



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:35 PM UTC

PDB ID : 3U9S / pdb_00003u9s
Title : Crystal structure of P. aeruginosa 3-methylcrotonyl-CoA carboxylase (MCC)
750 kD holoenzyme, CoA complex
Authors : Huang, C.S.; Tong, L.
Deposited on : 2011-10-19
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

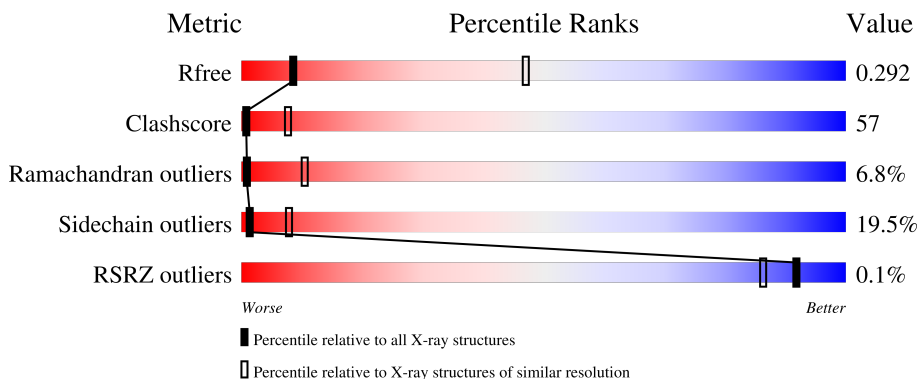
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	655	
1	C	655	
1	E	655	
1	G	655	
1	I	655	

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Mol	Chain	Length	Quality of chain
1	K	655	20%39%15%•24%
2	B	555	32%50%13%••
2	D	555	30%50%16%••
2	F	555	26%52%17%••
2	H	555	31%50%15%••
2	J	555	32%49%15%••
2	L	555	29%51%16%••

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 49939 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 Methylcrotonyl-CoA carboxylase, alpha-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	0	0	0
			4778	2978	892	886	22			
1	C	552	Total	C	N	O	S	0	0	0
			4280	2666	809	787	18			
1	E	552	Total	C	N	O	S	0	0	0
			4280	2666	809	787	18			
1	G	552	Total	C	N	O	S	0	0	0
			4280	2666	809	787	18			
1	I	498	Total	C	N	O	S	0	0	0
			3853	2399	731	707	16			
1	K	497	Total	C	N	O	S	0	0	0
			3844	2393	729	706	16			

- Molecule 2 is a protein called Methylcrotonyl-CoA carboxylase, beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	D	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	F	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	H	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	J	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	L	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	MET	-	expression tag	UNP Q9I297

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	GLY	-	expression tag	UNP Q9I297
B	10	SER	-	expression tag	UNP Q9I297
B	11	SER	-	expression tag	UNP Q9I297
B	12	HIS	-	expression tag	UNP Q9I297
B	13	HIS	-	expression tag	UNP Q9I297
B	14	HIS	-	expression tag	UNP Q9I297
B	15	HIS	-	expression tag	UNP Q9I297
B	16	HIS	-	expression tag	UNP Q9I297
B	17	HIS	-	expression tag	UNP Q9I297
B	18	SER	-	expression tag	UNP Q9I297
B	19	SER	-	expression tag	UNP Q9I297
B	20	GLY	-	expression tag	UNP Q9I297
B	21	LEU	-	expression tag	UNP Q9I297
B	22	VAL	-	expression tag	UNP Q9I297
B	23	PRO	-	expression tag	UNP Q9I297
B	24	ARG	-	expression tag	UNP Q9I297
B	25	GLY	-	expression tag	UNP Q9I297
B	26	SER	-	expression tag	UNP Q9I297
B	27	HIS	-	expression tag	UNP Q9I297
D	8	MET	-	expression tag	UNP Q9I297
D	9	GLY	-	expression tag	UNP Q9I297
D	10	SER	-	expression tag	UNP Q9I297
D	11	SER	-	expression tag	UNP Q9I297
D	12	HIS	-	expression tag	UNP Q9I297
D	13	HIS	-	expression tag	UNP Q9I297
D	14	HIS	-	expression tag	UNP Q9I297
D	15	HIS	-	expression tag	UNP Q9I297
D	16	HIS	-	expression tag	UNP Q9I297
D	17	HIS	-	expression tag	UNP Q9I297
D	18	SER	-	expression tag	UNP Q9I297
D	19	SER	-	expression tag	UNP Q9I297
D	20	GLY	-	expression tag	UNP Q9I297
D	21	LEU	-	expression tag	UNP Q9I297
D	22	VAL	-	expression tag	UNP Q9I297
D	23	PRO	-	expression tag	UNP Q9I297
D	24	ARG	-	expression tag	UNP Q9I297
D	25	GLY	-	expression tag	UNP Q9I297
D	26	SER	-	expression tag	UNP Q9I297
D	27	HIS	-	expression tag	UNP Q9I297
F	8	MET	-	expression tag	UNP Q9I297
F	9	GLY	-	expression tag	UNP Q9I297
F	10	SER	-	expression tag	UNP Q9I297

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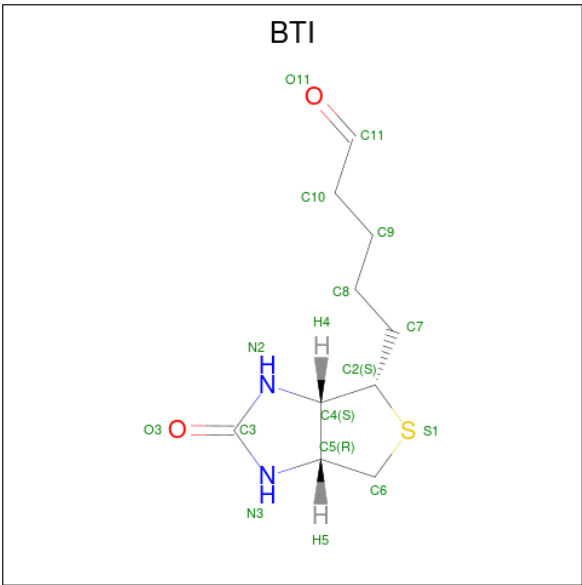
Chain	Residue	Modelled	Actual	Comment	Reference
F	11	SER	-	expression tag	UNP Q9I297
F	12	HIS	-	expression tag	UNP Q9I297
F	13	HIS	-	expression tag	UNP Q9I297
F	14	HIS	-	expression tag	UNP Q9I297
F	15	HIS	-	expression tag	UNP Q9I297
F	16	HIS	-	expression tag	UNP Q9I297
F	17	HIS	-	expression tag	UNP Q9I297
F	18	SER	-	expression tag	UNP Q9I297
F	19	SER	-	expression tag	UNP Q9I297
F	20	GLY	-	expression tag	UNP Q9I297
F	21	LEU	-	expression tag	UNP Q9I297
F	22	VAL	-	expression tag	UNP Q9I297
F	23	PRO	-	expression tag	UNP Q9I297
F	24	ARG	-	expression tag	UNP Q9I297
F	25	GLY	-	expression tag	UNP Q9I297
F	26	SER	-	expression tag	UNP Q9I297
F	27	HIS	-	expression tag	UNP Q9I297
H	8	MET	-	expression tag	UNP Q9I297
H	9	GLY	-	expression tag	UNP Q9I297
H	10	SER	-	expression tag	UNP Q9I297
H	11	SER	-	expression tag	UNP Q9I297
H	12	HIS	-	expression tag	UNP Q9I297
H	13	HIS	-	expression tag	UNP Q9I297
H	14	HIS	-	expression tag	UNP Q9I297
H	15	HIS	-	expression tag	UNP Q9I297
H	16	HIS	-	expression tag	UNP Q9I297
H	17	HIS	-	expression tag	UNP Q9I297
H	18	SER	-	expression tag	UNP Q9I297
H	19	SER	-	expression tag	UNP Q9I297
H	20	GLY	-	expression tag	UNP Q9I297
H	21	LEU	-	expression tag	UNP Q9I297
H	22	VAL	-	expression tag	UNP Q9I297
H	23	PRO	-	expression tag	UNP Q9I297
H	24	ARG	-	expression tag	UNP Q9I297
H	25	GLY	-	expression tag	UNP Q9I297
H	26	SER	-	expression tag	UNP Q9I297
H	27	HIS	-	expression tag	UNP Q9I297
J	8	MET	-	expression tag	UNP Q9I297
J	9	GLY	-	expression tag	UNP Q9I297
J	10	SER	-	expression tag	UNP Q9I297
J	11	SER	-	expression tag	UNP Q9I297
J	12	HIS	-	expression tag	UNP Q9I297

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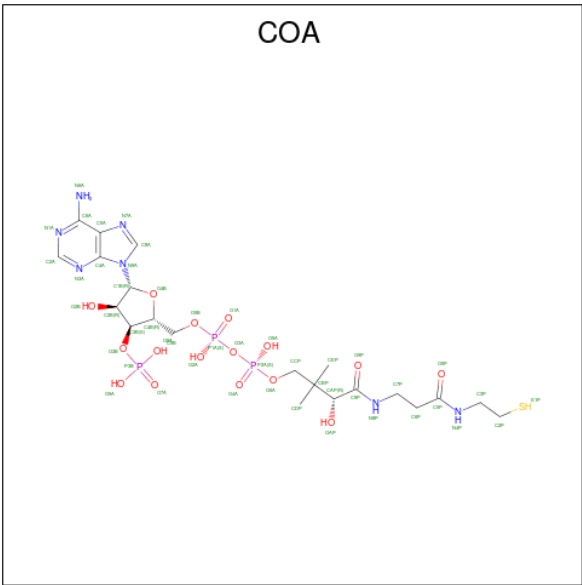
Chain	Residue	Modelled	Actual	Comment	Reference
J	13	HIS	-	expression tag	UNP Q9I297
J	14	HIS	-	expression tag	UNP Q9I297
J	15	HIS	-	expression tag	UNP Q9I297
J	16	HIS	-	expression tag	UNP Q9I297
J	17	HIS	-	expression tag	UNP Q9I297
J	18	SER	-	expression tag	UNP Q9I297
J	19	SER	-	expression tag	UNP Q9I297
J	20	GLY	-	expression tag	UNP Q9I297
J	21	LEU	-	expression tag	UNP Q9I297
J	22	VAL	-	expression tag	UNP Q9I297
J	23	PRO	-	expression tag	UNP Q9I297
J	24	ARG	-	expression tag	UNP Q9I297
J	25	GLY	-	expression tag	UNP Q9I297
J	26	SER	-	expression tag	UNP Q9I297
J	27	HIS	-	expression tag	UNP Q9I297
L	8	MET	-	expression tag	UNP Q9I297
L	9	GLY	-	expression tag	UNP Q9I297
L	10	SER	-	expression tag	UNP Q9I297
L	11	SER	-	expression tag	UNP Q9I297
L	12	HIS	-	expression tag	UNP Q9I297
L	13	HIS	-	expression tag	UNP Q9I297
L	14	HIS	-	expression tag	UNP Q9I297
L	15	HIS	-	expression tag	UNP Q9I297
L	16	HIS	-	expression tag	UNP Q9I297
L	17	HIS	-	expression tag	UNP Q9I297
L	18	SER	-	expression tag	UNP Q9I297
L	19	SER	-	expression tag	UNP Q9I297
L	20	GLY	-	expression tag	UNP Q9I297
L	21	LEU	-	expression tag	UNP Q9I297
L	22	VAL	-	expression tag	UNP Q9I297
L	23	PRO	-	expression tag	UNP Q9I297
L	24	ARG	-	expression tag	UNP Q9I297
L	25	GLY	-	expression tag	UNP Q9I297
L	26	SER	-	expression tag	UNP Q9I297
L	27	HIS	-	expression tag	UNP Q9I297

- Molecule 3 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	I	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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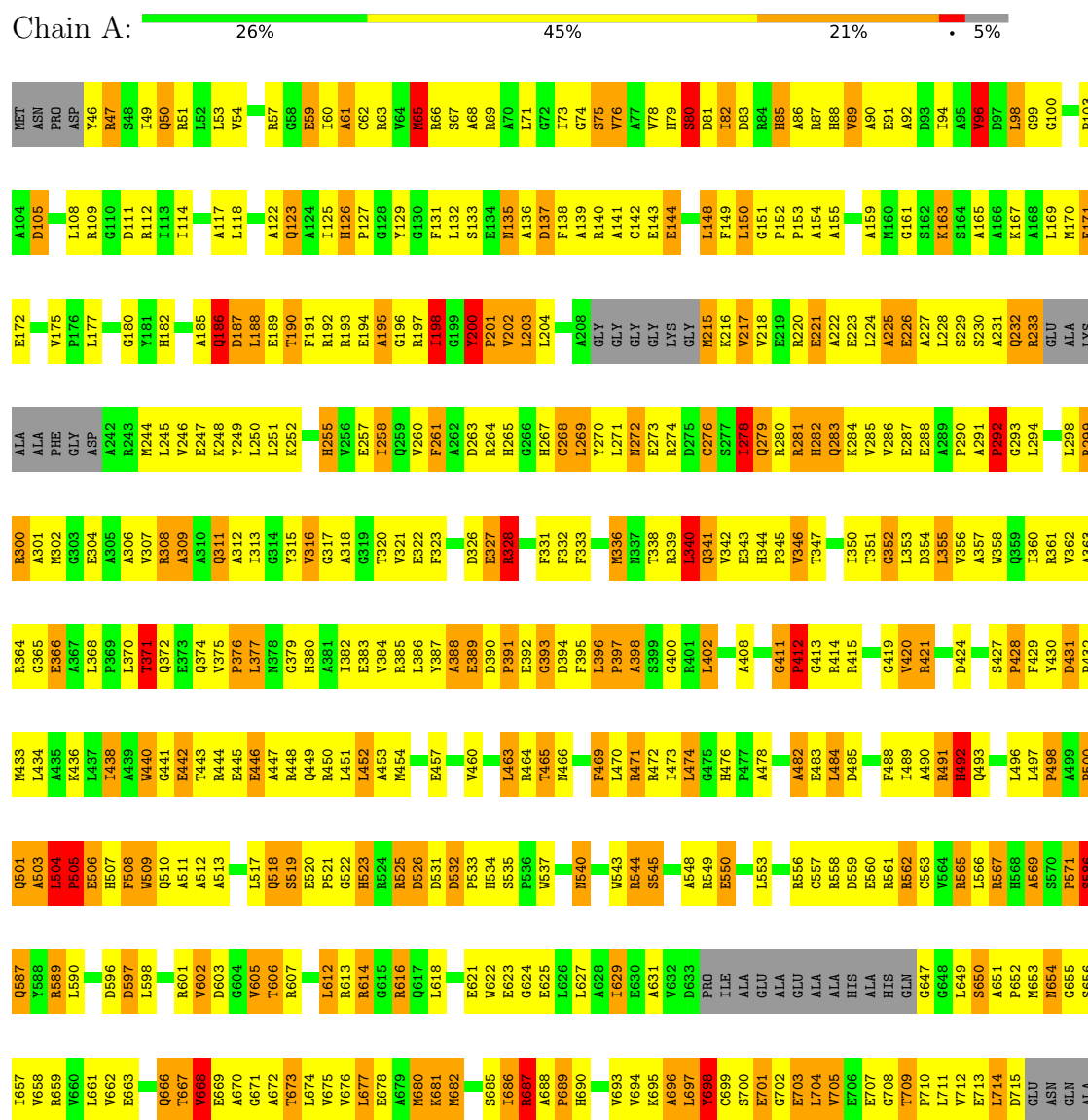
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	J	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

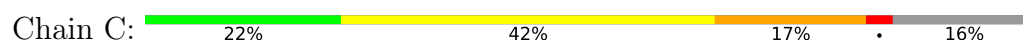
3 Residue-property plots

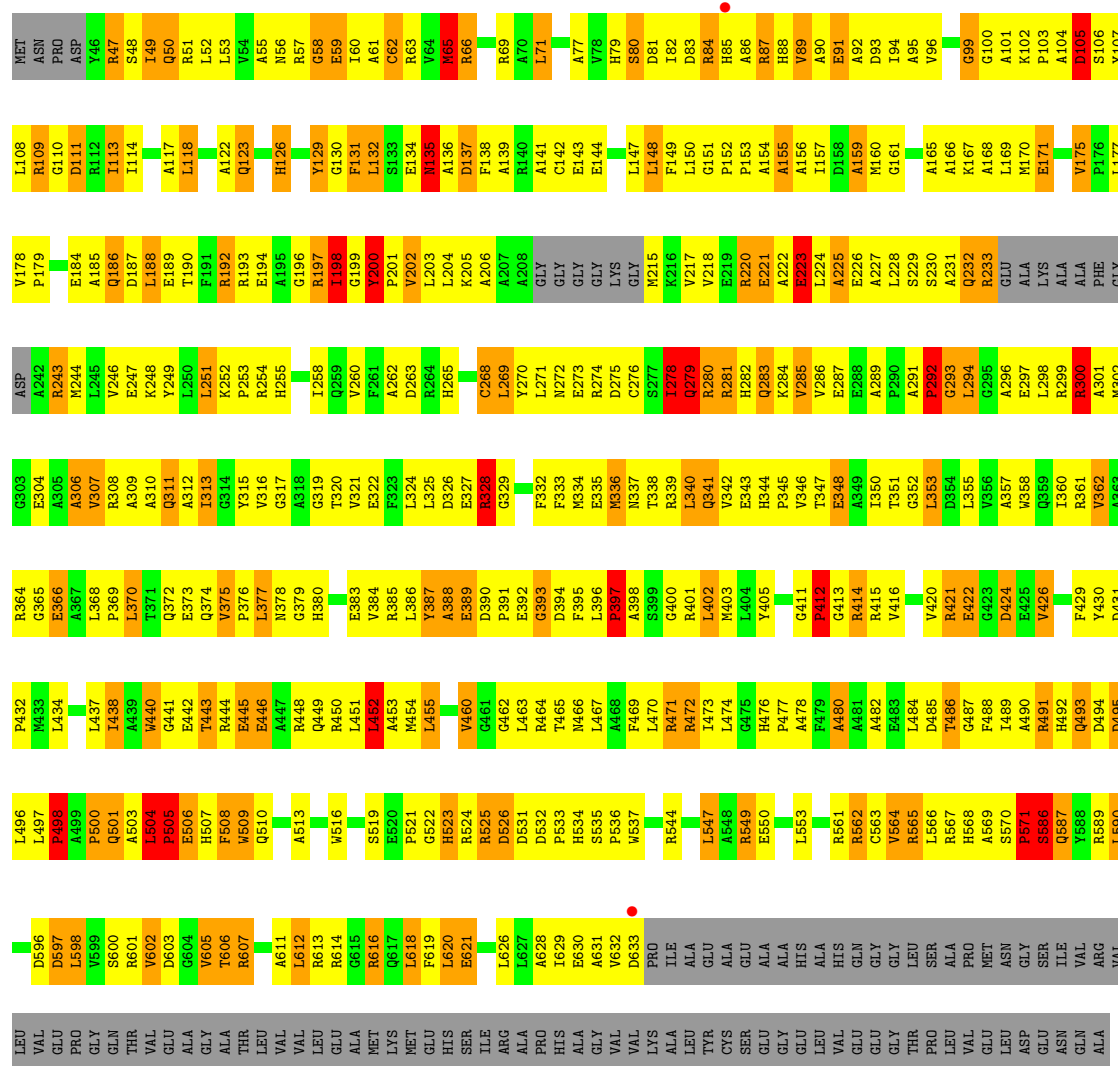
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

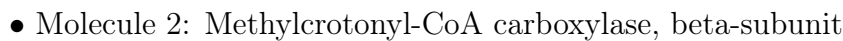
- Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

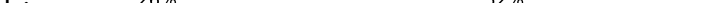


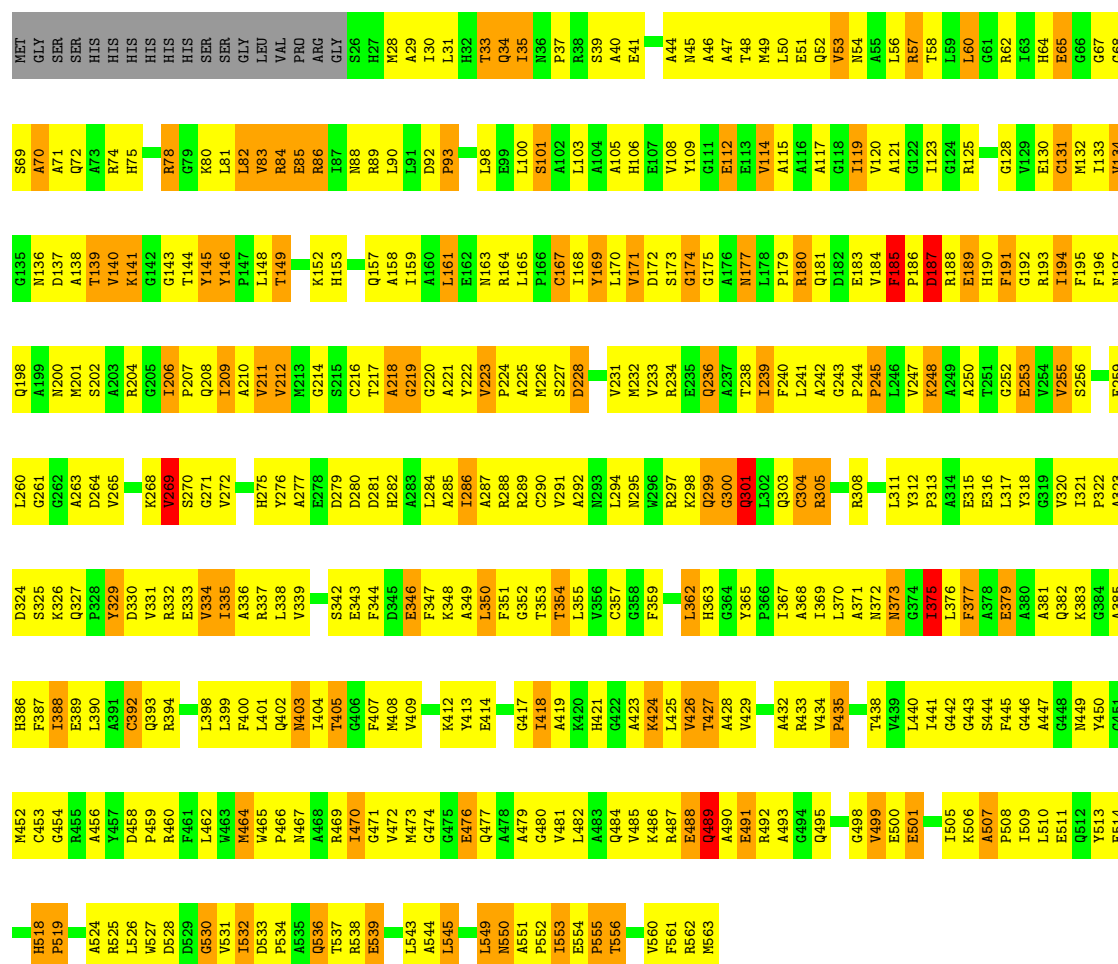
- Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit



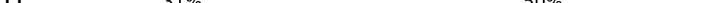


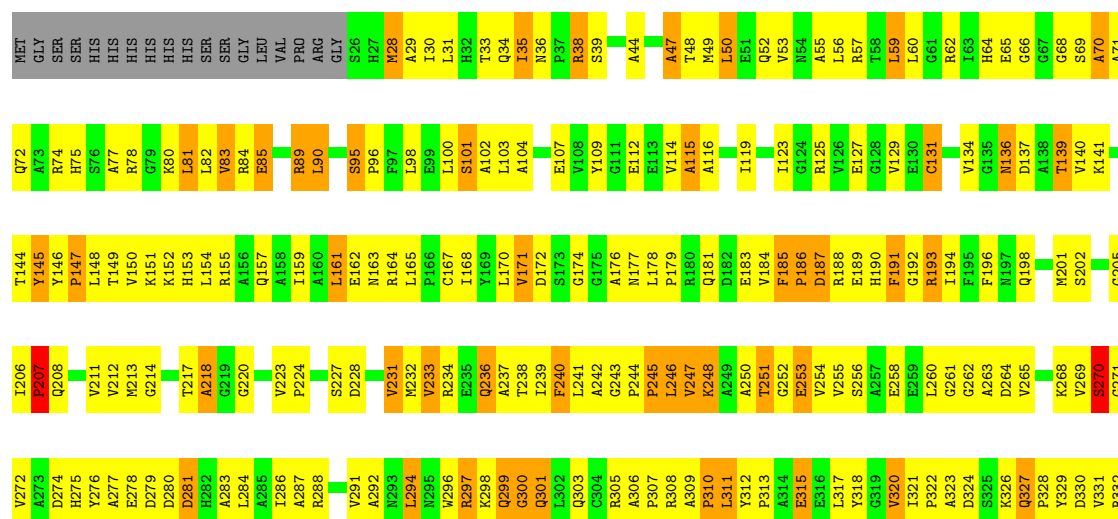


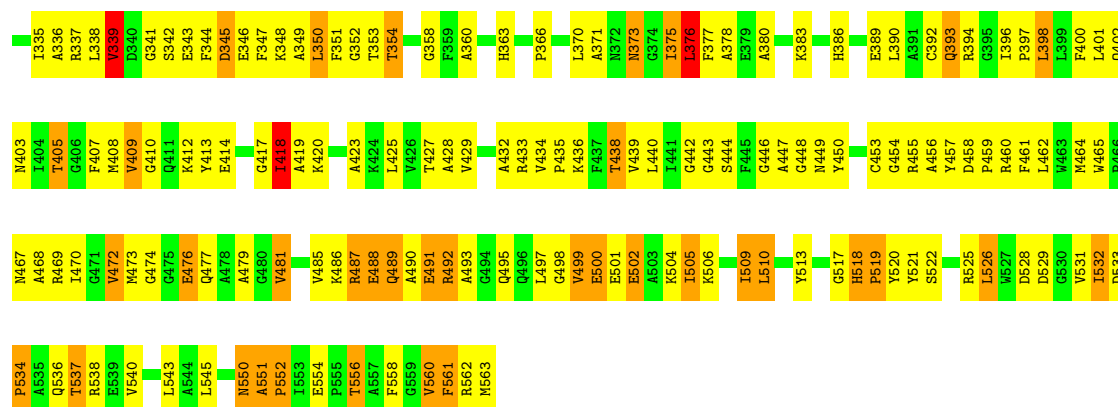
Chain F:  26% 52% 17% ..



- Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

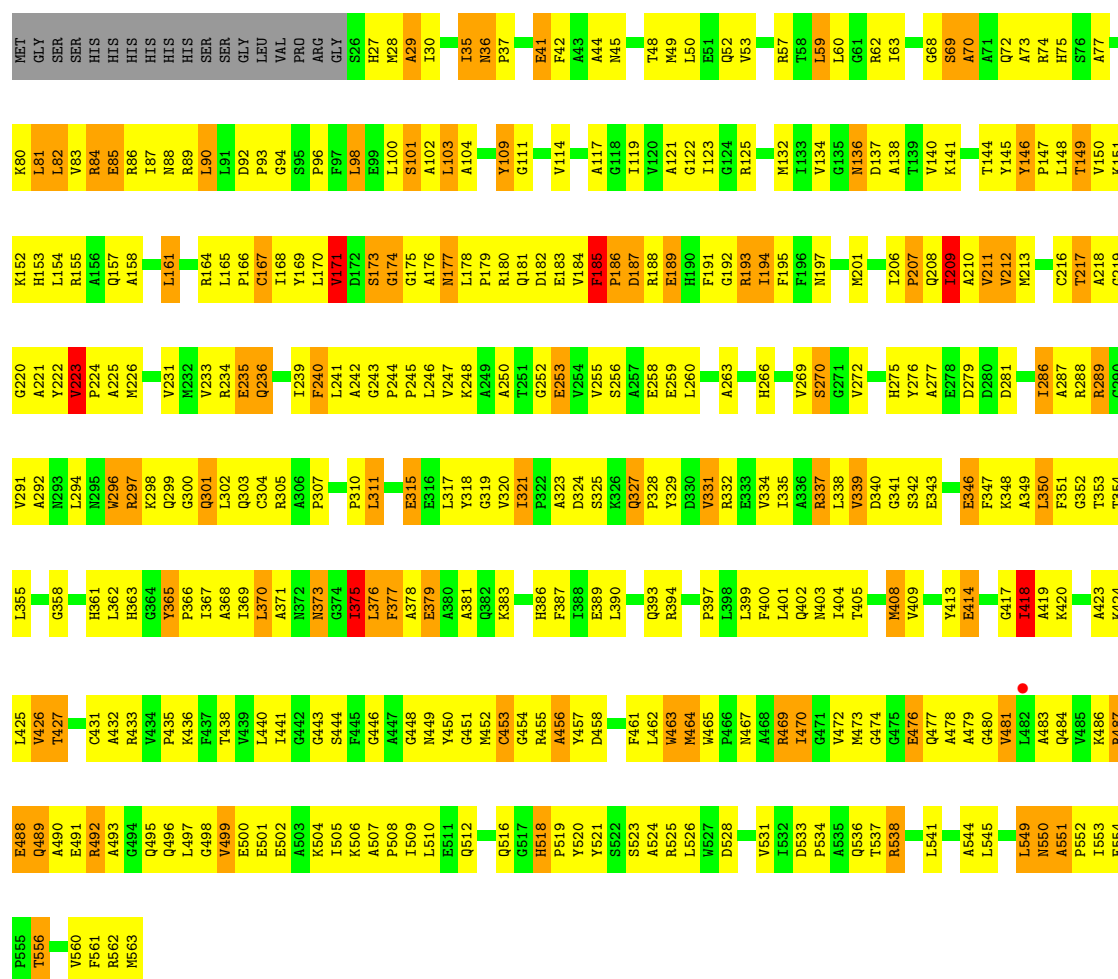
Chain H:  31% 50% 15% .





• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

Chain J: 32% 49% 15% . .



• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

Chain L: 29% 51% 16% . .

Q536	T537	R538	E539	V540	L541	A542	L543	A544	L545	L549	M550	A551	P552	I553	E554	P555	T556	A557	F558	G559	V560	F561	R562	M563																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
W465	L398	L399	L400	L401	Q402	N403	I404	T405	M408	G409	G410	Q411	K412	Y413	E414	G417	I418	A419	K420	H421	K424	L425	V426	T427	V429	A430	C431	A432	R433	V434	P435	K436	F437	T438	V439	L440	I441	G442	G443	S444	F445		Q516	G517	H518	P519	Y520	Y521	S522	S523	A524	R525	L526	W527	D528	P529	G530	V531	L462	W463	M464		D532																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
W465	L398	L399	L400	L401	Q402	N403	I404	T405	M408	G409	G410	Q411	K412	Y413	E414	G417	I418	A419	K420	H421	K424	L425	V426	T427	V429	A430	C431	A432	R433	V434	P435	K436	F437	T438	V439	L440	I441	G442	G443	S444	F445		Q516	G517	H518	P519	Y520	Y521	S522	S523	A524	R525	L526	W527	D528	P529	G530	V531	L462	W463	M464		D532																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
V331	R332	E333	V334	I335	A336	D274	H275	Y276	A277	E278	D279	D280	A283	L284	A285	Q286	R288	R289	C290	V291	S227	A292	N293	L294	M295	W296	R297	K298	Q299	G300	Q301	T302	I303	F304	C304	A371	N372	R373	T374	V375	L376	F377	A378	E379		Q382	E383	L384	H385	F387	I388	E389	L390	A391	G392	Q393	R394	G395	I396	P397		D330																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
I206	P207	Q208	I209	A210	V211	W212	M213	G214	S215	C216	T217	A218	G219	G220	A221	Y222	V223	P224	A225	M226	S227	D228	V231	M232	V233	R234	E235	Q236	A237	Q300	T301	T302	I303	F304	C304	A241	A242	G243	P244	P245	L246	V247	K248	A249	A250	T251	G252	E253	V254	V255	S256	A257	E258	E259	L260	A263	D264	V265	H266		D330																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
K141	T144	Y145	Y146	P147	K80	L81	L82	V83	R84	E85	R86	I87	N88	A156	Q157	I158	A159	A160	L161	R164	L165	P166	C167	I168	Y169	L170	V171	G174	G175	A105	H106	E107	N177	L178		Q181	E112	E113	V114		I119	V120	I123	G124	R125	V126	E127	G128	F195	N196	N197	E130	G131	M132	I133	V134	G135	A203	R204	C205		W140																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	S26	A29	I30	L31	H32	T33	N36	P37	R38	S39	A40	E41	F42	A43	A44	M45		T48	M49	L50	E51	Q52	V53	N54	A55	L56	R57	T58	L59	G60	R61	R62	I63	H64	E65	G68	S69	A70	A71																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.51Å 255.34Å 152.67Å 90.00° 95.74° 90.00°	Depositor
Resolution (Å)	48.90 – 3.50 48.90 – 3.50	Depositor EDS
% Data completeness (in resolution range)	83.0 (48.90-3.50) 83.0 (48.90-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 3.25Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.292 0.234 , 0.292	Depositor DCC
R_{free} test set	6800 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.971	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 79.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	49939	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.87	3/4866 (0.1%)	1.23	42/6581 (0.6%)
1	C	0.82	0/4362	1.22	39/5897 (0.7%)
1	E	0.80	1/4362 (0.0%)	1.21	35/5897 (0.6%)
1	G	0.83	2/4362 (0.0%)	1.23	40/5897 (0.7%)
1	I	0.82	3/3929 (0.1%)	1.23	37/5315 (0.7%)
1	K	0.89	8/3921 (0.2%)	1.22	28/5307 (0.5%)
2	B	0.88	2/4135 (0.0%)	1.26	30/5605 (0.5%)
2	D	0.85	0/4135	1.26	46/5605 (0.8%)
2	F	0.85	3/4135 (0.1%)	1.27	46/5605 (0.8%)
2	H	0.86	0/4135	1.22	25/5605 (0.4%)
2	J	0.90	2/4135 (0.0%)	1.27	41/5605 (0.7%)
2	L	0.87	2/4135 (0.0%)	1.25	39/5605 (0.7%)
All	All	0.85	26/50612 (0.1%)	1.24	448/68524 (0.7%)

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	E	0	1
1	G	0	2
1	I	0	1
2	B	0	1
2	H	0	1
2	J	0	2
All	All	0	9

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	28	MET	SD-CE	7.71	1.98	1.79
1	K	602	VAL	CA-CB	6.53	1.63	1.54
1	E	632	VAL	CA-CB	6.40	1.61	1.54
2	F	464	MET	SD-CE	6.32	1.95	1.79
1	K	178	VAL	CA-CB	6.27	1.62	1.54
1	K	443	THR	CA-CB	6.04	1.62	1.53
2	F	458	ASP	CA-C	-5.96	1.49	1.53
1	A	371	THR	CA-CB	-5.92	1.44	1.53
2	J	212	VAL	CA-CB	-5.90	1.47	1.54
1	I	606	THR	CA-CB	5.79	1.61	1.53
2	B	458	ASP	C-O	-5.72	1.21	1.23
2	L	481	VAL	CA-CB	5.70	1.60	1.54
1	G	321	VAL	CA-CB	-5.68	1.47	1.53
1	A	96	VAL	CA-CB	-5.34	1.47	1.54
1	G	82	ILE	CA-CB	5.33	1.61	1.54
1	K	256	VAL	CA-CB	5.32	1.60	1.54
2	B	458	ASP	CA-C	-5.31	1.49	1.53
2	J	209	ILE	CA-CB	-5.30	1.47	1.54
2	L	558	PHE	CA-C	-5.28	1.45	1.52
1	A	258	ILE	CA-CB	-5.10	1.48	1.54
1	I	65	MET	SD-CE	-5.09	1.66	1.79
1	K	426	VAL	CA-CB	5.09	1.58	1.53
1	K	78	VAL	CA-CB	5.08	1.61	1.54
1	I	632	VAL	CA-CB	5.07	1.60	1.54
1	K	489	ILE	CA-CB	5.04	1.60	1.54
1	K	113	ILE	CA-CB	5.00	1.60	1.54

All (448) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	506	GLU	N-CA-C	-16.31	93.10	113.97
1	C	506	GLU	N-CA-C	-14.73	93.60	112.90
1	I	506	GLU	N-CA-C	-13.79	96.53	113.50
1	K	506	GLU	N-CA-C	-13.08	97.01	113.23
1	A	200	TYR	CA-C-N	-12.93	103.68	119.84
1	A	200	TYR	C-N-CA	-12.93	103.68	119.84
1	A	506	GLU	N-CA-C	-12.88	97.25	113.23
1	G	506	GLU	N-CA-C	-12.29	97.99	113.23
1	E	545	SER	N-CA-C	11.90	124.33	111.36
1	G	545	SER	N-CA-C	11.81	123.70	111.07
2	F	193	ARG	N-CA-C	-11.15	99.68	113.28
2	D	193	ARG	N-CA-C	-11.14	99.34	113.16
2	L	550	ASN	N-CA-C	-11.04	99.19	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	545	SER	N-CA-C	10.87	124.28	111.02
1	G	200	TYR	CA-C-N	-10.76	106.39	119.84
1	G	200	TYR	C-N-CA	-10.76	106.39	119.84
2	B	193	ARG	N-CA-C	-10.26	100.76	113.28
1	E	200	TYR	CA-C-N	-10.14	107.16	119.84
1	E	200	TYR	C-N-CA	-10.14	107.16	119.84
1	I	545	SER	N-CA-C	10.02	121.79	111.07
2	D	551	ALA	CA-C-N	9.84	129.94	119.90
2	D	551	ALA	C-N-CA	9.84	129.94	119.90
2	H	193	ARG	N-CA-C	-9.84	101.28	113.18
2	J	427	THR	N-CA-C	-9.68	100.71	111.07
2	B	550	ASN	N-CA-C	-9.59	101.00	112.89
2	B	488	GLU	N-CA-C	-9.46	102.31	114.04
2	H	550	ASN	N-CA-C	-9.35	101.86	113.18
2	F	530	GLY	N-CA-C	9.23	121.40	112.08
2	J	550	ASN	N-CA-C	-9.04	101.69	112.89
2	F	346	GLU	N-CA-C	9.02	123.30	108.96
2	J	193	ARG	N-CA-C	-9.01	102.27	113.18
1	A	126	HIS	CA-C-N	8.93	129.11	119.28
1	A	126	HIS	C-N-CA	8.93	129.11	119.28
1	C	159	ALA	N-CA-C	-8.82	101.23	111.03
2	J	458	ASP	CA-C-N	-8.79	110.70	119.76
2	J	458	ASP	C-N-CA	-8.79	110.70	119.76
1	K	532	ASP	CA-C-N	8.61	127.92	118.97
1	K	532	ASP	C-N-CA	8.61	127.92	118.97
2	L	488	GLU	N-CA-C	-8.59	103.39	114.04
2	J	346	GLU	N-CA-C	8.55	122.33	109.25
1	A	442	GLU	N-CA-C	-8.40	103.03	113.28
1	E	348	GLU	N-CA-C	-8.39	102.21	111.36
2	D	158	ALA	N-CA-C	-8.36	100.46	111.24
2	J	492	ARG	N-CA-C	-8.17	103.78	112.93
2	J	171	VAL	N-CA-C	8.11	119.55	108.84
1	C	388	ALA	N-CA-C	-8.10	101.70	112.72
2	H	167	CYS	N-CA-C	8.10	122.11	109.07
1	K	126	HIS	CA-C-N	8.10	128.04	119.05
1	K	126	HIS	C-N-CA	8.10	128.04	119.05
2	H	551	ALA	CA-C-N	8.00	129.84	119.84
2	H	551	ALA	C-N-CA	8.00	129.84	119.84
2	F	323	ALA	N-CA-C	-7.98	103.69	113.50
2	B	551	ALA	CA-C-N	7.76	127.82	119.90
2	B	551	ALA	C-N-CA	7.76	127.82	119.90
1	C	200	TYR	CA-C-N	-7.71	110.20	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	TYR	C-N-CA	-7.71	110.20	119.84
2	B	346	GLU	N-CA-C	7.71	121.21	108.96
1	C	375	VAL	CA-C-N	7.69	129.45	119.84
1	C	375	VAL	C-N-CA	7.69	129.45	119.84
1	E	195	ALA	N-CA-C	-7.67	103.02	112.38
2	F	35	ILE	CB-CA-C	-7.67	101.40	110.91
2	H	270	SER	N-CA-C	7.66	119.53	111.03
1	A	474	LEU	N-CA-C	-7.64	104.11	113.50
2	J	286	ILE	N-CA-C	-7.63	103.10	110.42
2	H	346	GLU	N-CA-C	7.61	121.05	108.96
2	H	459	PRO	N-CA-C	-7.60	100.02	111.57
2	F	550	ASN	N-CA-C	-7.59	103.47	112.89
2	D	346	GLU	N-CA-C	7.53	120.77	109.25
2	F	459	PRO	N-CA-C	-7.51	99.44	111.38
2	L	193	ARG	N-CA-C	-7.49	103.87	113.16
2	F	83	VAL	N-CA-C	7.39	117.92	110.23
2	L	427	THR	N-CA-C	-7.39	103.16	111.07
2	H	418	ILE	N-CA-C	-7.34	103.44	112.76
1	A	605	VAL	N-CA-C	7.32	114.05	106.21
2	D	492	ARG	N-CA-C	-7.31	104.80	113.21
1	I	291	ALA	CA-C-N	7.31	128.97	119.84
1	I	291	ALA	C-N-CA	7.31	128.97	119.84
2	D	489	GLN	N-CA-C	-7.30	103.03	112.23
1	C	291	ALA	CA-C-N	7.29	128.95	119.84
1	C	291	ALA	C-N-CA	7.29	128.95	119.84
2	J	194	ILE	CB-CA-C	-7.25	102.53	112.02
1	I	273	GLU	N-CA-C	7.24	120.94	109.65
1	K	375	VAL	CA-C-N	7.22	128.87	119.84
1	K	375	VAL	C-N-CA	7.22	128.87	119.84
1	E	368	LEU	CA-C-N	7.18	127.80	120.04
1	E	368	LEU	C-N-CA	7.18	127.80	120.04
1	I	375	VAL	CA-C-N	7.17	128.14	120.11
1	I	375	VAL	C-N-CA	7.17	128.14	120.11
1	C	340	LEU	N-CA-C	-7.16	98.89	110.20
2	L	489	GLN	N-CA-C	-7.13	103.56	112.90
2	F	146	TYR	N-CA-C	-7.13	99.66	110.07
1	G	195	ALA	N-CA-C	-7.11	103.10	112.34
2	L	346	GLU	N-CA-C	7.10	119.68	108.67
2	D	550	ASN	N-CA-C	-7.08	103.90	112.54
2	J	551	ALA	CA-C-N	7.07	127.10	119.89
2	J	551	ALA	C-N-CA	7.07	127.10	119.89
2	F	488	GLU	N-CA-C	-7.05	105.30	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	459	PRO	N-CA-C	-7.01	100.23	111.38
2	D	29	ALA	N-CA-C	-7.00	105.16	113.21
2	D	92	ASP	CA-C-N	-6.99	111.87	119.98
2	D	92	ASP	C-N-CA	-6.99	111.87	119.98
2	F	286	ILE	N-CA-C	-6.98	103.97	110.53
2	F	492	ARG	N-CA-C	-6.96	104.87	113.15
2	B	270	SER	N-CA-C	6.95	118.51	111.07
1	K	545	SER	N-CA-C	6.89	122.66	111.37
2	D	402	GLN	N-CA-C	6.85	119.73	109.25
1	E	507	HIS	N-CA-C	-6.85	100.08	111.37
2	L	36	ASN	CA-C-N	6.84	126.54	119.56
2	L	36	ASN	C-N-CA	6.84	126.54	119.56
1	I	315	TYR	N-CA-C	6.84	120.15	110.23
2	F	507	ALA	CA-C-N	6.80	126.31	119.24
2	F	507	ALA	C-N-CA	6.80	126.31	119.24
1	K	311	GLN	N-CA-C	-6.79	103.95	111.82
2	B	327	GLN	CA-C-N	6.77	128.30	119.84
2	B	327	GLN	C-N-CA	6.77	128.30	119.84
1	C	589	ARG	N-CA-C	-6.77	100.21	109.95
1	I	453	ALA	N-CA-C	-6.76	103.53	111.03
1	A	279	GLN	N-CA-C	6.72	120.47	109.24
2	J	158	ALA	N-CA-C	-6.72	102.58	111.24
2	J	481	VAL	N-CA-C	6.71	117.47	110.62
2	H	492	ARG	N-CA-C	-6.70	105.43	112.93
2	D	36	ASN	CA-C-N	6.70	126.39	119.56
2	D	36	ASN	C-N-CA	6.70	126.39	119.56
2	H	191	PHE	N-CA-C	-6.70	101.66	110.43
2	F	518	HIS	CA-C-N	6.69	128.20	119.84
2	F	518	HIS	C-N-CA	6.69	128.20	119.84
1	K	569	ALA	N-CA-C	-6.68	105.28	113.50
2	L	551	ALA	CA-C-N	6.68	126.64	119.76
2	L	551	ALA	C-N-CA	6.68	126.64	119.76
1	C	442	GLU	N-CA-C	-6.67	105.30	113.50
2	J	488	GLU	N-CA-C	-6.67	105.71	114.31
2	D	458	ASP	CA-C-N	-6.67	113.07	120.14
2	D	458	ASP	C-N-CA	-6.67	113.07	120.14
2	F	489	GLN	N-CA-C	-6.61	103.91	112.23
2	B	149	THR	N-CA-C	-6.60	104.01	111.07
2	L	459	PRO	N-CA-C	-6.59	100.84	111.19
1	I	368	LEU	CA-C-N	6.59	126.17	119.19
1	I	368	LEU	C-N-CA	6.59	126.17	119.19
2	B	489	GLN	N-CA-C	-6.58	104.29	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	291	ALA	CA-C-N	6.57	128.06	119.84
1	G	291	ALA	C-N-CA	6.57	128.06	119.84
2	H	458	ASP	CA-C-N	-6.56	113.88	120.31
2	H	458	ASP	C-N-CA	-6.56	113.88	120.31
2	H	489	GLN	N-CA-C	-6.56	104.31	112.90
1	K	387	TYR	N-CA-C	6.55	120.71	110.17
1	A	411	GLY	CA-C-N	6.53	128.01	119.84
1	A	411	GLY	C-N-CA	6.53	128.01	119.84
1	K	315	TYR	N-CA-C	6.53	119.95	110.28
1	G	597	ASP	N-CA-C	6.53	119.10	108.26
1	E	340	LEU	N-CA-C	-6.53	99.89	110.20
2	B	204	ARG	N-CA-C	-6.53	105.62	112.93
1	A	603	ASP	N-CA-C	6.51	118.53	110.91
1	E	388	ALA	N-CA-C	-6.50	103.88	112.72
1	A	200	TYR	N-CA-C	6.49	124.15	109.81
1	E	321	VAL	CB-CA-C	-6.47	103.11	111.53
1	G	474	LEU	N-CA-C	-6.47	105.21	113.23
2	B	35	ILE	CB-CA-C	-6.42	101.92	110.98
2	L	248	LYS	N-CA-C	-6.42	103.79	111.69
1	I	589	ARG	N-CA-C	-6.42	100.48	110.17
1	C	597	ASP	N-CA-C	6.41	120.03	108.69
2	J	296	TRP	N-CA-C	6.40	119.56	109.96
1	E	159	ALA	N-CA-C	-6.39	104.00	110.97
1	E	514	GLU	N-CA-C	-6.39	103.44	111.11
2	L	492	ARG	N-CA-C	-6.39	105.54	113.15
1	G	504	LEU	CA-C-N	6.39	127.83	119.84
1	G	504	LEU	C-N-CA	6.39	127.83	119.84
1	A	689	PRO	N-CA-C	6.38	121.88	114.03
2	H	131	CYS	N-CA-C	6.36	119.90	109.85
2	D	507	ALA	CA-C-N	6.36	125.58	118.97
2	D	507	ALA	C-N-CA	6.36	125.58	118.97
2	F	145	TYR	N-CA-C	6.35	118.63	108.41
1	G	411	GLY	CA-C-N	6.34	127.76	119.84
1	G	411	GLY	C-N-CA	6.34	127.76	119.84
1	C	387	TYR	N-CA-C	6.33	120.15	109.76
1	A	532	ASP	CA-C-N	6.31	125.53	118.97
1	A	532	ASP	C-N-CA	6.31	125.53	118.97
1	I	474	LEU	N-CA-C	-6.30	105.75	113.50
2	L	286	ILE	N-CA-C	-6.30	104.36	110.72
2	F	427	THR	N-CA-C	-6.30	104.33	111.07
1	K	159	ALA	N-CA-C	-6.27	104.36	111.07
2	D	248	LYS	N-CA-C	-6.27	104.33	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	388	ALA	N-CA-C	-6.27	102.79	111.81
2	J	185	PHE	CA-C-N	6.26	127.67	119.84
2	J	185	PHE	C-N-CA	6.26	127.67	119.84
2	B	505	ILE	CB-CA-C	-6.25	104.06	111.94
2	F	458	ASP	CA-C-N	-6.24	113.55	119.85
2	F	458	ASP	C-N-CA	-6.24	113.55	119.85
2	F	34	GLN	N-CA-C	-6.23	103.34	113.19
1	C	426	VAL	CB-CA-C	-6.21	105.21	111.80
2	L	167	CYS	N-CA-C	6.21	119.06	109.07
1	C	126	HIS	CA-C-N	6.20	125.76	119.19
1	C	126	HIS	C-N-CA	6.20	125.76	119.19
2	J	223	VAL	CA-C-N	-6.19	112.10	119.84
2	J	223	VAL	C-N-CA	-6.19	112.10	119.84
1	K	605	VAL	N-CA-C	6.19	115.53	106.55
1	K	294	LEU	N-CA-C	6.17	123.93	110.80
1	I	143	GLU	N-CA-C	-6.16	105.26	112.89
2	F	187	ASP	N-CA-C	6.15	123.90	110.80
1	I	631	ALA	N-CA-C	6.14	119.91	110.20
1	G	340	LEU	N-CA-C	-6.14	100.50	110.20
1	I	484	LEU	N-CA-C	6.14	120.27	109.96
1	E	200	TYR	N-CA-C	6.13	123.37	109.81
2	B	518	HIS	N-CA-C	6.12	117.79	110.07
2	B	171	VAL	N-CA-C	6.12	116.92	108.84
1	I	308	ARG	N-CA-C	-6.12	103.93	111.40
2	L	367	ILE	N-CA-C	6.11	117.15	108.42
1	G	362	VAL	CB-CA-C	-6.09	102.72	112.16
2	J	489	GLN	N-CA-C	-6.09	104.20	111.69
2	B	540	VAL	N-CA-C	-6.08	104.92	110.82
1	E	442	GLU	N-CA-C	-6.08	104.94	112.90
2	L	239	ILE	CB-CA-C	-6.08	103.63	111.53
2	H	103	LEU	N-CA-C	-6.07	105.93	113.15
2	L	271	GLY	N-CA-C	-6.07	106.56	115.72
1	C	200	TYR	N-CA-C	6.06	123.20	109.81
1	A	89	VAL	N-CA-C	-6.05	104.08	112.50
2	D	171	VAL	N-CA-C	6.03	116.84	109.30
2	D	459	PRO	N-CA-C	-6.03	101.60	111.68
2	F	269	VAL	N-CA-C	6.03	121.88	109.34
1	A	484	LEU	N-CA-C	6.03	119.46	109.46
2	L	532	ILE	N-CA-C	6.02	116.16	108.82
2	D	270	SER	N-CA-C	6.01	117.52	110.97
1	I	340	LEU	N-CA-C	-6.00	100.22	109.76
2	D	176	ALA	N-CA-C	-5.99	99.94	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	209	ILE	CB-CA-C	-5.99	102.54	110.98
1	A	504	LEU	CA-C-N	5.96	127.29	119.84
1	A	504	LEU	C-N-CA	5.96	127.29	119.84
2	B	412	LYS	N-CA-C	-5.95	104.38	111.69
1	C	171	GLU	N-CA-C	-5.94	104.49	110.97
1	E	472	ARG	N-CA-C	5.92	120.35	113.18
1	I	388	ALA	N-CA-C	-5.91	104.68	112.72
2	F	171	VAL	N-CA-C	5.91	116.69	108.89
2	D	549	LEU	N-CA-C	-5.90	105.73	113.17
1	A	569	ALA	N-CA-C	-5.90	106.21	113.41
2	F	185	PHE	N-CA-C	5.89	122.83	109.81
1	G	520	GLU	CA-C-N	5.89	127.20	119.84
1	G	520	GLU	C-N-CA	5.89	127.20	119.84
2	J	270	SER	N-CA-C	5.89	117.56	111.03
2	J	531	VAL	N-CA-C	-5.88	99.95	108.71
1	E	356	VAL	CB-CA-C	-5.87	104.19	111.70
1	I	442	GLU	N-CA-C	-5.86	106.18	113.38
1	G	353	LEU	N-CA-C	5.86	119.02	109.59
1	C	89	VAL	N-CA-C	-5.85	104.62	111.00
2	D	518	HIS	N-CA-C	5.85	117.03	109.72
1	E	294	LEU	N-CA-C	5.84	123.25	110.80
1	E	597	ASP	N-CA-C	5.84	117.95	108.26
1	K	340	LEU	N-CA-C	-5.82	101.24	109.96
2	L	187	ASP	N-CA-C	5.82	123.19	110.80
2	D	83	VAL	N-CA-C	5.81	116.27	110.23
2	L	103	LEU	N-CA-C	-5.81	106.53	113.21
2	B	455	ARG	N-CA-C	5.80	118.35	111.33
2	J	244	PRO	N-CA-C	5.80	117.78	110.70
2	L	348	LYS	N-CA-C	-5.79	103.41	111.39
2	F	248	LYS	N-CA-C	-5.79	104.94	112.23
1	C	504	LEU	CA-C-N	5.78	127.07	119.84
1	C	504	LEU	C-N-CA	5.78	127.07	119.84
2	H	171	VAL	N-CA-C	5.78	116.47	108.84
2	L	126	VAL	N-CA-C	-5.76	99.82	108.12
1	A	396	LEU	CA-C-N	5.76	127.04	119.84
1	A	396	LEU	C-N-CA	5.76	127.04	119.84
1	G	388	ALA	N-CA-C	-5.75	103.52	111.81
1	K	279	GLN	N-CA-C	5.75	118.14	109.23
1	K	520	GLU	CA-C-N	5.75	127.03	119.84
1	K	520	GLU	C-N-CA	5.75	127.03	119.84
2	D	481	VAL	CB-CA-C	-5.74	104.64	111.81
1	I	396	LEU	CA-C-N	5.74	127.01	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	396	LEU	C-N-CA	5.74	127.01	119.84
1	G	417	ASP	N-CA-C	-5.74	99.38	108.73
2	J	404	ILE	N-CA-C	5.73	116.56	108.36
1	I	96	VAL	N-CA-C	5.72	117.59	108.89
2	D	185	PHE	N-CA-C	5.72	122.45	109.81
2	F	369	ILE	N-CA-C	5.71	117.22	108.71
2	D	146	TYR	N-CA-C	-5.68	102.75	110.36
2	B	85	GLU	N-CA-C	-5.68	104.47	111.40
2	H	323	ALA	N-CA-C	-5.68	106.19	113.23
2	D	115	ALA	N-CA-C	5.66	118.68	110.42
2	L	209	ILE	N-CA-C	5.65	117.14	108.71
1	K	507	HIS	N-CA-C	-5.64	98.78	110.80
1	A	171	GLU	N-CA-C	-5.64	105.05	111.14
1	K	308	ARG	N-CA-C	-5.63	104.78	111.03
2	B	286	ILE	N-CA-C	-5.63	105.24	110.53
2	H	34	GLN	N-CA-C	-5.62	104.64	113.02
2	H	518	HIS	N-CA-C	5.62	116.90	109.93
2	J	29	ALA	N-CA-C	-5.62	106.46	113.15
1	C	202	VAL	N-CA-C	5.61	117.49	108.85
2	J	470	ILE	N-CA-C	5.61	115.96	108.11
1	A	195	ALA	N-CA-C	-5.60	104.58	111.75
1	E	504	LEU	CA-C-N	5.60	126.84	119.84
1	E	504	LEU	C-N-CA	5.60	126.84	119.84
2	J	418	ILE	N-CA-C	-5.60	105.65	112.76
2	H	107	GLU	CA-C-N	-5.59	117.43	123.08
2	H	107	GLU	C-N-CA	-5.59	117.43	123.08
1	C	65	MET	N-CA-C	-5.59	105.09	111.07
1	C	379	GLY	N-CA-C	5.59	124.19	112.45
2	F	424	LYS	N-CA-C	-5.59	105.19	111.28
2	L	463	TRP	N-CA-C	5.59	118.36	110.14
1	G	96	VAL	N-CA-C	5.58	116.51	108.48
2	H	339	VAL	CB-CA-C	-5.58	102.14	111.29
2	D	209	ILE	N-CA-C	5.57	117.00	108.71
1	I	252	LYS	CA-C-N	5.57	125.33	119.76
1	I	252	LYS	C-N-CA	5.57	125.33	119.76
1	G	472	ARG	N-CA-C	5.56	119.33	112.54
2	B	323	ALA	N-CA-C	-5.56	106.63	113.41
2	F	64	HIS	N-CA-C	-5.55	106.48	113.20
1	A	589	ARG	N-CA-C	-5.55	101.98	110.14
2	L	181	GLN	N-CA-C	5.54	118.09	111.71
2	D	86	ARG	N-CA-C	-5.54	104.46	111.11
1	E	379	GLY	N-CA-C	5.54	126.31	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	28	MET	N-CA-C	-5.54	106.65	113.41
2	B	492	ARG	N-CA-C	-5.53	106.86	113.21
1	C	279	GLN	N-CA-C	5.52	118.45	109.06
2	F	403	ASN	N-CA-C	-5.51	99.06	110.80
1	G	589	ARG	N-CA-C	-5.50	101.86	110.17
1	I	265	HIS	N-CA-C	5.50	117.49	110.61
1	I	76	VAL	CB-CA-C	-5.50	104.38	111.53
2	L	146	TYR	N-CA-C	-5.49	102.15	110.39
1	A	291	ALA	CA-C-N	5.49	126.70	119.84
1	A	291	ALA	C-N-CA	5.49	126.70	119.84
1	K	597	ASP	N-CA-C	5.49	118.41	108.69
1	G	442	GLU	N-CA-C	-5.47	106.60	113.28
2	J	146	TYR	N-CA-C	-5.47	102.18	110.39
1	E	589	ARG	N-CA-C	-5.47	101.44	109.81
2	F	555	PRO	N-CA-C	-5.47	102.55	111.68
1	G	187	ASP	N-CA-C	5.47	115.34	108.45
2	D	412	LYS	N-CA-C	-5.47	106.45	113.23
1	C	480	ALA	N-CA-C	-5.47	105.01	110.97
1	A	76	VAL	CB-CA-C	-5.46	104.71	111.32
2	B	215	SER	N-CA-C	-5.46	103.33	110.53
1	G	143	GLU	N-CA-C	-5.45	106.63	113.28
1	C	80	SER	N-CA-C	-5.45	101.92	110.36
1	A	631	ALA	N-CA-C	5.44	117.57	109.25
1	I	504	LEU	CA-C-N	5.44	126.64	119.84
1	I	504	LEU	C-N-CA	5.44	126.64	119.84
1	A	388	ALA	N-CA-C	-5.43	103.99	111.81
2	F	470	ILE	N-CA-C	5.43	115.71	108.11
2	D	398	LEU	N-CA-C	5.42	118.08	109.24
1	K	631	ALA	N-CA-C	5.42	117.54	109.25
1	C	348	GLU	N-CA-C	-5.40	105.47	111.36
1	A	187	ASP	N-CA-C	5.40	115.15	108.19
1	C	199	GLY	N-CA-C	-5.39	100.39	113.18
1	A	61	ALA	N-CA-C	-5.39	105.48	111.36
2	B	369	ILE	N-CA-C	5.39	117.09	108.89
1	C	62	CYS	N-CA-C	-5.39	106.21	112.89
2	D	190	HIS	N-CA-C	5.38	118.19	109.86
1	G	89	VAL	N-CA-C	-5.38	105.03	112.50
1	E	202	VAL	N-CA-C	5.38	116.22	108.48
2	J	41	GLU	N-CA-C	-5.37	105.53	111.71
1	K	589	ARG	N-CA-C	-5.37	101.59	109.81
1	E	474	LEU	N-CA-C	-5.37	106.73	113.28
1	E	569	ALA	N-CA-C	-5.36	106.91	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	86	ARG	N-CA-C	-5.36	104.85	111.33
1	G	438	ILE	N-CA-C	5.36	116.44	108.46
1	A	80	SER	N-CA-C	-5.35	102.97	110.35
1	C	505	PRO	N-CA-C	5.35	123.49	112.47
1	I	520	GLU	CA-C-N	5.34	126.52	119.84
1	I	520	GLU	C-N-CA	5.34	126.52	119.84
1	K	171	GLU	N-CA-C	-5.34	105.37	111.14
2	D	167	CYS	N-CA-C	5.34	118.10	109.40
1	G	507	HIS	N-CA-C	-5.33	102.57	111.37
2	D	103	LEU	N-CA-C	-5.32	106.82	113.15
2	J	518	HIS	N-CA-C	5.32	116.53	109.93
1	E	375	VAL	CA-C-N	5.32	126.49	119.84
1	E	375	VAL	C-N-CA	5.32	126.49	119.84
2	D	145	TYR	N-CA-C	5.32	116.91	108.67
2	F	239	ILE	CB-CA-C	-5.30	104.90	111.32
1	E	156	ALA	N-CA-C	5.30	117.80	111.71
2	D	530	GLY	N-CA-C	5.29	117.43	112.08
1	A	309	ALA	N-CA-C	-5.29	106.08	112.54
1	K	514	GLU	N-CA-C	-5.29	104.93	111.33
2	L	426	VAL	N-CA-C	5.29	116.06	110.72
2	J	167	CYS	N-CA-C	5.28	118.01	109.40
1	G	279	GLN	N-CA-C	5.28	118.03	109.06
2	L	191	PHE	N-CA-C	-5.28	103.53	110.33
2	F	553	ILE	N-CA-C	-5.27	100.16	108.23
2	L	295	ASN	N-CA-C	-5.27	104.37	111.54
1	C	227	ALA	N-CA-C	-5.27	106.69	113.01
1	E	101	ALA	N-CA-C	5.27	119.03	111.02
1	A	264	ARG	N-CA-C	-5.26	106.05	113.20
2	L	234	ARG	N-CA-C	5.25	117.85	110.23
2	F	51	GLU	N-CA-C	-5.25	105.64	111.36
1	I	80	SER	N-CA-C	-5.24	102.24	110.36
1	I	597	ASP	N-CA-C	5.23	116.95	108.26
2	J	173	SER	N-CA-C	5.23	117.63	109.52
2	F	167	CYS	N-CA-C	5.23	117.43	108.90
2	D	552	PRO	N-CA-C	5.23	119.41	111.15
2	B	230	THR	N-CA-C	5.23	117.59	108.76
2	B	248	LYS	N-CA-C	-5.23	105.26	111.69
1	A	340	LEU	N-CA-C	-5.22	103.13	110.50
2	F	418	ILE	N-CA-C	-5.22	106.13	112.76
2	L	403	ASN	N-CA-C	-5.21	99.69	110.80
2	B	300	GLY	N-CA-C	-5.21	103.54	112.30
1	G	570	SER	CA-C-N	5.20	126.33	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	570	SER	C-N-CA	5.20	126.33	119.84
1	A	65	MET	N-CA-C	-5.19	105.51	111.07
1	C	452	LEU	N-CA-C	-5.19	106.21	112.54
1	G	157	ILE	N-CA-C	5.19	115.41	110.53
2	D	173	SER	N-CA-C	5.18	118.04	109.85
1	I	387	TYR	N-CA-C	5.18	118.56	110.32
2	L	210	ALA	N-CA-C	5.18	117.52	108.76
1	A	452	LEU	N-CA-C	-5.18	105.81	111.82
2	L	518	HIS	N-CA-C	5.18	116.18	109.65
2	J	456	ALA	N-CA-C	5.17	119.22	113.01
1	G	294	LEU	N-CA-C	5.17	121.81	110.80
2	L	171	VAL	N-CA-C	5.17	115.67	108.84
1	C	368	LEU	CA-C-N	5.17	124.67	119.19
1	C	368	LEU	C-N-CA	5.17	124.67	119.19
1	G	273	GLU	N-CA-C	5.16	115.19	108.07
1	K	480	ALA	N-CA-C	-5.16	105.35	110.97
2	L	145	TYR	N-CA-C	5.15	116.71	108.41
1	E	411	GLY	CA-C-N	5.15	126.28	119.84
1	E	411	GLY	C-N-CA	5.15	126.28	119.84
2	J	90	LEU	N-CA-C	5.14	116.89	111.28
1	A	190	THR	N-CA-C	-5.13	105.81	111.71
2	D	131	CYS	N-CA-C	5.13	117.93	109.72
2	L	29	ALA	N-CA-C	-5.13	107.00	113.20
1	G	630	GLU	N-CA-C	5.12	117.19	109.41
2	J	463	TRP	N-CA-C	5.12	117.94	109.85
1	C	87	ARG	N-CA-C	5.12	116.67	111.14
1	I	532	ASP	CA-C-N	5.11	124.72	119.05
1	I	532	ASP	C-N-CA	5.11	124.72	119.05
2	J	36	ASN	CA-C-N	5.11	124.72	119.56
2	J	36	ASN	C-N-CA	5.11	124.72	119.56
2	F	131	CYS	N-CA-C	5.10	118.06	109.95
1	E	315	TYR	N-CA-C	5.10	117.69	110.50
2	J	185	PHE	N-CA-C	5.10	121.07	109.81
2	F	210	ALA	N-CA-C	5.09	117.75	109.24
2	J	556	THR	N-CA-C	5.09	118.11	109.76
2	F	158	ALA	N-CA-C	-5.09	105.19	111.40
1	G	379	GLY	N-CA-C	5.09	125.24	113.18
1	I	514	GLU	N-CA-C	-5.09	105.63	111.07
1	A	308	ARG	N-CA-C	-5.08	104.72	112.04
1	C	306	ALA	N-CA-C	-5.08	105.65	111.14
1	G	199	GLY	N-CA-C	-5.08	101.14	113.18
2	J	358	GLY	N-CA-C	5.08	118.11	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	296	TRP	N-CA-C	5.07	117.88	109.46
2	H	300	GLY	N-CA-C	-5.06	103.80	112.30
2	L	441	ILE	CB-CA-C	-5.05	105.43	111.85
2	D	418	ILE	CB-CA-C	-5.05	103.01	111.29
2	D	456	ALA	N-CA-C	5.04	119.06	113.01
1	G	427	SER	N-CA-C	5.04	116.84	109.84
2	F	256	SER	N-CA-C	5.04	116.61	110.41
1	C	374	GLN	N-CA-C	-5.03	108.41	114.75
1	G	80	SER	N-CA-C	-5.03	102.07	109.86
2	D	396	ILE	N-CA-C	-5.02	102.42	107.89
2	F	115	ALA	N-CA-C	5.02	118.07	110.64
2	F	206	ILE	N-CA-C	-5.02	98.05	108.88
2	F	335	ILE	CB-CA-C	-5.01	105.38	112.14
2	B	422	GLY	N-CA-C	-5.01	106.72	112.73
1	E	61	ALA	N-CA-C	-5.00	105.92	112.23

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	698	TYR	Sidechain
2	B	109	TYR	Sidechain
1	E	129	TYR	Sidechain
1	G	129	TYR	Sidechain
1	G	588	TYR	Sidechain
2	H	145	TYR	Sidechain
1	I	129	TYR	Sidechain
2	J	109	TYR	Sidechain
2	J	365	TYR	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	4778	0	4730	603	0
1	C	4280	0	4227	567	0
1	E	4280	0	4227	551	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4280	0	4227	551	0
1	I	3853	0	3795	501	0
1	K	3844	0	3786	507	0
2	B	4051	0	4023	417	0
2	D	4051	0	4023	443	0
2	F	4051	0	4023	458	0
2	H	4051	0	4023	444	0
2	J	4051	0	4023	449	0
2	L	4051	0	4023	448	0
3	A	15	0	15	3	0
3	I	15	0	15	5	0
4	B	48	0	32	4	0
4	D	48	0	32	3	0
4	F	48	0	32	3	0
4	H	48	0	32	6	0
4	J	48	0	32	4	0
4	L	48	0	32	2	0
All	All	49939	0	49352	5697	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

