



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:04 PM UTC

PDB ID : 1I6V / pdb_00001i6v
Title : THERMUS AQUATICUS CORE RNA POLYMERASE-RIFAMPICIN COMPLEX
Authors : Campbell, E.A.; Korzheva, N.; Mustaev, A.; Murakami, K.; Goldfarb, A.; Darst, S.A.
Deposited on : 2001-03-05
Resolution : 3.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

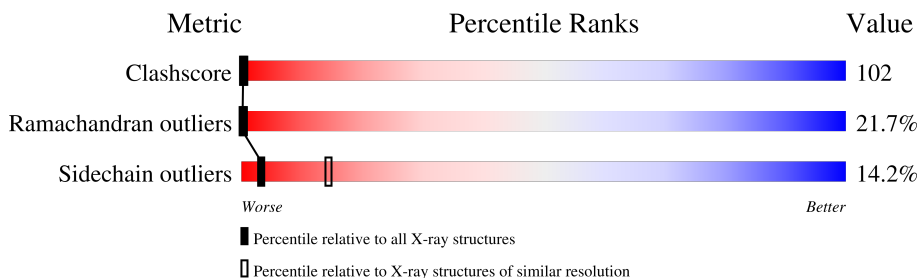
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	11% 39% 16% 5% 29%
1	B	314	10% 44% 18% • 27%
2	C	1118	11% 56% 29% •
3	D	1264	15% 49% 25% • 7%
4	E	99	17% 58% 23% ••

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21292 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 DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1741	1109	299	330	3			
1	B	230	Total	C	N	O	S	0	0	0
			1761	1122	299	337	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	VAL	GLY	conflict	UNP Q9KWU8
A	232	SER	LEU	conflict	UNP Q9KWU8
B	112	VAL	GLY	conflict	UNP Q9KWU8
B	232	SER	LEU	conflict	UNP Q9KWU8

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1113	Total	C	N	O	S	12	0	0
			8508	5386	1514	1585	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LYS	GLU	conflict	UNP Q9KWU7
C	?	-	GLU	deletion	UNP Q9KWU7
C	1111	VAL	ILE	conflict	UNP Q9KWU7

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1174	Total	C	N	O	S	17	0	0
			8502	5329	1550	1596	27			

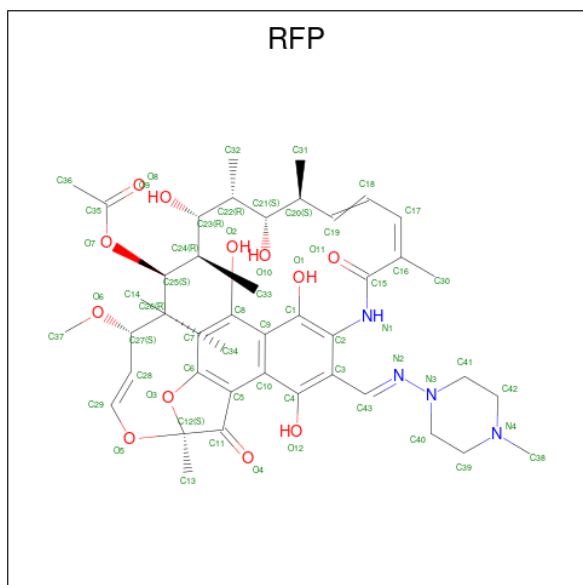
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	ALA	GLY	conflict	UNP Q9KWU6
D	77	ALA	GLY	conflict	UNP Q9KWU6
D	91	ALA	GLY	conflict	UNP Q9KWU6
D	113	ALA	GLY	conflict	UNP Q9KWU6
D	139	ALA	GLY	conflict	UNP Q9KWU6
D	144	ALA	GLY	conflict	UNP Q9KWU6
D	863	THR	VAL	conflict	UNP Q9KWU6
D	866	THR	VAL	conflict	UNP Q9KWU6
D	1009	ASN	LYS	conflict	UNP Q9KWU6

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	98	Total	C	N	O	S	0	0	0
			719	453	132	130	4			

- Molecule 5 is RIFAMPICIN (CCD ID: RFP) (formula: C₄₃H₅₈N₄O₁₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			59	43	4	12		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

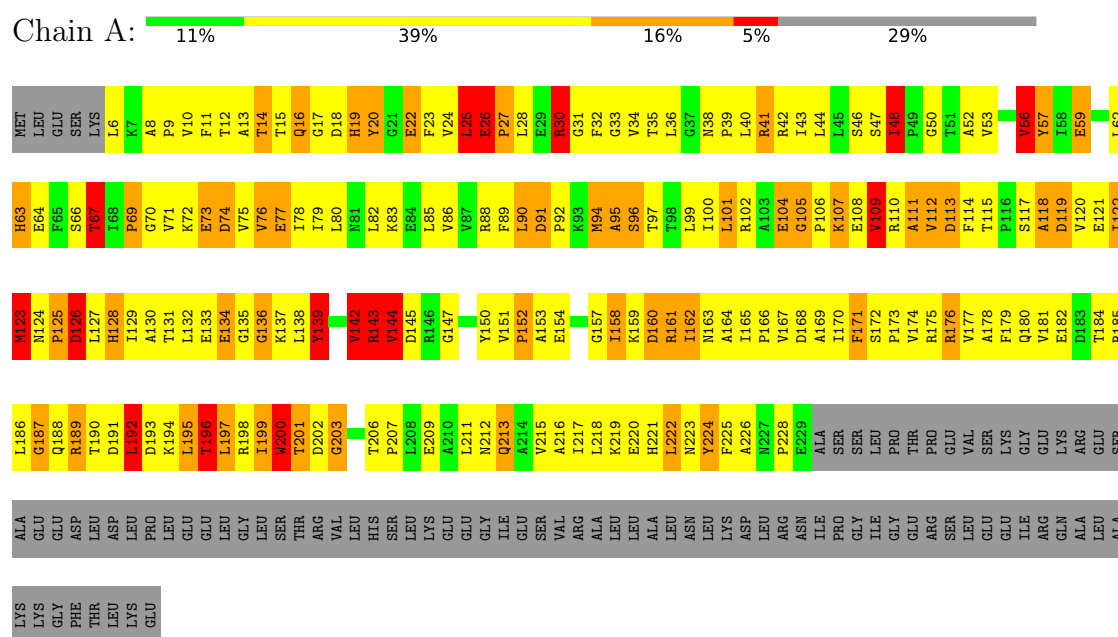
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

