46
1:C:468:ASN:OD1	1:C:470:ASN:HB2	2.16	0.46
1:D:301:ASP:CB	1:F:295:ARG:HH22	2.29	0.46
1:E:43:THR:CG2	1:E:49:HIS:O	2.64	0.46
1:E:628:ARG:O	1:E:630:ILE:HG13	2.16	0.46
1:F:34:ALA:O	1:F:109:ARG:NH2	2.48	0.46
1:A:177:ARG:HB2	1:A:178:GLU:H	1.26	0.46
1:A:406:LEU:HB2	1:A:639:VAL:HG11	1.98	0.46
1:B:13:ASP:O	1:B:14:ILE:C	2.54	0.46
1:B:40:LEU:N	1:B:40:LEU:HD13	2.31	0.46
1:B:363:LEU:C	1:B:364:PRO:O	2.49	0.46
1:C:39:PRO:HB3	1:C:102:ASN:HD21	1.81	0.46
1:C:56:LEU:CD1	1:C:110:MET:HE3	2.31	0.46
1:C:66:LEU:HD22	1:C:67:GLU:O	2.16	0.46
1:C:641:ASN:ND2	1:C:641:ASN:N	2.64	0.46
1:D:11:GLN:O	1:D:15:ASN:ND2	2.48	0.46
1:D:421:GLU:O	1:D:422:LEU:HB2	2.16	0.46
1:E:127:LYS:HD3	3:E:869:HOH:O	2.16	0.46
1:F:150:VAL:CG1	1:F:433:LEU:HD11	2.40	0.46
1:F:187:ASP:OD1	1:F:189:GLY:N	2.36	0.46
1:F:219:LEU:HD12	1:F:219:LEU:HA	1.78	0.46
1:F:396:ASP:O	1:F:629:ARG:NH1	2.47	0.46
1:A:374:ALA:O	1:A:375:THR:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:HD21	1:B:386:TYR:HE2	1.80	0.45
1:C:512:VAL:HG11	3:C:834:HOH:O	2.15	0.45
1:D:151:ILE:HD13	1:D:151:ILE:HA	1.80	0.45
1:D:413:VAL:HG12	1:D:643:LYS:HG2	1.97	0.45
1:E:215:ARG:O	1:E:216:LYS:C	2.55	0.45
1:F:573:SER:HA	1:F:578:MET:HE3	1.98	0.45
1:A:23:GLU:HA	1:A:24:PRO:HD2	1.67	0.45
1:A:53:VAL:O	1:A:55:THR:N	2.49	0.45
1:A:125:HIS:CG	1:A:211:TYR:HH	2.30	0.45
1:A:275:ILE:HD13	1:A:275:ILE:HG21	1.69	0.45
1:A:307:ASP:N	1:A:311:HIS:O	2.47	0.45
1:B:46:TYR:CE2	1:B:53:VAL:HG21	2.51	0.45
1:B:418:ILE:HG21	1:B:422:LEU:HD21	1.98	0.45
1:B:443:ILE:HD12	1:B:443:ILE:HA	1.87	0.45
1:C:295:ARG:HG2	1:C:339:TYR:CZ	2.50	0.45
1:C:506:ASP:OD2	1:C:521:ARG:NE	2.48	0.45
1:D:140:ILE:HG22	1:D:141:THR:HG23	1.98	0.45
1:D:239:TRP:CH2	1:D:574:LYS:CD	2.89	0.45
1:E:143:HIS:CE1	1:E:151:ILE:HG21	2.51	0.45
1:E:177:ARG:HH11	1:E:179:GLN:HG3	1.81	0.45
1:E:408:PHE:CA	1:E:641:ASN:OD1	2.64	0.45
1:E:594:GLU:HG2	1:E:594:GLU:O	2.16	0.45
1:F:69:ARG:HA	1:F:264:TYR:CD2	2.51	0.45
1:F:289:LEU:O	1:F:290:GLU:C	2.53	0.45
1:A:477:THR:CG2	1:A:509:PHE:CE1	2.99	0.45
1:A:560:ARG:HB2	3:A:819:HOH:O	2.15	0.45
1:A:578:MET:O	1:A:648:LYS:HA	2.16	0.45
1:B:256:PHE:C	1:B:256:PHE:HD1	2.17	0.45
1:B:374:ALA:O	1:B:376:ARG:N	2.49	0.45
1:B:510:GLN:HG2	1:B:519:ILE:HD13	1.97	0.45
1:D:368:MET:HE1	1:D:380:PHE:CD1	2.50	0.45
1:E:480:ILE:HA	1:E:583:TYR:O	2.17	0.45
1:A:23:GLU:O	1:A:24:PRO:C	2.55	0.45
1:A:51:ALA:O	1:A:52:ALA:O	2.35	0.45
1:A:213:LEU:CD1	1:A:213:LEU:N	2.79	0.45
1:A:291:ILE:HG23	1:A:291:ILE:HD13	1.55	0.45
1:B:16:HIS:NE2	1:B:27:TYR:CE2	2.84	0.45
1:B:45:ILE:O	1:B:94:LYS:CG	2.65	0.45
1:C:43:THR:CG2	1:C:49:HIS:O	2.64	0.45
1:D:47:ASN:C	1:D:92:GLN:HE21	2.20	0.45
1:F:66:LEU:HD23	1:F:67:GLU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:HIS:NE2	1:A:27:TYR:CE2	2.85	0.45
1:A:135:PRO:CG	1:A:536:PHE:CE1	3.00	0.45
1:A:588:ASP:O	1:A:588:ASP:OD1	2.35	0.45
1:C:89:VAL:O	1:C:90:LEU:C	2.55	0.45
1:C:475:LEU:HD23	1:C:476:ALA:N	2.31	0.45
1:D:620:ARG:C	1:D:621:PRO:O	2.55	0.45
1:E:27:TYR:HA	1:E:28:PRO:HD2	1.66	0.45
1:E:69:ARG:HA	1:E:264:TYR:CD2	2.52	0.45
1:E:289:LEU:O	1:E:290:GLU:C	2.54	0.45
1:E:419:ASP:HB3	1:E:461:THR:HG23	1.99	0.45
1:E:477:THR:HG23	1:E:509:PHE:CE1	2.51	0.45
1:F:125:HIS:HB3	1:F:211:TYR:OH	2.16	0.45
1:F:639:VAL:HG21	1:F:642:ILE:HD12	1.99	0.45
1:A:53:VAL:C	1:A:55:THR:N	2.70	0.45
1:A:195:VAL:CG1	1:A:372:GLU:HB3	2.46	0.45
1:A:255:GLY:CA	1:A:271:ARG:NH1	2.73	0.45
1:A:318:PRO:C	1:A:320:GLY:H	2.20	0.45
1:A:493:LEU:CB	1:A:497:GLU:HB2	2.43	0.45
1:A:592:ASP:C	1:A:594:GLU:N	2.70	0.45
1:B:5:THR:HB	1:B:10:LYS:HE3	1.99	0.45
1:B:38:ASN:C	1:B:40:LEU:H	2.20	0.45
1:B:275:ILE:HG23	1:B:276:HIS:N	2.31	0.45
1:B:405:ASN:HD22	1:B:405:ASN:HA	1.20	0.45
1:D:285:HIS:O	1:D:288:ASP:HB2	2.16	0.45
1:E:285:HIS:O	1:E:288:ASP:HB2	2.17	0.45
1:E:405:ASN:HD22	1:E:405:ASN:HA	1.56	0.45
1:F:78:ARG:NH1	1:F:82:GLU:OE2	2.49	0.45
1:A:260:THR:O	1:A:268:PHE:HD1	1.99	0.45
1:A:589:GLY:O	1:A:593:THR:OG1	2.33	0.45
1:B:572:LYS:O	1:B:573:SER:CB	2.60	0.45
1:C:43:THR:HG23	1:C:49:HIS:O	2.16	0.45
1:C:139:GLN:NE2	1:C:432:SER:H	2.15	0.45
1:D:578:MET:HE3	1:D:580:PHE:HZ	1.82	0.45
1:E:305:ILE:HG23	1:E:340:TYR:CE2	2.52	0.45
1:E:392:LYS:NZ	1:E:396:ASP:OD2	2.50	0.45
1:F:357:PRO:HB2	1:F:358:HIS:CE1	2.52	0.45
1:F:380:PHE:CE1	1:F:384:HIS:CE1	3.05	0.45
1:F:480:ILE:HA	1:F:583:TYR:O	2.17	0.45
1:A:178:GLU:C	1:A:180:ARG:H	2.19	0.45
1:A:253:ARG:NH1	1:A:253:ARG:HG3	2.30	0.45
1:A:330:SER:HB2	1:A:342:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:LYS:CD	1:A:578:MET:HE2	2.47	0.45
1:B:40:LEU:HD12	1:B:40:LEU:HA	1.55	0.45
1:B:158:LYS:CG	1:B:437:VAL:HG21	2.46	0.45
1:B:352:GLY:C	1:B:354:GLN:N	2.68	0.45
1:C:215:ARG:O	1:C:217:GLY:N	2.50	0.45
1:C:636:ILE:HG23	1:C:642:ILE:HG21	1.98	0.45
1:C:639:VAL:HG21	1:C:642:ILE:HD12	1.98	0.45
1:D:411:MET:CE	1:D:512:VAL:HB	2.45	0.45
1:D:628:ARG:O	1:D:630:ILE:HG13	2.16	0.45
1:E:56:LEU:HD11	1:E:65:LEU:HD21	1.99	0.45
1:E:215:ARG:O	1:E:217:GLY:N	2.50	0.45
1:E:256:PHE:CE2	1:E:377:ASP:HA	2.52	0.45
1:F:185:GLY:CA	1:F:375:THR:CG2	2.94	0.45
1:F:197:TRP:HZ2	1:F:219:LEU:HB3	1.81	0.45
1:F:207:ASP:OD2	1:F:212:HIS:CB	2.65	0.45
1:F:377:ASP:HA	1:F:378:PRO:HD3	1.90	0.45
1:A:284:ALA:O	1:A:350:MET:CE	2.65	0.45
1:A:489:ASN:HB3	1:A:491:ILE:HD11	1.97	0.45
1:A:491:ILE:HG12	1:F:175:LYS:HB2	1.98	0.45
1:B:147:ASN:ND2	1:B:149:GLU:HB3	2.26	0.45
1:B:403:HIS:C	1:B:405:ASN:N	2.70	0.45
1:C:285:HIS:O	1:C:288:ASP:HB2	2.17	0.45
1:C:413:VAL:HG12	1:C:643:LYS:HG3	1.99	0.45
1:C:573:SER:CB	1:C:649:ILE:HG22	2.47	0.45
1:D:305:ILE:HG23	1:D:340:TYR:CE2	2.51	0.45
1:E:197:TRP:HZ2	1:E:219:LEU:HB3	1.82	0.45
1:E:280:VAL:HG21	1:E:353:ARG:HG3	1.99	0.45
1:E:478:PHE:CZ	1:E:519:ILE:HD12	2.52	0.45
1:F:226:GLN:O	1:F:227:LEU:C	2.56	0.45
1:A:66:LEU:HD21	1:A:70:HIS:ND1	2.32	0.45
1:A:135:PRO:HG2	1:A:140:ILE:HD11	1.99	0.45
1:A:305:ILE:HB	1:A:313:ILE:HG13	1.99	0.45
1:A:378:PRO:C	1:A:380:PHE:N	2.71	0.45
1:A:631:PRO:HD2	3:A:818:HOH:O	2.17	0.45
1:B:272:PRO:CD	1:B:272:PRO:O	2.62	0.45
1:B:574:LYS:HA	1:B:575:PRO:HD3	1.87	0.45
1:C:31:LYS:HA	1:C:34:ALA:HB3	1.98	0.45
1:C:477:THR:HG23	1:C:509:PHE:CE1	2.52	0.45
1:D:89:VAL:C	1:D:91:ASN:N	2.66	0.45
1:D:147:ASN:HD22	1:D:149:GLU:HB3	1.82	0.45
1:E:56:LEU:HD11	1:E:110:MET:CE	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:GLU:O	1:E:116:VAL:HG23	2.18	0.45
1:E:125:HIS:HB3	1:E:211:TYR:OH	2.16	0.45
1:E:213:LEU:N	1:E:213:LEU:CD1	2.80	0.45
1:E:410:GLY:O	1:E:412:VAL:HG12	2.17	0.45
1:E:475:LEU:HD23	1:E:476:ALA:N	2.32	0.45
1:F:84:LEU:HD11	1:F:204:TRP:CE2	2.52	0.45
1:F:222:TRP:CD1	1:F:622:LEU:HD23	2.52	0.45
1:F:549:GLY:O	1:F:550:GLY:C	2.55	0.45
1:A:159:MET:HE1	1:B:155:TYR:CG	2.51	0.44
1:A:538:SER:O	1:A:542:GLN:HG3	2.18	0.44
1:A:574:LYS:HE3	1:A:578:MET:HE1	1.98	0.44
1:B:14:ILE:CD1	1:B:96:TRP:CZ2	3.00	0.44
1:B:42:ASP:OD1	1:B:44:SER:HB3	2.16	0.44
1:B:190:MET:C	1:B:192:ILE:N	2.67	0.44
1:B:473:GLU:O	1:B:474:ARG:HG2	2.17	0.44
1:C:125:HIS:HB3	1:C:211:TYR:OH	2.17	0.44
1:C:151:ILE:HD13	1:C:151:ILE:HA	1.76	0.44
1:C:573:SER:HB2	1:C:649:ILE:CG2	2.47	0.44
1:C:628:ARG:O	1:C:630:ILE:HG13	2.17	0.44
1:D:206:GLU:C	1:D:208:SER:H	2.21	0.44
1:D:568:MET:O	1:D:569:LEU:C	2.54	0.44
1:F:628:ARG:O	1:F:630:ILE:HG13	2.17	0.44
1:A:314:ASP:OD1	1:A:314:ASP:C	2.56	0.44
1:B:13:ASP:OD2	1:B:100:ARG:HD2	2.17	0.44
1:B:222:TRP:CD1	1:B:622:LEU:CD2	3.00	0.44
1:B:517:GLU:HG2	1:B:518:THR:H	1.81	0.44
1:C:143:HIS:CE1	1:C:151:ILE:HG21	2.52	0.44
1:C:305:ILE:HG23	1:C:340:TYR:CE2	2.53	0.44
1:C:433:LEU:HG	1:C:450:ALA:HB2	1.99	0.44
1:C:568:MET:O	1:C:569:LEU:C	2.55	0.44
1:C:573:SER:HB2	1:C:649:ILE:HG22	1.98	0.44
1:D:37:PHE:CE1	1:D:101:SER:HB3	2.52	0.44
1:D:89:VAL:O	1:D:90:LEU:C	2.55	0.44
1:D:433:LEU:HG	1:D:450:ALA:HB2	2.00	0.44
1:D:462:TYR:HB3	1:D:464:ILE:CD1	2.47	0.44
1:E:60:LEU:HD11	1:E:109:ARG:HG3	2.00	0.44
1:E:593:THR:C	1:E:595:GLY:H	2.20	0.44
1:F:285:HIS:O	1:F:288:ASP:HB2	2.17	0.44
1:A:304:TYR:CD1	1:A:312:THR:HB	2.53	0.44
1:A:305:ILE:HG21	1:A:305:ILE:HD13	1.68	0.44
1:A:521:ARG:HG2	1:A:522:SER:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:TYR:HD1	1:B:306:THR:HG22	1.82	0.44
1:C:197:TRP:HZ2	1:C:219:LEU:HB3	1.82	0.44
1:C:271:ARG:HA	1:C:272:PRO:HD3	1.81	0.44
1:C:408:PHE:CB	1:C:641:ASN:OD1	2.65	0.44
1:D:197:TRP:HZ2	1:D:219:LEU:HB3	1.82	0.44
1:D:480:ILE:HA	1:D:583:TYR:O	2.17	0.44
1:E:357:PRO:HB2	1:E:358:HIS:CE1	2.53	0.44
1:F:127:LYS:H	1:F:127:LYS:HG2	1.46	0.44
1:A:190:MET:CG	1:A:568:MET:HE2	2.42	0.44
1:A:559:GLU:H	1:A:559:GLU:HG2	1.70	0.44
1:B:47:ASN:N	1:B:92:GLN:O	2.49	0.44
1:B:48:ASP:OD2	1:B:52:ALA:N	2.49	0.44
1:B:496:ASP:H	1:B:498:ALA:H	1.66	0.44
1:C:300:ILE:HD11	1:C:390:ILE:HG22	2.00	0.44
1:C:316:ARG:HH21	1:E:338:GLN:NE2	2.16	0.44
1:C:330:SER:HB2	1:C:342:SER:CB	2.47	0.44
1:D:420:GLY:HA2	1:D:421:GLU:OE1	2.18	0.44
1:E:230:ARG:NH2	1:E:569:LEU:O	2.50	0.44
1:E:411:MET:CE	1:E:474:ARG:HB2	2.46	0.44
1:E:592:ASP:C	1:E:594:GLU:N	2.71	0.44
1:F:11:GLN:O	1:F:15:ASN:ND2	2.50	0.44
1:A:192:ILE:HD13	1:A:192:ILE:HA	1.93	0.44
1:A:199:MET:CE	3:A:774:HOH:O	2.65	0.44
1:B:34:ALA:O	1:B:109:ARG:NH2	2.50	0.44
1:B:84:LEU:HD21	1:B:204:TRP:CD2	2.53	0.44
1:B:319:LYS:HD3	1:B:319:LYS:HA	1.94	0.44
1:C:66:LEU:CD2	1:C:67:GLU:N	2.80	0.44
1:C:271:ARG:NH2	1:C:377:ASP:OD1	2.51	0.44
1:C:414:ASN:HD21	1:C:467:SER:H	1.64	0.44
1:C:480:ILE:HA	1:C:583:TYR:O	2.17	0.44
1:D:207:ASP:OD2	1:D:212:HIS:CB	2.65	0.44
1:D:220:PHE:CZ	1:D:329:GLU:HB2	2.52	0.44