All (5697) 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:I:170:MET:HE1	1:I:309:ALA:HB1	1.26	1.18
1:C:504:LEU:HB3	1:C:505:PRO:HD2	1.23	1.17
1:G:200:TYR:CE1	1:G:221:GLU:HA	1.82	1.15
2:J:201:MET:HE3	2:J:208:GLN:HE22	1.10	1.15
1:G:278:ILE:H	1:G:278:ILE:HD12	1.10	1.14
1:K:101:ALA:HB1	1:K:429:PHE:CE1	1.83	1.14
2:F:231:VAL:HG22	2:F:275:HIS:HB2	1.18	1.12
1:K:101:ALA:HB1	1:K:429:PHE:HE1	1.06	1.12
1:C:465:THR:HG22	1:C:467:LEU:H	1.13	1.11
2:L:231:VAL:HG22	2:L:275:HIS:HB2	1.32	1.11
1:I:605:VAL:HG12	1:K:96:VAL:HG12	1.26	1.11
1:A:396:LEU:HD12	1:A:464:ARG:HH12	1.15	1.11
1:C:400:GLY:H	1:C:463:LEU:HD21	1.04	1.11
2:D:217:THR:HG22	2:D:240:PHE:CE1	1.84	1.11
1:E:101:ALA:HB1	1:E:429:PHE:CE1	1.86	1.11
1:G:152:PRO:HD2	1:G:157:ILE:HD11	1.32	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:207:PRO:HG2	2:H:294:LEU:HD21	1.34	1.10
1:C:611:ALA:HB2	1:C:620:LEU:HD13	1.30	1.08
2:H:350:LEU:HD23	2:H:350:LEU:H	1.15	1.08
2:J:201:MET:HE3	2:J:208:GLN:NE2	1.67	1.08
2:D:217:THR:HG22	2:D:240:PHE:HE1	1.10	1.08
2:J:495:GLN:HG2	2:J:496:GLN:H	1.16	1.08
1:E:350:ILE:HA	1:E:440:TRP:HZ3	1.19	1.07
2:F:473:MET:HE2	2:F:477:GLN:HB3	1.36	1.07
1:A:525:ARG:HH11	1:A:525:ARG:HB3	1.19	1.07
1:C:334:MET:HE2	1:C:334:MET:HA	1.35	1.07
2:D:188:ARG:HB3	2:D:188:ARG:HH11	1.15	1.07
1:E:167:LYS:HE3	1:E:177:LEU:HD22	1.36	1.07
1:E:278:ILE:HD12	1:E:278:ILE:H	1.17	1.07
1:K:415:ARG:HD3	1:K:438:ILE:HD13	1.34	1.07
2:B:473:MET:HE1	2:L:246:LEU:HD21	1.35	1.07
2:D:444:SER:HB3	2:D:470:ILE:HG13	1.29	1.07
2:H:291:VAL:HA	2:H:294:LEU:HD12	1.38	1.05
1:I:562:ARG:HB3	1:I:562:ARG:HH11	1.20	1.04
1:A:562:ARG:HB3	1:A:562:ARG:HH11	1.17	1.04
2:B:33:THR:HG23	2:B:35:ILE:H	1.20	1.04
1:E:549:ARG:HG2	1:E:549:ARG:HH11	1.19	1.04
1:K:401:ARG:HB3	1:K:401:ARG:HH11	1.20	1.04
1:G:605:VAL:HG12	1:I:96:VAL:HG13	1.36	1.04
1:I:599:VAL:HG22	1:I:608:ARG:HB3	1.37	1.04
1:K:47:ARG:HB2	1:K:47:ARG:HH11	1.20	1.04
2:L:375:ILE:HB	2:L:377:PHE:HE1	1.19	1.04
1:E:101:ALA:HB1	1:E:429:PHE:HE1	1.23	1.03
1:E:550:GLU:HG3	1:E:567:ARG:HD2	1.33	1.03
2:H:161:LEU:HB2	2:H:201:MET:HE2	1.40	1.03
2:B:83:VAL:HG13	2:B:84:ARG:H	1.15	1.03
1:K:378:ASN:O	1:K:440:TRP:HH2	1.42	1.03
2:L:189:GLU:H	2:L:189:GLU:CD	1.63	1.03
1:G:47:ARG:HH11	1:G:47:ARG:HB2	1.22	1.02
2:H:444:SER:HB2	2:H:470:ILE:HG13	1.41	1.02
1:C:278:ILE:H	1:C:278:ILE:HD12	1.17	1.02
2:F:375:ILE:H	2:F:375:ILE:HD12	1.20	1.02
1:A:383:GLU:HG3	1:A:438:ILE:HG23	1.42	1.01
2:L:538:ARG:HH11	2:L:538:ARG:HG3	1.26	1.01
1:A:232:GLN:HG2	1:A:233:ARG:NH1	1.76	1.00
1:G:153:PRO:HD3	1:G:316:VAL:HG23	1.43	1.00
1:I:169:LEU:HD23	1:I:312:ALA:HB1	1.41	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:538:ARG:HG3	2:J:538:ARG:HH11	1.21	1.00
1:K:47:ARG:HB2	1:K:47:ARG:NH1	1.77	1.00
1:C:231:ALA:HB3	1:C:244:MET:SD	2.01	1.00
1:K:175:VAL:HG21	1:K:309:ALA:HB2	1.41	1.00
1:K:153:PRO:HD3	1:K:316:VAL:HG23	1.40	0.99
2:H:137:ASP:OD1	2:H:139:THR:HG23	1.62	0.99
1:G:251:LEU:HD22	1:G:328:ARG:HE	1.25	0.99
2:F:217:THR:HG22	2:F:240:PHE:HE1	1.24	0.99
1:G:175:VAL:HG21	1:G:309:ALA:HB2	1.43	0.99
2:F:137:ASP:HB3	2:F:140:VAL:HG23	1.45	0.99
1:I:278:ILE:H	1:I:278:ILE:HD12	1.24	0.99
2:L:403:ASN:ND2	2:L:442:GLY:HA3	1.78	0.99
1:K:66:ARG:HB2	1:K:66:ARG:HH11	1.26	0.99
2:B:137:ASP:HB3	2:B:140:VAL:HG23	1.43	0.98
1:E:304:GLU:O	1:E:307:VAL:HG12	1.62	0.98
1:G:185:ALA:CB	1:G:243:ARG:HG3	1.93	0.98
1:A:274:ARG:HH22	1:A:320:THR:HG21	1.29	0.98
1:A:544:ARG:HG2	1:A:544:ARG:HH11	1.25	0.98
2:B:82:LEU:H	2:B:82:LEU:HD12	1.29	0.98
1:E:251:LEU:HD12	1:E:251:LEU:H	1.26	0.98
2:H:375:ILE:HG22	2:H:376:LEU:H	1.26	0.97
1:I:596:ASP:OD1	1:I:612:LEU:HB3	1.64	0.97
1:E:562:ARG:HG2	1:E:562:ARG:HH11	1.26	0.97
1:G:63:ARG:HH21	1:G:356:VAL:HG23	1.28	0.97
1:E:53:LEU:HD13	1:E:117:ALA:HB2	1.47	0.97
1:C:232:GLN:H	1:C:233:ARG:NH2	1.63	0.97
1:E:505:PRO:HB3	1:E:507:HIS:HB2	1.47	0.97
1:C:203:LEU:HD23	1:C:205:LYS:NZ	1.79	0.97
1:C:285:VAL:HG12	1:C:286:VAL:HG23	1.47	0.97
1:E:465:THR:HG22	1:E:467:LEU:H	1.27	0.97
1:K:251:LEU:HD13	1:K:327:GLU:HB2	1.44	0.96
1:E:308:ARG:HH11	1:E:308:ARG:HG3	1.31	0.96
1:E:588:TYR:HB3	1:E:598:LEU:HD11	1.46	0.96
1:E:175:VAL:HG21	1:E:309:ALA:HB2	1.46	0.96
2:H:265:VAL:O	2:H:269:VAL:HB	1.66	0.96
1:I:550:GLU:HG2	1:I:567:ARG:HD2	1.46	0.96
2:F:440:LEU:HD12	2:F:464:MET:HE2	1.48	0.96
2:F:84:ARG:HG2	2:F:84:ARG:HH11	1.30	0.95
1:G:169:LEU:HD23	1:G:313:ILE:HG22	1.48	0.95
1:I:306:ALA:HB1	1:I:321:VAL:HG21	1.45	0.95
1:K:152:PRO:HG3	1:K:315:TYR:CZ	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:398:ALA:HB2	1:I:464:ARG:HE	1.30	0.95
1:A:200:TYR:CE1	1:A:221:GLU:HA	2.01	0.95
1:E:384:VAL:HG13	1:E:470:LEU:HD22	1.46	0.95
1:G:328:ARG:HH11	1:G:328:ARG:HG3	1.29	0.95
2:H:305:ARG:HB3	2:H:305:ARG:HH11	1.30	0.95
1:A:153:PRO:HD3	1:A:316:VAL:CG2	1.97	0.95
1:I:132:LEU:HD23	1:I:138:PHE:CD2	2.02	0.95
1:K:140:ARG:CZ	1:K:140:ARG:HB3	1.94	0.94
1:A:186:GLN:NE2	1:A:190:THR:H	1.65	0.94
1:A:278:ILE:H	1:A:278:ILE:HD12	1.31	0.94
1:A:186:GLN:HE22	1:A:190:THR:H	1.10	0.94
1:A:567:ARG:HG3	1:A:567:ARG:HH11	1.30	0.94
1:G:200:TYR:HE1	1:G:221:GLU:HA	1.28	0.94
2:H:232:MET:HE3	2:H:239:ILE:HG13	1.49	0.94
2:L:350:LEU:HD23	2:L:350:LEU:H	1.29	0.94
2:B:444:SER:HB3	2:B:449:ASN:HD22	1.32	0.94
2:D:338:LEU:O	2:D:538:ARG:HD2	1.67	0.94
1:C:344:HIS:ND1	1:C:345:PRO:HD3	1.83	0.94
1:I:562:ARG:HB3	1:I:562:ARG:NH1	1.81	0.94
2:F:180:ARG:HH11	2:F:180:ARG:HG3	1.32	0.94
2:L:191:PHE:HD2	2:L:192:GLY:H	1.16	0.94
1:A:605:VAL:HG12	1:C:96:VAL:HG13	1.47	0.93
2:B:89:ARG:HH21	2:B:89:ARG:HG3	1.33	0.93
1:E:252:LYS:HE3	1:E:491:ARG:NH2	1.83	0.93
2:H:90:LEU:HB2	2:H:284:LEU:HD22	1.50	0.93
1:C:400:GLY:N	1:C:463:LEU:HD21	1.83	0.93
1:E:504:LEU:HB3	1:E:505:PRO:HD2	1.49	0.93
1:K:321:VAL:HG22	1:K:336:MET:HG3	1.48	0.93
2:D:311:LEU:HD12	2:D:342:SER:HB2	1.49	0.93
2:J:350:LEU:HD12	2:J:350:LEU:H	1.32	0.93
2:F:433:ARG:NH2	2:F:554:GLU:HG3	1.83	0.93
2:J:464:MET:HE2	2:J:519:PRO:HG3	1.50	0.93
1:A:671:GLY:O	1:A:687:ARG:HB3	1.67	0.92
2:D:464:MET:HE2	2:D:519:PRO:HG3	1.50	0.92
2:J:469:ARG:HG2	2:J:469:ARG:HH21	1.34	0.92
1:K:304:GLU:HA	1:K:307:VAL:HG12	1.50	0.92
1:I:300:ARG:NH1	1:I:300:ARG:HB2	1.82	0.92
2:L:123:ILE:HD11	2:L:165:LEU:HD13	1.52	0.92
2:D:272:VAL:HG22	2:J:420:LYS:HB3	1.49	0.92
2:L:83:VAL:HG13	2:L:84:ARG:H	1.34	0.92
2:D:350:LEU:H	2:D:350:LEU:CD2	1.83	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:334:VAL:O	2:J:338:LEU:HD12	1.70	0.92
1:C:325:LEU:HD23	1:C:326:ASP:N	1.85	0.91
1:C:443:THR:HG23	1:C:446:GLU:HB2	1.51	0.91
2:D:161:LEU:HB2	2:D:201:MET:HE2	1.52	0.91
2:B:83:VAL:HG13	2:B:84:ARG:N	1.84	0.91
2:L:518:HIS:ND1	2:L:519:PRO:HD2	1.85	0.91
2:B:487:ARG:HB3	2:B:497:LEU:HD22	1.51	0.91
2:B:33:THR:HB	2:B:312:TYR:CE2	2.06	0.91
1:K:526:ASP:N	1:K:526:ASP:OD2	2.03	0.91
2:L:161:LEU:HD22	2:L:201:MET:HG2	1.52	0.91
1:A:586:SER:O	1:A:587:GLN:HB2	1.69	0.91
1:I:53:LEU:HD13	1:I:117:ALA:HB2	1.51	0.91
1:K:344:HIS:ND1	1:K:345:PRO:HD3	1.87	0.90
1:K:465:THR:HG22	1:K:467:LEU:H	1.34	0.90
1:A:186:GLN:HE21	1:A:187:ASP:H	0.96	0.90
1:G:559:ASP:O	1:G:560:GLU:HG3	1.70	0.90
1:A:653:MET:HG2	1:A:654:ASN:H	1.36	0.90
2:B:145:TYR:HD1	2:B:149:THR:HB	1.33	0.90
1:C:170:MET:HE1	1:C:309:ALA:HB1	1.53	0.90
2:F:408:MET:HE3	2:F:409:VAL:H	1.37	0.90
1:E:270:TYR:H	1:E:372:GLN:HE22	1.12	0.90
1:G:268:CYS:SG	1:G:307:VAL:HG23	2.12	0.90
2:J:119:ILE:HG23	2:J:152:LYS:HD3	1.52	0.90
2:B:518:HIS:ND1	2:B:519:PRO:HD2	1.86	0.90
1:K:270:TYR:H	1:K:372:GLN:HE22	1.12	0.90
1:E:400:GLY:H	1:E:463:LEU:HD11	1.35	0.89
1:G:328:ARG:HG3	1:G:328:ARG:NH1	1.83	0.89
2:D:350:LEU:H	2:D:350:LEU:HD23	1.34	0.89
1:G:185:ALA:HB3	1:G:243:ARG:HG3	1.52	0.89
2:H:297:ARG:HB2	2:L:303:GLN:HE21	1.38	0.89
1:C:504:LEU:HB3	1:C:505:PRO:CD	2.02	0.89
1:G:398:ALA:HB2	1:G:464:ARG:HE	1.36	0.89
2:J:117:ALA:O	2:J:149:THR:HG23	1.72	0.89
1:K:428:PRO:HG2	1:K:429:PHE:CD2	2.08	0.89
2:L:208:GLN:HA	2:L:208:GLN:HE21	1.38	0.89
2:L:375:ILE:HB	2:L:377:PHE:CE1	2.08	0.89
2:D:400:PHE:HB2	2:D:438:THR:HG23	1.55	0.89
2:F:212:VAL:HG23	2:F:231:VAL:O	1.73	0.89
2:J:81:LEU:HD22	2:J:85:GLU:HB3	1.54	0.88
1:C:270:TYR:H	1:C:372:GLN:HE22	1.20	0.88
2:D:188:ARG:HH11	2:D:188:ARG:CB	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:549:ARG:HH11	1:I:549:ARG:HG3	1.38	0.88
2:L:377:PHE:N	2:L:377:PHE:HD1	1.70	0.88
1:C:47:ARG:HB2	1:C:47:ARG:HH11	1.36	0.88
2:H:217:THR:HG22	2:H:240:PHE:HE1	1.36	0.88
2:L:375:ILE:HG21	2:L:408:MET:HE2	1.56	0.88
2:J:233:VAL:HG13	2:J:279:ASP:HA	1.53	0.88
1:E:232:GLN:HG2	1:E:233:ARG:NH1	1.87	0.88
2:J:231:VAL:HG22	2:J:275:HIS:HB2	1.55	0.88
1:C:49:ILE:CD1	1:C:364:ARG:HG2	2.03	0.88
2:F:217:THR:HG22	2:F:240:PHE:CE1	2.08	0.88
1:G:160:MET:HE2	1:G:313:ILE:HD13	1.55	0.88
1:A:186:GLN:NE2	1:A:187:ASP:H	1.72	0.87
1:G:110:GLY:O	1:G:114:ILE:HG22	1.73	0.87
1:C:505:PRO:HB3	1:C:507:HIS:HB2	1.53	0.87
1:A:398:ALA:HB2	1:A:464:ARG:HE	1.39	0.87
1:A:153:PRO:HD3	1:A:316:VAL:HG23	1.55	0.87
1:G:278:ILE:H	1:G:278:ILE:CD1	1.83	0.87
1:I:170:MET:CE	1:I:309:ALA:HB1	2.05	0.87
2:D:492:ARG:HH22	2:J:74:ARG:NH2	1.72	0.87
1:E:153:PRO:HD3	1:E:316:VAL:HG23	1.56	0.87
1:I:352:GLY:C	1:I:353:LEU:HD23	1.99	0.87
1:A:393:GLY:O	1:A:396:LEU:HG	1.75	0.87
1:C:53:LEU:HD13	1:C:117:ALA:HB2	1.57	0.86
1:C:203:LEU:HD23	1:C:205:LYS:HZ3	1.39	0.86
1:K:285:VAL:HG12	1:K:286:VAL:HG22	1.56	0.86
1:E:272:ASN:OD1	1:E:377:LEU:HD13	1.75	0.86
1:G:251:LEU:CD2	1:G:328:ARG:HE	1.87	0.86
1:E:112:ARG:HH11	1:E:112:ARG:HG3	1.39	0.86
2:F:137:ASP:OD1	2:F:139:THR:HG23	1.76	0.86
2:L:33:THR:HB	2:L:312:TYR:CE2	2.10	0.86
1:A:62:CYS:O	1:A:66:ARG:HG3	1.75	0.86
2:B:210:ALA:HB3	2:B:230:THR:HG23	1.57	0.86
1:E:350:ILE:HA	1:E:440:TRP:CZ3	2.09	0.86
2:D:119:ILE:HG23	2:D:152:LYS:HD3	1.58	0.86
1:E:179:PRO:HB2	1:E:198:ILE:HG12	1.57	0.86
1:G:586:SER:O	1:G:587:GLN:HB2	1.73	0.86
1:K:69:ARG:NH1	1:K:69:ARG:HB2	1.91	0.86
1:A:202:VAL:HG23	1:A:248:LYS:HA	1.56	0.86
1:E:339:ARG:HG3	1:E:339:ARG:HH11	1.40	0.86
2:B:33:THR:HB	2:B:312:TYR:HE2	1.39	0.85
1:E:232:GLN:HG2	1:E:233:ARG:HH12	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:560:VAL:HG23	2:H:202:SER:OG	1.76	0.85
2:F:82:LEU:HD12	2:F:83:VAL:H	1.40	0.85
2:B:81:LEU:HD11	2:B:89:ARG:NH2	1.90	0.85
1:E:613:ARG:O	1:E:614:ARG:HD2	1.76	0.85
1:I:612:LEU:N	1:I:612:LEU:HD12	1.90	0.85
2:L:81:LEU:HD13	2:L:280:ASP:HB2	1.58	0.85
2:L:231:VAL:CG2	2:L:275:HIS:HB2	2.06	0.85
1:E:562:ARG:HG2	1:E:562:ARG:NH1	1.88	0.85
1:A:188:LEU:HD23	1:A:228:LEU:HD23	1.59	0.85
1:C:451:LEU:O	1:C:455:LEU:HD12	1.75	0.85
2:H:161:LEU:O	2:H:161:LEU:HD12	1.77	0.85
2:H:207:PRO:HG2	2:H:294:LEU:CD2	2.06	0.85
1:I:412:PRO:HB2	1:I:450:ARG:HD3	1.59	0.85
2:J:83:VAL:HG13	2:J:84:ARG:H	1.42	0.85
2:L:53:VAL:O	2:L:57:ARG:HG3	1.76	0.85
1:K:264:ARG:HB3	1:K:264:ARG:HH11	1.41	0.85
2:B:467:ASN:H	2:B:467:ASN:HD22	1.21	0.84
1:I:607:ARG:HB3	1:I:607:ARG:HH11	1.41	0.84
2:F:62:ARG:O	2:F:65:GLU:HB2	1.77	0.84
2:J:440:LEU:HD12	2:J:464:MET:HG3	1.57	0.84
2:H:171:VAL:HG23	2:H:212:VAL:HA	1.59	0.84
1:I:519:SER:HB2	1:I:613:ARG:HE	1.41	0.84
1:I:605:VAL:HG12	1:K:96:VAL:CG1	2.07	0.84
1:K:150:LEU:HD23	1:K:359:GLN:HB3	1.59	0.84
1:K:309:ALA:O	1:K:312:ALA:HB3	1.75	0.84
1:K:57:ARG:HD2	1:K:107:TYR:CE2	2.12	0.84
1:C:569:ALA:O	1:C:571:PRO:HD3	1.78	0.84
1:E:198:ILE:HG23	1:E:248:LYS:HG2	1.59	0.84
2:B:311:LEU:HD12	2:B:342:SER:HB2	1.60	0.84
2:L:497:LEU:HD21	2:L:505:ILE:HD12	1.60	0.84
1:K:150:LEU:CD2	1:K:359:GLN:HB3	2.07	0.84
1:A:53:LEU:HD22	1:A:117:ALA:HB2	1.60	0.83
1:A:490:ALA:O	1:A:493:GLN:HB2	1.77	0.83
2:D:400:PHE:HB2	2:D:438:THR:CG2	2.07	0.83
2:L:189:GLU:CD	2:L:189:GLU:N	2.32	0.83
1:G:536:PRO:HB3	2:H:363:HIS:CE1	2.13	0.83
1:K:370:LEU:HD22	1:K:374:GLN:HB3	1.58	0.83
2:B:145:TYR:CD1	2:B:149:THR:HB	2.12	0.83
2:F:83:VAL:HG13	2:F:84:ARG:H	1.43	0.83
1:A:232:GLN:H	1:A:233:ARG:CZ	1.91	0.83
1:E:129:TYR:CE2	1:E:342:VAL:HA	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:ARG:NH1	1:E:300:ARG:HB2	1.93	0.83
1:G:380:HIS:NE2	1:G:444:ARG:HD2	1.94	0.83
2:L:525:ARG:HG3	2:L:525:ARG:HH11	1.42	0.83
2:H:213:MET:HE2	2:H:280:ASP:HA	1.59	0.83
2:J:444:SER:HB2	2:J:470:ILE:HG13	1.59	0.83
2:B:83:VAL:CG1	2:B:84:ARG:H	1.92	0.83
2:H:109:TYR:HE1	2:H:148:LEU:HD12	1.43	0.83
1:C:351:THR:OG1	1:C:352:GLY:N	2.07	0.83
2:D:230:THR:CG2	2:D:273:ALA:HA	2.08	0.83
1:G:251:LEU:HD22	1:G:328:ARG:NE	1.93	0.83
2:H:246:LEU:H	2:H:246:LEU:HD12	1.42	0.83
1:K:82:ILE:HD11	1:K:430:TYR:CE1	2.14	0.83
2:L:150:VAL:HG21	2:L:184:VAL:HG13	1.61	0.83
2:L:377:PHE:N	2:L:377:PHE:CD1	2.44	0.83
1:C:263:ASP:CB	1:C:362:VAL:HG12	2.09	0.83
2:D:41:GLU:O	2:D:44:ALA:HB3	1.78	0.83
2:D:164:ARG:HB3	2:D:551:ALA:HB2	1.61	0.83
1:G:496:LEU:O	1:G:497:LEU:HD23	1.79	0.83
2:H:231:VAL:CG2	2:H:275:HIS:HB2	2.08	0.83
1:A:269:LEU:HD12	1:A:375:VAL:HG22	1.61	0.82
1:A:396:LEU:HD12	1:A:464:ARG:NH1	1.93	0.82
1:A:203:LEU:HG	1:A:204:LEU:N	1.93	0.82
1:A:231:ALA:HB3	1:A:244:MET:HE3	1.59	0.82
2:F:305:ARG:CB	2:F:305:ARG:HH11	1.92	0.82
2:H:299:GLN:HB2	2:H:552:PRO:HD3	1.61	0.82
1:I:588:TYR:HB3	1:I:598:LEU:HD11	1.60	0.82
1:K:386:LEU:HD21	1:K:467:LEU:HD13	1.60	0.82
1:A:268:CYS:SG	1:A:307:VAL:HG23	2.18	0.82
1:C:496:LEU:O	1:C:497:LEU:HD23	1.78	0.82
1:E:187:ASP:OD1	1:E:189:GLU:HB2	1.79	0.82
2:H:350:LEU:H	2:H:350:LEU:CD2	1.91	0.82
1:A:269:LEU:HD12	1:A:375:VAL:CG2	2.09	0.82
1:G:313:ILE:HD11	1:G:315:TYR:HD2	1.43	0.82
2:H:433:ARG:H	2:H:556:THR:HG23	1.44	0.82
1:C:607:ARG:HB2	1:C:607:ARG:HH11	1.44	0.82
2:H:317:LEU:HA	2:H:320:VAL:HG23	1.60	0.82
2:L:207:PRO:HG2	2:L:294:LEU:HD22	1.59	0.82
2:D:278:GLU:HG2	2:D:282:HIS:ND1	1.93	0.82
2:D:375:ILE:HG22	2:D:376:LEU:H	1.45	0.82
1:A:200:TYR:HE1	1:A:221:GLU:HA	1.44	0.82
1:A:695:LYS:HB2	1:A:715:ASP:HB3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:PHE:HD2	2:B:192:GLY:H	1.28	0.82
1:E:285:VAL:HG12	1:E:286:VAL:HG23	1.60	0.82
1:E:490:ALA:O	1:E:493:GLN:HB2	1.80	0.82
1:G:186:GLN:NE2	1:G:190:THR:H	1.77	0.82
1:I:607:ARG:HG3	1:K:94:ILE:HG13	1.60	0.82
1:K:379:GLY:HA3	1:K:440:TRP:CZ2	2.15	0.82
1:C:108:LEU:HD23	1:C:132:LEU:CD1	2.09	0.82
1:C:611:ALA:CB	1:C:620:LEU:HD13	2.09	0.82
1:E:384:VAL:CG1	1:E:470:LEU:HD22	2.09	0.81
2:F:30:ILE:HD12	2:F:311:LEU:HD11	1.62	0.81
2:F:57:ARG:HH11	2:F:57:ARG:HG3	1.43	0.81
2:J:473:MET:HE2	2:J:477:GLN:HB3	1.62	0.81
2:B:460:ARG:NH1	2:B:548:ALA:HB1	1.95	0.81
1:G:201:PRO:HG2	1:G:328:ARG:HH21	1.44	0.81
1:I:525:ARG:HB3	1:I:525:ARG:HH11	1.46	0.81
2:B:486:LYS:HG3	2:B:497:LEU:HD11	1.61	0.81
1:I:344:HIS:HB2	1:I:355:LEU:HD12	1.62	0.81
2:J:495:GLN:HG2	2:J:496:GLN:N	1.89	0.81
2:H:164:ARG:HD3	2:H:550:ASN:O	1.81	0.81
1:A:103:PRO:O	1:A:108:LEU:HD12	1.80	0.81
1:C:561:ARG:HB3	1:C:561:ARG:NH1	1.96	0.81
2:J:375:ILE:HD12	2:J:375:ILE:H	1.45	0.81
2:J:518:HIS:ND1	2:J:519:PRO:HD2	1.94	0.81
2:L:62:ARG:HG2	2:L:62:ARG:HH11	1.45	0.81
1:A:249:TYR:HD2	1:A:250:LEU:H	1.23	0.81
2:D:472:VAL:HG22	2:D:473:MET:HG2	1.62	0.81
1:I:73:ILE:HD11	1:I:364:ARG:HH22	1.46	0.81
1:K:469:PHE:O	1:K:473:ILE:HG22	1.81	0.81
1:K:539:ARG:HH21	2:L:363:HIS:CE1	1.99	0.81
1:A:562:ARG:HH11	1:A:562:ARG:CB	1.94	0.81
1:C:201:PRO:HD2	1:C:328:ARG:NH2	1.95	0.81
2:F:48:THR:O	2:F:52:GLN:HG3	1.80	0.81
2:F:518:HIS:ND1	2:F:519:PRO:HD2	1.96	0.81
2:J:201:MET:CE	2:J:208:GLN:HE22	1.93	0.81
1:K:350:ILE:HA	1:K:440:TRP:HZ3	1.44	0.81
1:K:414:ARG:HB3	1:K:454:MET:HE3	1.63	0.81
2:B:420:LYS:HB3	2:L:272:VAL:HG22	1.60	0.80
2:D:230:THR:HG22	2:D:273:ALA:HA	1.63	0.80
1:G:232:GLN:HG2	1:G:233:ARG:NH1	1.95	0.80
1:K:53:LEU:HD13	1:K:117:ALA:HB2	1.62	0.80
1:A:442:GLU:OE2	1:A:446:GLU:HG2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ILE:HG23	1:C:488:PHE:HD2	1.44	0.80
1:E:251:LEU:HD12	1:E:251:LEU:N	1.96	0.80
2:J:444:SER:HB3	2:J:449:ASN:HD22	1.46	0.80
1:E:108:LEU:HA	1:E:132:LEU:HD21	1.63	0.80
2:F:490:ALA:O	2:F:495:GLN:HG3	1.80	0.80
1:I:476:HIS:ND1	1:I:477:PRO:HD2	1.97	0.80
1:A:292:PRO:HG2	1:A:484:LEU:HD11	1.63	0.80
2:F:161:LEU:HD22	2:F:201:MET:HG2	1.64	0.80
2:H:350:LEU:HD23	2:H:350:LEU:N	1.95	0.80
2:H:400:PHE:CE2	2:H:453:CYS:HB2	2.16	0.80
2:L:464:MET:HE1	2:L:522:SER:OG	1.81	0.80
1:C:218:VAL:HA	1:C:223:GLU:OE2	1.81	0.80
2:H:35:ILE:HD12	2:H:320:VAL:HG13	1.61	0.80
2:L:54:ASN:HA	2:L:57:ARG:HD3	1.64	0.80
1:A:469:PHE:HZ	1:A:489:ILE:HD11	1.47	0.80
2:B:375:ILE:HG22	2:B:376:LEU:H	1.46	0.80
2:B:473:MET:HE1	2:L:246:LEU:CD2	2.09	0.80
1:E:536:PRO:HB3	2:F:363:HIS:CE1	2.17	0.80
2:J:35:ILE:HD11	2:J:337:ARG:HH12	1.45	0.80
1:K:590:LEU:HD13	1:K:598:LEU:HD12	1.64	0.80
1:K:66:ARG:HH11	1:K:66:ARG:CB	1.94	0.80
1:K:405:TYR:HB3	1:K:422:GLU:HB2	1.64	0.80
1:A:492:HIS:ND1	1:A:492:HIS:N	2.29	0.80
2:B:439:VAL:HG22	2:B:463:TRP:HB2	1.63	0.80
1:G:257:GLU:O	1:G:273:GLU:HB2	1.82	0.80
1:K:490:ALA:O	1:K:493:GLN:HB2	1.82	0.80
2:B:138:ALA:HB2	2:B:172:ASP:OD2	1.80	0.80
1:C:186:GLN:NE2	1:C:190:THR:H	1.80	0.80
2:L:403:ASN:CG	2:L:442:GLY:HA3	2.06	0.80
1:C:469:PHE:CE2	1:C:473:ILE:HD12	2.17	0.79
1:K:69:ARG:HB2	1:K:69:ARG:HH11	1.44	0.79
1:K:384:VAL:CG1	1:K:470:LEU:HD22	2.11	0.79
2:J:331:VAL:HB	2:J:373:ASN:ND2	1.97	0.79
1:G:150:LEU:HD23	1:G:363:ALA:HB2	1.64	0.79
1:I:73:ILE:HD11	1:I:364:ARG:NH2	1.96	0.79
2:J:375:ILE:HG22	2:J:376:LEU:H	1.47	0.79
2:J:538:ARG:HG3	2:J:538:ARG:NH1	1.90	0.79
1:A:681:LYS:HG2	3:A:801:BTI:O11	1.83	0.79
1:K:463:LEU:HD22	1:K:464:ARG:H	1.47	0.79
1:K:505:PRO:CB	1:K:507:HIS:HB2	2.13	0.79
1:A:278:ILE:HG21	1:A:473:ILE:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ASP:O	1:C:84:ARG:HG2	1.81	0.79
2:H:172:ASP:OD1	2:H:214:GLY:HA3	1.83	0.79
1:A:440:TRP:CD1	1:A:440:TRP:C	2.60	0.79
1:C:501:GLN:HE21	1:C:504:LEU:HD23	1.46	0.79
1:E:395:PHE:O	1:E:397:PRO:HD3	1.81	0.79
1:G:231:ALA:HB3	1:G:244:MET:HE3	1.64	0.79
1:C:328:ARG:HG3	1:C:328:ARG:NH1	1.97	0.79
2:H:376:LEU:HD23	2:H:380:ALA:HB3	1.62	0.79
1:I:258:ILE:HD13	1:I:303:GLY:HA2	1.65	0.79
1:A:280:ARG:O	1:A:281:ARG:C	2.25	0.79
2:D:299:GLN:CB	2:D:552:PRO:HD3	2.13	0.79
1:E:252:LYS:HE3	1:E:491:ARG:HH22	1.45	0.79
1:G:70:ALA:O	1:K:450:ARG:HD3	1.82	0.79
2:H:212:VAL:O	2:H:233:VAL:HG23	1.81	0.79
1:C:605:VAL:HG23	1:C:605:VAL:O	1.81	0.79
2:F:35:ILE:HD12	2:F:337:ARG:NH2	1.97	0.79
2:H:231:VAL:HG23	2:H:275:HIS:HB2	1.65	0.79
1:I:602:VAL:HG23	1:I:605:VAL:HG23	1.63	0.79
1:K:63:ARG:HA	1:K:66:ARG:HD3	1.65	0.79
1:K:251:LEU:CD1	1:K:327:GLU:HB2	2.13	0.79
1:K:512:ALA:HB1	1:K:629:ILE:HD13	1.64	0.79
1:C:294:LEU:CD1	1:C:299:ARG:HH12	1.96	0.79
1:C:607:ARG:HH11	1:C:607:ARG:CB	1.96	0.79
1:A:605:VAL:HG23	1:A:605:VAL:O	1.83	0.78
1:C:334:MET:HA	1:C:334:MET:CE	2.12	0.78
1:G:605:VAL:HG23	1:G:605:VAL:O	1.81	0.78
1:K:279:GLN:HE21	1:K:282:HIS:HA	1.46	0.78
1:K:463:LEU:CD2	1:K:464:ARG:H	1.94	0.78
1:C:450:ARG:O	1:C:453:ALA:HB3	1.83	0.78
2:F:81:LEU:HD12	2:F:280:ASP:HB3	1.64	0.78
1:C:108:LEU:HD23	1:C:132:LEU:HD13	1.63	0.78
2:D:217:THR:CG2	2:D:240:PHE:HE1	1.94	0.78
2:J:332:ARG:HH11	2:J:332:ARG:HG3	1.47	0.78
2:L:193:ARG:HD2	2:L:196:PHE:HD2	1.47	0.78
1:A:682:MET:HA	2:F:326:LYS:HB3	1.66	0.78
2:H:305:ARG:HB3	2:H:305:ARG:NH1	1.99	0.78
1:I:279:GLN:O	1:I:489:ILE:HG21	1.81	0.78
2:J:300:GLY:HA3	2:J:549:LEU:HD23	1.64	0.78
1:I:255:HIS:CE1	1:I:322:GLU:HG2	2.18	0.78
1:G:186:GLN:HE22	1:G:190:THR:H	1.28	0.78
1:I:118:LEU:HD13	1:I:147:LEU:HD21	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:145:TYR:HD1	2:J:149:THR:HB	1.48	0.78
1:K:378:ASN:O	1:K:440:TRP:CH2	2.34	0.78
1:K:566:LEU:C	1:K:567:ARG:HD3	2.09	0.78
2:B:487:ARG:HB2	2:B:497:LEU:HB2	1.65	0.78
1:E:82:ILE:HD11	1:E:430:TYR:CE1	2.19	0.78
2:F:444:SER:HB2	2:F:470:ILE:HG13	1.64	0.78
1:I:473:ILE:HB	1:I:496:LEU:HD13	1.64	0.78
1:A:273:GLU:OE1	1:A:273:GLU:N	2.16	0.78
1:E:505:PRO:HB3	1:E:507:HIS:CB	2.14	0.78
1:K:109:ARG:HB3	1:K:109:ARG:HH11	1.48	0.78
1:A:186:GLN:HE21	1:A:187:ASP:N	1.80	0.78
2:B:346:GLU:OE1	2:B:356:VAL:HG13	1.82	0.78
1:E:150:LEU:HD22	1:E:359:GLN:HB3	1.66	0.78
2:H:311:LEU:HB2	2:H:342:SER:OG	1.84	0.78
2:B:467:ASN:HD22	2:B:467:ASN:N	1.82	0.77
1:E:264:ARG:HG2	1:E:264:ARG:HH11	1.49	0.77
2:H:307:PRO:HB3	2:H:363:HIS:HD2	1.47	0.77
1:K:46:TYR:HE1	1:K:366:GLU:HG3	1.47	0.77
1:K:274:ARG:HH11	1:K:347:THR:HB	1.49	0.77
2:B:425:LEU:O	2:B:429:VAL:HG23	1.83	0.77
1:C:251:LEU:HD11	1:C:328:ARG:HH21	1.50	0.77
1:G:185:ALA:HB2	1:G:243:ARG:HG3	1.67	0.77
1:G:249:TYR:HD2	1:G:250:LEU:N	1.81	0.77
1:K:105:ASP:O	1:K:109:ARG:HD2	1.84	0.77
2:L:365:TYR:HB2	2:L:545:LEU:HD13	1.65	0.77
2:B:117:ALA:O	2:B:149:THR:HG23	1.83	0.77
2:B:231:VAL:HG22	2:B:275:HIS:HB2	1.64	0.77
1:I:150:LEU:HD22	1:I:359:GLN:HB3	1.66	0.77
1:A:384:VAL:HG11	1:A:470:LEU:HD13	1.66	0.77
2:B:48:THR:O	2:B:52:GLN:HG3	1.85	0.77
1:C:294:LEU:HD11	1:C:299:ARG:HH12	1.49	0.77
2:D:389:GLU:HG2	2:H:560:VAL:HG13	1.66	0.77
1:A:380:HIS:NE2	1:A:444:ARG:HD2	1.99	0.77
1:C:53:LEU:HD13	1:C:117:ALA:CB	2.13	0.77
2:D:242:ALA:HB1	2:D:246:LEU:HD22	1.66	0.77
1:K:396:LEU:HD12	1:K:464:ARG:HH22	1.50	0.77
1:E:165:ALA:O	1:E:169:LEU:HD13	1.83	0.77
1:E:611:ALA:HB2	1:E:620:LEU:HD13	1.67	0.77
1:I:599:VAL:HG22	1:I:608:ARG:CB	2.14	0.77
2:L:464:MET:HE2	2:L:470:ILE:HD12	1.65	0.77
1:G:203:LEU:HD12	1:G:204:LEU:N	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:198:GLN:HG2	2:H:208:GLN:OE1	1.85	0.77
2:H:498:GLY:O	2:H:500:GLU:N	2.17	0.77
1:K:567:ARG:HH11	1:K:567:ARG:HG3	1.49	0.77
1:A:662:VAL:HG21	1:A:674:LEU:CD2	2.15	0.77
1:E:616:ARG:HG3	1:E:616:ARG:O	1.84	0.77
2:J:41:GLU:O	2:J:44:ALA:HB3	1.84	0.77
1:A:525:ARG:HB3	1:A:525:ARG:NH1	2.00	0.77
1:C:228:LEU:HD23	1:C:229:SER:N	1.99	0.77
1:G:182:HIS:HB3	1:G:245:LEU:CD2	2.14	0.77
2:H:81:LEU:CD2	2:H:85:GLU:HB3	2.15	0.77
1:I:602:VAL:O	1:I:605:VAL:HG22	1.85	0.77
1:K:397:PRO:HB3	1:K:432:PRO:HG3	1.65	0.77
2:L:161:LEU:HD22	2:L:201:MET:CG	2.14	0.77
1:A:395:PHE:O	1:A:397:PRO:HD3	1.85	0.76
1:C:501:GLN:NE2	1:C:504:LEU:HD23	2.00	0.76
2:H:217:THR:HG22	2:H:240:PHE:CE1	2.20	0.76
2:J:469:ARG:HG2	2:J:469:ARG:NH2	1.99	0.76
1:A:232:GLN:HG2	1:A:233:ARG:HH11	1.48	0.76
1:C:504:LEU:CB	1:C:505:PRO:HD2	2.12	0.76
2:D:441:ILE:HG22	2:D:465:TRP:CD2	2.21	0.76
2:J:289:ARG:O	2:J:292:ALA:HB3	1.85	0.76
1:A:662:VAL:HG22	1:A:674:LEU:HA	1.67	0.76
1:A:53:LEU:HD12	1:A:76:VAL:O	1.84	0.76
1:C:300:ARG:NH1	1:C:300:ARG:HB2	1.99	0.76
1:C:503:ALA:O	1:C:504:LEU:O	2.02	0.76
2:F:35:ILE:HD13	2:F:320:VAL:HG22	1.65	0.76
2:F:117:ALA:O	2:F:149:THR:HG23	1.84	0.76
2:F:202:SER:OG	2:H:560:VAL:HG23	1.84	0.76
1:G:170:MET:SD	1:G:309:ALA:HB1	2.25	0.76
2:H:275:HIS:HE1	2:L:347:PHE:HA	1.50	0.76
1:C:49:ILE:N	1:C:49:ILE:HD12	2.00	0.76
2:D:188:ARG:HB3	2:D:188:ARG:NH1	1.99	0.76
2:D:433:ARG:HG2	2:D:556:THR:HG23	1.67	0.76
2:F:390:LEU:O	2:F:394:ARG:HG3	1.85	0.76
2:H:498:GLY:C	2:H:500:GLU:H	1.93	0.76
2:L:74:ARG:NH2	2:L:78:ARG:HH12	1.83	0.76
2:B:155:ARG:O	2:B:159:ILE:HD13	1.85	0.76
1:I:278:ILE:HG21	1:I:473:ILE:HD11	1.67	0.76
1:A:544:ARG:HG2	1:A:544:ARG:NH1	1.94	0.76
1:C:383:GLU:HB2	1:C:438:ILE:HG23	1.67	0.76
2:D:89:ARG:HH21	2:D:89:ARG:HG3	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:SER:O	2:B:152:LYS:HE3	1.86	0.76
1:C:607:ARG:HB2	1:C:607:ARG:NH1	2.00	0.76
1:E:504:LEU:CB	1:E:505:PRO:HD2	2.14	0.76
1:G:526:ASP:OD2	1:G:526:ASP:N	2.18	0.76
2:H:417:GLY:C	2:H:419:ALA:H	1.94	0.76
2:L:483:ALA:HB3	2:L:506:LYS:HE2	1.68	0.76
1:I:152:PRO:HG2	1:I:338:THR:HB	1.68	0.76
1:K:257:GLU:O	1:K:273:GLU:HB2	1.85	0.76
1:K:605:VAL:HG23	1:K:605:VAL:O	1.85	0.76
1:C:440:TRP:CD1	1:C:440:TRP:C	2.64	0.76
1:E:387:TYR:CE1	1:E:433:MET:HB2	2.20	0.76
2:F:272:VAL:HG22	2:H:420:LYS:HB3	1.66	0.76
1:G:204:LEU:CD2	1:G:246:VAL:HG22	2.15	0.76
1:K:350:ILE:HA	1:K:440:TRP:CZ3	2.20	0.76
1:K:536:PRO:HD3	2:L:363:HIS:CD2	2.20	0.76
1:K:619:PHE:HB3	1:K:626:LEU:HD11	1.67	0.76
1:C:50:GLN:HB2	1:C:123:GLN:NE2	2.01	0.75
2:D:54:ASN:HA	2:D:57:ARG:HG3	1.68	0.75
1:G:473:ILE:HB	1:G:496:LEU:HD13	1.66	0.75
2:J:75:HIS:HE1	2:J:80:LYS:HE2	1.50	0.75
1:C:285:VAL:HG12	1:C:286:VAL:CG2	2.15	0.75
1:C:390:ASP:OD1	1:C:393:GLY:HA3	1.87	0.75
1:E:188:LEU:HD23	1:E:228:LEU:HD23	1.68	0.75
2:F:355:LEU:O	2:F:383:LYS:HE2	1.86	0.75
2:H:57:ARG:HG3	2:H:57:ARG:HH11	1.49	0.75
2:J:402:GLN:NE2	2:J:449:ASN:HA	2.01	0.75
1:A:201:PRO:HD2	1:A:328:ARG:HH21	1.50	0.75
1:A:697:LEU:HB3	1:A:712:VAL:HG22	1.68	0.75
2:D:422:GLY:O	2:D:426:VAL:HG23	1.87	0.75
2:F:72:GLN:HG3	2:F:82:LEU:HD21	1.68	0.75
2:F:168:ILE:HA	2:F:209:ILE:HG22	1.66	0.75
2:F:376:LEU:HG	2:F:404:ILE:CD1	2.15	0.75
2:F:525:ARG:HH11	2:F:525:ARG:HG3	1.51	0.75
2:H:109:TYR:CE1	2:H:148:LEU:HD12	2.21	0.75
1:I:104:ALA:HA	1:I:108:LEU:HD12	1.67	0.75
1:I:340:LEU:HD11	1:I:356:VAL:HG23	1.67	0.75
2:J:375:ILE:HD12	2:J:375:ILE:N	2.00	0.75
1:A:705:VAL:HG21	1:A:711:LEU:HD21	1.68	0.75
1:C:611:ALA:HB2	1:C:620:LEU:CD1	2.14	0.75
1:G:350:ILE:HD12	1:G:377:LEU:HD13	1.68	0.75
2:J:161:LEU:CD1	2:J:201:MET:HG2	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:561:ARG:H	1:E:561:ARG:HD2	1.51	0.75
1:G:190:THR:HG23	1:G:193:ARG:HH21	1.52	0.75
1:I:269:LEU:HA	1:I:372:GLN:NE2	2.02	0.75
2:L:441:ILE:HG22	2:L:465:TRP:CD2	2.22	0.75
1:G:150:LEU:CD2	1:G:363:ALA:HB2	2.16	0.75
2:L:299:GLN:OE1	2:L:552:PRO:HD3	1.86	0.75
1:C:395:PHE:O	1:C:397:PRO:HD3	1.86	0.75
1:E:278:ILE:HD11	1:E:484:LEU:HD23	1.69	0.75
2:F:161:LEU:HD22	2:F:201:MET:CG	2.17	0.75
1:G:254:ARG:HH12	1:G:293:GLY:H	1.32	0.75
1:G:280:ARG:O	1:G:281:ARG:C	2.30	0.75
1:A:666:GLN:O	1:A:693:VAL:HG13	1.87	0.74
1:E:170:MET:SD	1:E:309:ALA:HB1	2.27	0.74
2:F:218:ALA:O	2:F:221:ALA:HB3	1.87	0.74
1:A:525:ARG:HH11	1:A:525:ARG:CB	1.97	0.74
2:B:501:GLU:O	2:B:505:ILE:HG13	1.87	0.74
1:C:273:GLU:OE1	1:C:273:GLU:N	2.20	0.74
1:C:328:ARG:HG3	1:C:328:ARG:HH11	1.52	0.74
1:G:519:SER:HB3	1:G:613:ARG:HE	1.52	0.74
1:C:53:LEU:HD13	1:C:117:ALA:CA	2.17	0.74
1:G:440:TRP:C	1:G:440:TRP:CD1	2.65	0.74
2:J:35:ILE:HD11	2:J:337:ARG:NH1	2.02	0.74
1:C:233:ARG:HB3	1:C:233:ARG:HH11	1.52	0.74
1:C:315:TYR:OH	1:C:338:THR:HA	1.87	0.74
1:E:605:VAL:HG23	1:E:605:VAL:O	1.86	0.74
2:F:376:LEU:HG	2:F:404:ILE:HD11	1.67	0.74
2:H:375:ILE:HG22	2:H:376:LEU:N	2.03	0.74
2:H:476:GLU:HA	2:H:510:LEU:HD21	1.69	0.74
1:K:108:LEU:HD23	1:K:132:LEU:HD12	1.69	0.74
1:A:249:TYR:HD2	1:A:250:LEU:N	1.85	0.74
1:A:657:ILE:CD1	1:A:699:CYS:HB2	2.18	0.74
2:B:244:PRO:HA	2:B:247:VAL:HG12	1.69	0.74
1:C:135:ASN:OD1	1:C:135:ASN:O	2.05	0.74
1:G:204:LEU:HD23	1:G:246:VAL:HG22	1.69	0.74
1:G:519:SER:CB	1:G:613:ARG:HE	1.99	0.74
1:I:261:PHE:CE1	1:I:318:ALA:HB2	2.22	0.74
1:C:81:ASP:OD2	1:C:100:GLY:HA2	1.87	0.74
1:C:300:ARG:HB2	1:C:300:ARG:CZ	2.17	0.74
2:F:305:ARG:HH11	2:F:305:ARG:HB2	1.52	0.74
1:K:508:PHE:CZ	1:K:627:LEU:HD12	2.23	0.74
2:B:403:ASN:ND2	2:B:442:GLY:HA3	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:177:ASN:OD1	2:D:180:ARG:HG3	1.88	0.74
2:D:344:PHE:CZ	2:D:358:GLY:HA3	2.23	0.74
2:H:315:GLU:H	2:H:315:GLU:CD	1.95	0.74
1:A:491:ARG:HB3	1:A:492:HIS:ND1	2.03	0.74
1:C:169:LEU:CD2	1:C:313:ILE:HG12	2.18	0.74
1:K:452:LEU:CD2	1:K:474:LEU:HB3	2.17	0.74
2:F:225:ALA:O	2:H:562:ARG:HD2	1.87	0.74
2:F:432:ALA:HA	2:F:556:THR:HG21	1.69	0.74
1:K:270:TYR:N	1:K:372:GLN:HE22	1.85	0.74
1:K:408:ALA:HB2	1:K:457:GLU:HB2	1.69	0.74
1:E:251:LEU:HD11	1:E:328:ARG:CZ	2.17	0.73
2:F:241:LEU:HB2	2:H:414:GLU:OE2	1.88	0.73
1:G:607:ARG:NH1	1:G:607:ARG:HB2	2.02	0.73
1:K:302:MET:HG2	1:K:331:PHE:CD1	2.23	0.73
2:D:53:VAL:HG21	2:D:318:TYR:HE1	1.53	0.73
2:F:469:ARG:HG2	2:F:469:ARG:HH21	1.51	0.73
1:I:169:LEU:HD23	1:I:312:ALA:CB	2.19	0.73
2:F:109:TYR:CZ	2:F:148:LEU:HD12	2.23	0.73
2:F:243:GLY:O	2:F:247:VAL:HG23	1.88	0.73
1:G:383:GLU:HB2	1:G:438:ILE:HG23	1.68	0.73
1:K:287:GLU:HG2	1:K:343:GLU:HG3	1.70	0.73
1:K:549:ARG:HH21	1:K:571:PRO:HA	1.51	0.73
1:G:53:LEU:HD11	1:G:78:VAL:CG1	2.18	0.73
1:I:504:LEU:CD2	1:I:505:PRO:HD2	2.18	0.73
1:K:152:PRO:HG3	1:K:315:TYR:CE1	2.24	0.73
1:K:304:GLU:HA	1:K:307:VAL:CG1	2.17	0.73
1:A:496:LEU:O	1:A:497:LEU:HD23	1.89	0.73
1:C:322:GLU:OE2	1:C:337:ASN:ND2	2.21	0.73
2:F:433:ARG:HH22	2:F:554:GLU:HG3	1.52	0.73
1:G:452:LEU:CD2	1:G:474:LEU:HB3	2.19	0.73
1:A:339:ARG:HH11	1:A:339:ARG:HG3	1.53	0.73
1:A:655:GLY:N	2:H:251:THR:HB	2.04	0.73
2:D:178:LEU:CD1	2:J:478:ALA:HB1	2.19	0.73
1:G:390:ASP:OD1	1:G:393:GLY:HA3	1.89	0.73
1:I:358:TRP:O	1:I:362:VAL:HG22	1.89	0.73
2:L:432:ALA:HA	2:L:556:THR:HG21	1.69	0.73
1:A:267:HIS:HB3	1:A:368:LEU:HD12	1.69	0.73
1:C:258:ILE:HD11	1:C:302:MET:HB3	1.70	0.73
1:C:280:ARG:O	1:C:281:ARG:C	2.32	0.73
1:E:623:GLU:CD	1:E:623:GLU:N	2.47	0.73
2:F:375:ILE:H	2:F:375:ILE:CD1	1.94	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:ARG:HG3	1:E:48:SER:N	2.03	0.73
1:E:459:SER:HB3	1:E:621:GLU:OE1	1.89	0.73
1:G:169:LEU:CD2	1:G:313:ILE:HG22	2.19	0.73
1:I:278:ILE:H	1:I:278:ILE:CD1	2.00	0.73
1:I:280:ARG:O	1:I:280:ARG:HD3	1.88	0.73
1:K:550:GLU:HG2	1:K:567:ARG:NH1	2.03	0.73
1:I:491:ARG:HD2	1:I:492:HIS:CE1	2.23	0.73
2:J:490:ALA:HB1	2:J:495:GLN:OE1	1.88	0.73
1:K:505:PRO:HB2	1:K:507:HIS:HB2	1.68	0.73
1:K:543:TRP:HB3	2:L:96:PRO:HB3	1.71	0.73
1:C:232:GLN:N	1:C:233:ARG:NH2	2.36	0.73
2:D:507:ALA:N	2:D:508:PRO:HD2	2.03	0.73
1:E:390:ASP:CG	1:E:464:ARG:HD2	2.14	0.73
1:E:541:ASP:HB2	1:E:549:ARG:NH2	2.04	0.73
2:F:100:LEU:HD11	2:F:132:MET:HE1	1.71	0.73
1:I:272:ASN:CG	1:I:377:LEU:HD22	2.14	0.73
1:K:108:LEU:HD23	1:K:132:LEU:CD1	2.19	0.73
1:A:220:ARG:HB2	1:A:223:GLU:HB3	1.70	0.72
2:B:246:LEU:HG	2:L:481:VAL:HG21	1.70	0.72
1:C:263:ASP:HB3	1:C:362:VAL:HG12	1.70	0.72
2:D:420:LYS:HG3	2:D:421:HIS:N	2.03	0.72
1:G:47:ARG:HG2	1:G:148:LEU:HD11	1.71	0.72
1:G:567:ARG:HH11	1:G:567:ARG:HG3	1.51	0.72
1:A:96:VAL:CG1	1:E:605:VAL:HG12	2.19	0.72
2:D:472:VAL:HG11	2:J:181:GLN:CB	2.18	0.72
1:E:152:PRO:HG2	1:E:338:THR:HB	1.71	0.72
2:F:435:PRO:CD	2:F:553:ILE:HD12	2.19	0.72
1:G:395:PHE:O	1:G:397:PRO:HD3	1.89	0.72
1:I:601:ARG:HB3	1:I:601:ARG:HH11	1.53	0.72
2:L:215:SER:HA	2:L:238:THR:OG1	1.89	0.72
1:C:350:ILE:HA	1:C:440:TRP:HZ3	1.54	0.72
1:C:586:SER:O	1:C:587:GLN:HB2	1.89	0.72
1:I:308:ARG:HH11	1:I:308:ARG:HG3	1.53	0.72
1:A:654:ASN:HB2	2:H:251:THR:OG1	1.89	0.72
1:I:261:PHE:CE2	1:I:358:TRP:HB3	2.24	0.72
1:I:315:TYR:HE2	1:I:336:MET:HE1	1.54	0.72
2:J:484:GLN:HA	2:J:484:GLN:HE21	1.54	0.72
1:K:170:MET:SD	1:K:309:ALA:HB1	2.29	0.72
1:K:320:THR:HG21	1:K:341:GLN:HG3	1.71	0.72
2:L:82:LEU:H	2:L:82:LEU:HD12	1.54	0.72
2:L:234:ARG:HA	2:L:263:ALA:CB	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ALA:O	1:A:504:LEU:O	2.08	0.72
2:B:71:ALA:HA	2:B:74:ARG:HB3	1.70	0.72
2:D:164:ARG:CB	2:D:551:ALA:HB2	2.18	0.72
2:D:379:GLU:OE1	2:D:379:GLU:N	2.23	0.72
1:E:569:ALA:O	1:E:571:PRO:HD3	1.89	0.72
1:G:313:ILE:HD11	1:G:315:TYR:CD2	2.25	0.72
2:L:81:LEU:HD21	2:L:89:ARG:NH2	2.04	0.72
2:B:212:VAL:HG21	2:B:239:ILE:HD11	1.71	0.72
1:C:188:LEU:HG	1:C:228:LEU:HD22	1.70	0.72
1:C:465:THR:HG22	1:C:467:LEU:N	1.97	0.72
1:C:596:ASP:HB3	1:C:612:LEU:HD23	1.71	0.72
1:E:549:ARG:HG2	1:E:549:ARG:NH1	1.90	0.72
2:H:36:ASN:HD21	2:H:38:ARG:HD3	1.52	0.72
2:H:518:HIS:ND1	2:H:519:PRO:HD2	2.03	0.72
1:I:84:ARG:NH2	1:I:97:ASP:OD2	2.23	0.72
2:J:441:ILE:C	2:J:441:ILE:HD12	2.13	0.72
1:K:390:ASP:OD1	1:K:393:GLY:HA3	1.88	0.72
1:A:476:HIS:CE1	1:A:492:HIS:HD2	2.08	0.72
2:F:180:ARG:HG3	2:F:180:ARG:NH1	1.98	0.72
2:H:114:VAL:HG11	2:H:146:TYR:CZ	2.24	0.72
2:H:170:LEU:HD23	2:H:211:VAL:HB	1.72	0.72
1:I:54:VAL:HG12	1:I:54:VAL:O	1.89	0.72
1:I:421:ARG:HD3	1:I:424:ASP:OD2	1.90	0.72
2:J:438:THR:HB	2:J:462:LEU:HG	1.71	0.72
2:J:488:GLU:O	2:J:492:ARG:HG2	1.90	0.72
2:L:350:LEU:H	2:L:350:LEU:CD2	2.03	0.72
2:L:487:ARG:HG3	2:L:487:ARG:O	1.89	0.72
1:A:96:VAL:HG13	1:E:605:VAL:HG12	1.70	0.72
1:A:673:THR:HG21	1:A:676:VAL:HG22	1.72	0.72
1:G:326:ASP:OD1	1:G:328:ARG:HG2	1.89	0.72
1:G:504:LEU:HD13	1:G:622:TRP:HE1	1.55	0.72
1:K:401:ARG:HB3	1:K:401:ARG:NH1	2.00	0.72
1:A:150:LEU:CD2	1:A:363:ALA:HB2	2.19	0.72
1:E:525:ARG:HG2	1:E:525:ARG:HH11	1.55	0.72
1:I:346:VAL:O	1:I:349:ALA:HB3	1.89	0.72
2:L:53:VAL:HG12	2:L:57:ARG:HD2	1.72	0.72
1:A:351:THR:OG1	1:A:352:GLY:N	2.23	0.72
1:C:275:ASP:OD2	1:C:484:LEU:HD22	1.89	0.72
1:C:347:THR:O	1:C:351:THR:HG23	1.89	0.72
2:D:201:MET:HG2	2:D:206:ILE:HD12	1.70	0.72
2:D:351:PHE:CE2	2:D:379:GLU:HB3	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:472:VAL:CG1	2:J:181:GLN:HB2	2.20	0.72
1:E:467:LEU:HD12	1:E:467:LEU:O	1.90	0.72
1:I:251:LEU:HD11	1:I:328:ARG:NH2	2.03	0.72
1:I:505:PRO:CB	1:I:507:HIS:HB3	2.20	0.72
1:A:65:MET:HE3	1:A:92:ALA:HB2	1.72	0.71
1:E:53:LEU:HD13	1:E:117:ALA:CB	2.19	0.71
2:J:119:ILE:CG2	2:J:152:LYS:HD3	2.18	0.71
1:C:186:GLN:HE22	1:C:190:THR:H	1.37	0.71
1:C:526:ASP:OD2	1:C:526:ASP:N	2.10	0.71
2:F:75:HIS:CE1	2:F:80:LYS:HE2	2.25	0.71
1:I:81:ASP:HB2	1:I:100:GLY:HA2	1.72	0.71
2:J:486:LYS:HG2	2:J:505:ILE:HD12	1.70	0.71
1:C:320:THR:OG1	1:C:341:GLN:HG2	1.90	0.71
2:D:560:VAL:HG13	2:H:389:GLU:HB3	1.71	0.71
1:E:516:TRP:CD2	1:E:555:LEU:HD21	2.25	0.71
1:E:550:GLU:HG3	1:E:567:ARG:CD	2.16	0.71
2:F:231:VAL:HG22	2:F:275:HIS:CB	2.10	0.71
2:H:440:LEU:HD12	2:H:464:MET:HG3	1.72	0.71
2:L:218:ALA:O	2:L:221:ALA:HB3	1.91	0.71
2:B:194:ILE:N	2:B:194:ILE:HD12	2.03	0.71
1:C:50:GLN:H	1:C:123:GLN:HE21	1.39	0.71
1:C:198:ILE:HG23	1:C:248:LYS:HG2	1.72	0.71
1:G:393:GLY:O	1:G:396:LEU:HG	1.90	0.71
1:I:65:MET:HG3	1:I:75:SER:HB2	1.72	0.71
1:I:384:VAL:CG1	1:I:470:LEU:HD22	2.20	0.71
1:K:504:LEU:HD23	1:K:505:PRO:HD2	1.72	0.71
2:L:83:VAL:HG13	2:L:84:ARG:N	2.05	0.71
1:A:306:ALA:HB1	1:A:321:VAL:HG21	1.72	0.71
2:D:440:LEU:HB2	2:D:464:MET:HG3	1.70	0.71
1:G:473:ILE:HB	1:G:496:LEU:CD1	2.20	0.71
1:A:274:ARG:NH2	1:A:320:THR:HG21	2.04	0.71
1:C:613:ARG:O	1:C:614:ARG:HD2	1.90	0.71
1:E:553:LEU:O	1:E:564:VAL:HG22	1.89	0.71
1:K:54:VAL:CG1	1:K:64:VAL:HG11	2.20	0.71
1:E:218:VAL:O	1:E:218:VAL:HG23	1.89	0.71
1:E:261:PHE:CE1	1:E:318:ALA:HB2	2.26	0.71
1:E:344:HIS:ND1	1:E:345:PRO:HD3	2.05	0.71
1:E:525:ARG:HG2	1:E:525:ARG:NH1	2.03	0.71
1:C:61:ALA:O	1:C:65:MET:HB2	1.91	0.71
1:C:287:GLU:N	1:C:287:GLU:OE2	2.24	0.71
2:D:298:LYS:HE3	2:D:550:ASN:ND2	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:379:GLU:H	2:D:379:GLU:CD	1.97	0.71
2:D:472:VAL:HG11	2:J:181:GLN:HB2	1.73	0.71
1:I:280:ARG:O	1:I:281:ARG:C	2.32	0.71
1:K:153:PRO:HD3	1:K:316:VAL:CG2	2.19	0.71
1:K:428:PRO:HG2	1:K:429:PHE:CE2	2.25	0.71
1:A:261:PHE:CD1	1:A:358:TRP:HE3	2.09	0.71
2:D:331:VAL:O	2:D:334:VAL:HG23	1.90	0.71
2:F:207:PRO:HG2	2:F:294:LEU:HD22	1.71	0.71
2:H:62:ARG:O	2:H:65:GLU:HB2	1.90	0.71
2:J:152:LYS:HA	2:J:526:LEU:HD21	1.71	0.71
1:K:255:HIS:HE1	1:K:322:GLU:HG3	1.55	0.71
1:K:380:HIS:NE2	1:K:444:ARG:HG3	2.05	0.71
1:A:111:ASP:O	1:A:114:ILE:HG22	1.91	0.71
1:E:586:SER:O	1:E:587:GLN:HB2	1.90	0.71
1:I:270:TYR:H	1:I:372:GLN:HE22	1.39	0.71
1:I:504:LEU:HD23	1:I:505:PRO:HD2	1.71	0.71
1:I:681:LYS:HG2	3:I:801:BTI:O11	1.90	0.71
1:A:125:ILE:HD12	1:A:142:CYS:SG	2.31	0.70
1:A:344:HIS:ND1	1:A:345:PRO:HD3	2.06	0.70
1:I:144:GLU:HG2	1:I:144:GLU:O	1.90	0.70
2:J:476:GLU:CD	2:J:476:GLU:H	1.99	0.70
1:A:152:PRO:HG2	1:A:338:THR:HB	1.73	0.70
1:A:384:VAL:CG2	1:A:451:LEU:HD21	2.20	0.70
1:A:567:ARG:HG3	1:A:567:ARG:NH1	1.99	0.70
1:C:372:GLN:O	1:C:375:VAL:HG22	1.90	0.70
1:E:275:ASP:OD2	1:E:484:LEU:HD22	1.91	0.70
1:E:315:TYR:OH	1:E:338:THR:HA	1.92	0.70
1:E:503:ALA:O	1:E:504:LEU:O	2.10	0.70
1:I:440:TRP:CD1	1:I:440:TRP:C	2.69	0.70
2:J:408:MET:HE3	2:J:413:TYR:CE1	2.27	0.70
1:K:280:ARG:O	1:K:281:ARG:C	2.33	0.70
2:D:49:MET:HG3	2:D:318:TYR:HD1	1.56	0.70
1:E:279:GLN:O	1:E:489:ILE:HG21	1.91	0.70
1:E:333:PHE:O	1:E:334:MET:HE2	1.91	0.70
1:K:46:TYR:CE1	1:K:366:GLU:HG3	2.27	0.70
1:G:52:LEU:HD12	1:G:124:ALA:O	1.92	0.70
1:G:165:ALA:O	1:G:169:LEU:HD13	1.91	0.70
1:G:532:ASP:OD2	1:G:535:SER:HB2	1.91	0.70
1:A:562:ARG:HB3	1:A:562:ARG:NH1	2.00	0.70
2:D:299:GLN:HB2	2:D:552:PRO:HD3	1.72	0.70
1:E:200:TYR:O	1:E:202:VAL:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:390:ASP:OD1	1:E:464:ARG:HD2	1.90	0.70
2:H:405:THR:OG1	1:I:681:LYS:HG3	1.91	0.70
1:K:278:ILE:H	1:K:278:ILE:HD12	1.55	0.70
1:K:305:ALA:HA	1:K:308:ARG:HG3	1.73	0.70
1:G:218:VAL:HG11	1:G:224:LEU:HD13	1.74	0.70
1:G:588:TYR:HB3	1:G:598:LEU:HD11	1.72	0.70
2:H:533:ASP:HB3	2:H:536:GLN:HE21	1.57	0.70
1:I:444:ARG:HG2	1:I:444:ARG:HH11	1.55	0.70
1:I:586:SER:O	1:I:587:GLN:HB2	1.91	0.70
1:K:612:LEU:HD12	1:K:612:LEU:N	2.05	0.70
1:A:204:LEU:CD2	1:A:246:VAL:HG22	2.21	0.70
1:A:605:VAL:CG1	1:C:96:VAL:HG13	2.21	0.70
2:B:277:ALA:HB2	2:B:286:ILE:HD12	1.74	0.70
1:C:279:GLN:O	1:C:489:ILE:HG21	1.92	0.70
1:E:165:ALA:O	1:E:168:ALA:HB3	1.91	0.70
1:G:315:TYR:OH	1:G:338:THR:HA	1.92	0.70
1:I:150:LEU:HD21	1:I:359:GLN:O	1.92	0.70
1:I:452:LEU:HD23	1:I:474:LEU:HB3	1.74	0.70
1:I:608:ARG:HH22	1:K:90:ALA:HA	1.56	0.70
1:A:470:LEU:HA	1:A:473:ILE:HG22	1.73	0.70
1:G:517:LEU:HD22	1:G:553:LEU:HD11	1.74	0.70
2:H:444:SER:HB3	2:H:449:ASN:HD22	1.56	0.70
1:I:169:LEU:CD2	1:I:312:ALA:HB1	2.21	0.70
1:A:607:ARG:HG3	1:C:94:ILE:HG13	1.74	0.70
1:A:703:GLU:HG2	1:A:705:VAL:HG13	1.74	0.70
2:B:82:LEU:HD12	2:B:82:LEU:N	2.05	0.70
2:B:339:VAL:HG23	2:B:342:SER:HA	1.74	0.70
1:E:278:ILE:H	1:E:278:ILE:CD1	1.93	0.70
2:L:518:HIS:HD1	2:L:519:PRO:HD2	1.52	0.70
1:A:379:GLY:HA3	1:A:440:TRP:CH2	2.27	0.69
2:D:369:ILE:HG12	2:D:399:LEU:HD23	1.73	0.69
2:D:377:PHE:CE1	2:D:408:MET:HE2	2.26	0.69
1:G:302:MET:HG2	1:G:331:PHE:CE2	2.26	0.69
2:B:84:ARG:HG2	2:B:84:ARG:HH11	1.57	0.69
1:E:152:PRO:HG3	1:E:315:TYR:CZ	2.27	0.69
1:E:308:ARG:HG3	1:E:308:ARG:NH1	2.05	0.69
1:G:503:ALA:HB2	1:G:560:GLU:OE1	1.92	0.69
2:H:201:MET:HG2	2:H:206:ILE:HB	1.74	0.69
1:I:316:VAL:HG12	1:I:317:GLY:N	2.07	0.69
2:J:234:ARG:HA	2:J:263:ALA:CB	2.22	0.69
1:K:448:ARG:HD3	1:K:474:LEU:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:470:LEU:HA	1:K:473:ILE:CG2	2.22	0.69
1:K:496:LEU:O	1:K:497:LEU:HD23	1.90	0.69
1:A:200:TYR:O	1:A:202:VAL:N	2.25	0.69
1:A:384:VAL:HG23	1:A:451:LEU:HD21	1.74	0.69
2:D:315:GLU:OE1	2:D:315:GLU:N	2.24	0.69
1:E:118:LEU:CD1	1:E:147:LEU:HD21	2.22	0.69
1:E:160:MET:HE1	1:E:170:MET:HE3	1.74	0.69
2:F:83:VAL:HG13	2:F:84:ARG:N	2.05	0.69
2:L:81:LEU:HD13	2:L:280:ASP:CB	2.21	0.69
1:A:384:VAL:CG1	1:A:470:LEU:HD13	2.22	0.69
1:A:398:ALA:HB2	1:A:464:ARG:NE	2.08	0.69
2:H:350:LEU:CD2	2:H:350:LEU:N	2.54	0.69
1:I:607:ARG:HH11	1:I:607:ARG:CB	2.06	0.69
1:K:304:GLU:CA	1:K:307:VAL:HG12	2.20	0.69
2:B:188:ARG:N	2:L:455:ARG:HG3	2.08	0.69
1:C:405:TYR:HB3	1:C:422:GLU:HB2	1.74	0.69
1:E:300:ARG:NH1	1:E:300:ARG:CB	2.55	0.69
1:G:274:ARG:HH22	1:G:320:THR:HG21	1.57	0.69
2:H:375:ILE:CG2	2:H:376:LEU:H	2.00	0.69
1:A:261:PHE:CE2	1:A:318:ALA:HB2	2.28	0.69
1:A:470:LEU:HA	1:A:473:ILE:CG2	2.21	0.69
1:E:289:ALA:HB1	1:E:350:ILE:HD13	1.74	0.69
1:G:398:ALA:HB2	1:G:464:ARG:NE	2.07	0.69
1:I:278:ILE:CG2	1:I:489:ILE:HD13	2.22	0.69
2:J:441:ILE:HD12	2:J:441:ILE:O	1.93	0.69
1:K:153:PRO:O	1:K:157:ILE:HG13	1.92	0.69
1:K:393:GLY:O	1:K:396:LEU:HG	1.93	0.69
2:B:36:ASN:ND2	2:B:38:ARG:H	1.91	0.69
2:D:192:GLY:HA2	2:D:195:PHE:CD2	2.28	0.69
1:G:187:ASP:C	1:G:189:GLU:H	1.99	0.69
2:J:83:VAL:HG13	2:J:84:ARG:HG3	1.73	0.69
2:L:538:ARG:HG3	2:L:538:ARG:NH1	1.99	0.69
1:A:566:LEU:C	1:A:567:ARG:HD3	2.18	0.69
1:A:654:ASN:C	2:H:251:THR:HB	2.18	0.69
1:A:698:TYR:N	1:A:698:TYR:CD2	2.60	0.69
2:B:144:THR:HG22	2:B:175:GLY:H	1.58	0.69
2:B:297:ARG:HB3	2:B:297:ARG:HH11	1.57	0.69
2:B:465:TRP:HB3	2:B:467:ASN:ND2	2.07	0.69
1:C:47:ARG:HH11	1:C:47:ARG:CB	2.06	0.69
1:C:386:LEU:HD12	1:C:434:LEU:HB2	1.74	0.69
2:F:417:GLY:C	2:F:419:ALA:H	2.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:ARG:HD3	1:G:121:GLY:C	2.18	0.69
1:G:201:PRO:HG2	1:G:328:ARG:NH2	2.07	0.69
1:G:561:ARG:HH11	1:G:632:VAL:HG13	1.57	0.69
2:H:217:THR:CG2	2:H:240:PHE:HE1	2.03	0.69
2:H:326:LYS:NZ	1:I:681:LYS:HD3	2.08	0.69
2:H:402:GLN:NE2	2:H:449:ASN:HA	2.07	0.69
1:I:547:LEU:N	1:I:547:LEU:HD23	2.07	0.69
1:K:257:GLU:C	1:K:258:ILE:HD12	2.18	0.69
1:K:616:ARG:O	1:K:630:GLU:HB2	1.93	0.69
2:L:368:ALA:HB3	2:L:398:LEU:HD23	1.73	0.69
1:A:543:TRP:HB3	2:B:96:PRO:HB3	1.73	0.69
2:D:464:MET:CE	2:D:519:PRO:HG3	2.21	0.69
1:E:189:GLU:OE1	1:E:189:GLU:HA	1.92	0.69
1:G:278:ILE:HD12	1:G:278:ILE:N	1.95	0.69
2:H:35:ILE:CD1	2:H:320:VAL:HG13	2.23	0.69
2:H:90:LEU:HD12	2:H:90:LEU:O	1.93	0.69
2:B:33:THR:HG23	2:B:35:ILE:N	2.03	0.69
1:E:108:LEU:HD23	1:E:132:LEU:CD2	2.22	0.69
2:F:200:ASN:HD22	2:F:204:ARG:NH2	1.91	0.69
1:I:612:LEU:HD12	1:I:612:LEU:H	1.57	0.69
2:L:348:LYS:HB2	2:L:383:LYS:HE3	1.75	0.69
1:A:497:LEU:N	1:A:498:PRO:HD3	2.07	0.68
2:B:372:ASN:OD1	2:B:452:MET:HE2	1.92	0.68
2:B:81:LEU:HD11	2:B:89:ARG:HH22	1.56	0.68
2:B:311:LEU:C	2:B:312:TYR:CD1	2.71	0.68
2:D:71:ALA:HA	2:D:74:ARG:HB3	1.74	0.68
1:G:304:GLU:HA	1:G:307:VAL:CG1	2.24	0.68
2:H:81:LEU:HD21	2:H:85:GLU:HB3	1.74	0.68
2:J:235:GLU:HA	2:J:258:GLU:OE1	1.92	0.68
2:J:377:PHE:CD1	2:J:377:PHE:N	2.61	0.68
2:B:511:GLU:HG3	2:B:512:GLN:N	2.08	0.68
1:C:287:GLU:HG2	1:C:343:GLU:HG3	1.74	0.68
1:E:587:GLN:HB3	1:E:588:TYR:HD1	1.56	0.68
1:G:114:ILE:O	1:G:118:LEU:HB2	1.94	0.68
2:H:526:LEU:C	2:H:528:ASP:H	2.01	0.68
1:I:380:HIS:CD2	1:I:444:ARG:HD2	2.29	0.68
1:A:616:ARG:HG3	1:A:616:ARG:O	1.91	0.68
1:E:270:TYR:H	1:E:372:GLN:NE2	1.88	0.68
1:E:400:GLY:H	1:E:463:LEU:CD1	2.06	0.68
2:F:172:ASP:OD1	2:F:214:GLY:HA3	1.92	0.68
2:F:192:GLY:HA2	2:F:195:PHE:CD2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:75:HIS:CE1	2:J:80:LYS:HE2	2.27	0.68
2:J:146:TYR:HE1	2:J:180:ARG:NH1	1.90	0.68
1:K:129:TYR:OH	1:K:433:MET:HE1	1.94	0.68
2:L:473:MET:HE2	2:L:477:GLN:HB3	1.75	0.68
1:A:276:CYS:HB3	1:A:287:GLU:HG3	1.75	0.68
1:E:148:LEU:N	1:E:148:LEU:HD23	2.08	0.68
1:E:280:ARG:O	1:E:281:ARG:C	2.37	0.68
1:E:361:ARG:HG2	1:E:361:ARG:HH11	1.57	0.68
1:E:568:HIS:H	1:E:568:HIS:CD2	2.09	0.68
1:K:384:VAL:HG23	1:K:451:LEU:HD21	1.73	0.68
1:K:556:ARG:HD2	1:K:556:ARG:C	2.18	0.68
2:L:48:THR:O	2:L:52:GLN:HG3	1.92	0.68
2:L:74:ARG:HH21	2:L:78:ARG:HH12	1.40	0.68
1:C:107:TYR:O	1:C:132:LEU:HD21	1.93	0.68
1:C:353:LEU:HD23	1:C:353:LEU:N	2.09	0.68
1:C:452:LEU:HD23	1:C:474:LEU:HB3	1.76	0.68
1:I:300:ARG:HB2	1:I:300:ARG:CZ	2.24	0.68
1:I:504:LEU:HD23	1:I:505:PRO:CD	2.24	0.68
2:L:191:PHE:HD2	2:L:192:GLY:N	1.88	0.68
1:A:186:GLN:HE22	1:A:190:THR:N	1.88	0.68
2:B:417:GLY:C	2:B:419:ALA:H	2.02	0.68
2:D:233:VAL:HG13	2:D:279:ASP:HA	1.75	0.68
1:E:269:LEU:CD2	1:E:368:LEU:HD13	2.23	0.68
1:G:545:SER:O	2:H:536:GLN:NE2	2.26	0.68
2:D:440:LEU:HD21	2:D:444:SER:HB2	1.75	0.68
1:E:270:TYR:N	1:E:372:GLN:HE22	1.90	0.68
2:F:501:GLU:O	2:F:505:ILE:HG13	1.94	0.68
1:G:469:PHE:CE1	1:G:497:LEU:HD21	2.28	0.68
2:H:403:ASN:CG	2:H:442:GLY:HA3	2.19	0.68
1:I:278:ILE:HD12	1:I:278:ILE:N	2.05	0.68
1:I:339:ARG:NH1	1:I:341:GLN:HA	2.09	0.68
2:L:433:ARG:HH21	2:L:554:GLU:HG3	1.59	0.68
1:A:412:PRO:HB2	1:A:450:ARG:HD3	1.75	0.68
2:D:191:PHE:CD2	2:D:194:ILE:HD12	2.28	0.68
2:D:305:ARG:CB	2:D:305:ARG:HH11	2.07	0.68
1:G:315:TYR:CE2	1:G:338:THR:HG22	2.29	0.68
2:H:234:ARG:HD3	2:H:278:GLU:OE1	1.93	0.68
1:I:167:LYS:HB2	1:I:167:LYS:NZ	2.09	0.68
1:I:608:ARG:NH2	1:K:90:ALA:HA	2.09	0.68
1:K:269:LEU:HD21	1:K:368:LEU:HD13	1.76	0.68
1:A:150:LEU:HD23	1:A:363:ALA:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HG2	1:A:485:ASP:HB3	1.75	0.68
1:E:504:LEU:O	1:E:505:PRO:O	2.12	0.68
2:H:71:ALA:HA	2:H:74:ARG:HB3	1.76	0.68
2:H:473:MET:HE2	3:I:801:BTI:S1	2.34	0.68
1:I:607:ARG:CB	1:I:607:ARG:NH1	2.57	0.68
1:K:403:MET:HE2	1:K:462:GLY:HA3	1.75	0.68
1:K:439:ALA:HB3	1:K:451:LEU:HB2	1.74	0.68
1:E:547:LEU:N	1:E:547:LEU:HD23	2.09	0.67
1:G:341:GLN:OE1	1:G:342:VAL:HG23	1.93	0.67
1:I:65:MET:HE1	1:I:88:HIS:O	1.95	0.67
1:K:105:ASP:C	1:K:109:ARG:HD2	2.18	0.67
1:K:357:ALA:HA	1:K:360:ILE:HD11	1.76	0.67
2:L:444:SER:HB2	2:L:470:ILE:HG13	1.76	0.67
1:A:169:LEU:HD23	1:A:313:ILE:HG22	1.74	0.67
1:A:537:TRP:CE2	2:B:543:LEU:HD22	2.29	0.67
1:C:82:ILE:HD11	1:C:430:TYR:CE1	2.28	0.67
1:C:445:GLU:CD	1:C:448:ARG:NH2	2.52	0.67
2:D:481:VAL:HG12	2:J:245:PRO:HB2	1.77	0.67
1:E:132:LEU:HB3	1:E:138:PHE:CD2	2.30	0.67
2:F:84:ARG:HG2	2:F:84:ARG:NH1	2.06	0.67
2:F:173:SER:OG	2:F:174:GLY:N	2.23	0.67
1:G:607:ARG:CB	1:G:607:ARG:HH11	2.07	0.67
1:I:469:PHE:O	1:I:473:ILE:HG22	1.94	0.67
2:J:302:LEU:HD21	2:J:397:PRO:HD3	1.74	0.67
2:L:350:LEU:HD23	2:L:350:LEU:N	2.08	0.67
1:C:416:VAL:HG22	1:C:437:LEU:HD12	1.77	0.67
2:D:491:GLU:HA	2:D:495:GLN:O	1.95	0.67
1:E:465:THR:HG22	1:E:467:LEU:N	2.07	0.67
1:E:561:ARG:HG3	1:E:561:ARG:HH11	1.59	0.67
1:G:371:THR:OG1	1:G:374:GLN:HG3	1.95	0.67
2:H:164:ARG:HB2	2:H:551:ALA:HB2	1.75	0.67
2:H:207:PRO:CG	2:H:294:LEU:HD21	2.17	0.67
1:I:452:LEU:HD13	1:I:452:LEU:O	1.95	0.67
1:K:255:HIS:CE1	1:K:322:GLU:HG3	2.28	0.67
1:A:695:LYS:O	1:A:696:ALA:HB2	1.94	0.67
2:D:317:LEU:HD22	2:D:334:VAL:CG1	2.24	0.67
1:E:300:ARG:HB2	1:E:300:ARG:CZ	2.24	0.67
1:E:387:TYR:HE1	1:E:433:MET:HB2	1.59	0.67
1:G:114:ILE:HD11	1:G:145:ALA:HB3	1.75	0.67
2:H:232:MET:CE	2:H:239:ILE:HG13	2.23	0.67
1:I:605:VAL:HG23	1:I:605:VAL:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:233:VAL:CG1	2:J:279:ASP:HA	2.23	0.67
2:L:554:GLU:OE1	2:L:555:PRO:HD2	1.94	0.67
2:D:181:GLN:OE1	2:J:472:VAL:HG12	1.93	0.67
2:J:171:VAL:HG12	2:J:212:VAL:HG13	1.74	0.67
2:J:440:LEU:HD22	2:J:444:SER:OG	1.94	0.67
2:L:62:ARG:O	2:L:65:GLU:HB2	1.94	0.67
2:L:212:VAL:HG23	2:L:231:VAL:O	1.94	0.67
1:A:135:ASN:ND2	1:A:137:ASP:OD2	2.28	0.67
1:A:170:MET:SD	1:A:309:ALA:HB1	2.35	0.67
1:G:47:ARG:HH11	1:G:47:ARG:CB	2.03	0.67
2:H:75:HIS:HE1	2:H:80:LYS:HE2	1.59	0.67
1:I:391:PRO:HD3	1:I:465:THR:O	1.95	0.67
2:J:81:LEU:HD11	2:J:89:ARG:NH2	2.09	0.67
2:J:161:LEU:HD11	2:J:201:MET:HG2	1.75	0.67
2:B:189:GLU:OE1	2:B:189:GLU:N	2.28	0.67
2:B:293:ASN:HB3	2:F:359:PHE:HD1	1.59	0.67
1:C:200:TYR:OH	1:C:224:LEU:HD22	1.95	0.67
1:E:49:ILE:HD12	1:E:49:ILE:N	2.10	0.67
1:G:602:VAL:O	1:G:605:VAL:HG22	1.92	0.67
2:J:377:PHE:HA	2:J:418:ILE:HD11	1.77	0.67
2:J:525:ARG:HH11	2:J:525:ARG:HG3	1.59	0.67
1:K:264:ARG:HH11	1:K:264:ARG:CB	2.08	0.67
2:L:375:ILE:H	2:L:375:ILE:HD12	1.58	0.67
2:B:375:ILE:HG22	2:B:376:LEU:N	2.10	0.67
1:C:343:GLU:O	1:C:346:VAL:HG22	1.95	0.67
2:D:121:ALA:CB	2:D:134:VAL:HG22	2.24	0.67
1:E:104:ALA:HA	1:E:108:LEU:HD12	1.75	0.67
1:G:437:LEU:HD23	1:G:455:LEU:HD23	1.76	0.67
2:H:476:GLU:CA	2:H:510:LEU:HD21	2.25	0.67
1:I:251:LEU:HB2	1:I:327:GLU:HG3	1.74	0.67
2:B:155:ARG:NE	2:B:159:ILE:HD11	2.09	0.67
1:C:352:GLY:C	1:C:353:LEU:HD23	2.20	0.67
1:E:136:ALA:HB1	1:E:154:ALA:HB1	1.76	0.67
1:G:561:ARG:NH1	1:G:632:VAL:HG13	2.09	0.67
1:I:532:ASP:OD2	2:J:365:TYR:OH	2.12	0.67
1:I:607:ARG:HG3	1:K:94:ILE:CG1	2.24	0.67
1:K:165:ALA:O	1:K:168:ALA:HB3	1.95	0.67
2:L:114:VAL:HG11	2:L:146:TYR:CE2	2.29	0.67
2:L:486:LYS:HG2	2:L:505:ILE:HD13	1.77	0.67
1:C:200:TYR:O	1:C:202:VAL:N	2.27	0.67
1:E:257:GLU:O	1:E:273:GLU:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:201:MET:HE3	2:F:208:GLN:NE2	2.10	0.67
1:A:129:TYR:CE2	1:A:342:VAL:HA	2.30	0.66
1:A:350:ILE:HD12	1:A:377:LEU:HD13	1.76	0.66
1:A:673:THR:CG2	1:A:676:VAL:HG22	2.25	0.66
1:C:598:LEU:HD23	1:C:598:LEU:O	1.95	0.66
1:E:201:PRO:HD2	1:E:328:ARG:NH2	2.10	0.66
1:G:99:GLY:HA3	1:G:105:ASP:O	1.95	0.66
1:G:452:LEU:HD22	1:G:474:LEU:HB3	1.76	0.66
1:I:254:ARG:NH2	1:I:292:PRO:HB2	2.10	0.66
1:I:277:SER:O	1:I:279:GLN:HG3	1.95	0.66
1:A:469:PHE:CZ	1:A:489:ILE:HD11	2.30	0.66
2:B:177:ASN:OD1	2:B:180:ARG:NH1	2.28	0.66
1:C:315:TYR:CE2	1:C:336:MET:HE1	2.30	0.66
1:E:618:LEU:HD23	1:E:618:LEU:O	1.96	0.66
2:F:349:ALA:HB3	2:F:350:LEU:HD23	1.76	0.66
2:F:390:LEU:HD23	2:F:394:ARG:HH21	1.60	0.66
1:G:325:LEU:HD23	1:G:326:ASP:N	2.10	0.66
2:L:232:MET:HE3	2:L:239:ILE:HG13	1.77	0.66
2:B:137:ASP:HB3	2:B:140:VAL:CG2	2.24	0.66
1:E:118:LEU:HD12	1:E:147:LEU:HD21	1.75	0.66
1:E:269:LEU:HB2	1:E:372:GLN:NE2	2.10	0.66
1:G:50:GLN:NE2	1:G:123:GLN:NE2	2.43	0.66
1:G:618:LEU:HD23	1:G:629:ILE:HD13	1.78	0.66
2:H:305:ARG:NH1	2:H:305:ARG:CB	2.58	0.66
2:H:345:ASP:OD2	2:H:345:ASP:N	2.27	0.66
2:H:417:GLY:C	2:H:419:ALA:N	2.48	0.66
1:I:412:PRO:CB	1:I:450:ARG:HD3	2.25	0.66
1:K:63:ARG:HD3	1:K:417:ASP:OD1	1.96	0.66
1:K:140:ARG:HB3	1:K:140:ARG:NH1	2.09	0.66
1:K:144:GLU:O	1:K:144:GLU:HG2	1.93	0.66
2:L:90:LEU:O	2:L:288:ARG:NH2	2.28	0.66
1:A:377:LEU:HG	1:A:377:LEU:O	1.94	0.66
1:A:649:LEU:HD11	1:A:689:PRO:HG3	1.76	0.66
2:D:28:MET:C	2:D:30:ILE:H	2.02	0.66
1:G:261:PHE:CE2	1:G:318:ALA:HB2	2.31	0.66
1:G:513:ALA:HB2	1:G:564:VAL:HG21	1.76	0.66
2:H:317:LEU:HA	2:H:320:VAL:CG2	2.24	0.66
2:J:487:ARG:HD2	2:J:502:GLU:OE1	1.95	0.66
2:B:421:HIS:CE1	2:B:424:LYS:HZ1	2.13	0.66
1:C:500:PRO:O	1:C:501:GLN:HB3	1.95	0.66
2:D:433:ARG:HH11	2:D:433:ARG:HG3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:520:TYR:N	2:D:520:TYR:HD2	1.94	0.66
2:F:80:LYS:HG2	2:F:236:GLN:OE1	1.94	0.66
2:H:269:VAL:HG12	2:H:270:SER:N	2.09	0.66
1:I:62:CYS:O	1:I:66:ARG:HG3	1.94	0.66
1:I:135:ASN:O	1:I:135:ASN:OD1	2.13	0.66
1:E:250:LEU:HD21	1:E:332:PHE:HE1	1.60	0.66
2:F:207:PRO:HG2	2:F:294:LEU:CD2	2.25	0.66
1:G:302:MET:HE3	1:G:331:PHE:CB	2.26	0.66
2:B:50:LEU:HD23	2:B:54:ASN:HD21	1.61	0.66
2:B:78:ARG:HH11	2:B:78:ARG:HG3	1.61	0.66
2:D:350:LEU:CD2	2:D:350:LEU:N	2.56	0.66
1:E:186:GLN:NE2	1:E:187:ASP:OD1	2.29	0.66
2:H:326:LYS:CE	1:I:681:LYS:HD3	2.26	0.66
2:J:50:LEU:HD23	2:J:50:LEU:O	1.96	0.66
2:J:270:SER:OG	2:J:272:VAL:HG23	1.95	0.66
1:K:53:LEU:HD13	1:K:117:ALA:CB	2.26	0.66
1:C:251:LEU:HD11	1:C:328:ARG:NH2	2.10	0.66
1:C:384:VAL:CG1	1:C:470:LEU:HD13	2.26	0.66
1:E:469:PHE:O	1:E:473:ILE:HG22	1.96	0.66
2:F:377:PHE:HD1	2:F:377:PHE:H	1.42	0.66
2:F:377:PHE:N	2:F:377:PHE:CD1	2.63	0.66
1:I:51:ARG:HB2	1:I:122:ALA:HA	1.76	0.66
1:I:497:LEU:N	1:I:498:PRO:HD3	2.11	0.66
2:J:362:LEU:HB2	2:J:367:ILE:HD13	1.78	0.66
2:J:516:GLN:HA	2:J:521:TYR:CD2	2.30	0.66
1:K:357:ALA:HA	1:K:360:ILE:CD1	2.25	0.66
1:C:138:PHE:CD1	1:C:142:CYS:HB2	2.31	0.66
1:C:473:ILE:HA	1:C:496:LEU:HD21	1.76	0.66
1:E:392:GLU:C	1:E:394:ASP:H	2.04	0.66
1:E:519:SER:HB2	1:E:613:ARG:HE	1.60	0.66
1:G:335:GLU:HG3	1:G:336:MET:N	2.10	0.66
2:L:132:MET:HE3	2:L:156:ALA:CA	2.26	0.66
2:L:486:LYS:HG3	2:L:497:LEU:HD22	1.78	0.66
1:A:469:PHE:C	1:A:469:PHE:CD2	2.73	0.66
2:B:386:HIS:HD2	2:B:386:HIS:O	1.78	0.66
1:K:396:LEU:O	1:K:398:ALA:N	2.29	0.66
1:K:401:ARG:HH11	1:K:401:ARG:CB	2.04	0.66
1:A:167:LYS:HE3	1:A:177:LEU:HD12	1.77	0.65
2:B:84:ARG:HA	2:B:87:ILE:HD12	1.78	0.65
2:B:119:ILE:HG23	2:B:152:LYS:HD3	1.77	0.65
2:B:279:ASP:OD2	2:B:281:ASP:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:ARG:CB	2:B:497:LEU:HB2	2.26	0.65
2:D:441:ILE:HG22	2:D:465:TRP:CE2	2.30	0.65
2:F:209:ILE:HD11	2:F:290:CYS:CB	2.26	0.65
1:K:76:VAL:HG11	1:K:120:SER:OG	1.95	0.65
1:A:269:LEU:HB2	1:A:372:GLN:NE2	2.11	0.65
2:B:193:ARG:NH1	2:B:196:PHE:CD2	2.64	0.65
2:D:53:VAL:O	2:D:57:ARG:HG3	1.97	0.65
2:F:311:LEU:HG	2:F:342:SER:HB2	1.77	0.65
2:J:49:MET:HG3	2:J:318:TYR:CD1	2.32	0.65
2:J:191:PHE:CD2	2:J:194:ILE:HD13	2.31	0.65
1:K:471:ARG:HB2	1:K:471:ARG:HH11	1.60	0.65
1:A:698:TYR:N	1:A:698:TYR:HD2	1.94	0.65
1:G:298:LEU:O	1:G:301:ALA:HB3	1.96	0.65
1:I:178:VAL:HG13	1:I:332:PHE:CB	2.25	0.65
1:I:284:LYS:HD3	1:I:343:GLU:OE1	1.97	0.65
1:I:427:SER:OG	1:I:428:PRO:HD2	1.97	0.65
1:K:99:GLY:HA3	1:K:105:ASP:O	1.97	0.65
1:K:465:THR:HG22	1:K:467:LEU:N	2.08	0.65
2:L:123:ILE:CD1	2:L:165:LEU:HD13	2.26	0.65
2:L:144:THR:HG22	2:L:175:GLY:H	1.61	0.65
2:B:326:LYS:HZ3	2:B:405:THR:HG23	1.60	0.65
1:C:129:TYR:CE2	1:C:342:VAL:HA	2.31	0.65
1:E:250:LEU:HD21	1:E:332:PHE:CE1	2.32	0.65
2:F:498:GLY:C	2:F:500:GLU:H	2.05	0.65
1:I:271:LEU:HA	1:I:375:VAL:HG11	1.78	0.65
2:J:486:LYS:HA	2:J:489:GLN:HE21	1.61	0.65
2:L:389:GLU:HG2	2:L:558:PHE:HE1	1.61	0.65
1:A:652:PRO:HD3	1:A:686:ILE:CG2	2.26	0.65
2:D:282:HIS:O	2:D:286:ILE:HG13	1.96	0.65
1:E:300:ARG:CB	1:E:300:ARG:HH11	2.10	0.65
1:G:169:LEU:O	1:G:173:ALA:HB2	1.95	0.65
1:G:304:GLU:HA	1:G:307:VAL:HG12	1.78	0.65
2:J:525:ARG:HG3	2:J:525:ARG:NH1	2.10	0.65
2:L:303:GLN:OE1	2:L:303:GLN:HA	1.97	0.65
1:A:308:ARG:HH11	1:A:308:ARG:HG3	1.60	0.65
2:B:560:VAL:HG13	2:J:389:GLU:HB3	1.78	0.65
1:C:495:ASP:OD2	1:C:495:ASP:N	2.29	0.65
1:E:321:VAL:HG12	1:E:321:VAL:O	1.96	0.65
1:E:405:TYR:HB3	1:E:422:GLU:HB2	1.79	0.65
1:E:512:ALA:HB1	1:E:629:ILE:HD13	1.78	0.65
2:H:349:ALA:HB3	2:H:350:LEU:CD2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:ALA:HA	1:I:144:GLU:HB3	1.77	0.65
1:I:599:VAL:HG22	1:I:608:ARG:HD3	1.77	0.65
1:A:656:SER:OG	1:A:704:LEU:HD23	1.97	0.65
1:C:469:PHE:HZ	1:C:489:ILE:HD11	1.62	0.65
1:C:629:ILE:HD12	1:C:629:ILE:N	2.11	0.65
2:D:482:LEU:HD23	2:D:509:ILE:HG13	1.78	0.65
2:F:335:ILE:O	2:F:339:VAL:HG22	1.96	0.65
2:F:359:PHE:HE2	2:F:387:PHE:CE1	2.15	0.65
2:H:291:VAL:HA	2:H:294:LEU:CD1	2.22	0.65
2:H:378:ALA:H	2:H:418:ILE:HD11	1.62	0.65
1:K:273:GLU:OE2	1:K:291:ALA:N	2.30	0.65
1:A:383:GLU:HG3	1:A:438:ILE:CG2	2.22	0.65
1:A:559:ASP:O	1:A:560:GLU:HG3	1.97	0.65
2:B:270:SER:OG	2:B:272:VAL:HG23	1.96	0.65
1:C:93:ASP:C	1:C:94:ILE:HD12	2.22	0.65
1:E:123:GLN:O	1:E:148:LEU:HG	1.97	0.65
1:E:320:THR:HG21	1:E:341:GLN:HG3	1.78	0.65
1:G:503:ALA:O	1:G:504:LEU:O	2.14	0.65
2:H:207:PRO:HA	2:H:228:ASP:OD2	1.95	0.65
2:H:497:LEU:HD12	2:H:501:GLU:OE1	1.97	0.65
1:I:169:LEU:HD22	1:I:313:ILE:HG23	1.78	0.65
1:I:340:LEU:CD1	1:I:356:VAL:HG23	2.26	0.65
1:K:415:ARG:HG2	1:K:416:VAL:N	2.12	0.65
1:A:103:PRO:C	1:A:108:LEU:HD12	2.21	0.65
1:A:550:GLU:OE2	1:A:567:ARG:HD2	1.97	0.65
1:C:185:ALA:HB3	1:C:243:ARG:HB2	1.77	0.65
1:G:274:ARG:NH2	1:G:320:THR:HG21	2.12	0.65
1:G:380:HIS:CD2	1:G:444:ARG:HD2	2.31	0.65
1:I:344:HIS:N	1:I:345:PRO:CD	2.60	0.65
1:I:505:PRO:HB3	1:I:507:HIS:HB3	1.79	0.65
1:I:554:MET:HA	1:I:554:MET:HE3	1.79	0.65
2:J:28:MET:HE3	1:K:633:ASP:OD1	1.95	0.65
1:K:279:GLN:O	1:K:489:ILE:HG21	1.97	0.65
1:K:505:PRO:HB3	1:K:507:HIS:HB2	1.79	0.65
2:B:81:LEU:HD22	2:B:85:GLU:HB3	1.79	0.65
2:B:161:LEU:HD13	2:B:201:MET:HG3	1.79	0.65
2:B:181:GLN:OE1	2:L:472:VAL:HG12	1.96	0.65
1:C:523:HIS:ND1	1:C:524:ARG:N	2.45	0.65
1:C:561:ARG:HH12	1:C:632:VAL:HG22	1.61	0.65
2:D:516:GLN:HA	2:D:521:TYR:CD2	2.32	0.65
2:J:191:PHE:HD2	2:J:192:GLY:H	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ARG:NH1	1:E:63:ARG:O	2.30	0.64
1:E:339:ARG:HG3	1:E:339:ARG:NH1	2.12	0.64
2:F:375:ILE:HB	2:F:377:PHE:CE1	2.32	0.64
1:G:81:ASP:HB2	1:G:100:GLY:HA2	1.79	0.64
1:G:106:SER:OG	1:G:107:TYR:N	2.27	0.64
2:H:436:LYS:HD2	2:H:453:CYS:SG	2.37	0.64
1:I:108:LEU:HD23	1:I:132:LEU:CD1	2.27	0.64
1:I:569:ALA:O	1:I:571:PRO:HD3	1.98	0.64
2:J:194:ILE:H	2:J:194:ILE:HD12	1.61	0.64
1:A:204:LEU:O	1:A:215:MET:HA	1.96	0.64
2:B:250:ALA:O	2:B:252:GLY:N	2.30	0.64
2:B:375:ILE:H	2:B:375:ILE:HD12	1.62	0.64
2:D:101:SER:O	2:D:152:LYS:HE3	1.96	0.64
1:E:465:THR:HG22	1:E:466:ASN:N	2.11	0.64
2:F:209:ILE:HD11	2:F:290:CYS:HB3	1.77	0.64
2:F:234:ARG:HA	2:F:263:ALA:CB	2.27	0.64
1:I:350:ILE:HD12	1:I:377:LEU:CD1	2.28	0.64
2:J:151:LYS:HG2	2:J:526:LEU:HD22	1.80	0.64
2:L:339:VAL:HG23	2:L:340:ASP:N	2.12	0.64
1:A:705:VAL:CG1	1:A:709:THR:HG21	2.27	0.64
2:B:109:TYR:OH	2:B:147:PRO:HB2	1.97	0.64
1:E:522:GLY:O	1:E:523:HIS:HB2	1.96	0.64
1:G:203:LEU:HD21	1:G:247:GLU:OE2	1.96	0.64
1:G:361:ARG:HG2	1:G:366:GLU:OE1	1.98	0.64
2:H:330:ASP:OD1	2:H:332:ARG:HG3	1.97	0.64
1:A:249:TYR:CD2	1:A:250:LEU:N	2.64	0.64
2:B:31:LEU:CD1	2:B:336:ALA:HB2	2.27	0.64
1:C:443:THR:CG2	1:C:446:GLU:HB2	2.25	0.64
1:C:451:LEU:CD2	1:C:474:LEU:HD11	2.28	0.64
1:E:384:VAL:CG1	1:E:470:LEU:HD13	2.26	0.64
1:G:444:ARG:HG2	1:G:444:ARG:HH11	1.61	0.64
2:H:163:ASN:OD1	2:H:460:ARG:HD2	1.98	0.64
2:J:355:LEU:HD21	2:J:370:LEU:CD2	2.27	0.64
2:J:375:ILE:H	2:J:375:ILE:CD1	2.11	0.64
1:C:384:VAL:HG11	1:C:470:LEU:HD13	1.79	0.64
1:E:99:GLY:HA3	1:E:105:ASP:O	1.97	0.64
2:H:159:ILE:HD13	2:H:461:PHE:CE2	2.32	0.64
2:H:303:GLN:NE2	2:J:297:ARG:HG3	2.12	0.64
1:K:152:PRO:HG2	1:K:338:THR:HB	1.80	0.64
2:L:74:ARG:HH21	2:L:78:ARG:NH1	1.95	0.64
1:A:601:ARG:HG2	1:A:606:THR:HB	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:GLY:O	1:C:523:HIS:HB2	1.96	0.64
2:D:121:ALA:HB2	2:D:134:VAL:HG22	1.80	0.64
2:D:199:ALA:HB1	2:J:427:THR:HG23	1.79	0.64
2:F:465:TRP:NE1	2:F:534:PRO:HA	2.13	0.64
1:G:97:ASP:OD1	1:G:98:LEU:O	2.16	0.64
1:G:328:ARG:HH11	1:G:328:ARG:CG	2.03	0.64
1:I:53:LEU:HD13	1:I:117:ALA:CB	2.26	0.64
2:J:331:VAL:HB	2:J:373:ASN:HD21	1.61	0.64
2:J:486:LYS:HD2	2:J:489:GLN:HE21	1.63	0.64
1:A:204:LEU:HD22	1:A:245:LEU:O	1.96	0.64
1:C:350:ILE:HD12	1:C:351:THR:CG2	2.28	0.64
1:C:562:ARG:HB3	1:C:562:ARG:HH11	1.62	0.64
2:D:372:ASN:ND2	2:D:404:ILE:HB	2.13	0.64
2:F:81:LEU:HD12	2:F:280:ASP:CB	2.27	0.64
2:F:423:ALA:HA	2:F:426:VAL:HG23	1.80	0.64
2:F:498:GLY:O	2:F:500:GLU:N	2.30	0.64
1:K:353:LEU:HD22	1:K:358:TRP:CH2	2.33	0.64
1:K:465:THR:HG22	1:K:466:ASN:N	2.13	0.64
2:L:62:ARG:HG2	2:L:62:ARG:NH1	2.12	0.64
2:L:127:GLU:OE1	2:L:127:GLU:HA	1.98	0.64
1:A:540:ASN:HD22	1:A:540:ASN:C	2.06	0.64
2:B:119:ILE:CG2	2:B:152:LYS:HD3	2.28	0.64
1:E:49:ILE:HD13	1:E:364:ARG:HG2	1.80	0.64
1:E:285:VAL:HG12	1:E:286:VAL:CG2	2.26	0.64
1:G:132:LEU:HD23	1:G:138:PHE:CE2	2.33	0.64
1:G:426:VAL:HG21	1:G:463:LEU:HD11	1.80	0.64
2:H:476:GLU:CD	2:H:476:GLU:H	2.04	0.64
1:I:134:GLU:HG2	1:I:338:THR:OG1	1.98	0.64
1:I:503:ALA:O	1:I:504:LEU:O	2.14	0.64
1:I:522:GLY:O	1:I:523:HIS:HB2	1.97	0.64
2:J:240:PHE:CD2	2:J:260:LEU:HD23	2.33	0.64
1:K:286:VAL:HG21	1:K:473:ILE:HD11	1.80	0.64
1:C:393:GLY:O	1:C:396:LEU:HG	1.98	0.64
2:D:305:ARG:HH11	2:D:305:ARG:HB3	1.62	0.64
2:D:486:LYS:HG2	2:D:505:ILE:HD13	1.78	0.64
1:E:201:PRO:O	1:E:249:TYR:HB3	1.98	0.64
1:G:269:LEU:HD21	1:G:368:LEU:HD23	1.79	0.64
1:G:380:HIS:HE2	1:G:444:ARG:HD2	1.62	0.64
2:H:433:ARG:N	2:H:556:THR:HG23	2.11	0.64
1:I:47:ARG:HE	1:I:148:LEU:HD21	1.62	0.64
1:I:255:HIS:HE1	1:I:322:GLU:HG2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:476:HIS:CG	1:I:477:PRO:HD2	2.33	0.64
1:K:398:ALA:HB2	1:K:464:ARG:HE	1.63	0.64
2:L:435:PRO:HD3	2:L:553:ILE:HG23	1.78	0.64
1:A:473:ILE:HB	1:A:496:LEU:HD13	1.79	0.64
2:B:89:ARG:HG3	2:B:89:ARG:NH2	2.05	0.64
2:B:331:VAL:HG12	2:B:373:ASN:CG	2.23	0.64
2:B:393:GLN:O	2:B:393:GLN:HG2	1.98	0.64
1:C:294:LEU:HD12	1:C:294:LEU:O	1.98	0.64
2:H:438:THR:HG22	2:H:462:LEU:HG	1.80	0.64
1:I:392:GLU:C	1:I:394:ASP:H	2.06	0.64
1:I:540:ASN:HD22	1:I:540:ASN:C	2.06	0.64
1:K:503:ALA:O	1:K:504:LEU:O	2.16	0.64
2:L:465:TRP:HE3	2:L:467:ASN:HD21	1.43	0.64
1:C:274:ARG:HH22	1:C:320:THR:HG21	1.62	0.63
1:E:129:TYR:HE2	1:E:342:VAL:HA	1.59	0.63
2:F:53:VAL:CG1	2:F:57:ARG:NH1	2.61	0.63
2:H:464:MET:HE1	2:H:522:SER:OG	1.97	0.63
1:K:339:ARG:NH1	1:K:341:GLN:OE1	2.31	0.63
1:K:361:ARG:HA	1:K:366:GLU:OE1	1.97	0.63
2:L:91:LEU:HD22	2:L:95:SER:OG	1.98	0.63
2:B:487:ARG:HG3	2:B:487:ARG:O	1.97	0.63
1:G:280:ARG:HH11	1:G:283:GLN:HE22	1.46	0.63
1:G:315:TYR:HE2	1:G:338:THR:HG22	1.63	0.63
1:G:497:LEU:N	1:G:498:PRO:HD3	2.13	0.63
2:H:476:GLU:OE2	2:H:477:GLN:N	2.32	0.63
1:I:63:ARG:NH1	1:I:63:ARG:O	2.30	0.63
2:J:109:TYR:HE2	2:J:147:PRO:HD2	1.63	0.63
2:J:121:ALA:CB	2:J:134:VAL:HG12	2.28	0.63
2:J:335:ILE:O	2:J:339:VAL:HG22	1.99	0.63
1:K:387:TYR:HB3	1:K:389:GLU:HG3	1.80	0.63
1:K:522:GLY:O	1:K:523:HIS:HB2	1.97	0.63
2:L:316:GLU:OE2	2:L:337:ARG:NH2	2.29	0.63
1:A:657:ILE:HD13	1:A:699:CYS:HB2	1.79	0.63
1:A:662:VAL:HG21	1:A:674:LEU:HD23	1.80	0.63
1:C:205:LYS:HZ1	1:C:247:GLU:HG2	1.63	0.63
1:E:201:PRO:HD2	1:E:328:ARG:HH21	1.63	0.63
1:E:404:LEU:CD1	1:E:612:LEU:HD13	2.28	0.63
1:E:567:ARG:HH11	1:E:567:ARG:HG3	1.63	0.63
2:F:248:LYS:HA	2:F:252:GLY:O	1.99	0.63
2:F:491:GLU:C	2:F:493:ALA:H	2.05	0.63
2:H:245:PRO:HB2	2:H:246:LEU:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:49:MET:HG3	2:J:318:TYR:HD1	1.61	0.63
1:K:47:ARG:HE	1:K:148:LEU:CD2	2.11	0.63
1:A:390:ASP:OD1	1:A:393:GLY:HA3	1.99	0.63
1:A:677:LEU:HD23	1:A:686:ILE:HD11	1.80	0.63
2:D:440:LEU:CD2	2:D:444:SER:HB2	2.29	0.63
2:D:484:GLN:HG3	2:D:485:VAL:N	2.13	0.63
1:G:132:LEU:HD23	1:G:138:PHE:CD2	2.34	0.63
1:I:300:ARG:HB2	1:I:300:ARG:HH11	1.63	0.63
1:I:549:ARG:HH11	1:I:549:ARG:CG	2.10	0.63
1:C:272:ASN:CG	1:C:377:LEU:HD22	2.23	0.63
2:D:331:VAL:HG21	2:D:372:ASN:O	1.97	0.63
2:F:195:PHE:CE1	2:F:222:TYR:HB2	2.34	0.63
1:K:441:GLY:HA2	1:K:450:ARG:NH2	2.13	0.63
1:A:220:ARG:HB2	1:A:223:GLU:CB	2.28	0.63
1:A:344:HIS:N	1:A:345:PRO:CD	2.62	0.63
2:D:105:ALA:HA	2:D:108:VAL:HG21	1.79	0.63
2:F:198:GLN:OE1	2:F:223:VAL:HG13	1.99	0.63
2:H:83:VAL:CG1	2:H:84:ARG:N	2.60	0.63
2:H:444:SER:HB2	2:H:470:ILE:CG1	2.25	0.63
1:K:415:ARG:O	1:K:454:MET:HE1	1.99	0.63
2:L:486:LYS:HE3	2:L:497:LEU:HD13	1.81	0.63
1:A:668:VAL:HG12	1:A:669:GLU:H	1.64	0.63
1:C:308:ARG:HG3	1:C:308:ARG:HH11	1.63	0.63
1:C:315:TYR:CE2	1:C:338:THR:HG22	2.33	0.63
2:D:230:THR:HG21	2:D:273:ALA:HA	1.80	0.63
1:E:82:ILE:HD11	1:E:430:TYR:HE1	1.64	0.63
1:G:218:VAL:HG11	1:G:224:LEU:CD1	2.28	0.63
1:K:401:ARG:HG3	1:K:425:GLU:OE2	1.99	0.63
1:K:605:VAL:O	1:K:605:VAL:CG2	2.47	0.63
2:L:289:ARG:O	2:L:292:ALA:HB3	1.99	0.63
1:A:81:ASP:HB2	1:A:100:GLY:HA2	1.80	0.63
1:A:315:TYR:CE2	1:A:336:MET:HE1	2.33	0.63
1:A:652:PRO:HD3	1:A:686:ILE:HG21	1.81	0.63
2:B:31:LEU:HD12	2:B:336:ALA:HB2	1.80	0.63
2:B:308:ARG:HH22	2:B:343:GLU:CD	2.06	0.63
1:C:278:ILE:HG23	1:C:488:PHE:CD2	2.32	0.63
2:D:119:ILE:CG2	2:D:152:LYS:HD3	2.27	0.63
1:E:153:PRO:HD3	1:E:316:VAL:CG2	2.29	0.63
1:G:271:LEU:HA	1:G:375:VAL:HG11	1.79	0.63
1:G:345:PRO:CB	1:G:438:ILE:HD13	2.29	0.63
1:G:490:ALA:O	1:G:493:GLN:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:193:ARG:NH1	2:H:196:PHE:CD2	2.67	0.63
2:H:476:GLU:CD	2:H:476:GLU:N	2.57	0.63
1:A:136:ALA:O	1:A:137:ASP:C	2.41	0.63
2:B:29:ALA:O	2:B:343:GLU:HA	1.97	0.63
1:C:47:ARG:NE	1:C:148:LEU:HD21	2.14	0.63
1:C:51:ARG:HB2	1:C:122:ALA:HA	1.81	0.63
1:C:378:ASN:ND2	1:C:440:TRP:HH2	1.97	0.63
1:C:476:HIS:ND1	1:C:477:PRO:HD2	2.14	0.63
2:D:299:GLN:HB3	2:D:552:PRO:HD3	1.79	0.63
1:G:114:ILE:CD1	1:G:147:LEU:HD13	2.29	0.63
1:I:339:ARG:HH12	1:I:341:GLN:HA	1.64	0.63
1:I:386:LEU:HD21	1:I:467:LEU:CD1	2.29	0.63
2:J:248:LYS:HD2	2:J:248:LYS:O	1.99	0.63
1:K:455:LEU:CD1	1:K:474:LEU:HD12	2.29	0.63
1:K:587:GLN:C	1:K:588:TYR:HD1	2.07	0.63
1:A:365:GLY:O	1:A:366:GLU:O	2.17	0.62
2:B:312:TYR:HB2	2:B:337:ARG:HG2	1.81	0.62
1:C:350:ILE:HD12	1:C:351:THR:HG23	1.80	0.62
1:E:254:ARG:HH22	1:E:293:GLY:H	1.46	0.62
1:E:274:ARG:HH11	1:E:347:THR:HB	1.64	0.62
2:H:243:GLY:C	2:H:245:PRO:HD2	2.23	0.62
1:I:250:LEU:HD21	1:I:332:PHE:CE1	2.34	0.62
2:J:317:LEU:HD22	2:J:334:VAL:HG13	1.81	0.62
1:K:269:LEU:HD12	1:K:375:VAL:HG21	1.79	0.62
1:A:345:PRO:HB3	1:A:438:ILE:CD1	2.30	0.62
2:B:192:GLY:HA2	2:B:195:PHE:CD2	2.34	0.62
2:B:279:ASP:OD2	2:B:279:ASP:C	2.42	0.62
1:C:274:ARG:HD3	1:C:347:THR:OG1	2.00	0.62
1:E:85:HIS:ND1	1:E:86:ALA:N	2.47	0.62
1:E:109:ARG:O	1:E:113:ILE:HG13	1.99	0.62
2:F:347:PHE:O	2:F:383:LYS:NZ	2.32	0.62
1:G:611:ALA:HB2	1:G:620:LEU:HD13	1.82	0.62
1:I:254:ARG:HH22	1:I:292:PRO:HB2	1.64	0.62
2:B:49:MET:HG2	2:B:318:TYR:HA	1.81	0.62
1:C:232:GLN:HG2	1:C:233:ARG:HH22	1.64	0.62
2:F:425:LEU:O	2:F:429:VAL:HG23	1.99	0.62
1:K:136:ALA:HB1	1:K:154:ALA:HB1	1.81	0.62
2:L:197:ASN:O	2:L:201:MET:HG3	1.99	0.62
2:L:234:ARG:HG2	2:L:277:ALA:O	2.00	0.62
1:G:108:LEU:HD23	1:G:132:LEU:CD1	2.30	0.62