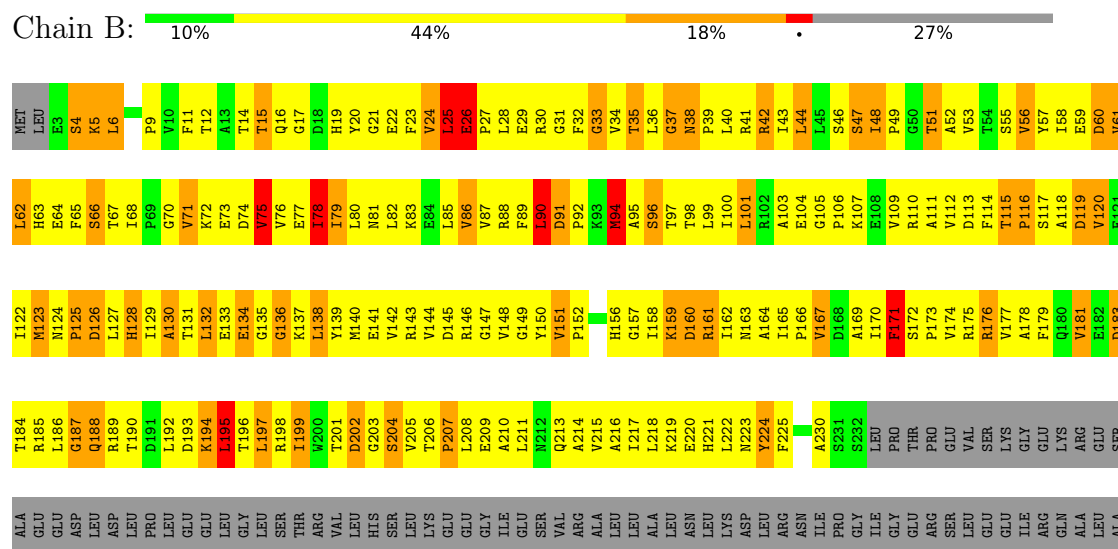
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: DNA-DIRECTED RNA POLYMERASE