1:D:256:PHE:HA	1:E:361:PHE:CE1	2.53	0.44
1:D:418:ILE:HD13	1:D:422:LEU:HD11	2.00	0.44
1:D:639:VAL:HG23	1:D:641:ASN:HD22	1.83	0.44
1:E:10:LYS:HA	1:E:96:TRP:NE1	2.32	0.44
1:E:323:LEU:HD11	3:E:849:HOH:O	2.17	0.44
1:F:39:PRO:HB3	1:F:102:ASN:HD21	1.82	0.44
1:F:89:VAL:O	1:F:90:LEU:C	2.55	0.44
1:A:56:LEU:HD11	1:A:65:LEU:HD21	2.00	0.44
1:A:461:THR:OG1	1:A:520:GLU:CG	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:PHE:CE1	1:A:593:THR:HG23	2.53	0.44
1:A:574:LYS:CG	1:A:578:MET:HE2	2.47	0.44
1:B:37:PHE:CE2	1:B:101:SER:CB	2.99	0.44
1:B:298:GLU:HG2	1:B:302:HIS:HD2	1.82	0.44
1:C:56:LEU:HD11	1:C:65:LEU:HD21	1.99	0.44
1:C:302:HIS:ND1	1:C:304:TYR:CZ	2.85	0.44
1:E:66:LEU:HD23	1:E:67:GLU:N	2.32	0.44
1:E:84:LEU:HD11	1:E:204:TRP:CE2	2.52	0.44
1:E:471:ASP:OD1	1:E:471:ASP:C	2.56	0.44
1:F:568:MET:O	1:F:569:LEU:C	2.56	0.44
1:A:307:ASP:C	1:A:307:ASP:OD1	2.55	0.44
1:B:296:ILE:HG21	1:B:390:ILE:HG21	1.98	0.44
1:B:484:PRO:HD2	1:B:498:ALA:HB1	2.00	0.44
1:C:84:LEU:HD11	1:C:204:TRP:CE2	2.52	0.44
1:D:40:LEU:HD12	1:D:53:VAL:CG1	2.42	0.44
1:D:71:TRP:CZ3	1:D:365:PRO:HG2	2.53	0.44
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.64	0.44
1:A:473:GLU:O	1:A:512:VAL:O	2.36	0.44
1:B:631:PRO:HD2	3:B:818:HOH:O	2.17	0.44
1:C:39:PRO:HB2	1:C:53:VAL:CG1	2.48	0.44
1:C:207:ASP:OD2	1:C:212:HIS:CB	2.65	0.44
1:C:226:GLN:O	1:C:227:LEU:C	2.56	0.44
1:D:46:TYR:CE2	1:D:53:VAL:HG21	2.51	0.44
1:E:157:ALA:HB3	1:E:448:ILE:CD1	2.47	0.44
1:E:301:ASP:OD2	1:E:393:LYS:NZ	2.50	0.44
1:E:554:ASP:C	1:E:556:SER:N	2.71	0.44
1:E:641:ASN:ND2	1:E:641:ASN:N	2.62	0.44
1:E:641:ASN:C	1:E:641:ASN:HD22	2.20	0.44
1:F:215:ARG:O	1:F:217:GLY:N	2.51	0.44
1:A:553:LEU:HD23	1:A:553:LEU:HA	1.81	0.44
1:B:295:ARG:NE	1:B:339:TYR:CE1	2.86	0.44
1:B:442:ASN:N	1:B:442:ASN:ND2	2.66	0.44
1:C:56:LEU:HD21	1:C:110:MET:CE	2.48	0.44
1:D:259:LEU:HD11	1:E:363:LEU:CD1	2.48	0.44
1:D:317:GLN:CB	1:D:318:PRO:HD2	2.28	0.44
1:D:385:LYS:HE2	3:D:750:HOH:O	2.17	0.44
1:D:393:LYS:HE3	1:D:393:LYS:HB3	1.82	0.44
1:E:639:VAL:HG21	1:E:642:ILE:HD12	1.99	0.44
1:F:56:LEU:HD21	1:F:110:MET:CE	2.48	0.44
1:F:125:HIS:CE1	1:F:200:ASP:O	2.71	0.44
1:A:82:GLU:OE1	1:A:114:GLU:OE2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:THR:O	1:A:147:ASN:O	2.35	0.43
1:A:508:PHE:HE2	3:A:864:HOH:O	1.94	0.43
1:B:367:VAL:O	1:B:373:THR:HG22	2.18	0.43
1:B:624:TYR:HA	1:B:625:PRO:HA	1.85	0.43
1:C:405:ASN:HD22	1:C:405:ASN:HA	1.53	0.43
1:D:165:THR:HG22	1:D:449:ASN:CB	2.25	0.43
1:D:195:VAL:CG2	1:D:196:THR:N	2.81	0.43
1:D:222:TRP:CH2	1:D:226:GLN:NE2	2.86	0.43
1:E:168:VAL:HG22	1:E:452:VAL:HA	2.00	0.43
1:E:178:GLU:HG3	1:E:178:GLU:O	2.18	0.43
1:E:464:ILE:O	1:E:519:ILE:N	2.51	0.43
1:F:43:THR:CG2	1:F:49:HIS:O	2.66	0.43
1:F:158:LYS:NZ	1:F:439:SER:HB2	2.33	0.43
1:F:305:ILE:HG23	1:F:340:TYR:CE2	2.53	0.43
1:F:424:THR:O	1:F:651:HIS:ND1	2.37	0.43
1:A:126:SER:O	1:A:128:LEU:N	2.51	0.43
1:A:296:ILE:HD11	1:A:340:TYR:HB3	2.00	0.43
1:A:416:VAL:CG1	1:A:643:LYS:HG3	2.48	0.43
1:A:424:THR:O	1:A:651:HIS:HA	2.18	0.43
1:A:618:ASP:OD1	1:A:620:ARG:N	2.51	0.43
1:B:158:LYS:HD3	1:B:446:VAL:HG11	1.99	0.43
1:B:177:ARG:NH1	1:B:179:GLN:CG	2.80	0.43
1:B:639:VAL:HG21	1:B:642:ILE:HD12	2.00	0.43
1:C:125:HIS:CE1	1:C:200:ASP:O	2.71	0.43
1:C:411:MET:HE3	1:C:512:VAL:HB	2.00	0.43
1:C:614:GLU:H	1:C:614:GLU:HG3	1.40	0.43
1:C:620:ARG:C	1:C:621:PRO:O	2.55	0.43
1:D:60:LEU:HD11	1:D:109:ARG:HG3	2.00	0.43
1:D:396:ASP:O	1:D:629:ARG:NH1	2.49	0.43
1:D:641:ASN:ND2	1:D:641:ASN:N	2.64	0.43
1:E:125:HIS:CE1	1:E:200:ASP:O	2.71	0.43
1:E:226:GLN:O	1:E:227:LEU:C	2.55	0.43
1:F:39:PRO:HB2	1:F:53:VAL:CG1	2.49	0.43
1:F:177:ARG:HH11	1:F:179:GLN:HG3	1.84	0.43
1:A:230:ARG:CZ	1:A:503:ILE:HD12	2.48	0.43
1:B:18:LEU:CD1	1:B:135:PRO:HG2	2.47	0.43
1:B:241:ASP:HA	1:B:242:PRO:HD3	1.87	0.43
1:C:140:ILE:HG22	1:C:141:THR:HG23	2.00	0.43
1:C:168:VAL:HG22	1:C:452:VAL:HA	1.99	0.43
1:C:411:MET:CE	1:C:512:VAL:HB	2.47	0.43
1:D:34:ALA:O	1:D:109:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LYS:O	1:D:85:MET:HG2	2.18	0.43
1:D:270:VAL:HG13	1:E:270:VAL:HG13	2.00	0.43
1:D:419:ASP:CB	1:D:463:LYS:HD2	2.47	0.43
1:E:207:ASP:OD2	1:E:212:HIS:CB	2.66	0.43
1:F:280:VAL:HG21	1:F:353:ARG:HG3	2.00	0.43
1:F:494:THR:H	1:F:497:GLU:HB2	1.83	0.43
1:F:591:LYS:NZ	1:F:591:LYS:CB	2.81	0.43
1:A:258:PRO:HG2	1:A:259:LEU:N	2.32	0.43
1:A:287:HIS:O	1:A:291:ILE:N	2.40	0.43
1:A:406:LEU:HA	1:A:406:LEU:HD23	1.69	0.43
1:A:419:ASP:OD1	1:A:463:LYS:NZ	2.40	0.43
1:A:475:LEU:HA	1:A:511:LYS:HA	2.00	0.43
1:A:495:LEU:HD13	1:A:583:TYR:OH	2.19	0.43
1:B:162:LYS:HA	1:B:163:PRO:HD3	1.77	0.43
1:B:195:VAL:HG11	1:B:372:GLU:HB3	1.99	0.43
1:B:433:LEU:HB2	1:B:448:ILE:CG2	2.48	0.43
1:B:639:VAL:HG23	1:B:641:ASN:HD22	1.83	0.43
1:C:219:LEU:HD12	1:C:219:LEU:HA	1.79	0.43
1:D:5:THR:CG2	1:D:6:GLY:H	2.18	0.43
1:D:86:LEU:HD23	1:D:86:LEU:O	2.19	0.43
1:D:150:VAL:HG21	1:D:168:VAL:CG1	2.30	0.43
1:D:159:MET:HE2	1:E:155:TYR:CB	2.47	0.43
1:D:200:ASP:OD2	1:D:609:CYS:SG	2.77	0.43
1:D:343:LEU:HD11	3:D:861:HOH:O	2.18	0.43
1:D:465:THR:HG23	1:D:518:THR:OG1	2.18	0.43
1:F:10:LYS:HA	1:F:96:TRP:NE1	2.34	0.43
1:F:127:LYS:HD3	3:F:869:HOH:O	2.18	0.43
1:A:60:LEU:HD22	1:A:106:PHE:CE1	2.50	0.43
1:A:124:ILE:HG22	1:A:611:VAL:HG11	2.00	0.43
1:A:411:MET:HE1	1:A:512:VAL:HG12	2.00	0.43
1:B:255:GLY:H	1:B:273:ASP:CB	2.29	0.43
1:B:271:ARG:HA	1:B:272:PRO:HD3	1.64	0.43
1:B:387:MET:HE2	1:B:387:MET:HB2	1.75	0.43
1:D:125:HIS:CE1	1:D:200:ASP:O	2.72	0.43
1:D:125:HIS:HB3	1:D:211:TYR:OH	2.19	0.43
1:D:271:ARG:HA	1:D:272:PRO:HD3	1.81	0.43
1:D:420:GLY:C	1:D:421:GLU:OE1	2.57	0.43
1:E:578:MET:HG3	1:E:580:PHE:CZ	2.53	0.43
1:F:215:ARG:O	1:F:216:LYS:C	2.55	0.43
1:F:323:LEU:HD11	3:F:849:HOH:O	2.19	0.43
1:F:324:LEU:HD23	1:F:324:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:PHE:CZ	1:A:377:ASP:HA	2.53	0.43
1:B:26:LYS:O	1:B:28:PRO:HD2	2.19	0.43
1:B:466:MET:CE	3:B:834:HOH:O	2.66	0.43
1:C:127:LYS:HD3	3:C:869:HOH:O	2.19	0.43
1:C:185:GLY:CA	1:C:375:THR:CG2	2.94	0.43
1:C:239:TRP:HH2	1:C:574:LYS:HD3	1.71	0.43
1:C:248:TRP:CZ3	1:C:289:LEU:HD13	2.54	0.43
1:C:256:PHE:CE2	1:C:377:ASP:HA	2.53	0.43
1:C:283:VAL:O	1:C:284:ALA:HB2	2.19	0.43
1:D:48:ASP:N	1:D:92:GLN:NE2	2.63	0.43
1:D:215:ARG:O	1:D:216:LYS:C	2.56	0.43
1:D:614:GLU:H	1:D:614:GLU:HG3	1.42	0.43
1:E:11:GLN:O	1:E:15:ASN:ND2	2.51	0.43
1:E:428:GLU:OE2	1:E:451:ARG:HD2	2.18	0.43
1:F:230:ARG:NH2	1:F:569:LEU:O	2.50	0.43
1:F:243:VAL:HG23	1:F:385:LYS:CD	2.48	0.43
1:F:300:ILE:HD11	1:F:390:ILE:HG22	2.00	0.43
1:F:442:ASN:HD22	1:F:442:ASN:N	2.17	0.43
1:F:641:ASN:ND2	1:F:641:ASN:N	2.64	0.43
1:A:11:GLN:HG3	1:A:15:ASN:ND2	2.26	0.43
1:A:69:ARG:HA	1:A:264:TYR:CD2	2.54	0.43
1:A:328:ILE:O	1:A:328:ILE:CG2	2.60	0.43
1:A:588:ASP:O	1:A:590:ASP:N	2.50	0.43
1:B:313:ILE:HD12	1:B:314:ASP:O	2.18	0.43
1:B:440:GLY:O	1:B:441:GLU:HG3	2.19	0.43
1:C:177:ARG:HH11	1:C:179:GLN:HG3	1.84	0.43
1:D:215:ARG:O	1:D:217:GLY:N	2.51	0.43
1:D:219:LEU:HD12	1:D:219:LEU:HA	1.79	0.43
1:D:364:PRO:HB2	1:D:365:PRO:CD	2.49	0.43
1:D:494:THR:O	1:D:495:LEU:C	2.56	0.43
1:E:60:LEU:HD22	1:E:106:PHE:HE1	1.84	0.43
1:E:413:VAL:HG12	1:E:643:LYS:HG3	2.00	0.43
1:F:27:TYR:HA	1:F:28:PRO:HD2	1.70	0.43
1:F:178:GLU:O	1:F:178:GLU:HG3	2.18	0.43
1:A:177:ARG:HD3	1:A:179:GLN:HB2	2.00	0.43
1:A:275:ILE:HG12	1:A:276:HIS:N	2.34	0.43
1:A:642:ILE:HD13	1:A:642:ILE:HG21	1.83	0.43
1:B:489:ASN:HB3	1:B:491:ILE:CG1	2.49	0.43
1:B:530:VAL:HA	1:B:531:PRO:HD2	1.90	0.43
1:C:364:PRO:HB2	1:C:365:PRO:CD	2.49	0.43
1:C:458:ASN:O	1:C:459:GLU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:LEU:C	1:D:343:LEU:CD2	2.87	0.43
1:E:185:GLY:CA	1:E:375:THR:CG2	2.93	0.43
1:F:43:THR:HG23	1:F:49:HIS:O	2.17	0.43
1:F:195:VAL:CG2	1:F:196:THR:N	2.82	0.43
1:A:424:THR:HA	1:A:456:ASN:O	2.19	0.43
1:A:588:ASP:O	1:A:589:GLY:C	2.56	0.43
1:A:633:GLU:C	1:A:635:VAL:H	2.20	0.43
1:B:27:TYR:O	1:B:30:LEU:N	2.52	0.43
1:B:39:PRO:O	1:B:46:TYR:HE2	2.01	0.43
1:B:68:GLN:HG2	1:B:110:MET:O	2.18	0.43
1:B:95:GLU:O	1:B:96:TRP:C	2.55	0.43
1:B:221:PHE:CG	1:B:222:TRP:N	2.86	0.43
1:C:259:LEU:HD11	1:F:363:LEU:CD1	2.49	0.43
1:C:260:THR:HG22	1:C:268:PHE:HE1	1.80	0.43
1:C:295:ARG:NE	1:C:339:TYR:CE1	2.87	0.43
1:D:553:LEU:HD22	1:D:555:LEU:HG	2.00	0.43
1:E:154:ALA:HB2	1:E:433:LEU:HD13	2.01	0.43
1:E:169:SER:O	1:E:170:PHE:CB	2.67	0.43
1:E:398:PHE:HB3	1:E:399:PRO:HD2	2.01	0.43
1:F:31:LYS:HA	1:F:34:ALA:HB3	2.00	0.43
1:F:256:PHE:CE2	1:F:377:ASP:HA	2.54	0.43
1:F:433:LEU:HG	1:F:450:ALA:HB2	2.01	0.43
1:F:639:VAL:HG23	1:F:641:ASN:HD22	1.84	0.43
1:A:48:ASP:OD1	1:A:50:GLY:CA	2.66	0.43
1:A:230:ARG:NH2	1:A:569:LEU:O	2.52	0.43
1:A:403:HIS:C	1:A:405:ASN:H	2.22	0.43
1:B:14:ILE:HD13	1:B:96:TRP:CZ2	2.53	0.43
1:B:226:GLN:O	1:B:227:LEU:C	2.56	0.43
1:B:279:ASP:OD1	1:B:286:VAL:N	2.44	0.43
1:B:403:HIS:HE1	1:B:407:GLU:HG2	1.82	0.43
1:C:248:TRP:CZ2	1:C:289:LEU:HD13	2.53	0.43
1:D:56:LEU:HD21	1:D:110:MET:CE	2.49	0.43
1:D:510:GLN:OE1	1:D:519:ILE:CG2	2.66	0.43
1:D:520:GLU:HG2	1:D:521:ARG:N	2.32	0.43
1:E:591:LYS:CA	1:E:594:GLU:HB2	2.48	0.43
1:A:122:SER:O	1:A:123:VAL:C	2.57	0.42
1:A:133:VAL:HG22	1:A:558:TYR:HB2	2.01	0.42
1:B:168:VAL:HG22	1:B:452:VAL:HA	2.01	0.42
1:B:570:LEU:HG	1:B:649:ILE:HD11	2.00	0.42
1:D:66:LEU:HD23	1:D:67:GLU:N	2.33	0.42
1:D:84:LEU:HD11	1:D:204:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:639:VAL:HG21	1:D:642:ILE:HD12	2.01	0.42
1:E:466:MET:HG3	1:E:466:MET:O	2.18	0.42