1:I:307:VAL:O	1:I:310:ALA:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:504:LEU:O	1:K:505:PRO:O	2.17	0.62
1:A:668:VAL:HG22	1:A:694:VAL:HG23	1.81	0.62
1:C:358:TRP:CZ2	1:C:369:PRO:HG2	2.34	0.62
1:E:264:ARG:HG2	1:E:264:ARG:NH1	2.12	0.62
1:E:269:LEU:HD23	1:E:368:LEU:HD13	1.80	0.62
1:E:358:TRP:O	1:E:362:VAL:HG22	2.00	0.62
1:G:63:ARG:NH2	1:G:356:VAL:HG23	2.07	0.62
1:G:391:PRO:HG3	1:G:466:ASN:HA	1.80	0.62
1:G:397:PRO:HB3	1:G:432:PRO:HG3	1.80	0.62
1:G:445:GLU:CD	1:G:448:ARG:NH2	2.58	0.62
1:I:546:ALA:HB3	2:J:60:LEU:HD12	1.80	0.62
1:K:271:LEU:HD23	1:K:375:VAL:HG21	1.82	0.62
2:L:298:LYS:HE3	2:L:550:ASN:ND2	2.14	0.62
1:A:201:PRO:HD2	1:A:328:ARG:NH2	2.15	0.62
1:A:218:VAL:HG23	1:A:218:VAL:O	1.99	0.62
1:A:605:VAL:HG12	1:C:96:VAL:CG1	2.26	0.62
2:B:245:PRO:HB2	2:L:481:VAL:HG13	1.82	0.62
1:C:402:LEU:HD23	1:C:463:LEU:HD12	1.81	0.62
1:E:252:LYS:CE	1:E:491:ARG:HH22	2.13	0.62
1:E:525:ARG:HH11	1:E:525:ARG:CG	2.12	0.62
2:F:487:ARG:HG2	2:F:487:ARG:O	1.99	0.62
1:G:186:GLN:HE21	1:G:187:ASP:H	1.46	0.62
1:G:270:TYR:H	1:G:372:GLN:HE22	1.47	0.62
1:I:504:LEU:HD13	1:I:622:TRP:HE1	1.63	0.62
2:J:102:ALA:C	2:J:104:ALA:H	2.07	0.62
1:A:412:PRO:CB	1:A:450:ARG:HD3	2.29	0.62
1:A:663:GLU:HG2	1:A:666:GLN:NE2	2.14	0.62
1:I:285:VAL:HG12	1:I:286:VAL:HG22	1.81	0.62
2:L:123:ILE:HD11	2:L:165:LEU:CD1	2.25	0.62
1:C:66:ARG:CB	1:C:66:ARG:HH11	2.13	0.62
1:C:294:LEU:CD1	1:C:299:ARG:NH1	2.63	0.62
1:E:361:ARG:HG2	1:E:361:ARG:NH1	2.15	0.62
2:F:417:GLY:C	2:F:419:ALA:N	2.53	0.62
2:F:507:ALA:N	2:F:508:PRO:HD2	2.14	0.62
2:B:65:GLU:HG2	2:B:68:GLY:HA2	1.82	0.62
1:C:49:ILE:HD13	1:C:364:ARG:HG2	1.82	0.62
1:C:201:PRO:HD2	1:C:328:ARG:HH22	1.64	0.62
2:D:199:ALA:HB2	2:D:226:MET:HE1	1.80	0.62
2:D:247:VAL:HG22	2:D:253:GLU:OE2	2.00	0.62
2:D:462:LEU:C	2:D:462:LEU:HD23	2.25	0.62
1:E:267:HIS:HB3	1:E:368:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:GLU:OE1	1:E:436:LYS:HG2	1.99	0.62
1:E:393:GLY:O	1:E:396:LEU:HG	2.00	0.62
1:E:503:ALA:HB2	1:E:560:GLU:OE1	1.99	0.62
1:I:613:ARG:O	1:I:614:ARG:HD2	2.00	0.62
2:J:72:GLN:O	2:J:75:HIS:HB3	1.99	0.62
1:K:129:TYR:CE2	1:K:342:VAL:HG13	2.35	0.62
1:K:567:ARG:HG3	1:K:567:ARG:NH1	2.09	0.62
2:L:305:ARG:CZ	2:L:305:ARG:HB2	2.29	0.62
1:A:469:PHE:C	1:A:469:PHE:HD2	2.08	0.62
2:B:347:PHE:O	2:B:348:LYS:C	2.42	0.62
2:B:481:VAL:HG13	2:L:245:PRO:CB	2.30	0.62
1:C:186:GLN:HG2	1:C:187:ASP:OD2	2.00	0.62
2:D:68:GLY:O	2:D:70:ALA:N	2.32	0.62
2:D:138:ALA:HB2	2:D:172:ASP:OD2	2.00	0.62
2:D:272:VAL:HG12	2:D:272:VAL:O	2.00	0.62
2:F:408:MET:HE3	2:F:409:VAL:N	2.11	0.62
1:I:46:TYR:HE1	1:I:364:ARG:HD3	1.65	0.62
2:J:45:ASN:OD1	2:J:323:ALA:N	2.33	0.62
2:J:473:MET:HE2	2:J:477:GLN:CB	2.30	0.62
1:K:82:ILE:HD11	1:K:430:TYR:HE1	1.62	0.62
1:K:270:TYR:CD1	1:K:372:GLN:NE2	2.68	0.62
2:L:29:ALA:O	2:L:343:GLU:HA	1.99	0.62
1:C:384:VAL:CG1	1:C:470:LEU:HD22	2.30	0.61
1:E:152:PRO:HG3	1:E:315:TYR:CE1	2.35	0.61
2:F:145:TYR:CD1	2:F:149:THR:HB	2.35	0.61
2:F:554:GLU:HB3	2:F:555:PRO:HD2	1.82	0.61
2:H:191:PHE:HD2	2:H:192:GLY:H	1.48	0.61
2:H:498:GLY:C	2:H:500:GLU:N	2.53	0.61
1:I:269:LEU:CA	1:I:372:GLN:HE22	2.13	0.61
2:J:243:GLY:H	2:J:246:LEU:HD13	1.64	0.61
2:J:332:ARG:HG3	2:J:332:ARG:NH1	2.07	0.61
1:K:600:SER:OG	1:K:602:VAL:HG23	2.00	0.61
2:L:198:GLN:NE2	2:L:226:MET:O	2.32	0.61
1:A:391:PRO:HG3	1:A:466:ASN:HA	1.82	0.61
1:A:556:ARG:HG3	1:A:561:ARG:HB3	1.81	0.61
1:C:274:ARG:HG2	1:C:289:ALA:HB2	1.82	0.61
1:E:255:HIS:HE1	1:E:322:GLU:HG2	1.64	0.61
2:F:109:TYR:CE1	2:F:148:LEU:HD12	2.35	0.61
1:G:176:PRO:C	1:G:177:LEU:HD23	2.25	0.61
2:H:315:GLU:CD	2:H:315:GLU:N	2.58	0.61
2:J:379:GLU:H	2:J:379:GLU:CD	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:208:GLN:HE21	2:L:208:GLN:CA	2.11	0.61
1:A:221:GLU:HG3	1:A:222:ALA:N	2.14	0.61
1:A:271:LEU:O	1:A:272:ASN:HB2	1.99	0.61
1:A:709:THR:HG23	1:A:710:PRO:HD2	1.81	0.61
2:B:460:ARG:HH12	2:B:548:ALA:HB1	1.62	0.61
1:C:309:ALA:O	1:C:312:ALA:HB3	2.00	0.61
1:C:353:LEU:HD13	1:C:358:TRP:CZ2	2.35	0.61
1:C:357:ALA:O	1:C:361:ARG:HG3	2.00	0.61
1:C:561:ARG:NH1	1:C:632:VAL:HG22	2.16	0.61
2:D:244:PRO:HA	2:D:247:VAL:HG12	1.82	0.61
2:D:393:GLN:HG2	2:D:393:GLN:O	2.00	0.61
1:G:104:ALA:HA	1:G:108:LEU:HD12	1.81	0.61
2:H:68:GLY:O	2:H:70:ALA:N	2.33	0.61
1:I:169:LEU:O	1:I:173:ALA:HB2	1.99	0.61
1:I:471:ARG:HH11	1:I:471:ARG:HB2	1.65	0.61
1:K:285:VAL:HG12	1:K:286:VAL:CG2	2.27	0.61
1:K:379:GLY:HA3	1:K:440:TRP:CH2	2.35	0.61
2:L:525:ARG:HG3	2:L:525:ARG:NH1	2.12	0.61
1:A:50:GLN:HE21	1:A:123:GLN:NE2	1.99	0.61
1:A:613:ARG:HG2	1:A:614:ARG:N	2.15	0.61
2:D:119:ILE:HD11	2:D:134:VAL:CG1	2.31	0.61
1:E:232:GLN:CG	1:E:233:ARG:HH12	2.12	0.61
2:F:56:LEU:HG	2:F:60:LEU:HD12	1.81	0.61
2:H:164:ARG:CB	2:H:551:ALA:HB2	2.29	0.61
2:H:303:GLN:NE2	2:J:297:ARG:HD2	2.16	0.61
2:H:465:TRP:HE3	2:H:467:ASN:HD21	1.48	0.61
2:H:521:TYR:CE1	2:H:525:ARG:CZ	2.83	0.61
2:J:83:VAL:HG13	2:J:84:ARG:N	2.11	0.61
2:J:86:ARG:HD3	2:J:213:MET:SD	2.40	0.61
1:K:497:LEU:N	1:K:498:PRO:HD3	2.15	0.61
2:L:74:ARG:CZ	2:L:78:ARG:HH12	2.13	0.61
2:L:486:LYS:HG2	2:L:505:ILE:CD1	2.31	0.61
1:A:662:VAL:HG21	1:A:674:LEU:HD22	1.80	0.61
2:F:29:ALA:O	2:F:343:GLU:HA	2.01	0.61
1:G:445:GLU:CD	1:G:448:ARG:HH21	2.08	0.61
1:I:111:ASP:O	1:I:114:ILE:HG22	2.01	0.61
1:I:613:ARG:HG2	1:I:614:ARG:N	2.14	0.61
2:J:59:LEU:HD12	2:J:59:LEU:O	1.99	0.61
2:L:390:LEU:O	2:L:394:ARG:HG3	2.00	0.61
2:L:464:MET:CE	2:L:470:ILE:HD12	2.29	0.61
2:L:476:GLU:HA	2:L:479:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HA	1:A:375:VAL:HG11	1.81	0.61
1:A:618:LEU:HD23	1:A:629:ILE:HD12	1.83	0.61
2:B:74:ARG:HG2	2:B:74:ARG:O	2.00	0.61
1:C:307:VAL:O	1:C:310:ALA:HB3	2.01	0.61
2:F:188:ARG:HA	2:H:456:ALA:HA	1.82	0.61
2:F:247:VAL:HG12	2:F:253:GLU:OE2	1.99	0.61
1:I:268:CYS:SG	1:I:307:VAL:HG22	2.41	0.61
1:I:328:ARG:NH1	1:I:328:ARG:HB2	2.16	0.61
2:J:486:LYS:HA	2:J:489:GLN:NE2	2.15	0.61
1:K:324:LEU:HB2	1:K:334:MET:SD	2.41	0.61
1:A:54:VAL:HG11	1:A:61:ALA:HA	1.81	0.61
1:A:315:TYR:HE2	1:A:338:THR:HG22	1.65	0.61
2:F:146:TYR:N	2:F:149:THR:OG1	2.34	0.61
2:F:563:MET:SD	2:L:424:LYS:HE3	2.40	0.61
1:G:513:ALA:HA	1:G:555:LEU:HD11	1.82	0.61
1:G:536:PRO:HB3	2:H:363:HIS:HE1	1.65	0.61
2:J:209:ILE:HG22	2:J:210:ALA:N	2.16	0.61
1:K:101:ALA:CB	1:K:429:PHE:HE1	1.98	0.61
1:K:320:THR:O	1:K:336:MET:HG2	2.00	0.61
2:L:403:ASN:HA	2:L:443:GLY:H	1.64	0.61
2:B:51:GLU:HA	2:B:54:ASN:HD22	1.65	0.61
2:B:75:HIS:CE1	2:B:80:LYS:HE2	2.35	0.61
2:B:231:VAL:CG2	2:B:275:HIS:HB2	2.31	0.61
1:C:263:ASP:OD1	1:C:265:HIS:HB2	2.00	0.61
1:C:294:LEU:HD13	1:C:299:ARG:NH1	2.15	0.61
1:E:101:ALA:HB1	1:E:429:PHE:CD1	2.36	0.61
1:E:273:GLU:OE2	1:E:291:ALA:N	2.34	0.61
1:E:328:ARG:HG3	1:E:328:ARG:HH11	1.65	0.61
2:F:194:ILE:O	2:F:198:GLN:HG3	2.01	0.61
2:F:219:GLY:C	2:F:221:ALA:H	2.08	0.61
1:G:200:TYR:O	1:G:202:VAL:N	2.34	0.61
1:G:448:ARG:HD3	1:G:474:LEU:O	2.00	0.61
1:G:612:LEU:HD12	1:G:612:LEU:O	1.99	0.61
1:K:269:LEU:CD2	1:K:368:LEU:HD13	2.31	0.61
1:K:307:VAL:O	1:K:310:ALA:HB3	2.01	0.61
2:B:87:ILE:CD1	2:B:120:VAL:HG11	2.31	0.61
2:B:403:ASN:HA	2:B:443:GLY:H	1.66	0.61
1:C:274:ARG:NH2	1:C:320:THR:HG21	2.16	0.61
2:D:376:LEU:HD23	2:D:380:ALA:HB3	1.82	0.61
1:E:131:PHE:H	1:E:131:PHE:HD1	1.47	0.61
1:E:344:HIS:N	1:E:345:PRO:CD	2.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:ARG:HB2	1:G:122:ALA:HA	1.83	0.61
1:I:108:LEU:HD23	1:I:132:LEU:HD12	1.82	0.61
1:K:612:LEU:HD12	1:K:612:LEU:H	1.65	0.61
1:K:613:ARG:HG2	1:K:614:ARG:N	2.16	0.61
2:L:90:LEU:HB2	2:L:284:LEU:HD22	1.82	0.61
1:A:300:ARG:O	1:A:304:GLU:OE2	2.19	0.61
1:C:50:GLN:HB2	1:C:123:GLN:HE22	1.64	0.61
2:D:432:ALA:HA	2:D:556:THR:HG21	1.83	0.61
1:E:340:LEU:HG	1:E:359:GLN:NE2	2.16	0.61
2:F:359:PHE:CE2	2:F:387:PHE:CE1	2.89	0.61
2:F:399:LEU:HD12	2:F:400:PHE:N	2.16	0.61
1:I:328:ARG:HB2	1:I:328:ARG:CZ	2.31	0.61
1:K:66:ARG:CB	1:K:66:ARG:NH1	2.62	0.61
2:L:194:ILE:N	2:L:194:ILE:HD12	2.15	0.61
1:A:431:ASP:C	1:A:431:ASP:OD2	2.44	0.60
2:B:202:SER:HB2	2:L:560:VAL:HG23	1.83	0.60
1:C:270:TYR:CD1	1:C:372:GLN:NE2	2.69	0.60
2:D:440:LEU:CD1	2:D:464:MET:HG3	2.31	0.60
1:E:602:VAL:O	1:E:602:VAL:HG12	2.00	0.60
1:G:71:LEU:CB	1:G:73:ILE:HD12	2.31	0.60
1:G:71:LEU:HB2	1:G:73:ILE:HD12	1.82	0.60
1:G:389:GLU:HA	1:G:397:PRO:HA	1.82	0.60
2:H:193:ARG:NH1	2:H:196:PHE:CE2	2.69	0.60
2:B:444:SER:CB	2:B:449:ASN:HD22	2.08	0.60
1:C:53:LEU:HD13	1:C:117:ALA:HA	1.82	0.60
1:C:278:ILE:H	1:C:278:ILE:CD1	1.95	0.60
2:D:109:TYR:OH	2:D:147:PRO:HB2	2.00	0.60
2:D:520:TYR:N	2:D:520:TYR:CD2	2.66	0.60
2:F:200:ASN:ND2	2:F:204:ARG:NH2	2.50	0.60
1:G:249:TYR:HD2	1:G:250:LEU:H	1.49	0.60
1:G:283:GLN:NE2	1:G:389:GLU:OE1	2.32	0.60
1:G:396:LEU:O	1:G:398:ALA:N	2.33	0.60
2:H:258:GLU:OE2	2:H:262:GLY:HA3	2.00	0.60
2:H:270:SER:OG	2:H:272:VAL:HG23	2.00	0.60
2:H:400:PHE:CD2	2:H:453:CYS:HB2	2.35	0.60
1:I:54:VAL:HG21	1:I:64:VAL:CG1	2.31	0.60
2:J:462:LEU:HD23	2:J:463:TRP:N	2.16	0.60
1:A:543:TRP:O	1:A:544:ARG:NH1	2.34	0.60
1:C:549:ARG:NE	1:C:571:PRO:HG3	2.16	0.60
2:D:300:GLY:O	2:D:301:GLN:HB2	2.00	0.60
1:E:112:ARG:HG3	1:E:112:ARG:NH1	2.12	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:LEU:HD23	1:E:269:LEU:H	1.65	0.60
1:E:320:THR:O	1:E:336:MET:HG2	2.01	0.60
2:F:484:GLN:HE22	2:F:487:ARG:NH1	1.98	0.60
1:G:379:GLY:HA3	1:G:440:TRP:CH2	2.37	0.60
1:G:488:PHE:C	1:G:488:PHE:CD2	2.79	0.60
1:I:505:PRO:HB2	1:I:507:HIS:HB3	1.82	0.60
2:J:351:PHE:O	2:J:383:LYS:HD2	2.01	0.60
1:K:269:LEU:HD12	1:K:375:VAL:CG2	2.32	0.60
1:A:196:GLY:O	1:A:198:ILE:N	2.34	0.60
1:A:267:HIS:CB	1:A:368:LEU:HD12	2.30	0.60
1:A:304:GLU:O	1:A:307:VAL:HG12	2.00	0.60
1:A:472:ARG:CZ	1:A:498:PRO:HD2	2.32	0.60
1:C:536:PRO:HB3	2:D:363:HIS:CD2	2.37	0.60
1:C:567:ARG:HH11	1:C:567:ARG:HG3	1.66	0.60
1:E:261:PHE:CZ	1:E:318:ALA:HB2	2.36	0.60
2:F:141:LYS:HE2	4:F:591:COA:O2B	2.01	0.60
1:G:47:ARG:HB2	1:G:47:ARG:NH1	2.06	0.60
1:G:250:LEU:H	1:G:250:LEU:HD12	1.66	0.60
1:G:618:LEU:O	1:G:629:ILE:HD12	2.01	0.60
2:H:30:ILE:HD13	2:H:343:GLU:HG2	1.81	0.60
2:H:500:GLU:OE1	2:H:500:GLU:HA	2.01	0.60
1:I:65:MET:HE3	1:I:92:ALA:HA	1.83	0.60
1:K:304:GLU:O	1:K:308:ARG:HG2	2.00	0.60
1:K:324:LEU:HB3	1:K:334:MET:HE3	1.82	0.60
1:K:550:GLU:HG2	1:K:567:ARG:CZ	2.32	0.60
2:L:81:LEU:HD21	2:L:89:ARG:HH21	1.64	0.60
2:L:375:ILE:HG22	2:L:376:LEU:H	1.66	0.60
2:L:462:LEU:C	2:L:462:LEU:HD23	2.26	0.60
1:A:667:THR:O	1:A:667:THR:HG22	2.01	0.60
2:B:50:LEU:O	2:B:54:ASN:ND2	2.35	0.60
2:B:84:ARG:HG2	2:B:84:ARG:NH1	2.15	0.60
2:B:417:GLY:C	2:B:419:ALA:N	2.57	0.60
1:C:55:ALA:HB1	1:C:113:ILE:HD13	1.82	0.60
1:C:94:ILE:HD12	1:C:94:ILE:N	2.16	0.60
1:C:341:GLN:OE1	1:C:342:VAL:HG23	2.01	0.60
1:C:384:VAL:HG23	1:C:451:LEU:HD21	1.83	0.60
2:D:233:VAL:CG1	2:D:279:ASP:HA	2.31	0.60
2:F:35:ILE:CD1	2:F:320:VAL:HG22	2.32	0.60
2:F:469:ARG:HG2	2:F:469:ARG:NH2	2.13	0.60
1:G:451:LEU:HA	1:G:454:MET:HG3	1.82	0.60
2:H:242:ALA:O	2:H:260:LEU:HD21	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:164:ARG:HD3	2:J:550:ASN:O	2.02	0.60
1:K:294:LEU:CB	1:K:298:LEU:HD22	2.31	0.60
1:K:620:LEU:HD12	1:K:621:GLU:N	2.16	0.60
1:A:272:ASN:ND2	1:A:377:LEU:HD22	2.17	0.60
1:A:493:GLN:HE22	1:A:497:LEU:HB2	1.65	0.60
2:B:464:MET:HE1	2:B:470:ILE:HG22	1.84	0.60
2:F:282:HIS:CE1	2:F:286:ILE:HD11	2.37	0.60
1:K:440:TRP:CD1	1:K:440:TRP:C	2.79	0.60
2:L:435:PRO:HG3	2:L:460:ARG:NH2	2.16	0.60
2:L:484:GLN:HG3	2:L:488:GLU:OE1	2.01	0.60
1:A:175:VAL:HG21	1:A:309:ALA:HB2	1.82	0.60
1:A:698:TYR:CE1	1:A:710:PRO:HB2	2.37	0.60
1:C:218:VAL:HG23	1:C:218:VAL:O	2.01	0.60
1:C:445:GLU:OE1	1:C:448:ARG:NH2	2.35	0.60
2:D:465:TRP:HB3	2:D:467:ASN:ND2	2.17	0.60
2:J:299:GLN:HB3	2:J:552:PRO:HD3	1.82	0.60
2:L:109:TYR:CE2	2:L:147:PRO:HD2	2.37	0.60
1:C:55:ALA:O	1:C:56:ASN:HB2	2.00	0.60
1:C:358:TRP:O	1:C:362:VAL:HG22	2.01	0.60
1:C:561:ARG:HB3	1:C:561:ARG:CZ	2.32	0.60
2:D:487:ARG:CG	2:D:487:ARG:O	2.49	0.60
1:E:197:ARG:O	1:E:198:ILE:HG13	2.02	0.60
2:F:191:PHE:HD2	2:F:192:GLY:H	1.47	0.60
2:F:507:ALA:HA	2:F:510:LEU:HD12	1.84	0.60
1:I:587:GLN:HB3	1:I:588:TYR:HD1	1.66	0.60
1:K:391:PRO:HD3	1:K:465:THR:O	2.02	0.60
1:C:304:GLU:HB3	1:C:308:ARG:NH2	2.17	0.60
1:C:387:TYR:HB2	1:C:466:ASN:ND2	2.17	0.60
1:E:169:LEU:HD12	1:E:169:LEU:N	2.17	0.60
1:I:148:LEU:N	1:I:148:LEU:HD23	2.17	0.60
1:I:587:GLN:OE1	1:I:587:GLN:HA	2.01	0.60
1:K:258:ILE:O	1:K:320:THR:HA	2.00	0.60
2:D:498:GLY:C	2:D:500:GLU:H	2.10	0.60
2:F:114:VAL:HG11	2:F:146:TYR:CZ	2.37	0.60
2:F:338:LEU:HD21	2:F:537:THR:HB	1.82	0.60
1:G:607:ARG:NH1	1:G:607:ARG:CB	2.65	0.60
2:J:49:MET:CG	2:J:318:TYR:HD1	2.15	0.60
1:A:220:ARG:HG3	1:A:223:GLU:OE1	2.02	0.59
1:A:450:ARG:O	1:A:453:ALA:HB3	2.02	0.59
1:A:491:ARG:C	1:A:493:GLN:H	2.10	0.59
1:A:596:ASP:HB3	1:A:612:LEU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:LEU:CD2	1:C:205:LYS:NZ	2.62	0.59
2:F:403:ASN:OD1	2:F:442:GLY:HA3	2.02	0.59
1:G:51:ARG:HD3	1:G:121:GLY:O	2.02	0.59
1:K:53:LEU:HD13	1:K:117:ALA:CA	2.32	0.59
1:K:132:LEU:HD23	1:K:138:PHE:CD2	2.37	0.59
1:K:346:VAL:HG13	1:K:383:GLU:HB2	1.84	0.59
1:K:361:ARG:HG2	1:K:361:ARG:HH11	1.67	0.59
1:K:559:ASP:O	1:K:560:GLU:HG3	2.02	0.59
2:L:365:TYR:CB	2:L:545:LEU:HD13	2.30	0.59
2:L:438:THR:HG22	2:L:462:LEU:HG	1.83	0.59
1:A:80:SER:OG	1:A:81:ASP:N	2.33	0.59
1:A:257:GLU:O	1:A:273:GLU:HB2	2.02	0.59
1:A:602:VAL:O	1:A:605:VAL:HG22	2.01	0.59
1:A:652:PRO:CD	1:A:686:ILE:HG12	2.32	0.59
2:B:35:ILE:HD11	2:B:337:ARG:NH1	2.17	0.59
2:B:191:PHE:HD2	2:B:192:GLY:N	1.99	0.59
1:C:455:LEU:O	1:C:471:ARG:NH1	2.34	0.59
2:D:317:LEU:HD22	2:D:334:VAL:HG12	1.84	0.59
1:E:63:ARG:NH1	1:E:356:VAL:HG21	2.17	0.59
1:G:178:VAL:HG22	1:G:332:PHE:CD1	2.37	0.59
1:I:104:ALA:HA	1:I:108:LEU:CD1	2.32	0.59
1:I:350:ILE:HD12	1:I:377:LEU:HD11	1.84	0.59
1:I:398:ALA:HB2	1:I:464:ARG:NE	2.10	0.59
2:L:218:ALA:O	2:L:221:ALA:CB	2.49	0.59
1:A:180:GLY:HA2	1:A:198:ILE:HD11	1.85	0.59
1:A:255:HIS:CE1	1:A:322:GLU:HG2	2.38	0.59
1:A:392:GLU:C	1:A:394:ASP:H	2.10	0.59
2:B:193:ARG:HD2	2:B:196:PHE:HD2	1.66	0.59
1:C:169:LEU:HD21	1:C:313:ILE:HG12	1.84	0.59
1:G:536:PRO:HG2	2:H:543:LEU:HD23	1.84	0.59
1:I:167:LYS:O	1:I:171:GLU:HB2	2.01	0.59
1:I:298:LEU:O	1:I:301:ALA:HB3	2.03	0.59
1:I:302:MET:HA	1:I:331:PHE:CE1	2.36	0.59
1:K:273:GLU:OE1	1:K:299:ARG:NH1	2.35	0.59
1:K:506:GLU:O	1:K:507:HIS:C	2.45	0.59
1:A:504:LEU:O	1:A:505:PRO:O	2.20	0.59
2:B:234:ARG:HA	2:B:263:ALA:CB	2.31	0.59
1:C:188:LEU:HD12	1:C:188:LEU:H	1.67	0.59
2:D:119:ILE:HD11	2:D:134:VAL:HG13	1.85	0.59
2:D:562:ARG:HH11	2:D:562:ARG:HG3	1.67	0.59
2:F:234:ARG:HA	2:F:263:ALA:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:270:SER:OG	2:F:271:GLY:N	2.33	0.59
2:J:533:ASP:O	2:J:534:PRO:C	2.45	0.59
1:K:587:GLN:C	1:K:588:TYR:CD1	2.81	0.59
2:L:208:GLN:HA	2:L:208:GLN:NE2	2.13	0.59
2:B:217:THR:HG22	2:B:240:PHE:CE1	2.37	0.59
1:C:63:ARG:O	1:C:63:ARG:NH1	2.35	0.59
2:F:218:ALA:O	2:F:221:ALA:CB	2.50	0.59
2:F:525:ARG:HG3	2:F:525:ARG:NH1	2.17	0.59
2:H:354:THR:HG21	2:H:375:ILE:HB	1.85	0.59
1:I:277:SER:HB3	1:I:485:ASP:O	2.01	0.59
1:I:549:ARG:HG3	1:I:549:ARG:NH1	2.14	0.59
2:J:486:LYS:HG2	2:J:505:ILE:CD1	2.31	0.59
2:J:507:ALA:HA	2:J:510:LEU:HD12	1.85	0.59
2:L:414:GLU:HA	2:L:418:ILE:HG22	1.83	0.59
1:A:288:GLU:HB3	1:A:382:ILE:HG12	1.85	0.59
1:C:452:LEU:CD2	1:C:474:LEU:HB3	2.32	0.59
2:D:82:LEU:N	2:D:82:LEU:HD12	2.18	0.59
2:D:305:ARG:CB	2:D:305:ARG:NH1	2.66	0.59
2:F:486:LYS:HG2	2:F:505:ILE:HD13	1.84	0.59
2:H:52:GLN:O	2:H:55:ALA:HB3	2.03	0.59
1:I:397:PRO:HB3	1:I:432:PRO:HG3	1.85	0.59
1:I:513:ALA:CB	1:I:564:VAL:HG11	2.33	0.59
1:K:152:PRO:CG	1:K:315:TYR:CZ	2.83	0.59
1:K:395:PHE:O	1:K:397:PRO:HD3	2.03	0.59
2:D:486:LYS:HE3	2:D:486:LYS:HA	1.84	0.59
1:E:108:LEU:HD23	1:E:132:LEU:HD22	1.85	0.59
1:E:365:GLY:O	1:E:366:GLU:O	2.21	0.59
1:G:76:VAL:HG13	1:G:94:ILE:HB	1.85	0.59
1:I:294:LEU:HD11	1:I:299:ARG:HH12	1.68	0.59
2:J:375:ILE:HG22	2:J:376:LEU:N	2.17	0.59
1:K:491:ARG:HD2	1:K:492:HIS:CE1	2.38	0.59
2:B:109:TYR:CD2	2:B:146:TYR:HD1	2.21	0.59
2:B:223:VAL:O	2:B:227:SER:OG	2.21	0.59
2:B:444:SER:HB3	2:B:449:ASN:ND2	2.12	0.59
1:C:99:GLY:HA3	1:C:105:ASP:O	2.02	0.59
1:E:607:ARG:HG3	1:E:607:ARG:HH11	1.68	0.59
1:I:315:TYR:OH	1:I:338:THR:HA	2.02	0.59
2:J:189:GLU:C	2:J:189:GLU:CD	2.71	0.59
2:J:509:ILE:HD13	2:J:512:GLN:OE1	2.01	0.59
2:L:350:LEU:CD2	2:L:350:LEU:N	2.65	0.59
2:B:90:LEU:O	2:B:288:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:TYR:CE2	2:B:147:PRO:HD2	2.38	0.59
2:D:345:ASP:OD1	2:F:289:ARG:NE	2.33	0.59
2:D:508:PRO:HG2	2:D:509:ILE:H	1.67	0.59
1:E:76:VAL:HG11	1:E:120:SER:OG	2.03	0.59
1:E:509:TRP:CZ3	1:E:562:ARG:HB2	2.38	0.59
2:F:245:PRO:CB	2:H:481:VAL:HG13	2.32	0.59
2:F:412:LYS:HE3	2:F:413:TYR:CE1	2.38	0.59
2:F:435:PRO:HD3	2:F:553:ILE:HG23	1.83	0.59
1:G:385:ARG:HB3	1:G:387:TYR:HE1	1.68	0.59
1:G:549:ARG:CG	1:G:549:ARG:HH11	2.16	0.59
2:H:533:ASP:CB	2:H:536:GLN:HE21	2.15	0.59
1:I:351:THR:OG1	1:I:352:GLY:N	2.36	0.59
1:I:504:LEU:HB3	1:I:505:PRO:HD2	1.84	0.59
1:K:169:LEU:O	1:K:173:ALA:HB2	2.03	0.59
1:K:279:GLN:HB2	1:K:283:GLN:O	2.02	0.59
1:K:452:LEU:HD21	1:K:474:LEU:HB3	1.83	0.59
1:A:482:ALA:O	1:A:484:LEU:N	2.30	0.59
1:A:512:ALA:HB1	1:A:629:ILE:HD13	1.85	0.59
1:A:676:VAL:HG13	1:A:685:SER:OG	2.03	0.59
1:C:465:THR:HG22	1:C:466:ASN:N	2.17	0.59
2:D:349:ALA:HB3	2:D:350:LEU:HD22	1.85	0.59
1:E:187:ASP:C	1:E:189:GLU:H	2.11	0.59
1:G:534:HIS:HB3	2:H:307:PRO:CG	2.33	0.59
2:H:300:GLY:O	2:H:301:GLN:HB2	2.02	0.59
1:I:343:GLU:C	1:I:345:PRO:HD2	2.28	0.59
2:J:35:ILE:CD1	2:J:320:VAL:HG22	2.33	0.59
2:J:141:LYS:NZ	2:J:177:ASN:HD21	2.00	0.59
2:J:311:LEU:HD12	2:J:341:GLY:O	2.03	0.59
1:K:271:LEU:HA	1:K:375:VAL:HG11	1.84	0.59
1:A:496:LEU:C	1:A:498:PRO:HD3	2.27	0.58
1:A:697:LEU:CB	1:A:712:VAL:HG22	2.32	0.58
1:C:160:MET:HE2	1:C:336:MET:HB3	1.85	0.58
1:C:389:GLU:HG2	1:C:397:PRO:HG3	1.85	0.58
2:D:331:VAL:H	2:D:373:ASN:HD21	1.50	0.58
1:G:53:LEU:HD11	1:G:78:VAL:HG13	1.83	0.58
1:G:416:VAL:HG22	1:G:437:LEU:HD12	1.85	0.58
2:H:48:THR:O	2:H:52:GLN:HG3	2.03	0.58
2:H:297:ARG:HB2	2:L:303:GLN:NE2	2.14	0.58
2:L:167:CYS:HB2	2:L:208:GLN:NE2	2.18	0.58
2:B:481:VAL:HG13	2:L:245:PRO:HB3	1.86	0.58
2:D:248:LYS:HA	2:D:252:GLY:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:553:LEU:HB2	1:E:564:VAL:CG2	2.34	0.58
2:F:441:ILE:HG22	2:F:465:TRP:CD2	2.38	0.58
1:G:274:ARG:HH22	1:G:320:THR:CG2	2.16	0.58
1:G:308:ARG:HH11	1:G:308:ARG:HG3	1.68	0.58
2:J:491:GLU:C	2:J:493:ALA:H	2.09	0.58
2:J:512:GLN:O	2:J:516:GLN:HG3	2.04	0.58
1:K:396:LEU:HD12	1:K:464:ARG:NH2	2.19	0.58
2:L:155:ARG:O	2:L:159:ILE:HD12	2.03	0.58
1:C:508:PHE:O	1:C:510:GLN:N	2.37	0.58
1:C:516:TRP:CZ2	1:C:631:ALA:HB2	2.38	0.58
1:C:570:SER:O	1:C:570:SER:OG	2.21	0.58
2:F:300:GLY:HA3	2:F:549:LEU:HD23	1.85	0.58
1:G:187:ASP:O	1:G:189:GLU:N	2.36	0.58
1:I:315:TYR:HE2	1:I:336:MET:CE	2.15	0.58
2:J:89:ARG:HH21	2:J:89:ARG:HG3	1.67	0.58
2:J:191:PHE:HA	2:J:194:ILE:HD11	1.84	0.58
2:J:390:LEU:O	2:J:394:ARG:HG3	2.03	0.58
1:K:470:LEU:O	1:K:473:ILE:HG23	2.03	0.58
2:L:234:ARG:HA	2:L:263:ALA:HB3	1.85	0.58
2:L:247:VAL:O	2:L:250:ALA:HB3	2.03	0.58
1:A:444:ARG:O	1:A:447:ALA:HB3	2.02	0.58
1:A:654:ASN:HB2	2:H:251:THR:CB	2.34	0.58
2:D:151:LYS:HG2	2:D:526:LEU:HD13	1.86	0.58
1:E:358:TRP:HA	1:E:361:ARG:HD2	1.84	0.58
1:G:223:GLU:HG2	1:G:223:GLU:O	2.02	0.58
1:G:567:ARG:HG3	1:G:567:ARG:NH1	2.15	0.58
2:H:153:HIS:ND1	2:H:194:ILE:HD13	2.18	0.58
2:H:398:LEU:HD12	2:H:434:VAL:CG2	2.33	0.58
1:I:46:TYR:CE1	1:I:364:ARG:HD3	2.37	0.58
1:I:71:LEU:HD23	1:I:71:LEU:O	2.03	0.58
1:I:274:ARG:HD3	1:I:346:VAL:CG2	2.34	0.58
1:I:623:GLU:OE1	1:I:623:GLU:HA	2.03	0.58
2:J:324:ASP:O	2:J:327:GLN:HB2	2.04	0.58
1:A:53:LEU:HD12	1:A:76:VAL:HB	1.85	0.58
1:A:65:MET:HG3	1:A:75:SER:CB	2.33	0.58
1:A:298:LEU:O	1:A:301:ALA:HB3	2.04	0.58
2:B:50:LEU:CD2	2:B:54:ASN:HD21	2.16	0.58
2:D:516:GLN:OE1	2:J:181:GLN:NE2	2.35	0.58
1:G:108:LEU:HD23	1:G:132:LEU:HD13	1.86	0.58
1:G:189:GLU:OE1	1:G:193:ARG:HD3	2.03	0.58
2:J:302:LEU:HD12	2:J:549:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:533:ASP:HB3	2:J:536:GLN:HE21	1.68	0.58
2:L:239:ILE:O	2:L:266:HIS:NE2	2.34	0.58
2:B:33:THR:HG23	2:B:34:GLN:N	2.19	0.58
2:B:78:ARG:HG3	2:B:78:ARG:NH1	2.18	0.58
2:D:264:ASP:OD2	2:D:268:LYS:HE3	2.04	0.58
1:E:232:GLN:O	1:E:233:ARG:HG2	2.02	0.58
2:H:50:LEU:O	2:H:50:LEU:HD23	2.04	0.58
2:H:170:LEU:CD2	2:H:211:VAL:HB	2.33	0.58
1:C:274:ARG:NH1	1:C:347:THR:OG1	2.26	0.58
1:C:360:ILE:O	1:C:364:ARG:HD2	2.03	0.58
2:D:305:ARG:NH1	2:D:305:ARG:HB2	2.19	0.58
2:D:418:ILE:HG13	2:D:418:ILE:O	2.03	0.58
1:E:108:LEU:HD23	1:E:132:LEU:HD21	1.86	0.58
1:E:109:ARG:HD3	1:E:112:ARG:NH2	2.18	0.58
1:E:315:TYR:HE2	1:E:336:MET:HE1	1.68	0.58
1:E:440:TRP:C	1:E:440:TRP:CD1	2.81	0.58
2:F:57:ARG:HG3	2:F:57:ARG:NH1	2.17	0.58
1:G:199:GLY:O	1:G:201:PRO:N	2.36	0.58
1:G:501:GLN:HE21	1:G:504:LEU:HG	1.69	0.58
1:G:550:GLU:HG3	1:G:567:ARG:HD2	1.85	0.58
1:G:559:ASP:C	1:G:560:GLU:HG3	2.28	0.58
2:H:33:THR:HB	2:H:312:TYR:CE2	2.38	0.58
2:J:521:TYR:CE1	2:J:525:ARG:NH2	2.71	0.58
1:K:250:LEU:HD21	1:K:332:PHE:HE1	1.69	0.58
1:K:258:ILE:HD12	1:K:258:ILE:N	2.19	0.58
1:K:294:LEU:HB3	1:K:298:LEU:HD22	1.85	0.58
1:K:437:LEU:HD22	1:K:455:LEU:HD23	1.86	0.58
1:A:51:ARG:HB2	1:A:122:ALA:HA	1.85	0.58
2:B:155:ARG:O	2:B:159:ILE:CD1	2.51	0.58
2:B:484:GLN:HA	2:B:484:GLN:HE21	1.69	0.58
2:D:151:LYS:HE3	2:D:526:LEU:HB2	1.86	0.58
1:G:201:PRO:CG	1:G:328:ARG:HH21	2.15	0.58
1:G:280:ARG:NH1	1:G:389:GLU:OE1	2.36	0.58
2:H:449:ASN:OD1	2:H:454:GLY:HA3	2.03	0.58
1:I:386:LEU:HD21	1:I:467:LEU:HD12	1.85	0.58
1:K:268:CYS:SG	1:K:307:VAL:HG23	2.43	0.58
1:K:388:ALA:HB3	1:K:432:PRO:HB2	1.85	0.58
1:C:271:LEU:O	1:C:272:ASN:HB2	2.03	0.58
1:C:272:ASN:OD1	1:C:377:LEU:HD22	2.04	0.58
1:C:489:ILE:HG23	1:C:490:ALA:N	2.18	0.58
2:D:444:SER:OG	2:D:449:ASN:ND2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:HIS:CE1	1:E:322:GLU:HG2	2.38	0.58
1:E:341:GLN:OE1	1:E:342:VAL:HG23	2.04	0.58
2:H:268:LYS:HE3	2:L:350:LEU:HD12	1.85	0.58
2:H:324:ASP:O	2:H:327:GLN:HB2	2.03	0.58
2:H:327:GLN:OE1	2:H:328:PRO:HD2	2.03	0.58
2:J:195:PHE:CE1	2:J:222:TYR:HB2	2.39	0.58
2:J:218:ALA:O	2:J:221:ALA:HB3	2.04	0.58
1:K:393:GLY:O	1:K:396:LEU:CG	2.52	0.58
1:A:99:GLY:HA3	1:A:105:ASP:O	2.03	0.58
2:D:195:PHE:CE1	2:D:222:TYR:HB2	2.39	0.58
2:D:242:ALA:CB	2:D:246:LEU:HD22	2.34	0.58
2:D:370:LEU:HD11	2:D:387:PHE:HD2	1.68	0.58
1:E:299:ARG:O	1:E:301:ALA:N	2.37	0.58
1:E:562:ARG:HH11	1:E:562:ARG:CG	2.06	0.58
1:E:611:ALA:HB2	1:E:620:LEU:CD1	2.33	0.58
2:F:247:VAL:HG13	2:H:409:VAL:HG23	1.83	0.58
1:G:59:GLU:OE1	1:G:129:TYR:OH	2.22	0.58
1:I:465:THR:HG22	1:I:467:LEU:H	1.69	0.58
1:I:466:ASN:O	1:I:470:LEU:HG	2.04	0.58
1:I:491:ARG:C	1:I:493:GLN:H	2.11	0.58
1:I:607:ARG:HB3	1:I:607:ARG:NH1	2.14	0.58
2:J:48:THR:O	2:J:52:GLN:HG3	2.04	0.58
2:L:404:ILE:HG23	2:L:404:ILE:O	2.04	0.58
1:A:299:ARG:O	1:A:301:ALA:N	2.37	0.57
2:B:33:THR:HG23	2:B:35:ILE:HG13	1.84	0.57
2:B:159:ILE:H	2:B:159:ILE:HD12	1.68	0.57
2:B:293:ASN:HB3	2:F:359:PHE:CD1	2.39	0.57
2:D:351:PHE:O	2:D:383:LYS:HD2	2.04	0.57
2:F:331:VAL:H	2:F:373:ASN:HD21	1.52	0.57
2:H:432:ALA:HA	2:H:556:THR:HG21	1.84	0.57
2:J:303:GLN:NE2	2:L:297:ARG:HB2	2.18	0.57
2:L:195:PHE:CE1	2:L:222:TYR:HB2	2.39	0.57
1:A:274:ARG:HH22	1:A:320:THR:CG2	2.09	0.57
1:A:279:GLN:O	1:A:489:ILE:HG21	2.04	0.57
1:A:653:MET:HG2	1:A:654:ASN:N	2.13	0.57
2:D:237:ALA:O	2:D:238:THR:HG23	2.04	0.57
2:F:31:LEU:HD21	2:F:344:PHE:HB3	1.86	0.57
2:F:89:ARG:HG3	2:F:89:ARG:HH21	1.69	0.57
1:G:170:MET:SD	1:G:309:ALA:CB	2.90	0.57
1:I:306:ALA:HB1	1:I:321:VAL:CG2	2.29	0.57
1:K:539:ARG:HH21	2:L:363:HIS:HE1	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:302:LEU:HD22	2:L:366:PRO:HG2	1.85	0.57
1:A:300:ARG:CZ	1:A:304:GLU:OE1	2.52	0.57
1:A:493:GLN:NE2	1:A:497:LEU:HB2	2.19	0.57
1:A:504:LEU:HD13	1:A:622:TRP:HE1	1.68	0.57
1:A:525:ARG:HD2	2:B:125:ARG:HH21	1.69	0.57
2:B:95:SER:HB2	2:B:125:ARG:HB2	1.86	0.57
1:C:94:ILE:HG22	1:C:95:ALA:N	2.20	0.57
1:C:101:ALA:HB1	1:C:429:PHE:CE1	2.39	0.57
1:C:333:PHE:CE1	1:C:335:GLU:HA	2.38	0.57
1:G:515:ALA:HB2	1:G:598:LEU:HD22	1.86	0.57
1:I:270:TYR:N	1:I:372:GLN:HE22	2.01	0.57
4:J:591:COA:H122	4:J:591:COA:O1A	2.04	0.57
1:K:78:VAL:HB	1:K:98:LEU:HD21	1.86	0.57
2:L:42:PHE:HA	2:L:45:ASN:HD22	1.69	0.57
2:L:346:GLU:HG2	2:L:349:ALA:HA	1.86	0.57
2:L:351:PHE:O	2:L:383:LYS:HD2	2.02	0.57
2:L:375:ILE:HD12	2:L:375:ILE:N	2.18	0.57
1:A:361:ARG:HH11	1:A:361:ARG:CG	2.16	0.57
1:C:344:HIS:HB2	1:C:355:LEU:HD12	1.86	0.57
1:C:561:ARG:NH1	1:C:561:ARG:CB	2.66	0.57
1:C:605:VAL:O	1:C:605:VAL:CG2	2.50	0.57
2:D:62:ARG:O	2:D:65:GLU:HB2	2.03	0.57
2:F:41:GLU:O	2:F:44:ALA:HB3	2.04	0.57
2:F:90:LEU:HB2	2:F:284:LEU:HD22	1.86	0.57
1:G:258:ILE:HD12	1:G:306:ALA:HB2	1.86	0.57
1:G:263:ASP:OD2	1:G:367:ALA:HA	2.04	0.57
1:G:302:MET:HG2	1:G:331:PHE:CD2	2.40	0.57
1:I:300:ARG:HH11	1:I:300:ARG:CB	2.16	0.57
1:I:428:PRO:HG2	1:I:429:PHE:CD1	2.39	0.57
1:K:279:GLN:NE2	1:K:282:HIS:HA	2.19	0.57
1:A:195:ALA:HB1	1:A:200:TYR:HE2	1.69	0.57
2:B:397:PRO:HG2	2:B:545:LEU:HD21	1.85	0.57
1:C:508:PHE:O	1:C:509:TRP:C	2.47	0.57
1:E:298:LEU:O	1:E:301:ALA:HB3	2.04	0.57
1:E:546:ALA:O	2:F:57:ARG:NE	2.31	0.57
2:F:33:THR:HG22	2:F:312:TYR:CZ	2.39	0.57
1:G:165:ALA:O	1:G:168:ALA:HB3	2.04	0.57
1:G:474:LEU:HD23	1:G:479:PHE:CE1	2.39	0.57
2:H:44:ALA:O	2:H:47:ALA:HB3	2.04	0.57
2:J:491:GLU:HA	2:J:495:GLN:O	2.04	0.57
2:L:195:PHE:HB3	2:L:226:MET:HE1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:MET:HG2	1:A:331:PHE:CD2	2.40	0.57
2:D:211:VAL:HG13	2:D:231:VAL:HB	1.85	0.57
1:E:47:ARG:HH11	1:E:47:ARG:HB2	1.69	0.57
1:E:437:LEU:CD2	1:E:455:LEU:HD23	2.34	0.57
2:F:185:PHE:CE2	2:H:472:VAL:HA	2.40	0.57
2:F:484:GLN:HE22	2:F:487:ARG:CZ	2.17	0.57
1:G:611:ALA:HB2	1:G:620:LEU:CD1	2.34	0.57
2:H:485:VAL:CG2	2:H:486:LYS:N	2.68	0.57
1:K:516:TRP:HA	1:K:618:LEU:HD13	1.86	0.57
2:L:30:ILE:HD12	2:L:311:LEU:HD11	1.87	0.57
1:A:678:GLU:O	1:A:678:GLU:CD	2.48	0.57
2:B:89:ARG:HH21	2:B:89:ARG:CG	2.14	0.57
2:B:561:PHE:CD2	2:J:563:MET:HE1	2.39	0.57
2:D:50:LEU:HD23	2:D:54:ASN:ND2	2.19	0.57
1:E:531:ASP:HB3	2:F:298:LYS:HB2	1.87	0.57
2:F:435:PRO:CG	2:F:553:ILE:HD12	2.34	0.57
2:F:526:LEU:C	2:F:528:ASP:H	2.10	0.57
1:G:194:GLU:C	1:G:196:GLY:N	2.60	0.57
1:I:167:LYS:HB2	1:I:167:LYS:HZ2	1.68	0.57
1:I:278:ILE:HG23	1:I:489:ILE:HD13	1.86	0.57
1:I:607:ARG:NH1	1:I:607:ARG:HB2	2.20	0.57
1:K:305:ALA:CA	1:K:308:ARG:HG3	2.34	0.57
1:K:536:PRO:O	1:K:539:ARG:HG2	2.05	0.57
2:L:305:ARG:CZ	2:L:305:ARG:CB	2.82	0.57
2:L:305:ARG:HB3	2:L:305:ARG:NH1	2.19	0.57
1:A:347:THR:O	1:A:351:THR:HG23	2.05	0.57
2:B:52:GLN:O	2:B:55:ALA:HB3	2.05	0.57
2:B:245:PRO:CB	2:L:481:VAL:HG13	2.34	0.57
1:C:243:ARG:O	1:C:243:ARG:HG2	2.04	0.57
1:C:544:ARG:HH21	2:D:88:ASN:ND2	2.03	0.57
1:E:47:ARG:HG3	1:E:48:SER:H	1.69	0.57
1:E:500:PRO:O	1:E:501:GLN:HB3	2.05	0.57
1:E:563:CYS:SG	1:E:565:ARG:NH2	2.78	0.57
2:F:180:ARG:HH11	2:F:180:ARG:CG	2.12	0.57
2:F:255:VAL:HG22	2:F:259:GLU:OE1	2.04	0.57
1:G:109:ARG:HB3	1:G:109:ARG:HH11	1.69	0.57
1:G:135:ASN:O	1:G:135:ASN:OD1	2.22	0.57
1:G:228:LEU:HG	1:G:229:SER:N	2.18	0.57
1:G:385:ARG:HB3	1:G:387:TYR:CE1	2.39	0.57
1:I:69:ARG:NH2	1:I:91:GLU:O	2.38	0.57
1:I:99:GLY:HA3	1:I:105:ASP:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:365:GLY:O	1:I:366:GLU:O	2.22	0.57
2:J:462:LEU:HD23	2:J:462:LEU:C	2.29	0.57
1:K:105:ASP:OD2	1:K:105:ASP:N	2.32	0.57
2:L:161:LEU:CD2	2:L:201:MET:HG2	2.29	0.57
1:A:195:ALA:HB1	1:A:200:TYR:CE2	2.40	0.57
1:C:220:ARG:HB2	1:C:223:GLU:HB3	1.86	0.57
1:C:325:LEU:HD23	1:C:326:ASP:H	1.68	0.57
2:F:330:ASP:OD1	2:F:332:ARG:HB2	2.05	0.57
1:G:220:ARG:HB2	1:G:223:GLU:HB3	1.87	0.57
1:G:550:GLU:CG	1:G:567:ARG:HD2	2.34	0.57
1:G:587:GLN:HA	1:G:587:GLN:OE1	2.04	0.57
2:H:56:LEU:HD12	2:H:56:LEU:O	2.05	0.57
2:H:476:GLU:OE2	2:H:477:GLN:HG2	2.04	0.57
1:I:269:LEU:CA	1:I:372:GLN:NE2	2.67	0.57
1:I:504:LEU:CB	1:I:505:PRO:HD2	2.34	0.57
1:I:618:LEU:C	1:I:618:LEU:HD12	2.29	0.57
2:J:144:THR:HG21	4:J:591:COA:C5A	2.35	0.57
1:K:251:LEU:HD22	1:K:327:GLU:OE2	2.04	0.57
1:A:377:LEU:O	1:A:377:LEU:CG	2.51	0.57
1:A:675:VAL:HG11	1:A:711:LEU:HD13	1.85	0.57
1:C:114:ILE:CD1	1:C:147:LEU:HD12	2.35	0.57
1:C:141:ALA:HA	1:C:144:GLU:HB3	1.86	0.57
1:C:287:GLU:HG2	1:C:343:GLU:CG	2.35	0.57
1:E:223:GLU:O	1:E:223:GLU:HG2	2.04	0.57
1:E:248:LYS:HE3	1:E:328:ARG:HH12	1.70	0.57
2:F:241:LEU:HD12	2:H:418:ILE:HG23	1.87	0.57
2:F:386:HIS:O	2:F:390:LEU:HD12	2.05	0.57
1:G:205:LYS:HE2	1:G:245:LEU:HD13	1.87	0.57
1:G:365:GLY:O	1:G:366:GLU:O	2.22	0.57
2:H:485:VAL:HG23	2:H:486:LYS:N	2.20	0.57
2:H:521:TYR:O	2:H:525:ARG:HG3	2.05	0.57
1:I:65:MET:HE3	1:I:92:ALA:CA	2.35	0.57
1:I:107:TYR:HB2	1:I:131:PHE:CE1	2.40	0.57
1:I:289:ALA:HB1	1:I:350:ILE:HD13	1.87	0.57
1:I:374:GLN:O	1:I:376:PRO:HD3	2.03	0.57
1:I:549:ARG:CG	1:I:549:ARG:NH1	2.67	0.57
2:J:185:PHE:N	2:J:186:PRO:HD2	2.20	0.57
1:K:321:VAL:HG22	1:K:336:MET:CG	2.29	0.57
2:B:265:VAL:O	2:B:269:VAL:HB	2.05	0.56
2:D:449:ASN:OD1	2:D:454:GLY:HA3	2.05	0.56
1:E:186:GLN:HG3	1:E:190:THR:OG1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:CYS:HB2	1:E:284:LYS:NZ	2.20	0.56
1:E:404:LEU:HD13	1:E:612:LEU:HD13	1.86	0.56
2:F:146:TYR:N	2:F:149:THR:HG1	2.03	0.56
2:F:308:ARG:HH22	2:F:343:GLU:HG3	1.69	0.56
2:F:331:VAL:HA	2:F:334:VAL:HG23	1.87	0.56
1:I:269:LEU:HA	1:I:372:GLN:HE22	1.70	0.56
1:I:504:LEU:O	1:I:505:PRO:O	2.23	0.56
1:K:500:PRO:O	1:K:501:GLN:HB3	2.05	0.56
2:L:54:ASN:O	2:L:58:THR:HG23	2.05	0.56
2:L:235:GLU:HA	2:L:258:GLU:OE1	2.03	0.56
2:L:311:LEU:HB2	2:L:312:TYR:CE1	2.40	0.56
1:A:563:CYS:SG	1:A:565:ARG:NH2	2.77	0.56
2:B:193:ARG:NH1	2:B:196:PHE:CE2	2.74	0.56
2:B:457:TYR:N	2:B:457:TYR:CD2	2.71	0.56
1:C:395:PHE:C	1:C:397:PRO:HD3	2.30	0.56
2:D:45:ASN:OD1	2:D:323:ALA:N	2.38	0.56
1:E:561:ARG:H	1:E:561:ARG:CD	2.18	0.56
2:F:334:VAL:O	2:F:338:LEU:HD12	2.05	0.56
1:G:469:PHE:CD1	1:G:497:LEU:HD21	2.40	0.56
2:H:246:LEU:HD12	2:H:246:LEU:N	2.18	0.56
2:H:400:PHE:CD2	2:H:453:CYS:CB	2.88	0.56
2:H:521:TYR:CD1	2:H:525:ARG:NH1	2.72	0.56
1:I:47:ARG:HH21	1:I:148:LEU:HD22	1.70	0.56
1:I:299:ARG:O	1:I:301:ALA:N	2.38	0.56
2:J:334:VAL:O	2:J:338:LEU:CD1	2.50	0.56
2:J:498:GLY:O	2:J:500:GLU:N	2.38	0.56
2:J:523:SER:HA	2:J:528:ASP:OD2	2.06	0.56
1:K:109:ARG:HB3	1:K:109:ARG:NH1	2.18	0.56
1:K:302:MET:HG2	1:K:331:PHE:CE1	2.40	0.56
1:A:231:ALA:HA	1:A:233:ARG:HH22	1.71	0.56
1:A:269:LEU:HD23	1:A:269:LEU:H	1.69	0.56
2:B:217:THR:HG22	2:B:240:PHE:HE1	1.71	0.56
1:C:384:VAL:CG2	1:C:451:LEU:HD21	2.34	0.56
1:C:415:ARG:HD3	1:C:438:ILE:CD1	2.35	0.56
1:C:516:TRP:O	1:C:519:SER:OG	2.23	0.56
1:C:536:PRO:HB3	2:D:363:HIS:NE2	2.19	0.56
2:D:48:THR:O	2:D:52:GLN:HG3	2.04	0.56
2:D:62:ARG:HG2	2:D:62:ARG:HH11	1.71	0.56
2:D:476:GLU:OE2	2:D:477:GLN:N	2.38	0.56
1:E:169:LEU:CD1	1:E:169:LEU:H	2.19	0.56
1:E:378:ASN:O	1:E:440:TRP:CH2	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:613:ARG:HG2	1:E:614:ARG:N	2.21	0.56
2:F:82:LEU:HD12	2:F:83:VAL:N	2.16	0.56
2:F:433:ARG:H	2:F:556:THR:HG23	1.71	0.56
2:F:561:PHE:HB3	2:F:563:MET:HE3	1.87	0.56
1:G:96:VAL:HG11	1:G:116:ALA:HB1	1.87	0.56
1:G:469:PHE:CE2	1:G:473:ILE:HG21	2.41	0.56
1:I:77:ALA:HB1	1:I:88:HIS:HD2	1.70	0.56
1:K:387:TYR:CE2	1:K:433:MET:HB2	2.40	0.56
2:L:191:PHE:HE2	2:L:195:PHE:CZ	2.23	0.56
2:L:388:ILE:O	2:L:392:CYS:HB2	2.05	0.56
1:A:251:LEU:HD11	1:A:328:ARG:CZ	2.36	0.56
1:A:345:PRO:HB3	1:A:438:ILE:HD13	1.87	0.56
2:B:170:LEU:HD22	2:B:211:VAL:HB	1.86	0.56
1:C:188:LEU:HG	1:C:228:LEU:CD2	2.35	0.56
1:C:613:ARG:O	1:C:614:ARG:CD	2.53	0.56
1:E:508:PHE:HB2	1:E:622:TRP:CE2	2.41	0.56
2:F:109:TYR:OH	2:F:148:LEU:HD12	2.06	0.56
2:F:435:PRO:CD	2:F:553:ILE:HG23	2.34	0.56
1:G:150:LEU:HD21	1:G:363:ALA:CB	2.36	0.56
1:G:326:ASP:OD1	1:G:327:GLU:N	2.38	0.56
2:H:279:ASP:OD2	2:H:279:ASP:C	2.48	0.56
1:I:96:VAL:HG21	1:I:116:ALA:HB1	1.86	0.56
1:I:341:GLN:OE1	1:I:342:VAL:HG23	2.06	0.56
1:I:531:ASP:OD2	2:J:298:LYS:HB2	2.05	0.56
1:K:54:VAL:HG11	1:K:64:VAL:HG11	1.85	0.56
1:K:54:VAL:HG13	1:K:64:VAL:HG11	1.85	0.56
1:K:400:GLY:H	1:K:463:LEU:HD11	1.70	0.56
2:L:421:HIS:HA	2:L:424:LYS:HD2	1.87	0.56
1:A:169:LEU:CD2	1:A:313:ILE:HG22	2.36	0.56
2:D:362:LEU:C	2:D:362:LEU:HD23	2.29	0.56
2:F:84:ARG:HH11	2:F:84:ARG:CG	2.11	0.56
1:G:141:ALA:HA	1:G:144:GLU:HB3	1.87	0.56
1:G:259:GLN:OE1	1:G:320:THR:HG22	2.05	0.56
1:G:270:TYR:CE2	1:G:303:GLY:HA3	2.40	0.56
1:G:508:PHE:O	1:G:509:TRP:C	2.48	0.56
2:H:447:ALA:H	3:I:801:BTI:HN3	1.52	0.56
2:J:476:GLU:OE2	2:J:477:GLN:HG3	2.06	0.56
2:J:521:TYR:CE1	2:J:525:ARG:CZ	2.89	0.56
1:K:590:LEU:HD13	1:K:598:LEU:CD1	2.35	0.56
1:A:152:PRO:HG3	1:A:315:TYR:CZ	2.40	0.56
1:A:204:LEU:HD22	1:A:246:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:GLU:HG3	1:A:666:GLN:HB2	1.87	0.56
2:B:218:ALA:O	2:B:221:ALA:HB3	2.05	0.56
2:B:498:GLY:O	2:B:500:GLU:N	2.38	0.56
1:C:373:GLU:OE1	1:C:373:GLU:N	2.36	0.56
1:C:378:ASN:ND2	1:C:440:TRP:CH2	2.74	0.56
2:D:202:SER:OG	2:J:560:VAL:HG23	2.06	0.56
2:D:278:GLU:HG2	2:D:282:HIS:CE1	2.39	0.56
2:D:476:GLU:HA	2:D:510:LEU:HD21	1.86	0.56
1:E:185:ALA:O	1:E:186:GLN:O	2.24	0.56
1:E:397:PRO:HB3	1:E:432:PRO:HG3	1.87	0.56
2:F:347:PHE:O	2:F:348:LYS:C	2.47	0.56
2:F:362:LEU:HD12	2:F:367:ILE:HD13	1.88	0.56
1:G:138:PHE:CE1	1:G:142:CYS:HB2	2.40	0.56
1:G:543:TRP:HB3	2:H:96:PRO:HB3	1.88	0.56
2:H:349:ALA:HB3	2:H:350:LEU:HD22	1.88	0.56
1:I:289:ALA:O	1:I:350:ILE:HG21	2.05	0.56
2:J:68:GLY:O	2:J:70:ALA:N	2.39	0.56
2:J:185:PHE:H	2:J:186:PRO:HD2	1.69	0.56
2:J:484:GLN:HA	2:J:484:GLN:NE2	2.19	0.56
1:K:602:VAL:HG12	1:K:602:VAL:O	2.06	0.56
2:L:313:PRO:HB2	2:L:316:GLU:HG3	1.88	0.56
1:A:607:ARG:HB3	1:A:607:ARG:HH11	1.70	0.56
2:B:246:LEU:HD11	4:B:591:COA:O5P	2.06	0.56
2:B:402:GLN:OE1	2:B:452:MET:HB2	2.05	0.56
1:C:278:ILE:HD11	1:C:484:LEU:CD2	2.35	0.56
1:C:387:TYR:H	1:C:466:ASN:ND2	2.03	0.56
1:C:516:TRP:CH2	1:C:631:ALA:HB2	2.40	0.56
1:C:562:ARG:HH11	1:C:562:ARG:CB	2.19	0.56
1:E:328:ARG:HG3	1:E:328:ARG:NH1	2.19	0.56
1:E:533:PRO:C	1:E:535:SER:H	2.13	0.56
2:F:119:ILE:HG21	2:F:149:THR:HG22	1.87	0.56
2:F:440:LEU:HB2	2:F:464:MET:HG3	1.88	0.56
1:G:281:ARG:HH21	1:G:395:PHE:HD2	1.53	0.56
1:I:251:LEU:O	1:I:327:GLU:HG2	2.05	0.56
1:K:51:ARG:HB2	1:K:122:ALA:HA	1.87	0.56
1:K:250:LEU:HD21	1:K:332:PHE:CE1	2.41	0.56
1:K:392:GLU:C	1:K:394:ASP:H	2.14	0.56
2:L:53:VAL:HG12	2:L:57:ARG:CD	2.36	0.56
2:L:102:ALA:C	2:L:104:ALA:H	2.11	0.56
1:A:81:ASP:HB3	1:A:100:GLY:O	2.05	0.56
1:A:429:PHE:O	1:A:430:TYR:CD2	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:TYR:HE2	2:B:147:PRO:HD2	1.71	0.56
2:B:146:TYR:N	2:B:149:THR:OG1	2.39	0.56
2:B:248:LYS:CG	2:B:254:VAL:HG22	2.36	0.56
2:B:248:LYS:HA	2:B:252:GLY:O	2.06	0.56
2:B:424:LYS:HG2	2:J:563:MET:HE3	1.88	0.56
2:D:234:ARG:HA	2:D:263:ALA:CB	2.36	0.56
2:D:562:ARG:HG3	2:D:562:ARG:NH1	2.20	0.56
1:E:607:ARG:HG3	1:E:607:ARG:NH1	2.21	0.56
2:F:389:GLU:OE2	2:L:560:VAL:HG12	2.05	0.56
1:G:345:PRO:HB2	1:G:438:ILE:HD13	1.87	0.56
2:H:234:ARG:HA	2:H:263:ALA:CB	2.36	0.56
1:I:289:ALA:HA	1:I:290:PRO:C	2.30	0.56
2:J:49:MET:HG2	2:J:318:TYR:HA	1.88	0.56
2:L:294:LEU:O	2:L:295:ASN:C	2.45	0.56
1:A:345:PRO:CB	1:A:438:ILE:HD13	2.36	0.56
1:A:672:ALA:O	1:A:674:LEU:HG	2.06	0.56
2:B:159:ILE:HD12	2:B:159:ILE:N	2.21	0.56
2:B:178:LEU:HD12	2:L:482:LEU:HD13	1.87	0.56
1:C:175:VAL:O	1:C:177:LEU:HD12	2.06	0.56
1:C:342:VAL:HG11	1:C:385:ARG:CZ	2.36	0.56
1:E:263:ASP:HA	1:E:362:VAL:HG12	1.86	0.56
1:E:519:SER:HB2	1:E:613:ARG:NE	2.21	0.56
1:G:269:LEU:CD2	1:G:368:LEU:HD23	2.35	0.56
1:G:378:ASN:O	1:G:440:TRP:CZ3	2.59	0.56
2:H:233:VAL:CG1	2:H:279:ASP:HA	2.36	0.56
2:H:561:PHE:HB3	2:H:563:MET:HE2	1.87	0.56
1:K:251:LEU:HG	1:K:328:ARG:NH1	2.20	0.56
1:A:384:VAL:CG1	1:A:470:LEU:HD22	2.36	0.56
1:A:695:LYS:O	1:A:695:LYS:HG2	2.04	0.56
2:B:119:ILE:HD11	2:B:153:HIS:ND1	2.21	0.56
2:D:484:GLN:HG2	2:J:245:PRO:HB3	1.88	0.56
1:E:184:GLU:C	1:E:184:GLU:CD	2.74	0.56
1:G:384:VAL:HB	1:G:470:LEU:HD13	1.87	0.56
1:G:537:TRP:CE2	2:H:543:LEU:HD22	2.41	0.56
2:H:412:LYS:HG3	2:H:413:TYR:N	2.21	0.56
2:J:305:ARG:HH21	2:J:361:HIS:CG	2.24	0.56
2:J:444:SER:CB	2:J:470:ILE:HG13	2.34	0.56
2:J:449:ASN:OD1	2:J:454:GLY:HA3	2.05	0.56
2:L:164:ARG:HG2	2:L:164:ARG:O	2.06	0.56
1:A:497:LEU:N	1:A:498:PRO:CD	2.69	0.55
1:C:47:ARG:CB	1:C:47:ARG:NH1	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ILE:CD1	1:C:364:ARG:CG	2.80	0.55
2:D:224:PRO:HG3	2:D:239:ILE:HD13	1.88	0.55
1:E:596:ASP:HB3	1:E:612:LEU:HD23	1.88	0.55
1:G:50:GLN:HE21	1:G:123:GLN:NE2	2.03	0.55
2:J:121:ALA:HB2	2:J:134:VAL:HG12	1.87	0.55
2:J:243:GLY:N	2:J:246:LEU:HD13	2.20	0.55
2:B:194:ILE:N	2:B:194:ILE:CD1	2.68	0.55
1:C:387:TYR:C	1:C:389:GLU:H	2.14	0.55
2:D:526:LEU:C	2:D:528:ASP:H	2.14	0.55
1:E:150:LEU:CD2	1:E:359:GLN:HB3	2.34	0.55
1:E:388:ALA:HB2	1:E:434:LEU:HD11	1.89	0.55
1:G:52:LEU:HD22	1:G:360:ILE:HD11	1.87	0.55
1:G:611:ALA:CB	1:G:620:LEU:HD13	2.37	0.55
2:H:244:PRO:N	2:H:245:PRO:CD	2.69	0.55
2:H:291:VAL:CA	2:H:294:LEU:HD12	2.26	0.55
1:I:65:MET:CE	1:I:92:ALA:HB2	2.36	0.55
1:I:302:MET:HG2	1:I:331:PHE:CG	2.40	0.55
2:J:340:ASP:OD2	2:J:538:ARG:NH2	2.38	0.55
1:K:408:ALA:HB1	1:K:457:GLU:OE1	2.05	0.55
1:A:346:VAL:HG12	1:A:383:GLU:HB2	1.88	0.55
2:B:247:VAL:HG22	2:B:253:GLU:OE2	2.07	0.55
1:C:260:VAL:HG22	1:C:319:GLY:O	2.06	0.55
2:D:71:ALA:CB	2:D:74:ARG:HD3	2.36	0.55
2:D:83:VAL:HG13	2:D:84:ARG:H	1.71	0.55
2:D:193:ARG:NH1	2:J:456:ALA:O	2.36	0.55
2:F:331:VAL:O	2:F:334:VAL:HG23	2.07	0.55
2:F:357:CYS:SG	2:F:370:LEU:HD23	2.46	0.55
1:G:251:LEU:O	1:G:252:LYS:C	2.50	0.55
1:I:159:ALA:C	1:I:161:GLY:H	2.14	0.55
1:I:469:PHE:HD1	1:I:497:LEU:HD21	1.70	0.55
2:J:189:GLU:CD	2:J:189:GLU:O	2.50	0.55
2:L:193:ARG:HG3	2:L:193:ARG:O	2.05	0.55
1:A:448:ARG:HD3	1:A:474:LEU:O	2.07	0.55
1:A:504:LEU:HB3	1:A:505:PRO:HD2	1.87	0.55
1:A:519:SER:HB2	1:A:613:ARG:HE	1.71	0.55
1:A:589:ARG:HG2	1:A:590:LEU:H	1.70	0.55
1:C:448:ARG:HG2	1:C:474:LEU:HD22	1.88	0.55
1:C:561:ARG:CB	1:C:561:ARG:HH11	2.19	0.55
1:C:596:ASP:CB	1:C:612:LEU:HD23	2.35	0.55
2:D:50:LEU:HD23	2:D:50:LEU:O	2.07	0.55
2:F:362:LEU:HD12	2:F:367:ILE:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:TYR:OH	1:G:224:LEU:HD23	2.05	0.55
1:G:607:ARG:HH11	1:G:607:ARG:HB3	1.71	0.55
1:G:613:ARG:O	1:G:614:ARG:HD3	2.07	0.55
2:H:231:VAL:HG22	2:H:275:HIS:HB2	1.88	0.55
2:H:476:GLU:HA	2:H:510:LEU:CD2	2.36	0.55
1:I:525:ARG:HH11	1:I:525:ARG:CB	2.16	0.55
2:J:479:ALA:O	2:J:506:LYS:HE2	2.06	0.55
2:L:288:ARG:HG2	2:L:288:ARG:HH21	1.71	0.55
2:L:435:PRO:HG3	2:L:460:ARG:HH22	1.71	0.55
2:B:239:ILE:O	2:B:266:HIS:CE1	2.59	0.55
1:C:398:ALA:HB2	1:C:464:ARG:NE	2.21	0.55
1:C:446:GLU:OE1	1:E:71:LEU:HD22	2.07	0.55
1:E:308:ARG:HH11	1:E:308:ARG:CG	2.11	0.55
2:F:398:LEU:CD1	2:F:434:VAL:HG21	2.35	0.55
1:I:79:HIS:HD2	1:I:80:SER:O	1.89	0.55
1:I:449:GLN:OE1	1:K:364:ARG:NH2	2.40	0.55
1:K:504:LEU:HD23	1:K:505:PRO:CD	2.35	0.55
1:A:508:PHE:O	1:A:509:TRP:C	2.48	0.55
2:B:386:HIS:O	2:B:386:HIS:CD2	2.59	0.55
1:C:47:ARG:HE	1:C:148:LEU:HD21	1.72	0.55
1:E:108:LEU:HA	1:E:132:LEU:CD2	2.34	0.55
2:F:189:GLU:OE1	2:F:189:GLU:N	2.30	0.55
2:F:388:ILE:HD11	2:F:429:VAL:HG22	1.89	0.55
1:G:182:HIS:HB3	1:G:245:LEU:HD21	1.89	0.55
2:H:427:THR:HB	2:H:561:PHE:HE2	1.71	0.55
2:J:170:LEU:HD23	2:J:211:VAL:CG2	2.36	0.55
2:J:420:LYS:HE3	2:J:563:MET:O	2.07	0.55
1:K:66:ARG:HB2	1:K:66:ARG:NH1	2.08	0.55
1:K:169:LEU:HD12	1:K:169:LEU:N	2.22	0.55
1:K:411:GLY:O	1:K:412:PRO:C	2.49	0.55
1:K:429:PHE:CD2	1:K:429:PHE:N	2.71	0.55
1:A:427:SER:OG	1:A:428:PRO:HD2	2.07	0.55
1:A:534:HIS:O	2:B:363:HIS:HE1	1.90	0.55
2:B:89:ARG:HD2	2:B:281:ASP:OD1	2.06	0.55
2:B:264:ASP:OD1	2:B:276:TYR:HE1	1.90	0.55
1:C:513:ALA:HB2	1:C:564:VAL:HG11	1.89	0.55
2:D:371:ALA:HB2	2:D:401:LEU:HD12	1.89	0.55
2:D:375:ILE:HG22	2:D:376:LEU:N	2.18	0.55
1:E:300:ARG:HH11	1:E:300:ARG:HB3	1.71	0.55
1:G:103:PRO:O	1:G:108:LEU:HD12	2.06	0.55
1:I:278:ILE:HG22	1:I:489:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:531:ASP:HB3	2:J:298:LYS:HB2	1.88	0.55
2:J:173:SER:OG	2:J:174:GLY:N	2.39	0.55
2:J:191:PHE:HA	2:J:194:ILE:CD1	2.37	0.55
2:J:234:ARG:C	2:J:235:GLU:HG2	2.31	0.55
1:A:361:ARG:HH11	1:A:361:ARG:HG2	1.71	0.55
1:A:532:ASP:O	1:A:535:SER:HB2	2.07	0.55
2:B:157:GLN:HB3	2:B:201:MET:HE1	1.88	0.55
1:C:263:ASP:HB3	1:C:362:VAL:CG1	2.35	0.55
2:D:191:PHE:CE2	2:D:194:ILE:HD12	2.42	0.55
1:E:276:CYS:HB2	1:E:284:LYS:HZ2	1.72	0.55
1:E:401:ARG:HG2	1:E:401:ARG:HH11	1.71	0.55
2:F:121:ALA:HB2	2:F:134:VAL:HG13	1.89	0.55
2:F:412:LYS:HG3	2:F:413:TYR:N	2.22	0.55
1:G:364:ARG:HD2	1:G:366:GLU:OE1	2.07	0.55
1:G:426:VAL:HG21	1:G:463:LEU:CD1	2.36	0.55
1:I:47:ARG:HE	1:I:148:LEU:CD2	2.20	0.55
1:I:47:ARG:HB2	1:I:47:ARG:HH11	1.71	0.55
1:K:163:LYS:HE2	1:K:167:LYS:NZ	2.22	0.55
1:K:448:ARG:HG2	1:K:474:LEU:HD22	1.89	0.55
1:K:586:SER:O	1:K:587:GLN:HB2	2.06	0.55
2:L:167:CYS:HB2	2:L:208:GLN:HE22	1.72	0.55
1:A:302:MET:HG2	1:A:331:PHE:CE2	2.42	0.55
1:A:647:GLY:N	1:A:714:LEU:HB2	2.22	0.55
1:A:671:GLY:HA2	1:A:688:ALA:H	1.71	0.55
2:B:418:ILE:HG13	2:B:418:ILE:O	2.07	0.55
1:C:328:ARG:HH11	1:C:328:ARG:CG	2.19	0.55
1:C:549:ARG:HD3	1:C:568:HIS:O	2.07	0.55
2:D:164:ARG:HG2	2:D:164:ARG:O	2.05	0.55
2:D:178:LEU:HD12	2:J:478:ALA:HB1	1.88	0.55
2:D:192:GLY:HA2	2:D:195:PHE:HD2	1.68	0.55
2:D:498:GLY:O	2:D:500:GLU:N	2.40	0.55
1:E:621:GLU:HG3	1:E:626:LEU:HB2	1.88	0.55
1:G:138:PHE:CD1	1:G:138:PHE:C	2.85	0.55
1:G:153:PRO:HD2	1:G:156:ALA:HB3	1.89	0.55
2:H:102:ALA:C	2:H:104:ALA:H	2.14	0.55
2:H:344:PHE:CZ	2:H:358:GLY:HA3	2.42	0.55
1:I:299:ARG:C	1:I:301:ALA:N	2.65	0.55
2:J:161:LEU:HD13	2:J:201:MET:HG2	1.87	0.55
1:K:320:THR:CG2	1:K:341:GLN:HG3	2.36	0.55
1:K:519:SER:HB2	1:K:613:ARG:HE	1.72	0.55
1:C:134:GLU:O	1:C:135:ASN:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:303:GLN:HE21	2:F:297:ARG:HB2	1.71	0.55
1:E:307:VAL:O	1:E:310:ALA:HB3	2.07	0.55
1:G:150:LEU:CD2	1:G:359:GLN:O	2.55	0.55
1:G:159:ALA:C	1:G:161:GLY:H	2.15	0.55
1:G:201:PRO:CG	1:G:328:ARG:NH2	2.70	0.55
2:H:211:VAL:HG12	2:H:211:VAL:O	2.07	0.55
2:H:275:HIS:CE1	2:L:347:PHE:HA	2.36	0.55
2:H:317:LEU:O	2:H:318:TYR:C	2.49	0.55
1:I:103:PRO:C	1:I:108:LEU:HD12	2.31	0.55
1:I:263:ASP:HB3	1:I:362:VAL:HG12	1.88	0.55
1:I:273:GLU:OE1	1:I:273:GLU:N	2.40	0.55
2:J:538:ARG:HH11	2:J:538:ARG:CG	2.05	0.55
1:K:65:MET:SD	1:K:75:SER:HB3	2.47	0.55
1:C:225:ALA:O	1:C:228:LEU:HB3	2.07	0.54
1:C:263:ASP:C	1:C:265:HIS:H	2.15	0.54
1:C:601:ARG:HE	1:C:606:THR:HG23	1.71	0.54
1:E:350:ILE:HD12	1:E:377:LEU:CD1	2.37	0.54
1:E:357:ALA:O	1:E:361:ARG:HG3	2.08	0.54
1:E:541:ASP:HB2	1:E:549:ARG:HH21	1.70	0.54
1:G:160:MET:HE2	1:G:313:ILE:HG21	1.88	0.54
1:I:299:ARG:C	1:I:301:ALA:H	2.15	0.54
1:K:61:ALA:O	1:K:65:MET:HB2	2.07	0.54
1:K:254:ARG:HH22	1:K:292:PRO:HB2	1.71	0.54
1:A:217:VAL:CG2	1:A:249:TYR:HD1	2.20	0.54
1:C:135:ASN:O	1:C:135:ASN:CG	2.50	0.54
1:C:169:LEU:HD23	1:C:313:ILE:HG12	1.87	0.54
1:C:278:ILE:HD11	1:C:484:LEU:HD21	1.89	0.54
1:C:613:ARG:HG2	1:C:614:ARG:N	2.23	0.54
2:D:317:LEU:HD22	2:D:334:VAL:HG13	1.89	0.54
1:E:516:TRP:CG	1:E:555:LEU:HD11	2.42	0.54
2:F:138:ALA:HB2	2:F:172:ASP:OD2	2.07	0.54
2:F:187:ASP:OD2	2:H:151:LYS:NZ	2.32	0.54
2:F:324:ASP:C	2:F:324:ASP:OD1	2.50	0.54
1:I:328:ARG:NH1	1:I:328:ARG:CB	2.70	0.54
2:J:164:ARG:CB	2:J:551:ALA:HB2	2.37	0.54
2:J:417:GLY:C	2:J:419:ALA:N	2.61	0.54
1:K:384:VAL:HG13	1:K:470:LEU:HD22	1.87	0.54
1:K:557:CYS:O	1:K:558:ARG:C	2.50	0.54
2:L:441:ILE:HG22	2:L:465:TRP:CE3	2.42	0.54
1:A:463:LEU:CD2	1:A:464:ARG:H	2.21	0.54
1:C:375:VAL:O	1:C:375:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:469:ARG:HD2	2:D:517:GLY:O	2.07	0.54
2:D:491:GLU:C	2:D:493:ALA:H	2.15	0.54
1:E:264:ARG:C	1:E:265:HIS:HD2	2.16	0.54
1:E:384:VAL:HG11	1:E:470:LEU:HD13	1.89	0.54
1:E:558:ARG:HD2	1:E:560:GLU:OE2	2.07	0.54
2:F:245:PRO:HB3	2:H:481:VAL:HG13	1.88	0.54
1:G:81:ASP:C	1:G:83:ASP:H	2.15	0.54
2:H:59:LEU:HD12	2:H:59:LEU:O	2.07	0.54
1:I:302:MET:HG2	1:I:331:PHE:CD1	2.43	0.54
2:J:141:LYS:HG3	2:J:141:LYS:O	2.07	0.54
1:K:47:ARG:HE	1:K:148:LEU:HD21	1.71	0.54
1:K:108:LEU:HA	1:K:132:LEU:HD11	1.88	0.54
2:L:74:ARG:NE	2:L:78:ARG:HH12	2.05	0.54
2:L:83:VAL:CG1	2:L:84:ARG:H	2.16	0.54
2:L:103:LEU:O	2:L:524:ALA:HA	2.07	0.54
2:L:402:GLN:HE22	2:L:449:ASN:ND2	2.05	0.54
1:A:85:HIS:NE2	1:A:424:ASP:OD1	2.40	0.54
1:A:109:ARG:NE	1:A:112:ARG:NH2	2.56	0.54
1:A:251:LEU:HD12	1:A:326:ASP:OD2	2.08	0.54
1:A:681:LYS:NZ	2:F:474:GLY:H	2.05	0.54
1:C:509:TRP:CZ2	1:C:562:ARG:HG3	2.43	0.54
2:D:402:GLN:HE22	2:D:444:SER:CB	2.20	0.54
1:E:262:ALA:O	1:E:362:VAL:HG11	2.08	0.54
1:G:218:VAL:HG21	1:G:224:LEU:HD13	1.89	0.54
1:G:391:PRO:HD3	1:G:465:THR:O	2.07	0.54
2:H:274:ASP:OD1	2:L:348:LYS:HE2	2.07	0.54
1:I:589:ARG:HG2	1:I:590:LEU:H	1.71	0.54
1:K:172:GLU:O	1:K:172:GLU:OE2	2.24	0.54
2:L:144:THR:HG21	4:L:591:COA:C5A	2.38	0.54
1:A:71:LEU:HD23	1:A:71:LEU:O	2.06	0.54
1:A:496:LEU:C	1:A:497:LEU:HD23	2.32	0.54
2:B:56:LEU:O	2:B:60:LEU:HG	2.08	0.54
2:B:225:ALA:O	2:L:562:ARG:HD2	2.07	0.54
1:C:129:TYR:CD2	1:C:342:VAL:HA	2.43	0.54
2:D:66:GLY:C	2:D:68:GLY:H	2.16	0.54
1:E:605:VAL:O	1:E:605:VAL:CG2	2.54	0.54
2:F:294:LEU:O	2:F:295:ASN:C	2.50	0.54
2:F:325:SER:HB3	2:F:326:LYS:NZ	2.23	0.54
1:G:362:VAL:CG2	1:G:363:ALA:N	2.71	0.54
2:H:247:VAL:HG22	2:H:253:GLU:OE2	2.07	0.54
2:J:103:LEU:O	2:J:524:ALA:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:161:LEU:HD13	2:J:201:MET:SD	2.48	0.54
2:L:444:SER:HB3	2:L:449:ASN:HD22	1.72	0.54
1:A:446:GLU:O	1:A:450:ARG:HB2	2.08	0.54
1:A:446:GLU:OE1	1:C:71:LEU:HD21	2.08	0.54
1:A:681:LYS:HG3	1:A:681:LYS:O	2.06	0.54
2:B:375:ILE:HG21	2:B:408:MET:HB2	1.90	0.54
2:B:420:LYS:HE3	2:B:563:MET:O	2.06	0.54
2:B:465:TRP:HB3	2:B:467:ASN:HD21	1.70	0.54
1:C:165:ALA:O	1:C:168:ALA:HB3	2.08	0.54
1:C:254:ARG:HH12	1:C:293:GLY:H	1.56	0.54
2:D:89:ARG:HG3	2:D:89:ARG:NH2	2.19	0.54
2:D:233:VAL:HG13	2:D:279:ASP:CA	2.38	0.54
2:D:339:VAL:CG2	2:D:342:SER:HA	2.37	0.54
1:E:587:GLN:HB3	1:E:588:TYR:CD1	2.40	0.54
2:F:408:MET:O	2:F:418:ILE:HD13	2.08	0.54
1:G:103:PRO:C	1:G:108:LEU:HD12	2.33	0.54
1:G:186:GLN:HE22	1:G:189:GLU:HB3	1.73	0.54
2:H:119:ILE:CG2	2:H:152:LYS:HD3	2.38	0.54
1:K:270:TYR:H	1:K:372:GLN:NE2	1.94	0.54
2:L:98:LEU:HD21	2:L:463:TRP:HZ2	1.71	0.54
1:A:280:ARG:O	1:A:280:ARG:HG2	2.07	0.54
2:B:271:GLY:O	2:F:348:LYS:NZ	2.33	0.54
1:E:129:TYR:CD2	1:E:342:VAL:HA	2.43	0.54
1:E:169:LEU:N	1:E:169:LEU:CD1	2.71	0.54
1:E:450:ARG:O	1:E:453:ALA:HB3	2.07	0.54
2:F:233:VAL:HG11	2:F:236:GLN:NE2	2.23	0.54
1:G:607:ARG:HG3	1:I:94:ILE:HG12	1.89	0.54
2:J:90:LEU:HD21	2:J:168:ILE:HD13	1.89	0.54
2:J:234:ARG:HA	2:J:263:ALA:HB3	1.87	0.54
2:J:277:ALA:HB2	2:J:286:ILE:HD12	1.90	0.54
2:J:366:PRO:O	2:J:397:PRO:HD2	2.08	0.54
1:K:69:ARG:HH11	1:K:69:ARG:CB	2.18	0.54
1:K:175:VAL:CG2	1:K:309:ALA:HB2	2.27	0.54
1:A:136:ALA:HB1	1:A:154:ALA:HB1	1.90	0.54
1:A:414:ARG:HB2	1:A:454:MET:SD	2.48	0.54
1:A:689:PRO:O	1:A:690:HIS:ND1	2.40	0.54
1:E:114:ILE:O	1:E:118:LEU:HB2	2.07	0.54
1:E:188:LEU:CD2	1:E:228:LEU:HD23	2.38	0.54
1:E:271:LEU:O	1:E:272:ASN:HB2	2.08	0.54
1:E:392:GLU:O	1:E:394:ASP:N	2.41	0.54
2:F:362:LEU:HD21	2:F:538:ARG:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:ASP:C	1:G:189:GLU:N	2.65	0.54
2:J:432:ALA:HA	2:J:556:THR:HG21	1.88	0.54
1:K:365:GLY:O	1:K:366:GLU:O	2.26	0.54
2:L:87:ILE:N	2:L:87:ILE:HD12	2.23	0.54
2:L:136:ASN:OD1	2:L:136:ASN:N	2.41	0.54
2:L:429:VAL:CG1	2:L:430:ALA:N	2.70	0.54
1:A:313:ILE:HD11	1:A:315:TYR:HD2	1.72	0.54
2:B:212:VAL:O	2:B:233:VAL:HG23	2.08	0.54
2:D:487:ARG:NH2	2:D:502:GLU:OE2	2.41	0.54
1:E:114:ILE:HD11	1:E:138:PHE:CE1	2.43	0.54
1:E:611:ALA:CB	1:E:620:LEU:HD13	2.36	0.54
2:F:44:ALA:O	2:F:47:ALA:HB3	2.07	0.54
2:F:57:ARG:HH11	2:F:57:ARG:CG	2.16	0.54
2:F:153:HIS:ND1	2:F:194:ILE:HD13	2.23	0.54
2:F:184:VAL:O	2:F:191:PHE:HB2	2.08	0.54
1:G:331:PHE:O	1:G:332:PHE:CD2	2.61	0.54
2:H:178:LEU:HD12	4:H:591:COA:N6A	2.22	0.54
2:J:536:GLN:O	2:J:537:THR:C	2.49	0.54
1:K:391:PRO:HG3	1:K:466:ASN:HA	1.89	0.54
1:A:170:MET:SD	1:A:309:ALA:CB	2.96	0.54
2:B:423:ALA:HB1	2:L:226:MET:HG3	1.89	0.54
1:C:200:TYR:O	1:C:202:VAL:HG12	2.07	0.54
1:C:397:PRO:HB3	1:C:432:PRO:HG3	1.89	0.54
1:E:504:LEU:HB3	1:E:505:PRO:CD	2.31	0.54
2:F:74:ARG:O	2:F:74:ARG:HG2	2.07	0.54
2:F:388:ILE:HG21	2:F:428:ALA:HB1	1.90	0.54
1:G:156:ALA:O	1:G:159:ALA:HB3	2.08	0.54
1:I:505:PRO:HB3	1:I:507:HIS:CB	2.37	0.54
1:I:509:TRP:CH2	1:I:562:ARG:HG3	2.43	0.54
1:K:351:THR:OG1	1:K:352:GLY:N	2.41	0.54
1:K:415:ARG:CD	1:K:438:ILE:HD13	2.23	0.54
1:K:590:LEU:HD12	1:K:597:ASP:O	2.07	0.54
1:A:79:HIS:HD2	1:A:80:SER:O	1.91	0.53
1:A:513:ALA:CB	1:A:566:LEU:HD21	2.39	0.53
2:B:154:LEU:HD23	2:B:157:GLN:NE2	2.22	0.53
1:C:505:PRO:CB	1:C:507:HIS:HB2	2.34	0.53
1:E:123:GLN:CD	1:E:123:GLN:N	2.66	0.53
1:E:270:TYR:CD1	1:E:372:GLN:NE2	2.76	0.53
1:E:378:ASN:O	1:E:440:TRP:HH2	1.91	0.53
2:H:335:ILE:O	2:H:339:VAL:HG22	2.08	0.53
2:H:425:LEU:O	2:H:429:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:272:VAL:O	2:J:272:VAL:HG12	2.07	0.53
2:J:476:GLU:CD	2:J:476:GLU:N	2.66	0.53
1:K:508:PHE:HB2	1:K:622:TRP:CE2	2.42	0.53
2:L:378:ALA:O	2:L:379:GLU:C	2.49	0.53
1:A:290:PRO:HD2	1:A:380:HIS:ND1	2.23	0.53
1:A:354:ASP:CG	1:A:357:ALA:HB2	2.34	0.53
2:B:381:ALA:HB1	2:B:425:LEU:HB2	1.90	0.53
1:C:154:ALA:O	1:C:155:ALA:C	2.51	0.53
1:C:443:THR:HG23	1:C:446:GLU:H	1.73	0.53
1:E:258:ILE:O	1:E:320:THR:HA	2.07	0.53
1:E:278:ILE:HG21	1:E:473:ILE:HD11	1.89	0.53
1:E:418:SER:HB2	1:E:435:ALA:HB2	1.89	0.53
1:E:596:ASP:CG	1:E:612:LEU:HD23	2.33	0.53
1:E:600:SER:O	1:E:606:THR:HA	2.08	0.53
1:G:448:ARG:HG3	1:G:479:PHE:CE1	2.43	0.53
1:G:487:GLY:O	1:G:490:ALA:HB3	2.08	0.53
1:I:60:ILE:O	1:I:64:VAL:HG12	2.08	0.53
1:I:621:GLU:HG3	1:I:625:GLU:O	2.08	0.53
2:J:145:TYR:CD2	2:J:191:PHE:HE1	2.26	0.53
2:J:329:TYR:OH	2:J:441:ILE:HD13	2.07	0.53
2:L:332:ARG:HH22	2:L:353:THR:HG22	1.72	0.53
1:A:445:GLU:OE2	1:A:448:ARG:NH2	2.41	0.53
2:B:421:HIS:HA	2:B:424:LYS:HE3	1.90	0.53
1:C:148:LEU:N	1:C:148:LEU:HD23	2.23	0.53
1:C:203:LEU:HD23	1:C:205:LYS:HZ2	1.67	0.53
1:C:350:ILE:HA	1:C:440:TRP:CZ3	2.39	0.53
1:E:280:ARG:HH11	1:E:389:GLU:CD	2.16	0.53
2:F:192:GLY:HA2	2:F:195:PHE:HD2	1.72	0.53
1:I:106:SER:O	1:I:108:LEU:N	2.41	0.53
1:I:414:ARG:HB3	1:I:454:MET:SD	2.48	0.53
2:J:50:LEU:HD23	2:J:50:LEU:C	2.33	0.53
1:K:384:VAL:HG11	1:K:470:LEU:HD22	1.88	0.53
2:B:56:LEU:HG	2:B:60:LEU:HD11	1.91	0.53
1:C:108:LEU:HD23	1:C:132:LEU:HD11	1.88	0.53
1:C:547:LEU:N	1:C:547:LEU:HD23	2.23	0.53
2:D:68:GLY:O	2:D:69:SER:C	2.52	0.53
1:E:520:GLU:O	1:E:522:GLY:N	2.41	0.53
2:F:313:PRO:HB2	2:F:316:GLU:HG3	1.89	0.53
2:F:375:ILE:HD12	2:F:375:ILE:N	2.05	0.53
2:F:484:GLN:O	2:F:488:GLU:HG3	2.08	0.53
2:H:36:ASN:ND2	2:H:38:ARG:HD3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:49:MET:CE	2:H:321:ILE:HG21	2.38	0.53
2:J:298:LYS:HD3	2:J:550:ASN:HA	1.89	0.53
2:J:414:GLU:OE1	2:J:414:GLU:HA	2.07	0.53
2:J:499:VAL:HG12	2:J:499:VAL:O	2.08	0.53
2:L:192:GLY:HA2	2:L:195:PHE:CD2	2.43	0.53
2:L:445:PHE:HA	2:L:471:GLY:O	2.08	0.53
1:A:699:CYS:HA	1:A:703:GLU:CD	2.34	0.53
2:B:289:ARG:O	2:B:292:ALA:HB3	2.09	0.53
2:B:326:LYS:NZ	2:B:405:THR:HG23	2.23	0.53
1:C:131:PHE:HB3	1:C:132:LEU:HD22	1.90	0.53
1:C:388:ALA:HB3	1:C:432:PRO:HB2	1.91	0.53
2:D:400:PHE:HB2	2:D:438:THR:HG22	1.86	0.53
1:E:489:ILE:HG23	1:E:490:ALA:N	2.24	0.53
2:H:306:ALA:O	2:H:308:ARG:HG3	2.08	0.53
2:H:502:GLU:O	2:H:502:GLU:HG2	2.08	0.53
1:I:49:ILE:HD12	1:I:49:ILE:N	2.22	0.53
2:J:109:TYR:N	2:J:109:TYR:CD1	2.77	0.53
2:J:465:TRP:HB3	2:J:467:ASN:ND2	2.24	0.53
1:K:108:LEU:HA	1:K:132:LEU:CD1	2.39	0.53
1:K:129:TYR:CD2	1:K:342:VAL:HA	2.44	0.53
1:K:344:HIS:CE1	1:K:345:PRO:HD3	2.43	0.53
1:K:358:TRP:HD1	1:K:361:ARG:HD2	1.72	0.53
1:K:613:ARG:O	1:K:614:ARG:HD2	2.08	0.53
2:L:440:LEU:HD12	2:L:464:MET:HE2	1.89	0.53
1:A:361:ARG:CG	1:A:361:ARG:NH1	2.72	0.53
1:C:411:GLY:O	1:C:412:PRO:C	2.51	0.53
2:D:431:CYS:HB2	2:D:558:PHE:HD2	1.74	0.53
2:F:57:ARG:NH1	2:F:57:ARG:CG	2.72	0.53
2:F:78:ARG:HH22	2:H:492:ARG:NH1	2.06	0.53
2:H:57:ARG:HG3	2:H:57:ARG:NH1	2.16	0.53
1:I:255:HIS:C	1:I:255:HIS:ND1	2.67	0.53
1:K:336:MET:HE3	1:K:337:ASN:O	2.08	0.53
1:A:138:PHE:CD1	1:A:138:PHE:C	2.87	0.53
1:A:172:GLU:O	1:A:172:GLU:OE2	2.26	0.53
1:A:292:PRO:HG2	1:A:484:LEU:CD1	2.38	0.53
1:A:360:ILE:O	1:A:364:ARG:HG3	2.08	0.53
2:B:75:HIS:C	2:B:77:ALA:N	2.64	0.53
1:C:178:VAL:HG22	1:C:332:PHE:HB3	1.89	0.53
1:C:197:ARG:O	1:C:198:ILE:HG13	2.09	0.53
2:D:476:GLU:H	2:D:476:GLU:CD	2.17	0.53
2:F:376:LEU:HG	2:F:404:ILE:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:LEU:O	1:G:272:ASN:HB2	2.07	0.53
2:H:378:ALA:H	2:H:418:ILE:CD1	2.21	0.53
2:J:464:MET:CE	2:J:519:PRO:HG3	2.33	0.53
1:K:55:ALA:HB1	1:K:113:ILE:HD13	1.89	0.53
1:K:140:ARG:CZ	1:K:140:ARG:CB	2.79	0.53
1:K:405:TYR:HD1	1:K:460:VAL:HG13	1.73	0.53
2:L:155:ARG:NE	2:L:159:ILE:HD11	2.24	0.53
1:A:545:SER:O	2:B:536:GLN:NE2	2.28	0.53
1:A:586:SER:O	1:A:587:GLN:CB	2.48	0.53
2:D:224:PRO:CG	2:D:239:ILE:HD13	2.38	0.53
1:E:181:TYR:CD1	1:E:182:HIS:N	2.76	0.53
1:E:444:ARG:NH2	1:E:479:PHE:CE1	2.77	0.53
2:F:67:GLY:N	2:F:139:THR:OG1	2.35	0.53
1:G:232:GLN:HG2	1:G:233:ARG:CZ	2.39	0.53
1:I:611:ALA:HB2	1:I:620:LEU:HD13	1.90	0.53
2:J:123:ILE:HD13	2:J:165:LEU:HD11	1.91	0.53
2:L:520:TYR:H	2:L:520:TYR:HD2	1.57	0.53
1:A:191:PHE:CE2	1:A:228:LEU:HD11	2.44	0.53
1:A:299:ARG:C	1:A:301:ALA:N	2.65	0.53
1:A:380:HIS:CD2	1:A:444:ARG:HD2	2.44	0.53
1:A:391:PRO:HD3	1:A:465:THR:O	2.08	0.53
2:B:85:GLU:OE1	2:B:85:GLU:HA	2.09	0.53
1:C:478:ALA:CB	1:C:488:PHE:HE1	2.21	0.53
2:D:45:ASN:OD1	2:D:322:PRO:HA	2.08	0.53
2:D:188:ARG:HH11	2:D:188:ARG:CG	2.22	0.53
1:E:63:ARG:HH12	1:E:356:VAL:HG21	1.73	0.53
1:E:251:LEU:H	1:E:251:LEU:CD1	2.10	0.53
2:F:65:GLU:O	2:F:72:GLN:NE2	2.41	0.53
2:F:192:GLY:HA3	2:H:450:TYR:CZ	2.44	0.53
1:G:65:MET:HG3	1:G:75:SER:CB	2.38	0.53
1:G:516:TRP:CD1	1:G:553:LEU:HD22	2.44	0.53
2:H:521:TYR:CE1	2:H:525:ARG:NH1	2.77	0.53
1:I:451:LEU:HD12	1:I:454:MET:HE2	1.91	0.53
2:J:145:TYR:CD1	2:J:149:THR:HB	2.37	0.53
2:J:178:LEU:HG	4:J:591:COA:H61A	1.73	0.53
2:J:461:PHE:CD1	2:J:544:ALA:HB1	2.44	0.53
1:K:278:ILE:HG23	1:K:488:PHE:HD2	1.73	0.53
1:K:482:ALA:C	1:K:484:LEU:HD12	2.34	0.53
1:K:567:ARG:HD3	1:K:567:ARG:N	2.24	0.53
2:L:132:MET:HE3	2:L:156:ALA:C	2.33	0.53
2:L:369:ILE:C	2:L:370:LEU:HD12	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:425:LEU:HD21	2:L:451:GLY:O	2.09	0.53
2:L:536:GLN:O	2:L:540:VAL:HG23	2.08	0.53
1:A:76:VAL:HG13	1:A:94:ILE:HB	1.91	0.53
1:C:296:ALA:O	1:C:300:ARG:HG2	2.09	0.53
2:D:437:PHE:HE1	2:D:544:ALA:HB1	1.74	0.53
2:H:109:TYR:OH	2:H:147:PRO:HB2	2.09	0.53
2:H:213:MET:HA	2:H:233:VAL:CG2	2.39	0.53
1:I:103:PRO:O	1:I:108:LEU:HD12	2.09	0.53
1:I:150:LEU:HD21	1:I:359:GLN:C	2.34	0.53
2:L:334:VAL:HG12	2:L:338:LEU:HD11	1.91	0.53
1:A:138:PHE:CE1	1:A:142:CYS:HB2	2.44	0.52
1:A:694:VAL:HG11	1:A:697:LEU:HD22	1.91	0.52
1:C:47:ARG:O	1:C:364:ARG:HB3	2.08	0.52
1:C:421:ARG:HG2	1:C:424:ASP:OD2	2.09	0.52
1:C:451:LEU:HD23	1:C:474:LEU:HD11	1.90	0.52
2:D:345:ASP:CG	2:F:289:ARG:HH21	2.17	0.52
1:E:550:GLU:HA	1:E:567:ARG:CD	2.39	0.52
2:F:484:GLN:HE22	2:F:487:ARG:NH2	2.07	0.52
1:G:152:PRO:CD	1:G:157:ILE:HD11	2.22	0.52
1:G:254:ARG:NH2	1:G:292:PRO:HD2	2.22	0.52
1:G:344:HIS:N	1:G:345:PRO:CD	2.73	0.52
1:G:386:LEU:CD1	1:G:386:LEU:C	2.82	0.52
1:G:482:ALA:O	1:G:484:LEU:HD12	2.09	0.52
1:G:508:PHE:HA	1:G:622:TRP:CZ3	2.44	0.52
2:H:390:LEU:O	2:H:394:ARG:HG3	2.09	0.52
1:I:517:LEU:HD11	2:J:94:GLY:HA3	1.90	0.52
2:L:288:ARG:NH2	2:L:288:ARG:HG2	2.24	0.52
1:A:150:LEU:HD21	1:A:363:ALA:CB	2.38	0.52
1:A:203:LEU:O	1:A:204:LEU:HD23	2.07	0.52
1:A:304:GLU:HA	1:A:307:VAL:HG12	1.91	0.52
1:A:506:GLU:OE1	1:A:506:GLU:HA	2.09	0.52
2:B:230:THR:OG1	2:L:562:ARG:NH2	2.41	0.52
1:C:201:PRO:O	1:C:249:TYR:HB3	2.09	0.52
2:F:402:GLN:HE22	2:F:449:ASN:HA	1.72	0.52
1:G:299:ARG:C	1:G:301:ALA:H	2.17	0.52
2:J:211:VAL:CG1	2:J:231:VAL:HB	2.39	0.52
1:K:52:LEU:HD11	1:K:126:HIS:HB2	1.90	0.52
1:A:194:GLU:C	1:A:196:GLY:N	2.63	0.52
1:A:309:ALA:O	1:A:312:ALA:HB3	2.09	0.52
2:B:83:VAL:HG13	2:B:84:ARG:HG3	1.92	0.52
2:B:312:TYR:CD1	2:B:312:TYR:N	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:LEU:HD12	2:D:82:LEU:H	1.72	0.52
2:D:324:ASP:O	2:D:327:GLN:HB2	2.09	0.52
2:D:400:PHE:CB	2:D:438:THR:CG2	2.83	0.52
1:E:486:THR:O	1:E:486:THR:HG22	2.09	0.52
2:F:157:GLN:NE2	2:F:197:ASN:HB2	2.25	0.52
2:F:201:MET:HE3	2:F:208:GLN:HE22	1.72	0.52
2:F:354:THR:HG22	2:F:375:ILE:N	2.24	0.52
1:G:152:PRO:HG2	1:G:338:THR:HB	1.91	0.52
1:G:491:ARG:C	1:G:493:GLN:H	2.17	0.52
1:G:519:SER:HB2	1:G:613:ARG:HE	1.72	0.52
1:I:251:LEU:HD21	1:I:328:ARG:HH22	1.74	0.52
2:L:59:LEU:HD22	2:L:520:TYR:CE1	2.44	0.52
1:A:135:ASN:O	1:A:135:ASN:CG	2.52	0.52
1:A:557:CYS:O	1:A:558:ARG:C	2.52	0.52
2:B:201:MET:HB3	2:B:208:GLN:HE21	1.72	0.52
1:C:308:ARG:HG3	1:C:308:ARG:NH1	2.24	0.52
1:E:520:GLU:C	1:E:522:GLY:H	2.17	0.52
2:F:352:GLY:HA3	2:F:379:GLU:HB3	1.90	0.52
1:G:404:LEU:CD2	1:G:612:LEU:HD11	2.40	0.52
2:H:30:ILE:HG22	2:H:31:LEU:N	2.24	0.52
2:H:81:LEU:HD23	2:H:82:LEU:H	1.75	0.52
2:H:309:ALA:O	2:H:310:PRO:O	2.27	0.52
1:I:400:GLY:H	1:I:463:LEU:HD11	1.75	0.52
2:J:486:LYS:HD2	2:J:489:GLN:NE2	2.24	0.52
2:L:49:MET:HE1	2:L:467:ASN:HB3	1.90	0.52
1:A:153:PRO:CD	1:A:316:VAL:HG23	2.36	0.52
1:A:268:CYS:O	1:A:307:VAL:HG21	2.09	0.52
2:B:82:LEU:H	2:B:82:LEU:CD1	2.09	0.52
2:B:231:VAL:CG2	2:B:286:ILE:HG21	2.40	0.52
1:C:485:ASP:OD2	1:C:487:GLY:N	2.37	0.52
1:C:590:LEU:C	1:C:590:LEU:HD12	2.34	0.52
2:D:44:ALA:O	2:D:47:ALA:HB3	2.09	0.52
2:D:397:PRO:HA	2:D:434:VAL:CG2	2.39	0.52
2:D:431:CYS:O	2:D:556:THR:HG23	2.10	0.52
1:E:598:LEU:HD12	1:E:599:VAL:N	2.24	0.52
2:F:181:GLN:OE1	2:H:472:VAL:HG12	2.10	0.52
2:F:289:ARG:O	2:F:292:ALA:HB3	2.09	0.52
1:G:152:PRO:HB2	1:G:157:ILE:HG12	1.92	0.52
1:G:196:GLY:O	1:G:198:ILE:N	2.41	0.52
1:G:523:HIS:ND1	1:G:524:ARG:N	2.58	0.52
1:I:438:ILE:N	1:I:438:ILE:HD12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:562:ARG:HH11	1:I:562:ARG:CB	2.08	0.52
2:L:114:VAL:HG11	2:L:146:TYR:CZ	2.44	0.52
2:L:114:VAL:HG12	2:L:140:VAL:CG1	2.39	0.52
2:L:277:ALA:HB2	2:L:286:ILE:CD1	2.40	0.52
2:L:498:GLY:C	2:L:500:GLU:H	2.17	0.52
1:A:165:ALA:O	1:A:169:LEU:HD13	2.09	0.52
1:A:556:ARG:HG2	1:A:556:ARG:HH11	1.74	0.52
2:B:303:GLN:NE2	2:D:297:ARG:HB2	2.25	0.52
1:C:465:THR:CG2	1:C:466:ASN:N	2.72	0.52
1:E:470:LEU:HA	1:E:473:ILE:CG2	2.40	0.52
1:E:491:ARG:HD2	1:E:492:HIS:CE1	2.45	0.52
2:F:71:ALA:HA	2:F:74:ARG:HB3	1.90	0.52
1:G:302:MET:HE3	1:G:331:PHE:HB2	1.92	0.52
1:G:504:LEU:O	1:G:505:PRO:O	2.28	0.52
2:H:234:ARG:HA	2:H:263:ALA:HB3	1.92	0.52
1:I:154:ALA:HA	1:I:157:ILE:HD12	1.91	0.52
2:J:28:MET:C	2:J:30:ILE:H	2.16	0.52
1:K:269:LEU:N	1:K:269:LEU:HD23	2.24	0.52
2:L:155:ARG:HE	2:L:159:ILE:HD11	1.74	0.52
1:A:263:ASP:C	1:A:265:HIS:H	2.17	0.52
1:A:346:VAL:CG2	1:A:347:THR:N	2.72	0.52
1:C:69:ARG:HB3	1:C:69:ARG:HH11	1.74	0.52
1:C:421:ARG:O	1:C:422:GLU:C	2.52	0.52
2:D:313:PRO:HD2	2:D:316:GLU:OE1	2.10	0.52
1:E:531:ASP:OD2	2:F:298:LYS:HG3	2.10	0.52
1:E:547:LEU:N	1:E:547:LEU:CD2	2.73	0.52
2:F:339:VAL:HG23	2:F:342:SER:HA	1.90	0.52
2:F:476:GLU:HA	2:F:479:ALA:HB3	1.92	0.52
2:J:29:ALA:O	2:J:343:GLU:HA	2.09	0.52
2:J:211:VAL:HG13	2:J:231:VAL:HB	1.89	0.52
2:J:381:ALA:HA	2:J:425:LEU:HD22	1.92	0.52
1:K:135:ASN:HD21	1:K:138:PHE:HB2	1.74	0.52
1:K:508:PHE:O	1:K:509:TRP:C	2.53	0.52
2:L:109:TYR:OH	2:L:147:PRO:HB2	2.08	0.52
1:A:444:ARG:NH1	1:A:444:ARG:HG2	2.24	0.52
2:B:432:ALA:HA	2:B:556:THR:HG21	1.91	0.52
1:C:566:LEU:C	1:C:567:ARG:HD3	2.35	0.52
1:C:605:VAL:HG12	1:E:96:VAL:CG1	2.39	0.52
2:D:239:ILE:O	2:D:266:HIS:NE2	2.39	0.52
2:D:252:GLY:O	2:D:253:GLU:HB3	2.09	0.52
2:D:472:VAL:HG12	2:J:181:GLN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:481:VAL:HG12	2:J:245:PRO:CB	2.39	0.52
1:E:169:LEU:HD23	1:E:313:ILE:HG22	1.91	0.52
2:F:508:PRO:O	2:F:511:GLU:HG3	2.09	0.52
1:G:217:VAL:HG23	1:G:249:TYR:HD1	1.74	0.52
2:H:171:VAL:CG2	2:H:212:VAL:HA	2.36	0.52
1:K:408:ALA:CB	1:K:457:GLU:HB2	2.37	0.52
2:L:265:VAL:O	2:L:269:VAL:HG23	2.09	0.52
2:L:338:LEU:HD22	2:L:537:THR:HG22	1.92	0.52
1:A:605:VAL:O	1:A:605:VAL:CG2	2.56	0.52
2:B:201:MET:HB3	2:B:208:GLN:NE2	2.25	0.52
1:C:251:LEU:CD2	1:C:328:ARG:HE	2.23	0.52
2:D:324:ASP:HB3	2:D:327:GLN:HB2	1.91	0.52
1:E:160:MET:CE	1:E:170:MET:HE3	2.39	0.52
1:E:333:PHE:CD1	1:E:333:PHE:C	2.88	0.52
1:E:396:LEU:O	1:E:398:ALA:N	2.43	0.52
2:F:74:ARG:NH2	2:F:78:ARG:NH1	2.58	0.52
1:G:302:MET:HG2	1:G:331:PHE:CZ	2.44	0.52
2:H:231:VAL:HG11	2:H:283:ALA:HB1	1.92	0.52
1:I:391:PRO:HG2	1:I:468:ALA:HB3	1.91	0.52
2:J:300:GLY:O	2:J:301:GLN:HB2	2.10	0.52
1:K:123:GLN:O	1:K:148:LEU:HG	2.10	0.52
1:K:302:MET:HG2	1:K:331:PHE:CG	2.45	0.52
1:A:251:LEU:O	1:A:252:LYS:C	2.52	0.52
1:C:203:LEU:HG	1:C:204:LEU:N	2.25	0.52
1:C:252:LYS:CG	1:C:485:ASP:HB3	2.40	0.52
2:D:526:LEU:C	2:D:528:ASP:N	2.68	0.52
2:F:54:ASN:O	2:F:58:THR:HG23	2.10	0.52
2:F:449:ASN:OD1	2:F:454:GLY:HA3	2.11	0.52
1:G:136:ALA:O	1:G:137:ASP:C	2.53	0.52
2:H:75:HIS:CE1	2:H:80:LYS:HE2	2.43	0.52
2:H:220:GLY:O	2:H:224:PRO:HD2	2.10	0.52
2:H:440:LEU:HD12	2:H:464:MET:HE2	1.92	0.52
2:H:491:GLU:C	2:H:493:ALA:H	2.17	0.52
1:I:344:HIS:N	1:I:345:PRO:HD3	2.25	0.52
1:I:623:GLU:OE1	1:I:623:GLU:CA	2.58	0.52
2:J:297:ARG:HB3	2:J:297:ARG:NH1	2.25	0.52
1:K:455:LEU:HD12	1:K:474:LEU:HD12	1.90	0.52
1:A:135:ASN:O	1:A:136:ALA:C	2.53	0.51
1:A:217:VAL:HG21	1:A:249:TYR:CD1	2.45	0.51
1:A:622:TRP:CD1	1:A:622:TRP:O	2.63	0.51
2:B:274:ASP:OD1	2:F:348:LYS:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:449:ASN:OD1	2:B:454:GLY:HA3	2.09	0.51
1:C:469:PHE:HE2	1:C:473:ILE:HD12	1.68	0.51
2:D:351:PHE:HE2	2:D:379:GLU:HB3	1.75	0.51
2:D:498:GLY:C	2:D:500:GLU:N	2.69	0.51
1:G:78:VAL:HB	1:G:98:LEU:HD21	1.92	0.51
2:H:303:GLN:NE2	2:J:297:ARG:CD	2.73	0.51
1:I:54:VAL:HG21	1:I:64:VAL:HG13	1.92	0.51
1:I:269:LEU:HB3	1:I:372:GLN:NE2	2.25	0.51
2:J:417:GLY:C	2:J:419:ALA:H	2.16	0.51
1:K:537:TRP:HB3	2:L:125:ARG:HG2	1.91	0.51
2:L:402:GLN:HE22	2:L:449:ASN:HD22	1.58	0.51
1:A:201:PRO:CD	1:A:328:ARG:HH21	2.19	0.51
1:A:358:TRP:CH2	1:A:370:LEU:HD12	2.45	0.51
1:C:152:PRO:HG2	1:C:338:THR:HB	1.91	0.51
1:C:278:ILE:HD12	1:C:278:ILE:N	2.03	0.51
1:C:339:ARG:HH11	1:C:339:ARG:HG3	1.74	0.51
2:D:211:VAL:CG1	2:D:231:VAL:HB	2.39	0.51
2:D:248:LYS:HZ2	2:D:254:VAL:CG2	2.23	0.51
1:E:278:ILE:HG23	1:E:488:PHE:CD2	2.45	0.51
1:E:623:GLU:CD	1:E:623:GLU:H	2.18	0.51
2:F:185:PHE:CD2	2:H:472:VAL:HA	2.45	0.51
2:F:227:SER:O	2:F:228:ASP:C	2.53	0.51
2:F:398:LEU:N	2:F:398:LEU:HD12	2.25	0.51
1:G:446:GLU:HG3	1:I:71:LEU:HD21	1.91	0.51
2:H:50:LEU:HD23	2:H:50:LEU:C	2.35	0.51
2:H:407:PHE:CE1	2:H:447:ALA:HB3	2.45	0.51
1:I:599:VAL:CG2	1:I:608:ARG:HD3	2.41	0.51
2:J:369:ILE:HG12	2:J:399:LEU:HD23	1.92	0.51
2:L:82:LEU:HD12	2:L:82:LEU:N	2.24	0.51
1:C:175:VAL:HG21	1:C:309:ALA:HB2	1.92	0.51
1:C:289:ALA:O	1:C:350:ILE:HG21	2.10	0.51
1:C:319:GLY:HA2	1:C:339:ARG:O	2.10	0.51