• Molecule 1: DNA-DIRECTED RNA POLYMERASE

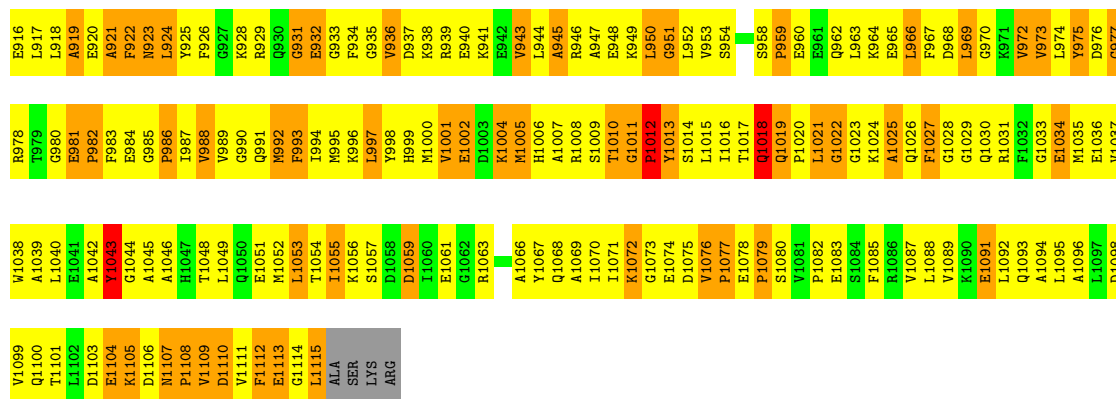


LYS
LYS
GLY
PHE
THR
LEU
LYS
GLU

• Molecule 2: DNA-DIRECTED RNA POLYMERASE

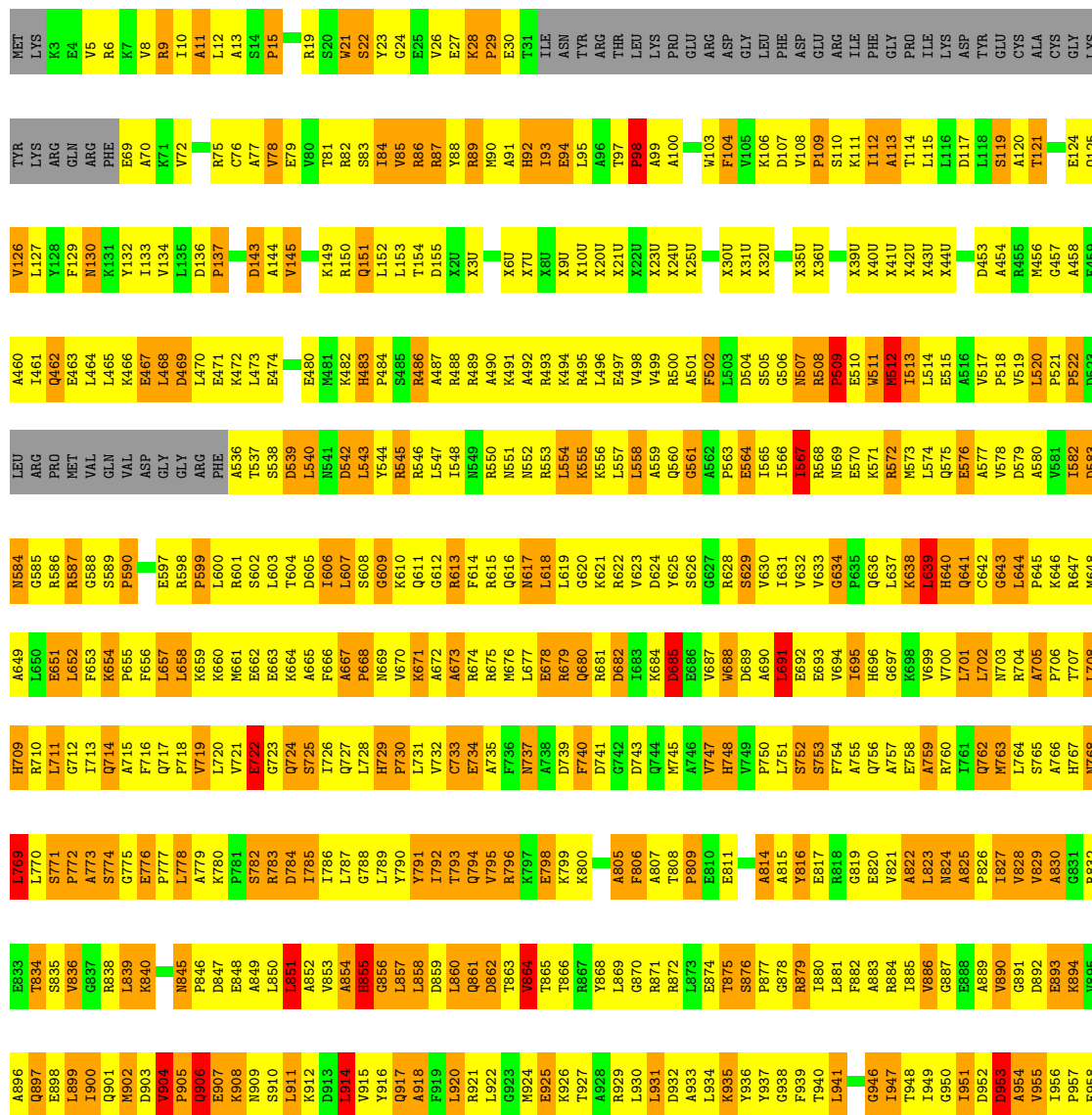
Chain C: 11% 56% 29%

E886	E796	A732	M871	T609	F549	T487	V427	L367	T306	P244	T183	M121	K61	NET
E887	G797	A733	B672	B610	L550	A488	R428	T368	L307	G245	M184	T122	G62	K2
E888	G798	L734	B673	B611	E551	S489	D429	T369	L308	T246	K185	E123	G63	I3
E889	E799	R735	B674	A612	H552	E490	H430	A370	Y309	P247	R186	G124	L64	K4
E890	K800	D736	A675	B613	D553	E491	V431	K371	L310	P248	K187	G125	V65	R5
E891	L801	R737	L676	B614	D554	D492	R432	L372	F311	K249	S126	S126	L66	F6
E892	G802	L738	M677	B615	A555	R493	T433	T373	A312	K250	K190	F127	D67	G7
E893	R803	E739	B678	B616	N556	E494	H434	K374	L313	D251	F191	T128	F68	R8
E894	L804		F679	D617	R557	T495	Y435	S375	T314	K252	P192	E129	L69	R19
E895	R805	I742	G681	B618	A558	L496	G436	A376	E70	A253	R195	K130	E70	R15
E896	L806	V743	G681	B619	L559	A497	R437	P377	G316	L254	V194	Y71	Y71	E11
E897	R807	R744	G682	L620	M560	Q498	I438	L378	L195	A255	R196	R72	R72	E12
E898	R808	I745	M683	B621	G561	A499	C439	E379	F318	Y256	L196	I73	I73	E13
E899	G809	G746	B623	H623	S562	N500	V440	A380	G319	L257	L197	G135	G74	F15
E900	D810	A747	G684	B624	N563	T501	V441	A381	H320	F258	R198	I136	D75	P16
E901	P811	E748	G686	L625	M564	R502	E442	L382	V321	G259	V199	V137	P76	P17
E902	G812	V749	A687	B626	G565	L503	T443	R383	V322	L260	K200	S138	P77	P18
E903	V813	K750	L688	B627	T566	L503	P444	F384	D323	L261	G201	Q139	F78	I18
E904	E814		E689	Y628	Q567	R507	E445	F385	D324	A262	Y202	I140	S79	T19
E905	L815	D753	B690	A629	L589	I508	G446	F386	L325	D263	D203	H41	Q80	E20
E906	B766	I754	S691	B630	V569	A509	I754	S387	D326	P264	Q204	R142	D81	I21
E907	P817	K816	L755	S631	P570	T510	N448	R388	H327	K265	E205	S143	E82	Q22
E908	G818	V756	E693	B632	L571	D511	I449	S389	L328	R266	K206	P144	G83	V23
E909	V819	G757	L694	D633	L572	R512	G450	Q390	G329	Y267	L207	G145	R84	E24
E910	R820	R758	L695	G634	R573	V513	L451	L391	N330	D268	V208	V146	E85	S25
E911	E821	T759	G696	T635	A574	V514	I452	S392	R331	L269	R209	I147	K96	Z26
E912	R822	S760	R697	A636	Q575	A515	T453	Q393	R332	G270	E210	F148	D87	Y27
E913	R823	F761	G698	F637	A576	R516	S454	F394	L333	L289	S212	T149	L88	X26
E914	R824	K762	F699	D638	P577	R517	L455	K395	R334	G273	K211	P150	T69	A29
E915	R825	G763	F700	Q1639	V578	R518	A456	D396	T335	R274	A213	D151	Y90	L30
E916	E826		T701	R640	M579	G519	A457	E397	V336	Y275	Y214	P152	Q91	Q31
E917	R827		R702	B641	E590	E520	Y458	T398	E337	K276	G215	A153	A92	A32
E918	R828	T768	L703	H642	T581	P521	A459	L404	F344	G284	L222	K160	Q99	R38
E919	G829	R769	H704	B643	G582	V522	R460	L405	E338	R285	L222	R345	G99	R39
E920	K830	E770	L705	B644	L583	I523	V461	H406	L339	L217	L216	P154	P34	E40
E921	R831	E771	E706	B645	E584	V524	F466	K407	V346	S286	E224	I162	I101	R41
E922	K832	R772	R707	G646	E585	A525	D462	L408	A341	G287	A225	I163	H02	V42
E923	L833	L773		G647	R586	E526	P526	L409	L348	R288	V226	P164	K103	G43
E924	E834			B648	L587	R528	F467	R409	L349	T289	L227	L165	I04	L44
E925	R835	R774	L711		S588	V529	R468	L410	F345	L290	A228	P166	G105	Q45
E926	G836	R775	L712	B651	R589	E529	V467	A411	R350	V291	G106	K167	T105	A46
E927	R837	S776	A713	G651	V590	E530	R469	L412	A352	R292	R230	R168	L107	A47
E928	K838	I777	R713	G652	D590	E530	F468	L413	R353	F293	P231	G169	F48	F48
E929	R839	R778	D714	B653	L591	F531	T469	L414	R354	E294	E232	P170	K109	R49
E930	G840	G779	L715	L654	S592	M532	P470	L415	F355	D295	E233	W71	E50	E50
E931	R900	R780	K716	L655	A593	D533	Y471	G416	V356	G296	A234	D111	D111	T51
E932	N901	N841	L717	A656	E594	V534	R472	A412	R357	E297	R235	D173	F52	E52
E933	R842	K781	L718	D657	L595	S535	R473	L413	R358	F298	V236	L174	V113	P53
E934	H843	R782	G718	G658	L596	E536	V474	L414	K359	D299	R237	E175	F114	L54
E935	E844	E783	P719	G659	R597	P537	V475	F415	V360	D300	L116	E176	L116	L55
E936	N904	R784	R720	B659	L598	K543	R476	F416	E421	G301	E301	V177	G177	E56
E937	N905	R785	R721	A660	E598	N543	N476	G417	V356	E296	L238	E178	L118	R57
E938	F906	K786	L722	B661	E599	V539	G477	G418	R356	G297	R239	D172	D111	T51
E939	D907	G847	R723	B662	R601	F540	V478	L418	E357	F298	V236	L174	V113	P53
E940	G948	T788	R724	E663	G601	S541	V479	T419	R358	D299	R237	E175	F114	L54
E941	N908	S789	D725	G664	E602	L542	T480	R420	K359	D300	L116	E176	L116	L55
E942	T910	R790	I726	F665	R603	N543	E481	E421	V360	E301	L238	E177	L118	R57
E943	R851	R791	T727	L666	V604	T544	E482	R422	G362	F302	L239	V177	G177	E56
E944	P912	I852	H728	A667	K605	N545	V483	A423	S363	F303	L241	E177	L118	R57
E945	E913	T793	L729	L668	R606	L546	V484	G424	S363	F303	L241	E177	L118	R57
E946	R854	P794	E730	G669	D607	V547	V485	G424	S364	L304	L242	E177	L118	R57
E947	E914	E795	S731	E670	E668	D549	V486	G425	P364	D205	E242	E177	L118	R57