1:E:468:ASN:HD21	1:E:474:ARG:CG	2.30	0.42
1:F:168:VAL:HG22	1:F:452:VAL:HA	2.00	0.42
1:F:620:ARG:C	1:F:621:PRO:O	2.55	0.42
1:A:37:PHE:CE2	1:A:101:SER:HB3	2.54	0.42
1:A:86:LEU:HB3	1:A:118:ALA:CB	2.50	0.42
1:A:219:LEU:HD12	1:A:219:LEU:HA	1.91	0.42
1:A:461:THR:OG1	1:A:520:GLU:HG2	2.18	0.42
1:A:479:ARG:NH1	1:A:587:THR:CG2	2.82	0.42
1:A:480:ILE:HD13	1:A:480:ILE:HG21	1.47	0.42
1:B:23:GLU:OE2	1:B:439:SER:O	2.37	0.42
1:B:151:ILE:HD13	1:B:151:ILE:HA	1.88	0.42
1:B:151:ILE:HD13	1:B:433:LEU:HD22	2.00	0.42
1:C:135:PRO:CB	1:C:140:ILE:HD11	2.48	0.42
1:C:177:ARG:HD2	1:F:360:LYS:HB3	2.01	0.42
1:C:239:TRP:CH2	1:C:574:LYS:CD	2.90	0.42
1:C:538:SER:O	1:C:542:GLN:HG3	2.18	0.42
1:D:233:PHE:O	1:D:236:LEU:HB3	2.19	0.42
1:E:45:ILE:HB	1:E:98:CYS:HB2	2.01	0.42
1:F:46:TYR:CD2	1:F:53:VAL:HG21	2.53	0.42
1:F:271:ARG:NH2	1:F:377:ASP:OD1	2.52	0.42
1:F:283:VAL:O	1:F:284:ALA:HB2	2.19	0.42
1:F:414:ASN:HD21	1:F:467:SER:H	1.66	0.42
1:A:427:ASP:CB	1:A:567:ARG:NH1	2.78	0.42
1:A:508:PHE:CD2	1:A:521:ARG:CD	3.01	0.42
1:B:192:ILE:HD12	1:B:192:ILE:HG23	1.82	0.42
1:B:197:TRP:HZ2	1:B:219:LEU:HB3	1.85	0.42
1:B:479:ARG:HD2	1:B:587:THR:CG2	2.49	0.42
1:B:570:LEU:HG	1:B:649:ILE:CD1	2.49	0.42
1:C:215:ARG:O	1:C:216:LYS:C	2.55	0.42
1:C:494:THR:O	1:C:495:LEU:C	2.57	0.42
1:D:323:LEU:HD11	3:D:849:HOH:O	2.20	0.42
1:D:408:PHE:CE2	1:D:411:MET:SD	3.12	0.42
1:F:12:GLN:OE1	1:F:547:VAL:HG11	2.19	0.42
1:F:428:GLU:OE2	1:F:451:ARG:HD2	2.19	0.42
1:F:458:ASN:O	1:F:459:GLU:C	2.56	0.42
1:F:636:ILE:HG23	1:F:642:ILE:HG21	2.01	0.42
1:A:169:SER:O	1:A:170:PHE:CB	2.65	0.42
1:A:454:ARG:NH1	1:A:567:ARG:CD	2.82	0.42
1:A:529:THR:CG2	1:A:566:ASP:HA	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ASP:C	1:A:634:ARG:N	2.73	0.42
1:B:201:PHE:CD1	1:B:201:PHE:N	2.88	0.42
1:B:295:ARG:HH11	1:B:295:ARG:HD2	1.34	0.42
1:B:296:ILE:HA	1:B:296:ILE:HD13	1.65	0.42
1:B:517:GLU:HG2	1:B:518:THR:N	2.34	0.42
1:C:46:TYR:CD2	1:C:53:VAL:HG21	2.54	0.42
1:C:146:THR:HG21	1:C:433:LEU:HD21	2.00	0.42
1:D:283:VAL:O	1:D:284:ALA:HB2	2.19	0.42
1:D:300:ILE:HD11	1:D:390:ILE:HG22	2.01	0.42
1:D:317:GLN:CB	1:D:318:PRO:CD	2.96	0.42
1:D:485:ILE:O	1:D:492:THR:HA	2.18	0.42
1:D:636:ILE:HG23	1:D:642:ILE:HG21	2.01	0.42
1:E:554:ASP:C	1:E:556:SER:H	2.23	0.42
1:E:568:MET:O	1:E:569:LEU:C	2.57	0.42
1:F:5:THR:HG22	1:F:6:GLY:N	2.28	0.42
1:F:86:LEU:O	1:F:86:LEU:HD23	2.20	0.42
1:F:641:ASN:HD22	1:F:641:ASN:C	2.23	0.42
1:A:80:ARG:O	1:A:80:ARG:HG2	2.19	0.42
1:B:26:LYS:O	1:B:28:PRO:CD	2.68	0.42
1:B:126:SER:O	1:B:127:LYS:C	2.56	0.42
1:B:301:ASP:CG	1:B:393:LYS:NZ	2.71	0.42
1:B:350:MET:O	1:B:354:GLN:HG2	2.19	0.42
1:C:178:GLU:O	1:C:178:GLU:HG3	2.20	0.42
1:C:517:GLU:HG2	1:C:518:THR:N	2.33	0.42
1:D:41:GLY:O	1:D:42:ASP:HB2	2.19	0.42
1:E:185:GLY:CA	1:E:375:THR:HG22	2.49	0.42
1:E:639:VAL:HG23	1:E:641:ASN:HD22	1.83	0.42
1:F:19:ASP:O	1:F:20:LYS:C	2.57	0.42
1:F:66:LEU:HD23	1:F:67:GLU:N	2.34	0.42
1:F:408:PHE:CB	1:F:641:ASN:OD1	2.66	0.42
1:A:43:THR:HG23	1:A:49:HIS:C	2.40	0.42
1:A:89:VAL:O	1:A:90:LEU:C	2.58	0.42
1:A:177:ARG:HH12	1:A:256:PHE:HB2	1.84	0.42
1:A:222:TRP:CZ3	1:A:623:GLY:HA3	2.55	0.42
1:A:271:ARG:HA	1:A:272:PRO:HD3	1.83	0.42
1:A:292:THR:O	1:A:296:ILE:HG12	2.19	0.42
1:A:578:MET:O	1:A:648:LYS:HG3	2.20	0.42
1:A:628:ARG:O	1:A:630:ILE:HG13	2.20	0.42
1:B:428:GLU:OE2	1:B:451:ARG:HD2	2.20	0.42
1:C:398:PHE:HB3	1:C:399:PRO:HD2	2.01	0.42
1:D:43:THR:HG23	1:D:49:HIS:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:LEU:HD11	1:D:580:PHE:HB2	2.02	0.42
1:D:573:SER:OG	1:D:574:LYS:N	2.48	0.42
1:E:591:LYS:HB2	1:E:591:LYS:HZ2	1.85	0.42
1:F:135:PRO:CB	1:F:140:ILE:HD11	2.50	0.42
1:F:634:ARG:HH11	1:F:634:ARG:CG	2.25	0.42
1:A:197:TRP:HZ2	1:A:219:LEU:HB3	1.85	0.42
1:A:591:LYS:CA	1:A:594:GLU:HB2	2.40	0.42
1:A:593:THR:C	1:A:595:GLY:H	2.22	0.42
1:A:606:HIS:HB3	1:A:608:GLN:H	1.83	0.42
1:C:5:THR:HG22	1:C:6:GLY:N	2.29	0.42
1:C:302:HIS:ND1	1:C:304:TYR:OH	2.53	0.42
1:C:591:LYS:NZ	1:C:591:LYS:CB	2.82	0.42
1:D:256:PHE:CE2	1:D:377:ASP:HA	2.54	0.42
1:E:634:ARG:HG2	1:E:634:ARG:NH1	2.20	0.42
1:B:419:ASP:CB	1:B:463:LYS:HD3	2.50	0.42
1:B:479:ARG:HH11	1:B:587:THR:CG2	2.33	0.42
1:C:78:ARG:NH1	1:C:82:GLU:OE2	2.49	0.42
1:C:127:LYS:H	1:C:127:LYS:HG2	1.48	0.42
1:C:493:LEU:HB2	1:C:497:GLU:HB2	2.02	0.42
1:E:151:ILE:HD13	1:E:151:ILE:HA	1.77	0.42
1:E:283:VAL:O	1:E:284:ALA:HB2	2.20	0.42
1:E:364:PRO:HB2	1:E:365:PRO:CD	2.50	0.42
1:E:533:MET:H	1:E:533:MET:HE2	1.84	0.42
1:E:624:TYR:HA	1:E:625:PRO:HA	1.82	0.42
1:A:64:ARG:O	1:A:78:ARG:NH1	2.53	0.42
1:A:244:ASP:OD1	1:A:382:ARG:HD3	2.20	0.42
1:A:313:ILE:HG13	1:A:313:ILE:O	2.19	0.42
1:A:391:PHE:O	1:A:392:LYS:C	2.57	0.42
1:A:406:LEU:HD23	1:A:406:LEU:N	2.32	0.42
1:A:466:MET:HE3	1:A:466:MET:HB2	1.90	0.42
1:A:573:SER:HA	1:A:578:MET:HE3	2.02	0.42
3:A:678:HOH:O	1:B:266:GLY:CA	2.66	0.42
1:B:14:ILE:HD13	1:B:96:TRP:HZ2	1.85	0.42
1:B:418:ILE:HD11	1:B:462:TYR:HE1	1.83	0.42
1:B:485:ILE:HG13	1:B:581:ASN:HD22	1.83	0.42
1:B:577:GLY:HA2	1:B:649:ILE:O	2.20	0.42
1:C:233:PHE:O	1:C:236:LEU:HB3	2.20	0.42
1:D:39:PRO:HB2	1:D:53:VAL:CG1	2.50	0.42
1:D:177:ARG:HH11	1:D:179:GLN:HG3	1.83	0.42
1:E:256:PHE:C	1:E:256:PHE:HD1	2.20	0.42
1:E:295:ARG:NE	1:E:339:TYR:CE1	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:ILE:HD11	1:E:390:ILE:HG22	2.00	0.42
1:E:385:LYS:HE2	3:E:750:HOH:O	2.20	0.42
1:E:610:GLY:HA2	1:E:614:GLU:HB2	2.01	0.42
1:F:222:TRP:CH2	1:F:226:GLN:NE2	2.88	0.42
1:B:489:ASN:CB	1:B:491:ILE:HD11	2.42	0.42
1:B:553:LEU:O	1:B:554:ASP:CB	2.58	0.42
1:C:185:GLY:CA	1:C:375:THR:HG22	2.49	0.42
1:D:72:TYR:HD2	1:D:79:GLN:HB3	1.83	0.42
1:D:226:GLN:O	1:D:227:LEU:C	2.56	0.42
1:D:237:SER:HA	1:D:574:LYS:CE	2.47	0.42
1:D:295:ARG:NE	1:D:339:TYR:CE1	2.88	0.42
1:D:553:LEU:CD2	1:D:555:LEU:HG	2.50	0.42
1:D:591:LYS:CA	1:D:594:GLU:HB2	2.50	0.42
1:E:148:SER:HB2	1:E:259:LEU:O	2.19	0.42
1:F:60:LEU:HD22	1:F:106:PHE:HE1	1.85	0.42
1:F:139:GLN:NE2	1:F:432:SER:H	2.17	0.42
1:F:364:PRO:HB2	1:F:365:PRO:CD	2.50	0.42
1:F:582:LEU:CD2	1:F:584:VAL:HG23	2.49	0.42
1:A:197:TRP:NE1	1:A:223:VAL:HG21	2.35	0.41
1:A:246:LEU:HD11	1:A:277:PHE:CE2	2.54	0.41
1:B:301:ASP:CB	1:D:295:ARG:NH2	2.82	0.41
1:B:399:PRO:HA	1:B:400:PRO:HD3	1.94	0.41
1:B:474:ARG:HH11	1:B:474:ARG:HD2	1.44	0.41
1:C:222:TRP:CH2	1:C:226:GLN:NE2	2.88	0.41
1:D:78:ARG:NH1	1:D:82:GLU:OE2	2.51	0.41
1:E:78:ARG:NH1	1:E:82:GLU:OE2	2.49	0.41
1:E:305:ILE:HB	1:E:313:ILE:HG13	2.02	0.41
1:F:151:ILE:HD13	1:F:151:ILE:HA	1.76	0.41
1:F:398:PHE:HB3	1:F:399:PRO:HD2	2.02	0.41
1:F:578:MET:HG3	1:F:580:PHE:CZ	2.55	0.41
1:F:610:GLY:HA2	1:F:614:GLU:HB2	2.02	0.41
1:F:624:TYR:HA	1:F:625:PRO:HA	1.82	0.41
1:A:222:TRP:CH2	1:A:623:GLY:CA	3.03	0.41
1:A:222:TRP:CD1	1:A:622:LEU:HD23	2.55	0.41
1:A:247:HIS:HB2	1:A:250:ARG:CG	2.50	0.41
1:A:353:ARG:NE	1:A:369:GLU:OE2	2.53	0.41
1:A:630:ILE:HD13	1:A:630:ILE:HG21	1.70	0.41
1:B:45:ILE:HB	1:B:98:CYS:HB2	2.02	0.41
1:B:287:HIS:C	1:B:289:LEU:N	2.73	0.41
1:B:555:LEU:C	1:B:557:ALA:N	2.73	0.41
1:C:86:LEU:O	1:C:86:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:GLY:O	1:C:593:THR:OG1	2.35	0.41
1:D:168:VAL:HG22	1:D:452:VAL:HA	2.02	0.41
1:D:222:TRP:CD1	1:D:622:LEU:HD23	2.55	0.41
1:D:248:TRP:CZ2	1:D:289:LEU:HD13	2.54	0.41
1:D:499:ARG:NE	1:D:628:ARG:O	2.53	0.41
1:D:541:GLU:O	1:D:545:ASN:HB2	2.20	0.41
1:E:56:LEU:HD21	1:E:110:MET:CE	2.50	0.41
1:E:175:LYS:O	1:E:176:ASN:HB2	2.20	0.41
1:E:248:TRP:CZ3	1:E:289:LEU:HD13	2.55	0.41
1:E:411:MET:CE	1:E:512:VAL:HB	2.51	0.41
1:E:636:ILE:HG23	1:E:642:ILE:HG21	2.00	0.41
1:F:143:HIS:CE1	1:F:151:ILE:CG2	3.04	0.41
1:F:295:ARG:NE	1:F:339:TYR:CE1	2.88	0.41
1:A:377:ASP:OD1	1:A:378:PRO:HD2	2.20	0.41
1:A:413:VAL:HA	1:A:466:MET:HB2	2.02	0.41
1:B:13:ASP:OD1	1:B:100:ARG:NE	2.51	0.41
1:B:66:LEU:HD22	1:B:111:ASN:HD22	1.85	0.41
1:B:157:ALA:HB3	1:B:448:ILE:HG12	2.02	0.41
1:B:184:PHE:CD1	1:B:184:PHE:C	2.94	0.41
1:C:9:GLN:O	1:C:10:LYS:C	2.59	0.41
1:C:573:SER:N	3:C:857:HOH:O	2.53	0.41
1:C:634:ARG:HH11	1:C:634:ARG:CG	2.24	0.41
1:D:127:LYS:HD3	3:D:869:HOH:O	2.20	0.41
1:D:195:VAL:HG22	1:D:196:THR:N	2.36	0.41
1:D:255:GLY:O	1:E:361:PHE:HZ	2.02	0.41
1:E:139:GLN:NE2	1:E:432:SER:H	2.18	0.41
1:E:195:VAL:CG2	1:E:196:THR:N	2.82	0.41
1:E:200:ASP:OD2	1:E:609:CYS:SG	2.79	0.41
1:E:322:GLU:O	1:E:325:GLY:N	2.53	0.41
1:F:200:ASP:OD2	1:F:609:CYS:SG	2.79	0.41
1:A:18:LEU:CD2	1:A:119:LEU:HD23	2.48	0.41
1:A:76:ASN:HD22	1:A:79:GLN:H	1.66	0.41
1:A:215:ARG:O	1:A:217:GLY:N	2.53	0.41
1:A:350:MET:O	1:A:350:MET:HG3	2.19	0.41
1:A:465:THR:O	1:A:466:MET:CB	2.68	0.41
1:A:639:VAL:O	1:A:639:VAL:HG22	2.20	0.41
1:B:322:GLU:C	1:B:324:LEU:N	2.72	0.41
1:B:594:GLU:CG	1:B:594:GLU:O	2.68	0.41
1:C:368:MET:CE	1:C:380:PHE:HA	2.22	0.41
1:D:178:GLU:O	1:D:178:GLU:HG3	2.19	0.41
1:D:185:GLY:HA2	1:D:375:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:LEU:HD11	1:D:277:PHE:HE2	1.85	0.41
1:D:300:ILE:HD13	1:D:390:ILE:O	2.20	0.41
1:D:305:ILE:HB	1:D:313:ILE:HG13	2.03	0.41
1:E:278:GLU:H	1:E:354:GLN:NE2	2.16	0.41
1:E:317:GLN:CB	1:E:318:PRO:CD	2.96	0.41
1:E:456:ASN:ND2	1:E:457:HIS:N	2.43	0.41
1:F:37:PHE:CD2	1:F:101:SER:HB3	2.55	0.41
1:F:135:PRO:HB3	1:F:536:PHE:CD1	2.56	0.41
1:F:533:MET:HB3	1:F:534:PRO:CD	2.49	0.41
1:A:95:GLU:CG	1:A:96:TRP:N	2.82	0.41
1:A:291:ILE:HD12	1:A:291:ILE:HG21	1.53	0.41
1:A:295:ARG:CZ	1:A:339:TYR:CE1	3.04	0.41
1:A:305:ILE:HG22	1:A:306:THR:N	2.35	0.41
1:A:338:GLN:NE2	1:E:316:ARG:HH21	2.18	0.41