1:C:333:PHE:CD1	1:C:333:PHE:C	2.88	0.51
2:D:289:ARG:O	2:D:292:ALA:HB3	2.10	0.51
2:D:339:VAL:HG22	2:D:342:SER:HA	1.91	0.51
2:D:472:VAL:CG1	2:J:181:GLN:CB	2.83	0.51
1:G:47:ARG:HG3	1:G:48:SER:N	2.25	0.51
1:G:189:GLU:HG3	1:G:190:THR:N	2.24	0.51
2:H:248:LYS:HA	2:H:252:GLY:O	2.10	0.51
2:H:392:CYS:SG	2:H:556:THR:HG21	2.50	0.51
1:I:380:HIS:NE2	1:I:444:ARG:HD2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:620:LEU:C	1:I:620:LEU:HD12	2.36	0.51
2:J:36:ASN:HD22	2:J:37:PRO:HD2	1.74	0.51
2:J:87:ILE:HG22	2:J:88:ASN:N	2.26	0.51
2:J:424:LYS:NZ	2:J:562:ARG:O	2.43	0.51
1:K:63:ARG:NH2	1:K:356:VAL:CG2	2.73	0.51
1:A:67:SER:O	1:A:68:ALA:C	2.53	0.51
1:A:150:LEU:CD2	1:A:363:ALA:CB	2.88	0.51
1:A:283:GLN:NE2	1:A:389:GLU:OE1	2.44	0.51
1:A:339:ARG:HG3	1:A:339:ARG:NH1	2.23	0.51
1:A:360:ILE:O	1:A:360:ILE:HG22	2.10	0.51
2:D:190:HIS:C	2:D:191:PHE:O	2.53	0.51
2:D:386:HIS:HD2	2:D:386:HIS:O	1.93	0.51
1:E:229:SER:O	1:E:231:ALA:N	2.42	0.51
1:E:350:ILE:HD12	1:E:377:LEU:HD11	1.92	0.51
2:F:408:MET:HG3	2:F:413:TYR:CE2	2.45	0.51
1:G:114:ILE:HD11	1:G:145:ALA:CB	2.40	0.51
1:G:202:VAL:CG2	1:G:247:GLU:O	2.59	0.51
2:H:339:VAL:HG11	2:H:360:ALA:CB	2.40	0.51
2:H:378:ALA:N	2:H:418:ILE:HD11	2.25	0.51
2:H:532:ILE:O	2:H:534:PRO:HD3	2.10	0.51
1:I:104:ALA:CA	1:I:108:LEU:HD12	2.37	0.51
1:I:274:ARG:NH1	1:I:347:THR:OG1	2.40	0.51
1:I:390:ASP:OD1	1:I:393:GLY:HA3	2.09	0.51
1:I:543:TRP:HB3	2:J:96:PRO:HB3	1.92	0.51
1:K:489:ILE:HG23	1:K:490:ALA:N	2.26	0.51
2:L:132:MET:HE3	2:L:156:ALA:O	2.09	0.51
2:L:152:LYS:HA	2:L:526:LEU:HD21	1.93	0.51
1:A:186:GLN:NE2	1:A:187:ASP:N	2.50	0.51
1:A:255:HIS:HE1	1:A:322:GLU:HG2	1.75	0.51
1:A:346:VAL:CG1	1:A:383:GLU:HB2	2.41	0.51
2:B:248:LYS:HG2	2:B:254:VAL:HG22	1.92	0.51
2:B:386:HIS:CD2	2:B:386:HIS:C	2.89	0.51
1:C:47:ARG:HG3	1:C:48:SER:N	2.24	0.51
1:C:156:ALA:O	1:C:159:ALA:HB3	2.10	0.51
1:C:405:TYR:HD1	1:C:460:VAL:HG13	1.76	0.51
1:C:506:GLU:O	1:C:507:HIS:C	2.53	0.51
1:E:280:ARG:HD3	1:E:283:GLN:NE2	2.26	0.51
2:F:484:GLN:NE2	2:F:487:ARG:NH1	2.58	0.51
1:G:134:GLU:O	1:G:135:ASN:HB3	2.10	0.51
1:G:354:ASP:OD2	1:G:357:ALA:HB2	2.11	0.51
2:H:354:THR:HG21	2:H:375:ILE:C	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:444:ARG:HH11	1:I:444:ARG:CG	2.23	0.51
1:I:509:TRP:CD2	1:I:562:ARG:HD3	2.45	0.51
2:J:171:VAL:CG1	2:J:212:VAL:HG13	2.41	0.51
2:J:467:ASN:ND2	2:J:467:ASN:H	2.09	0.51
2:J:483:ALA:HB3	2:J:506:LYS:HE3	1.91	0.51
1:K:164:SER:OG	1:K:165:ALA:N	2.43	0.51
1:A:221:GLU:CG	1:A:222:ALA:N	2.74	0.51
1:A:508:PHE:O	1:A:510:GLN:N	2.44	0.51
1:A:590:LEU:HD12	1:A:597:ASP:O	2.10	0.51
2:B:500:GLU:O	2:B:504:LYS:HD3	2.11	0.51
1:C:71:LEU:O	1:C:71:LEU:HD23	2.11	0.51
1:C:344:HIS:CG	1:C:345:PRO:HD3	2.44	0.51
1:C:497:LEU:N	1:C:498:PRO:HD3	2.25	0.51
2:D:487:ARG:HA	2:D:497:LEU:HD13	1.91	0.51
2:F:433:ARG:N	2:F:556:THR:HG23	2.25	0.51
1:G:378:ASN:O	1:G:440:TRP:HZ3	1.94	0.51
2:H:161:LEU:HD22	2:H:201:MET:HG3	1.93	0.51
2:H:486:LYS:HG2	2:H:505:ILE:CD1	2.40	0.51
2:J:217:THR:HG22	2:J:240:PHE:HE1	1.76	0.51
2:J:486:LYS:HG3	2:J:497:LEU:HD22	1.93	0.51
1:K:143:GLU:HA	1:K:147:LEU:O	2.10	0.51
1:K:554:MET:HA	1:K:554:MET:HE3	1.92	0.51
2:L:347:PHE:CE2	2:L:348:LYS:HG2	2.45	0.51
1:A:187:ASP:OD1	1:A:189:GLU:N	2.44	0.51
1:A:269:LEU:HD23	1:A:368:LEU:HD13	1.93	0.51
1:A:273:GLU:HG2	1:A:274:ARG:N	2.25	0.51
1:A:695:LYS:O	1:A:696:ALA:CB	2.58	0.51
2:B:89:ARG:NH2	2:B:89:ARG:CG	2.70	0.51
2:B:231:VAL:HG21	2:B:286:ILE:CG2	2.41	0.51
2:B:284:LEU:O	2:B:287:ALA:HB3	2.10	0.51
2:B:533:ASP:HB3	2:B:536:GLN:HE21	1.76	0.51
1:C:138:PHE:CE1	1:C:142:CYS:HB2	2.45	0.51
1:C:563:CYS:SG	1:C:565:ARG:NH2	2.83	0.51
2:D:389:GLU:CG	2:H:560:VAL:HG13	2.39	0.51
2:F:506:LYS:HZ3	2:F:506:LYS:HB2	1.76	0.51
1:G:114:ILE:HD11	1:G:147:LEU:HD13	1.93	0.51
1:G:249:TYR:CD2	1:G:250:LEU:N	2.69	0.51
1:G:299:ARG:C	1:G:301:ALA:N	2.67	0.51
2:H:457:TYR:N	2:H:457:TYR:CD2	2.78	0.51
2:J:435:PRO:HD3	2:J:553:ILE:HG23	1.92	0.51
1:K:140:ARG:NH1	1:K:140:ARG:CB	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:304:GLU:O	1:K:307:VAL:HG12	2.10	0.51
1:K:357:ALA:O	1:K:361:ARG:HG3	2.11	0.51
2:B:479:ALA:HB2	2:B:509:ILE:CG2	2.40	0.51
1:C:522:GLY:O	1:C:523:HIS:CB	2.57	0.51
2:D:192:GLY:HA3	2:J:450:TYR:CZ	2.46	0.51
1:E:387:TYR:HB2	1:E:466:ASN:ND2	2.25	0.51
2:F:45:ASN:OD1	2:F:322:PRO:HA	2.10	0.51
1:G:231:ALA:HB3	1:G:244:MET:CE	2.36	0.51
2:H:191:PHE:HD2	2:H:192:GLY:N	2.09	0.51
2:J:299:GLN:HG2	2:J:552:PRO:HB3	1.93	0.51
2:L:298:LYS:HG2	2:L:550:ASN:HA	1.92	0.51
1:A:148:LEU:N	1:A:148:LEU:HD23	2.25	0.51
1:C:101:ALA:HB1	1:C:429:PHE:CD1	2.46	0.51
1:C:299:ARG:O	1:C:301:ALA:N	2.44	0.51
1:C:344:HIS:CE1	1:C:345:PRO:HD3	2.46	0.51
1:C:348:GLU:OE1	1:C:415:ARG:NH1	2.40	0.51
2:D:216:CYS:SG	2:D:220:GLY:O	2.69	0.51
2:D:317:LEU:O	2:D:318:TYR:C	2.54	0.51
2:D:403:ASN:HA	2:D:443:GLY:H	1.76	0.51
2:D:457:TYR:N	2:D:457:TYR:CD2	2.79	0.51
2:D:486:LYS:HG2	2:D:505:ILE:CD1	2.41	0.51
2:F:217:THR:CG2	2:F:240:PHE:HE1	2.10	0.51
2:F:331:VAL:HG21	2:F:371:ALA:HB1	1.92	0.51
1:G:150:LEU:CD2	1:G:363:ALA:CB	2.85	0.51
1:G:320:THR:HG21	1:G:341:GLN:HB2	1.93	0.51
1:G:473:ILE:CB	1:G:496:LEU:HD13	2.39	0.51
2:H:246:LEU:H	2:H:246:LEU:CD1	2.18	0.51
2:H:298:LYS:HE3	2:H:550:ASN:ND2	2.26	0.51
1:I:251:LEU:HD11	1:I:328:ARG:HH22	1.72	0.51
1:I:469:PHE:C	1:I:469:PHE:CD2	2.88	0.51
1:I:497:LEU:N	1:I:498:PRO:CD	2.74	0.51
1:I:602:VAL:HG23	1:I:605:VAL:O	2.11	0.51
2:J:299:GLN:CG	2:J:552:PRO:HD3	2.40	0.51
2:L:441:ILE:HG22	2:L:465:TRP:CE2	2.46	0.51
1:A:65:MET:CE	1:A:88:HIS:O	2.58	0.51
1:C:62:CYS:HB3	1:C:91:GLU:OE1	2.11	0.51
1:C:252:LYS:HG3	1:C:485:ASP:HB3	1.92	0.51
2:D:206:ILE:O	2:D:207:PRO:C	2.53	0.51
2:D:258:GLU:HG3	2:D:258:GLU:O	2.10	0.51
2:D:440:LEU:HD12	2:D:464:MET:HG3	1.91	0.51
2:F:192:GLY:HA3	2:H:450:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:216:CYS:HB3	2:F:239:ILE:HA	1.91	0.51
2:F:346:GLU:HG3	2:F:357:CYS:O	2.11	0.51
1:G:179:PRO:O	1:G:248:LYS:HB2	2.10	0.51
1:G:448:ARG:HG3	1:G:479:PHE:HE1	1.74	0.51
2:H:420:LYS:O	2:H:423:ALA:HB3	2.10	0.51
1:K:307:VAL:O	1:K:311:GLN:NE2	2.44	0.51
2:L:308:ARG:NH2	2:L:343:GLU:OE1	2.44	0.51
1:A:78:VAL:HB	1:A:98:LEU:HD21	1.94	0.50
1:A:159:ALA:C	1:A:161:GLY:H	2.19	0.50
1:A:278:ILE:H	1:A:278:ILE:CD1	2.06	0.50
1:A:320:THR:HG21	1:A:341:GLN:HB2	1.93	0.50
2:B:326:LYS:NZ	2:B:405:THR:CG2	2.74	0.50
1:C:431:ASP:OD1	1:C:432:PRO:HD2	2.11	0.50
2:D:59:LEU:O	2:D:63:ILE:HG13	2.11	0.50
1:E:437:LEU:HD23	1:E:455:LEU:HD23	1.93	0.50
2:F:108:VAL:HG11	2:F:148:LEU:CD1	2.40	0.50
1:G:411:GLY:H	1:G:414:ARG:HG3	1.76	0.50
2:J:171:VAL:HG12	2:J:171:VAL:O	2.09	0.50
1:K:76:VAL:HA	1:K:94:ILE:O	2.10	0.50
2:L:147:PRO:HA	2:L:184:VAL:HG22	1.93	0.50
1:A:263:ASP:HB3	1:A:362:VAL:HG12	1.92	0.50
2:D:53:VAL:O	2:D:57:ARG:CG	2.59	0.50
2:D:357:CYS:SG	2:D:370:LEU:HG	2.51	0.50
1:E:541:ASP:CB	1:E:549:ARG:NH2	2.74	0.50
2:F:247:VAL:O	2:F:250:ALA:HB3	2.12	0.50
2:F:491:GLU:C	2:F:493:ALA:N	2.70	0.50
1:G:51:ARG:CD	1:G:121:GLY:O	2.59	0.50
1:G:306:ALA:C	1:G:308:ARG:H	2.19	0.50
1:G:437:LEU:HD23	1:G:455:LEU:CD2	2.41	0.50
2:H:227:SER:O	2:H:228:ASP:C	2.54	0.50
2:J:100:LEU:O	2:J:101:SER:C	2.54	0.50
1:K:353:LEU:HD22	1:K:358:TRP:CZ2	2.47	0.50
1:K:466:ASN:ND2	1:K:470:LEU:HD11	2.26	0.50
1:A:258:ILE:O	1:A:320:THR:HA	2.10	0.50
2:B:33:THR:CG2	2:B:35:ILE:HG13	2.40	0.50
1:C:273:GLU:H	1:C:273:GLU:CD	2.17	0.50
2:D:476:GLU:CD	2:D:477:GLN:H	2.19	0.50
1:E:167:LYS:HE3	1:E:177:LEU:CD2	2.24	0.50
1:E:193:ARG:HG2	1:E:193:ARG:HH11	1.76	0.50
1:E:323:PHE:CE1	1:E:331:PHE:HD1	2.30	0.50
1:E:541:ASP:CB	1:E:549:ARG:HH21	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:614:ARG:HB2	1:E:619:PHE:HE1	1.77	0.50
2:F:83:VAL:CG1	2:F:84:ARG:H	2.20	0.50
2:F:190:HIS:C	2:F:191:PHE:O	2.53	0.50
1:G:135:ASN:ND2	1:G:137:ASP:OD2	2.44	0.50
1:G:328:ARG:HB2	1:G:330:GLN:OE1	2.11	0.50
2:H:317:LEU:CA	2:H:320:VAL:HG23	2.37	0.50
2:H:472:VAL:HG22	2:H:473:MET:HG2	1.94	0.50
1:I:315:TYR:HD1	1:I:316:VAL:N	2.09	0.50
2:J:179:PRO:CD	4:J:591:COA:H2A	2.40	0.50
2:J:191:PHE:HD2	2:J:192:GLY:N	2.08	0.50
2:J:252:GLY:O	2:J:253:GLU:O	2.29	0.50
2:J:498:GLY:C	2:J:500:GLU:H	2.19	0.50
1:K:54:VAL:HG11	1:K:61:ALA:HA	1.93	0.50
1:K:315:TYR:OH	1:K:338:THR:HA	2.12	0.50
1:K:516:TRP:CD2	1:K:555:LEU:HD21	2.47	0.50
1:A:81:ASP:HB3	1:A:100:GLY:C	2.37	0.50
1:A:187:ASP:C	1:A:189:GLU:H	2.20	0.50
2:B:87:ILE:HD11	2:B:120:VAL:CG1	2.42	0.50
2:B:187:ASP:O	2:B:190:HIS:HB2	2.11	0.50
2:B:232:MET:HE2	2:B:263:ALA:HA	1.93	0.50
1:C:136:ALA:O	1:C:137:ASP:C	2.53	0.50
2:D:49:MET:HE1	2:D:467:ASN:HB3	1.93	0.50
2:D:247:VAL:HG22	2:D:253:GLU:CD	2.36	0.50
2:D:417:GLY:C	2:D:419:ALA:N	2.64	0.50
2:D:440:LEU:HD13	2:D:464:MET:SD	2.51	0.50
2:F:219:GLY:C	2:F:221:ALA:N	2.68	0.50
1:G:289:ALA:O	1:G:350:ILE:HG21	2.11	0.50
2:H:68:GLY:C	2:H:70:ALA:N	2.66	0.50
2:H:403:ASN:ND2	2:H:442:GLY:HA3	2.27	0.50
1:I:254:ARG:HH22	1:I:293:GLY:H	1.59	0.50
1:I:285:VAL:HG12	1:I:286:VAL:CG2	2.41	0.50
2:J:59:LEU:O	2:J:63:ILE:HG13	2.11	0.50
2:J:484:GLN:HE21	2:J:484:GLN:CA	2.18	0.50
1:K:141:ALA:HA	1:K:144:GLU:CD	2.37	0.50
1:K:613:ARG:O	1:K:614:ARG:CD	2.59	0.50
2:L:49:MET:HE1	2:L:467:ASN:ND2	2.26	0.50
2:L:417:GLY:C	2:L:419:ALA:N	2.68	0.50
1:A:427:SER:OG	1:A:428:PRO:N	2.45	0.50
1:C:292:PRO:HG2	1:C:484:LEU:CD1	2.42	0.50
2:D:26:SER:CB	2:F:289:ARG:NH1	2.75	0.50
2:D:161:LEU:HD12	2:D:161:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:488:GLU:O	2:D:492:ARG:HG2	2.11	0.50
1:E:166:ALA:C	1:E:168:ALA:N	2.69	0.50
1:E:263:ASP:HA	1:E:362:VAL:CG1	2.41	0.50
1:E:380:HIS:CE1	1:E:444:ARG:HD2	2.47	0.50
1:E:555:LEU:HD22	1:E:629:ILE:HG22	1.94	0.50
2:F:90:LEU:HD12	2:F:288:ARG:HG3	1.92	0.50
1:G:400:GLY:H	1:G:463:LEU:HD21	1.77	0.50
2:H:277:ALA:HB2	2:H:286:ILE:HD12	1.92	0.50
1:I:258:ILE:CD1	1:I:303:GLY:HA2	2.38	0.50
2:J:206:ILE:O	2:J:206:ILE:HG22	2.12	0.50
1:K:280:ARG:HG3	1:K:395:PHE:CD2	2.46	0.50
2:L:157:GLN:NE2	2:L:197:ASN:CB	2.75	0.50
2:L:255:VAL:HG13	2:L:259:GLU:OE1	2.11	0.50
2:B:50:LEU:HD23	2:B:54:ASN:ND2	2.26	0.50
2:B:268:LYS:HB2	2:B:268:LYS:HZ2	1.76	0.50
1:C:276:CYS:CB	1:C:284:LYS:HD3	2.42	0.50
2:D:78:ARG:HH22	2:J:492:ARG:HH22	1.59	0.50
1:E:123:GLN:CD	1:E:123:GLN:H	2.19	0.50
1:E:315:TYR:CE2	1:E:336:MET:HE1	2.45	0.50
1:E:371:THR:O	1:E:372:GLN:C	2.53	0.50
2:F:485:VAL:HA	2:F:488:GLU:OE1	2.12	0.50
1:G:140:ARG:NH1	1:G:144:GLU:OE2	2.44	0.50
1:G:460:VAL:O	1:G:626:LEU:HD23	2.11	0.50
1:G:605:VAL:O	1:G:605:VAL:CG2	2.53	0.50
1:K:107:TYR:HB2	1:K:131:PHE:CE1	2.46	0.50
1:K:129:TYR:O	1:K:129:TYR:HD1	1.94	0.50
2:L:321:ILE:HD13	2:L:329:TYR:CE2	2.47	0.50
2:L:426:VAL:O	2:L:429:VAL:HG12	2.11	0.50
1:A:204:LEU:HD21	1:A:246:VAL:HG22	1.93	0.50
1:A:281:ARG:HH21	1:A:395:PHE:HD2	1.60	0.50
1:A:365:GLY:O	1:A:366:GLU:C	2.54	0.50
1:C:77:ALA:O	1:C:95:ALA:HA	2.11	0.50
1:C:414:ARG:HB3	1:C:454:MET:HE3	1.93	0.50
1:C:544:ARG:HH21	2:D:88:ASN:HD21	1.58	0.50
2:D:521:TYR:CD1	2:D:525:ARG:NH1	2.80	0.50
1:E:351:THR:OG1	1:E:352:GLY:N	2.45	0.50
1:E:440:TRP:CG	1:E:441:GLY:N	2.79	0.50
1:G:177:LEU:HD23	1:G:177:LEU:N	2.26	0.50
1:I:178:VAL:HG13	1:I:332:PHE:HB3	1.93	0.50
1:I:343:GLU:C	1:I:345:PRO:CD	2.85	0.50
2:J:98:LEU:C	2:J:98:LEU:HD12	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:109:TYR:CE2	2:J:147:PRO:HD2	2.45	0.50
2:J:317:LEU:O	2:J:318:TYR:C	2.55	0.50
1:K:50:GLN:HB2	1:K:123:GLN:OE1	2.11	0.50
1:K:141:ALA:HA	1:K:144:GLU:OE2	2.11	0.50
1:K:441:GLY:HA2	1:K:450:ARG:HH21	1.75	0.50
2:B:35:ILE:HD12	2:B:337:ARG:NH2	2.26	0.50
2:B:87:ILE:HD11	2:B:120:VAL:HG11	1.93	0.50
2:B:362:LEU:HD21	2:B:541:LEU:HB2	1.94	0.50
2:D:331:VAL:HG11	2:D:371:ALA:HB1	1.93	0.50
2:D:487:ARG:O	2:D:487:ARG:HG3	2.12	0.50
2:F:242:ALA:HB2	2:H:409:VAL:HG11	1.93	0.50
2:F:393:GLN:O	2:F:393:GLN:HG2	2.10	0.50
2:F:487:ARG:O	2:F:487:ARG:CG	2.58	0.50
2:H:272:VAL:O	2:H:272:VAL:HG12	2.11	0.50
1:I:343:GLU:H	1:I:343:GLU:CD	2.19	0.50
1:I:469:PHE:HA	1:I:472:ARG:HE	1.76	0.50
2:J:189:GLU:C	2:J:189:GLU:OE1	2.55	0.50
2:J:518:HIS:CD2	2:J:520:TYR:H	2.29	0.50
1:K:324:LEU:HB3	1:K:334:MET:CE	2.41	0.50
2:L:61:GLY:O	2:L:62:ARG:C	2.54	0.50
2:L:498:GLY:C	2:L:500:GLU:N	2.70	0.50
1:A:59:GLU:HB3	1:A:419:GLY:N	2.26	0.50
1:A:699:CYS:HA	1:A:703:GLU:OE1	2.11	0.50
2:B:36:ASN:OD1	2:B:39:SER:N	2.45	0.50
2:B:466:PRO:HD3	2:B:532:ILE:O	2.12	0.50
2:D:154:LEU:HA	2:D:157:GLN:HG3	1.94	0.50
2:D:457:TYR:N	2:D:457:TYR:HD2	2.08	0.50
1:E:131:PHE:HD1	1:E:131:PHE:N	2.09	0.50
1:E:139:ALA:O	1:E:143:GLU:HB2	2.11	0.50
1:E:229:SER:C	1:E:231:ALA:H	2.20	0.50
1:E:346:VAL:HG13	1:E:383:GLU:HB2	1.94	0.50
2:F:241:LEU:HD12	2:H:418:ILE:CG2	2.41	0.50
2:F:476:GLU:OE2	2:F:477:GLN:N	2.45	0.50
1:G:205:LYS:CE	1:G:245:LEU:HD13	2.41	0.50
1:I:107:TYR:O	1:I:113:ILE:HD11	2.12	0.50
1:I:352:GLY:O	1:I:353:LEU:HD23	2.11	0.50
1:I:392:GLU:O	1:I:394:ASP:N	2.44	0.50
2:J:375:ILE:O	2:J:376:LEU:HB2	2.12	0.50
1:K:63:ARG:HH22	1:K:356:VAL:HG23	1.77	0.50
1:K:412:PRO:CB	1:K:450:ARG:HH11	2.25	0.50
1:K:508:PHE:HB2	1:K:622:TRP:CZ2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:618:LEU:HD23	1:K:618:LEU:O	2.11	0.50
2:L:87:ILE:HD12	2:L:87:ILE:H	1.76	0.50
2:L:324:ASP:O	2:L:327:GLN:HB2	2.12	0.50
1:A:65:MET:HE1	1:A:88:HIS:O	2.11	0.49
1:A:76:VAL:HG13	1:A:94:ILE:CG2	2.41	0.49
1:A:569:ALA:O	1:A:571:PRO:HD3	2.12	0.49
2:B:161:LEU:HB2	2:B:201:MET:HE2	1.93	0.49
2:B:240:PHE:CE1	2:B:243:GLY:HA2	2.47	0.49
1:C:269:LEU:HD13	1:C:375:VAL:CG1	2.42	0.49
2:D:389:GLU:CD	2:H:561:PHE:H	2.20	0.49
2:D:397:PRO:HA	2:D:434:VAL:HG23	1.94	0.49
2:D:456:ALA:C	2:D:457:TYR:HD2	2.20	0.49
1:E:299:ARG:C	1:E:301:ALA:N	2.70	0.49
2:F:46:ALA:O	2:F:50:LEU:HB2	2.13	0.49
2:F:372:ASN:ND2	2:F:404:ILE:HD13	2.27	0.49
2:F:487:ARG:CB	2:F:487:ARG:HH11	2.25	0.49
1:G:160:MET:CE	1:G:313:ILE:HG21	2.42	0.49
1:G:446:GLU:O	1:G:450:ARG:HB2	2.12	0.49
1:I:274:ARG:HG2	1:I:289:ALA:HB2	1.94	0.49
2:L:194:ILE:N	2:L:194:ILE:CD1	2.74	0.49
1:A:257:GLU:OE1	1:A:343:GLU:OE2	2.30	0.49
1:A:445:GLU:O	1:A:449:GLN:HB2	2.12	0.49
1:A:677:LEU:HD21	1:A:711:LEU:HD11	1.94	0.49
1:A:702:GLY:O	1:A:704:LEU:HG	2.12	0.49
1:C:149:PHE:CE1	1:C:151:GLY:HA3	2.47	0.49
1:C:553:LEU:HD12	1:C:566:LEU:HD11	1.93	0.49
1:E:297:GLU:O	1:E:300:ARG:HG3	2.13	0.49
2:F:298:LYS:HE3	2:F:550:ASN:ND2	2.27	0.49
2:F:525:ARG:O	2:F:526:LEU:HB2	2.12	0.49
2:F:528:ASP:C	2:F:530:GLY:H	2.21	0.49
1:G:339:ARG:HG3	1:G:340:LEU:O	2.12	0.49
1:I:135:ASN:O	1:I:135:ASN:CG	2.55	0.49
1:I:153:PRO:O	1:I:154:ALA:C	2.55	0.49
1:I:289:ALA:CB	1:I:350:ILE:HD13	2.41	0.49
1:K:63:ARG:NH1	1:K:356:VAL:HG21	2.26	0.49
1:K:132:LEU:HD23	1:K:138:PHE:CE2	2.46	0.49
1:K:516:TRP:HA	1:K:618:LEU:CD1	2.43	0.49
1:A:549:ARG:HH11	1:A:549:ARG:HG3	1.77	0.49
1:A:613:ARG:O	1:A:614:ARG:HD3	2.11	0.49
2:B:44:ALA:O	2:B:47:ALA:HB3	2.12	0.49
2:D:71:ALA:HB1	2:D:74:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:ASN:OD1	2:D:460:ARG:NH1	2.43	0.49
2:D:324:ASP:O	2:D:325:SER:C	2.54	0.49
2:D:418:ILE:HG23	2:D:419:ALA:N	2.26	0.49
1:E:550:GLU:HA	1:E:567:ARG:HD3	1.94	0.49
2:F:301:GLN:HE21	2:F:301:GLN:HA	1.77	0.49
2:F:476:GLU:O	2:F:480:GLY:N	2.45	0.49
1:G:306:ALA:C	1:G:308:ARG:N	2.69	0.49
1:G:569:ALA:O	1:G:571:PRO:HD3	2.12	0.49
2:H:205:GLY:O	2:H:207:PRO:HD3	2.13	0.49
2:H:403:ASN:HA	2:H:443:GLY:H	1.76	0.49
1:I:308:ARG:HG3	1:I:308:ARG:NH1	2.22	0.49
2:J:242:ALA:O	2:J:260:LEU:HD21	2.13	0.49
1:K:253:PRO:HB2	1:K:324:LEU:HG	1.93	0.49
1:K:321:VAL:HA	1:K:336:MET:HG2	1.94	0.49
1:K:407:GLU:HA	1:K:458:THR:HG22	1.93	0.49
2:L:538:ARG:NH1	2:L:538:ARG:CG	2.70	0.49
1:A:501:GLN:HE21	1:A:504:LEU:HG	1.77	0.49
1:C:50:GLN:OE1	1:C:50:GLN:N	2.45	0.49
1:C:320:THR:HG21	1:C:341:GLN:HB2	1.94	0.49
1:C:365:GLY:O	1:C:366:GLU:O	2.30	0.49
2:D:227:SER:O	2:D:228:ASP:C	2.56	0.49
1:E:63:ARG:NH1	1:E:63:ARG:HG3	2.28	0.49
1:E:333:PHE:CE1	1:E:335:GLU:HA	2.48	0.49
1:E:516:TRP:O	1:E:519:SER:OG	2.25	0.49
1:E:532:ASP:O	1:E:535:SER:HB2	2.13	0.49
2:F:225:ALA:O	2:H:562:ARG:CD	2.59	0.49
2:F:264:ASP:OD2	2:F:268:LYS:HE3	2.12	0.49
2:F:311:LEU:CG	2:F:342:SER:HB2	2.41	0.49
2:F:324:ASP:CG	2:F:327:GLN:HB2	2.38	0.49
1:G:54:VAL:O	1:G:54:VAL:HG12	2.13	0.49
1:G:220:ARG:HA	1:G:220:ARG:HE	1.77	0.49
1:G:287:GLU:HG2	1:G:343:GLU:HG3	1.95	0.49
1:G:519:SER:HB2	1:G:613:ARG:HH21	1.78	0.49
1:G:546:ALA:HB3	2:H:60:LEU:HD12	1.93	0.49
2:J:538:ARG:NH1	2:J:538:ARG:CG	2.66	0.49
1:K:125:ILE:HG13	1:K:147:LEU:HD13	1.92	0.49
2:L:74:ARG:HH21	2:L:78:ARG:NH2	2.10	0.49
2:L:248:LYS:HA	2:L:252:GLY:O	2.11	0.49
2:L:312:TYR:O	2:L:313:PRO:C	2.55	0.49
1:A:187:ASP:O	1:A:191:PHE:HB2	2.13	0.49
1:A:508:PHE:CE1	1:A:627:LEU:HD12	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:CYS:O	2:B:433:ARG:HG2	2.12	0.49
1:C:416:VAL:HG23	1:C:454:MET:HE1	1.95	0.49
2:D:272:VAL:O	2:D:272:VAL:CG1	2.59	0.49
2:D:476:GLU:CD	2:D:476:GLU:N	2.70	0.49
1:E:49:ILE:N	1:E:49:ILE:CD1	2.74	0.49
1:E:101:ALA:CB	1:E:429:PHE:HE1	2.10	0.49
2:F:284:LEU:O	2:F:287:ALA:HB3	2.13	0.49
1:I:47:ARG:HB2	1:I:47:ARG:NH1	2.26	0.49
1:I:496:LEU:O	1:I:497:LEU:HD23	2.12	0.49
1:K:403:MET:HE2	1:K:462:GLY:CA	2.39	0.49
1:A:261:PHE:CD1	1:A:358:TRP:CE3	2.96	0.49
2:B:81:LEU:HD11	2:B:89:ARG:HH21	1.77	0.49
1:C:403:MET:CE	1:C:462:GLY:HA3	2.43	0.49
2:D:201:MET:CG	2:D:206:ILE:HD12	2.41	0.49
2:D:347:PHE:HA	2:F:275:HIS:HE1	1.76	0.49
2:D:441:ILE:HG22	2:D:465:TRP:CE3	2.48	0.49
1:E:107:TYR:HB3	1:E:131:PHE:HD2	1.78	0.49
1:E:131:PHE:N	1:E:131:PHE:CD1	2.81	0.49
1:E:135:ASN:CG	1:E:135:ASN:O	2.55	0.49
1:E:232:GLN:C	1:E:233:ARG:HG2	2.37	0.49
1:E:389:GLU:HA	1:E:397:PRO:HA	1.94	0.49
1:E:440:TRP:CD1	1:E:441:GLY:N	2.80	0.49
2:F:250:ALA:O	2:F:252:GLY:N	2.45	0.49
1:G:217:VAL:CG2	1:G:249:TYR:HD1	2.25	0.49
1:G:566:LEU:C	1:G:567:ARG:HD3	2.38	0.49
2:H:123:ILE:HA	2:H:131:CYS:O	2.12	0.49
1:I:79:HIS:CD2	1:I:80:SER:O	2.66	0.49
1:I:384:VAL:HG13	1:I:470:LEU:HD22	1.95	0.49
2:J:176:ALA:O	2:J:178:LEU:N	2.46	0.49
2:J:219:GLY:C	2:J:221:ALA:H	2.21	0.49
2:J:377:PHE:CA	2:J:418:ILE:HD11	2.41	0.49
1:K:466:ASN:HD21	1:K:470:LEU:HD11	1.78	0.49
1:A:513:ALA:HB1	1:A:566:LEU:HD21	1.94	0.49
2:B:189:GLU:CD	2:B:189:GLU:H	2.16	0.49
2:B:247:VAL:HG23	2:L:409:VAL:HG23	1.94	0.49
2:B:403:ASN:CG	2:B:442:GLY:HA3	2.38	0.49
1:C:344:HIS:N	1:C:345:PRO:CD	2.76	0.49
1:C:619:PHE:CE2	1:C:628:ALA:HB2	2.47	0.49
2:D:102:ALA:C	2:D:104:ALA:H	2.21	0.49
2:D:232:MET:O	2:D:277:ALA:HB3	2.12	0.49
1:E:46:TYR:CE1	1:E:364:ARG:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:ASN:ND2	1:E:60:ILE:HG21	2.27	0.49
1:E:125:ILE:CD1	1:E:147:LEU:HD13	2.42	0.49
1:E:465:THR:CG2	1:E:467:LEU:H	2.11	0.49
1:G:261:PHE:CZ	1:G:318:ALA:HB2	2.47	0.49
1:G:261:PHE:CD1	1:G:358:TRP:CE3	2.99	0.49
2:H:444:SER:CB	2:H:449:ASN:HD22	2.25	0.49
1:I:102:LYS:HD3	1:I:429:PHE:HD2	1.78	0.49
1:I:333:PHE:CE1	1:I:335:GLU:HA	2.48	0.49
2:J:408:MET:HG2	2:J:413:TYR:CD1	2.47	0.49
1:K:101:ALA:HB1	1:K:429:PHE:CD1	2.45	0.49
1:A:63:ARG:NH2	1:A:356:VAL:HG23	2.27	0.49
1:A:299:ARG:C	1:A:301:ALA:H	2.21	0.49
1:A:589:ARG:O	1:A:598:LEU:HD12	2.12	0.49
1:A:671:GLY:HA2	1:A:688:ALA:N	2.28	0.49
2:B:185:PHE:H	2:B:186:PRO:HD2	1.78	0.49
1:C:269:LEU:CD2	1:C:370:LEU:O	2.61	0.49
1:C:446:GLU:O	1:C:450:ARG:HB2	2.12	0.49
1:C:491:ARG:HD2	1:C:492:HIS:CE1	2.48	0.49
2:D:440:LEU:CB	2:D:464:MET:HG3	2.42	0.49
1:E:251:LEU:HD11	1:E:328:ARG:NH2	2.27	0.49
2:F:338:LEU:HD21	2:F:537:THR:CG2	2.42	0.49
2:F:446:GLY:O	2:F:447:ALA:C	2.53	0.49
1:G:168:ALA:O	1:G:171:GLU:HB2	2.13	0.49
1:G:198:ILE:O	1:G:248:LYS:NZ	2.40	0.49
1:G:534:HIS:HB3	2:H:307:PRO:HG2	1.94	0.49
2:H:305:ARG:HH11	2:H:305:ARG:CB	2.08	0.49
2:H:335:ILE:HD13	2:H:344:PHE:CE1	2.47	0.49
2:H:520:TYR:CD2	2:H:520:TYR:N	2.80	0.49
1:I:82:ILE:HG13	1:I:83:ASP:OD1	2.13	0.49
1:I:114:ILE:HD11	1:I:142:CYS:HA	1.94	0.49
1:I:389:GLU:O	1:I:390:ASP:HB2	2.12	0.49
2:J:36:ASN:HD22	2:J:37:PRO:CD	2.25	0.49
1:K:278:ILE:H	1:K:278:ILE:CD1	2.19	0.49
1:K:383:GLU:HG2	1:K:384:VAL:N	2.28	0.49
1:A:278:ILE:HG23	1:A:488:PHE:HD2	1.78	0.49
1:A:353:LEU:HD13	1:A:358:TRP:CH2	2.48	0.49
1:A:607:ARG:CB	1:A:607:ARG:NH1	2.76	0.49
3:A:801:BTI:O3	2:F:407:PHE:HD1	1.96	0.49
2:B:100:LEU:HD22	2:B:529:ASP:HB3	1.94	0.49
2:B:324:ASP:O	2:B:327:GLN:HB2	2.13	0.49
2:B:324:ASP:O	2:B:325:SER:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:554:GLU:OE2	2:B:555:PRO:HD2	2.13	0.49
1:C:200:TYR:OH	1:C:224:LEU:CD2	2.59	0.49
1:E:55:ALA:O	1:E:56:ASN:HB2	2.13	0.49
1:E:107:TYR:HB2	1:E:131:PHE:CE2	2.48	0.49
1:E:549:ARG:NH1	1:E:549:ARG:CG	2.69	0.49
2:F:74:ARG:HH22	2:F:78:ARG:NH1	2.10	0.49
2:F:242:ALA:CB	2:H:409:VAL:HG11	2.42	0.49
2:F:435:PRO:HG2	2:F:553:ILE:HD12	1.94	0.49
1:G:344:HIS:ND1	1:G:345:PRO:HD3	2.27	0.49
1:G:371:THR:O	1:G:372:GLN:C	2.54	0.49
2:H:154:LEU:HD23	2:H:157:GLN:NE2	2.27	0.49
2:J:351:PHE:O	2:J:352:GLY:C	2.54	0.49
2:J:463:TRP:HH2	2:J:544:ALA:HB2	1.78	0.49
1:K:274:ARG:HG2	1:K:289:ALA:HB2	1.95	0.49
1:K:320:THR:HG21	1:K:341:GLN:CG	2.41	0.49
1:K:408:ALA:H	1:K:458:THR:CG2	2.26	0.49
1:K:588:TYR:CD1	1:K:588:TYR:N	2.81	0.49
2:L:74:ARG:HH21	2:L:78:ARG:HH22	1.60	0.49
2:L:347:PHE:CZ	2:L:348:LYS:HG2	2.48	0.49
2:L:491:GLU:C	2:L:493:ALA:H	2.18	0.49
1:A:83:ASP:C	1:A:85:HIS:N	2.69	0.49
1:A:548:ALA:O	1:A:550:GLU:OE1	2.31	0.49
1:A:612:LEU:HD12	1:A:612:LEU:O	2.13	0.49
1:A:654:ASN:OD1	2:H:251:THR:HG21	2.13	0.49
2:B:75:HIS:HE1	2:B:80:LYS:HE2	1.78	0.49
2:B:170:LEU:CD2	2:B:211:VAL:HB	2.43	0.49
1:C:478:ALA:HB1	1:C:488:PHE:HE1	1.78	0.49
1:C:618:LEU:HG	1:C:618:LEU:O	2.09	0.49
2:D:487:ARG:HD3	2:D:497:LEU:HB2	1.94	0.49
1:E:296:ALA:O	1:E:300:ARG:HG2	2.13	0.49
1:E:384:VAL:HG12	1:E:470:LEU:HD13	1.95	0.49
1:E:421:ARG:O	1:E:422:GLU:C	2.55	0.49
1:E:434:LEU:HD12	1:E:434:LEU:N	2.27	0.49
1:E:557:CYS:HB2	1:E:629:ILE:HG12	1.95	0.49
2:H:161:LEU:HD12	2:H:161:LEU:C	2.38	0.49
2:H:162:GLU:OE1	2:H:460:ARG:HA	2.13	0.49
1:I:263:ASP:C	1:I:265:HIS:H	2.21	0.49
1:I:289:ALA:HA	1:I:290:PRO:O	2.13	0.49
1:I:353:LEU:HD23	1:I:353:LEU:N	2.28	0.49
1:K:400:GLY:H	1:K:463:LEU:CD1	2.26	0.49
2:L:244:PRO:N	2:L:245:PRO:CD	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:O	1:A:471:ARG:C	2.55	0.48
2:B:411:GLN:NE2	2:B:411:GLN:O	2.46	0.48
1:C:221:GLU:HG3	1:C:222:ALA:N	2.28	0.48
1:C:549:ARG:HH11	1:C:549:ARG:CG	2.26	0.48
2:D:28:MET:HE2	1:E:633:ASP:OD1	2.13	0.48
2:F:354:THR:CG2	2:F:375:ILE:N	2.76	0.48
1:G:65:MET:HE1	1:G:88:HIS:HB2	1.95	0.48
2:H:335:ILE:O	2:H:339:VAL:CG2	2.61	0.48
2:H:339:VAL:CG1	2:H:360:ALA:HB1	2.43	0.48
2:H:449:ASN:ND2	2:H:470:ILE:HD11	2.28	0.48
1:I:307:VAL:O	1:I:307:VAL:CG1	2.56	0.48
2:J:140:VAL:O	2:J:141:LYS:C	2.55	0.48
2:J:141:LYS:NZ	2:J:177:ASN:ND2	2.59	0.48
2:J:207:PRO:HG2	2:J:294:LEU:HD13	1.95	0.48
1:K:269:LEU:HB2	1:K:372:GLN:NE2	2.28	0.48
2:L:185:PHE:HB3	2:L:186:PRO:CD	2.43	0.48
2:L:191:PHE:CD2	2:L:192:GLY:N	2.74	0.48
2:L:233:VAL:HG13	2:L:279:ASP:HA	1.95	0.48
2:B:30:ILE:HD13	2:B:343:GLU:HG2	1.94	0.48
2:B:137:ASP:OD1	2:B:139:THR:HG23	2.12	0.48
2:B:375:ILE:O	2:B:376:LEU:HB2	2.13	0.48
1:C:476:HIS:CG	1:C:477:PRO:HD2	2.48	0.48
1:C:549:ARG:CZ	1:C:571:PRO:HG3	2.43	0.48
2:D:119:ILE:HG23	2:D:119:ILE:O	2.12	0.48
2:D:536:GLN:O	2:D:537:THR:C	2.55	0.48
2:F:331:VAL:O	2:F:334:VAL:N	2.41	0.48
2:F:479:ALA:HB1	2:F:506:LYS:CG	2.43	0.48
1:G:197:ARG:O	1:G:198:ILE:HG13	2.13	0.48
1:G:534:HIS:HB3	2:H:307:PRO:HG3	1.93	0.48
2:H:394:ARG:HB2	2:H:396:ILE:HD12	1.95	0.48
2:H:413:TYR:O	2:H:418:ILE:HB	2.13	0.48
2:H:432:ALA:HA	2:H:556:THR:CG2	2.43	0.48
2:H:562:ARG:NH1	2:H:562:ARG:HG3	2.27	0.48
1:I:135:ASN:O	1:I:136:ALA:C	2.56	0.48
1:I:166:ALA:C	1:I:168:ALA:N	2.69	0.48
1:I:618:LEU:HG	1:I:618:LEU:O	2.13	0.48
2:J:197:ASN:O	2:J:201:MET:HG3	2.12	0.48
2:J:371:ALA:HB2	2:J:401:LEU:HD12	1.94	0.48
1:K:333:PHE:CD1	1:K:333:PHE:C	2.91	0.48
1:K:389:GLU:HA	1:K:397:PRO:HA	1.94	0.48
1:A:261:PHE:CZ	1:A:318:ALA:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLY:H	1:A:463:LEU:HD11	1.78	0.48
1:A:700:SER:O	1:A:701:GLU:C	2.56	0.48
2:B:193:ARG:HD2	2:B:196:PHE:CD2	2.47	0.48
1:C:83:ASP:HB3	1:C:86:ALA:HB2	1.94	0.48
1:C:315:TYR:HE2	1:C:338:THR:HG22	1.76	0.48
1:C:470:LEU:O	1:C:473:ILE:HG22	2.14	0.48
1:C:602:VAL:HG12	1:C:602:VAL:O	2.13	0.48
1:E:598:LEU:HD12	1:E:598:LEU:C	2.38	0.48
2:F:71:ALA:O	2:F:74:ARG:HB3	2.13	0.48
2:F:141:LYS:HG3	2:F:141:LYS:O	2.13	0.48
2:F:485:VAL:HG11	4:H:591:COA:OAP	2.13	0.48
1:G:258:ILE:CD1	1:G:306:ALA:HB2	2.43	0.48
1:G:469:PHE:HE1	1:G:497:LEU:HD21	1.75	0.48
1:I:65:MET:HG3	1:I:75:SER:CB	2.43	0.48
2:J:166:PRO:HD3	2:J:296:TRP:CZ2	2.48	0.48
2:J:355:LEU:HD21	2:J:370:LEU:HD23	1.93	0.48
2:J:440:LEU:CD1	2:J:464:MET:HG3	2.37	0.48
2:J:470:ILE:HG23	2:J:470:ILE:O	2.13	0.48
1:K:79:HIS:CD2	1:K:84:ARG:HA	2.47	0.48
2:L:140:VAL:O	2:L:141:LYS:C	2.56	0.48
2:L:482:LEU:HD23	2:L:509:ILE:HG13	1.94	0.48
1:A:298:LEU:O	1:A:298:LEU:HG	2.12	0.48
1:A:491:ARG:HB3	1:A:492:HIS:CE1	2.49	0.48
1:A:659:ARG:HG2	1:A:676:VAL:HB	1.95	0.48
1:C:231:ALA:CB	1:C:244:MET:SD	2.90	0.48
1:C:389:GLU:HA	1:C:397:PRO:HA	1.95	0.48
1:C:596:ASP:CG	1:C:612:LEU:HD23	2.38	0.48
2:D:86:ARG:HA	2:D:284:LEU:HD11	1.93	0.48
2:D:218:ALA:O	2:D:221:ALA:HB3	2.14	0.48
2:D:316:GLU:CB	2:D:337:ARG:HE	2.27	0.48
2:D:331:VAL:C	2:D:333:GLU:N	2.71	0.48
1:E:165:ALA:O	1:E:169:LEU:CD1	2.59	0.48
1:E:304:GLU:C	1:E:307:VAL:HG12	2.36	0.48
2:F:287:ALA:O	2:F:288:ARG:C	2.56	0.48
2:F:300:GLY:O	2:F:301:GLN:HB2	2.14	0.48
2:F:533:ASP:HB3	2:F:536:GLN:HE21	1.79	0.48
1:G:85:HIS:NE2	1:G:424:ASP:OD1	2.47	0.48
2:H:243:GLY:C	2:H:245:PRO:CD	2.87	0.48
2:H:469:ARG:HH21	2:H:469:ARG:HG2	1.78	0.48
2:J:414:GLU:OE1	2:J:414:GLU:CA	2.61	0.48
2:J:521:TYR:O	2:J:525:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:61:ALA:HA	1:K:64:VAL:HG12	1.95	0.48
1:K:380:HIS:CD2	1:K:444:ARG:HG3	2.48	0.48
1:K:536:PRO:HD3	2:L:363:HIS:HD2	1.75	0.48
2:L:86:ARG:HD3	2:L:213:MET:SD	2.54	0.48
2:L:100:LEU:O	2:L:101:SER:C	2.57	0.48
2:L:237:ALA:C	2:L:238:THR:HG23	2.37	0.48
1:A:537:TRP:CD2	2:B:543:LEU:HD22	2.49	0.48
2:B:83:VAL:CG1	2:B:84:ARG:N	2.55	0.48
2:D:100:LEU:O	2:D:101:SER:C	2.55	0.48
2:D:431:CYS:HB2	2:D:558:PHE:CD2	2.48	0.48
1:E:320:THR:CG2	1:E:341:GLN:HG3	2.43	0.48
2:F:421:HIS:CE1	2:F:424:LYS:HZ2	2.32	0.48
2:F:533:ASP:O	2:F:534:PRO:C	2.54	0.48
1:G:536:PRO:HB3	2:H:363:HIS:ND1	2.26	0.48
1:I:254:ARG:O	1:I:256:VAL:HG23	2.13	0.48
2:J:350:LEU:H	2:J:350:LEU:CD1	2.03	0.48
2:L:83:VAL:O	2:L:87:ILE:CD1	2.62	0.48
2:L:132:MET:HE3	2:L:156:ALA:HA	1.93	0.48
2:L:470:ILE:O	2:L:470:ILE:HG22	2.13	0.48
1:A:284:LYS:NZ	1:A:341:GLN:NE2	2.61	0.48
1:A:345:PRO:HG2	1:A:436:LYS:HE2	1.94	0.48
2:B:65:GLU:O	2:B:72:GLN:NE2	2.47	0.48
2:B:297:ARG:HB3	2:B:297:ARG:NH1	2.26	0.48
1:C:49:ILE:HD13	1:C:364:ARG:CG	2.42	0.48
1:C:505:PRO:HB3	1:C:507:HIS:CB	2.36	0.48
2:F:279:ASP:OD2	2:F:279:ASP:N	2.44	0.48
1:G:325:LEU:HD23	1:G:325:LEU:C	2.38	0.48
1:G:345:PRO:HB3	1:G:438:ILE:HD13	1.95	0.48
1:I:54:VAL:HG21	1:I:64:VAL:HG11	1.95	0.48
1:I:519:SER:CB	1:I:613:ARG:HE	2.19	0.48
1:I:532:ASP:OD2	1:I:535:SER:HB2	2.13	0.48
1:I:602:VAL:HG23	1:I:605:VAL:CG2	2.40	0.48
2:J:119:ILE:HG23	2:J:119:ILE:O	2.14	0.48
2:J:386:HIS:HD2	2:J:386:HIS:O	1.96	0.48
2:L:154:LEU:HD21	2:L:194:ILE:HD12	1.95	0.48
2:L:429:VAL:HG13	2:L:430:ALA:N	2.28	0.48
1:A:200:TYR:CD1	1:A:221:GLU:HA	2.45	0.48
2:B:232:MET:CE	2:B:263:ALA:HA	2.44	0.48
1:C:351:THR:HG1	1:C:352:GLY:H	1.58	0.48
2:D:35:ILE:HD12	2:D:320:VAL:HG22	1.95	0.48
2:D:199:ALA:CB	2:J:427:THR:HG23	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:289:ARG:HD2	2:D:289:ARG:HA	1.62	0.48
2:D:479:ALA:HB2	2:D:509:ILE:CG2	2.44	0.48
1:E:109:ARG:CD	1:E:112:ARG:NH2	2.76	0.48
1:E:263:ASP:OD2	1:E:267:HIS:HB2	2.14	0.48
1:G:279:GLN:HB2	1:G:283:GLN:O	2.14	0.48
1:G:507:HIS:HB3	1:G:622:TRP:HH2	1.77	0.48
2:H:248:LYS:HG2	2:H:254:VAL:HG22	1.95	0.48
2:H:446:GLY:C	2:H:448:GLY:N	2.70	0.48
1:I:85:HIS:ND1	1:I:86:ALA:N	2.62	0.48
1:K:54:VAL:HG11	1:K:64:VAL:CG1	2.43	0.48
1:K:474:LEU:HA	1:K:479:PHE:HD1	1.79	0.48
2:L:311:LEU:C	2:L:312:TYR:CD1	2.92	0.48
2:L:402:GLN:NE2	2:L:444:SER:OG	2.45	0.48
1:A:269:LEU:CD2	1:A:368:LEU:HD13	2.44	0.48
2:B:412:LYS:HE2	2:B:413:TYR:CE2	2.49	0.48
1:C:504:LEU:CB	1:C:505:PRO:CD	2.76	0.48
2:D:119:ILE:O	2:D:152:LYS:NZ	2.45	0.48
2:D:209:ILE:HG22	2:D:210:ALA:N	2.29	0.48
2:D:367:ILE:O	2:D:367:ILE:HG13	2.13	0.48
2:D:434:VAL:HG23	2:D:435:PRO:N	2.27	0.48
2:D:472:VAL:HG11	2:J:181:GLN:HB3	1.91	0.48
1:E:78:VAL:CG1	1:E:96:VAL:HG23	2.44	0.48
1:E:169:LEU:CD2	1:E:313:ILE:HG22	2.44	0.48
1:E:389:GLU:HG2	1:E:397:PRO:HG3	1.95	0.48
1:E:401:ARG:O	1:E:403:MET:HE2	2.13	0.48
1:E:439:ALA:HB3	1:E:451:LEU:HB2	1.96	0.48
2:H:303:GLN:NE2	2:J:297:ARG:CG	2.76	0.48
2:H:347:PHE:O	2:H:348:LYS:C	2.56	0.48
2:J:191:PHE:HE2	2:J:195:PHE:CZ	2.32	0.48
2:L:536:GLN:O	2:L:537:THR:C	2.57	0.48
1:A:340:LEU:CD2	1:A:344:HIS:HB3	2.44	0.48
1:A:491:ARG:HD2	1:A:492:HIS:CE1	2.49	0.48
1:A:549:ARG:O	1:A:567:ARG:HA	2.13	0.48
2:B:102:ALA:C	2:B:104:ALA:H	2.20	0.48
2:B:330:ASP:OD2	2:B:332:ARG:NH1	2.46	0.48
2:D:241:LEU:HD12	2:J:418:ILE:HG23	1.96	0.48
2:D:317:LEU:CD2	2:D:334:VAL:CG1	2.92	0.48
1:E:63:ARG:NH2	1:E:356:VAL:HG23	2.28	0.48
1:E:135:ASN:O	1:E:136:ALA:C	2.57	0.48
1:E:616:ARG:HG3	1:E:630:GLU:HB2	1.95	0.48
2:F:403:ASN:HA	2:F:443:GLY:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:476:GLU:H	2:F:476:GLU:CD	2.22	0.48
1:G:135:ASN:ND2	1:G:137:ASP:HB2	2.28	0.48
1:G:202:VAL:HG23	1:G:248:LYS:HA	1.96	0.48
1:G:470:LEU:O	1:G:471:ARG:C	2.56	0.48
1:G:473:ILE:HG13	1:G:473:ILE:O	2.13	0.48
1:G:496:LEU:C	1:G:497:LEU:HD23	2.39	0.48
1:G:513:ALA:HB1	1:G:566:LEU:HD11	1.94	0.48
1:G:536:PRO:CB	2:H:363:HIS:HE1	2.26	0.48
2:H:68:GLY:C	2:H:70:ALA:H	2.21	0.48
1:I:302:MET:HA	1:I:331:PHE:CZ	2.49	0.48
1:I:491:ARG:HH11	1:I:492:HIS:CE1	2.32	0.48
1:K:77:ALA:O	1:K:95:ALA:HA	2.13	0.48
1:K:269:LEU:CB	1:K:372:GLN:NE2	2.76	0.48
1:K:335:GLU:HG3	1:K:336:MET:N	2.29	0.48
1:A:217:VAL:CG2	1:A:249:TYR:CD1	2.97	0.48
1:A:350:ILE:HA	1:A:440:TRP:HZ3	1.79	0.48
1:C:52:LEU:HD12	1:C:53:LEU:N	2.29	0.48
1:C:327:GLU:O	1:C:329:GLY:N	2.47	0.48
1:C:501:GLN:NE2	1:C:504:LEU:CD2	2.73	0.48
2:D:414:GLU:C	2:D:416:GLY:H	2.21	0.48
1:E:71:LEU:HA	1:E:71:LEU:HD23	1.70	0.48
1:E:327:GLU:O	1:E:329:GLY:N	2.47	0.48
1:E:504:LEU:CB	1:E:505:PRO:CD	2.90	0.48
2:F:84:ARG:NH1	2:F:84:ARG:CG	2.72	0.48
2:F:315:GLU:C	2:F:317:LEU:N	2.69	0.48
1:G:53:LEU:HG	1:G:54:VAL:N	2.29	0.48
1:G:360:ILE:O	1:G:364:ARG:HG3	2.13	0.48
1:G:504:LEU:HB3	1:G:505:PRO:HD2	1.95	0.48
1:I:167:LYS:HG3	1:I:177:LEU:HD13	1.95	0.48
1:I:309:ALA:O	1:I:312:ALA:HB3	2.14	0.48
2:J:98:LEU:C	2:J:98:LEU:CD1	2.87	0.48
2:J:299:GLN:CB	2:J:552:PRO:HD3	2.42	0.48
2:J:436:LYS:HD2	2:J:453:CYS:SG	2.54	0.48
2:J:507:ALA:N	2:J:508:PRO:HD2	2.28	0.48
2:L:255:VAL:CG1	2:L:256:SER:N	2.77	0.48
2:L:408:MET:HG3	2:L:413:TYR:CD2	2.48	0.48
2:L:474:GLY:HA3	2:L:477:GLN:NE2	2.28	0.48
1:A:556:ARG:HG2	1:A:556:ARG:NH1	2.29	0.47
1:C:138:PHE:O	1:C:139:ALA:C	2.57	0.47
1:C:202:VAL:HG21	1:C:246:VAL:HG13	1.96	0.47
1:C:380:HIS:NE2	1:C:444:ARG:HG3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:LYS:HG3	1:E:177:LEU:CD2	2.44	0.47
1:E:278:ILE:HG23	1:E:488:PHE:HD2	1.79	0.47
1:E:313:ILE:HD11	1:E:315:TYR:HD2	1.79	0.47
2:F:424:LYS:HB3	2:L:563:MET:CE	2.43	0.47
1:G:218:VAL:CG1	1:G:224:LEU:HD13	2.43	0.47
1:G:421:ARG:NE	1:G:424:ASP:OD2	2.46	0.47
1:G:452:LEU:HD22	1:G:474:LEU:CB	2.42	0.47
1:G:612:LEU:HD12	1:G:612:LEU:N	2.29	0.47
2:H:53:VAL:O	2:H:57:ARG:HG2	2.14	0.47
2:H:398:LEU:HD12	2:H:434:VAL:HG21	1.96	0.47
2:H:490:ALA:HA	2:H:493:ALA:HB3	1.95	0.47
1:I:82:ILE:HD13	1:I:101:ALA:HB1	1.96	0.47
2:J:248:LYS:HD2	2:J:248:LYS:C	2.40	0.47
2:J:500:GLU:O	2:J:504:LYS:HG3	2.14	0.47
1:K:324:LEU:CB	1:K:334:MET:HE3	2.43	0.47
1:K:516:TRP:CZ2	1:K:631:ALA:HB2	2.48	0.47
1:A:693:VAL:O	1:A:714:LEU:HD22	2.14	0.47
1:C:262:ALA:O	1:C:316:VAL:O	2.32	0.47
2:D:31:LEU:HD12	2:D:336:ALA:HB2	1.97	0.47
2:D:155:ARG:HD2	2:D:155:ARG:O	2.13	0.47
2:D:176:ALA:HB1	2:D:184:VAL:HG11	1.95	0.47
2:D:424:LYS:HD2	2:H:563:MET:SD	2.54	0.47
2:D:444:SER:HG	2:D:449:ASN:ND2	2.12	0.47
1:E:248:LYS:C	1:E:248:LYS:HD3	2.39	0.47
1:E:269:LEU:HD23	1:E:269:LEU:N	2.29	0.47
1:E:308:ARG:NH1	1:E:308:ARG:CG	2.72	0.47
1:E:429:PHE:N	1:E:429:PHE:CD2	2.81	0.47
2:F:206:ILE:O	2:F:207:PRO:C	2.57	0.47
1:G:86:ALA:HB3	1:G:89:VAL:HG23	1.96	0.47
1:G:518:GLN:CB	1:G:590:LEU:HD23	2.43	0.47
1:G:613:ARG:HG2	1:G:614:ARG:N	2.29	0.47
2:H:321:ILE:HD13	2:H:329:TYR:CE1	2.49	0.47
2:H:386:HIS:HD2	2:H:386:HIS:O	1.97	0.47
1:I:138:PHE:O	1:I:139:ALA:C	2.57	0.47
2:J:81:LEU:HD11	2:J:89:ARG:HH21	1.80	0.47
2:J:136:ASN:OD1	2:J:136:ASN:N	2.46	0.47
2:J:248:LYS:HA	2:J:252:GLY:O	2.14	0.47
2:J:499:VAL:O	2:J:499:VAL:CG1	2.63	0.47
1:K:440:TRP:CD1	1:K:441:GLY:N	2.82	0.47
2:L:498:GLY:O	2:L:500:GLU:N	2.47	0.47
2:B:68:GLY:O	2:B:70:ALA:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:GLU:OE2	2:B:379:GLU:N	2.44	0.47
2:B:498:GLY:C	2:B:500:GLU:N	2.71	0.47
1:C:201:PRO:CD	1:C:328:ARG:NH2	2.71	0.47
1:C:392:GLU:O	1:C:394:ASP:N	2.45	0.47
2:D:357:CYS:HB2	2:D:383:LYS:HE2	1.96	0.47
2:F:100:LEU:O	2:F:152:LYS:HE3	2.14	0.47
2:F:212:VAL:HG21	2:F:232:MET:CG	2.44	0.47
1:G:49:ILE:HD11	1:G:148:LEU:CD1	2.44	0.47
1:G:143:GLU:HA	1:G:147:LEU:O	2.15	0.47
1:G:197:ARG:O	1:G:198:ILE:CG1	2.62	0.47
2:H:81:LEU:HD22	2:H:85:GLU:HB3	1.96	0.47
1:I:76:VAL:HG11	1:I:120:SER:OG	2.14	0.47
1:K:62:CYS:O	1:K:66:ARG:HG3	2.14	0.47
1:K:305:ALA:C	1:K:308:ARG:HG3	2.39	0.47
1:A:186:GLN:NE2	1:A:190:THR:N	2.47	0.47
1:A:396:LEU:CD1	1:A:464:ARG:HH12	2.05	0.47
2:B:161:LEU:HD22	2:B:201:MET:HE2	1.97	0.47
2:B:178:LEU:CD1	2:L:482:LEU:HD13	2.43	0.47
2:B:220:GLY:O	2:B:224:PRO:HD2	2.15	0.47
2:B:244:PRO:HA	2:B:247:VAL:CG1	2.42	0.47
2:B:268:LYS:NZ	2:B:268:LYS:CB	2.77	0.47
2:B:498:GLY:C	2:B:500:GLU:H	2.21	0.47
1:C:251:LEU:O	1:C:252:LYS:C	2.58	0.47
1:C:262:ALA:HB2	1:C:268:CYS:HB2	1.96	0.47
1:C:280:ARG:O	1:C:280:ARG:NE	2.40	0.47
1:C:388:ALA:HB2	1:C:434:LEU:HD11	1.97	0.47
1:C:549:ARG:HG2	1:C:549:ARG:NH1	2.29	0.47
2:D:338:LEU:O	2:D:538:ARG:CD	2.51	0.47
1:E:77:ALA:O	1:E:95:ALA:HA	2.14	0.47
1:E:324:LEU:HD22	1:E:334:MET:SD	2.54	0.47
1:E:407:GLU:HA	1:E:458:THR:HG23	1.96	0.47
1:E:426:VAL:O	1:E:426:VAL:HG12	2.15	0.47
2:F:195:PHE:HB3	2:F:226:MET:HE1	1.96	0.47
2:F:527:TRP:CH2	2:H:186:PRO:HG3	2.49	0.47
1:G:522:GLY:O	1:G:523:HIS:HB2	2.14	0.47
1:G:549:ARG:CG	1:G:549:ARG:NH1	2.77	0.47
2:H:497:LEU:HD11	2:H:501:GLU:HB2	1.96	0.47
1:I:620:LEU:HD12	1:I:621:GLU:N	2.28	0.47
2:J:339:VAL:HG23	2:J:342:SER:HA	1.97	0.47
1:K:148:LEU:N	1:K:148:LEU:HD23	2.30	0.47
1:K:414:ARG:HD3	1:K:454:MET:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:109:TYR:CZ	2:L:147:PRO:HD2	2.49	0.47
2:L:431:CYS:O	2:L:556:THR:HG23	2.15	0.47
1:A:144:GLU:HG2	1:A:144:GLU:O	2.12	0.47
1:A:163:LYS:O	1:A:167:LYS:HB2	2.13	0.47
1:A:376:PRO:O	1:A:377:LEU:HB2	2.14	0.47
1:A:565:ARG:HG2	1:A:567:ARG:CZ	2.44	0.47
1:A:652:PRO:HD3	1:A:686:ILE:HG12	1.96	0.47
1:A:680:MET:O	1:A:681:LYS:C	2.57	0.47
1:C:232:GLN:H	1:C:233:ARG:CZ	2.27	0.47
2:D:400:PHE:CB	2:D:438:THR:HG22	2.44	0.47
2:D:435:PRO:HD3	2:D:553:ILE:HG23	1.97	0.47
1:E:53:LEU:HD13	1:E:117:ALA:CA	2.44	0.47
1:E:346:VAL:O	1:E:349:ALA:HB3	2.13	0.47
1:E:384:VAL:HG23	1:E:451:LEU:HD21	1.97	0.47
2:F:137:ASP:C	2:F:139:THR:N	2.73	0.47
1:G:60:ILE:HD12	1:G:63:ARG:HB3	1.96	0.47
1:I:440:TRP:CG	1:I:441:GLY:N	2.82	0.47
1:I:501:GLN:C	1:I:504:LEU:H	2.22	0.47
2:J:146:TYR:HE1	2:J:180:ARG:HH11	1.62	0.47
1:K:46:TYR:C	1:K:46:TYR:CD2	2.92	0.47
1:K:437:LEU:HD22	1:K:455:LEU:CD2	2.43	0.47
1:K:470:LEU:HA	1:K:473:ILE:HG21	1.93	0.47
1:K:505:PRO:HB2	1:K:507:HIS:CB	2.40	0.47
2:L:526:LEU:C	2:L:528:ASP:H	2.23	0.47
1:A:154:ALA:O	1:A:155:ALA:C	2.57	0.47
1:A:229:SER:C	1:A:231:ALA:H	2.22	0.47
2:B:178:LEU:HB2	2:L:482:LEU:HD13	1.97	0.47
2:B:518:HIS:ND1	2:B:519:PRO:CD	2.69	0.47
1:C:185:ALA:CB	1:C:243:ARG:HB2	2.43	0.47
1:C:188:LEU:CG	1:C:228:LEU:HD22	2.43	0.47
2:D:240:PHE:CE1	2:D:243:GLY:HA2	2.50	0.47
2:D:492:ARG:NH2	2:J:74:ARG:NH2	2.53	0.47
2:F:45:ASN:HB3	2:F:321:ILE:O	2.14	0.47
2:F:119:ILE:CG2	2:F:149:THR:HG22	2.45	0.47
1:G:520:GLU:OE1	1:G:613:ARG:NH2	2.47	0.47
2:H:248:LYS:CG	2:H:254:VAL:HG22	2.44	0.47
1:I:386:LEU:HD21	1:I:467:LEU:HD13	1.96	0.47
2:J:114:VAL:HG11	2:J:146:TYR:CE2	2.49	0.47
2:J:164:ARG:NH1	2:J:296:TRP:CZ2	2.83	0.47
1:K:250:LEU:CD1	1:K:324:LEU:HD23	2.44	0.47
1:K:561:ARG:O	1:K:562:ARG:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:49:MET:HE1	2:L:467:ASN:HD22	1.78	0.47
2:L:386:HIS:HD2	2:L:386:HIS:O	1.97	0.47
1:A:263:ASP:OD2	1:A:368:LEU:N	2.38	0.47
2:B:486:LYS:HG2	2:B:505:ILE:CD1	2.44	0.47
1:C:114:ILE:HD12	1:C:147:LEU:HD12	1.94	0.47
1:C:440:TRP:CD1	1:C:441:GLY:N	2.82	0.47
1:C:523:HIS:ND1	1:C:523:HIS:C	2.72	0.47
2:D:30:ILE:HG22	2:D:31:LEU:N	2.30	0.47
2:D:36:ASN:HB3	2:D:39:SER:HB2	1.97	0.47
2:D:92:ASP:HB2	2:D:95:SER:HB2	1.96	0.47
2:D:145:TYR:CE1	2:D:149:THR:HG22	2.50	0.47
2:D:164:ARG:HB2	2:D:551:ALA:HB2	1.97	0.47
2:D:237:ALA:O	2:D:238:THR:CG2	2.62	0.47
2:D:350:LEU:HD23	2:D:350:LEU:N	2.14	0.47
2:D:420:LYS:O	2:D:423:ALA:HB3	2.14	0.47
2:D:462:LEU:HD23	2:D:462:LEU:O	2.14	0.47
2:D:472:VAL:HG22	2:D:473:MET:CG	2.40	0.47
1:E:207:ALA:HB2	1:E:243:ARG:NH1	2.30	0.47
1:E:287:GLU:HG2	1:E:343:GLU:HG3	1.96	0.47
1:E:451:LEU:HD23	1:E:474:LEU:HD13	1.97	0.47
1:E:465:THR:CG2	1:E:466:ASN:N	2.77	0.47
1:E:508:PHE:O	1:E:509:TRP:C	2.57	0.47
1:E:533:PRO:C	1:E:535:SER:N	2.72	0.47
1:E:561:ARG:HH11	1:E:561:ARG:CG	2.26	0.47
2:F:53:VAL:HG12	2:F:57:ARG:NH1	2.29	0.47
2:F:526:LEU:C	2:F:528:ASP:N	2.70	0.47
1:G:398:ALA:CB	1:G:464:ARG:HE	2.18	0.47
1:G:536:PRO:CA	2:H:363:HIS:HE1	2.28	0.47
2:H:339:VAL:HG11	2:H:360:ALA:HB1	1.95	0.47
2:H:551:ALA:HA	2:H:552:PRO:HD2	1.67	0.47
1:I:272:ASN:ND2	1:I:377:LEU:HD22	2.29	0.47
1:I:315:TYR:CD1	1:I:316:VAL:N	2.82	0.47
1:I:392:GLU:OE2	1:I:498:PRO:O	2.32	0.47
1:I:439:ALA:HB3	1:I:451:LEU:HB2	1.96	0.47
1:I:622:TRP:O	1:I:622:TRP:CD1	2.68	0.47
2:J:311:LEU:HB2	2:J:342:SER:OG	2.14	0.47
2:J:375:ILE:N	2:J:375:ILE:CD1	2.69	0.47
1:K:322:GLU:OE2	1:K:337:ASN:ND2	2.48	0.47
2:L:39:SER:OG	2:L:40:ALA:N	2.47	0.47
2:L:444:SER:HB2	2:L:470:ILE:CG1	2.44	0.47
1:A:60:ILE:HD12	1:A:60:ILE:HA	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ALA:O	1:C:167:LYS:C	2.58	0.47
1:C:525:ARG:NH1	1:C:531:ASP:CG	2.73	0.47
1:C:525:ARG:NH1	1:C:531:ASP:OD1	2.48	0.47
1:C:544:ARG:NH2	2:D:88:ASN:ND2	2.61	0.47
1:E:148:LEU:N	1:E:148:LEU:CD2	2.78	0.47
1:E:451:LEU:HD23	1:E:474:LEU:CD1	2.44	0.47
1:E:627:LEU:H	1:E:627:LEU:HD12	1.80	0.47
2:F:108:VAL:HG11	2:F:148:LEU:HD11	1.96	0.47
2:H:311:LEU:HD12	2:H:341:GLY:O	2.15	0.47
2:H:497:LEU:CD2	2:H:502:GLU:HB2	2.45	0.47
1:I:531:ASP:OD2	2:J:298:LYS:CB	2.63	0.47
2:J:68:GLY:C	2:J:70:ALA:N	2.72	0.47
1:K:142:CYS:SG	1:K:149:PHE:HD2	2.38	0.47
1:K:263:ASP:N	1:K:263:ASP:OD1	2.47	0.47
1:K:395:PHE:HZ	1:K:469:PHE:CE1	2.33	0.47
1:K:407:GLU:OE1	1:K:416:VAL:HG11	2.15	0.47
2:L:41:GLU:O	2:L:44:ALA:HB3	2.14	0.47
2:L:169:TYR:HE2	2:L:208:GLN:HE22	1.63	0.47
2:L:209:ILE:HD11	2:L:290:CYS:HB2	1.97	0.47
2:L:324:ASP:O	2:L:325:SER:C	2.58	0.47
1:A:340:LEU:HD22	1:A:344:HIS:HB3	1.96	0.47
1:A:402:LEU:HD11	1:A:420:VAL:HG21	1.96	0.47
1:A:471:ARG:NH2	1:A:624:GLY:O	2.47	0.47
2:B:344:PHE:CE2	2:B:346:GLU:HG3	2.50	0.47
2:B:388:ILE:O	2:B:392:CYS:HB2	2.15	0.47
1:C:189:GLU:O	1:C:192:ARG:HB3	2.15	0.47
1:C:489:ILE:CG2	1:C:490:ALA:N	2.78	0.47
1:C:491:ARG:C	1:C:493:GLN:H	2.22	0.47
2:D:409:VAL:HB	2:J:247:VAL:HG22	1.96	0.47
1:E:361:ARG:HH11	1:E:361:ARG:CG	2.26	0.47
1:E:436:LYS:C	1:E:437:LEU:HD12	2.40	0.47
1:E:608:ARG:O	1:E:608:ARG:HG3	2.14	0.47
2:F:333:GLU:O	2:F:337:ARG:NH1	2.48	0.47
1:G:170:MET:HE1	1:G:309:ALA:HB1	1.97	0.47
1:G:201:PRO:HD2	1:G:328:ARG:NH2	2.30	0.47
1:G:516:TRP:CE3	1:G:613:ARG:NH2	2.83	0.47
2:H:30:ILE:CD1	2:H:343:GLU:HG2	2.44	0.47
1:I:300:ARG:NH1	1:I:300:ARG:CB	2.62	0.47
1:I:365:GLY:O	1:I:366:GLU:C	2.57	0.47
1:I:412:PRO:CB	1:I:450:ARG:HH11	2.28	0.47
1:I:545:SER:O	2:J:536:GLN:NE2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:393:GLN:O	2:J:393:GLN:HG2	2.15	0.47
1:K:118:LEU:HD22	1:K:147:LEU:HD11	1.97	0.47
1:K:379:GLY:CA	1:K:440:TRP:CH2	2.98	0.47
2:L:54:ASN:HA	2:L:57:ARG:CD	2.41	0.47
2:L:59:LEU:HD22	2:L:520:TYR:HE1	1.79	0.47
2:L:74:ARG:HH21	2:L:78:ARG:CZ	2.27	0.47
2:L:157:GLN:NE2	2:L:197:ASN:OD1	2.48	0.47
2:L:302:LEU:CD2	2:L:366:PRO:HG2	2.44	0.47
2:L:373:ASN:HD22	2:L:373:ASN:HA	1.57	0.47
2:L:377:PHE:O	2:L:378:ALA:C	2.58	0.47
1:A:540:ASN:HA	2:B:94:GLY:O	2.16	0.47
2:B:224:PRO:CG	2:B:239:ILE:HD13	2.46	0.47
2:B:331:VAL:C	2:B:333:GLU:N	2.72	0.47
2:B:430:ALA:HB1	2:L:196:PHE:HD1	1.80	0.47
1:C:178:VAL:HG22	1:C:332:PHE:CB	2.44	0.47
1:C:203:LEU:CD2	1:C:205:LYS:HZ2	2.26	0.47
1:C:392:GLU:C	1:C:394:ASP:H	2.22	0.47
2:D:338:LEU:HD22	2:D:537:THR:HG22	1.97	0.47
2:D:354:THR:CG2	2:D:375:ILE:N	2.78	0.47
2:D:470:ILE:O	2:D:470:ILE:CG2	2.63	0.47
2:D:499:VAL:O	2:D:499:VAL:HG12	2.14	0.47
2:D:527:TRP:CZ2	2:J:186:PRO:HG3	2.50	0.47
1:E:181:TYR:HD1	1:E:182:HIS:H	1.62	0.47
1:E:400:GLY:N	1:E:463:LEU:HD11	2.17	0.47
1:E:404:LEU:HD11	1:E:612:LEU:HD13	1.94	0.47
1:E:508:PHE:HB2	1:E:622:TRP:CZ2	2.49	0.47
2:F:83:VAL:CG1	2:F:84:ARG:N	2.76	0.47
2:F:190:HIS:O	2:F:191:PHE:O	2.33	0.47
2:F:392:CYS:SG	2:F:556:THR:HG21	2.54	0.47
1:G:167:LYS:HE3	1:G:167:LYS:HB2	1.64	0.47
1:G:201:PRO:HD2	1:G:328:ARG:HH22	1.79	0.47
2:J:378:ALA:H	2:J:418:ILE:HD12	1.80	0.47
2:J:462:LEU:C	2:J:462:LEU:CD2	2.88	0.47
1:K:71:LEU:O	1:K:71:LEU:HD23	2.14	0.47
1:K:103:PRO:O	1:K:108:LEU:HD12	2.15	0.47
2:L:33:THR:HB	2:L:312:TYR:HE2	1.72	0.47
2:L:354:THR:HG22	2:L:375:ILE:N	2.30	0.47
1:A:269:LEU:HB2	1:A:372:GLN:HE21	1.80	0.46
2:B:481:VAL:HG13	2:L:245:PRO:HB2	1.97	0.46
1:C:135:ASN:O	1:C:136:ALA:C	2.58	0.46
1:C:194:GLU:C	1:C:196:GLY:N	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ARG:HH21	1:C:275:ASP:CG	2.23	0.46
2:D:85:GLU:O	2:D:86:ARG:C	2.58	0.46
2:D:145:TYR:HB2	2:D:176:ALA:HA	1.97	0.46
2:D:330:ASP:OD1	2:D:332:ARG:HG3	2.14	0.46
1:E:166:ALA:C	1:E:168:ALA:H	2.22	0.46
1:E:271:LEU:HD23	1:E:375:VAL:HG21	1.96	0.46
1:E:339:ARG:HH11	1:E:339:ARG:CG	2.17	0.46
1:E:526:ASP:OD2	1:E:526:ASP:N	2.46	0.46
1:G:67:SER:O	1:G:68:ALA:C	2.58	0.46
1:G:395:PHE:HZ	1:G:469:PHE:CE1	2.32	0.46
1:G:411:GLY:N	1:G:414:ARG:HG3	2.30	0.46
2:H:119:ILE:CG2	2:H:119:ILE:O	2.63	0.46
2:H:428:ALA:HA	2:H:558:PHE:CE2	2.50	0.46
2:H:446:GLY:O	2:H:448:GLY:N	2.47	0.46
1:I:402:LEU:HD21	1:I:434:LEU:HD21	1.97	0.46
2:J:102:ALA:C	2:J:104:ALA:N	2.73	0.46
2:J:413:TYR:O	2:J:418:ILE:HB	2.15	0.46
2:J:526:LEU:C	2:J:528:ASP:H	2.22	0.46
1:K:346:VAL:HG13	1:K:438:ILE:HG23	1.97	0.46
1:K:463:LEU:HD22	1:K:464:ARG:N	2.23	0.46
1:K:549:ARG:HH21	1:K:571:PRO:CA	2.25	0.46
1:K:590:LEU:CD1	1:K:598:LEU:HD12	2.42	0.46
2:L:98:LEU:HD21	2:L:463:TRP:CZ2	2.49	0.46
1:A:354:ASP:OD1	1:A:357:ALA:HB2	2.15	0.46
2:B:59:LEU:HD22	2:B:520:TYR:CE1	2.50	0.46
1:C:114:ILE:O	1:C:118:LEU:HB2	2.15	0.46
1:C:251:LEU:HB3	1:C:327:GLU:OE2	2.16	0.46
1:C:260:VAL:CG2	1:C:319:GLY:O	2.64	0.46
1:C:384:VAL:HG12	1:C:470:LEU:HD13	1.96	0.46
1:C:405:TYR:HB3	1:C:422:GLU:CB	2.45	0.46
1:C:513:ALA:CB	1:C:564:VAL:HG11	2.46	0.46
1:C:565:ARG:CG	1:C:567:ARG:NH2	2.78	0.46
1:C:620:LEU:HD12	1:C:621:GLU:N	2.31	0.46
2:D:39:SER:HB3	2:D:42:PHE:HB2	1.97	0.46
2:D:230:THR:HG22	2:D:273:ALA:CA	2.41	0.46
1:E:167:LYS:HG3	1:E:177:LEU:HD21	1.97	0.46
1:E:506:GLU:O	1:E:507:HIS:C	2.58	0.46
1:G:138:PHE:CD1	1:G:142:CYS:HB2	2.50	0.46
1:G:362:VAL:HG23	1:G:363:ALA:N	2.30	0.46
1:G:386:LEU:C	1:G:386:LEU:HD13	2.41	0.46
1:G:520:GLU:C	1:G:522:GLY:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:302:MET:HB3	1:I:323:PHE:CE2	2.50	0.46
2:J:74:ARG:HG2	2:J:74:ARG:O	2.15	0.46
2:J:431:CYS:O	2:J:556:THR:HG23	2.15	0.46
1:K:51:ARG:HA	1:K:74:GLY:O	2.15	0.46
1:K:251:LEU:HD13	1:K:327:GLU:CB	2.31	0.46
1:K:258:ILE:HD13	1:K:323:PHE:CD2	2.50	0.46
1:K:320:THR:HG21	1:K:341:GLN:HB2	1.96	0.46
1:K:504:LEU:HB3	1:K:505:PRO:HD2	1.97	0.46
2:L:83:VAL:HG22	2:L:84:ARG:N	2.30	0.46
2:L:127:GLU:O	2:L:129:VAL:HG23	2.15	0.46
2:L:219:GLY:C	2:L:221:ALA:H	2.23	0.46
1:A:607:ARG:CZ	1:A:607:ARG:HB2	2.45	0.46
2:B:159:ILE:CD1	2:B:159:ILE:H	2.28	0.46
1:C:69:ARG:NH1	1:C:69:ARG:CB	2.78	0.46
1:C:152:PRO:HG3	1:C:315:TYR:CZ	2.50	0.46
2:D:373:ASN:HD22	2:D:373:ASN:HA	1.52	0.46
1:E:102:LYS:HB2	1:E:105:ASP:OD1	2.15	0.46
1:E:218:VAL:O	1:E:218:VAL:CG2	2.58	0.46
1:E:221:GLU:HG3	1:E:222:ALA:N	2.31	0.46
2:F:218:ALA:HB1	3:I:801:BTI:H5	1.96	0.46
2:F:368:ALA:HB1	2:F:387:PHE:CE2	2.50	0.46
2:F:421:HIS:CE1	2:F:424:LYS:NZ	2.83	0.46
1:G:270:TYR:CE1	1:G:372:GLN:CD	2.94	0.46
2:H:366:PRO:O	2:H:397:PRO:HD2	2.14	0.46
2:J:191:PHE:C	2:J:193:ARG:H	2.24	0.46
2:J:195:PHE:CZ	2:J:222:TYR:HB2	2.51	0.46
2:J:427:THR:HB	2:J:561:PHE:HE2	1.81	0.46
1:K:321:VAL:HA	1:K:336:MET:CG	2.44	0.46
1:K:429:PHE:O	1:K:430:TYR:CD2	2.68	0.46
2:L:234:ARG:HE	2:L:234:ARG:HB2	1.32	0.46
2:L:338:LEU:HD22	2:L:537:THR:CG2	2.46	0.46
2:L:402:GLN:HE21	2:L:444:SER:CB	2.29	0.46
1:A:76:VAL:HG13	1:A:94:ILE:HG22	1.97	0.46
1:A:420:VAL:HG23	1:A:421:ARG:N	2.29	0.46
2:B:487:ARG:HA	2:B:497:LEU:HD13	1.98	0.46
1:C:111:ASP:O	1:C:114:ILE:HG22	2.15	0.46
1:C:255:HIS:HA	1:C:324:LEU:HD12	1.98	0.46
1:C:272:ASN:OD1	1:C:377:LEU:HB2	2.16	0.46
1:C:602:VAL:O	1:C:605:VAL:HG22	2.15	0.46
2:D:35:ILE:CD1	2:D:320:VAL:HG22	2.46	0.46
2:D:248:LYS:HG2	2:D:253:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:520:TYR:HD2	2:D:520:TYR:H	1.61	0.46
1:E:189:GLU:OE1	1:E:189:GLU:CA	2.61	0.46
1:E:365:GLY:O	1:E:366:GLU:C	2.58	0.46
1:E:437:LEU:HD22	1:E:455:LEU:CD2	2.45	0.46
1:E:596:ASP:CB	1:E:612:LEU:HD23	2.45	0.46
2:F:304:CYS:HB3	2:F:365:TYR:HD1	1.79	0.46
2:F:351:PHE:CZ	2:F:379:GLU:HG3	2.51	0.46
2:F:433:ARG:CZ	2:F:554:GLU:HG3	2.45	0.46
1:G:339:ARG:NH1	1:G:341:GLN:OE1	2.47	0.46
2:H:72:GLN:O	2:H:75:HIS:HB3	2.15	0.46
2:H:100:LEU:O	2:H:101:SER:C	2.57	0.46
2:H:251:THR:OG1	2:H:251:THR:O	2.29	0.46
1:I:450:ARG:O	1:I:453:ALA:HB3	2.15	0.46
1:I:469:PHE:HD2	1:I:470:LEU:N	2.13	0.46
1:K:163:LYS:HE2	1:K:167:LYS:HZ2	1.80	0.46
1:K:630:GLU:HG3	1:K:631:ALA:N	2.30	0.46
2:L:464:MET:O	2:L:531:VAL:HG13	2.15	0.46
1:A:203:LEU:HG	1:A:204:LEU:H	1.74	0.46
1:A:411:GLY:O	1:A:412:PRO:C	2.58	0.46
2:B:30:ILE:HG22	2:B:31:LEU:N	2.31	0.46
2:B:231:VAL:HG21	2:B:286:ILE:HG21	1.96	0.46
2:B:491:GLU:C	2:B:493:ALA:H	2.21	0.46
1:C:87:ARG:O	1:C:90:ALA:HB3	2.16	0.46
1:C:414:ARG:HG2	1:C:414:ARG:NH1	2.29	0.46
2:D:347:PHE:HA	2:F:275:HIS:CE1	2.50	0.46
1:E:252:LYS:HG3	1:E:485:ASP:HB3	1.98	0.46
1:E:395:PHE:C	1:E:397:PRO:HD3	2.39	0.46
1:E:602:VAL:O	1:E:605:VAL:HG22	2.16	0.46
2:F:53:VAL:CG1	2:F:57:ARG:HH12	2.27	0.46
1:G:185:ALA:O	1:G:186:GLN:O	2.33	0.46
1:G:258:ILE:O	1:G:320:THR:HA	2.15	0.46
1:G:506:GLU:O	1:G:507:HIS:C	2.59	0.46
1:G:515:ALA:HB2	1:G:598:LEU:CD2	2.45	0.46
2:H:83:VAL:HG12	2:H:84:ARG:N	2.29	0.46
2:H:375:ILE:HG21	2:H:408:MET:HB2	1.96	0.46
1:I:260:VAL:HG23	1:I:319:GLY:O	2.15	0.46
1:I:525:ARG:HH11	1:I:525:ARG:CG	2.29	0.46
1:I:619:PHE:CE2	1:I:628:ALA:HB2	2.51	0.46
2:J:68:GLY:O	2:J:69:SER:C	2.58	0.46
2:J:81:LEU:CD2	2:J:85:GLU:HB3	2.35	0.46
2:J:338:LEU:HD21	2:J:537:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:389:GLU:O	1:K:390:ASP:HB2	2.14	0.46
1:K:512:ALA:HB1	1:K:629:ILE:CD1	2.41	0.46
2:L:53:VAL:CG1	2:L:57:ARG:HD2	2.44	0.46
2:L:68:GLY:C	2:L:70:ALA:N	2.72	0.46
2:L:184:VAL:HG12	2:L:184:VAL:O	2.15	0.46
1:A:427:SER:OG	1:A:428:PRO:CD	2.63	0.46
2:B:123:ILE:HA	2:B:131:CYS:O	2.15	0.46
2:B:137:ASP:CB	2:B:140:VAL:HG23	2.31	0.46
1:E:76:VAL:HA	1:E:94:ILE:O	2.15	0.46
1:E:76:VAL:HG22	1:E:94:ILE:HB	1.97	0.46
2:F:331:VAL:C	2:F:333:GLU:N	2.73	0.46
2:F:533:ASP:C	2:F:533:ASP:OD2	2.59	0.46
1:G:150:LEU:HD21	1:G:363:ALA:HB2	1.94	0.46
1:G:299:ARG:O	1:G:301:ALA:N	2.48	0.46
1:G:304:GLU:CA	1:G:307:VAL:HG12	2.46	0.46
1:I:427:SER:HG	1:I:428:PRO:HD2	1.79	0.46
1:I:532:ASP:OD1	2:J:298:LYS:NZ	2.48	0.46
2:J:220:GLY:O	2:J:224:PRO:HD2	2.15	0.46
1:K:262:ALA:O	1:K:316:VAL:O	2.33	0.46
1:K:371:THR:O	1:K:374:GLN:HB2	2.16	0.46
2:L:398:LEU:HB2	2:L:436:LYS:HG2	1.98	0.46
2:L:414:GLU:HA	2:L:418:ILE:CG2	2.46	0.46
2:L:516:GLN:HG2	2:L:521:TYR:CZ	2.51	0.46
2:B:201:MET:HG2	2:B:206:ILE:HD12	1.97	0.46
1:C:170:MET:CE	1:C:309:ALA:HB1	2.36	0.46
1:C:280:ARG:HD3	1:C:283:GLN:NE2	2.31	0.46
1:C:298:LEU:O	1:C:298:LEU:HG	2.16	0.46
1:C:403:MET:HE2	1:C:462:GLY:HA3	1.97	0.46
1:C:549:ARG:CG	1:C:549:ARG:NH1	2.78	0.46
2:D:105:ALA:HA	2:D:108:VAL:CG2	2.45	0.46
2:D:238:THR:HA	2:D:261:GLY:O	2.15	0.46
2:D:481:VAL:CG1	2:J:245:PRO:HB2	2.44	0.46
1:E:132:LEU:HD12	1:E:138:PHE:HD2	1.81	0.46
2:F:105:ALA:HA	2:F:108:VAL:HG21	1.96	0.46
2:F:513:TYR:CZ	2:H:181:GLN:HG2	2.50	0.46
1:G:52:LEU:CD2	1:G:360:ILE:HD11	2.46	0.46
1:G:166:ALA:C	1:G:168:ALA:N	2.73	0.46
1:G:351:THR:OG1	1:G:352:GLY:N	2.47	0.46
1:G:383:GLU:HG3	1:G:438:ILE:HG12	1.97	0.46
2:H:119:ILE:O	2:H:119:ILE:HG23	2.16	0.46
1:I:273:GLU:H	1:I:273:GLU:CD	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:181:GLN:NE2	2:J:182:ASP:N	2.64	0.46
2:J:291:VAL:O	2:J:291:VAL:HG12	2.16	0.46
1:K:290:PRO:HD2	1:K:380:HIS:ND1	2.31	0.46
1:K:465:THR:CG2	1:K:467:LEU:H	2.17	0.46
2:L:68:GLY:O	2:L:70:ALA:N	2.48	0.46
2:L:270:SER:OG	2:L:271:GLY:N	2.46	0.46
2:L:302:LEU:HD22	2:L:366:PRO:CG	2.46	0.46
2:L:324:ASP:C	2:L:324:ASP:OD2	2.59	0.46
2:L:501:GLU:N	2:L:501:GLU:OE2	2.47	0.46
2:B:31:LEU:HD12	2:B:336:ALA:CB	2.46	0.46
2:B:275:HIS:HE1	2:F:347:PHE:HA	1.80	0.46
2:B:389:GLU:HG2	2:B:558:PHE:HE1	1.81	0.46
1:C:63:ARG:NH1	1:C:63:ARG:HG3	2.30	0.46
1:C:153:PRO:O	1:C:154:ALA:C	2.58	0.46
1:C:482:ALA:C	1:C:484:LEU:H	2.23	0.46
2:D:62:ARG:HG2	2:D:62:ARG:NH1	2.31	0.46
2:D:291:VAL:HA	2:D:294:LEU:HG	1.96	0.46
2:D:379:GLU:N	2:D:379:GLU:CD	2.71	0.46
1:E:269:LEU:CB	1:E:372:GLN:NE2	2.78	0.46
1:E:343:GLU:C	1:E:345:PRO:HD2	2.41	0.46
2:F:39:SER:OG	2:F:40:ALA:N	2.49	0.46
2:F:103:LEU:O	2:F:524:ALA:HA	2.15	0.46
1:G:96:VAL:HG11	1:G:116:ALA:CB	2.46	0.46
1:G:302:MET:HE3	1:G:331:PHE:CG	2.51	0.46
2:H:145:TYR:HB2	2:H:176:ALA:HA	1.98	0.46
2:H:433:ARG:H	2:H:556:THR:CG2	2.23	0.46
1:I:112:ARG:HH11	1:I:112:ARG:HG3	1.80	0.46
1:I:251:LEU:HD11	1:I:328:ARG:CZ	2.45	0.46
1:I:274:ARG:HD3	1:I:346:VAL:HG23	1.98	0.46
1:I:294:LEU:CD1	1:I:299:ARG:NH1	2.79	0.46
2:L:207:PRO:HG2	2:L:294:LEU:CD2	2.39	0.46
2:L:216:CYS:HB3	2:L:238:THR:O	2.16	0.46
2:L:400:PHE:O	2:L:401:LEU:HD23	2.15	0.46
2:L:438:THR:CG2	2:L:462:LEU:HG	2.46	0.46
1:A:47:ARG:CZ	1:A:148:LEU:HD22	2.46	0.46
1:A:713:GLU:O	1:A:714:LEU:O	2.32	0.46
2:B:77:ALA:C	2:B:79:GLY:H	2.24	0.46
2:B:171:VAL:HG11	2:B:216:CYS:SG	2.56	0.46
2:B:184:VAL:O	2:B:184:VAL:HG12	2.15	0.46
2:B:316:GLU:O	2:B:320:VAL:HG23	2.15	0.46
2:B:377:PHE:CD1	2:B:377:PHE:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ALA:HB2	1:C:464:ARG:HE	1.80	0.46
1:C:570:SER:O	1:C:586:SER:N	2.49	0.46
2:D:83:VAL:HG13	2:D:84:ARG:N	2.29	0.46
2:D:317:LEU:CD2	2:D:334:VAL:HG12	2.46	0.46
1:E:311:GLN:O	1:E:312:ALA:C	2.59	0.46
1:E:396:LEU:HD12	1:E:464:ARG:HH12	1.81	0.46
1:G:226:GLU:OE1	1:G:226:GLU:N	2.49	0.46
1:G:251:LEU:N	1:G:251:LEU:CD1	2.79	0.46
2:H:213:MET:HA	2:H:233:VAL:HG23	1.98	0.46
2:H:351:PHE:O	2:H:352:GLY:C	2.59	0.46
2:J:155:ARG:HD2	2:J:155:ARG:O	2.16	0.46
2:J:338:LEU:O	2:J:538:ARG:NH1	2.48	0.46
2:J:390:LEU:CD2	2:L:228:ASP:HB3	2.46	0.46
2:J:498:GLY:C	2:J:500:GLU:N	2.74	0.46
1:K:358:TRP:O	1:K:361:ARG:HB2	2.16	0.46
2:L:191:PHE:HE2	2:L:195:PHE:HZ	1.63	0.46
2:L:376:LEU:HD12	2:L:404:ILE:HD13	1.98	0.46
1:A:653:MET:CG	1:A:654:ASN:H	2.17	0.46
2:B:215:SER:HA	2:B:238:THR:OG1	2.16	0.46
1:C:167:LYS:HG3	1:C:177:LEU:CD2	2.46	0.46
1:C:204:LEU:O	1:C:215:MET:HA	2.15	0.46
1:C:416:VAL:HG23	1:C:454:MET:CE	2.46	0.46
1:C:567:ARG:HG3	1:C:567:ARG:NH1	2.29	0.46
1:E:202:VAL:HG21	1:E:246:VAL:HG13	1.98	0.46
1:E:249:TYR:CD2	1:E:250:LEU:N	2.84	0.46
1:E:336:MET:CE	1:E:338:THR:HG22	2.46	0.46
1:E:414:ARG:HD3	1:E:454:MET:HG2	1.97	0.46
2:F:487:ARG:NH1	2:F:487:ARG:HB3	2.31	0.46
2:H:36:ASN:HD21	2:H:38:ARG:CD	2.24	0.46
2:H:223:VAL:O	2:H:227:SER:OG	2.34	0.46
2:H:231:VAL:CG1	2:H:283:ALA:HB1	2.44	0.46
2:H:298:LYS:HG2	2:H:550:ASN:HA	1.97	0.46
2:H:317:LEU:HD23	2:H:337:ARG:HD2	1.98	0.46
2:H:400:PHE:CE2	2:H:453:CYS:CB	2.96	0.46
1:I:476:HIS:CD2	1:I:496:LEU:HD21	2.51	0.46
1:I:548:ALA:O	1:I:550:GLU:HG3	2.16	0.46
2:J:170:LEU:HD23	2:J:211:VAL:HG23	1.98	0.46
1:K:107:TYR:CB	1:K:131:PHE:CE1	2.99	0.46
1:K:261:PHE:CZ	1:K:358:TRP:HB3	2.51	0.46
1:K:485:ASP:CG	1:K:491:ARG:NH2	2.74	0.46
1:K:547:LEU:H	1:K:547:LEU:HG	1.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ALA:O	1:A:186:GLN:O	2.33	0.45
1:A:189:GLU:O	1:A:193:ARG:HD3	2.17	0.45
1:A:263:ASP:OD1	1:A:265:HIS:HB2	2.16	0.45
1:A:558:ARG:HE	1:A:627:LEU:HD22	1.81	0.45
2:B:188:ARG:H	2:L:455:ARG:HG3	1.80	0.45
2:B:227:SER:O	2:B:228:ASP:C	2.59	0.45
1:C:170:MET:HE1	1:C:309:ALA:CB	2.37	0.45
1:C:274:ARG:HH11	1:C:347:THR:HG1	1.57	0.45
1:C:299:ARG:C	1:C:301:ALA:N	2.75	0.45
1:C:396:LEU:O	1:C:398:ALA:N	2.48	0.45
1:C:516:TRP:CZ3	1:C:613:ARG:NH1	2.83	0.45
1:C:550:GLU:HG2	1:C:567:ARG:HD2	1.97	0.45
2:D:347:PHE:O	2:D:348:LYS:C	2.58	0.45
1:E:109:ARG:NH1	1:E:111:ASP:OD2	2.49	0.45
2:F:144:THR:HG21	4:F:591:COA:C5A	2.46	0.45
2:F:408:MET:HG3	2:F:413:TYR:CD2	2.50	0.45
2:F:449:ASN:ND2	2:F:470:ILE:HD11	2.31	0.45
2:F:456:ALA:HA	2:H:188:ARG:HA	1.97	0.45
2:H:455:ARG:HH22	2:H:529:ASP:CG	2.24	0.45
2:H:486:LYS:HD2	2:H:489:GLN:HE21	1.81	0.45
1:K:384:VAL:CG1	1:K:470:LEU:HD13	2.46	0.45
2:L:240:PHE:CE1	2:L:243:GLY:CA	3.00	0.45
2:L:483:ALA:HB2	2:L:505:ILE:HG22	1.97	0.45
1:A:87:ARG:O	1:A:90:ALA:HB3	2.15	0.45
1:A:258:ILE:HD12	1:A:306:ALA:HB2	1.98	0.45
1:A:654:ASN:O	2:H:251:THR:CG2	2.64	0.45
2:B:339:VAL:CG2	2:B:342:SER:HA	2.46	0.45
2:B:348:LYS:O	2:B:383:LYS:HE2	2.16	0.45
2:B:487:ARG:HB3	2:B:497:LEU:CD2	2.36	0.45
1:C:160:MET:HE2	1:C:336:MET:CB	2.46	0.45
1:C:201:PRO:CG	1:C:328:ARG:HH21	2.29	0.45
2:D:331:VAL:C	2:D:333:GLU:H	2.24	0.45
2:D:518:HIS:CD2	2:D:520:TYR:H	2.33	0.45
1:E:289:ALA:CB	1:E:350:ILE:HD13	2.45	0.45
1:E:298:LEU:HD21	1:E:325:LEU:CD1	2.46	0.45
2:F:81:LEU:HD21	2:F:89:ARG:HH22	1.81	0.45
2:F:125:ARG:HD2	2:F:128:GLY:HA2	1.99	0.45
2:F:141:LYS:HZ3	2:F:177:ASN:HD21	1.64	0.45
2:F:189:GLU:H	2:F:189:GLU:CD	2.20	0.45
2:F:563:MET:HE1	2:L:563:MET:SD	2.57	0.45
1:G:128:GLY:O	1:G:133:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:GLU:C	1:G:184:GLU:CD	2.83	0.45
1:G:202:VAL:HG23	1:G:247:GLU:O	2.16	0.45
1:G:416:VAL:HG13	1:G:437:LEU:HD12	1.96	0.45
1:G:543:TRP:CH2	2:H:540:VAL:HG22	2.51	0.45
2:H:66:GLY:C	2:H:68:GLY:H	2.24	0.45
2:H:270:SER:HG	2:H:272:VAL:HG23	1.80	0.45
1:I:302:MET:HE2	1:I:323:PHE:HD2	1.82	0.45
1:I:358:TRP:CZ2	1:I:369:PRO:HG2	2.51	0.45
1:I:540:ASN:C	1:I:540:ASN:ND2	2.74	0.45
2:J:218:ALA:O	2:J:221:ALA:CB	2.64	0.45
2:J:457:TYR:N	2:J:457:TYR:CD2	2.83	0.45
1:K:532:ASP:OD2	2:L:365:TYR:OH	2.26	0.45
2:L:375:ILE:H	2:L:375:ILE:CD1	2.29	0.45
1:A:482:ALA:C	1:A:484:LEU:H	2.21	0.45
1:A:562:ARG:HH11	1:A:562:ARG:CG	2.29	0.45
2:B:26:SER:C	2:B:28:MET:H	2.23	0.45
2:B:75:HIS:C	2:B:77:ALA:H	2.23	0.45
2:B:335:ILE:O	2:B:339:VAL:HG22	2.17	0.45
1:C:327:GLU:C	1:C:329:GLY:N	2.74	0.45
2:F:440:LEU:HD12	2:F:464:MET:CE	2.32	0.45
1:G:350:ILE:HD12	1:G:377:LEU:CD1	2.41	0.45
1:G:485:ASP:OD2	1:G:491:ARG:NH2	2.48	0.45
2:H:188:ARG:NH1	2:H:188:ARG:HG2	2.31	0.45
2:H:277:ALA:CB	2:H:283:ALA:HB2	2.46	0.45
2:H:488:GLU:O	2:H:492:ARG:HG2	2.15	0.45
1:I:275:ASP:C	1:I:275:ASP:OD2	2.60	0.45
1:I:391:PRO:CD	1:I:465:THR:O	2.65	0.45
1:I:438:ILE:HD12	1:I:438:ILE:H	1.80	0.45
1:I:452:LEU:HD23	1:I:474:LEU:CB	2.45	0.45
1:I:601:ARG:HB3	1:I:601:ARG:NH1	2.25	0.45
2:J:161:LEU:HD13	2:J:201:MET:CG	2.46	0.45
2:J:332:ARG:NH1	2:J:332:ARG:CG	2.75	0.45
1:K:305:ALA:O	1:K:308:ARG:HG3	2.16	0.45
1:K:386:LEU:CD2	1:K:467:LEU:HD13	2.41	0.45
1:K:465:THR:CG2	1:K:466:ASN:N	2.78	0.45
2:L:244:PRO:HD3	2:L:260:LEU:HD23	1.98	0.45
2:L:283:ALA:HA	2:L:286:ILE:HD12	1.99	0.45
1:A:217:VAL:HG21	1:A:249:TYR:CE1	2.52	0.45
1:A:280:ARG:O	1:A:282:HIS:N	2.49	0.45
2:B:268:LYS:HB2	2:B:268:LYS:NZ	2.31	0.45
2:B:375:ILE:HD12	2:B:375:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:562:ARG:HD2	2:L:225:ALA:O	2.17	0.45
1:C:222:ALA:C	1:C:224:LEU:N	2.72	0.45
1:C:222:ALA:O	1:C:224:LEU:N	2.49	0.45
2:D:221:ALA:C	2:D:224:PRO:HD2	2.41	0.45
2:D:423:ALA:HB1	2:J:226:MET:CG	2.45	0.45
2:D:437:PHE:CE1	2:D:544:ALA:HB1	2.50	0.45
2:D:449:ASN:ND2	2:D:470:ILE:HD11	2.31	0.45
1:E:51:ARG:NH1	1:E:121:GLY:O	2.50	0.45
1:E:132:LEU:HD22	1:E:132:LEU:N	2.32	0.45
1:E:411:GLY:O	1:E:412:PRO:C	2.59	0.45
2:F:385:ALA:O	2:F:389:GLU:HG3	2.16	0.45
2:F:432:ALA:HA	2:F:556:THR:CG2	2.40	0.45
1:G:65:MET:HG3	1:G:75:SER:HB2	1.98	0.45
1:G:138:PHE:C	1:G:138:PHE:HD1	2.22	0.45
1:G:160:MET:HG3	1:G:336:MET:HB3	1.99	0.45
1:G:249:TYR:CE2	1:G:250:LEU:O	2.70	0.45
2:H:187:ASP:O	2:H:190:HIS:HB2	2.16	0.45
2:H:417:GLY:O	2:H:419:ALA:N	2.50	0.45
2:H:486:LYS:HG2	2:H:505:ILE:HD11	1.97	0.45
1:I:136:ALA:O	1:I:137:ASP:C	2.58	0.45
1:I:163:LYS:HG2	1:I:167:LYS:NZ	2.32	0.45
1:I:294:LEU:CD1	1:I:299:ARG:HH12	2.29	0.45
1:I:383:GLU:HB2	1:I:438:ILE:HG23	1.98	0.45
2:J:164:ARG:HB3	2:J:551:ALA:HB2	1.98	0.45
2:J:346:GLU:HG2	2:J:349:ALA:HA	1.97	0.45
1:K:89:VAL:O	1:K:89:VAL:HG12	2.16	0.45
1:K:468:ALA:O	1:K:471:ARG:HB3	2.17	0.45
2:L:31:LEU:HD12	2:L:336:ALA:HB2	1.98	0.45
1:A:231:ALA:HA	1:A:233:ARG:NH2	2.31	0.45
1:A:431:ASP:OD2	1:A:433:MET:N	2.50	0.45
2:B:75:HIS:O	2:B:77:ALA:N	2.49	0.45
2:B:158:ALA:O	2:B:159:ILE:C	2.60	0.45
2:B:385:ALA:O	2:B:389:GLU:HG3	2.16	0.45
1:C:345:PRO:HB3	1:C:415:ARG:NH1	2.32	0.45
1:C:616:ARG:HD2	1:C:630:GLU:OE1	2.16	0.45
2:D:221:ALA:O	2:D:224:PRO:HD2	2.16	0.45
2:D:465:TRP:HB3	2:D:467:ASN:HD21	1.80	0.45
1:E:125:ILE:HD11	1:E:147:LEU:HD13	1.97	0.45
2:F:308:ARG:NH2	2:F:343:GLU:HG3	2.31	0.45
2:F:445:PHE:HA	2:F:471:GLY:O	2.16	0.45
1:G:156:ALA:HB1	1:G:313:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:277:SER:HB3	1:G:485:ASP:O	2.16	0.45
1:G:354:ASP:HB3	1:G:357:ALA:HB3	1.98	0.45
2:H:83:VAL:HG13	2:H:84:ARG:N	2.31	0.45
2:H:179:PRO:HD2	4:H:591:COA:H2A	1.97	0.45
1:I:251:LEU:O	1:I:252:LYS:C	2.59	0.45
2:J:45:ASN:HB3	2:J:321:ILE:O	2.16	0.45
2:J:109:TYR:HE1	2:J:148:LEU:HD12	1.82	0.45
2:J:368:ALA:HB1	2:J:387:PHE:CZ	2.52	0.45
1:K:408:ALA:H	1:K:458:THR:HG22	1.82	0.45
2:L:412:LYS:H	2:L:412:LYS:HG3	1.55	0.45
1:A:152:PRO:HA	1:A:316:VAL:HG23	1.98	0.45
1:A:271:LEU:O	1:A:272:ASN:CB	2.65	0.45
1:A:659:ARG:HG3	1:A:676:VAL:CG2	2.47	0.45
2:B:42:PHE:C	2:B:42:PHE:CD2	2.94	0.45
2:B:178:LEU:HG	4:B:591:COA:H61A	1.81	0.45
2:B:469:ARG:NH2	2:B:519:PRO:CD	2.80	0.45
2:B:472:VAL:CG1	2:L:181:GLN:HG2	2.47	0.45
2:B:500:GLU:N	2:B:500:GLU:OE2	2.48	0.45
1:C:102:LYS:O	1:C:106:SER:OG	2.26	0.45
1:C:229:SER:C	1:C:231:ALA:H	2.25	0.45
1:E:322:GLU:OE2	1:E:337:ASN:ND2	2.50	0.45
2:F:100:LEU:HD13	2:F:159:ILE:CD1	2.45	0.45
2:F:190:HIS:O	2:F:191:PHE:C	2.59	0.45
2:F:321:ILE:O	2:F:321:ILE:HG22	2.17	0.45
2:F:438:THR:O	2:F:462:LEU:HA	2.16	0.45
1:G:198:ILE:HG23	1:G:248:LYS:HG2	1.98	0.45
1:G:452:LEU:CD2	1:G:474:LEU:CB	2.93	0.45
1:G:516:TRP:CG	1:G:555:LEU:HD21	2.52	0.45
1:G:536:PRO:C	1:G:538:SER:H	2.24	0.45
1:G:605:VAL:HG12	1:I:96:VAL:CG1	2.26	0.45
2:H:83:VAL:CG2	2:H:136:ASN:O	2.65	0.45
2:H:154:LEU:HD23	2:H:157:GLN:HE21	1.81	0.45
2:H:402:GLN:HE22	2:H:449:ASN:HA	1.78	0.45
1:I:343:GLU:O	1:I:346:VAL:HG22	2.17	0.45
1:I:346:VAL:CG1	1:I:383:GLU:HB2	2.46	0.45
1:I:421:ARG:O	1:I:422:GLU:C	2.60	0.45
2:J:73:ALA:C	2:J:75:HIS:N	2.74	0.45
2:J:378:ALA:H	2:J:418:ILE:CD1	2.30	0.45
1:K:135:ASN:O	1:K:136:ALA:C	2.58	0.45
1:K:392:GLU:O	1:K:394:ASP:N	2.50	0.45
1:K:516:TRP:HZ3	1:K:630:GLU:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:222:TYR:O	2:L:223:VAL:C	2.60	0.45
1:A:50:GLN:NE2	1:A:123:GLN:HE21	2.15	0.45
1:A:506:GLU:O	1:A:507:HIS:C	2.60	0.45
1:A:677:LEU:CD2	1:A:711:LEU:HD11	2.47	0.45
2:B:470:ILE:O	2:B:517:GLY:HA2	2.17	0.45
2:B:497:LEU:HA	2:B:501:GLU:OE2	2.17	0.45
1:C:110:GLY:O	1:C:114:ILE:HG22	2.17	0.45
1:C:132:LEU:HD22	1:C:132:LEU:N	2.31	0.45
1:C:504:LEU:O	1:C:505:PRO:O	2.34	0.45
1:C:605:VAL:HG12	1:E:96:VAL:HG12	1.98	0.45
2:D:56:LEU:O	2:D:57:ARG:C	2.59	0.45
2:D:72:GLN:O	2:D:75:HIS:HB3	2.17	0.45
1:E:126:HIS:NE2	1:E:359:GLN:OE1	2.49	0.45
1:E:387:TYR:HB3	1:E:389:GLU:HG3	1.98	0.45
2:F:303:GLN:OE1	2:F:303:GLN:HA	2.16	0.45
2:F:507:ALA:HB3	2:F:508:PRO:CD	2.46	0.45
1:G:52:LEU:HD12	1:G:124:ALA:C	2.42	0.45
1:G:67:SER:O	1:G:71:LEU:CD1	2.65	0.45
1:G:270:TYR:H	1:G:372:GLN:NE2	2.12	0.45
1:G:356:VAL:HA	1:G:359:GLN:OE1	2.17	0.45
2:H:145:TYR:CE1	2:H:149:THR:HG22	2.52	0.45
2:H:561:PHE:CB	2:H:563:MET:HE2	2.46	0.45
1:I:589:ARG:HG2	1:I:590:LEU:N	2.32	0.45
2:L:74:ARG:HE	2:L:78:ARG:HH12	1.64	0.45
2:L:308:ARG:NH2	2:L:343:GLU:CD	2.75	0.45
1:A:140:ARG:HD3	1:A:140:ARG:C	2.42	0.45
1:A:170:MET:HE2	1:A:170:MET:N	2.32	0.45
1:A:534:HIS:O	2:B:363:HIS:CE1	2.69	0.45
1:A:656:SER:O	1:A:678:GLU:HG3	2.17	0.45
1:A:659:ARG:HG3	1:A:659:ARG:O	2.16	0.45
1:A:713:GLU:C	1:A:714:LEU:O	2.60	0.45
2:B:248:LYS:HG3	2:B:254:VAL:HG22	1.97	0.45
2:B:277:ALA:HB2	2:B:286:ILE:CD1	2.44	0.45
1:C:375:VAL:HA	1:C:376:PRO:HD2	1.76	0.45
1:C:441:GLY:HA3	1:C:446:GLU:HB3	1.99	0.45
1:C:470:LEU:O	1:C:471:ARG:C	2.57	0.45
1:C:561:ARG:NH1	1:C:632:VAL:CG2	2.79	0.45
2:D:255:VAL:HG22	2:D:256:SER:N	2.32	0.45
2:D:320:VAL:O	2:D:322:PRO:HD3	2.17	0.45
2:D:507:ALA:N	2:D:508:PRO:CD	2.76	0.45
2:D:507:ALA:HB3	2:D:508:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:GLU:O	1:E:135:ASN:HB3	2.16	0.45
1:E:164:SER:OG	1:E:165:ALA:N	2.50	0.45
1:E:360:ILE:O	1:E:364:ARG:HG3	2.17	0.45
2:F:242:ALA:O	2:F:260:LEU:HD21	2.17	0.45
2:F:252:GLY:O	2:F:253:GLU:O	2.34	0.45
1:G:170:MET:CE	1:G:309:ALA:HB1	2.47	0.45
1:G:306:ALA:O	1:G:308:ARG:N	2.49	0.45
1:G:307:VAL:O	1:G:310:ALA:HB3	2.17	0.45
2:H:29:ALA:O	2:H:343:GLU:HA	2.17	0.45
2:H:161:LEU:HD13	2:H:206:ILE:CD1	2.47	0.45
2:H:331:VAL:O	2:H:331:VAL:HG22	2.16	0.45
4:H:591:COA:H122	4:H:591:COA:O1A	2.17	0.45
1:I:108:LEU:HA	1:I:132:LEU:CD1	2.47	0.45
1:I:280:ARG:NH1	1:I:283:GLN:OE1	2.50	0.45
1:I:299:ARG:HH11	1:I:299:ARG:HG3	1.81	0.45
2:J:144:THR:HG22	2:J:175:GLY:H	1.82	0.45
2:J:231:VAL:HG21	2:J:286:ILE:HG22	1.99	0.45
2:J:433:ARG:HB3	2:J:554:GLU:HB2	1.99	0.45
2:J:446:GLY:C	2:J:448:GLY:N	2.75	0.45
2:J:472:VAL:O	2:J:472:VAL:HG22	2.17	0.45
1:K:497:LEU:N	1:K:498:PRO:CD	2.80	0.45
1:K:549:ARG:NH2	1:K:571:PRO:HB3	2.32	0.45
1:A:123:GLN:OE1	1:A:123:GLN:N	2.49	0.45
1:C:130:GLY:O	1:C:131:PHE:C	2.60	0.45
1:C:298:LEU:HD21	1:C:325:LEU:CD1	2.47	0.45
1:C:416:VAL:HG22	1:C:437:LEU:HA	1.98	0.45
1:C:452:LEU:CD2	1:C:474:LEU:CB	2.95	0.45
1:E:252:LYS:HB3	1:E:327:GLU:HG3	1.98	0.45
2:F:89:ARG:HG3	2:F:89:ARG:NH2	2.31	0.45
2:F:100:LEU:HD13	2:F:159:ILE:HD12	1.99	0.45
2:F:527:TRP:CZ3	2:H:186:PRO:HG3	2.52	0.45
1:G:275:ASP:OD1	1:G:484:LEU:HD22	2.17	0.45
1:G:295:GLY:O	1:G:296:ALA:C	2.60	0.45
1:G:558:ARG:HB3	1:G:559:ASP:H	1.42	0.45
1:G:612:LEU:O	1:G:612:LEU:CD1	2.64	0.45
2:H:462:LEU:HD23	2:H:462:LEU:C	2.42	0.45
1:I:412:PRO:HB3	1:I:450:ARG:NH1	2.32	0.45