• Molecule 3: DNA-DIRECTED RNA POLYMERASE

Chain D: 15% 49% 25% 7%



- Molecule 4: DNA-DIRECTED RNA POLYMERASE

Chain E: 17% 58% 23%

[illegible]

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	199.45Å 199.45Å 289.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.276 , 0.359	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21292	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, RFP

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	0.56	0/1775	1.11	12/2417 (0.5%)
1	B	0.59	1/1795 (0.1%)	1.16	13/2447 (0.5%)
2	C	0.54	0/8672	1.21	107/11752 (0.9%)
3	D	0.60	2/8439 (0.0%)	1.30	123/11447 (1.1%)
4	E	0.47	0/730	1.15	7/991 (0.7%)
All	All	0.57	3/21411 (0.0%)	1.23	262/29054 (0.9%)

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
2	C	0	1
3	D	0	3
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1270	ALA	C-N	-19.61	1.06	1.33
1	B	94	MET	SD-CE	12.20	2.10	1.79
3	D	1268	PRO	C-N	5.74	1.41	1.33

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270	ALA	O-C-N	-22.83	92.23	122.59
3	D	1270	ALA	CA-C-N	17.97	155.87	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270	ALA	C-N-CA	17.97	155.87	121.54
3	D	775	GLY	N-CA-C	17.26	127.55	111.67
3	D	834	THR	N-CA-C	-14.30	95.86	114.31
3	D	1069	GLU	N-CA-C	-13.55	96.79	113.18
3	D	1204	CYS	N-CA-C	-12.49	98.19	114.31
3	D	1010	ASN	N-CA-C	-11.79	98.43	111.28
2	C	255	ALA	N-CA-C	-11.24	99.53	113.02
2	C	736	ASP	N-CA-C	-11.05	99.75	113.01
2	C	809	GLY	N-CA-C	-11.02	101.57	114.69
2	C	267	TYR	N-CA-C	-10.89	101.43	112.97
3	D	1326	THR	N-CA-C	-10.78	98.98	112.88
3	D	1205	TYR	N-CA-C	-10.31	100.88	113.15
2	C	7	GLY	N-CA-C	10.24	124.40	110.58
3	D	1278	ASP	N-CA-C	-10.22	100.75	113.02
2	C	256	TYR	N-CA-C	-9.94	100.84	113.16
3	D	677	LEU	N-CA-C	-9.92	101.17	113.38
3	D	966	GLU	N-CA-C	-9.79	100.61	111.28
2	C	919	ALA	N-CA-C	-9.56	100.84	111.07
3	D	1065	LEU	N-CA-C	-9.34	99.39	110.41
3	D	1297	GLU	N-CA-C	-9.32	101.92	113.38
3	D	1388	ARG	N-CA-C	9.30	124.82	113.38
3	D	955	VAL	N-CA-C	9.28	121.29	107.75
2	C	590	ASP	N-CA-C	-9.19	102.07	113.38
3	D	1267	ARG	CA-C-N	9.18	131.31	119.84
3	D	1267	ARG	C-N-CA	9.18	131.31	119.84
2	C	379	GLU	N-CA-C	-9.01	97.13	110.46
3	D	27	GLU	N-CA-C	-8.95	102.50	113.15
2	C	580	MET	N-CA-C	8.95	129.85	110.80
3	D	1018	ASN	CA-C-N	-8.81	108.83	119.84
3	D	1018	ASN	C-N-CA	-8.81	108.83	119.84
2	C	950	LEU	N-CA-C	-8.62	101.48	113.20
2	C	923	ASN	N-CA-C	-8.62	102.94	113.19
2	C	218	VAL	N-CA-C	8.58	119.19	111.81
1	A	117	SER	N-CA-C	8.48	122.23	108.32
3	D	814	ALA	N-CA-C	-8.41	102.11	111.28
2	C	1108	PRO	N-CA-C	-8.32	105.02	114.92
2	C	721	ARG	N-CA-C	8.17	122.71	109.40
2	C	29	ALA	N-CA-C	-8.13	103.30	113.55
3	D	897	GLN	N-CA-C	-8.07	103.44	113.28
2	C	999	HIS	N-CA-C	7.88	119.77	111.03
2	C	785	VAL	N-CA-C	7.85	118.71	108.35
1	B	25	LEU	N-CA-C	-7.84	97.81	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	763	MET	N-CA-C	7.81	122.12	112.59
2	C	467	ILE	N-CA-C	7.79	125.54	109.34
2	C	831	ARG	N-CA-C	7.79	122.09	112.59
3	D	1213	ARG	CA-C-N	-7.78	111.59	119.99
3	D	1213	ARG	C-N-CA	-7.78	111.59	119.99
2	C	861	LEU	N-CA-C	-7.76	98.73	110.07
2	C	459	ALA	N-CA-C	7.71	121.41	110.23
3	D	1423	GLY	N-CA-C	-7.70	102.68	112.54
3	D	785	ILE	N-CA-C	-7.61	103.44	110.82
3	D	954	ALA	N-CA-C	-7.54	95.16	108.13
3	D	649	ALA	N-CA-C	-7.52	102.44	111.69
2	C	729	LEU	N-CA-C	-7.46	104.06	113.01
2	C	1011	GLY	CA-C-N	7.45	129.15	119.84
2	C	1011	GLY	C-N-CA	7.45	129.15	119.84
3	D	671	LYS	N-CA-C	-7.42	103.13	111.07
3	D	1031	ASN	CA-C-N	7.41	126.93	118.85
3	D	1031	ASN	C-N-CA	7.41	126.93	118.85
1	A	25	LEU	N-CA-C	-7.39	95.05	110.80
1	A	171	PHE	N-CA-C	7.36	120.38	111.40
1	B	33	GLY	N-CA-C	-7.36	103.60	113.24
2	C	582	GLY	N-CA-C	7.34	123.03	113.27
3	D	618	LEU	N-CA-C	-7.32	103.30	111.28
2	C	351	LEU	N-CA-C	-7.26	103.06	110.97
3	D	972	ARG	N-CA-C	-7.23	103.56	112.38
2	C	737	LEU	N-CA-C	-7.22	100.18	108.49
3	D	918	ALA	N-CA-C	-7.22	103.48	112.72
1	B	26	GLU	N-CA-C	7.21	125.75	109.81