1:A:465:THR:HG23	1:A:518:THR:OG1	2.20	0.41
1:B:82:GLU:O	1:B:83:ALA:C	2.59	0.41
1:B:258:PRO:CG	1:B:259:LEU:N	2.82	0.41
1:B:432:SER:O	1:B:434:ILE:N	2.54	0.41
1:B:503:ILE:HG21	1:B:503:ILE:HD13	1.40	0.41
1:B:591:LYS:HA	1:B:594:GLU:HB2	2.03	0.41
1:B:634:ARG:HH11	1:B:634:ARG:CG	2.24	0.41
1:C:66:LEU:HD23	1:C:67:GLU:H	1.85	0.41
1:C:305:ILE:CG1	1:C:315:ILE:HG21	2.48	0.41
1:C:373:THR:O	1:C:373:THR:HG23	2.21	0.41
1:C:424:THR:HA	1:C:457:HIS:HA	2.01	0.41
1:C:499:ARG:NE	1:C:628:ARG:O	2.54	0.41
1:C:591:LYS:CA	1:C:594:GLU:HB2	2.50	0.41
1:D:185:GLY:CA	1:D:375:THR:CG2	2.94	0.41
1:D:271:ARG:NH2	1:D:377:ASP:OD1	2.53	0.41
1:D:303:GLY:O	1:D:315:ILE:HG12	2.20	0.41
1:D:624:TYR:HA	1:D:625:PRO:HA	1.83	0.41
1:E:469:ASN:HD22	1:E:469:ASN:HA	1.67	0.41
1:E:591:LYS:O	1:E:594:GLU:HB2	2.20	0.41
1:F:353:ARG:NE	1:F:369:GLU:OE2	2.54	0.41
1:F:494:THR:O	1:F:495:LEU:C	2.58	0.41
1:A:14:ILE:HG23	1:A:18:LEU:HD11	2.02	0.41
1:A:43:THR:O	1:A:43:THR:CG2	2.67	0.41
1:B:398:PHE:HB3	1:B:399:PRO:CD	2.46	0.41
1:B:433:LEU:HG	1:B:450:ALA:HB2	2.01	0.41
1:D:133:VAL:HG22	1:D:558:TYR:HB2	2.03	0.41
1:D:589:GLY:O	1:D:593:THR:OG1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:633:GLU:C	1:D:635:VAL:N	2.74	0.41
1:E:16:HIS:HB3	1:E:30:LEU:CD1	2.49	0.41
1:E:313:ILE:HD12	1:E:314:ASP:O	2.21	0.41
1:A:37:PHE:HE2	1:A:97:TYR:HH	1.64	0.41
1:A:251:ILE:HD11	3:A:700:HOH:O	2.20	0.41
1:A:281:ASP:CG	1:A:358:HIS:HA	2.40	0.41
1:A:295:ARG:HH22	1:E:301:ASP:CB	2.34	0.41
1:A:422:LEU:HD22	1:A:570:LEU:CG	2.50	0.41
1:C:413:VAL:HG12	1:C:643:LYS:CG	2.51	0.41
1:D:106:PHE:O	1:D:107:ARG:C	2.59	0.41
1:D:248:TRP:CZ3	1:D:289:LEU:HD13	2.54	0.41
1:D:322:GLU:O	1:D:325:GLY:N	2.54	0.41
1:D:533:MET:CE	1:D:533:MET:N	2.81	0.41
1:E:233:PHE:O	1:E:236:LEU:HB3	2.20	0.41
1:F:154:ALA:HB2	1:F:433:LEU:HD13	2.03	0.41
1:F:248:TRP:CZ2	1:F:289:LEU:HD13	2.55	0.41
1:F:313:ILE:HD12	1:F:314:ASP:O	2.20	0.41
1:F:345:ASN:O	1:F:348:HIS:HB2	2.21	0.41
1:F:423:ILE:HA	1:F:650:VAL:O	2.19	0.41
1:A:351:LEU:HD23	1:A:351:LEU:HA	1.58	0.41
1:A:399:PRO:HA	1:A:400:PRO:HD3	1.78	0.41
1:A:564:ILE:CB	1:A:565:PRO:CD	2.99	0.41
1:A:629:ARG:HH11	1:A:629:ARG:CG	2.31	0.41
1:A:632:ASP:CG	1:A:634:ARG:HB2	2.40	0.41
1:B:120:TYR:CE2	1:B:134:LEU:HD13	2.52	0.41
1:B:353:ARG:HH11	1:B:353:ARG:HD2	1.16	0.41
1:B:636:ILE:HG23	1:B:642:ILE:HG21	2.02	0.41
1:C:71:TRP:CZ3	1:C:365:PRO:CG	3.04	0.41
1:C:357:PRO:HB2	1:C:358:HIS:CE1	2.56	0.41
1:C:403:HIS:C	1:C:405:ASN:N	2.73	0.41
1:C:610:GLY:HA2	1:C:614:GLU:HB2	2.03	0.41
1:E:158:LYS:NZ	1:E:439:SER:HB2	2.35	0.41
1:E:345:ASN:O	1:E:348:HIS:HB2	2.21	0.41
1:E:494:THR:O	1:E:495:LEU:C	2.58	0.41
1:F:148:SER:HB2	1:F:259:LEU:O	2.20	0.41
1:A:100:ARG:HH11	1:A:100:ARG:HD3	1.69	0.41
1:A:403:HIS:O	1:A:405:ASN:N	2.53	0.41
1:A:483:CYS:CB	3:A:763:HOH:O	2.69	0.41
1:A:536:PHE:O	1:A:540:LYS:N	2.54	0.41
1:B:9:GLN:O	1:B:10:LYS:O	2.38	0.41
1:B:14:ILE:HD11	1:B:96:TRP:HH2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LYS:O	1:B:34:ALA:HB3	2.21	0.41
1:B:83:ALA:HA	1:B:114:GLU:HB3	2.02	0.41
1:B:222:TRP:CG	1:B:622:LEU:HD23	2.55	0.41
1:B:300:ILE:CD1	1:B:390:ILE:HG22	2.47	0.41
1:B:403:HIS:C	1:B:405:ASN:H	2.24	0.41
1:C:158:LYS:HD3	1:C:446:VAL:HG12	2.03	0.41
1:C:200:ASP:OD2	1:C:609:CYS:SG	2.79	0.41
1:C:300:ILE:HD13	1:C:390:ILE:O	2.19	0.41
1:D:16:HIS:HB3	1:D:30:LEU:CD1	2.51	0.41
1:D:185:GLY:CA	1:D:375:THR:HG22	2.51	0.41
1:D:610:GLY:HA2	1:D:614:GLU:HB2	2.03	0.41
1:E:8:ALA:O	1:E:547:VAL:HG21	2.20	0.41
1:E:197:TRP:CE3	1:E:197:TRP:O	2.73	0.41
1:E:222:TRP:CH2	1:E:226:GLN:NE2	2.88	0.41
1:E:248:TRP:CZ2	1:E:289:LEU:HD13	2.54	0.41
1:E:410:GLY:O	1:E:411:MET:C	2.59	0.41
1:E:493:LEU:HB2	1:E:497:GLU:HB2	2.03	0.41
1:E:509:PHE:CZ	1:E:593:THR:CG2	3.04	0.41
1:E:522:SER:C	1:E:524:LYS:N	2.74	0.41
1:E:620:ARG:C	1:E:621:PRO:O	2.57	0.41
1:F:16:HIS:HB3	1:F:30:LEU:CD1	2.50	0.41
1:F:300:ILE:HD13	1:F:390:ILE:O	2.20	0.41
1:F:303:GLY:O	1:F:315:ILE:HG12	2.21	0.41
1:F:322:GLU:O	1:F:325:GLY:N	2.54	0.41
1:A:284:ALA:HB1	1:A:285:HIS:H	1.70	0.41
1:A:287:HIS:O	1:A:290:GLU:HB2	2.21	0.41
1:A:367:VAL:O	1:A:373:THR:CG2	2.68	0.41
1:A:380:PHE:CD1	1:A:380:PHE:C	2.94	0.41
1:A:468:ASN:ND2	1:A:514:SER:HA	2.31	0.41
1:A:591:LYS:HB2	1:A:591:LYS:NZ	2.36	0.41
1:A:630:ILE:CD1	1:A:636:ILE:HD11	2.51	0.41
1:B:45:ILE:HG12	1:B:45:ILE:H	1.17	0.41
1:B:46:TYR:CZ	1:B:53:VAL:HG21	2.56	0.41
1:B:285:HIS:HB2	1:B:288:ASP:OD2	2.20	0.41
1:B:301:ASP:HB3	1:D:295:ARG:NH2	2.37	0.41
1:B:400:PRO:HB3	1:B:629:ARG:O	2.21	0.41
1:B:493:LEU:HA	1:B:497:GLU:OE1	2.21	0.41
1:B:528:VAL:O	1:B:528:VAL:HG23	2.20	0.41
1:B:614:GLU:H	1:B:614:GLU:HG3	1.35	0.41
1:B:620:ARG:HG3	1:B:624:TYR:CD1	2.54	0.41
1:C:252:ILE:HB	1:C:275:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:CD1	1:D:57:MET:HG3	2.49	0.41
1:D:246:LEU:HD11	1:D:277:PHE:CE2	2.56	0.41
1:D:357:PRO:HB2	1:D:358:HIS:CE1	2.55	0.41
1:D:533:MET:HB3	1:D:534:PRO:CD	2.50	0.41
1:E:86:LEU:O	1:E:86:LEU:HD23	2.21	0.41
1:F:5:THR:CG2	1:F:10:LYS:HE3	2.51	0.41
1:F:72:TYR:CD1	1:F:72:TYR:C	2.95	0.41
1:F:443:ILE:HD12	1:F:443:ILE:HA	1.97	0.41
1:A:59:GLU:OE1	1:A:64:ARG:CD	2.67	0.40
1:A:236:LEU:C	1:A:238:ASN:N	2.74	0.40
1:A:393:LYS:HB3	1:A:393:LYS:HE3	1.69	0.40
1:A:491:ILE:HG22	1:A:491:ILE:O	2.21	0.40
1:B:86:LEU:HD22	1:B:90:LEU:CD2	2.50	0.40
1:B:222:TRP:CH2	1:B:623:GLY:HA2	2.56	0.40
1:B:533:MET:HB3	1:B:534:PRO:HG2	2.02	0.40
1:C:133:VAL:HG21	1:C:555:LEU:HD23	2.02	0.40
1:C:639:VAL:HG23	1:C:641:ASN:HD22	1.84	0.40
1:D:9:GLN:O	1:D:10:LYS:C	2.59	0.40
1:D:48:ASP:CB	1:D:92:GLN:HE21	2.34	0.40
1:E:256:PHE:HD1	1:E:256:PHE:O	2.04	0.40
1:F:192:ILE:HD13	1:F:192:ILE:HA	1.89	0.40
1:F:197:TRP:CE3	1:F:197:TRP:O	2.74	0.40
1:F:373:THR:O	1:F:373:THR:HG23	2.22	0.40
1:F:456:ASN:ND2	1:F:457:HIS:N	2.42	0.40
1:F:499:ARG:NE	1:F:628:ARG:O	2.54	0.40
1:A:626:LEU:N	1:A:626:LEU:HD23	2.35	0.40
1:B:316:ARG:HH21	1:D:338:GLN:NE2	2.17	0.40
1:B:366:GLY:O	1:B:367:VAL:C	2.58	0.40
1:B:498:ALA:O	1:B:499:ARG:C	2.60	0.40
1:B:630:ILE:HG23	1:B:636:ILE:HD13	2.03	0.40
1:C:16:HIS:HB3	1:C:30:LEU:CD1	2.50	0.40
1:C:154:ALA:HB2	1:C:433:LEU:HD13	2.04	0.40
1:C:205:TRP:NE1	1:C:213:LEU:HD13	2.36	0.40
1:C:322:GLU:O	1:C:325:GLY:N	2.54	0.40
1:C:641:ASN:HD22	1:C:641:ASN:C	2.23	0.40
1:D:487:ASP:OD1	1:D:487:ASP:O	2.40	0.40
1:E:106:PHE:O	1:E:107:ARG:C	2.59	0.40
1:E:121:VAL:HG23	1:E:199:MET:HG2	2.04	0.40
1:E:237:SER:OG	1:E:578:MET:HE1	2.20	0.40
1:E:631:PRO:HD2	3:E:818:HOH:O	2.21	0.40
1:F:134:LEU:HA	1:F:135:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:ILE:HG22	1:F:141:THR:HG23	2.02	0.40
1:F:385:LYS:HE2	3:F:750:HOH:O	2.21	0.40
1:B:11:GLN:O	1:B:12:GLN:C	2.57	0.40
1:B:17:LEU:HD23	1:B:17:LEU:HA	1.86	0.40
1:B:30:LEU:HD23	1:B:30:LEU:HA	1.74	0.40
1:B:48:ASP:CA	1:B:92:GLN:HE21	2.33	0.40
1:B:582:LEU:HD23	1:B:582:LEU:C	2.42	0.40
1:C:5:THR:CG2	1:C:10:LYS:HE3	2.51	0.40
1:C:41:GLY:O	1:C:42:ASP:HB2	2.22	0.40
1:C:106:PHE:O	1:C:107:ARG:C	2.59	0.40
1:C:633:GLU:C	1:C:635:VAL:N	2.74	0.40
1:D:76:ASN:ND2	1:D:79:GLN:HG3	2.36	0.40
1:D:278:GLU:H	1:D:354:GLN:NE2	2.20	0.40
1:D:408:PHE:CZ	1:D:411:MET:SD	3.15	0.40
1:E:39:PRO:CB	1:E:53:VAL:CG1	2.99	0.40
1:E:143:HIS:CE1	1:E:151:ILE:CG2	3.04	0.40
1:E:269:PRO:CB	1:E:363:LEU:HD23	2.40	0.40
1:E:634:ARG:HH11	1:E:634:ARG:CG	2.24	0.40
1:A:395:THR:HG21	1:A:500:TRP:CZ3	2.56	0.40
1:B:375:THR:HB	3:B:747:HOH:O	2.21	0.40
1:B:461:THR:HG1	1:B:462:TYR:N	2.16	0.40
1:B:594:GLU:O	1:B:594:GLU:HG2	2.22	0.40
1:D:60:LEU:HD22	1:D:106:PHE:HE1	1.87	0.40
1:D:84:LEU:HD12	1:D:84:LEU:HA	1.93	0.40
1:D:211:TYR:CD1	1:D:211:TYR:N	2.89	0.40
1:D:485:ILE:HG12	1:D:581:ASN:ND2	2.36	0.40
1:E:30:LEU:HD23	1:E:30:LEU:HA	1.94	0.40
1:E:324:LEU:HD23	1:E:324:LEU:HA	1.80	0.40
1:E:578:MET:HE3	1:E:580:PHE:HZ	1.85	0.40
1:E:588:ASP:OD1	1:E:588:ASP:O	2.39	0.40
1:F:5:THR:CG2	1:F:6:GLY:H	2.20	0.40
1:F:8:ALA:CB	1:F:553:LEU:HD12	2.51	0.40
1:F:248:TRP:CZ3	1:F:289:LEU:HD13	2.56	0.40
1:A:60:LEU:HA	1:A:65:LEU:HD22	2.04	0.40
1:A:124:ILE:HG22	1:A:611:VAL:CG1	2.51	0.40
1:A:195:VAL:CG2	1:A:196:THR:N	2.82	0.40
1:A:307:ASP:OD1	1:A:310:GLY:N	2.54	0.40
1:A:471:ASP:O	1:A:514:SER:HB2	2.21	0.40
1:A:560:ARG:CB	3:A:819:HOH:O	2.70	0.40
1:A:620:ARG:C	1:A:621:PRO:O	2.60	0.40
1:B:14:ILE:HD11	1:B:96:TRP:CH2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:O	1:B:57:MET:C	2.60	0.40
1:B:222:TRP:CG	1:B:622:LEU:CD2	3.04	0.40
1:B:224:HIS:O	1:B:225:HIS:C	2.59	0.40
1:B:330:SER:HB2	1:B:342:SER:HG	1.83	0.40
1:C:385:LYS:HE2	3:C:750:HOH:O	2.21	0.40
1:C:399:PRO:HA	1:C:400:PRO:HD3	1.91	0.40
1:D:176:ASN:HD22	1:D:176:ASN:HA	1.79	0.40
1:D:205:TRP:NE1	1:D:213:LEU:HD13	2.37	0.40
1:D:230:ARG:NH2	1:D:503:ILE:HD12	2.37	0.40
1:D:377:ASP:HA	1:D:378:PRO:HD3	1.88	0.40
1:E:427:ASP:HB3	1:E:567:ARG:HH12	1.86	0.40
1:F:478:PHE:CZ	1:F:519:ILE:CD1	3.05	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:B:309:ASP:OD1	1:C:49:HIS:CD2[2_647]	1.85	0.35
1:C:594:GLU:OE1	1:F:471:ASP:CB[2_657]	2.13	0.07
1:C:474:ARG:NH2	1:D:41:GLY:O[2_656]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	626/657 (95%)	501 (80%)	97 (16%)	28 (4%)	2	18
1	B	626/657 (95%)	506 (81%)	89 (14%)	31 (5%)	2	16
1	C	626/657 (95%)	517 (83%)	95 (15%)	14 (2%)	6	35
1	D	626/657 (95%)	516 (82%)	91 (14%)	19 (3%)	4	28
1	E	626/657 (95%)	512 (82%)	95 (15%)	19 (3%)	4	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	626/657 (95%)	503 (80%)	102 (16%)	21 (3%)	3	24
All	All	3756/3942 (95%)	3055 (81%)	569 (15%)	132 (4%)	3	24