1:I:455:LEU:HD23	1:I:467:LEU:HD11	1.99	0.45
1:I:519:SER:HB2	1:I:613:ARG:NE	2.20	0.45
1:I:598:LEU:C	1:I:598:LEU:HD12	2.41	0.45
2:J:315:GLU:CD	2:J:315:GLU:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:344:HIS:N	1:K:345:PRO:CD	2.80	0.45
1:K:384:VAL:CG2	1:K:451:LEU:HD21	2.43	0.45
2:L:83:VAL:O	2:L:87:ILE:HD13	2.17	0.45
2:L:223:VAL:N	2:L:224:PRO:HD2	2.32	0.45
2:L:424:LYS:NZ	2:L:563:MET:HA	2.31	0.45
1:A:396:LEU:O	1:A:398:ALA:N	2.50	0.45
1:A:675:VAL:HG21	1:A:699:CYS:SG	2.56	0.45
2:B:554:GLU:CD	2:B:555:PRO:HD2	2.42	0.45
2:B:562:ARG:HG3	2:B:562:ARG:NH1	2.31	0.45
1:C:66:ARG:HH11	1:C:66:ARG:HB2	1.82	0.45
1:C:69:ARG:CZ	1:C:69:ARG:HB2	2.46	0.45
1:C:473:ILE:CA	1:C:496:LEU:HD21	2.47	0.45
2:D:348:LYS:O	2:D:383:LYS:HE3	2.17	0.45
2:D:409:VAL:O	2:D:413:TYR:HD2	2.00	0.45
2:D:456:ALA:HA	2:J:188:ARG:HA	1.99	0.45
1:E:339:ARG:NH1	1:E:339:ARG:CG	2.79	0.45
1:E:601:ARG:HE	1:E:601:ARG:HB3	1.52	0.45
2:F:168:ILE:HG23	2:F:209:ILE:CG2	2.47	0.45
1:G:232:GLN:CG	1:G:233:ARG:NH1	2.75	0.45
1:G:274:ARG:HD3	1:G:347:THR:OG1	2.17	0.45
1:G:340:LEU:HD22	1:G:344:HIS:HB3	1.99	0.45
1:G:496:LEU:C	1:G:498:PRO:HD3	2.42	0.45
2:H:464:MET:O	2:H:531:VAL:HA	2.17	0.45
2:H:562:ARG:HG3	2:H:562:ARG:HH11	1.81	0.45
1:I:392:GLU:C	1:I:394:ASP:N	2.74	0.45
1:I:500:PRO:O	1:I:501:GLN:HB3	2.17	0.45
2:J:121:ALA:HB1	2:J:134:VAL:HG12	1.98	0.45
2:J:141:LYS:HZ1	2:J:177:ASN:HD21	1.65	0.45
2:J:371:ALA:CB	2:J:401:LEU:HB2	2.47	0.45
1:K:382:ILE:HD12	1:K:448:ARG:N	2.32	0.45
1:K:548:ALA:HB1	1:K:568:HIS:O	2.17	0.45
2:L:206:ILE:O	2:L:207:PRO:C	2.60	0.45
2:L:549:LEU:CD2	2:L:553:ILE:HD11	2.47	0.45
2:L:549:LEU:HD23	2:L:553:ILE:HD11	1.99	0.45
1:A:82:ILE:C	1:A:83:ASP:OD1	2.60	0.44
1:A:537:TRP:CZ2	2:B:543:LEU:HD22	2.52	0.44
1:A:607:ARG:HB3	1:A:607:ARG:NH1	2.32	0.44
2:B:68:GLY:C	2:B:70:ALA:N	2.74	0.44
2:B:367:ILE:HG21	2:B:545:LEU:HD11	1.98	0.44
2:B:465:TRP:CB	2:B:467:ASN:HD21	2.28	0.44
1:C:612:LEU:HD12	1:C:612:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:345:ASP:OD2	2:D:345:ASP:N	2.49	0.44
2:D:487:ARG:HB2	2:D:497:LEU:HD22	1.99	0.44
2:D:533:ASP:O	2:D:534:PRO:C	2.61	0.44
1:E:481:ALA:C	1:E:483:GLU:H	2.25	0.44
2:F:35:ILE:O	2:F:37:PRO:HD3	2.17	0.44
2:F:414:GLU:OE2	2:H:240:PHE:HA	2.17	0.44
1:G:309:ALA:O	1:G:312:ALA:HB3	2.17	0.44
2:H:186:PRO:O	2:H:187:ASP:O	2.36	0.44
2:H:238:THR:HA	2:H:261:GLY:O	2.17	0.44
1:I:342:VAL:HG21	1:I:385:ARG:NH2	2.32	0.44
2:J:167:CYS:HB3	2:J:169:TYR:CE2	2.52	0.44
2:J:220:GLY:HA2	2:J:223:VAL:HG23	1.99	0.44
1:K:491:ARG:C	1:K:493:GLN:H	2.26	0.44
1:K:516:TRP:CH2	1:K:631:ALA:HB2	2.52	0.44
2:L:75:HIS:NE2	2:L:80:LYS:HE2	2.32	0.44
2:L:347:PHE:CE2	2:L:348:LYS:CG	3.00	0.44
1:A:649:LEU:HD11	1:A:689:PRO:CG	2.45	0.44
1:A:651:ALA:H	1:A:711:LEU:HD12	1.82	0.44
2:B:191:PHE:CD2	2:B:192:GLY:N	2.83	0.44
2:B:320:VAL:HG11	2:B:333:GLU:HB3	1.98	0.44
2:B:534:PRO:O	2:B:537:THR:OG1	2.35	0.44
2:D:188:ARG:HG3	2:J:455:ARG:O	2.17	0.44
2:D:237:ALA:C	2:D:238:THR:HG23	2.42	0.44
2:D:470:ILE:O	2:D:470:ILE:HG23	2.17	0.44
2:F:106:HIS:O	2:F:108:VAL:HG23	2.17	0.44
2:F:130:GLU:OE2	2:F:130:GLU:N	2.42	0.44
1:G:76:VAL:HA	1:G:94:ILE:O	2.17	0.44
1:G:450:ARG:O	1:G:453:ALA:HB3	2.17	0.44
1:G:497:LEU:N	1:G:498:PRO:CD	2.78	0.44
1:G:533:PRO:HD2	1:G:534:HIS:CD2	2.52	0.44
2:H:102:ALA:C	2:H:104:ALA:N	2.75	0.44
1:I:416:VAL:HG22	1:I:437:LEU:HA	1.99	0.44
1:I:448:ARG:HG2	1:I:474:LEU:HD22	1.99	0.44
2:J:206:ILE:O	2:J:207:PRO:C	2.58	0.44
2:J:287:ALA:O	2:J:288:ARG:C	2.59	0.44
2:J:481:VAL:HA	2:J:484:GLN:HB3	1.98	0.44
2:J:497:LEU:HG	2:J:501:GLU:HB2	1.99	0.44
1:K:175:VAL:O	1:K:177:LEU:HD23	2.17	0.44
1:K:348:GLU:HG2	1:K:353:LEU:O	2.17	0.44
1:K:620:LEU:HD12	1:K:620:LEU:C	2.42	0.44
2:L:56:LEU:HD11	2:L:60:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASP:OD2	1:A:368:LEU:HG	2.17	0.44
1:A:470:LEU:CA	1:A:473:ILE:HG22	2.42	0.44
1:A:650:SER:HB2	1:A:711:LEU:H	1.82	0.44
1:A:708:GLY:O	1:A:709:THR:C	2.58	0.44
1:C:281:ARG:NH2	1:C:395:PHE:HD2	2.16	0.44
2:D:89:ARG:HH21	2:D:89:ARG:CG	2.26	0.44
2:D:377:PHE:CZ	2:D:408:MET:HE2	2.52	0.44
2:D:386:HIS:O	2:D:386:HIS:CD2	2.71	0.44
2:D:433:ARG:HH11	2:D:433:ARG:CG	2.27	0.44
1:E:371:THR:HG23	1:E:374:GLN:HG3	1.98	0.44
2:F:332:ARG:HG3	2:F:332:ARG:HH11	1.81	0.44
2:F:417:GLY:O	2:F:419:ALA:N	2.50	0.44
2:F:476:GLU:CD	2:F:476:GLU:N	2.75	0.44
1:G:71:LEU:HB3	1:G:73:ILE:HD12	2.00	0.44
1:G:104:ALA:HA	1:G:108:LEU:CD1	2.47	0.44
1:G:139:ALA:HA	1:G:142:CYS:HB3	1.99	0.44
1:G:333:PHE:O	1:G:334:MET:HE2	2.17	0.44
2:H:513:TYR:N	2:H:513:TYR:CD1	2.85	0.44
1:I:106:SER:C	1:I:108:LEU:N	2.76	0.44
1:I:440:TRP:CD1	1:I:441:GLY:N	2.85	0.44
1:K:47:ARG:HG2	1:K:148:LEU:HD11	1.99	0.44
1:K:294:LEU:HB2	1:K:298:LEU:HD22	1.98	0.44
1:K:304:GLU:C	1:K:307:VAL:HG12	2.42	0.44
1:K:437:LEU:HD12	1:K:437:LEU:N	2.33	0.44
2:L:402:GLN:NE2	2:L:449:ASN:HD22	2.15	0.44
1:A:270:TYR:CE1	1:A:372:GLN:CD	2.95	0.44
1:A:306:ALA:HB1	1:A:321:VAL:CG2	2.46	0.44
1:A:343:GLU:C	1:A:345:PRO:HD2	2.43	0.44
2:B:180:ARG:HG3	2:B:180:ARG:HH11	1.81	0.44
2:B:285:ALA:O	2:B:289:ARG:HG2	2.16	0.44
2:D:351:PHE:C	2:D:351:PHE:CD2	2.95	0.44
1:E:107:TYR:CB	1:E:131:PHE:CD2	3.00	0.44
1:E:201:PRO:CD	1:E:328:ARG:HH21	2.30	0.44
1:E:327:GLU:C	1:E:329:GLY:N	2.73	0.44
2:F:365:TYR:CB	2:F:545:LEU:HD13	2.47	0.44
1:G:60:ILE:HD12	1:G:60:ILE:O	2.16	0.44
1:G:114:ILE:HD12	1:G:147:LEU:HD13	1.98	0.44
1:G:395:PHE:C	1:G:397:PRO:HD3	2.41	0.44
1:G:466:ASN:O	1:G:469:PHE:HB3	2.16	0.44
1:G:547:LEU:HD11	2:H:64:HIS:CE1	2.51	0.44
2:H:81:LEU:HD23	2:H:82:LEU:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:287:GLU:HG2	1:I:343:GLU:HG3	2.00	0.44
1:I:445:GLU:HB3	1:I:448:ARG:HH21	1.83	0.44
1:I:605:VAL:O	1:I:605:VAL:CG2	2.63	0.44
2:J:362:LEU:HD21	2:J:538:ARG:HG2	1.99	0.44
1:K:412:PRO:HB3	1:K:450:ARG:HH11	1.83	0.44
2:L:125:ARG:HD2	2:L:128:GLY:HA2	1.99	0.44
1:A:188:LEU:HD23	1:A:228:LEU:CD2	2.39	0.44
1:A:358:TRP:HH2	1:A:370:LEU:HD12	1.81	0.44
1:A:388:ALA:HB2	1:A:434:LEU:HD11	2.00	0.44
1:A:413:GLY:N	1:A:450:ARG:HH11	2.15	0.44
1:A:705:VAL:HG12	1:A:709:THR:HG21	2.00	0.44
2:B:186:PRO:HG3	2:L:527:TRP:CH2	2.52	0.44
2:B:246:LEU:H	2:B:246:LEU:HD12	1.82	0.44
2:B:507:ALA:HB3	2:B:508:PRO:CD	2.47	0.44
2:D:287:ALA:O	2:D:288:ARG:C	2.61	0.44
2:D:303:GLN:NE2	2:F:297:ARG:HD2	2.33	0.44
2:D:378:ALA:HB3	2:D:379:GLU:OE1	2.18	0.44
2:D:396:ILE:O	2:D:434:VAL:HG21	2.18	0.44
1:E:105:ASP:O	1:E:109:ARG:HD2	2.17	0.44
1:E:170:MET:SD	1:E:309:ALA:CB	3.03	0.44
1:E:289:ALA:O	1:E:350:ILE:HG21	2.16	0.44
1:E:389:GLU:O	1:E:390:ASP:HB2	2.17	0.44
1:E:470:LEU:HA	1:E:473:ILE:HG23	1.98	0.44
2:F:100:LEU:O	2:F:101:SER:C	2.59	0.44
2:F:234:ARG:HD2	2:F:276:TYR:OH	2.17	0.44
1:G:201:PRO:CB	1:G:251:LEU:HD11	2.47	0.44
1:G:261:PHE:O	1:G:368:LEU:HD21	2.16	0.44
1:G:607:ARG:HB2	1:G:607:ARG:CZ	2.47	0.44
2:H:307:PRO:HB3	2:H:363:HIS:CD2	2.38	0.44
2:H:348:LYS:O	2:H:383:LYS:HE3	2.17	0.44
1:I:53:LEU:C	1:I:53:LEU:HD23	2.42	0.44
1:I:112:ARG:HG3	1:I:112:ARG:NH1	2.33	0.44
1:I:270:TYR:H	1:I:372:GLN:NE2	2.12	0.44
1:I:278:ILE:CG2	1:I:473:ILE:HD11	2.42	0.44
1:I:294:LEU:HD12	1:I:294:LEU:O	2.17	0.44
1:I:320:THR:O	1:I:336:MET:HG2	2.18	0.44
1:I:371:THR:O	1:I:374:GLN:HB2	2.17	0.44
1:I:446:GLU:HG2	1:I:450:ARG:HH21	1.82	0.44
1:I:516:TRP:CD2	1:I:613:ARG:NH2	2.85	0.44
1:I:546:ALA:HB3	2:J:60:LEU:CD1	2.48	0.44
1:I:596:ASP:HB3	1:I:612:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:157:GLN:OE1	2:J:194:ILE:HG23	2.17	0.44
2:J:220:GLY:O	2:J:223:VAL:HG23	2.17	0.44
2:J:484:GLN:NE2	2:J:484:GLN:CA	2.75	0.44
2:J:486:LYS:CG	2:J:497:LEU:HD22	2.48	0.44
1:K:85:HIS:NE2	1:K:424:ASP:OD1	2.50	0.44
1:K:135:ASN:HB2	1:K:137:ASP:OD1	2.17	0.44
1:K:588:TYR:HD1	1:K:588:TYR:N	2.14	0.44
2:L:316:GLU:CB	2:L:337:ARG:HE	2.31	0.44
2:L:518:HIS:O	2:L:521:TYR:N	2.51	0.44
2:L:525:ARG:NH1	2:L:525:ARG:CG	2.75	0.44
1:A:500:PRO:O	1:A:501:GLN:HB3	2.17	0.44
2:B:28:MET:HG2	1:C:633:ASP:OD2	2.17	0.44
2:B:81:LEU:HA	2:B:81:LEU:HD23	1.69	0.44
2:B:489:GLN:HA	2:B:492:ARG:HE	1.82	0.44
1:C:325:LEU:HD23	1:C:325:LEU:C	2.40	0.44
2:D:68:GLY:C	2:D:70:ALA:N	2.72	0.44
2:D:176:ALA:H	4:D:591:COA:H21	1.81	0.44
2:D:289:ARG:O	2:D:293:ASN:ND2	2.51	0.44
2:D:300:GLY:O	2:D:301:GLN:CB	2.66	0.44
1:E:396:LEU:HD12	1:E:464:ARG:NH1	2.33	0.44
2:F:373:ASN:HD22	2:F:373:ASN:HA	1.43	0.44
1:G:59:GLU:HB3	1:G:419:GLY:N	2.32	0.44
1:G:191:PHE:CE2	1:G:228:LEU:HD13	2.53	0.44
1:G:200:TYR:OH	1:G:224:LEU:CD2	2.65	0.44
1:G:217:VAL:HG21	1:G:249:TYR:CD1	2.53	0.44
1:G:365:GLY:O	1:G:366:GLU:C	2.60	0.44
1:G:518:GLN:HB2	1:G:590:LEU:HD23	2.00	0.44
2:H:499:VAL:O	2:H:499:VAL:HG12	2.18	0.44
1:I:93:ASP:OD2	1:I:93:ASP:N	2.50	0.44
1:I:536:PRO:HD3	2:J:363:HIS:CD2	2.53	0.44
2:J:141:LYS:HZ3	2:J:177:ASN:ND2	2.14	0.44
1:K:289:ALA:HB1	1:K:350:ILE:HD13	1.98	0.44
2:L:270:SER:OG	2:L:272:VAL:HG23	2.18	0.44
2:L:286:ILE:O	2:L:289:ARG:HB2	2.17	0.44
2:L:365:TYR:HB2	2:L:545:LEU:CD1	2.42	0.44
2:L:455:ARG:HD3	2:L:455:ARG:HA	1.77	0.44
2:L:516:GLN:HA	2:L:521:TYR:CD2	2.53	0.44
1:A:202:VAL:HA	1:A:249:TYR:H	1.83	0.44
1:A:261:PHE:CE1	1:A:358:TRP:HB3	2.53	0.44
2:B:311:LEU:C	2:B:312:TYR:HD1	2.24	0.44
2:B:311:LEU:HB2	2:B:312:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:546:SER:HA	2:B:549:LEU:HD12	2.00	0.44
1:C:60:ILE:O	1:C:63:ARG:HB3	2.17	0.44
1:C:202:VAL:HA	1:C:249:TYR:H	1.82	0.44
1:C:342:VAL:HG11	1:C:385:ARG:NH2	2.33	0.44
1:C:345:PRO:HB3	1:C:438:ILE:HD13	1.99	0.44
2:D:108:VAL:HG11	2:D:148:LEU:HD11	1.98	0.44
2:D:170:LEU:HD23	2:D:211:VAL:CG2	2.47	0.44
2:D:234:ARG:HA	2:D:263:ALA:HB3	1.98	0.44
4:D:591:COA:H62	4:D:591:COA:H62A	1.83	0.44
1:E:47:ARG:CG	1:E:48:SER:N	2.77	0.44
1:E:54:VAL:HG13	1:E:64:VAL:HG11	2.00	0.44
1:E:205:LYS:HB3	1:E:206:ALA:H	1.61	0.44
1:E:500:PRO:O	1:E:501:GLN:CB	2.65	0.44
1:E:603:ASP:O	1:E:605:VAL:HG13	2.17	0.44
1:G:170:MET:HE2	1:G:170:MET:N	2.32	0.44
1:G:451:LEU:HD23	1:G:474:LEU:HD21	2.00	0.44
2:H:401:LEU:HD23	2:H:439:VAL:HB	2.00	0.44
2:H:435:PRO:HG3	2:H:460:ARG:NH2	2.33	0.44
1:I:47:ARG:NH2	1:I:148:LEU:HD22	2.33	0.44
1:I:252:LYS:HB2	1:I:327:GLU:CD	2.43	0.44
1:I:473:ILE:HG12	1:I:473:ILE:O	2.17	0.44
2:J:53:VAL:HG12	2:J:57:ARG:NH1	2.33	0.44
2:J:473:MET:HE3	2:J:473:MET:HB2	1.75	0.44
1:K:78:VAL:HG12	1:K:96:VAL:HG23	1.99	0.44
1:K:114:ILE:HD13	1:K:138:PHE:CE2	2.52	0.44
1:K:296:ALA:O	1:K:299:ARG:HB3	2.18	0.44
1:K:396:LEU:HB2	1:K:464:ARG:NH2	2.33	0.44
2:L:169:TYR:CD2	2:L:169:TYR:N	2.85	0.44
2:L:169:TYR:N	2:L:169:TYR:HD2	2.15	0.44
2:L:338:LEU:O	2:L:538:ARG:NH1	2.51	0.44
1:A:127:PRO:HB2	1:A:133:SER:HB3	2.00	0.44
1:A:522:GLY:O	1:A:523:HIS:HB2	2.18	0.44
1:A:586:SER:HB2	1:A:587:GLN:H	1.52	0.44
1:C:49:ILE:CD1	1:C:49:ILE:N	2.72	0.44
1:C:152:PRO:HD2	1:C:157:ILE:HD11	1.99	0.44
1:C:306:ALA:HB1	1:C:321:VAL:HG21	2.00	0.44
1:C:415:ARG:HD3	1:C:438:ILE:HD12	2.00	0.44
1:C:416:VAL:HG22	1:C:437:LEU:CD1	2.47	0.44
1:C:497:LEU:N	1:C:498:PRO:CD	2.81	0.44
2:D:101:SER:CB	2:D:526:LEU:HD23	2.47	0.44
2:D:521:TYR:CE1	2:D:525:ARG:NH1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:549:LEU:HD23	2:D:549:LEU:HA	1.73	0.44
1:E:186:GLN:NE2	1:E:189:GLU:HB2	2.33	0.44
1:E:272:ASN:CG	1:E:377:LEU:HD13	2.42	0.44
1:E:299:ARG:C	1:E:301:ALA:H	2.26	0.44
1:E:320:THR:OG1	1:E:341:GLN:HG3	2.16	0.44
2:F:106:HIS:HB3	2:F:524:ALA:HB2	1.99	0.44
2:F:301:GLN:HA	2:F:301:GLN:NE2	2.32	0.44
2:F:311:LEU:HG	2:F:342:SER:CB	2.45	0.44
2:F:402:GLN:OE1	2:F:452:MET:HB2	2.18	0.44
2:F:491:GLU:HA	2:F:495:GLN:O	2.17	0.44
1:G:232:GLN:HB2	1:G:233:ARG:H	1.66	0.44
1:G:525:ARG:HB3	1:G:531:ASP:OD1	2.18	0.44
1:G:550:GLU:HG2	1:G:567:ARG:CZ	2.48	0.44
1:I:171:GLU:HB2	1:I:177:LEU:HD11	2.00	0.44
1:I:320:THR:HG21	1:I:341:GLN:HB2	1.99	0.44
1:I:376:PRO:O	1:I:377:LEU:HB2	2.17	0.44
2:J:42:PHE:CE1	2:J:319:GLY:HA3	2.51	0.44
2:J:220:GLY:HA2	2:J:223:VAL:CG2	2.48	0.44
2:J:329:TYR:OH	2:J:441:ILE:CD1	2.66	0.44
2:J:469:ARG:HH21	2:J:469:ARG:CG	2.12	0.44
1:K:340:LEU:CD1	1:K:359:GLN:HE22	2.31	0.44
2:L:248:LYS:C	2:L:250:ALA:H	2.26	0.44
2:L:344:PHE:CZ	2:L:358:GLY:HA3	2.52	0.44
2:L:528:ASP:C	2:L:530:GLY:H	2.25	0.44
1:A:306:ALA:C	1:A:308:ARG:H	2.25	0.44
1:A:371:THR:O	1:A:372:GLN:C	2.60	0.44
1:A:451:LEU:CD2	1:A:474:LEU:HD11	2.48	0.44
2:B:191:PHE:HA	2:B:194:ILE:HD13	2.00	0.44
2:B:242:ALA:O	2:B:260:LEU:HD21	2.18	0.44
2:B:294:LEU:HD23	2:B:294:LEU:HA	1.55	0.44
2:B:393:GLN:HE21	2:B:393:GLN:HB3	1.59	0.44
2:B:467:ASN:N	2:B:467:ASN:ND2	2.52	0.44
1:C:186:GLN:HE21	1:C:187:ASP:CG	2.26	0.44
1:C:253:PRO:HG2	1:C:486:THR:OG1	2.18	0.44
1:C:273:GLU:N	1:C:273:GLU:CD	2.75	0.44
1:C:466:ASN:OD1	1:C:466:ASN:C	2.60	0.44
1:E:179:PRO:HD2	1:E:248:LYS:CB	2.48	0.44
1:E:194:GLU:C	1:E:196:GLY:N	2.75	0.44
1:G:127:PRO:HB2	1:G:133:SER:HA	2.00	0.44
1:G:217:VAL:CG2	1:G:249:TYR:CD1	3.01	0.44
1:G:251:LEU:N	1:G:251:LEU:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:GLU:N	1:G:273:GLU:OE1	2.51	0.44
1:G:414:ARG:CB	1:G:454:MET:SD	3.06	0.44
1:G:440:TRP:CD1	1:G:441:GLY:N	2.86	0.44
1:G:612:LEU:HD12	1:G:612:LEU:H	1.83	0.44
2:H:409:VAL:HG23	2:H:410:GLY:N	2.30	0.44
1:I:126:HIS:HE2	1:I:356:VAL:HG22	1.83	0.44
1:I:336:MET:CE	1:I:338:THR:HG23	2.47	0.44
1:I:615:GLY:C	1:I:617:GLN:H	2.26	0.44
2:J:137:ASP:O	2:J:138:ALA:C	2.61	0.44
2:J:239:ILE:O	2:J:266:HIS:NE2	2.51	0.44
2:J:321:ILE:HD13	2:J:321:ILE:HA	1.83	0.44
1:K:114:ILE:O	1:K:118:LEU:HD23	2.18	0.44
1:K:130:GLY:O	1:K:131:PHE:C	2.61	0.44
2:L:74:ARG:NH2	2:L:78:ARG:NH1	2.54	0.44
2:L:250:ALA:O	2:L:252:GLY:N	2.51	0.44
1:A:203:LEU:CG	1:A:204:LEU:N	2.73	0.43
1:A:442:GLU:OE2	1:A:442:GLU:N	2.45	0.43
2:B:59:LEU:O	2:B:63:ILE:HG13	2.18	0.43
2:B:155:ARG:CZ	2:B:159:ILE:HD11	2.48	0.43
2:B:190:HIS:C	2:B:191:PHE:O	2.61	0.43
2:B:507:ALA:N	2:B:508:PRO:HD2	2.33	0.43
1:C:60:ILE:HD13	1:C:129:TYR:CZ	2.53	0.43
2:D:140:VAL:O	2:D:141:LYS:C	2.61	0.43
1:E:132:LEU:CB	1:E:138:PHE:CD2	3.00	0.43
1:E:136:ALA:O	1:E:137:ASP:C	2.60	0.43
1:E:154:ALA:O	1:E:155:ALA:C	2.60	0.43
2:F:400:PHE:CE2	2:F:453:CYS:HB2	2.52	0.43
1:G:194:GLU:C	1:G:196:GLY:H	2.26	0.43
1:G:278:ILE:HD13	1:G:286:VAL:O	2.18	0.43
1:G:295:GLY:O	1:G:297:GLU:N	2.51	0.43
1:G:350:ILE:HG13	1:G:351:THR:N	2.32	0.43
2:H:83:VAL:HG12	2:H:84:ARG:H	1.82	0.43
2:H:218:ALA:HB2	2:H:241:LEU:O	2.18	0.43
1:I:51:ARG:O	1:I:122:ALA:HB1	2.18	0.43
1:I:65:MET:HE1	1:I:92:ALA:HB2	1.99	0.43
2:J:302:LEU:CD1	2:J:549:LEU:HD11	2.47	0.43
2:J:324:ASP:O	2:J:325:SER:C	2.60	0.43
2:J:423:ALA:O	2:J:426:VAL:HG23	2.18	0.43
2:J:426:VAL:HG13	2:J:451:GLY:HA2	2.00	0.43
1:K:469:PHE:C	1:K:469:PHE:CD2	2.96	0.43
2:L:71:ALA:HA	2:L:74:ARG:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:99:GLU:C	2:L:100:LEU:HD23	2.44	0.43
1:A:83:ASP:C	1:A:85:HIS:H	2.25	0.43
1:A:251:LEU:HD11	1:A:328:ARG:NH2	2.33	0.43
1:A:278:ILE:HG23	1:A:488:PHE:CD2	2.53	0.43
1:A:344:HIS:CG	1:A:345:PRO:HD3	2.53	0.43
1:A:497:LEU:O	1:A:498:PRO:O	2.36	0.43
2:B:72:GLN:O	2:B:75:HIS:HB3	2.18	0.43
2:B:287:ALA:O	2:B:288:ARG:C	2.61	0.43
1:C:57:ARG:HH21	1:C:83:ASP:CG	2.27	0.43
1:C:138:PHE:HD1	1:C:142:CYS:HB2	1.78	0.43
1:C:300:ARG:NH1	1:C:300:ARG:CB	2.76	0.43
1:C:350:ILE:HD12	1:C:351:THR:N	2.34	0.43
1:C:587:GLN:OE1	1:C:587:GLN:HA	2.18	0.43
2:D:75:HIS:C	2:D:77:ALA:N	2.76	0.43
1:E:60:ILE:HD12	1:E:60:ILE:HA	1.70	0.43
1:E:613:ARG:C	1:E:614:ARG:HD2	2.43	0.43
2:F:123:ILE:HA	2:F:131:CYS:O	2.18	0.43
2:F:223:VAL:N	2:F:224:PRO:HD2	2.33	0.43
2:F:509:ILE:HD13	2:F:509:ILE:N	2.32	0.43
1:G:64:VAL:HG21	1:G:126:HIS:CD2	2.53	0.43
1:G:291:ALA:HA	1:G:292:PRO:HD3	1.82	0.43
1:G:421:ARG:O	1:G:422:GLU:C	2.61	0.43
2:H:489:GLN:O	2:H:493:ALA:HB2	2.18	0.43
1:I:65:MET:HE3	1:I:92:ALA:CB	2.48	0.43
1:I:170:MET:SD	1:I:309:ALA:CB	3.06	0.43
1:I:170:MET:SD	1:I:309:ALA:HB1	2.57	0.43
1:I:328:ARG:CB	1:I:328:ARG:HH11	2.31	0.43
1:I:416:VAL:HG22	1:I:437:LEU:HG	2.00	0.43
1:I:486:THR:HG22	1:I:486:THR:O	2.17	0.43
2:J:119:ILE:O	2:J:152:LYS:NZ	2.49	0.43
2:J:255:VAL:HG22	2:J:256:SER:N	2.33	0.43
2:J:288:ARG:HH21	2:J:288:ARG:HG2	1.83	0.43
2:J:486:LYS:HE2	2:J:497:LEU:HD13	2.01	0.43
1:K:439:ALA:CB	1:K:451:LEU:HB2	2.45	0.43
2:B:125:ARG:HD2	2:B:128:GLY:HA2	2.00	0.43
2:B:194:ILE:CD1	2:B:194:ILE:H	2.31	0.43
1:C:186:GLN:CD	1:C:190:THR:HG1	2.23	0.43
2:D:60:LEU:O	2:D:64:HIS:ND1	2.46	0.43
2:D:87:ILE:HG22	2:D:88:ASN:N	2.33	0.43
2:D:316:GLU:HB2	2:D:337:ARG:HE	1.83	0.43
2:D:338:LEU:C	2:D:538:ARG:HD2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:ILE:HD12	1:E:278:ILE:N	2.03	0.43
1:E:340:LEU:HA	1:E:340:LEU:HD23	1.49	0.43
1:E:437:LEU:HD12	1:E:437:LEU:N	2.32	0.43
1:E:489:ILE:HG23	1:E:490:ALA:H	1.83	0.43
2:F:212:VAL:CG2	2:F:232:MET:HG2	2.48	0.43
1:G:186:GLN:CD	1:G:190:THR:OG1	2.61	0.43
1:G:390:ASP:CG	1:G:464:ARG:HD2	2.43	0.43
1:G:444:ARG:HG2	1:G:444:ARG:NH1	2.27	0.43
2:H:144:THR:HG21	4:H:591:COA:C5A	2.48	0.43
2:H:338:LEU:HD23	2:H:538:ARG:HB2	2.00	0.43
2:H:533:ASP:HB3	2:H:536:GLN:NE2	2.29	0.43
1:I:476:HIS:ND1	1:I:477:PRO:CD	2.77	0.43
2:J:317:LEU:O	2:J:320:VAL:N	2.47	0.43
1:K:58:GLY:O	1:K:60:ILE:N	2.52	0.43
2:L:45:ASN:HB3	2:L:321:ILE:O	2.18	0.43
2:L:242:ALA:HA	2:L:246:LEU:HD12	2.01	0.43
2:L:300:GLY:O	2:L:301:GLN:HG3	2.17	0.43
1:A:300:ARG:NH2	1:A:304:GLU:OE1	2.51	0.43
1:A:311:GLN:OE1	1:A:311:GLN:HA	2.18	0.43
2:B:51:GLU:HA	2:B:54:ASN:ND2	2.32	0.43
1:C:136:ALA:HB1	1:C:154:ALA:HB1	2.00	0.43
1:C:350:ILE:HD12	1:C:351:THR:HG22	1.99	0.43
1:E:413:GLY:HA3	1:E:450:ARG:NH1	2.33	0.43
2:F:31:LEU:HD12	2:F:336:ALA:HB2	2.00	0.43
2:F:321:ILE:HD13	2:F:329:TYR:CE2	2.53	0.43
2:F:338:LEU:HD21	2:F:537:THR:CB	2.47	0.43
2:F:435:PRO:HD2	2:F:553:ILE:HD12	2.00	0.43
1:G:198:ILE:HG23	1:G:248:LYS:CG	2.49	0.43
1:G:384:VAL:HB	1:G:470:LEU:CD1	2.49	0.43
1:G:404:LEU:HD21	1:G:612:LEU:HD11	2.01	0.43
2:H:244:PRO:HA	2:H:247:VAL:HG12	2.01	0.43
1:I:166:ALA:O	1:I:167:LYS:C	2.61	0.43
1:I:512:ALA:HB2	1:I:620:LEU:HD23	2.00	0.43
1:I:540:ASN:HA	2:J:94:GLY:O	2.19	0.43
2:J:73:ALA:C	2:J:75:HIS:H	2.25	0.43
2:J:403:ASN:HA	2:J:443:GLY:H	1.84	0.43
1:K:59:GLU:OE2	1:K:436:LYS:NZ	2.51	0.43
1:K:500:PRO:O	1:K:501:GLN:CB	2.64	0.43
1:K:549:ARG:NH2	1:K:571:PRO:CB	2.82	0.43
2:L:190:HIS:C	2:L:191:PHE:O	2.60	0.43
2:L:277:ALA:HB2	2:L:286:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:412:LYS:HB2	2:L:412:LYS:HE3	1.78	0.43
1:A:149:PHE:O	1:A:151:GLY:N	2.51	0.43
1:A:169:LEU:HD12	1:A:169:LEU:N	2.33	0.43
1:A:225:ALA:O	1:A:228:LEU:HB3	2.18	0.43
1:A:392:GLU:O	1:A:394:ASP:N	2.51	0.43
1:A:463:LEU:HD22	1:A:464:ARG:H	1.84	0.43
1:A:549:ARG:HH11	1:A:549:ARG:CG	2.32	0.43
2:B:49:MET:O	2:B:52:GLN:HB2	2.18	0.43
2:B:255:VAL:HG22	2:B:256:SER:N	2.33	0.43
2:B:272:VAL:O	2:B:272:VAL:HG12	2.19	0.43
2:B:412:LYS:CG	2:B:413:TYR:N	2.82	0.43
1:C:77:ALA:HB1	1:C:88:HIS:HD2	1.84	0.43
1:C:228:LEU:O	1:C:244:MET:HE3	2.19	0.43
1:C:384:VAL:HG13	1:C:470:LEU:HD22	2.00	0.43
1:C:445:GLU:OE1	1:C:445:GLU:HA	2.17	0.43
2:D:28:MET:C	2:D:30:ILE:N	2.69	0.43
2:D:371:ALA:CB	2:D:401:LEU:HB2	2.49	0.43
1:E:203:LEU:HG	1:E:204:LEU:N	2.34	0.43
1:E:251:LEU:HD11	1:E:328:ARG:NH1	2.33	0.43
1:E:288:GLU:HB3	1:E:382:ILE:HG12	1.99	0.43
1:E:452:LEU:CD1	1:E:452:LEU:O	2.66	0.43
1:E:534:HIS:O	1:E:535:SER:C	2.60	0.43
1:E:549:ARG:HH11	1:E:549:ARG:CG	2.05	0.43
2:F:157:GLN:HE21	2:F:197:ASN:CB	2.32	0.43
2:F:238:THR:HA	2:F:261:GLY:O	2.18	0.43
2:F:282:HIS:O	2:F:285:ALA:HB3	2.18	0.43
2:F:375:ILE:CD1	2:F:375:ILE:N	2.73	0.43
2:F:382:GLN:OE1	2:F:421:HIS:CE1	2.71	0.43
2:F:507:ALA:HB3	2:F:508:PRO:HD3	2.00	0.43
1:G:169:LEU:N	1:G:169:LEU:HD12	2.33	0.43
2:H:212:VAL:HG12	2:H:237:ALA:HB1	2.00	0.43
2:H:407:PHE:N	2:H:407:PHE:CD1	2.86	0.43
1:I:108:LEU:HA	1:I:132:LEU:HD11	1.99	0.43
1:I:294:LEU:HD11	1:I:299:ARG:NH1	2.31	0.43
1:I:375:VAL:HA	1:I:376:PRO:HD2	1.70	0.43
1:I:508:PHE:O	1:I:511:ALA:N	2.51	0.43
2:J:216:CYS:O	2:J:216:CYS:SG	2.76	0.43
2:J:370:LEU:HD11	2:J:387:PHE:HD2	1.83	0.43
1:K:276:CYS:HB2	1:K:284:LYS:HE2	2.01	0.43
1:K:384:VAL:HG11	1:K:470:LEU:HD13	2.00	0.43
1:K:516:TRP:CZ3	1:K:630:GLU:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:223:VAL:O	2:L:227:SER:OG	2.36	0.43
1:A:69:ARG:NH2	1:A:91:GLU:O	2.47	0.43
1:A:190:THR:HA	1:A:193:ARG:HD3	1.99	0.43
1:A:224:LEU:O	1:A:224:LEU:HD23	2.19	0.43
1:A:263:ASP:C	1:A:265:HIS:N	2.77	0.43
1:A:304:GLU:HB3	1:A:308:ARG:NH2	2.34	0.43
1:A:491:ARG:C	1:A:493:GLN:N	2.76	0.43
2:B:180:ARG:NH1	2:B:180:ARG:HG3	2.33	0.43
2:B:248:LYS:C	2:B:250:ALA:H	2.25	0.43
2:B:469:ARG:HD3	2:B:518:HIS:HA	2.00	0.43
1:C:138:PHE:CD1	1:C:138:PHE:C	2.96	0.43
2:D:90:LEU:O	2:D:288:ARG:NH2	2.51	0.43
2:D:121:ALA:HB1	2:D:134:VAL:HG22	1.98	0.43
1:E:169:LEU:O	1:E:173:ALA:HB2	2.18	0.43
1:E:437:LEU:CD2	1:E:455:LEU:CD2	2.97	0.43
1:E:516:TRP:CE2	1:E:613:ARG:NH2	2.86	0.43
2:F:92:ASP:O	2:F:93:PRO:C	2.61	0.43
2:F:170:LEU:HD23	2:F:211:VAL:HB	2.01	0.43
2:F:381:ALA:HA	2:F:425:LEU:HD13	1.99	0.43
1:G:232:GLN:H	1:G:233:ARG:CZ	2.32	0.43
1:G:275:ASP:OD2	1:G:277:SER:OG	2.23	0.43
1:G:516:TRP:CD1	1:G:555:LEU:HD21	2.53	0.43
1:I:384:VAL:HG11	1:I:470:LEU:HD22	1.99	0.43
1:I:553:LEU:HD12	1:I:566:LEU:CD1	2.48	0.43
2:J:59:LEU:HD12	2:J:59:LEU:C	2.44	0.43
2:J:100:LEU:HG	2:J:122:GLY:HA2	2.00	0.43
2:J:150:VAL:HG21	2:J:184:VAL:HG13	2.01	0.43
2:J:341:GLY:O	2:J:343:GLU:HG2	2.19	0.43
1:K:488:PHE:CE1	1:K:492:HIS:ND1	2.81	0.43
2:L:313:PRO:HD2	2:L:316:GLU:OE1	2.19	0.43
2:L:478:ALA:O	2:L:482:LEU:HB2	2.19	0.43
1:A:138:PHE:O	1:A:139:ALA:C	2.61	0.43
1:A:361:ARG:NH2	1:E:442:GLU:OE2	2.51	0.43
1:A:673:THR:HA	1:A:687:ARG:HA	1.99	0.43
2:B:74:ARG:O	2:B:77:ALA:HB3	2.19	0.43
2:B:351:PHE:O	2:B:383:LYS:HD2	2.18	0.43
1:C:443:THR:OG1	1:C:444:ARG:N	2.51	0.43
1:C:536:PRO:HD3	2:D:363:HIS:HD2	1.83	0.43
2:D:375:ILE:CG2	2:D:376:LEU:H	2.20	0.43
2:D:417:GLY:C	2:D:419:ALA:H	2.27	0.43
2:D:476:GLU:CA	2:D:510:LEU:HD21	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:SER:C	1:E:49:ILE:HD12	2.43	0.43
1:E:289:ALA:HB1	1:E:350:ILE:CD1	2.44	0.43
1:E:351:THR:HA	1:E:376:PRO:HG2	2.01	0.43
1:E:392:GLU:OE2	1:E:500:PRO:HD3	2.18	0.43
1:E:412:PRO:HB3	1:E:450:ARG:CZ	2.48	0.43
1:E:613:ARG:HG2	1:E:614:ARG:H	1.83	0.43
2:F:167:CYS:HB3	2:F:169:TYR:CE2	2.54	0.43
2:F:536:GLN:HA	2:F:539:GLU:HG3	2.00	0.43
1:G:150:LEU:HD21	1:G:363:ALA:HB3	2.01	0.43
2:H:115:ALA:O	2:H:116:ALA:C	2.61	0.43
2:H:127:GLU:OE2	2:H:292:ALA:HB2	2.19	0.43
2:H:184:VAL:O	2:H:184:VAL:HG12	2.18	0.43
2:H:270:SER:OG	2:H:271:GLY:N	2.51	0.43
1:I:65:MET:HE3	1:I:92:ALA:HB2	1.99	0.43
1:I:111:ASP:C	1:I:114:ILE:HG22	2.42	0.43
1:I:339:ARG:HH11	1:I:339:ARG:HG3	1.83	0.43
1:I:428:PRO:HG2	1:I:429:PHE:N	2.34	0.43
1:I:534:HIS:HB3	2:J:307:PRO:CG	2.48	0.43
2:J:347:PHE:O	2:J:348:LYS:C	2.61	0.43
1:A:663:GLU:CG	1:A:666:GLN:HB2	2.49	0.43
1:A:669:GLU:HB3	1:A:670:ALA:H	1.69	0.43
1:A:673:THR:HG21	1:A:685:SER:OG	2.18	0.43
2:B:224:PRO:HB2	2:B:230:THR:HG21	2.01	0.43
2:B:375:ILE:H	2:B:375:ILE:CD1	2.29	0.43
1:C:69:ARG:HB3	1:C:69:ARG:NH1	2.34	0.43
1:C:194:GLU:C	1:C:196:GLY:H	2.27	0.43
1:C:254:ARG:HH22	1:C:292:PRO:HD2	1.83	0.43
1:C:619:PHE:HB3	1:C:626:LEU:HD11	2.00	0.43
2:D:355:LEU:HB2	2:D:380:ALA:HB1	2.01	0.43
2:D:377:PHE:CD1	2:D:377:PHE:N	2.82	0.43
2:F:100:LEU:CD1	2:F:132:MET:HE1	2.46	0.43
2:F:248:LYS:C	2:F:250:ALA:H	2.27	0.43
1:G:517:LEU:C	1:G:519:SER:H	2.26	0.43
2:H:75:HIS:C	2:H:77:ALA:N	2.77	0.43
2:H:476:GLU:CB	2:H:510:LEU:HD21	2.49	0.43
1:I:81:ASP:HB2	1:I:100:GLY:CA	2.47	0.43
1:I:160:MET:SD	1:I:160:MET:N	2.92	0.43
1:I:508:PHE:O	1:I:509:TRP:C	2.61	0.43
1:I:517:LEU:HD22	1:I:566:LEU:CD1	2.49	0.43
2:J:83:VAL:CG1	2:J:84:ARG:H	2.23	0.43
1:K:114:ILE:CD1	1:K:138:PHE:CZ	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:140:ARG:O	1:K:144:GLU:HB3	2.19	0.43
1:K:251:LEU:O	1:K:252:LYS:C	2.62	0.43
1:K:336:MET:HE3	1:K:337:ASN:C	2.44	0.43
1:K:541:ASP:O	1:K:549:ARG:HG2	2.18	0.43
2:L:197:ASN:HD22	2:L:197:ASN:HA	1.65	0.43
2:L:315:GLU:C	2:L:317:LEU:N	2.74	0.43
1:A:501:GLN:C	1:A:504:LEU:H	2.27	0.43
1:A:598:LEU:HD12	1:A:598:LEU:HA	1.79	0.43
2:B:308:ARG:NH2	2:B:343:GLU:CD	2.76	0.43
2:B:402:GLN:HE21	2:B:402:GLN:HB3	1.57	0.43
2:B:441:ILE:HB	2:B:465:TRP:CE3	2.54	0.43
1:C:274:ARG:HH22	1:C:320:THR:CG2	2.30	0.43
1:C:513:ALA:CB	1:C:566:LEU:HD21	2.49	0.43
1:C:569:ALA:C	1:C:571:PRO:HD3	2.42	0.43
2:D:476:GLU:O	2:D:480:GLY:N	2.52	0.43
1:E:204:LEU:O	1:E:215:MET:HA	2.19	0.43
1:E:553:LEU:HB2	1:E:564:VAL:HG22	2.01	0.43
1:E:567:ARG:HH11	1:E:567:ARG:CG	2.26	0.43
2:F:181:GLN:C	2:F:183:GLU:H	2.25	0.43
2:F:191:PHE:HD2	2:F:192:GLY:N	2.16	0.43
2:F:299:GLN:CB	2:F:552:PRO:HD3	2.49	0.43
2:F:375:ILE:HD13	2:F:377:PHE:HE1	1.84	0.43
1:G:202:VAL:HG22	1:G:247:GLU:O	2.19	0.43
1:G:251:LEU:HD11	1:G:328:ARG:HH21	1.84	0.43
2:H:65:GLU:O	2:H:72:GLN:NE2	2.52	0.43
2:H:155:ARG:NH2	2:H:460:ARG:O	2.52	0.43
2:H:536:GLN:O	2:H:537:THR:C	2.60	0.43
1:I:98:LEU:HA	1:I:98:LEU:HD23	1.64	0.43
1:I:324:LEU:HB2	1:I:334:MET:HG3	2.00	0.43
2:J:109:TYR:O	2:J:111:GLY:C	2.60	0.43
2:L:148:LEU:HD23	2:L:148:LEU:HA	1.80	0.43
2:L:533:ASP:C	2:L:533:ASP:OD2	2.61	0.43
1:A:331:PHE:O	1:A:332:PHE:CD2	2.71	0.43
1:A:704:LEU:HG	1:A:704:LEU:H	1.69	0.43
2:B:36:ASN:ND2	2:B:36:ASN:C	2.76	0.43
2:B:194:ILE:O	2:B:198:GLN:HB2	2.18	0.43
2:B:260:LEU:HD12	2:L:411:GLN:HA	2.00	0.43
2:B:370:LEU:HD11	2:B:387:PHE:HD2	1.83	0.43
1:C:159:ALA:C	1:C:161:GLY:H	2.27	0.43
1:C:251:LEU:O	1:C:327:GLU:HG3	2.19	0.43
2:D:309:ALA:HB1	2:D:310:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ARG:HG3	1:E:63:ARG:HH11	1.84	0.43
1:E:187:ASP:C	1:E:189:GLU:N	2.76	0.43
1:E:454:MET:HE2	1:E:454:MET:HB3	1.87	0.43
1:E:505:PRO:CB	1:E:507:HIS:CB	2.92	0.43
2:F:114:VAL:HG11	2:F:146:TYR:CE2	2.53	0.43
2:F:325:SER:HB3	2:F:326:LYS:HZ2	1.83	0.43
2:F:332:ARG:HG3	2:F:332:ARG:NH1	2.34	0.43
1:G:404:LEU:HD22	1:G:612:LEU:HD11	1.99	0.43
2:H:248:LYS:HD2	2:H:248:LYS:C	2.44	0.43
1:I:261:PHE:CE1	1:I:318:ALA:CB	2.99	0.43
1:I:320:THR:OG1	1:I:341:GLN:HG3	2.19	0.43
2:J:75:HIS:C	2:J:77:ALA:N	2.77	0.43
2:J:192:GLY:HA2	2:J:195:PHE:CD2	2.54	0.43
2:J:377:PHE:N	2:J:377:PHE:HD1	2.14	0.43
2:J:440:LEU:HB2	2:J:464:MET:HG3	2.01	0.43
1:K:255:HIS:CE1	1:K:322:GLU:CG	2.99	0.43
2:L:57:ARG:HG2	2:L:57:ARG:HH11	1.84	0.43
2:L:91:LEU:HD23	2:L:125:ARG:O	2.19	0.43
2:L:462:LEU:C	2:L:462:LEU:CD2	2.92	0.43
1:A:223:GLU:O	1:A:227:ALA:HB2	2.19	0.42
1:A:283:GLN:O	1:A:285:VAL:HG23	2.19	0.42
1:A:326:ASP:O	1:A:327:GLU:C	2.60	0.42
1:A:714:LEU:HB3	1:A:715:ASP:H	1.61	0.42
2:B:331:VAL:O	2:B:333:GLU:N	2.52	0.42
2:B:526:LEU:C	2:B:528:ASP:H	2.25	0.42
1:C:126:HIS:HB2	1:C:150:LEU:HD12	2.00	0.42
1:C:263:ASP:HB2	1:C:362:VAL:HG12	1.97	0.42
1:C:279:GLN:HE21	1:C:279:GLN:HB3	1.62	0.42
2:D:75:HIS:NE2	2:D:80:LYS:HE2	2.34	0.42
2:D:199:ALA:HB2	2:D:226:MET:CE	2.46	0.42
2:D:433:ARG:HG3	2:D:433:ARG:NH1	2.29	0.42
1:E:590:LEU:HD12	1:E:597:ASP:O	2.19	0.42
2:F:223:VAL:O	2:F:227:SER:OG	2.34	0.42
2:F:350:LEU:HD23	2:F:350:LEU:N	2.34	0.42
2:F:370:LEU:HD12	2:F:398:LEU:HD23	2.00	0.42
1:G:64:VAL:HG13	1:G:65:MET:N	2.34	0.42
1:G:71:LEU:HD22	1:G:360:ILE:HG21	2.01	0.42
1:G:136:ALA:HB1	1:G:154:ALA:HB1	2.00	0.42
1:G:189:GLU:O	1:G:192:ARG:N	2.51	0.42
1:G:509:TRP:HB3	1:G:564:VAL:HG11	2.01	0.42
2:H:30:ILE:CG2	2:H:31:LEU:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:393:GLN:HE21	2:H:393:GLN:HB3	1.55	0.42
1:I:59:GLU:CD	1:I:60:ILE:N	2.77	0.42
1:I:306:ALA:CB	1:I:321:VAL:HG21	2.31	0.42
1:I:356:VAL:O	1:I:359:GLN:HB2	2.18	0.42
1:I:396:LEU:O	1:I:398:ALA:N	2.52	0.42
1:I:534:HIS:HB3	2:J:307:PRO:HG3	2.00	0.42
2:J:373:ASN:HD22	2:J:373:ASN:HA	1.49	0.42
1:K:261:PHE:O	1:K:268:CYS:HA	2.19	0.42
2:L:205:GLY:O	2:L:207:PRO:HD3	2.19	0.42
2:L:240:PHE:CE1	2:L:243:GLY:HA2	2.54	0.42
2:L:335:ILE:O	2:L:339:VAL:HG13	2.19	0.42
1:A:307:VAL:HG22	1:A:307:VAL:O	2.20	0.42
2:B:354:THR:HG21	2:B:375:ILE:C	2.44	0.42
2:B:479:ALA:HB2	2:B:509:ILE:HG21	2.01	0.42
2:B:487:ARG:O	2:B:491:GLU:HB2	2.19	0.42
1:C:103:PRO:O	1:C:108:LEU:HD12	2.19	0.42
1:C:297:GLU:O	1:C:300:ARG:HG3	2.18	0.42
2:D:512:GLN:HE21	2:D:512:GLN:HB3	1.61	0.42
2:D:560:VAL:HG13	2:H:389:GLU:CB	2.43	0.42
1:E:81:ASP:C	1:E:83:ASP:H	2.27	0.42
1:E:179:PRO:HD2	1:E:248:LYS:HB3	2.01	0.42
2:F:137:ASP:C	2:F:139:THR:H	2.28	0.42
2:F:291:VAL:O	2:F:291:VAL:HG12	2.18	0.42
1:G:199:GLY:C	1:G:201:PRO:CD	2.92	0.42
1:G:476:HIS:ND1	1:G:477:PRO:HD2	2.34	0.42
1:G:501:GLN:NE2	1:G:504:LEU:HG	2.34	0.42
2:H:140:VAL:O	2:H:141:LYS:C	2.61	0.42
2:H:513:TYR:N	2:H:513:TYR:HD1	2.17	0.42
2:H:520:TYR:N	2:H:520:TYR:HD2	2.16	0.42
1:I:607:ARG:HB2	1:I:607:ARG:CZ	2.49	0.42
2:J:327:GLN:HA	2:J:328:PRO:HD3	1.80	0.42
1:K:133:SER:OG	1:K:339:ARG:HG2	2.19	0.42
1:K:365:GLY:O	1:K:366:GLU:C	2.62	0.42
1:K:463:LEU:CD2	1:K:464:ARG:N	2.74	0.42
1:K:463:LEU:HD23	1:K:464:ARG:H	1.78	0.42
2:L:189:GLU:C	2:L:189:GLU:OE1	2.63	0.42
2:L:279:ASP:CG	2:L:280:ASP:N	2.73	0.42
2:L:400:PHE:C	2:L:401:LEU:HD23	2.44	0.42
2:L:440:LEU:HG	2:L:463:TRP:O	2.20	0.42
1:A:218:VAL:O	1:A:218:VAL:CG2	2.65	0.42
1:A:440:TRP:CD1	1:A:441:GLY:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLN:HE21	1:A:497:LEU:HG	1.85	0.42
1:A:517:LEU:HB2	1:A:553:LEU:HD11	2.00	0.42
3:A:801:BTI:O3	2:F:407:PHE:N	2.51	0.42
2:B:144:THR:HG21	4:B:591:COA:C5A	2.50	0.42
2:B:172:ASP:OD1	2:B:214:GLY:HA3	2.20	0.42
2:B:412:LYS:HG3	2:B:413:TYR:N	2.34	0.42
2:B:487:ARG:CA	2:B:497:LEU:HD13	2.49	0.42
1:C:365:GLY:O	1:C:366:GLU:C	2.63	0.42
1:C:387:TYR:C	1:C:389:GLU:N	2.76	0.42
2:D:240:PHE:CD1	2:D:243:GLY:HA2	2.54	0.42
2:D:418:ILE:CG2	2:D:419:ALA:N	2.82	0.42
2:D:436:LYS:HE3	2:D:436:LYS:HB2	1.88	0.42
1:E:134:GLU:HG2	1:E:338:THR:OG1	2.19	0.42
2:F:197:ASN:O	2:F:201:MET:HG3	2.19	0.42
1:G:602:VAL:O	1:G:603:ASP:HB2	2.18	0.42
2:H:236:GLN:OE1	2:H:280:ASP:OD1	2.37	0.42
2:H:278:GLU:O	2:H:279:ASP:HB3	2.18	0.42
1:I:256:VAL:HG13	1:I:274:ARG:O	2.18	0.42
1:I:472:ARG:H	1:I:472:ARG:HG2	1.59	0.42
1:I:587:GLN:HB3	1:I:588:TYR:CD1	2.50	0.42
2:J:85:GLU:OE1	2:J:85:GLU:HA	2.19	0.42
2:J:164:ARG:O	2:J:164:ARG:HG2	2.18	0.42
2:J:305:ARG:HH21	2:J:361:HIS:CE1	2.38	0.42
2:J:441:ILE:C	2:J:441:ILE:CD1	2.82	0.42
2:J:489:GLN:O	2:J:493:ALA:HB2	2.19	0.42
2:J:491:GLU:C	2:J:493:ALA:N	2.76	0.42
2:J:501:GLU:CD	2:J:501:GLU:N	2.77	0.42
1:K:280:ARG:O	1:K:282:HIS:N	2.52	0.42
1:K:298:LEU:HD11	1:K:325:LEU:HD11	2.01	0.42
1:K:361:ARG:HG2	1:K:361:ARG:NH1	2.32	0.42
1:K:421:ARG:O	1:K:422:GLU:C	2.61	0.42
1:K:470:LEU:CA	1:K:473:ILE:CG2	2.95	0.42
1:A:129:TYR:CD2	1:A:342:VAL:HA	2.53	0.42
1:A:200:TYR:OH	1:A:224:LEU:HD13	2.19	0.42
1:A:346:VAL:HG23	1:A:347:THR:N	2.32	0.42
1:A:531:ASP:N	1:A:531:ASP:OD1	2.52	0.42
2:B:36:ASN:HD21	2:B:38:ARG:HB2	1.84	0.42
2:B:190:HIS:O	2:B:191:PHE:O	2.37	0.42
2:B:533:ASP:HB3	2:B:536:GLN:HB2	2.01	0.42
1:C:270:TYR:N	1:C:372:GLN:HE22	2.02	0.42
2:D:31:LEU:HD12	2:D:336:ALA:CA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:LEU:HD22	2:D:100:LEU:HA	1.74	0.42
2:D:507:ALA:HB3	2:D:508:PRO:HD3	2.02	0.42
2:D:521:TYR:CE1	2:D:525:ARG:CZ	3.02	0.42
1:E:79:HIS:CD2	1:E:84:ARG:HA	2.55	0.42
1:E:188:LEU:HD23	1:E:228:LEU:CD2	2.46	0.42
2:F:140:VAL:O	2:F:143:GLY:N	2.41	0.42
2:F:181:GLN:C	2:F:183:GLU:N	2.77	0.42
2:F:219:GLY:O	2:F:221:ALA:N	2.52	0.42
2:F:464:MET:O	2:F:531:VAL:HA	2.19	0.42
2:F:467:ASN:ND2	2:F:467:ASN:H	2.17	0.42
2:F:498:GLY:C	2:F:500:GLU:N	2.64	0.42
1:G:67:SER:O	1:G:71:LEU:HD12	2.18	0.42
1:G:136:ALA:O	1:G:140:ARG:HB2	2.19	0.42
1:G:414:ARG:HB2	1:G:454:MET:SD	2.59	0.42
2:H:30:ILE:C	2:H:31:LEU:HD23	2.45	0.42
2:H:150:VAL:HG21	2:H:184:VAL:HG13	2.00	0.42
2:H:188:ARG:HG2	2:H:188:ARG:HH11	1.84	0.42
2:H:509:ILE:HD13	2:H:509:ILE:HA	1.69	0.42
4:H:591:COA:H62A	4:H:591:COA:H62	1.84	0.42
1:I:114:ILE:CD1	1:I:142:CYS:HA	2.49	0.42
1:I:444:ARG:CG	1:I:444:ARG:NH1	2.82	0.42
1:K:47:ARG:HE	1:K:148:LEU:HD22	1.80	0.42
1:K:55:ALA:HA	1:K:78:VAL:HG21	2.02	0.42
1:K:307:VAL:HG22	1:K:311:GLN:HE22	1.84	0.42
1:K:402:LEU:CD2	1:K:460:VAL:HG12	2.50	0.42
2:L:372:ASN:OD1	2:L:452:MET:HE2	2.20	0.42
1:A:232:GLN:H	1:A:233:ARG:NH2	2.14	0.42
1:A:463:LEU:HD23	1:A:464:ARG:H	1.84	0.42
1:A:526:ASP:OD2	1:A:526:ASP:N	2.34	0.42
2:B:305:ARG:O	2:B:364:GLY:HA2	2.18	0.42
1:C:160:MET:SD	1:C:313:ILE:HD13	2.60	0.42
1:C:269:LEU:HD13	1:C:375:VAL:HG11	2.01	0.42
1:C:537:TRP:CH2	2:D:123:ILE:HG22	2.54	0.42
1:C:565:ARG:CG	1:C:567:ARG:CZ	2.98	0.42
2:D:295:ASN:O	2:D:295:ASN:ND2	2.53	0.42
2:D:306:ALA:HA	2:D:307:PRO:HD3	1.84	0.42
2:D:438:THR:HG21	2:D:453:CYS:O	2.20	0.42
1:E:56:ASN:HD22	1:E:128:GLY:HA3	1.85	0.42
1:E:191:PHE:HZ	1:E:244:MET:O	2.03	0.42
1:E:264:ARG:C	1:E:265:HIS:CD2	2.97	0.42
1:E:512:ALA:CB	1:E:629:ILE:HD13	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:567:ARG:CG	1:E:567:ARG:NH1	2.80	0.42
2:F:81:LEU:HD21	2:F:89:ARG:NH2	2.34	0.42
2:F:401:LEU:HD23	2:F:401:LEU:HA	1.71	0.42
1:G:549:ARG:NH1	1:G:549:ARG:HG2	2.33	0.42
2:H:525:ARG:O	2:H:526:LEU:HB2	2.19	0.42
1:I:251:LEU:HD12	1:I:327:GLU:HB2	2.00	0.42
1:I:315:TYR:CE2	1:I:336:MET:HE1	2.43	0.42
1:I:403:MET:HE2	1:I:403:MET:HB2	1.93	0.42
1:I:465:THR:HG22	1:I:466:ASN:N	2.35	0.42
1:I:531:ASP:OD2	2:J:298:LYS:HG3	2.19	0.42
2:J:164:ARG:HB2	2:J:551:ALA:HB2	2.00	0.42
2:J:441:ILE:O	2:J:441:ILE:CD1	2.64	0.42
2:J:533:ASP:HB3	2:J:536:GLN:HG3	2.00	0.42
1:K:284:LYS:O	1:K:385:ARG:NH1	2.53	0.42
1:K:387:TYR:HE2	1:K:433:MET:HB2	1.81	0.42
2:L:49:MET:CE	2:L:321:ILE:HG21	2.49	0.42
2:L:130:GLU:O	2:L:165:LEU:HD22	2.20	0.42
2:L:331:VAL:HG21	2:L:371:ALA:HB1	2.01	0.42
1:A:126:HIS:HA	1:A:127:PRO:HD2	1.83	0.42
1:A:268:CYS:SG	1:A:307:VAL:CG2	2.99	0.42
1:A:306:ALA:C	1:A:308:ARG:N	2.77	0.42
2:B:31:LEU:HD13	2:B:336:ALA:HB2	2.01	0.42
1:C:280:ARG:HD3	1:C:283:GLN:CD	2.44	0.42
1:C:477:PRO:O	1:C:480:ALA:HB3	2.19	0.42
1:C:508:PHE:C	1:C:510:GLN:N	2.78	0.42
2:D:190:HIS:O	2:D:191:PHE:C	2.61	0.42
2:D:331:VAL:O	2:D:333:GLU:N	2.53	0.42
1:E:78:VAL:HG13	1:E:96:VAL:HG23	2.02	0.42
1:E:114:ILE:O	1:E:114:ILE:CG2	2.67	0.42
1:E:508:PHE:O	1:E:511:ALA:N	2.53	0.42
2:F:164:ARG:CB	2:F:551:ALA:HB2	2.49	0.42
2:F:412:LYS:CG	2:F:413:TYR:N	2.82	0.42
1:G:47:ARG:CG	1:G:148:LEU:HD11	2.47	0.42
2:H:213:MET:HA	2:H:233:VAL:HG21	2.01	0.42
2:H:470:ILE:O	2:H:517:GLY:HA2	2.19	0.42
2:H:476:GLU:CD	2:H:477:GLN:N	2.77	0.42
2:J:386:HIS:CD2	2:J:386:HIS:C	2.97	0.42
2:J:401:LEU:HA	2:J:401:LEU:HD23	1.83	0.42
2:J:518:HIS:NE2	2:J:520:TYR:CG	2.87	0.42
1:K:47:ARG:HG3	1:K:48:SER:N	2.34	0.42
1:K:536:PRO:HG2	2:L:543:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:285:ALA:O	2:L:289:ARG:HG2	2.20	0.42
2:L:367:ILE:O	2:L:367:ILE:HG13	2.19	0.42
1:A:299:ARG:HB2	1:A:299:ARG:CZ	2.50	0.42
1:A:362:VAL:HG23	1:A:363:ALA:N	2.35	0.42
1:A:444:ARG:HG2	1:A:444:ARG:HH11	1.85	0.42
1:A:693:VAL:O	1:A:714:LEU:CD2	2.68	0.42
2:B:206:ILE:O	2:B:207:PRO:C	2.63	0.42
2:B:235:GLU:HA	2:B:235:GLU:OE2	2.20	0.42
2:B:247:VAL:HG23	2:L:409:VAL:CG2	2.50	0.42
1:C:59:GLU:CD	1:C:129:TYR:HH	2.26	0.42
1:C:311:GLN:O	1:C:312:ALA:C	2.63	0.42
2:D:145:TYR:CD1	2:D:149:THR:HG22	2.55	0.42
2:D:317:LEU:HD21	2:D:334:VAL:HA	2.02	0.42
2:D:411:GLN:HA	2:J:260:LEU:HD12	2.02	0.42
1:E:178:VAL:HA	1:E:179:PRO:HD3	1.79	0.42
1:E:269:LEU:HD12	1:E:375:VAL:HG23	2.02	0.42
1:E:491:ARG:C	1:E:493:GLN:H	2.28	0.42
1:E:549:ARG:O	1:E:567:ARG:HA	2.20	0.42
2:F:487:ARG:HH11	2:F:487:ARG:HB3	1.85	0.42
1:G:57:ARG:HH11	1:G:57:ARG:HG3	1.85	0.42
1:G:596:ASP:OD1	1:G:596:ASP:N	2.52	0.42
2:H:185:PHE:H	2:H:186:PRO:HD2	1.84	0.42
2:H:351:PHE:O	2:H:383:LYS:HD2	2.20	0.42
1:I:302:MET:HG2	1:I:331:PHE:CD2	2.53	0.42
1:I:596:ASP:CG	1:I:612:LEU:HD23	2.45	0.42
2:J:89:ARG:NH2	2:J:89:ARG:HG3	2.35	0.42
2:J:234:ARG:HB3	2:J:276:TYR:CZ	2.55	0.42
1:K:250:LEU:HD13	1:K:324:LEU:HD23	2.01	0.42
1:K:331:PHE:CD2	1:K:331:PHE:N	2.88	0.42
1:K:395:PHE:CZ	1:K:469:PHE:CE1	3.07	0.42
2:L:403:ASN:ND2	2:L:442:GLY:CA	2.66	0.42
2:L:476:GLU:O	2:L:480:GLY:N	2.45	0.42
1:A:224:LEU:HD23	1:A:224:LEU:C	2.45	0.42
1:A:476:HIS:CE1	1:A:478:ALA:HB2	2.54	0.42
2:B:455:ARG:HG3	2:L:188:ARG:N	2.34	0.42
1:C:47:ARG:HB2	1:C:47:ARG:NH1	2.15	0.42
1:C:123:GLN:CD	1:C:123:GLN:N	2.78	0.42
1:C:132:LEU:HD22	1:C:132:LEU:H	1.85	0.42
1:C:205:LYS:HB3	1:C:206:ALA:H	1.74	0.42
1:C:390:ASP:CG	1:C:393:GLY:HA3	2.45	0.42
1:C:426:VAL:HG21	1:C:463:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:LEU:HD23	1:C:470:LEU:HA	1.78	0.42
2:D:270:SER:OG	2:D:272:VAL:HG23	2.20	0.42
1:E:569:ALA:C	1:E:571:PRO:HD3	2.43	0.42
2:F:121:ALA:HA	2:F:133:ILE:O	2.20	0.42
2:F:362:LEU:CD2	2:F:538:ARG:HG3	2.50	0.42
2:F:424:LYS:HB3	2:L:563:MET:HE3	2.01	0.42
1:G:50:GLN:HE21	1:G:123:GLN:HE22	1.66	0.42
1:G:110:GLY:O	1:G:114:ILE:CG2	2.58	0.42
1:G:153:PRO:O	1:G:154:ALA:C	2.61	0.42
1:G:218:VAL:CB	1:G:224:LEU:HD13	2.49	0.42
2:H:321:ILE:O	2:H:321:ILE:HG22	2.18	0.42
2:H:375:ILE:CG2	2:H:408:MET:HB2	2.50	0.42
2:H:457:TYR:N	2:H:457:TYR:HD2	2.16	0.42
1:I:170:MET:HB3	1:I:177:LEU:HD21	2.01	0.42
1:I:289:ALA:HB1	1:I:350:ILE:CD1	2.49	0.42
1:I:387:TYR:C	1:I:389:GLU:H	2.28	0.42
1:I:452:LEU:HD22	1:I:452:LEU:HA	1.71	0.42
1:I:557:CYS:O	1:I:558:ARG:C	2.62	0.42
2:J:379:GLU:OE1	2:J:379:GLU:N	2.52	0.42
2:L:155:ARG:NE	2:L:159:ILE:CD1	2.83	0.42
2:L:186:PRO:O	2:L:187:ASP:O	2.38	0.42
2:L:305:ARG:CB	2:L:305:ARG:NH1	2.82	0.42
2:L:311:LEU:HB2	2:L:312:TYR:CD1	2.55	0.42
2:L:404:ILE:O	2:L:404:ILE:CG2	2.68	0.42
1:A:79:HIS:CD2	1:A:80:SER:O	2.73	0.42
1:A:371:THR:O	1:A:374:GLN:HB2	2.20	0.42
1:A:446:GLU:OE2	1:C:361:ARG:NH1	2.48	0.42
1:A:650:SER:HA	1:A:711:LEU:HB2	2.01	0.42
1:A:654:ASN:HD22	1:A:707:GLU:HG2	1.84	0.42
1:A:658:VAL:O	1:A:658:VAL:HG12	2.19	0.42
2:B:213:MET:HE2	2:B:280:ASP:HA	2.02	0.42
2:B:341:GLY:O	2:B:343:GLU:HG2	2.19	0.42
1:C:184:GLU:C	1:C:184:GLU:CD	2.86	0.42
1:C:298:LEU:HD21	1:C:325:LEU:HD11	2.01	0.42
1:C:413:GLY:N	1:C:450:ARG:HH11	2.17	0.42
1:C:460:VAL:O	1:C:626:LEU:HD23	2.20	0.42
1:C:494:ASP:O	1:C:498:PRO:HD3	2.20	0.42
1:C:565:ARG:HG2	1:C:567:ARG:CZ	2.50	0.42
2:D:400:PHE:CD2	2:D:453:CYS:HB2	2.55	0.42
2:D:481:VAL:HG23	2:D:482:LEU:H	1.85	0.42
1:E:460:VAL:O	1:E:626:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:ILE:HD12	2:F:337:ARG:CZ	2.49	0.42
2:F:68:GLY:O	2:F:70:ALA:N	2.53	0.42
2:F:74:ARG:HH22	2:F:78:ARG:HH11	1.67	0.42
2:F:244:PRO:N	2:F:245:PRO:CD	2.83	0.42
1:G:251:LEU:HD22	1:G:328:ARG:CD	2.50	0.42
1:G:274:ARG:HG2	1:G:289:ALA:HB2	2.01	0.42
1:G:601:ARG:HE	1:G:601:ARG:HB3	1.35	0.42
2:H:171:VAL:HG23	2:H:171:VAL:O	2.19	0.42
2:H:377:PHE:CE1	2:H:408:MET:HE2	2.55	0.42
1:I:411:GLY:O	1:I:412:PRO:C	2.63	0.42
1:I:463:LEU:CD2	1:I:464:ARG:H	2.33	0.42
1:I:491:ARG:C	1:I:493:GLN:N	2.78	0.42
2:J:242:ALA:HA	2:J:246:LEU:HD22	2.02	0.42
2:J:331:VAL:H	2:J:373:ASN:HD21	1.68	0.42
1:K:534:HIS:O	2:L:363:HIS:NE2	2.53	0.42
1:K:537:TRP:O	2:L:125:ARG:HG3	2.20	0.42
2:L:42:PHE:CE1	2:L:319:GLY:HA3	2.55	0.42
2:L:63:ILE:O	2:L:63:ILE:HG22	2.20	0.42
2:L:227:SER:O	2:L:228:ASP:C	2.61	0.42
2:L:519:PRO:O	2:L:520:TYR:C	2.62	0.42
1:A:71:LEU:HD21	1:E:446:GLU:HG2	2.02	0.42
1:A:267:HIS:O	1:A:268:CYS:HB2	2.19	0.42
1:A:695:LYS:HD3	1:A:715:ASP:CB	2.50	0.42
2:B:35:ILE:HD11	2:B:337:ARG:HH12	1.83	0.42
2:B:157:GLN:HE22	2:B:194:ILE:HA	1.85	0.42
2:B:161:LEU:HD13	2:B:206:ILE:HD12	2.00	0.42
2:B:186:PRO:O	2:B:187:ASP:O	2.38	0.42
2:B:242:ALA:HB2	2:L:409:VAL:HG11	2.02	0.42
2:B:481:VAL:O	2:B:484:GLN:N	2.53	0.42
2:B:532:ILE:HD11	2:B:537:THR:HG23	2.02	0.42
1:C:58:GLY:O	1:C:60:ILE:N	2.53	0.42
1:C:524:ARG:HD2	1:C:533:PRO:O	2.20	0.42
1:C:536:PRO:HD3	2:D:363:HIS:CD2	2.55	0.42
2:D:169:TYR:CD2	2:D:169:TYR:N	2.88	0.42
2:D:192:GLY:HA3	2:J:450:TYR:CE1	2.55	0.42
1:E:299:ARG:O	1:E:300:ARG:C	2.62	0.42
1:E:503:ALA:CB	1:E:560:GLU:OE1	2.66	0.42
1:E:568:HIS:H	1:E:568:HIS:HD2	1.61	0.42
2:F:185:PHE:CD1	2:F:185:PHE:C	2.98	0.42
2:F:245:PRO:HB2	2:H:481:VAL:HG13	2.02	0.42
2:F:490:ALA:HA	2:F:493:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:ALA:CA	1:G:108:LEU:HD12	2.48	0.42
1:G:172:GLU:OE1	1:G:172:GLU:HA	2.20	0.42
1:G:343:GLU:O	1:G:346:VAL:HG22	2.19	0.42
1:G:421:ARG:HD3	1:G:421:ARG:N	2.35	0.42
1:G:440:TRP:CG	1:G:441:GLY:N	2.86	0.42
2:H:109:TYR:CE2	2:H:147:PRO:HD2	2.55	0.42
2:H:161:LEU:CD2	2:H:201:MET:HE2	2.50	0.42
2:H:339:VAL:CG1	2:H:360:ALA:CB	2.98	0.42
2:H:487:ARG:HB3	2:H:497:LEU:CB	2.50	0.42
1:I:132:LEU:HD23	1:I:138:PHE:CE2	2.51	0.42
1:I:328:ARG:HH11	1:I:328:ARG:HB3	1.85	0.42
1:I:350:ILE:HA	1:I:440:TRP:HZ3	1.85	0.42
1:I:360:ILE:O	1:I:364:ARG:HG3	2.19	0.42
1:I:513:ALA:HB2	1:I:564:VAL:HG11	2.02	0.42
2:J:250:ALA:O	2:J:252:GLY:N	2.53	0.42
2:J:400:PHE:CD2	2:J:453:CYS:HB2	2.54	0.42
1:K:63:ARG:CZ	1:K:356:VAL:HG21	2.50	0.42
1:K:114:ILE:O	1:K:118:LEU:HB2	2.19	0.42
1:K:294:LEU:CD1	1:K:299:ARG:NH2	2.83	0.42
1:A:313:ILE:HD11	1:A:315:TYR:CD2	2.52	0.41
1:A:342:VAL:HB	1:A:385:ARG:NH2	2.35	0.41
1:A:520:GLU:OE1	1:A:613:ARG:NH2	2.53	0.41
1:A:709:THR:CG2	1:A:710:PRO:HD2	2.48	0.41
2:B:163:ASN:OD1	2:B:460:ARG:NH1	2.50	0.41
2:B:264:ASP:OD1	2:B:276:TYR:CE1	2.71	0.41
2:B:331:VAL:C	2:B:333:GLU:H	2.28	0.41
2:B:486:LYS:HG2	2:B:505:ILE:HD11	2.00	0.41
1:C:299:ARG:C	1:C:301:ALA:H	2.28	0.41
1:C:415:ARG:HD3	1:C:438:ILE:HD13	2.00	0.41
1:C:532:ASP:CG	1:C:535:SER:HB2	2.45	0.41
1:C:619:PHE:CD2	1:C:628:ALA:HB2	2.55	0.41
1:E:159:ALA:C	1:E:161:GLY:H	2.26	0.41
1:E:619:PHE:HB3	1:E:626:LEU:HD11	2.02	0.41
2:F:144:THR:HG22	2:F:175:GLY:H	1.85	0.41
2:F:433:ARG:H	2:F:556:THR:CG2	2.32	0.41
2:F:466:PRO:HD3	2:F:532:ILE:O	2.20	0.41
1:G:471:ARG:HH22	1:G:621:GLU:CD	2.28	0.41
2:H:89:ARG:HD3	2:H:281:ASP:OD1	2.20	0.41
2:H:347:PHE:HA	2:J:275:HIS:HE1	1.85	0.41
1:I:251:LEU:HB2	1:I:327:GLU:CG	2.47	0.41
1:I:516:TRP:CD1	1:I:516:TRP:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:152:LYS:O	2:J:153:HIS:C	2.63	0.41
2:J:191:PHE:CD2	2:J:192:GLY:N	2.86	0.41
2:J:222:TYR:O	2:J:223:VAL:C	2.61	0.41
2:J:256:SER:OG	2:J:259:GLU:HB2	2.20	0.41
1:K:71:LEU:HD21	1:K:364:ARG:HH12	1.85	0.41
1:K:135:ASN:ND2	1:K:138:PHE:HB2	2.34	0.41
1:K:440:TRP:CG	1:K:441:GLY:N	2.86	0.41
2:L:82:LEU:H	2:L:82:LEU:CD1	2.27	0.41
2:L:83:VAL:CG2	2:L:120:VAL:HG11	2.50	0.41
2:L:437:PHE:CD2	2:L:437:PHE:N	2.88	0.41
1:A:46:TYR:CD2	1:A:46:TYR:O	2.73	0.41
1:A:139:ALA:HB2	1:A:149:PHE:CE1	2.55	0.41
1:A:202:VAL:HG22	1:A:247:GLU:O	2.20	0.41
2:B:140:VAL:O	2:B:141:LYS:C	2.63	0.41
2:B:497:LEU:HD23	2:B:502:GLU:HB2	2.02	0.41
1:C:66:ARG:HA	1:C:69:ARG:NH1	2.35	0.41
1:C:218:VAL:O	1:C:218:VAL:CG2	2.68	0.41
1:C:270:TYR:CE1	1:C:372:GLN:NE2	2.88	0.41
1:C:346:VAL:HG23	1:C:347:THR:N	2.36	0.41
1:C:351:THR:HB	1:C:376:PRO:HG2	2.02	0.41
2:D:164:ARG:O	2:D:164:ARG:CG	2.68	0.41
2:D:351:PHE:O	2:D:352:GLY:C	2.61	0.41
1:E:51:ARG:HA	1:E:74:GLY:O	2.20	0.41
1:E:186:GLN:HB3	1:E:187:ASP:H	1.56	0.41
1:E:321:VAL:HG11	1:E:323:PHE:CE2	2.55	0.41
1:G:289:ALA:HA	1:G:290:PRO:C	2.45	0.41
1:G:488:PHE:C	1:G:488:PHE:HD2	2.26	0.41
2:H:349:ALA:HB3	2:H:350:LEU:HD23	2.02	0.41
2:H:442:GLY:O	2:H:468:ALA:HA	2.20	0.41
1:I:371:THR:O	1:I:372:GLN:C	2.61	0.41
1:I:414:ARG:HH22	1:I:453:ALA:HB1	1.85	0.41
1:I:613:ARG:O	1:I:614:ARG:CD	2.66	0.41
2:J:82:LEU:H	2:J:82:LEU:HD12	1.83	0.41
1:K:282:HIS:N	1:K:282:HIS:ND1	2.67	0.41
1:K:325:LEU:C	1:K:325:LEU:HD23	2.45	0.41
2:L:176:ALA:O	2:L:178:LEU:N	2.52	0.41
2:L:433:ARG:NH2	2:L:554:GLU:HG3	2.33	0.41
2:L:520:TYR:CD2	2:L:520:TYR:N	2.88	0.41
2:B:198:GLN:HG3	2:B:208:GLN:OE1	2.20	0.41
2:B:462:LEU:HD12	2:B:463:TRP:N	2.35	0.41
1:C:222:ALA:C	1:C:224:LEU:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:ARG:HD3	1:C:474:LEU:O	2.21	0.41
1:C:513:ALA:HB1	1:C:566:LEU:HD21	2.02	0.41
2:D:414:GLU:C	2:D:416:GLY:N	2.78	0.41
2:D:472:VAL:C	2:D:473:MET:HG2	2.45	0.41
1:E:109:ARG:NH1	1:E:109:ARG:HG2	2.34	0.41
1:E:354:ASP:OD2	1:E:354:ASP:C	2.63	0.41
2:F:311:LEU:CD1	2:F:342:SER:HB2	2.50	0.41
2:F:544:ALA:O	2:F:545:LEU:C	2.63	0.41
2:H:49:MET:HE3	2:H:321:ILE:HG21	2.01	0.41
2:H:250:ALA:O	2:H:252:GLY:N	2.52	0.41
2:H:287:ALA:O	2:H:288:ARG:C	2.61	0.41
2:H:308:ARG:HH22	2:H:343:GLU:CD	2.28	0.41
1:I:130:GLY:O	1:I:131:PHE:C	2.62	0.41
1:I:140:ARG:HD3	1:I:141:ALA:N	2.35	0.41
1:I:342:VAL:HB	1:I:343:GLU:OE1	2.20	0.41
1:I:446:GLU:O	1:I:450:ARG:HB2	2.20	0.41
1:K:269:LEU:CD1	1:K:375:VAL:CG2	2.98	0.41
1:K:270:TYR:CE2	1:K:303:GLY:HA3	2.55	0.41
1:K:349:ALA:CB	1:K:381:ALA:HB2	2.50	0.41
1:K:360:ILE:H	1:K:360:ILE:HG13	1.35	0.41
2:L:396:ILE:HA	2:L:397:PRO:HD3	1.89	0.41
1:A:73:ILE:HG22	1:A:74:GLY:N	2.34	0.41
1:A:249:TYR:O	1:A:250:LEU:HD23	2.20	0.41
1:A:308:ARG:HG3	1:A:308:ARG:NH1	2.31	0.41
1:A:550:GLU:OE2	1:A:567:ARG:HB3	2.20	0.41
2:B:376:LEU:HD23	2:B:380:ALA:HB3	2.01	0.41
1:C:175:VAL:O	1:C:175:VAL:HG12	2.18	0.41
1:C:321:VAL:HG22	1:C:336:MET:HG3	2.02	0.41
2:D:129:VAL:HG13	2:D:296:TRP:CD1	2.54	0.41
2:D:224:PRO:HG2	2:D:225:ALA:N	2.35	0.41
2:D:354:THR:CG2	2:D:375:ILE:H	2.34	0.41
2:D:354:THR:HG22	2:D:375:ILE:N	2.35	0.41
2:D:492:ARG:HH22	2:J:74:ARG:CZ	2.31	0.41
2:D:537:THR:HG22	2:D:538:ARG:N	2.34	0.41
1:E:186:GLN:CB	1:E:190:THR:HB	2.50	0.41
1:E:196:GLY:O	1:E:198:ILE:N	2.53	0.41
1:E:269:LEU:HB2	1:E:372:GLN:HE22	1.85	0.41
1:E:497:LEU:N	1:E:498:PRO:HD3	2.36	0.41
1:E:618:LEU:HD23	1:E:629:ILE:HB	2.02	0.41
2:F:134:VAL:HG11	2:F:153:HIS:HD2	1.85	0.41
2:F:212:VAL:HG21	2:F:232:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:489:GLN:O	2:F:493:ALA:HB2	2.20	0.41
1:G:132:LEU:HD23	1:G:138:PHE:HD2	1.84	0.41
1:G:144:GLU:HG2	1:G:144:GLU:O	2.20	0.41
1:G:174:GLY:C	1:G:308:ARG:HD2	2.46	0.41
1:G:205:LYS:HD3	1:G:247:GLU:OE2	2.20	0.41
1:G:516:TRP:CH2	1:G:631:ALA:HB2	2.55	0.41
1:G:622:TRP:CD1	1:G:622:TRP:O	2.73	0.41
2:H:134:VAL:HG11	2:H:153:HIS:CD2	2.56	0.41
2:H:373:ASN:HD22	2:H:373:ASN:HA	1.58	0.41
2:H:518:HIS:CD2	2:H:520:TYR:H	2.38	0.41
2:J:154:LEU:HD23	2:J:157:GLN:NE2	2.36	0.41
2:J:348:LYS:HE2	2:L:274:ASP:OD1	2.19	0.41
2:J:483:ALA:HB3	2:J:506:LYS:CE	2.49	0.41
1:K:112:ARG:HH11	1:K:112:ARG:HG3	1.85	0.41
1:K:298:LEU:HD23	1:K:298:LEU:O	2.19	0.41
1:K:349:ALA:HB3	1:K:381:ALA:CB	2.51	0.41
2:L:126:VAL:HG12	2:L:291:VAL:HG11	2.01	0.41
2:L:132:MET:CE	2:L:156:ALA:O	2.69	0.41
2:L:195:PHE:HB3	2:L:226:MET:CE	2.48	0.41
1:A:187:ASP:C	1:A:189:GLU:N	2.79	0.41
1:A:415:ARG:HB3	1:A:438:ILE:HG13	2.02	0.41
1:A:440:TRP:CG	1:A:441:GLY:N	2.86	0.41
1:A:589:ARG:HG2	1:A:590:LEU:N	2.35	0.41
1:A:653:MET:CG	1:A:654:ASN:N	2.80	0.41
2:B:525:ARG:HH11	2:B:525:ARG:HG3	1.86	0.41
2:B:536:GLN:O	2:B:539:GLU:HG2	2.20	0.41
1:C:79:HIS:CD2	1:C:80:SER:O	2.74	0.41
1:C:201:PRO:HB2	1:C:251:LEU:HD11	2.02	0.41
1:C:401:ARG:HH11	1:C:401:ARG:HG2	1.86	0.41
2:D:188:ARG:HA	2:J:456:ALA:HA	2.03	0.41
2:D:309:ALA:O	2:D:310:PRO:O	2.38	0.41
2:D:464:MET:O	2:D:531:VAL:HA	2.20	0.41
2:D:472:VAL:CG2	2:D:473:MET:HG2	2.43	0.41
1:E:63:ARG:HH22	1:E:356:VAL:HG23	1.85	0.41
1:E:298:LEU:HD21	1:E:325:LEU:HD11	2.01	0.41
1:E:514:GLU:OE1	1:E:568:HIS:CE1	2.74	0.41
2:F:201:MET:CE	2:F:208:GLN:HE22	2.32	0.41
1:G:351:THR:HA	1:G:376:PRO:HG2	2.02	0.41
1:G:445:GLU:OE2	1:G:448:ARG:NH2	2.53	0.41
1:G:553:LEU:HD12	1:G:566:LEU:HD12	2.02	0.41
2:H:95:SER:HB2	2:H:125:ARG:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:526:LEU:C	2:H:528:ASP:N	2.68	0.41
1:I:277:SER:O	1:I:279:GLN:N	2.54	0.41
1:I:412:PRO:HB2	1:I:450:ARG:HH11	1.85	0.41
2:J:219:GLY:C	2:J:221:ALA:N	2.78	0.41
1:K:340:LEU:HD12	1:K:359:GLN:OE1	2.20	0.41
2:L:45:ASN:HA	2:L:323:ALA:HB2	2.02	0.41
2:L:231:VAL:HG21	2:L:286:ILE:CG2	2.51	0.41
1:A:140:ARG:HD3	1:A:141:ALA:N	2.35	0.41
1:A:198:ILE:O	1:A:248:LYS:HE2	2.20	0.41
1:A:232:GLN:HE21	1:A:232:GLN:HB3	1.66	0.41
1:A:298:LEU:HA	1:A:298:LEU:HD12	1.64	0.41
1:A:323:PHE:HD1	1:A:332:PHE:C	2.29	0.41
1:A:393:GLY:O	1:A:396:LEU:CG	2.58	0.41
1:A:562:ARG:NH1	1:A:562:ARG:CG	2.82	0.41
1:A:566:LEU:O	1:A:567:ARG:HD3	2.20	0.41
1:A:678:GLU:O	1:A:678:GLU:CG	2.68	0.41
2:B:35:ILE:HD12	2:B:337:ARG:CZ	2.50	0.41
2:B:119:ILE:HG23	2:B:119:ILE:O	2.19	0.41
1:C:129:TYR:HE2	1:C:342:VAL:HA	1.80	0.41
1:C:602:VAL:O	1:C:603:ASP:HB2	2.21	0.41
2:D:175:GLY:HA3	4:D:591:COA:HN4	1.84	0.41
1:E:107:TYR:HB3	1:E:131:PHE:CD2	2.56	0.41
1:E:608:ARG:O	1:E:608:ARG:CG	2.68	0.41
2:F:40:ALA:O	2:F:41:GLU:C	2.64	0.41
2:F:265:VAL:O	2:F:269:VAL:HG23	2.20	0.41
2:F:479:ALA:HB1	2:F:506:LYS:HG3	2.01	0.41
1:G:59:GLU:HB3	1:G:418:SER:C	2.45	0.41
1:G:135:ASN:O	1:G:135:ASN:CG	2.62	0.41
1:G:482:ALA:C	1:G:484:LEU:H	2.28	0.41
1:G:520:GLU:O	1:G:522:GLY:N	2.54	0.41
2:H:31:LEU:HD12	2:H:336:ALA:HB2	2.03	0.41
2:H:36:ASN:ND2	2:H:36:ASN:C	2.77	0.41
1:I:67:SER:O	1:I:68:ALA:C	2.63	0.41
1:I:334:MET:O	1:I:335:GLU:HB3	2.20	0.41
1:I:359:GLN:O	1:I:362:VAL:HG23	2.20	0.41
2:J:258:GLU:O	2:J:258:GLU:HG3	2.20	0.41
1:K:85:HIS:HD1	1:K:86:ALA:N	2.18	0.41
1:K:325:LEU:HD23	1:K:326:ASP:N	2.36	0.41
1:K:386:LEU:HB3	1:K:435:ALA:H	1.85	0.41
1:K:558:ARG:NH2	1:K:625:GLU:OE1	2.54	0.41
1:A:53:LEU:HD11	1:A:78:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:MET:HG3	1:A:75:SER:HB2	2.01	0.41
1:A:138:PHE:CD1	1:A:142:CYS:HB2	2.55	0.41
1:A:229:SER:O	1:A:231:ALA:N	2.53	0.41
1:A:385:ARG:HB3	1:A:387:TYR:CE1	2.56	0.41
2:B:306:ALA:HA	2:B:307:PRO:HD3	1.86	0.41
2:B:338:LEU:O	2:B:538:ARG:NH1	2.47	0.41
1:C:109:ARG:NH1	1:C:111:ASP:OD2	2.54	0.41
1:C:152:PRO:HG3	1:C:315:TYR:CE1	2.56	0.41
1:C:166:ALA:C	1:C:168:ALA:N	2.77	0.41
1:C:384:VAL:HG11	1:C:470:LEU:HD22	2.02	0.41
2:D:351:PHE:CE1	2:F:271:GLY:HA3	2.56	0.41
2:D:442:GLY:O	2:D:468:ALA:HA	2.20	0.41
2:F:137:ASP:CB	2:F:140:VAL:HG23	2.32	0.41
2:F:277:ALA:HB2	2:F:286:ILE:HD12	2.02	0.41
2:F:365:TYR:HB2	2:F:545:LEU:HD13	2.02	0.41
2:F:400:PHE:CD2	2:F:453:CYS:HB3	2.56	0.41
2:F:543:LEU:HD23	2:F:543:LEU:HA	1.75	0.41
4:F:591:COA:H62A	4:F:591:COA:H62	1.86	0.41
1:G:284:LYS:NZ	1:G:322:GLU:OE2	2.52	0.41
1:G:539:ARG:HB2	1:G:541:ASP:OD2	2.21	0.41
2:H:49:MET:HG2	2:H:318:TYR:HA	2.03	0.41
1:I:370:LEU:HD22	1:I:374:GLN:HB3	2.03	0.41
1:I:404:LEU:O	1:I:460:VAL:HA	2.20	0.41
2:J:223:VAL:HG23	2:J:223:VAL:H	1.45	0.41
2:J:476:GLU:O	2:J:480:GLY:N	2.49	0.41
1:K:53:LEU:HD11	1:K:78:VAL:CG1	2.51	0.41
1:K:170:MET:HG3	1:K:333:PHE:CE2	2.56	0.41
1:K:358:TRP:HZ2	1:K:369:PRO:HG2	1.85	0.41
1:K:555:LEU:HD23	1:K:555:LEU:HA	1.91	0.41
2:L:393:GLN:O	2:L:393:GLN:HG2	2.20	0.41
1:A:170:MET:HG3	1:A:333:PHE:CE1	2.56	0.41
1:A:708:GLY:O	1:A:709:THR:O	2.39	0.41
2:B:193:ARG:NH1	2:L:458:ASP:OD1	2.43	0.41
2:B:244:PRO:N	2:B:245:PRO:CD	2.84	0.41
1:C:47:ARG:NE	1:C:148:LEU:CD2	2.83	0.41
1:C:47:ARG:HE	1:C:148:LEU:CD2	2.33	0.41
1:C:90:ALA:O	1:C:92:ALA:N	2.54	0.41
1:C:228:LEU:HD23	1:C:229:SER:H	1.81	0.41
1:C:389:GLU:HB3	1:C:390:ASP:H	1.50	0.41
1:C:620:LEU:HD12	1:C:620:LEU:C	2.45	0.41
2:D:36:ASN:OD1	2:D:39:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:LEU:HD12	2:D:280:ASP:HB3	2.02	0.41
2:D:508:PRO:O	2:D:511:GLU:HG3	2.21	0.41
1:E:56:ASN:OD1	1:E:57:ARG:N	2.44	0.41
1:E:107:TYR:HB2	1:E:131:PHE:CD2	2.55	0.41
1:E:348:GLU:HG2	1:E:355:LEU:HG	2.02	0.41
1:E:448:ARG:HD3	1:E:474:LEU:O	2.20	0.41
2:F:49:MET:HG2	2:F:318:TYR:HA	2.02	0.41
2:F:362:LEU:HB2	2:F:367:ILE:HD13	2.03	0.41
2:F:424:LYS:HE2	2:F:562:ARG:O	2.20	0.41
1:G:251:LEU:N	1:G:326:ASP:OD2	2.50	0.41
2:H:28:MET:HE2	1:I:633:ASP:C	2.46	0.41
2:H:247:VAL:HG11	2:H:255:VAL:HG12	2.03	0.41
2:H:311:LEU:C	2:H:312:TYR:CD1	2.99	0.41
1:I:262:ALA:O	1:I:316:VAL:O	2.38	0.41
1:I:308:ARG:NH1	1:I:308:ARG:CG	2.84	0.41
2:J:351:PHE:CE1	2:L:271:GLY:HA3	2.55	0.41
1:K:47:ARG:NE	1:K:148:LEU:HD21	2.35	0.41
1:K:136:ALA:O	1:K:140:ARG:HB2	2.21	0.41
1:K:302:MET:HA	1:K:305:ALA:HB3	2.01	0.41
2:L:376:LEU:HB2	2:L:404:ILE:HD11	2.02	0.41
2:L:507:ALA:HA	2:L:510:LEU:HD12	2.02	0.41
1:A:150:LEU:HD23	1:A:150:LEU:HA	1.67	0.41
1:A:226:GLU:C	1:A:228:LEU:N	2.77	0.41
1:A:354:ASP:O	1:A:357:ALA:HB3	2.21	0.41
1:A:408:ALA:HB2	1:A:457:GLU:HB2	2.02	0.41
1:A:508:PHE:O	1:A:511:ALA:N	2.53	0.41
1:A:533:PRO:C	1:A:535:SER:H	2.29	0.41
2:B:169:TYR:N	2:B:169:TYR:CD2	2.89	0.41
2:B:240:PHE:CD1	2:B:243:GLY:HA2	2.55	0.41
2:B:367:ILE:CG2	2:B:545:LEU:HD11	2.50	0.41
2:B:417:GLY:O	2:B:419:ALA:N	2.54	0.41
2:B:420:LYS:O	2:B:423:ALA:HB3	2.21	0.41
1:C:263:ASP:HA	1:C:362:VAL:CG1	2.51	0.41
1:C:337:ASN:HD22	1:C:341:GLN:HE21	1.68	0.41
1:C:469:PHE:O	1:C:472:ARG:HG3	2.21	0.41
1:C:525:ARG:HH11	1:C:525:ARG:CB	2.34	0.41
2:D:41:GLU:O	2:D:44:ALA:CB	2.60	0.41
2:D:434:VAL:HG23	2:D:435:PRO:CD	2.51	0.41
2:D:483:ALA:O	2:D:486:LYS:HB3	2.21	0.41
1:E:53:LEU:C	1:E:53:LEU:HD23	2.46	0.41
1:E:263:ASP:OD1	1:E:263:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:557:CYS:SG	1:E:627:LEU:HD23	2.61	0.41
1:E:601:ARG:HA	1:E:606:THR:HG23	2.02	0.41
2:F:106:HIS:H	2:F:524:ALA:HB1	1.86	0.41
2:F:195:PHE:O	2:F:196:PHE:C	2.61	0.41
2:F:216:CYS:CB	2:F:238:THR:O	2.68	0.41
2:F:247:VAL:HG12	2:F:247:VAL:O	2.20	0.41
2:F:317:LEU:O	2:F:318:TYR:C	2.64	0.41
2:F:350:LEU:HD23	2:F:350:LEU:H	1.86	0.41
2:F:400:PHE:CD2	2:F:453:CYS:CB	3.04	0.41
1:G:109:ARG:NH1	1:G:111:ASP:OD2	2.54	0.41
1:G:280:ARG:HD3	1:G:283:GLN:NE2	2.36	0.41
1:G:344:HIS:N	1:G:345:PRO:HD3	2.35	0.41
1:G:534:HIS:CD2	1:G:534:HIS:H	2.36	0.41
2:H:49:MET:HE3	2:H:321:ILE:CG2	2.51	0.41
2:H:49:MET:HE1	2:H:321:ILE:HG21	2.02	0.41
2:H:114:VAL:HG11	2:H:146:TYR:CE2	2.55	0.41
2:H:234:ARG:HD2	2:H:276:TYR:OH	2.21	0.41
2:H:326:LYS:HE3	1:I:681:LYS:HD3	2.02	0.41
2:H:400:PHE:HB2	2:H:438:THR:OG1	2.20	0.41
2:H:500:GLU:O	2:H:504:LYS:HG2	2.21	0.41
1:I:128:GLY:O	1:I:133:SER:HB3	2.21	0.41
1:I:258:ILE:HD12	1:I:302:MET:O	2.21	0.41
1:I:414:ARG:NH1	1:I:457:GLU:OE1	2.54	0.41
1:I:455:LEU:HB3	1:I:471:ARG:HD3	2.02	0.41
1:I:522:GLY:O	1:I:523:HIS:CB	2.64	0.41
2:J:92:ASP:O	2:J:93:PRO:C	2.63	0.41
2:J:186:PRO:O	2:J:187:ASP:O	2.38	0.41
2:J:220:GLY:C	2:J:223:VAL:HG23	2.46	0.41
2:J:537:THR:HG22	2:J:541:LEU:CD1	2.50	0.41
1:K:136:ALA:O	1:K:137:ASP:C	2.63	0.41
1:K:373:GLU:N	1:K:373:GLU:CD	2.79	0.41
1:K:380:HIS:CE1	1:K:444:ARG:HG3	2.56	0.41
1:K:504:LEU:CD2	1:K:505:PRO:HD2	2.45	0.41
1:K:537:TRP:CH2	2:L:123:ILE:HG22	2.56	0.41
1:K:543:TRP:C	1:K:544:ARG:HG2	2.45	0.41
2:L:49:MET:HG2	2:L:318:TYR:HA	2.03	0.41
2:L:102:ALA:C	2:L:104:ALA:N	2.76	0.41
2:L:209:ILE:O	2:L:209:ILE:HG22	2.18	0.41
2:L:324:ASP:HB3	2:L:327:GLN:HB2	2.03	0.41
1:A:71:LEU:HD21	1:A:364:ARG:HH22	1.85	0.41
1:A:182:HIS:HA	1:A:245:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:GLU:HG2	1:A:663:GLU:H	1.50	0.41
1:A:689:PRO:C	1:A:690:HIS:ND1	2.79	0.41
2:B:61:GLY:O	2:B:64:HIS:HB2	2.20	0.41
2:B:234:ARG:O	2:B:235:GLU:HB2	2.20	0.41
1:C:269:LEU:HD12	1:C:271:LEU:HD21	2.03	0.41
1:C:320:THR:CG2	1:C:341:GLN:HB2	2.50	0.41
1:C:473:ILE:HG21	1:C:473:ILE:HD13	1.86	0.41
1:C:516:TRP:CD2	1:C:613:ARG:NH2	2.87	0.41
1:C:534:HIS:O	1:C:535:SER:C	2.63	0.41
2:D:198:GLN:HG2	2:D:208:GLN:OE1	2.20	0.41
2:D:244:PRO:O	2:D:245:PRO:C	2.64	0.41
2:D:394:ARG:HB2	2:D:396:ILE:CD1	2.51	0.41
2:D:418:ILE:HG23	2:J:241:LEU:HD12	2.02	0.41
2:D:433:ARG:CG	2:D:433:ARG:NH1	2.82	0.41
1:E:57:ARG:HD2	1:E:107:TYR:CE2	2.56	0.41
1:E:132:LEU:HA	1:E:132:LEU:HD13	1.87	0.41
1:E:207:ALA:CB	1:E:243:ARG:NH1	2.83	0.41
1:E:470:LEU:O	1:E:471:ARG:C	2.64	0.41
1:E:622:TRP:HB3	1:E:627:LEU:HD13	2.03	0.41
2:F:212:VAL:CG2	2:F:232:MET:CG	2.99	0.41
2:F:479:ALA:HB1	2:F:506:LYS:HG2	2.02	0.41
1:G:165:ALA:O	1:G:169:LEU:CD1	2.67	0.41
1:G:178:VAL:HG23	1:G:332:PHE:HB3	2.02	0.41
1:G:501:GLN:O	1:G:501:GLN:HG3	2.20	0.41
1:G:536:PRO:CB	2:H:363:HIS:CE1	2.94	0.41
2:H:309:ALA:HB1	2:H:310:PRO:CD	2.50	0.41
2:H:322:PRO:CD	2:H:329:TYR:CD1	3.04	0.41
2:H:378:ALA:HB2	2:H:418:ILE:HD12	2.02	0.41
1:I:60:ILE:HD12	1:I:60:ILE:HA	1.77	0.41
2:J:334:VAL:HG12	2:J:338:LEU:HD11	2.02	0.41
2:J:516:GLN:HB3	2:J:521:TYR:CE2	2.56	0.41
1:K:503:ALA:O	1:K:504:LEU:C	2.63	0.41
1:K:544:ARG:HH21	2:L:88:ASN:ND2	2.19	0.41
1:K:555:LEU:HD22	1:K:629:ILE:HG22	2.02	0.41
1:K:569:ALA:O	1:K:571:PRO:HD3	2.21	0.41
2:L:132:MET:HE3	2:L:156:ALA:HB1	2.02	0.41
2:L:204:ARG:HE	2:L:204:ARG:HB2	1.17	0.41
4:L:591:COA:H62	4:L:591:COA:H62A	1.85	0.41
1:A:382:ILE:HG22	1:A:383:GLU:N	2.35	0.40
1:A:518:GLN:HB3	1:A:590:LEU:HD23	2.03	0.40
1:A:622:TRP:CD1	1:A:622:TRP:C	2.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:THR:O	1:A:668:VAL:O	2.39	0.40
1:A:695:LYS:HD3	1:A:715:ASP:HB2	2.03	0.40
2:B:321:ILE:O	2:B:321:ILE:HG22	2.21	0.40
2:D:212:VAL:HG23	2:D:231:VAL:O	2.22	0.40
1:E:520:GLU:C	1:E:522:GLY:N	2.79	0.40
1:E:615:GLY:C	1:E:617:GLN:H	2.27	0.40
2:F:163:ASN:OD1	2:F:460:ARG:HD2	2.21	0.40
2:F:545:LEU:HA	2:F:545:LEU:HD23	1.65	0.40
1:G:57:ARG:HG3	1:G:58:GLY:N	2.36	0.40
1:G:84:ARG:H	1:G:84:ARG:HG2	1.66	0.40
1:G:203:LEU:HD12	1:G:204:LEU:C	2.46	0.40
1:G:389:GLU:HG2	1:G:397:PRO:HG3	2.03	0.40
1:G:603:ASP:C	1:G:605:VAL:H	2.29	0.40
1:I:127:PRO:HG3	1:I:149:PHE:CE2	2.56	0.40
1:I:385:ARG:HD3	1:I:387:TYR:HE1	1.86	0.40
1:I:452:LEU:O	1:I:452:LEU:CD1	2.65	0.40
1:I:469:PHE:CD2	1:I:470:LEU:N	2.90	0.40
3:I:801:BTI:HN2	3:I:801:BTI:H72	1.60	0.40
2:J:100:LEU:HD11	2:J:132:MET:HE1	2.03	0.40
2:J:222:TYR:HA	2:J:225:ALA:HB3	2.03	0.40
2:L:112:GLU:H	2:L:112:GLU:HG2	1.55	0.40
2:L:157:GLN:NE2	2:L:197:ASN:HB2	2.36	0.40
2:L:192:GLY:HA2	2:L:195:PHE:HD2	1.83	0.40
2:L:215:SER:HA	2:L:238:THR:HG1	1.85	0.40
2:L:420:LYS:HE3	2:L:563:MET:O	2.21	0.40
1:A:49:ILE:HD11	1:A:148:LEU:CD1	2.51	0.40
1:A:57:ARG:HH11	1:A:57:ARG:HG3	1.86	0.40
1:A:323:PHE:CD1	1:A:333:PHE:HA	2.56	0.40
1:A:398:ALA:HB3	1:A:464:ARG:HB2	2.03	0.40
1:A:489:ILE:HD12	1:A:489:ILE:HA	1.70	0.40
2:B:186:PRO:HG3	2:L:527:TRP:CZ2	2.57	0.40
2:B:331:VAL:HG12	2:B:373:ASN:ND2	2.36	0.40
1:C:613:ARG:HG2	1:C:614:ARG:H	1.85	0.40
2:D:191:PHE:HD2	2:D:192:GLY:H	1.69	0.40
2:D:240:PHE:CE1	2:D:243:GLY:CA	3.04	0.40
2:D:423:ALA:HB1	2:J:226:MET:HG3	2.02	0.40
2:D:476:GLU:OE2	2:D:477:GLN:HB2	2.21	0.40
1:E:387:TYR:C	1:E:389:GLU:H	2.29	0.40
2:F:408:MET:CG	2:F:413:TYR:CE2	3.04	0.40
2:F:481:VAL:HG13	2:H:245:PRO:HB3	2.02	0.40
2:F:482:LEU:HD21	2:H:179:PRO:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:327:GLU:O	1:G:329:GLY:N	2.55	0.40
1:G:371:THR:HG1	1:G:374:GLN:HG3	1.84	0.40
1:G:615:GLY:C	1:G:617:GLN:H	2.30	0.40
2:H:164:ARG:C	2:H:165:LEU:HD23	2.47	0.40
2:H:312:TYR:O	2:H:313:PRO:C	2.63	0.40
2:H:486:LYS:HD2	2:H:489:GLN:NE2	2.35	0.40
1:I:169:LEU:HD22	1:I:313:ILE:CG2	2.48	0.40
1:I:537:TRP:HB3	2:J:125:ARG:HG2	2.01	0.40
2:J:465:TRP:HB3	2:J:467:ASN:HD21	1.87	0.40
1:K:112:ARG:HG3	1:K:112:ARG:NH1	2.36	0.40
1:K:170:MET:SD	1:K:309:ALA:CB	3.04	0.40
1:K:508:PHE:O	1:K:510:GLN:N	2.54	0.40
2:L:164:ARG:O	2:L:164:ARG:CG	2.67	0.40
2:L:213:MET:HE1	2:L:284:LEU:HG	2.02	0.40
2:L:247:VAL:O	2:L:247:VAL:HG12	2.19	0.40
1:A:109:ARG:CZ	1:A:112:ARG:HH22	2.34	0.40
1:A:271:LEU:CD1	1:A:355:LEU:HD21	2.51	0.40
1:A:384:VAL:HG13	1:A:470:LEU:HD22	2.03	0.40
2:B:467:ASN:H	2:B:467:ASN:ND2	1.96	0.40
1:C:190:THR:HG23	1:C:193:ARG:NH1	2.36	0.40
1:C:320:THR:HG21	1:C:341:GLN:CG	2.51	0.40
1:C:333:PHE:CZ	1:C:335:GLU:HA	2.55	0.40
2:D:170:LEU:HD23	2:D:211:VAL:HG23	2.02	0.40
1:E:150:LEU:HD21	1:E:359:GLN:O	2.21	0.40
1:E:186:GLN:HB3	1:E:190:THR:HB	2.02	0.40
1:E:607:ARG:HH11	1:E:607:ARG:CG	2.35	0.40
2:F:450:TYR:CE1	2:H:192:GLY:HA3	2.55	0.40
1:G:83:ASP:O	1:G:89:VAL:HG21	2.22	0.40
1:G:359:GLN:O	1:G:362:VAL:HG22	2.21	0.40
1:G:411:GLY:O	1:G:412:PRO:C	2.63	0.40
2:H:405:THR:HG23	1:I:681:LYS:HG2	2.03	0.40
2:H:479:ALA:O	2:H:506:LYS:HG2	2.21	0.40
1:I:256:VAL:O	1:I:323:PHE:HB2	2.21	0.40
2:J:27:HIS:CB	1:K:616:ARG:NH2	2.85	0.40
2:J:473:MET:CE	2:J:477:GLN:HB3	2.43	0.40
1:K:274:ARG:NH2	1:K:320:THR:HG21	2.37	0.40
1:K:532:ASP:O	1:K:535:SER:HB2	2.21	0.40
2:L:106:HIS:O	2:L:107:GLU:HB2	2.22	0.40
2:L:222:TYR:HE2	2:L:241:LEU:HD21	1.86	0.40
2:L:362:LEU:HD23	2:L:362:LEU:C	2.47	0.40
1:A:112:ARG:NH1	1:A:112:ARG:HG3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ARG:CB	1:A:454:MET:SD	3.09	0.40
1:A:531:ASP:HB3	2:B:298:LYS:HB2	2.02	0.40
1:A:682:MET:SD	2:F:405:THR:HG21	2.62	0.40
2:B:241:LEU:HA	2:B:241:LEU:HD23	1.67	0.40
2:B:242:ALA:CB	2:L:409:VAL:HG11	2.52	0.40
2:B:457:TYR:N	2:B:457:TYR:HD2	2.19	0.40
4:B:591:COA:OAP	2:L:485:VAL:HG11	2.21	0.40
1:C:179:PRO:HB2	1:C:198:ILE:HG12	2.03	0.40
1:C:340:LEU:HD21	1:C:344:HIS:CG	2.57	0.40
2:D:165:LEU:HD21	2:D:547:ALA:O	2.21	0.40
2:D:394:ARG:HB2	2:D:396:ILE:HD12	2.04	0.40
1:E:309:ALA:O	1:E:312:ALA:HB3	2.20	0.40
1:E:340:LEU:HG	1:E:359:GLN:HE22	1.84	0.40
2:F:161:LEU:CD2	2:F:201:MET:HG2	2.43	0.40
1:G:518:GLN:HB3	1:G:590:LEU:HD23	2.03	0.40
2:H:101:SER:O	2:H:152:LYS:HE3	2.22	0.40
2:H:112:GLU:H	2:H:112:GLU:CD	2.30	0.40
2:H:164:ARG:NH1	2:H:296:TRP:CZ2	2.90	0.40
2:H:331:VAL:HG21	2:H:371:ALA:HB1	2.03	0.40
2:H:491:GLU:HA	2:H:495:GLN:O	2.21	0.40
1:I:374:GLN:O	1:I:376:PRO:CD	2.68	0.40
1:K:373:GLU:CD	1:K:373:GLU:H	2.29	0.40
2:L:68:GLY:C	2:L:70:ALA:H	2.30	0.40
2:L:305:ARG:HB3	2:L:305:ARG:HH11	1.85	0.40
2:L:376:LEU:HD12	2:L:404:ILE:CD1	2.52	0.40
2:L:507:ALA:N	2:L:508:PRO:HD2	2.36	0.40
1:A:187:ASP:O	1:A:189:GLU:N	2.55	0.40
1:A:248:LYS:NZ	1:A:328:ARG:HH12	2.20	0.40
1:A:299:ARG:O	1:A:300:ARG:C	2.64	0.40
1:A:562:ARG:CB	1:A:562:ARG:NH1	2.74	0.40
1:A:672:ALA:O	1:A:674:LEU:N	2.54	0.40
2:B:247:VAL:O	2:B:250:ALA:HB3	2.21	0.40
2:B:320:VAL:O	2:B:322:PRO:HD3	2.22	0.40
2:B:541:LEU:HD23	2:B:541:LEU:HA	1.80	0.40
1:C:519:SER:HB2	1:C:613:ARG:HE	1.86	0.40
2:D:89:ARG:NH2	2:D:89:ARG:CG	2.82	0.40
1:E:255:HIS:ND1	1:E:255:HIS:C	2.79	0.40
1:E:259:GLN:C	1:E:260:VAL:CG2	2.93	0.40
1:E:279:GLN:HB2	1:E:283:GLN:O	2.21	0.40
1:E:384:VAL:CG1	1:E:470:LEU:CD2	2.91	0.40
1:E:516:TRP:CE3	1:E:555:LEU:HD21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:544:ARG:HG3	1:E:550:GLU:OE1	2.21	0.40
2:F:85:GLU:O	2:F:86:ARG:C	2.64	0.40
2:F:119:ILE:HG22	2:F:149:THR:CG2	2.51	0.40
2:F:484:GLN:NE2	2:F:487:ARG:HH12	2.19	0.40
2:F:508:PRO:HG2	2:F:509:ILE:H	1.85	0.40
1:G:114:ILE:HD11	1:G:147:LEU:CD1	2.51	0.40
1:G:182:HIS:CB	1:G:245:LEU:CD2	2.93	0.40
1:G:199:GLY:O	1:G:201:PRO:CD	2.69	0.40
1:G:386:LEU:HD11	1:G:465:THR:CG2	2.52	0.40
1:G:387:TYR:N	1:G:466:ASN:OD1	2.54	0.40
2:H:338:LEU:HD21	2:H:537:THR:HB	2.04	0.40
2:H:446:GLY:O	2:H:447:ALA:C	2.64	0.40
1:I:543:TRP:O	1:I:544:ARG:NH1	2.55	0.40
2:J:424:LYS:H	2:J:424:LYS:HG3	1.64	0.40
1:K:47:ARG:HB2	1:K:47:ARG:CZ	2.47	0.40
1:K:85:HIS:ND1	1:K:86:ALA:N	2.70	0.40
1:K:282:HIS:O	1:K:283:GLN:HB2	2.22	0.40
1:K:298:LEU:O	1:K:301:ALA:HB3	2.22	0.40
1:K:340:LEU:HD12	1:K:359:GLN:HE22	1.86	0.40
1:K:405:TYR:HB3	1:K:422:GLU:CB	2.42	0.40
2:L:146:TYR:O	2:L:147:PRO:C	2.64	0.40
2:L:247:VAL:O	2:L:247:VAL:CG1	2.69	0.40
2:L:382:GLN:HE21	2:L:382:GLN:HB2	1.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	613/655 (94%)	427 (70%)	114 (19%)	72 (12%)	0 4
1	C	546/655 (83%)	382 (70%)	113 (21%)	51 (9%)	0 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	546/655 (83%)	384 (70%)	109 (20%)	53 (10%)	0	6
1	G	546/655 (83%)	381 (70%)	113 (21%)	52 (10%)	0	6
1	I	493/655 (75%)	353 (72%)	101 (20%)	39 (8%)	1	8
1	K	493/655 (75%)	364 (74%)	88 (18%)	41 (8%)	0	7
2	B	535/555 (96%)	448 (84%)	63 (12%)	24 (4%)	2	17
2	D	535/555 (96%)	456 (85%)	62 (12%)	17 (3%)	3	24
2	F	535/555 (96%)	439 (82%)	73 (14%)	23 (4%)	2	18
2	H	535/555 (96%)	450 (84%)	60 (11%)	25 (5%)	2	17
2	J	535/555 (96%)	452 (84%)	65 (12%)	18 (3%)	3	23
2	L	535/555 (96%)	438 (82%)	76 (14%)	21 (4%)	2	20
All	All	6447/7260 (89%)	4974 (77%)	1037 (16%)	436 (7%)	1	10