3	D	606	ILE	N-CA-C	-7.19	103.65	113.00
3	D	512	MET	N-CA-C	-7.17	95.53	110.80
2	C	390	GLN	N-CA-C	-7.11	104.21	113.17
2	C	544	THR	N-CA-C	-7.08	102.77	111.40
2	C	209	ARG	N-CA-C	-7.07	104.61	113.23
3	D	979	GLU	N-CA-C	-7.00	104.85	113.19
1	A	22	GLU	N-CA-C	-6.99	100.10	110.23
2	C	464	LEU	N-CA-C	6.98	121.11	107.98
2	C	540	PHE	N-CA-C	6.98	119.55	109.14
2	C	611	ILE	N-CA-C	-6.89	99.74	108.84
3	D	1082	ALA	N-CA-C	-6.88	103.86	111.36
3	D	1042	ARG	N-CA-C	-6.87	96.86	108.26
2	C	1076	VAL	CA-C-N	6.86	128.41	119.84
2	C	1076	VAL	C-N-CA	6.86	128.41	119.84
3	D	1437	ALA	N-CA-C	-6.85	104.89	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	555	LYS	N-CA-C	-6.83	104.95	113.28
1	B	61	VAL	N-CA-C	6.82	118.64	108.54
3	D	545	ARG	N-CA-C	-6.81	103.78	111.07
3	D	508	ARG	N-CA-C	-6.80	94.79	109.81
3	D	976	GLN	N-CA-C	-6.77	105.65	114.04
3	D	973	GLN	N-CA-C	-6.71	105.08	113.20
2	C	465	GLY	N-CA-C	-6.67	103.85	113.86
3	D	137	PRO	N-CA-CB	6.67	110.26	103.25
3	D	1439	SER	N-CA-C	-6.67	104.04	111.71
2	C	792	VAL	CA-C-N	6.67	127.25	120.38
2	C	792	VAL	C-N-CA	6.67	127.25	120.38
2	C	876	VAL	CA-C-N	-6.65	111.53	119.84
2	C	876	VAL	C-N-CA	-6.65	111.53	119.84
2	C	920	GLU	N-CA-C	-6.61	102.00	110.19
1	B	187	GLY	N-CA-C	-6.61	101.78	111.03
2	C	233	GLU	N-CA-C	-6.58	103.33	111.75
2	C	662	GLU	N-CA-C	-6.58	102.34	111.81
3	D	929	ARG	N-CA-C	-6.58	103.00	111.02
2	C	344	PHE	N-CA-C	-6.57	103.95	112.23
2	C	307	LEU	N-CA-C	-6.57	103.39	111.33
2	C	888	THR	N-CA-C	-6.56	103.97	112.23
3	D	729	HIS	N-CA-C	6.54	120.19	108.47
2	C	774	LEU	N-CA-C	-6.54	103.26	111.11
1	B	186	LEU	N-CA-C	-6.51	103.88	110.97
3	D	1079	LYS	N-CA-C	-6.50	104.23	111.71
3	D	967	ALA	N-CA-C	-6.46	103.51	111.33
2	C	21	ILE	N-CA-C	-6.45	104.04	110.62
2	C	801	VAL	N-CA-C	6.44	119.10	111.05
3	D	1280	VAL	N-CA-C	6.42	118.17	108.80
3	D	1281	VAL	N-CA-C	6.41	122.67	109.34
3	D	1125	MET	N-CA-C	6.39	119.60	109.50
2	C	1053	LEU	N-CA-C	-6.39	104.27	113.21
2	C	468	ARG	N-CA-C	6.37	124.37	110.80
3	D	462	GLN	N-CA-C	-6.35	103.28	111.02
3	D	1294	VAL	N-CA-C	-6.31	99.11	108.45
3	D	950	GLY	N-CA-C	-6.31	102.99	113.02
4	E	37	ASN	N-CA-C	-6.30	103.23	113.19
4	E	77	GLU	N-CA-C	-6.28	104.78	112.88
3	D	92	HIS	N-CA-C	6.27	120.71	111.87
3	D	1040	GLY	N-CA-C	-6.27	104.05	112.14
3	D	1086	LEU	N-CA-C	-6.26	105.70	113.15
1	B	91	ASP	CA-C-N	6.25	126.44	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ASP	C-N-CA	6.25	126.44	119.32
2	C	997	LEU	N-CA-C	6.24	118.83	110.35
2	C	1639	GLN	N-CA-C	6.23	118.58	107.80
3	D	98	PRO	N-CA-CB	6.21	109.78	103.25
3	D	151	GLN	N-CA-C	-6.21	103.23	111.24
2	C	830	LYS	N-CA-C	-6.21	100.47	109.59
3	D	971	LEU	N-CA-C	-6.19	103.82	112.12
3	D	1195	GLN	N-CA-C	6.19	120.30	112.87
2	C	836	GLY	N-CA-C	-6.17	98.55	113.18
3	D	520	LEU	CA-C-N	-6.16	114.04	120.38
3	D	520	LEU	C-N-CA	-6.16	114.04	120.38
3	D	29	PRO	N-CA-CB	6.14	109.69	103.25
2	C	756	VAL	CA-C-N	-6.13	117.85	122.33
2	C	756	VAL	C-N-CA	-6.13	117.85	122.33
3	D	1180	ALA	N-CA-C	-6.13	104.90	112.38
3	D	964	LEU	N-CA-C	-6.13	102.43	110.33
3	D	851	LEU	N-CA-C	-6.09	104.72	111.36
2	C	82	GLU	N-CA-C	-6.09	105.11	112.54
3	D	870	GLY	N-CA-C	-6.09	106.03	116.01
3	D	1062	ARG	N-CA-C	-6.09	103.81	111.11
3	D	782	SER	N-CA-C	6.08	116.58	108.38
3	D	1282	ARG	N-CA-C	6.06	123.71	110.80
3	D	1464	GLU	N-CA-C	-6.05	102.30	111.56
2	C	900	ARG	N-CA-C	-6.04	101.05	110.42
3	D	826	PRO	N-CA-CB	6.02	109.57	103.25
3	D	109	PRO	N-CA-CB	6.02	109.50	103.48
2	C	41	ASN	N-CA-C	6.01	118.35	109.69
3	D	1179	GLU	N-CA-C	-5.98	105.64	113.12
2	C	941	LYS	N-CA-C	-5.97	104.69	111.14
3	D	505	SER	CB-CA-C	-5.97	108.69	115.79
2	C	115	LEU	N-CA-C	5.96	115.88	108.19
1	B	101	LEU	N-CA-C	5.95	118.22	109.24
2	C	627	ARG	N-CA-C	5.93	118.62	109.07
1	A	94	MET	N-CA-C	5.89	118.06	108.63
4	E	48	MET	N-CA-C	5.89	113.61	108.78
1	B	78	ILE	N-CA-C	-5.88	104.60	110.30
2	C	97	ARG	N-CA-C	5.88	117.61	109.15
2	C	327	HIS	N-CA-C	-5.87	101.35	110.10
2	C	579	VAL	N-CA-C	-5.87	99.85	109.12