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	147	ASN
1	A	176	ASN
1	A	441	GLU
1	A	471	ASP
1	B	176	ASN
1	B	472	GLY
1	B	514	SER
1	B	556	SER
1	C	176	ASN
1	D	176	ASN
1	E	176	ASN
1	F	176	ASN
1	A	6	GLY
1	A	7	ASN
1	A	90	LEU
1	A	104	ALA
1	A	242	PRO
1	A	472	GLY
1	A	488	ASN
1	A	555	LEU
1	A	557	ALA
1	A	560	ARG
1	A	589	GLY
1	A	611	VAL
1	B	7	ASN
1	B	147	ASN
1	B	427	ASP
1	B	488	ASN
1	B	489	ASN
1	B	569	LEU
1	B	594	GLU
1	B	611	VAL
1	C	7	ASN
1	C	42	ASP
1	D	7	ASN

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Mol	Chain	Res	Type
1	D	42	ASP
1	D	557	ALA
1	E	7	ASN
1	E	44	SER
1	E	492	THR
1	F	7	ASN
1	F	42	ASP
1	F	557	ALA
1	A	54	GLU
1	A	427	ASP
1	A	569	LEU
1	A	634	ARG
1	B	8	ALA
1	B	42	ASP
1	B	44	SER
1	B	90	LEU
1	B	523	SER
1	B	593	THR
1	B	595	GLY
1	C	44	SER
1	C	90	LEU
1	C	104	ALA
1	C	320	GLY
1	C	569	LEU
1	C	595	GLY
1	D	44	SER
1	D	90	LEU
1	D	104	ALA
1	D	320	GLY
1	D	489	ASN
1	D	514	SER
1	D	569	LEU
1	D	595	GLY
1	E	42	ASP
1	E	90	LEU
1	E	104	ALA
1	E	320	GLY
1	E	489	ASN
1	E	557	ALA
1	E	569	LEU
1	F	44	SER
1	F	90	LEU