All (436) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	225	ALA
1	A	230	SER
1	A	294	LEU
1	A	366	GLU
1	A	377	LEU
1	A	397	PRO
1	A	412	PRO
1	A	498	PRO
1	A	504	LEU
1	A	505	PRO
1	A	586	SER
1	A	587	GLN
1	A	661	LEU
1	A	666	GLN
1	A	668	VAL
1	A	696	ALA
1	A	701	GLU
1	A	703	GLU
1	A	705	VAL
1	A	714	LEU
2	B	70	ALA
2	B	186	PRO

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Mol	Chain	Res	Type
2	B	187	ASP
2	B	375	ILE
2	B	376	LEU
2	B	474	GLY
1	C	186	GLN
1	C	225	ALA
1	C	292	PRO
1	C	294	LEU
1	C	366	GLU
1	C	377	LEU
1	C	397	PRO
1	C	412	PRO
1	C	501	GLN
1	C	504	LEU
1	C	505	PRO
1	C	523	HIS
2	D	70	ALA
2	D	186	PRO
2	D	187	ASP
2	D	310	PRO
1	E	86	ALA
1	E	186	GLN
1	E	225	ALA
1	E	278	ILE
1	E	294	LEU
1	E	366	GLU
1	E	397	PRO
1	E	412	PRO
1	E	501	GLN
1	E	504	LEU
1	E	505	PRO
2	F	70	ALA
2	F	186	PRO
2	F	187	ASP
2	F	375	ILE
1	G	186	GLN
1	G	188	LEU
1	G	200	TYR
1	G	225	ALA
1	G	294	LEU
1	G	366	GLU
1	G	397	PRO