2	C	74	GLY	N-CA-C	5.86	118.50	110.58
3	D	554	LEU	N-CA-C	-5.86	105.98	114.12
3	D	1398	TRP	N-CA-C	-5.85	104.99	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	393	GLN	N-CA-C	5.84	118.07	110.53
2	C	206	THR	N-CA-C	-5.82	105.44	112.54
3	D	759	ALA	N-CA-C	-5.81	106.09	112.72
4	E	21	VAL	N-CA-C	5.81	116.00	110.42
4	E	69	LEU	N-CA-C	-5.79	106.18	113.18
3	D	15	PRO	N-CA-C	-5.78	106.33	113.84
2	C	11	GLU	N-CA-C	5.77	119.13	111.75
3	D	1432	LYS	N-CA-C	5.76	123.07	110.80
3	D	1085	ALA	N-CA-C	-5.75	105.43	113.37
3	D	769	LEU	N-CA-C	-5.75	104.42	112.12
3	D	641	GLN	N-CA-C	5.74	118.91	110.59
3	D	691	LEU	N-CA-C	-5.74	105.03	111.28
1	A	151	VAL	CA-C-N	5.73	127.00	119.84
1	A	151	VAL	C-N-CA	5.73	127.00	119.84
2	C	1006	HIS	N-CA-C	-5.72	98.61	110.80
2	C	814	GLU	N-CA-C	-5.71	99.87	109.07
2	C	648	ARG	N-CA-C	5.70	118.36	111.40
1	A	142	VAL	N-CA-C	5.68	116.73	106.61
3	D	559	ALA	N-CA-C	-5.68	106.06	112.87
3	D	1134	LEU	N-CA-C	-5.66	100.99	109.15
2	C	226	VAL	N-CA-C	-5.66	104.17	110.62
3	D	1029	ARG	N-CA-C	5.65	117.08	110.41
2	C	651	LYS	N-CA-C	-5.65	106.34	113.23
3	D	904	VAL	N-CA-C	5.63	121.05	108.88
3	D	1277	ILE	CB-CA-C	-5.63	104.04	111.70
1	A	95	ALA	N-CA-C	-5.63	105.23	111.71
2	C	892	LEU	N-CA-C	-5.62	105.30	111.82
1	B	181	VAL	N-CA-C	5.61	114.69	106.55
3	D	1389	LEU	N-CA-C	5.61	116.77	108.86
2	C	615	TYR	N-CA-C	5.60	122.73	110.80
2	C	394	PHE	N-CA-C	-5.60	103.14	110.53
2	C	163	ILE	CA-C-N	5.59	126.83	119.84
2	C	163	ILE	C-N-CA	5.59	126.83	119.84
3	D	692	GLU	N-CA-C	-5.55	106.21	112.87
2	C	329	GLY	N-CA-C	-5.55	100.02	113.18
1	A	76	VAL	N-CA-C	-5.55	104.92	110.30
2	C	69	LEU	CB-CA-C	-5.53	108.46	116.54
2	C	1091	GLU	N-CA-C	-5.50	107.57	114.56
3	D	1268	PRO	O-C-N	-5.49	115.22	122.64
2	C	421	GLU	N-CA-C	-5.49	102.78	110.35
3	D	1435	LEU	N-CA-C	5.47	117.70	111.02
2	C	485	TYR	N-CA-C	-5.45	104.08	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	SER	N-CA-C	5.45	115.32	108.45
2	C	391	LEU	N-CA-C	-5.45	106.00	113.30
2	C	884	GLN	N-CA-C	-5.45	106.61	113.20
2	C	35	PRO	CA-C-N	5.44	126.64	119.84
2	C	35	PRO	C-N-CA	5.44	126.64	119.84
2	C	932	GLU	N-CA-C	-5.42	105.76	112.38
2	C	19	THR	N-CA-C	-5.42	105.35	112.72
3	D	1032	PRO	N-CA-C	5.39	120.62	113.40
1	B	171	PHE	N-CA-C	5.36	117.04	108.41
3	D	852	ALA	N-CA-C	-5.34	105.57	111.71
3	D	639	LEU	N-CA-C	-5.34	99.43	110.80
2	C	907	ASP	N-CA-C	5.32	117.33	107.60
2	C	717	LEU	N-CA-C	-5.31	106.57	114.64
3	D	119	SER	N-CA-C	-5.31	106.64	113.23
2	C	1092	LEU	N-CA-C	-5.30	105.95	112.90
3	D	771	SER	CA-C-N	5.30	126.47	119.84
3	D	771	SER	C-N-CA	5.30	126.47	119.84
2	C	345	ARG	N-CA-C	-5.29	105.42	111.14
2	C	73	ILE	N-CA-C	-5.28	98.35	109.34
3	D	1360	GLY	N-CA-C	5.27	121.01	114.37
2	C	542	LEU	N-CA-C	5.27	117.70	111.33
4	E	82	GLU	N-CA-C	-5.26	105.66	111.71
2	C	1004	LYS	N-CA-C	-5.26	102.22	110.17
3	D	1021	TYR	N-CA-C	-5.25	105.19	113.02
3	D	1172	HIS	N-CA-C	-5.25	103.53	111.56
3	D	1431	THR	N-CA-C	5.25	121.98	110.80
2	C	889	HIS	N-CA-C	-5.20	104.54	111.24
3	D	1362	LYS	N-CA-C	5.16	119.15	111.87
2	C	186	VAL	N-CA-C	-5.15	102.20	109.21
2	C	154	ARG	CA-C-N	5.14	126.27	119.84
2	C	154	ARG	C-N-CA	5.14	126.27	119.84
3	D	1118	ILE	N-CA-C	-5.13	98.66	109.34
3	D	1142	SER	N-CA-C	-5.12	106.54	112.89
1	A	56	VAL	N-CA-C	5.12	115.64	108.17
3	D	914	LEU	N-CA-C	-5.10	104.79	111.02
2	C	72	ARG	N-CA-C	5.09	117.27	107.44
3	D	708	LEU	N-CA-C	-5.08	100.42	109.06
3	D	1185	GLU	N-CA-C	-5.08	101.83	109.85
3	D	960	LYS	N-CA-C	-5.08	105.21	111.40
3	D	1186	VAL	CA-C-N	5.07	126.17	119.84
3	D	1186	VAL	C-N-CA	5.07	126.17	119.84
3	D	1468	LEU	N-CA-C	-5.07	107.39	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1231	GLU	N-CA-C	-5.05	105.30	112.17
1	A	104	GLU	N-CA-C	5.02	117.28	110.35
2	C	726	ILE	CA-C-N	5.02	125.30	119.93
2	C	726	ILE	C-N-CA	5.02	125.30	119.93
3	D	121	THR	N-CA-C	5.01	116.74	111.28
3	D	13	ALA	N-CA-C	5.01	116.85	107.99
2	C	221	LEU	N-CA-C	-5.00	107.24	113.19
4	E	48	MET	CB-CA-C	-5.00	109.87	117.07