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Mol	Chain	Res	Type
1	F	104	ALA
1	F	320	GLY
1	F	489	ASN
1	F	569	LEU
1	F	595	GLY
1	A	24	PRO
1	A	474	ARG
1	A	523	SER
1	A	556	SER
1	A	595	GLY
1	B	101	SER
1	B	411	MET
1	B	433	LEU
1	B	492	THR
1	B	496	ASP
1	B	516	PRO
1	B	589	GLY
1	B	592	ASP
1	C	496	ASP
1	D	427	ASP
1	D	496	ASP
1	D	561	SER
1	E	496	ASP
1	E	595	GLY
1	F	473	GLU
1	F	492	THR
1	F	496	ASP
1	A	473	GLU
1	B	43	THR
1	B	320	GLY
1	C	242	PRO
1	C	427	ASP
1	D	242	PRO
1	D	354	GLN
1	E	242	PRO
1	E	427	ASP
1	E	554	ASP
1	F	242	PRO
1	F	427	ASP
1	A	489	ASN
1	B	192	ILE
1	C	593	THR

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Mol	Chain	Res	Type
1	C	594	GLU
1	D	593	THR
1	E	516	PRO
1	E	592	ASP
1	F	592	ASP
1	F	593	THR
1	F	594	GLU
1	F	472	GLY
1	F	563	GLY
1	B	242	PRO
1	D	28	PRO
1	E	611	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	564/580 (97%)	438 (78%)	126 (22%)	1	4
1	B	564/580 (97%)	450 (80%)	114 (20%)	1	6
1	C	564/580 (97%)	494 (88%)	70 (12%)	4	21
1	D	564/580 (97%)	489 (87%)	75 (13%)	4	18
1	E	564/580 (97%)	498 (88%)	66 (12%)	5	23
1	F	564/580 (97%)	498 (88%)	66 (12%)	5	23
All	All	3384/3480 (97%)	2867 (85%)	517 (15%)	2	13