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Mol	Chain	Res	Type
1	G	412	PRO
1	G	504	LEU
1	G	505	PRO
1	G	586	SER
1	G	587	GLN
2	H	177	ASN
2	H	186	PRO
2	H	187	ASP
2	H	218	ALA
2	H	310	PRO
2	H	375	ILE
2	H	499	VAL
1	I	278	ILE
1	I	292	PRO
1	I	366	GLU
1	I	397	PRO
1	I	412	PRO
1	I	504	LEU
1	I	505	PRO
1	I	523	HIS
1	I	586	SER
2	J	70	ALA
2	J	177	ASN
2	J	186	PRO
2	J	187	ASP
2	J	253	GLU
2	J	499	VAL
1	K	59	GLU
1	K	366	GLU
1	K	412	PRO
1	K	501	GLN
1	K	504	LEU
1	K	505	PRO
1	K	586	SER
2	L	70	ALA
2	L	177	ASN
2	L	186	PRO
2	L	187	ASP
2	L	375	ILE
1	A	82	ILE
1	A	86	ALA
1	A	150	LEU

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Mol	Chain	Res	Type
1	A	188	LEU
1	A	198	ILE
1	A	268	CYS
1	A	281	ARG
1	A	283	GLN
1	A	293	GLY
1	A	317	GLY
1	A	482	ALA
1	A	509	TRP
1	A	650	SER
1	A	680	MET
1	A	687	ARG
2	B	69	SER
2	B	174	GLY
2	B	177	ASN
2	B	191	PHE
2	B	253	GLU
2	B	499	VAL
1	C	59	GLU
1	C	105	ASP
1	C	135	ASN
1	C	188	LEU
1	C	198	ILE
1	C	230	SER
1	C	278	ILE
1	C	281	ARG
1	C	283	GLN
1	C	293	GLY
1	C	317	GLY
1	C	328	ARG
1	C	393	GLY
1	C	402	LEU
1	C	509	TRP
1	C	571	PRO
1	C	586	SER
1	C	587	GLN
2	D	69	SER
2	D	101	SER
2	D	177	ASN
2	D	301	GLN
2	D	375	ILE
2	D	499	VAL