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
2	C	1013	TYR	Sidechain
3	D	1165	TYR	Sidechain
3	D	1268	PRO	Mainchain
3	D	1270	ALA	Mainchain

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	1741	0	1747	367	0
1	B	1761	0	1754	336	0
2	C	8508	0	8421	1917	0
3	D	8502	0	8002	1758	0
4	E	719	0	685	142	0
5	C	59	0	56	6	0
6	D	1	0	0	0	0
7	D	1	0	0	0	0
All	All	21292	0	20665	4262	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 102.

All (4262) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:MET:CE	1:B:94:MET:SD	2.10	1.39
2:C:690:ILE:HB	2:C:852:ILE:HG22	1.19	1.18
2:C:565:GLN:HG3	2:C:995:MET:HE1	1.25	1.16
3:D:1280:VAL:HG12	3:D:1281:VAL:HG23	1.25	1.16
2:C:491:GLU:HA	2:C:531:PHE:HA	1.29	1.15
3:D:772:PRO:HG3	3:D:778:LEU:HB2	1.28	1.14
2:C:861:LEU:HG	2:C:862:PRO:HD2	1.23	1.14
3:D:1280:VAL:HG13	3:D:1315:ASP:HA	1.25	1.13
2:C:613:VAL:HG21	2:C:619:ARG:HG2	1.31	1.13
2:C:208:VAL:HG11	2:C:218:VAL:HG11	1.27	1.12
3:D:129:PHE:HA	3:D:454:ALA:HB1	1.24	1.12
1:A:96:SER:HB3	1:A:145:ASP:HA	1.16	1.11
2:C:399:ASN:C	2:C:399:ASN:HD22	1.59	1.11
3:D:890:VAL:HG12	3:D:891:GLY:H	1.12	1.10
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.33	1.10
3:D:1015:TYR:HB3	3:D:1019:PRO:HD3	1.33	1.10
3:D:483:HIS:H	3:D:484:PRO:HD2	1.00	1.09
2:C:17:PRO:HD2	2:C:20:GLU:HB2	1.32	1.09
2:C:261:LEU:HG	2:C:263:ASP:HB3	1.33	1.09
2:C:262:ALA:HB1	2:C:266:ARG:HD3	1.15	1.08
1:A:26:GLU:HB3	1:A:27:PRO:CD	1.81	1.08
2:C:129:ILE:HG21	2:C:387:SER:HB2	1.36	1.08
3:D:691:LEU:H	3:D:691:LEU:HD12	1.18	1.08
3:D:728:LEU:HD22	3:D:745:MET:HE1	1.32	1.07
2:C:12:VAL:HG12	2:C:13:ILE:H	1.17	1.07
2:C:115:LEU:HD12	2:C:116:GLY:H	1.12	1.06
3:D:876:SER:H	3:D:879:ARG:HG3	1.20	1.06
3:D:772:PRO:CG	3:D:778:LEU:HB2	1.86	1.06
1:A:30:ARG:HD2	1:A:191:ASP:HB3	1.37	1.05
2:C:376:ARG:H	2:C:377:PRO:HD2	1.20	1.05
2:C:873:PRO:O	2:C:877:PRO:HD2	1.56	1.05
3:D:1019:PRO:HB2	3:D:1022:VAL:HG23	1.37	1.05
3:D:1154:GLU:HB3	3:D:1159:ARG:HG2	1.38	1.05
2:C:333:ILE:HD11	2:C:468:ARG:HE	1.20	1.05
2:C:474:VAL:HG22	2:C:530:GLU:HA	1.37	1.04
2:C:1008:ARG:HD3	2:C:1029:GLY:H	1.19	1.04
3:D:1273:VAL:HG23	3:D:1324:PRO:HG3	1.37	1.04
3:D:886:VAL:HG11	3:D:900:ILE:HD11	1.36	1.03
2:C:253:ALA:HA	2:C:256:TYR:HB2	1.36	1.03
3:D:811:GLU:HA	3:D:814:ALA:HB3	1.34	1.03
3:D:126:VAL:H	3:D:456:MET:HE2	1.23	1.03
2:C:456:ALA:HB3	2:C:459:ALA:HB2	1.34	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:879:ARG:NH2	3:D:904:VAL:HA	1.75	1.02
2:C:710:ILE:HD11	2:C:790:LEU:HD22	1.05	1.02
1:B:195:LEU:HD11	1:B:197:LEU:HD13	1.42	1.02
2:C:140:ILE:HG22	2:C:333:ILE:HG12	1.40	1.01
1:B:26:GLU:HG3	1:B:194:LYS:HD2	1.38	1.01
1:A:26:GLU:HB3	1:A:27:PRO:HD3	1.43	1.01
1:B:97:THR:CG2	1:B:120:VAL:HG21	1.91	1.00
3:D:521:PRO:HG2	3:D:522:PRO:HD3	1.41	1.00
3:D:89:ARG:C	3:D:520:LEU:HD21	1.85	1.00
1:A:131:THR:HG23	2:C:644:ARG:HH21	1.24	1.00
1:A:158:ILE:HD11	1:A:161:ARG:HE	1.23	1.00
2:C:525:ALA:HB1	2:C:526:PRO:HD2	1.44	1.00
3:D:1045:MET:HA	3:D:1045:MET:HE3	1.42	1.00
2:C:1045:ALA:HB1	2:C:1048:THR:HB	1.40	0.99
1:B:97:THR:HG21	1:B:120:VAL:HG21	1.42	0.99
2:C:72:ARG:HD3	2:C:112:GLU:OE1	1.62	0.99
3:D:772:PRO:HD2	3:D:776:GLU:O	1.62	0.99
3:D:1236:LEU:HB2	3:D:1256:LEU:HB2	1.45	0.99
2:C:755:LEU:HD12	2:C:790:LEU:HD23	1.41	0.99
3:D:1141:GLU:HA	3:D:1171:VAL:HG11	1.42	0.98
3:D:1353:GLN:HE21	3:D:1368:ILE:HD11	1.24	0.98
3:D:1092:GLY:HA2	3:D:1096:ARG:HE	1.29	0.98
3:D:860:LEU:HA	3:D:877:PRO:HG2	1.43	0.98
1:A:143:ARG:HE	1:A:159:LYS:HE2	1.24	0.98
2:C:110:GLU:HG2	2:C:369:PRO:HG2	1.44	0.98
3:D:483:HIS:H	3:D:484:PRO:CD	1.75	0.98
3:D:699:VAL:HB	3:D:716:PHE:O	1.63	0.97
3:D:721:VAL:HG12	3:D:722:GLU:H	1.28	0.97
2:C:1055:ILE:H	2:C:1055:ILE:HD12	1.26	0.97
2:C:384:GLU:O	2:C:388:ARG:HB2	1.65	0.97