All (517) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	12	GLN
1	A	15	ASN
1	A	23	GLU
1	A	25	THR
1	A	31	LYS

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Mol	Chain	Res	Type
1	A	32	ASP
1	A	45	ILE
1	A	53	VAL
1	A	56	LEU
1	A	63	HIS
1	A	64	ARG
1	A	66	LEU
1	A	72	TYR
1	A	77	THR
1	A	85	MET
1	A	90	LEU
1	A	108	GLU
1	A	110	MET
1	A	112	GLU
1	A	127	LYS
1	A	139	GLN
1	A	151	ILE
1	A	156	SER
1	A	159	MET
1	A	163	PRO
1	A	165	THR
1	A	175	LYS
1	A	176	ASN
1	A	179	GLN
1	A	180	ARG
1	A	195	VAL
1	A	216	LYS
1	A	219	LEU
1	A	221	PHE
1	A	235	ARG
1	A	242	PRO
1	A	243	VAL
1	A	244	ASP
1	A	252	ILE
1	A	256	PHE
1	A	258	PRO
1	A	259	LEU
1	A	263	LYS
1	A	270	VAL
1	A	279	ASP
1	A	280	VAL
1	A	281	ASP

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Mol	Chain	Res	Type
1	A	291	ILE
1	A	297	HIS
1	A	306	THR
1	A	308	SER
1	A	313	ILE
1	A	315	ILE
1	A	316	ARG
1	A	322	GLU
1	A	329	GLU
1	A	330	SER
1	A	334	SER
1	A	335	SER
1	A	343	LEU
1	A	365	PRO
1	A	373	THR
1	A	375	THR
1	A	376	ARG
1	A	378	PRO
1	A	382	ARG
1	A	395	THR
1	A	397	SER
1	A	407	GLU
1	A	409	SER
1	A	411	MET
1	A	412	VAL
1	A	416	VAL
1	A	418	ILE
1	A	423	ILE
1	A	427	ASP
1	A	438	ASP
1	A	441	GLU
1	A	442	ASN
1	A	444	GLU
1	A	445	ASP
1	A	446	VAL
1	A	453	HIS
1	A	456	ASN
1	A	461	THR
1	A	465	THR
1	A	466	MET
1	A	467	SER
1	A	475	LEU

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Mol	Chain	Res	Type
1	A	477	THR
1	A	492	THR
1	A	493	LEU
1	A	499	ARG
1	A	501	PHE
1	A	513	PRO
1	A	517	GLU
1	A	518	THR
1	A	519	ILE
1	A	523	SER
1	A	532	ASP
1	A	533	MET
1	A	535	SER
1	A	544	ASP
1	A	547	VAL
1	A	556	SER
1	A	559	GLU
1	A	560	ARG
1	A	567	ARG
1	A	574	LYS
1	A	578	MET
1	A	579	GLU
1	A	586	VAL
1	A	587	THR
1	A	596	HIS
1	A	606	HIS
1	A	609	CYS
1	A	620	ARG
1	A	626	LEU
1	A	634	ARG
1	A	636	ILE
1	A	639	VAL
1	A	641	ASN
1	A	643	LYS
1	A	646	VAL
1	A	650	VAL
1	B	11	GLN
1	B	18	LEU
1	B	23	GLU
1	B	29	ASP
1	B	31	LYS
1	B	40	LEU

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Mol	Chain	Res	Type
1	B	45	ILE
1	B	53	VAL
1	B	56	LEU
1	B	63	HIS
1	B	64	ARG
1	B	66	LEU
1	B	69	ARG
1	B	72	TYR
1	B	77	THR
1	B	85	MET
1	B	86	LEU
1	B	90	LEU
1	B	108	GLU
1	B	151	ILE
1	B	156	SER
1	B	159	MET
1	B	165	THR
1	B	175	LYS
1	B	176	ASN
1	B	179	GLN
1	B	208	SER
1	B	211	TYR
1	B	213	LEU
1	B	219	LEU
1	B	221	PHE
1	B	233	PHE
1	B	242	PRO
1	B	244	ASP
1	B	251	ILE
1	B	253	ARG
1	B	256	PHE
1	B	258	PRO
1	B	259	LEU
1	B	261	SER
1	B	270	VAL
1	B	275	ILE
1	B	279	ASP
1	B	280	VAL
1	B	281	ASP
1	B	291	ILE
1	B	297	HIS
1	B	306	THR

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Mol	Chain	Res	Type
1	B	309	ASP
1	B	313	ILE
1	B	316	ARG
1	B	322	GLU
1	B	330	SER
1	B	343	LEU
1	B	364	PRO
1	B	365	PRO
1	B	369	GLU
1	B	372	GLU
1	B	373	THR
1	B	375	THR
1	B	376	ARG
1	B	382	ARG
1	B	395	THR
1	B	405	ASN
1	B	409	SER
1	B	411	MET
1	B	412	VAL
1	B	416	VAL
1	B	427	ASP
1	B	437	VAL
1	B	438	ASP
1	B	453	HIS
1	B	454	ARG
1	B	456	ASN
1	B	463	LYS
1	B	467	SER
1	B	469	ASN
1	B	473	GLU
1	B	475	LEU
1	B	487	ASP
1	B	491	ILE
1	B	493	LEU
1	B	499	ARG
1	B	501	PHE
1	B	510	GLN
1	B	511	LYS
1	B	514	SER
1	B	516	PRO
1	B	519	ILE
1	B	523	SER