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Mol	Chain	Res	Type
1	E	59	GLU
1	E	131	PHE
1	E	135	ASN
1	E	188	LEU
1	E	198	ILE
1	E	230	SER
1	E	293	GLY
1	E	299	ARG
1	E	300	ARG
1	E	328	ARG
1	E	391	PRO
1	E	521	PRO
1	E	523	HIS
1	E	539	ARG
1	E	586	SER
1	E	587	GLN
1	E	602	VAL
2	F	253	GLU
2	F	301	GLN
2	F	499	VAL
1	G	82	ILE
1	G	99	GLY
1	G	135	ASN
1	G	150	LEU
1	G	282	HIS
1	G	283	GLN
1	G	293	GLY
1	G	317	GLY
1	G	328	ARG
1	G	501	GLN
1	G	571	PRO
2	H	47	ALA
2	H	69	SER
2	H	70	ALA
2	H	101	SER
2	H	236	GLN
2	H	253	GLU
2	H	301	GLN
2	H	376	LEU
2	H	474	GLY
1	I	59	GLU
1	I	107	TYR

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Mol	Chain	Res	Type
1	I	282	HIS
1	I	283	GLN
1	I	293	GLY
1	I	294	LEU
1	I	501	GLN
1	I	587	GLN
2	J	69	SER
2	J	101	SER
2	J	375	ILE
2	J	376	LEU
1	K	135	ASN
1	K	278	ILE
1	K	281	ARG
1	K	283	GLN
1	K	293	GLY
1	K	294	LEU
1	K	317	GLY
1	K	397	PRO
1	K	491	ARG
1	K	523	HIS
1	K	587	GLN
1	K	602	VAL
2	L	101	SER
2	L	474	GLY
2	L	499	VAL
1	A	59	GLU
1	A	135	ASN
1	A	292	PRO
1	A	300	ARG
1	A	398	ALA
1	A	402	LEU
1	A	483	GLU
1	A	491	ARG
1	A	501	GLN
1	A	503	ALA
1	A	623	GLU
1	A	673	THR
1	A	681	LYS
2	B	236	GLN
1	C	91	GLU
1	C	155	ALA
1	C	282	HIS

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Mol	Chain	Res	Type
1	C	300	ARG
1	C	391	PRO
1	C	498	PRO
1	C	508	PHE
1	C	521	PRO
1	C	602	VAL
2	D	207	PRO
2	D	253	GLU
1	E	281	ARG
1	E	283	GLN
1	E	292	PRO
1	E	377	LEU
1	E	393	GLY
1	E	422	GLU
1	E	500	PRO
1	E	503	ALA
1	E	534	HIS
1	E	603	ASP
2	F	69	SER
2	F	177	ASN
2	F	191	PHE
2	F	218	ALA
2	F	236	GLN
1	G	59	GLU
1	G	131	PHE
1	G	268	CYS
1	G	292	PRO
1	G	296	ALA
1	G	377	LEU
1	G	391	PRO
1	G	398	ALA
1	G	521	PRO
2	H	115	ALA
1	I	82	ILE
1	I	86	ALA
1	I	135	ASN
1	I	300	ARG
1	I	377	LEU
1	I	393	GLY
1	I	482	ALA
1	I	491	ARG
1	I	498	PRO

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Mol	Chain	Res	Type
1	I	571	PRO
2	J	301	GLN
1	K	292	PRO
1	K	498	PRO
1	K	521	PRO
1	K	603	ASP
2	L	69	SER
2	L	141	LYS
2	L	174	GLY
2	L	236	GLN
2	L	253	GLU
1	A	98	LEU
1	A	131	PHE
1	A	389	GLU
1	A	508	PHE
1	A	523	HIS
1	A	571	PRO
2	B	76	SER
2	B	141	LYS
2	B	251	THR
2	B	403	ASN
1	C	104	ALA
1	C	131	PHE
1	C	389	GLU
1	C	500	PRO
2	D	47	ALA
1	E	99	GLY
1	E	268	CYS
1	E	282	HIS
1	E	571	PRO
1	E	623	GLU
2	F	101	SER
2	F	141	LYS
1	G	86	ALA
1	G	160	MET
1	G	171	GLU
1	G	198	ILE
1	G	389	GLU
1	G	463	LEU
1	G	482	ALA
1	G	491	ARG
2	H	39	SER

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Mol	Chain	Res	Type
2	H	207	PRO
2	H	537	THR
1	I	255	HIS
1	I	391	PRO
1	I	503	ALA
1	I	509	TRP
2	J	207	PRO
2	J	236	GLN
1	K	150	LEU
1	K	155	ALA
1	K	282	HIS
1	K	301	ALA
1	K	482	ALA
1	K	500	PRO
1	K	509	TRP
1	K	571	PRO
1	A	272	ASN
1	A	282	HIS
1	A	299	ARG
1	A	328	ARG
1	A	391	PRO
1	A	393	GLY
2	B	83	VAL
2	B	93	PRO
2	B	185	PHE
2	B	325	SER
1	C	137	ASP
1	C	223	GLU
1	C	268	CYS
1	C	422	GLU
1	C	491	ARG
2	D	27	HIS
2	D	39	SER
2	D	174	GLY
2	D	236	GLN
1	E	150	LEU
1	E	349	ALA
1	E	389	GLU
1	E	498	PRO
1	E	509	TRP
2	F	93	PRO
2	F	228	ASP

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Mol	Chain	Res	Type
1	G	248	LYS
1	G	281	ARG
1	G	432	PRO
1	G	483	GLU
1	G	498	PRO
1	G	523	HIS
2	H	174	GLY
2	H	185	PHE
2	H	245	PRO
1	I	105	ASP
1	I	154	ALA
1	I	296	ALA
2	J	103	LEU
1	K	131	PHE
1	K	391	PRO
1	K	503	ALA
2	L	185	PHE
2	L	218	ALA
2	L	376	LEU
1	A	492	HIS
1	A	521	PRO
1	A	625	GLU
2	B	101	SER
2	B	115	ALA
1	C	58	GLY
1	C	99	GLY
1	C	109	ARG
1	E	482	ALA
2	F	112	GLU
2	F	245	PRO
2	F	300	GLY
1	G	58	GLY
1	I	428	PRO
1	I	500	PRO
1	I	521	PRO
2	J	174	GLY
2	J	310	PRO
1	K	105	ASP
1	K	377	LEU
1	A	278	ILE
1	A	428	PRO
1	A	500	PRO

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Mol	Chain	Res	Type
1	A	709	THR
1	E	82	ILE
1	E	317	GLY
1	E	432	PRO
2	F	220	GLY
2	J	474	GLY
2	L	93	PRO
2	L	207	PRO
1	A	200	TYR
2	B	310	PRO
2	F	174	GLY
1	G	393	GLY
1	I	390	ASP
1	K	82	ILE
1	K	428	PRO
1	A	376	PRO
1	A	432	PRO
1	E	379	GLY
2	F	185	PHE
2	F	219	GLY
1	G	278	ILE
1	G	307	VAL
1	G	500	PRO
1	I	432	PRO
2	J	185	PHE
1	K	58	GLY
1	K	390	ASP
1	K	393	GLY
2	L	245	PRO
1	G	352	GLY
2	H	534	PRO
2	H	552	PRO
2	L	178	LEU
1	A	352	GLY
2	L	310	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	477/496 (96%)	380 (80%)	97 (20%)	1	7
1	C	423/496 (85%)	330 (78%)	93 (22%)	1	5
1	E	423/496 (85%)	327 (77%)	96 (23%)	1	5
1	G	423/496 (85%)	325 (77%)	98 (23%)	1	5
1	I	382/496 (77%)	306 (80%)	76 (20%)	1	7
1	K	381/496 (77%)	296 (78%)	85 (22%)	1	5
2	B	401/418 (96%)	338 (84%)	63 (16%)	2	15
2	D	401/418 (96%)	323 (80%)	78 (20%)	1	8
2	F	401/418 (96%)	330 (82%)	71 (18%)	2	10
2	H	401/418 (96%)	329 (82%)	72 (18%)	2	10
2	J	401/418 (96%)	345 (86%)	56 (14%)	3	19
2	L	401/418 (96%)	329 (82%)	72 (18%)	2	10
All	All	4915/5484 (90%)	3958 (80%)	957 (20%)	1	8

All (957) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	50	GLN
1	A	65	MET
1	A	75	SER
1	A	80	SER
1	A	85	HIS
1	A	89	VAL
1	A	96	VAL
1	A	105	ASP
1	A	118	LEU
1	A	123	GLN
1	A	132	LEU
1	A	137	ASP
1	A	143	GLU
1	A	144	GLU
1	A	148	LEU
1	A	163	LYS
1	A	171	GLU
1	A	186	GLN
1	A	192	ARG

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Mol	Chain	Res	Type
1	A	197	ARG
1	A	198	ILE
1	A	200	TYR
1	A	201	PRO
1	A	202	VAL
1	A	203	LEU
1	A	215	MET
1	A	216	LYS
1	A	217	VAL
1	A	221	GLU
1	A	226	GLU
1	A	232	GLN
1	A	233	ARG
1	A	255	HIS
1	A	260	VAL
1	A	261	PHE
1	A	269	LEU
1	A	276	CYS
1	A	278	ILE
1	A	286	VAL
1	A	292	PRO
1	A	311	GLN
1	A	316	VAL
1	A	327	GLU
1	A	328	ARG
1	A	336	MET
1	A	340	LEU
1	A	341	GLN
1	A	346	VAL
1	A	355	LEU
1	A	371	THR
1	A	386	LEU
1	A	412	PRO
1	A	420	VAL
1	A	421	ARG
1	A	431	ASP
1	A	438	ILE
1	A	440	TRP
1	A	443	THR
1	A	446	GLU
1	A	452	LEU
1	A	460	VAL

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Mol	Chain	Res	Type
1	A	463	LEU
1	A	465	THR
1	A	469	PHE
1	A	471	ARG
1	A	492	HIS
1	A	505	PRO
1	A	518	GLN
1	A	519	SER
1	A	525	ARG
1	A	526	ASP
1	A	540	ASN
1	A	544	ARG
1	A	550	GLU
1	A	562	ARG
1	A	565	ARG
1	A	567	ARG
1	A	586	SER
1	A	597	ASP
1	A	602	VAL
1	A	606	THR
1	A	612	LEU
1	A	614	ARG
1	A	616	ARG
1	A	621	GLU
1	A	629	ILE
1	A	654	ASN
1	A	667	THR
1	A	668	VAL
1	A	677	LEU
1	A	682	MET
1	A	686	ILE
1	A	687	ARG
1	A	697	LEU
1	A	698	TYR
1	A	704	LEU
2	B	28	MET
2	B	33	THR
2	B	34	GLN
2	B	35	ILE
2	B	36	ASN
2	B	62	ARG
2	B	63	ILE

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Mol	Chain	Res	Type
2	B	64	HIS
2	B	69	SER
2	B	81	LEU
2	B	85	GLU
2	B	89	ARG
2	B	93	PRO
2	B	98	LEU
2	B	99	GLU
2	B	112	GLU
2	B	114	VAL
2	B	120	VAL
2	B	139	THR
2	B	140	VAL
2	B	147	PRO
2	B	149	THR
2	B	151	LYS
2	B	161	LEU
2	B	162	GLU
2	B	189	GLU
2	B	227	SER
2	B	230	THR
2	B	231	VAL
2	B	247	VAL
2	B	256	SER
2	B	268	LYS
2	B	281	ASP
2	B	308	ARG
2	B	312	TYR
2	B	327	GLN
2	B	331	VAL
2	B	350	LEU
2	B	353	THR
2	B	354	THR
2	B	362	LEU
2	B	370	LEU
2	B	373	ASN
2	B	392	CYS
2	B	393	GLN
2	B	409	VAL
2	B	429	VAL
2	B	466	PRO
2	B	467	ASN

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Mol	Chain	Res	Type
2	B	473	MET
2	B	476	GLU
2	B	481	VAL
2	B	484	GLN
2	B	487	ARG
2	B	491	GLU
2	B	497	LEU
2	B	499	VAL
2	B	502	GLU
2	B	510	LEU
2	B	511	GLU
2	B	537	THR
2	B	545	LEU
2	B	553	ILE
1	C	47	ARG
1	C	49	ILE
1	C	50	GLN
1	C	65	MET
1	C	66	ARG
1	C	71	LEU
1	C	84	ARG
1	C	85	HIS
1	C	89	VAL
1	C	105	ASP
1	C	111	ASP
1	C	113	ILE
1	C	118	LEU
1	C	123	GLN
1	C	129	TYR
1	C	132	LEU
1	C	135	ASN
1	C	143	GLU
1	C	148	LEU
1	C	171	GLU
1	C	175	VAL
1	C	192	ARG
1	C	197	ARG
1	C	198	ILE
1	C	200	TYR
1	C	217	VAL
1	C	220	ARG
1	C	221	GLU

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Mol	Chain	Res	Type
1	C	223	GLU
1	C	226	GLU
1	C	232	GLN
1	C	233	ARG
1	C	243	ARG
1	C	251	LEU
1	C	269	LEU
1	C	278	ILE
1	C	279	GLN
1	C	280	ARG
1	C	285	VAL
1	C	292	PRO
1	C	300	ARG
1	C	307	VAL
1	C	311	GLN
1	C	313	ILE
1	C	328	ARG
1	C	336	MET
1	C	341	GLN
1	C	353	LEU
1	C	362	VAL
1	C	370	LEU
1	C	397	PRO
1	C	412	PRO
1	C	414	ARG
1	C	420	VAL
1	C	421	ARG
1	C	424	ASP
1	C	438	ILE
1	C	440	TRP
1	C	443	THR
1	C	445	GLU
1	C	446	GLU
1	C	449	GLN
1	C	452	LEU
1	C	455	LEU
1	C	460	VAL
1	C	471	ARG
1	C	472	ARG
1	C	486	THR
1	C	493	GLN
1	C	495	ASP

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Mol	Chain	Res	Type
1	C	498	PRO
1	C	505	PRO
1	C	525	ARG
1	C	526	ASP
1	C	547	LEU
1	C	549	ARG
1	C	562	ARG
1	C	564	VAL
1	C	565	ARG
1	C	571	PRO
1	C	586	SER
1	C	590	LEU
1	C	597	ASP
1	C	598	LEU
1	C	600	SER
1	C	605	VAL
1	C	606	THR
1	C	607	ARG
1	C	612	LEU
1	C	616	ARG
1	C	618	LEU
1	C	620	LEU
1	C	621	GLU
2	D	41	GLU
2	D	50	LEU
2	D	57	ARG
2	D	65	GLU
2	D	74	ARG
2	D	78	ARG
2	D	81	LEU
2	D	85	GLU
2	D	89	ARG
2	D	98	LEU
2	D	100	LEU
2	D	129	VAL
2	D	136	ASN
2	D	147	PRO
2	D	157	GLN
2	D	168	ILE
2	D	178	LEU
2	D	179	PRO
2	D	180	ARG

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Mol	Chain	Res	Type
2	D	188	ARG
2	D	189	GLU
2	D	197	ASN
2	D	198	GLN
2	D	201	MET
2	D	207	PRO
2	D	211	VAL
2	D	212	VAL
2	D	213	MET
2	D	230	THR
2	D	235	GLU
2	D	245	PRO
2	D	247	VAL
2	D	248	LYS
2	D	260	LEU
2	D	270	SER
2	D	281	ASP
2	D	293	ASN
2	D	294	LEU
2	D	297	ARG
2	D	304	CYS
2	D	326	LYS
2	D	327	GLN
2	D	334	VAL
2	D	339	VAL
2	D	345	ASP
2	D	350	LEU
2	D	351	PHE
2	D	353	THR
2	D	354	THR
2	D	357	CYS
2	D	370	LEU
2	D	373	ASN
2	D	376	LEU
2	D	379	GLU
2	D	398	LEU
2	D	402	GLN
2	D	405	THR
2	D	434	VAL
2	D	438	THR
2	D	441	ILE
2	D	453	CYS

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Mol	Chain	Res	Type
2	D	464	MET
2	D	472	VAL
2	D	473	MET
2	D	476	GLU
2	D	481	VAL
2	D	484	GLN
2	D	486	LYS
2	D	488	GLU
2	D	489	GLN
2	D	505	ILE
2	D	511	GLU
2	D	512	GLN
2	D	519	PRO
2	D	520	TYR
2	D	525	ARG
2	D	532	ILE
2	D	534	PRO
1	E	49	ILE
1	E	52	LEU
1	E	60	ILE
1	E	66	ARG
1	E	78	VAL
1	E	84	ARG
1	E	85	HIS
1	E	96	VAL
1	E	105	ASP
1	E	111	ASP
1	E	112	ARG
1	E	123	GLN
1	E	129	TYR
1	E	148	LEU
1	E	169	LEU
1	E	177	LEU
1	E	178	VAL
1	E	184	GLU
1	E	186	GLN
1	E	189	GLU
1	E	193	ARG
1	E	197	ARG
1	E	198	ILE
1	E	200	TYR
1	E	205	LYS

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Mol	Chain	Res	Type
1	E	217	VAL
1	E	221	GLU
1	E	233	ARG
1	E	243	ARG
1	E	251	LEU
1	E	261	PHE
1	E	269	LEU
1	E	278	ILE
1	E	285	VAL
1	E	288	GLU
1	E	292	PRO
1	E	300	ARG
1	E	308	ARG
1	E	311	GLN
1	E	326	ASP
1	E	328	ARG
1	E	335	GLU
1	E	340	LEU
1	E	341	GLN
1	E	342	VAL
1	E	345	PRO
1	E	347	THR
1	E	362	VAL
1	E	371	THR
1	E	376	PRO
1	E	378	ASN
1	E	386	LEU
1	E	392	GLU
1	E	397	PRO
1	E	406	ARG
1	E	412	PRO
1	E	418	SER
1	E	421	ARG
1	E	429	PHE
1	E	440	TRP
1	E	443	THR
1	E	452	LEU
1	E	459	SER
1	E	460	VAL
1	E	463	LEU
1	E	467	LEU
1	E	473	ILE

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Mol	Chain	Res	Type
1	E	505	PRO
1	E	510	GLN
1	E	519	SER
1	E	520	GLU
1	E	525	ARG
1	E	526	ASP
1	E	541	ASP
1	E	547	LEU
1	E	549	ARG
1	E	550	GLU
1	E	554	MET
1	E	556	ARG
1	E	560	GLU
1	E	561	ARG
1	E	562	ARG
1	E	564	VAL
1	E	568	HIS
1	E	571	PRO
1	E	589	ARG
1	E	591	ASP
1	E	601	ARG
1	E	605	VAL
1	E	606	THR
1	E	612	LEU
1	E	616	ARG
1	E	617	GLN
1	E	618	LEU
1	E	621	GLU
1	E	623	GLU
2	F	33	THR
2	F	34	GLN
2	F	53	VAL
2	F	57	ARG
2	F	60	LEU
2	F	65	GLU
2	F	78	ARG
2	F	82	LEU
2	F	84	ARG
2	F	85	GLU
2	F	88	ASN
2	F	98	LEU
2	F	112	GLU

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Mol	Chain	Res	Type
2	F	114	VAL
2	F	119	ILE
2	F	120	VAL
2	F	134	VAL
2	F	136	ASN
2	F	139	THR
2	F	140	VAL
2	F	149	THR
2	F	161	LEU
2	F	165	LEU
2	F	169	TYR
2	F	171	VAL
2	F	179	PRO
2	F	180	ARG
2	F	187	ASP
2	F	189	GLU
2	F	194	ILE
2	F	209	ILE
2	F	211	VAL
2	F	212	VAL
2	F	223	VAL
2	F	255	VAL
2	F	269	VAL
2	F	281	ASP
2	F	299	GLN
2	F	301	GLN
2	F	304	CYS
2	F	305	ARG
2	F	329	TYR
2	F	334	VAL
2	F	350	LEU
2	F	353	THR
2	F	354	THR
2	F	362	LEU
2	F	373	ASN
2	F	375	ILE
2	F	377	PHE
2	F	379	GLU
2	F	388	ILE
2	F	392	CYS
2	F	405	THR
2	F	426	VAL

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Mol	Chain	Res	Type
2	F	427	THR
2	F	435	PRO
2	F	472	VAL
2	F	476	GLU
2	F	489	GLN
2	F	491	GLU
2	F	499	VAL
2	F	501	GLU
2	F	514	GLU
2	F	519	PRO
2	F	532	ILE
2	F	536	GLN
2	F	539	GLU
2	F	545	LEU
2	F	549	LEU
2	F	556	THR
1	G	47	ARG
1	G	50	GLN
1	G	59	GLU
1	G	65	MET
1	G	66	ARG
1	G	81	ASP
1	G	83	ASP
1	G	85	HIS
1	G	91	GLU
1	G	102	LYS
1	G	105	ASP
1	G	109	ARG
1	G	112	ARG
1	G	118	LEU
1	G	126	HIS
1	G	132	LEU
1	G	135	ASN
1	G	143	GLU
1	G	157	ILE
1	G	172	GLU
1	G	177	LEU
1	G	186	GLN
1	G	197	ARG
1	G	200	TYR
1	G	203	LEU
1	G	216	LYS

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Mol	Chain	Res	Type
1	G	217	VAL
1	G	219	GLU
1	G	220	ARG
1	G	221	GLU
1	G	226	GLU
1	G	228	LEU
1	G	232	GLN
1	G	233	ARG
1	G	247	GLU
1	G	249	TYR
1	G	250	LEU
1	G	251	LEU
1	G	260	VAL
1	G	261	PHE
1	G	269	LEU
1	G	276	CYS
1	G	278	ILE
1	G	311	GLN
1	G	328	ARG
1	G	330	GLN
1	G	335	GLU
1	G	336	MET
1	G	338	THR
1	G	340	LEU
1	G	341	GLN
1	G	346	VAL
1	G	355	LEU
1	G	356	VAL
1	G	360	ILE
1	G	378	ASN
1	G	386	LEU
1	G	397	PRO
1	G	421	ARG
1	G	437	LEU
1	G	438	ILE
1	G	440	TRP
1	G	443	THR
1	G	444	ARG
1	G	446	GLU
1	G	452	LEU
1	G	454	MET
1	G	459	SER

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Mol	Chain	Res	Type
1	G	460	VAL
1	G	463	LEU
1	G	471	ARG
1	G	473	ILE
1	G	484	LEU
1	G	485	ASP
1	G	489	ILE
1	G	495	ASP
1	G	505	PRO
1	G	517	LEU
1	G	518	GLN
1	G	526	ASP
1	G	540	ASN
1	G	541	ASP
1	G	547	LEU
1	G	549	ARG
1	G	552	ASP
1	G	554	MET
1	G	559	ASP
1	G	562	ARG
1	G	565	ARG
1	G	571	PRO
1	G	601	ARG
1	G	602	VAL
1	G	606	THR
1	G	612	LEU
1	G	618	LEU
1	G	621	GLU
1	G	625	GLU
1	G	629	ILE
2	H	35	ILE
2	H	38	ARG
2	H	50	LEU
2	H	59	LEU
2	H	78	ARG
2	H	81	LEU
2	H	83	VAL
2	H	85	GLU
2	H	89	ARG
2	H	90	LEU
2	H	95	SER
2	H	98	LEU

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Mol	Chain	Res	Type
2	H	129	VAL
2	H	136	ASN
2	H	139	THR
2	H	147	PRO
2	H	161	LEU
2	H	168	ILE
2	H	183	GLU
2	H	189	GLU
2	H	207	PRO
2	H	231	VAL
2	H	233	VAL
2	H	240	PHE
2	H	246	LEU
2	H	247	VAL
2	H	248	LYS
2	H	251	THR
2	H	256	SER
2	H	264	ASP
2	H	270	SER
2	H	281	ASP
2	H	294	LEU
2	H	297	ARG
2	H	299	GLN
2	H	311	LEU
2	H	315	GLU
2	H	320	VAL
2	H	327	GLN
2	H	339	VAL
2	H	345	ASP
2	H	350	LEU
2	H	353	THR
2	H	354	THR
2	H	370	LEU
2	H	373	ASN
2	H	376	LEU
2	H	393	GLN
2	H	398	LEU
2	H	405	THR
2	H	409	VAL
2	H	418	ILE
2	H	438	THR
2	H	472	VAL

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Mol	Chain	Res	Type
2	H	476	GLU
2	H	481	VAL
2	H	487	ARG
2	H	488	GLU
2	H	491	GLU
2	H	500	GLU
2	H	502	GLU
2	H	505	ILE
2	H	509	ILE
2	H	510	LEU
2	H	519	PRO
2	H	526	LEU
2	H	532	ILE
2	H	545	LEU
2	H	554	GLU
2	H	556	THR
2	H	560	VAL
2	H	561	PHE
1	I	50	GLN
1	I	54	VAL
1	I	65	MET
1	I	71	LEU
1	I	85	HIS
1	I	96	VAL
1	I	111	ASP
1	I	123	GLN
1	I	135	ASN
1	I	147	LEU
1	I	148	LEU
1	I	150	LEU
1	I	160	MET
1	I	167	LYS
1	I	169	LEU
1	I	178	VAL
1	I	179	PRO
1	I	251	LEU
1	I	255	HIS
1	I	260	VAL
1	I	261	PHE
1	I	269	LEU
1	I	278	ILE
1	I	280	ARG

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Mol	Chain	Res	Type
1	I	286	VAL
1	I	300	ARG
1	I	307	VAL
1	I	311	GLN
1	I	325	LEU
1	I	335	GLU
1	I	338	THR
1	I	340	LEU
1	I	341	GLN
1	I	353	LEU
1	I	356	VAL
1	I	362	VAL
1	I	386	LEU
1	I	421	ARG
1	I	438	ILE
1	I	440	TRP
1	I	443	THR
1	I	444	ARG
1	I	449	GLN
1	I	452	LEU
1	I	455	LEU
1	I	459	SER
1	I	463	LEU
1	I	465	THR
1	I	469	PHE
1	I	471	ARG
1	I	473	ILE
1	I	474	LEU
1	I	483	GLU
1	I	489	ILE
1	I	504	LEU
1	I	505	PRO
1	I	519	SER
1	I	525	ARG
1	I	526	ASP
1	I	538	SER
1	I	539	ARG
1	I	540	ASN
1	I	541	ASP
1	I	554	MET
1	I	560	GLU
1	I	561	ARG

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Mol	Chain	Res	Type
1	I	565	ARG
1	I	571	PRO
1	I	589	ARG
1	I	597	ASP
1	I	598	LEU
1	I	601	ARG
1	I	612	LEU
1	I	618	LEU
1	I	620	LEU
1	I	623	GLU
2	J	35	ILE
2	J	59	LEU
2	J	62	ARG
2	J	81	LEU
2	J	82	LEU
2	J	84	ARG
2	J	85	GLU
2	J	98	LEU
2	J	136	ASN
2	J	149	THR
2	J	161	LEU
2	J	171	VAL
2	J	183	GLU
2	J	189	GLU
2	J	209	ILE
2	J	211	VAL
2	J	217	THR
2	J	223	VAL
2	J	235	GLU
2	J	236	GLN
2	J	240	PHE
2	J	269	VAL
2	J	281	ASP
2	J	289	ARG
2	J	297	ARG
2	J	304	CYS
2	J	311	LEU
2	J	315	GLU
2	J	321	ILE
2	J	327	GLN
2	J	331	VAL
2	J	337	ARG

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Mol	Chain	Res	Type
2	J	339	VAL
2	J	350	LEU
2	J	353	THR
2	J	354	THR
2	J	370	LEU
2	J	373	ASN
2	J	375	ILE
2	J	377	PHE
2	J	379	GLU
2	J	405	THR
2	J	408	MET
2	J	409	VAL
2	J	414	GLU
2	J	418	ILE
2	J	426	VAL
2	J	452	MET
2	J	453	CYS
2	J	464	MET
2	J	469	ARG
2	J	476	GLU
2	J	487	ARG
2	J	538	ARG
2	J	545	LEU
2	J	549	LEU
1	K	47	ARG
1	K	52	LEU
1	K	59	GLU
1	K	66	ARG
1	K	71	LEU
1	K	85	HIS
1	K	91	GLU
1	K	96	VAL
1	K	114	ILE
1	K	118	LEU
1	K	123	GLN
1	K	129	TYR
1	K	137	ASP
1	K	140	ARG
1	K	144	GLU
1	K	148	LEU
1	K	150	LEU
1	K	251	LEU

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Mol	Chain	Res	Type
1	K	263	ASP
1	K	264	ARG
1	K	269	LEU
1	K	273	GLU
1	K	278	ILE
1	K	280	ARG
1	K	282	HIS
1	K	285	VAL
1	K	286	VAL
1	K	288	GLU
1	K	292	PRO
1	K	308	ARG
1	K	311	GLN
1	K	322	GLU
1	K	335	GLU
1	K	336	MET
1	K	341	GLN
1	K	347	THR
1	K	356	VAL
1	K	358	TRP
1	K	359	GLN
1	K	360	ILE
1	K	386	LEU
1	K	392	GLU
1	K	401	ARG
1	K	412	PRO
1	K	421	ARG
1	K	429	PHE
1	K	438	ILE
1	K	443	THR
1	K	445	GLU
1	K	446	GLU
1	K	452	LEU
1	K	460	VAL
1	K	463	LEU
1	K	471	ARG
1	K	473	ILE
1	K	479	PHE
1	K	504	LEU
1	K	505	PRO
1	K	507	HIS
1	K	510	GLN

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Mol	Chain	Res	Type
1	K	518	GLN
1	K	524	ARG
1	K	525	ARG
1	K	526	ASP
1	K	540	ASN
1	K	547	LEU
1	K	552	ASP
1	K	560	GLU
1	K	565	ARG
1	K	566	LEU
1	K	567	ARG
1	K	588	TYR
1	K	591	ASP
1	K	597	ASP
1	K	598	LEU
1	K	600	SER
1	K	605	VAL
1	K	606	THR
1	K	612	LEU
1	K	618	LEU
1	K	620	LEU
1	K	625	GLU
1	K	626	LEU
1	K	627	LEU
1	K	630	GLU
2	L	31	LEU
2	L	38	ARG
2	L	50	LEU
2	L	60	LEU
2	L	62	ARG
2	L	63	ILE
2	L	65	GLU
2	L	78	ARG
2	L	82	LEU
2	L	83	VAL
2	L	84	ARG
2	L	95	SER
2	L	98	LEU
2	L	99	GLU
2	L	100	LEU
2	L	114	VAL
2	L	119	ILE

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Mol	Chain	Res	Type
2	L	133	ILE
2	L	134	VAL
2	L	136	ASN
2	L	159	ILE
2	L	161	LEU
2	L	169	TYR
2	L	171	VAL
2	L	188	ARG
2	L	189	GLU
2	L	198	GLN
2	L	200	ASN
2	L	202	SER
2	L	204	ARG
2	L	206	ILE
2	L	208	GLN
2	L	209	ILE
2	L	212	VAL
2	L	217	THR
2	L	234	ARG
2	L	269	VAL
2	L	279	ASP
2	L	302	LEU
2	L	304	CYS
2	L	305	ARG
2	L	315	GLU
2	L	327	GLN
2	L	329	TYR
2	L	335	ILE
2	L	339	VAL
2	L	350	LEU
2	L	353	THR
2	L	354	THR
2	L	373	ASN
2	L	375	ILE
2	L	376	LEU
2	L	377	PHE
2	L	392	CYS
2	L	405	THR
2	L	409	VAL
2	L	412	LYS
2	L	414	GLU
2	L	426	VAL

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Mol	Chain	Res	Type
2	L	434	VAL
2	L	438	THR
2	L	455	ARG
2	L	470	ILE
2	L	472	VAL
2	L	476	GLU
2	L	499	VAL
2	L	519	PRO
2	L	520	TYR
2	L	532	ILE
2	L	538	ARG
2	L	541	LEU
2	L	560	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (202) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	79	HIS
1	A	186	GLN
1	A	232	GLN
1	A	255	HIS
1	A	272	ASN
1	A	279	GLN
1	A	372	GLN
1	A	492	HIS
1	A	493	GLN
1	A	501	GLN
1	A	540	ASN
1	A	666	GLN
1	A	684	HIS
2	B	36	ASN
2	B	54	ASN
2	B	64	HIS
2	B	72	GLN
2	B	75	HIS
2	B	106	HIS
2	B	136	ASN
2	B	157	GLN
2	B	190	HIS
2	B	197	ASN
2	B	198	GLN

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Mol	Chain	Res	Type
2	B	200	ASN
2	B	266	HIS
2	B	303	GLN
2	B	363	HIS
2	B	373	ASN
2	B	386	HIS
2	B	393	GLN
2	B	402	GLN
2	B	403	ASN
2	B	411	GLN
2	B	449	ASN
2	B	467	ASN
2	B	496	GLN
2	B	512	GLN
2	B	515	HIS
2	B	536	GLN
1	C	79	HIS
1	C	123	GLN
1	C	186	GLN
1	C	232	GLN
1	C	279	GLN
1	C	311	GLN
1	C	330	GLN
1	C	337	ASN
1	C	372	GLN
1	C	378	ASN
1	C	492	HIS
1	C	501	GLN
1	C	510	GLN
1	C	617	GLN
2	D	52	GLN
2	D	54	ASN
2	D	88	ASN
2	D	197	ASN
2	D	200	ASN
2	D	236	GLN
2	D	293	ASN
2	D	303	GLN
2	D	372	ASN
2	D	373	ASN
2	D	382	GLN
2	D	386	HIS

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Mol	Chain	Res	Type
2	D	402	GLN
2	D	403	ASN
2	D	411	GLN
2	D	449	ASN
2	D	467	ASN
2	D	484	GLN
2	D	512	GLN
2	D	536	GLN
1	E	50	GLN
1	E	79	HIS
1	E	88	HIS
1	E	186	GLN
1	E	265	HIS
1	E	279	GLN
1	E	283	GLN
1	E	372	GLN
1	E	380	HIS
1	E	501	GLN
1	E	510	GLN
1	E	534	HIS
1	E	568	HIS
1	E	617	GLN
2	F	36	ASN
2	F	72	GLN
2	F	75	HIS
2	F	88	ASN
2	F	177	ASN
2	F	197	ASN
2	F	200	ASN
2	F	236	GLN
2	F	275	HIS
2	F	301	GLN
2	F	303	GLN
2	F	327	GLN
2	F	363	HIS
2	F	373	ASN
2	F	386	HIS
2	F	393	GLN
2	F	402	GLN
2	F	421	HIS
2	F	467	ASN
2	F	484	GLN

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Mol	Chain	Res	Type
2	F	489	GLN
2	F	495	GLN
2	F	536	GLN
1	G	50	GLN
1	G	79	HIS
1	G	186	GLN
1	G	232	GLN
1	G	279	GLN
1	G	282	HIS
1	G	283	GLN
1	G	372	GLN
1	G	501	GLN
1	G	507	HIS
1	G	518	GLN
1	G	534	HIS
1	G	540	ASN
1	G	617	GLN
2	H	36	ASN
2	H	72	GLN
2	H	75	HIS
2	H	106	HIS
2	H	157	GLN
2	H	190	HIS
2	H	197	ASN
2	H	200	ASN
2	H	236	GLN
2	H	275	HIS
2	H	303	GLN
2	H	373	ASN
2	H	382	GLN
2	H	386	HIS
2	H	393	GLN
2	H	402	GLN
2	H	403	ASN
2	H	449	ASN
2	H	467	ASN
2	H	489	GLN
2	H	536	GLN
1	I	79	HIS
1	I	88	HIS
1	I	272	ASN
1	I	279	GLN

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Mol	Chain	Res	Type
1	I	311	GLN
1	I	359	GLN
1	I	372	GLN
1	I	492	HIS
1	I	501	GLN
1	I	540	ASN
2	J	36	ASN
2	J	72	GLN
2	J	75	HIS
2	J	157	GLN
2	J	177	ASN
2	J	181	GLN
2	J	198	GLN
2	J	236	GLN
2	J	363	HIS
2	J	373	ASN
2	J	382	GLN
2	J	386	HIS
2	J	402	GLN
2	J	403	ASN
2	J	449	ASN
2	J	467	ASN
2	J	484	GLN
2	J	489	GLN
1	K	50	GLN
1	K	79	HIS
1	K	255	HIS
1	K	259	GLN
1	K	267	HIS
1	K	279	GLN
1	K	311	GLN
1	K	337	ASN
1	K	372	GLN
1	K	501	GLN
2	L	36	ASN
2	L	54	ASN
2	L	106	HIS
2	L	153	HIS
2	L	157	GLN
2	L	197	ASN
2	L	208	GLN
2	L	275	HIS

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Mol	Chain	Res	Type
2	L	303	GLN
2	L	327	GLN
2	L	373	ASN
2	L	382	GLN
2	L	386	HIS
2	L	402	GLN
2	L	403	ASN
2	L	449	ASN
2	L	467	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	COA	F	591	-	47,50,50	0.98	3 (6%)	69,75,75	1.43	9 (13%)
4	COA	H	591	-	47,50,50	1.02	3 (6%)	69,75,75	1.43	9 (13%)
4	COA	D	591	-	47,50,50	1.04	4 (8%)	69,75,75	1.48	8 (11%)
4	COA	B	591	-	47,50,50	1.03	4 (8%)	69,75,75	1.45	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	COA	L	591	-	47,50,50	0.98	3 (6%)	69,75,75	1.51	9 (13%)
4	COA	J	591	-	47,50,50	1.02	3 (6%)	69,75,75	1.42	8 (11%)
3	BTI	A	801	1	15,16,16	1.68	1 (6%)	20,21,21	2.34	7 (35%)
3	BTI	I	801	1	15,16,16	1.69	1 (6%)	20,21,21	2.30	7 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	COA	F	591	-	-	13/48/64/64	0/3/3/3
4	COA	H	591	-	-	13/48/64/64	0/3/3/3
4	COA	D	591	-	-	12/48/64/64	0/3/3/3
4	COA	B	591	-	-	12/48/64/64	0/3/3/3
4	COA	L	591	-	-	15/48/64/64	0/3/3/3
4	COA	J	591	-	-	14/48/64/64	0/3/3/3
3	BTI	A	801	1	-	5/6/27/27	0/2/2/2
3	BTI	I	801	1	-	5/6/27/27	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	801	BTI	O3-C3	6.16	1.36	1.23
3	A	801	BTI	O3-C3	6.12	1.36	1.23
4	L	591	COA	C5A-N7A	-3.14	1.33	1.39
4	B	591	COA	C5A-N7A	-3.13	1.33	1.39
4	D	591	COA	C5A-N7A	-3.12	1.33	1.39
4	J	591	COA	C5A-N7A	-3.10	1.33	1.39
4	F	591	COA	C5A-N7A	-3.08	1.33	1.39
4	H	591	COA	C5A-N7A	-3.04	1.33	1.39
4	L	591	COA	C8A-N9A	-2.42	1.33	1.37
4	D	591	COA	C8A-N9A	-2.36	1.33	1.37
4	H	591	COA	C8A-N9A	-2.35	1.33	1.37
4	B	591	COA	C8A-N9A	-2.32	1.33	1.37
4	J	591	COA	C8A-N9A	-2.32	1.33	1.37
4	F	591	COA	C8A-N9A	-2.28	1.33	1.37
4	L	591	COA	C4A-N9A	-2.24	1.33	1.37
4	D	591	COA	C4A-N9A	-2.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	591	COA	C4A-N9A	-2.11	1.33	1.37
4	B	591	COA	C4A-N9A	-2.10	1.33	1.37
4	H	591	COA	C4A-N9A	-2.07	1.33	1.37
4	D	591	COA	P2A-O3A	2.02	1.61	1.59
4	J	591	COA	C4A-N9A	-2.02	1.33	1.37
4	B	591	COA	P1A-O3A	2.00	1.61	1.59

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	591	COA	C5A-C4A-N3A	-5.47	119.18	126.72
4	L	591	COA	C5A-C4A-N3A	-5.30	119.42	126.72
4	B	591	COA	C5A-C4A-N3A	-5.27	119.47	126.72
4	J	591	COA	C5A-C4A-N3A	-5.14	119.64	126.72
3	A	801	BTI	C4-N2-C3	-4.99	106.36	112.56
4	H	591	COA	C5A-C4A-N3A	-4.87	120.02	126.72
4	D	591	COA	N3A-C2A-N1A	-4.77	121.36	128.58
4	F	591	COA	C5A-C4A-N3A	-4.69	120.26	126.72
4	J	591	COA	N3A-C2A-N1A	-4.63	121.58	128.58
4	L	591	COA	N3A-C2A-N1A	-4.60	121.62	128.58
4	B	591	COA	N3A-C2A-N1A	-4.55	121.69	128.58
4	F	591	COA	N3A-C2A-N1A	-4.50	121.77	128.58
4	H	591	COA	N3A-C2A-N1A	-4.35	121.99	128.58
3	A	801	BTI	C6-S1-C2	4.34	99.01	89.98
3	I	801	BTI	C4-N2-C3	-4.30	107.22	112.56
3	A	801	BTI	C6-C5-N3	-4.27	107.68	113.18
3	I	801	BTI	C6-S1-C2	4.25	98.82	89.98
3	I	801	BTI	C6-C5-N3	-4.23	107.73	113.18
3	I	801	BTI	N2-C3-N3	3.88	113.33	108.85
4	D	591	COA	N3A-C4A-N9A	3.82	133.66	127.17
4	B	591	COA	N3A-C4A-N9A	3.71	133.47	127.17
4	D	591	COA	C2A-N3A-C4A	3.71	120.89	111.83
4	H	591	COA	N3A-C4A-N9A	3.69	133.44	127.17
4	L	591	COA	N3A-C4A-N9A	3.69	133.44	127.17
4	J	591	COA	N3A-C4A-N9A	3.68	133.43	127.17
4	L	591	COA	C2A-N3A-C4A	3.61	120.66	111.83
4	B	591	COA	C2A-N3A-C4A	3.55	120.49	111.83
4	J	591	COA	C2A-N3A-C4A	3.53	120.45	111.83
3	A	801	BTI	N2-C3-N3	3.50	112.89	108.85
4	H	591	COA	N9A-C8A-N7A	-3.34	109.20	113.94
4	L	591	COA	N9A-C8A-N7A	-3.31	109.23	113.94
4	F	591	COA	N3A-C4A-N9A	3.30	132.78	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	591	COA	C2A-N3A-C4A	3.30	119.88	111.83
4	H	591	COA	C2A-N3A-C4A	3.27	119.82	111.83
4	D	591	COA	N9A-C8A-N7A	-3.16	109.46	113.94
4	B	591	COA	N9A-C8A-N7A	-3.05	109.61	113.94
4	F	591	COA	N9A-C8A-N7A	-3.00	109.67	113.94
4	L	591	COA	C4A-C5A-N7A	-2.96	107.20	110.58
4	L	591	COA	C5A-N7A-C8A	2.96	108.10	103.45
4	J	591	COA	N9A-C8A-N7A	-2.93	109.78	113.94
4	D	591	COA	C4A-C5A-N7A	-2.92	107.24	110.58
4	D	591	COA	C5A-N7A-C8A	2.88	107.98	103.45
3	I	801	BTI	C5-N3-C3	-2.86	108.18	112.38
4	H	591	COA	C5A-N7A-C8A	2.85	107.94	103.45
4	H	591	COA	C4A-N9A-C8A	2.85	108.73	105.74
4	B	591	COA	C5A-N7A-C8A	2.77	107.81	103.45
3	A	801	BTI	C5-N3-C3	-2.77	108.31	112.38
4	B	591	COA	C4A-C5A-N7A	-2.73	107.46	110.58
4	F	591	COA	C5A-N7A-C8A	2.64	107.60	103.45
4	J	591	COA	C5A-N7A-C8A	2.62	107.56	103.45
4	H	591	COA	C4A-C5A-N7A	-2.61	107.60	110.58
4	F	591	COA	C4A-C5A-N7A	-2.54	107.68	110.58
4	J	591	COA	C4A-C5A-N7A	-2.51	107.72	110.58
4	L	591	COA	C4A-N9A-C8A	2.45	108.31	105.74
3	A	801	BTI	C2-C4-C5	2.39	111.82	108.89
4	D	591	COA	C4A-N9A-C8A	2.31	108.16	105.74
3	A	801	BTI	C5-C6-S1	-2.26	102.96	106.06
4	F	591	COA	C4A-N9A-C8A	2.24	108.09	105.74
3	I	801	BTI	C2-C4-C5	2.22	111.61	108.89
4	B	591	COA	C4A-N9A-C8A	2.21	108.06	105.74
4	L	591	COA	C4B-O4B-C1B	-2.21	104.59	109.47
4	F	591	COA	P3B-O3B-C3B	-2.20	117.54	123.43
4	J	591	COA	C4A-N9A-C8A	2.17	108.02	105.74
4	H	591	COA	C4B-O4B-C1B	-2.10	104.84	109.47
3	I	801	BTI	C5-C6-S1	-2.09	103.18	106.06

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	BTI	C11-C10-C9-C8
3	A	801	BTI	S1-C2-C7-C8
3	A	801	BTI	C4-C2-C7-C8
3	I	801	BTI	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
3	I	801	BTI	S1-C2-C7-C8
3	I	801	BTI	C4-C2-C7-C8
4	B	591	COA	O4B-C4B-C5B-O5B
4	B	591	COA	C5B-O5B-P1A-O2A
4	B	591	COA	C5B-O5B-P1A-O3A
4	B	591	COA	CCP-O6A-P2A-O3A
4	B	591	COA	CCP-O6A-P2A-O4A
4	B	591	COA	CCP-O6A-P2A-O5A
4	B	591	COA	CDP-CBP-CCP-O6A
4	B	591	COA	CEP-CBP-CCP-O6A
4	B	591	COA	CAP-CBP-CCP-O6A
4	B	591	COA	S1P-C2P-C3P-N4P
4	D	591	COA	O4B-C4B-C5B-O5B
4	D	591	COA	C5B-O5B-P1A-O1A
4	D	591	COA	C5B-O5B-P1A-O2A
4	D	591	COA	C5B-O5B-P1A-O3A
4	D	591	COA	CCP-O6A-P2A-O3A
4	D	591	COA	CCP-O6A-P2A-O4A
4	D	591	COA	CCP-O6A-P2A-O5A
4	D	591	COA	CDP-CBP-CCP-O6A
4	D	591	COA	CEP-CBP-CCP-O6A
4	D	591	COA	CAP-CBP-CCP-O6A
4	D	591	COA	S1P-C2P-C3P-N4P
4	F	591	COA	O4B-C4B-C5B-O5B
4	F	591	COA	C5B-O5B-P1A-O2A
4	F	591	COA	C5B-O5B-P1A-O3A
4	F	591	COA	CCP-O6A-P2A-O3A
4	F	591	COA	CCP-O6A-P2A-O4A
4	F	591	COA	CCP-O6A-P2A-O5A
4	F	591	COA	CDP-CBP-CCP-O6A
4	F	591	COA	CEP-CBP-CCP-O6A
4	F	591	COA	CAP-CBP-CCP-O6A
4	F	591	COA	S1P-C2P-C3P-N4P
4	H	591	COA	O4B-C4B-C5B-O5B
4	H	591	COA	C5B-O5B-P1A-O2A
4	H	591	COA	C5B-O5B-P1A-O3A
4	H	591	COA	CCP-O6A-P2A-O3A
4	H	591	COA	CCP-O6A-P2A-O4A
4	H	591	COA	CCP-O6A-P2A-O5A
4	H	591	COA	CDP-CBP-CCP-O6A
4	H	591	COA	CEP-CBP-CCP-O6A
4	H	591	COA	CAP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
4	H	591	COA	S1P-C2P-C3P-N4P
4	J	591	COA	O4B-C4B-C5B-O5B
4	J	591	COA	C5B-O5B-P1A-O2A
4	J	591	COA	C5B-O5B-P1A-O3A
4	J	591	COA	CCP-O6A-P2A-O3A
4	J	591	COA	CCP-O6A-P2A-O4A
4	J	591	COA	CCP-O6A-P2A-O5A
4	J	591	COA	CDP-CBP-CCP-O6A
4	J	591	COA	CEP-CBP-CCP-O6A
4	J	591	COA	CAP-CBP-CCP-O6A
4	J	591	COA	S1P-C2P-C3P-N4P
4	L	591	COA	O4B-C4B-C5B-O5B
4	L	591	COA	C5B-O5B-P1A-O2A
4	L	591	COA	C5B-O5B-P1A-O3A
4	L	591	COA	CCP-O6A-P2A-O3A
4	L	591	COA	CCP-O6A-P2A-O4A
4	L	591	COA	CCP-O6A-P2A-O5A
4	L	591	COA	CDP-CBP-CCP-O6A
4	L	591	COA	CEP-CBP-CCP-O6A
4	L	591	COA	CAP-CBP-CCP-O6A
4	L	591	COA	S1P-C2P-C3P-N4P
4	B	591	COA	C3B-C4B-C5B-O5B
4	D	591	COA	C3B-C4B-C5B-O5B
4	J	591	COA	C3B-C4B-C5B-O5B
4	L	591	COA	C3B-C4B-C5B-O5B
4	F	591	COA	C3B-C4B-C5B-O5B
4	H	591	COA	C3B-C4B-C5B-O5B
3	A	801	BTI	C2-C7-C8-C9
3	I	801	BTI	C2-C7-C8-C9
3	I	801	BTI	C7-C8-C9-C10
4	L	591	COA	O5P-C5P-N4P-C3P
3	A	801	BTI	C7-C8-C9-C10
4	J	591	COA	C2P-C3P-N4P-C5P
4	B	591	COA	C5B-O5B-P1A-O1A
4	F	591	COA	C5B-O5B-P1A-O1A
4	H	591	COA	C5B-O5B-P1A-O1A
4	J	591	COA	C5B-O5B-P1A-O1A
4	L	591	COA	C5B-O5B-P1A-O1A
4	F	591	COA	C5P-C6P-C7P-N8P
4	J	591	COA	C5P-C6P-C7P-N8P
4	L	591	COA	C5P-C6P-C7P-N8P
4	L	591	COA	C6P-C5P-N4P-C3P

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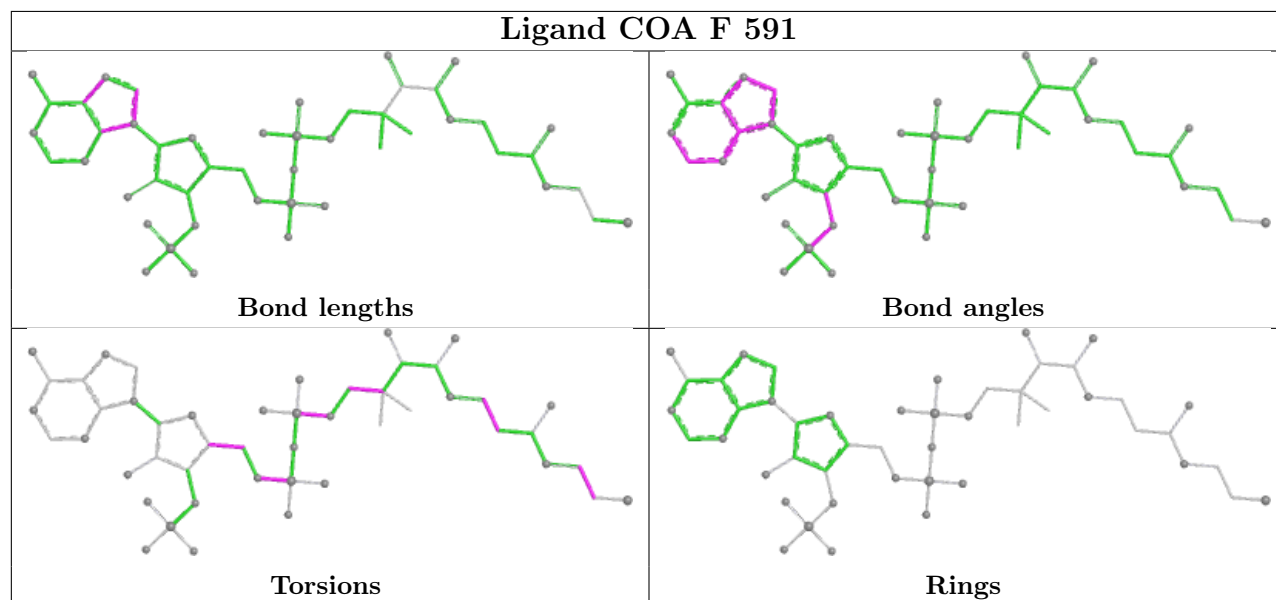
Mol	Chain	Res	Type	Atoms
4	H	591	COA	C5P-C6P-C7P-N8P

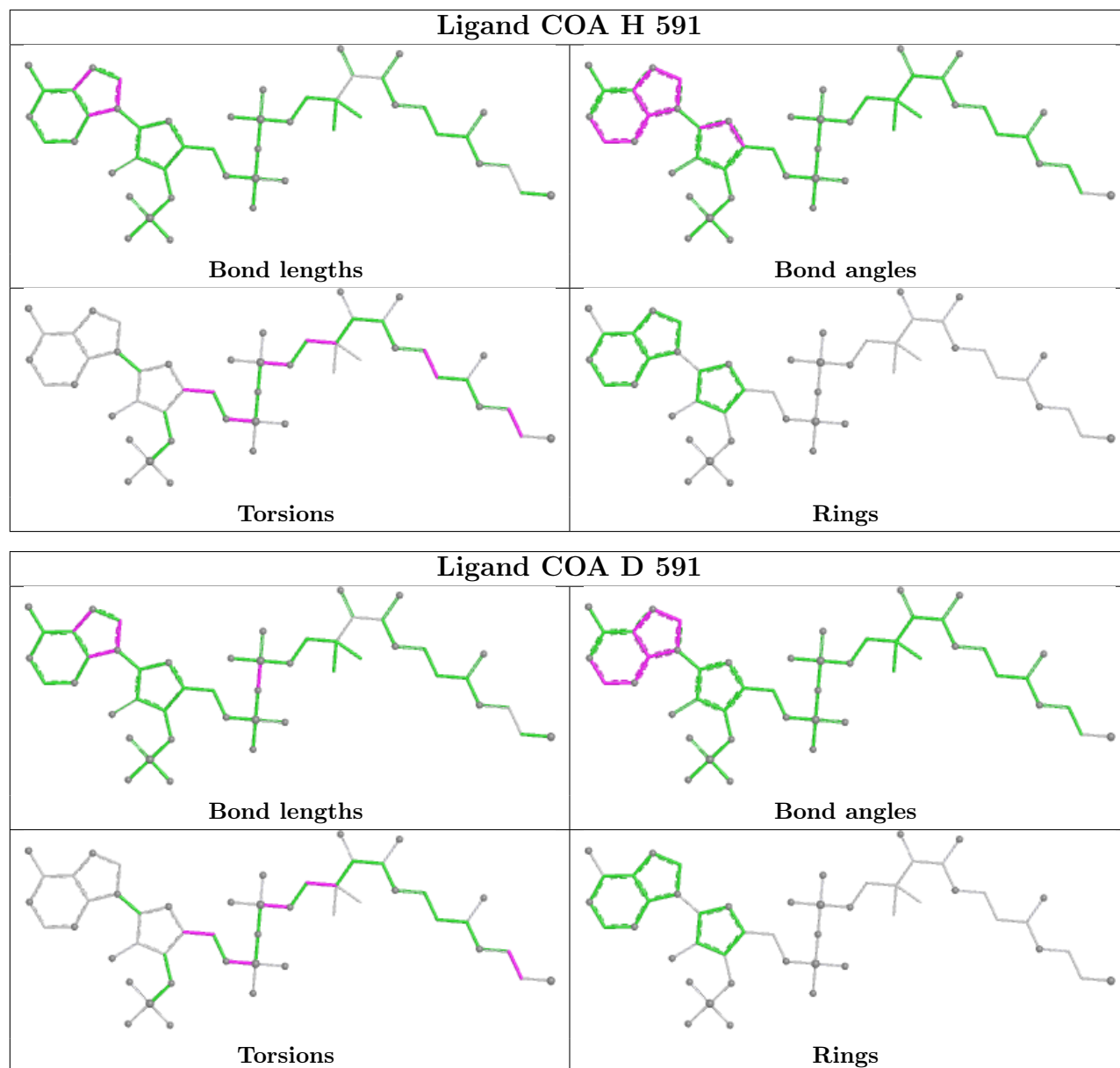
There are no ring outliers.

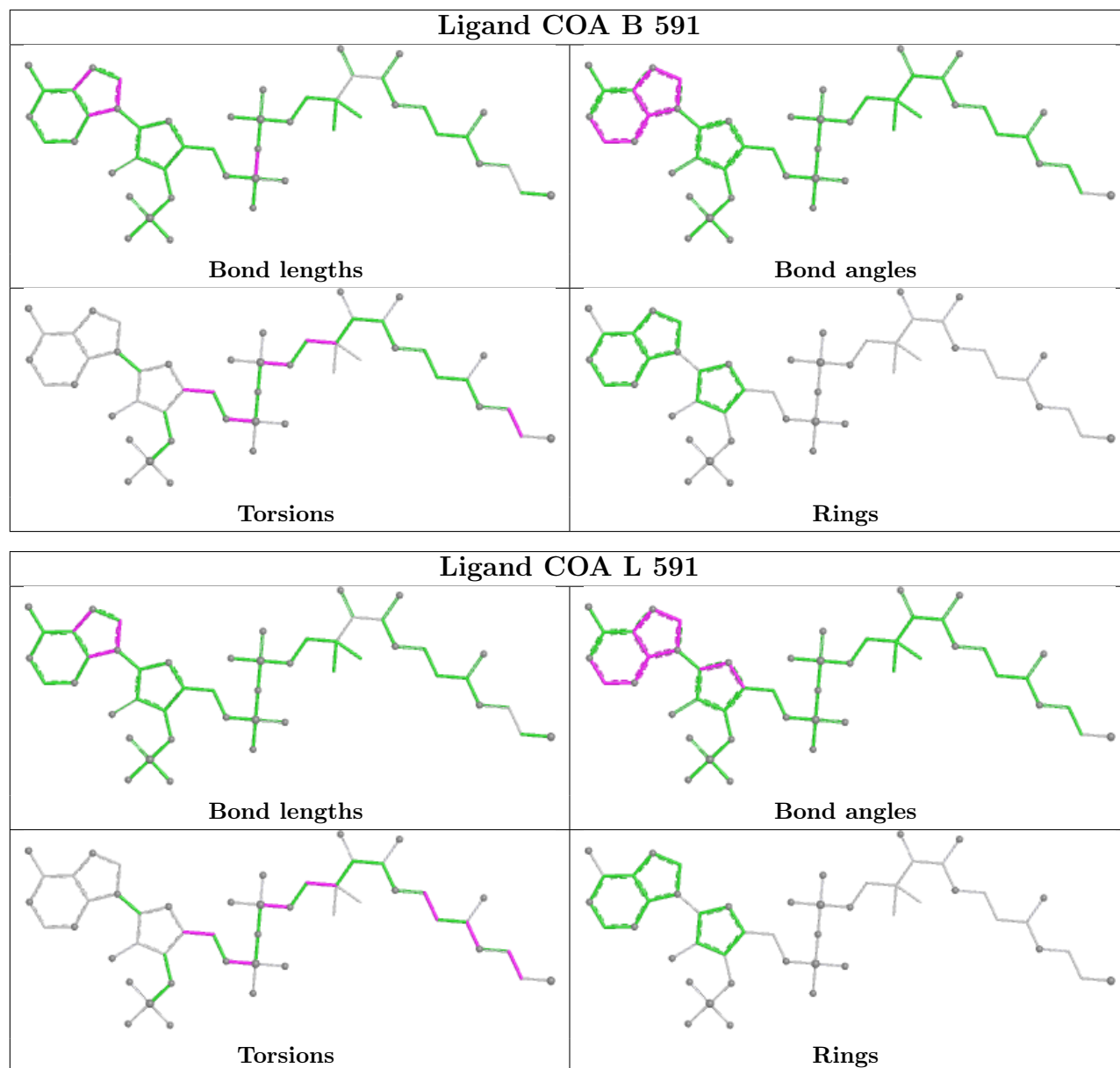
8 monomers are involved in 30 short contacts:

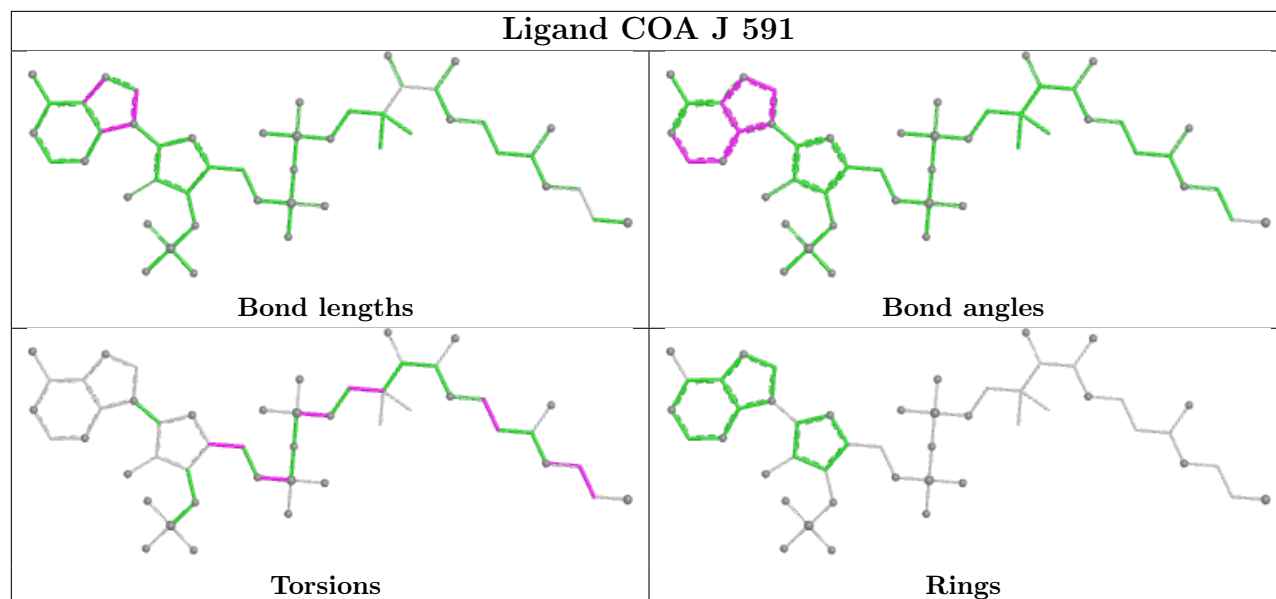
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	591	COA	3	0
4	H	591	COA	6	0
4	D	591	COA	3	0
4	B	591	COA	4	0
4	L	591	COA	2	0
4	J	591	COA	4	0
3	A	801	BTI	3	0
3	I	801	BTI	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	621/655 (94%)	0.05	0 100 100	71, 115, 170, 200	0
1	C	552/655 (84%)	-0.03	2 (0%) 88 72	69, 113, 154, 187	0
1	E	552/655 (84%)	0.01	1 (0%) 91 82	71, 113, 154, 189	0
1	G	552/655 (84%)	0.07	0 100 100	76, 112, 155, 187	0
1	I	498/655 (76%)	0.02	2 (0%) 88 72	73, 113, 146, 193	0
1	K	497/655 (75%)	0.11	2 (0%) 88 72	65, 115, 146, 187	0
2	B	537/555 (96%)	-0.21	0 100 100	60, 87, 140, 169	0
2	D	537/555 (96%)	-0.21	0 100 100	58, 89, 143, 171	0
2	F	537/555 (96%)	-0.19	0 100 100	58, 88, 142, 167	0
2	H	537/555 (96%)	-0.19	0 100 100	59, 88, 138, 169	0
2	J	537/555 (96%)	-0.21	1 (0%) 91 82	55, 88, 142, 168	0
2	L	537/555 (96%)	-0.19	0 100 100	57, 88, 139, 167	0
All	All	6494/7260 (89%)	-0.08	8 (0%) 92 86	55, 103, 153, 200	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	55	ALA	3.0
1	C	633	ASP	2.6
1	I	504	LEU	2.5
2	J	482	LEU	2.2
1	C	85	HIS	2.2
1	K	568	HIS	2.1
1	E	242	ALA	2.1
1	I	180	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

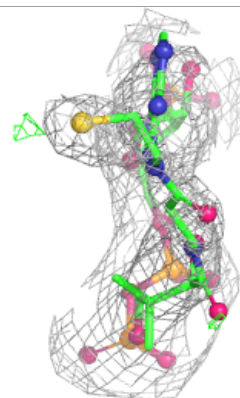
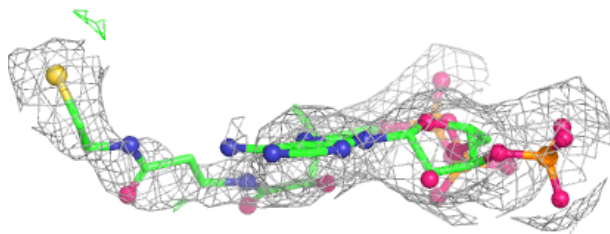
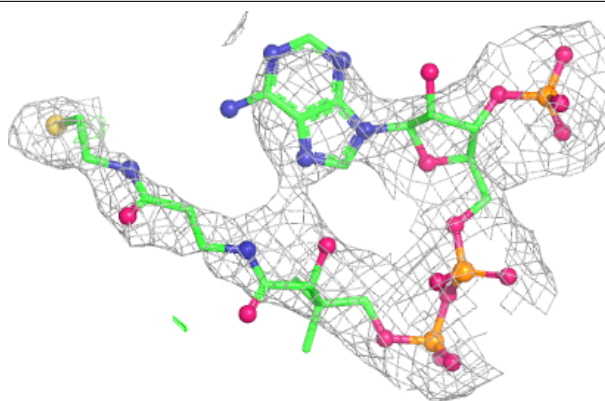
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	COA	B	591	48/48	0.88	0.13	103,129,139,142	0
4	COA	D	591	48/48	0.88	0.11	102,129,142,145	0
4	COA	H	591	48/48	0.90	0.11	102,128,137,139	0
4	COA	J	591	48/48	0.90	0.12	101,127,136,137	0
3	BTI	A	801	15/15	0.91	0.23	140,152,154,155	0
4	COA	F	591	48/48	0.91	0.14	97,124,134,135	0
3	BTI	I	801	15/15	0.92	0.17	142,152,155,158	0
4	COA	L	591	48/48	0.93	0.12	98,125,132,135	0

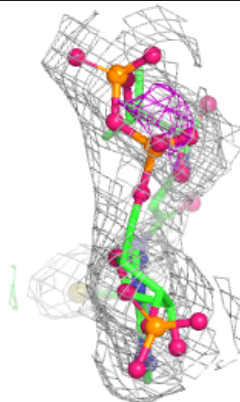
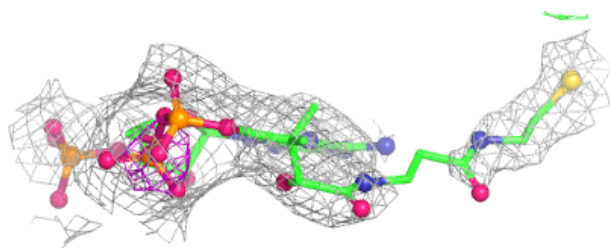
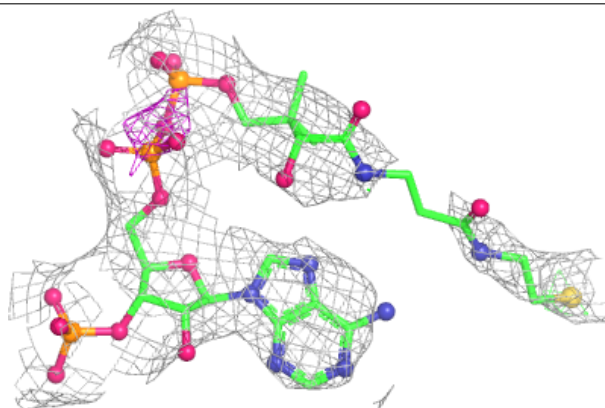
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around COA B 591:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

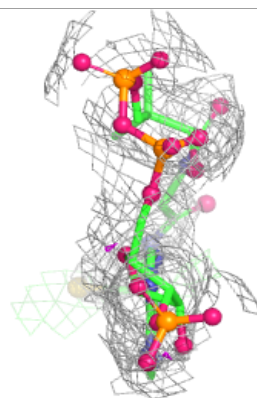
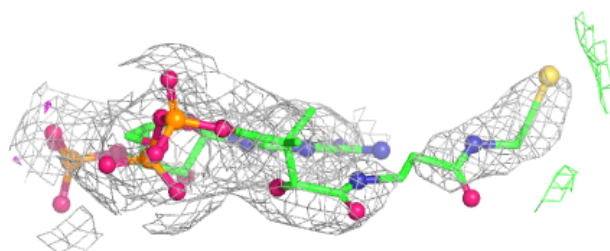
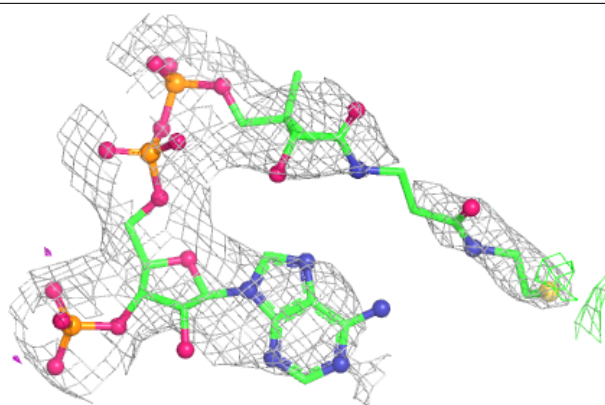
**Electron density around COA D 591:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

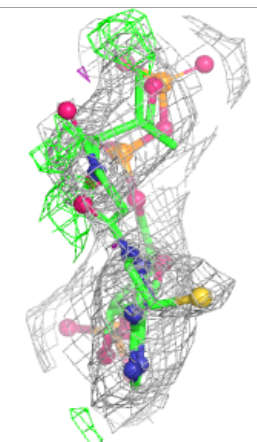
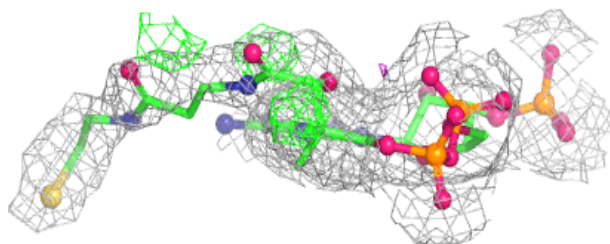
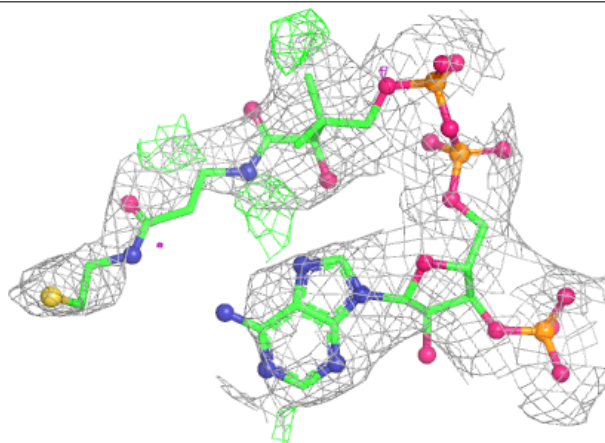


Electron density around COA H 591:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

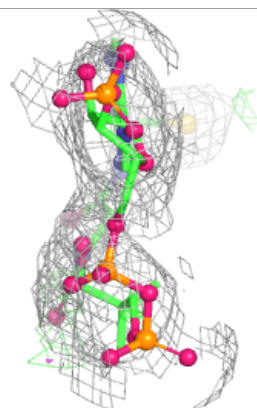
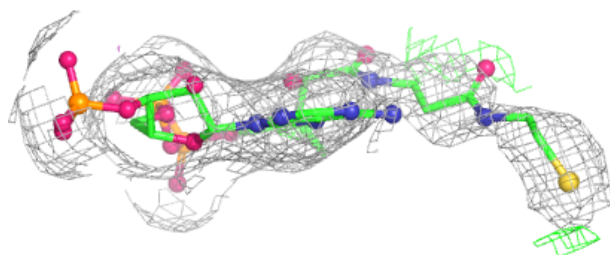
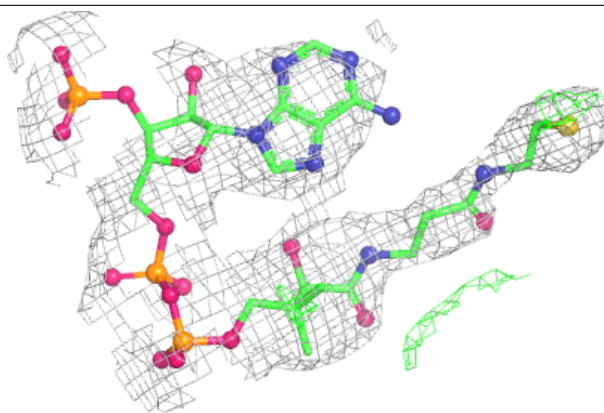
**Electron density around COA J 591:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

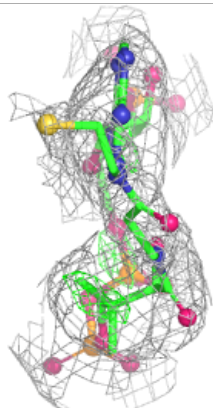
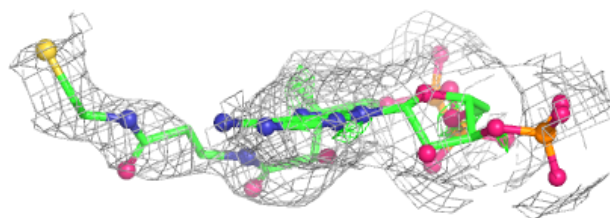
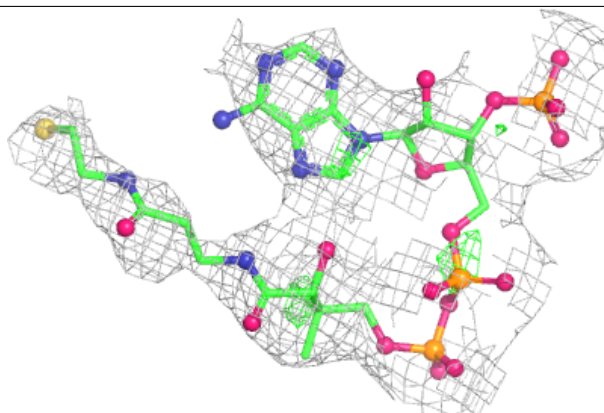


Electron density around COA F 591:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around COA L 591:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.