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Mol	Chain	Res	Type
1	B	532	ASP
1	B	533	MET
1	B	535	SER
1	B	544	ASP
1	B	548	ASN
1	B	553	LEU
1	B	554	ASP
1	B	555	LEU
1	B	556	SER
1	B	559	GLU
1	B	560	ARG
1	B	561	SER
1	B	567	ARG
1	B	570	LEU
1	B	576	GLU
1	B	578	MET
1	B	586	VAL
1	B	596	HIS
1	B	606	HIS
1	B	609	CYS
1	B	620	ARG
1	B	634	ARG
1	B	641	ASN
1	B	643	LYS
1	C	23	GLU
1	C	63	HIS
1	C	64	ARG
1	C	66	LEU
1	C	72	TYR
1	C	77	THR
1	C	85	MET
1	C	92	GLN
1	C	108	GLU
1	C	153	LYS
1	C	175	LYS
1	C	176	ASN
1	C	179	GLN
1	C	195	VAL
1	C	219	LEU
1	C	233	PHE
1	C	244	ASP
1	C	249	ASP

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Mol	Chain	Res	Type
1	C	256	PHE
1	C	259	LEU
1	C	270	VAL
1	C	273	ASP
1	C	279	ASP
1	C	280	VAL
1	C	281	ASP
1	C	297	HIS
1	C	306	THR
1	C	313	ILE
1	C	316	ARG
1	C	322	GLU
1	C	330	SER
1	C	343	LEU
1	C	351	LEU
1	C	367	VAL
1	C	372	GLU
1	C	373	THR
1	C	376	ARG
1	C	382	ARG
1	C	395	THR
1	C	405	ASN
1	C	411	MET
1	C	412	VAL
1	C	416	VAL
1	C	427	ASP
1	C	430	GLN
1	C	438	ASP
1	C	453	HIS
1	C	454	ARG
1	C	456	ASN
1	C	461	THR
1	C	474	ARG
1	C	492	THR
1	C	493	LEU
1	C	499	ARG
1	C	501	PHE
1	C	519	ILE
1	C	532	ASP
1	C	533	MET
1	C	547	VAL
1	C	548	ASN

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Mol	Chain	Res	Type
1	C	555	LEU
1	C	567	ARG
1	C	586	VAL
1	C	596	HIS
1	C	606	HIS
1	C	609	CYS
1	C	620	ARG
1	C	634	ARG
1	C	641	ASN
1	C	643	LYS
1	D	29	ASP
1	D	56	LEU
1	D	63	HIS
1	D	64	ARG
1	D	66	LEU
1	D	72	TYR
1	D	77	THR
1	D	85	MET
1	D	92	GLN
1	D	108	GLU
1	D	153	LYS
1	D	175	LYS
1	D	176	ASN
1	D	179	GLN
1	D	219	LEU
1	D	233	PHE
1	D	242	PRO
1	D	244	ASP
1	D	249	ASP
1	D	256	PHE
1	D	259	LEU
1	D	270	VAL
1	D	273	ASP
1	D	279	ASP
1	D	280	VAL
1	D	281	ASP
1	D	297	HIS
1	D	306	THR
1	D	313	ILE
1	D	316	ARG
1	D	322	GLU
1	D	330	SER

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Mol	Chain	Res	Type
1	D	343	LEU
1	D	351	LEU
1	D	367	VAL
1	D	372	GLU
1	D	373	THR
1	D	376	ARG
1	D	382	ARG
1	D	395	THR
1	D	411	MET
1	D	413	VAL
1	D	416	VAL
1	D	419	ASP
1	D	427	ASP
1	D	430	GLN
1	D	438	ASP
1	D	445	ASP
1	D	449	ASN
1	D	453	HIS
1	D	454	ARG
1	D	456	ASN
1	D	461	THR
1	D	465	THR
1	D	470	ASN
1	D	493	LEU
1	D	499	ARG
1	D	501	PHE
1	D	519	ILE
1	D	523	SER
1	D	532	ASP
1	D	533	MET
1	D	545	ASN
1	D	553	LEU
1	D	554	ASP
1	D	558	TYR
1	D	567	ARG
1	D	586	VAL
1	D	596	HIS
1	D	606	HIS
1	D	609	CYS
1	D	620	ARG
1	D	634	ARG
1	D	641	ASN

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Mol	Chain	Res	Type
1	D	643	LYS
1	E	63	HIS
1	E	64	ARG
1	E	66	LEU
1	E	72	TYR
1	E	77	THR
1	E	85	MET
1	E	92	GLN
1	E	108	GLU
1	E	151	ILE
1	E	153	LYS
1	E	175	LYS
1	E	176	ASN
1	E	179	GLN
1	E	195	VAL
1	E	219	LEU
1	E	233	PHE
1	E	244	ASP
1	E	249	ASP
1	E	256	PHE
1	E	259	LEU
1	E	270	VAL
1	E	273	ASP
1	E	279	ASP
1	E	280	VAL
1	E	281	ASP
1	E	306	THR
1	E	313	ILE
1	E	316	ARG
1	E	322	GLU
1	E	330	SER
1	E	343	LEU
1	E	351	LEU
1	E	367	VAL
1	E	372	GLU
1	E	373	THR
1	E	376	ARG
1	E	382	ARG
1	E	395	THR
1	E	405	ASN
1	E	411	MET
1	E	412	VAL

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Mol	Chain	Res	Type
1	E	416	VAL
1	E	427	ASP
1	E	430	GLN
1	E	438	ASP
1	E	453	HIS
1	E	454	ARG
1	E	456	ASN
1	E	461	THR
1	E	493	LEU
1	E	499	ARG
1	E	501	PHE
1	E	519	ILE
1	E	523	SER
1	E	532	ASP
1	E	533	MET
1	E	559	GLU
1	E	567	ARG
1	E	586	VAL
1	E	596	HIS
1	E	606	HIS
1	E	609	CYS
1	E	620	ARG
1	E	634	ARG
1	E	641	ASN
1	E	643	LYS
1	F	63	HIS
1	F	64	ARG
1	F	66	LEU
1	F	72	TYR
1	F	77	THR
1	F	85	MET
1	F	92	GLN
1	F	108	GLU
1	F	153	LYS
1	F	175	LYS
1	F	176	ASN
1	F	179	GLN
1	F	195	VAL
1	F	219	LEU
1	F	233	PHE
1	F	244	ASP
1	F	249	ASP

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Mol	Chain	Res	Type
1	F	256	PHE
1	F	259	LEU
1	F	270	VAL
1	F	273	ASP
1	F	279	ASP
1	F	280	VAL
1	F	281	ASP
1	F	297	HIS
1	F	306	THR
1	F	313	ILE
1	F	316	ARG
1	F	322	GLU
1	F	330	SER
1	F	343	LEU
1	F	351	LEU
1	F	367	VAL
1	F	372	GLU
1	F	373	THR
1	F	376	ARG
1	F	382	ARG
1	F	395	THR
1	F	405	ASN
1	F	411	MET
1	F	412	VAL
1	F	416	VAL
1	F	427	ASP
1	F	430	GLN
1	F	438	ASP
1	F	453	HIS
1	F	454	ARG
1	F	456	ASN
1	F	461	THR
1	F	493	LEU
1	F	499	ARG
1	F	501	PHE
1	F	519	ILE
1	F	532	ASP
1	F	533	MET
1	F	547	VAL
1	F	558	TYR
1	F	567	ARG
1	F	586	VAL

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Mol	Chain	Res	Type
1	F	596	HIS
1	F	606	HIS
1	F	609	CYS
1	F	620	ARG
1	F	634	ARG
1	F	641	ASN
1	F	643	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (158) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	16	HIS
1	A	47	ASN
1	A	61	ASN
1	A	76	ASN
1	A	92	GLN
1	A	102	ASN
1	A	143	HIS
1	A	191	ASN
1	A	212	HIS
1	A	225	HIS
1	A	336	ASN
1	A	338	GLN
1	A	354	GLN
1	A	389	ASN
1	A	405	ASN
1	A	414	ASN
1	A	449	ASN
1	A	453	HIS
1	A	456	ASN
1	A	545	ASN
1	A	548	ASN
1	A	581	ASN
1	A	606	HIS
1	A	612	HIS
1	B	15	ASN
1	B	47	ASN
1	B	61	ASN
1	B	63	HIS
1	B	76	ASN
1	B	92	GLN

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Mol	Chain	Res	Type
1	B	102	ASN
1	B	143	HIS
1	B	147	ASN
1	B	176	ASN
1	B	191	ASN
1	B	225	HIS
1	B	302	HIS
1	B	311	HIS
1	B	338	GLN
1	B	354	GLN
1	B	389	ASN
1	B	403	HIS
1	B	405	ASN
1	B	414	ASN
1	B	435	ASN
1	B	442	ASN
1	B	453	HIS
1	B	456	ASN
1	B	457	HIS
1	B	470	ASN
1	B	488	ASN
1	B	548	ASN
1	B	581	ASN
1	B	606	HIS
1	B	612	HIS
1	C	11	GLN
1	C	15	ASN
1	C	61	ASN
1	C	63	HIS
1	C	76	ASN
1	C	92	GLN
1	C	102	ASN
1	C	143	HIS
1	C	147	ASN
1	C	176	ASN
1	C	191	ASN
1	C	336	ASN
1	C	338	GLN
1	C	354	GLN
1	C	389	ASN
1	C	405	ASN
1	C	414	ASN

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Mol	Chain	Res	Type
1	C	435	ASN
1	C	442	ASN
1	C	453	HIS
1	C	456	ASN
1	C	469	ASN
1	C	606	HIS
1	C	612	HIS
1	D	11	GLN
1	D	15	ASN
1	D	61	ASN
1	D	63	HIS
1	D	76	ASN
1	D	92	GLN
1	D	102	ASN
1	D	143	HIS
1	D	147	ASN
1	D	176	ASN
1	D	191	ASN
1	D	336	ASN
1	D	338	GLN
1	D	354	GLN
1	D	389	ASN
1	D	414	ASN
1	D	435	ASN
1	D	442	ASN
1	D	449	ASN
1	D	453	HIS
1	D	456	ASN
1	D	606	HIS
1	D	612	HIS
1	E	11	GLN
1	E	15	ASN
1	E	61	ASN
1	E	63	HIS
1	E	76	ASN
1	E	92	GLN
1	E	102	ASN
1	E	143	HIS
1	E	147	ASN
1	E	161	GLN
1	E	176	ASN
1	E	191	ASN

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Mol	Chain	Res	Type
1	E	336	ASN
1	E	338	GLN
1	E	354	GLN
1	E	389	ASN
1	E	394	HIS
1	E	405	ASN
1	E	414	ASN
1	E	435	ASN
1	E	442	ASN
1	E	449	ASN
1	E	453	HIS
1	E	456	ASN
1	E	468	ASN
1	E	469	ASN
1	E	548	ASN
1	E	606	HIS
1	E	612	HIS
1	F	7	ASN
1	F	11	GLN
1	F	15	ASN
1	F	61	ASN
1	F	63	HIS
1	F	76	ASN
1	F	92	GLN
1	F	102	ASN
1	F	143	HIS
1	F	147	ASN
1	F	161	GLN
1	F	176	ASN
1	F	191	ASN
1	F	336	ASN
1	F	338	GLN
1	F	354	GLN
1	F	389	ASN
1	F	405	ASN
1	F	414	ASN
1	F	435	ASN
1	F	442	ASN
1	F	449	ASN
1	F	453	HIS
1	F	456	ASN
1	F	606	HIS

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Mol	Chain	Res	Type
1	F	612	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.