1:A:96:SER:CB	1:A:145:ASP:HA	1.95	0.97
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.44	0.96
2:C:946:ARG:HE	3:D:861:GLN:HE22	1.10	0.96
3:D:836:VAL:O	3:D:865:THR:HG23	1.65	0.96
1:B:106:PRO:HA	1:B:133:GLU:HA	1.46	0.96
2:C:159:ILE:HD11	2:C:310:LEU:HB2	1.48	0.96
3:D:860:LEU:C	3:D:862:ASP:H	1.69	0.96
2:C:195:LEU:HD13	2:C:227:LEU:HD13	1.48	0.96
2:C:497:ALA:HA	2:C:502:PRO:HG3	1.47	0.96
2:C:165:LEU:HD22	2:C:334:ARG:HD3	1.48	0.95
2:C:564:MET:HE1	2:C:846:LYS:HG2	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:710:ILE:HG13	2:C:790:LEU:HD13	1.46	0.95
3:D:1310:ARG:HA	3:D:1323:GLN:O	1.66	0.94
3:D:483:HIS:HA	3:D:489:ARG:HG3	1.49	0.94
2:C:438:ILE:HD13	2:C:470:PRO:HD3	1.49	0.94
2:C:1001:VAL:HG11	3:D:724:GLN:HB3	1.49	0.94
1:B:106:PRO:HB3	1:B:133:GLU:HG3	1.51	0.93
2:C:1038:TRP:NE1	3:D:1099:VAL:HG11	1.82	0.93
3:D:639:LEU:H	3:D:729:HIS:CD2	1.83	0.93
3:D:899:LEU:O	3:D:900:ILE:HG13	1.66	0.93
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.49	0.93
1:B:26:GLU:HB3	1:B:27:PRO:HD3	1.48	0.93
3:D:857:LEU:HD12	3:D:858:LEU:H	1.34	0.93
3:D:1118:ILE:HD13	3:D:1190:SER:HB3	1.51	0.93
2:C:585:GLU:HG2	2:C:665:PHE:HE2	1.33	0.92
2:C:710:ILE:HD11	2:C:790:LEU:CD2	1.97	0.92
2:C:115:LEU:HD12	2:C:116:GLY:N	1.83	0.92
1:A:30:ARG:H	1:A:30:ARG:HD3	1.35	0.92
2:C:690:ILE:CB	2:C:852:ILE:HG22	1.99	0.92
3:D:1236:LEU:HD11	3:D:1356:TYR:HE2	1.31	0.92
1:B:25:LEU:HD11	1:B:28:LEU:HD11	1.51	0.92
2:C:946:ARG:HE	3:D:861:GLN:NE2	1.67	0.92
2:C:613:VAL:HG13	2:C:620:LEU:H	1.33	0.92
3:D:704:ARG:HH12	3:D:743:ASP:CG	1.78	0.92
3:D:806:PHE:H	3:D:827:ILE:HA	1.35	0.92
2:C:198:ARG:HG2	2:C:228:ALA:HA	1.52	0.92
2:C:585:GLU:HG2	2:C:665:PHE:CE2	2.05	0.91
1:A:38:ASN:ND2	2:C:980:GLY:HA2	1.84	0.91
3:D:699:VAL:H	3:D:756:GLN:NE2	1.68	0.91
3:D:900:ILE:HG22	3:D:902:MET:H	1.35	0.91
1:A:41:ARG:HB3	1:A:41:ARG:NH1	1.85	0.91
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.52	0.91
1:A:197:LEU:HD23	1:A:197:LEU:H	1.35	0.91
3:D:1147:ARG:NH1	3:D:1190:SER:HB2	1.86	0.91
2:C:605:LYS:HG2	2:C:607:ASP:H	1.33	0.90
2:C:749:VAL:HG11	2:C:792:VAL:HG21	1.53	0.90
2:C:852:ILE:HD13	2:C:852:ILE:N	1.84	0.90
3:D:615:ARG:HA	3:D:618:LEU:HD12	1.52	0.90
2:C:31:GLN:OE1	2:C:39:ARG:HB3	1.71	0.90
3:D:1019:PRO:C	3:D:1021:TYR:H	1.77	0.90
2:C:203:ASP:O	2:C:206:THR:HG22	1.72	0.90
3:D:1261:GLU:CD	3:D:1268:PRO:HB3	1.97	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:483:HIS:N	3:D:484:PRO:HD2	1.86	0.90
2:C:564:MET:SD	2:C:840:ALA:HB1	2.12	0.90
3:D:552:ASN:HA	3:D:555:LYS:HB3	1.53	0.90
2:C:323:ASP:C	2:C:325:ILE:H	1.79	0.90
3:D:643:GLY:HA3	3:D:727:GLN:H	1.37	0.90
3:D:1278:ASP:HA	3:D:1318:TYR:HA	1.54	0.90
2:C:256:TYR:HA	2:C:260:LEU:HD13	1.54	0.89
4:E:31:LEU:HD12	4:E:35:PHE:HA	1.54	0.89
3:D:901:GLN:HB2	3:D:905:PRO:HG3	1.52	0.89
1:A:88:ARG:HD3	1:A:121:GLU:OE2	1.72	0.89
1:A:15:THR:HG22	1:B:230:ALA:HB1	1.53	0.89
1:A:160:ASP:O	1:A:162:ILE:HG22	1.72	0.89
3:D:1321:ALA:O	3:D:1323:GLN:N	2.05	0.89
2:C:99:GLN:HB3	2:C:109:LYS:HG2	1.54	0.89
3:D:1253:THR:HA	3:D:1258:ARG:HD2	1.53	0.89
2:C:246:ASP:HB3	2:C:247:PRO:HD2	1.54	0.89
2:C:1103:ASP:HB2	2:C:1108:PRO:HB2	1.55	0.89
3:D:1008:PHE:HE1	3:D:1035:ILE:HG13	1.37	0.89
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.53	0.89
2:C:1095:LEU:HD12	3:D:603:LEU:HD23	1.55	0.89
1:B:78:ILE:HG13	1:B:130:ALA:HB2	1.52	0.89
2:C:159:ILE:HD13	2:C:306:THR:HG23	1.55	0.89
2:C:260:LEU:O	2:C:261:LEU:HD23	1.73	0.89
1:A:72:LYS:HA	2:C:607:ASP:HB3	1.55	0.88
3:D:1024:ALA:HA	3:D:1028:ALA:HB3	1.51	0.88
2:C:110:GLU:CG	2:C:369:PRO:HG2	2.03	0.88
2:C:701:THR:HG22	2:C:832:LYS:HA	1.56	0.88
2:C:1017:THR:O	2:C:1018:GLN:HB2	1.71	0.88
2:C:257:LEU:HD23	2:C:261:LEU:HD21	1.54	0.88
2:C:726:ILE:HD12	2:C:726:ILE:H	1.37	0.88
3:D:699:VAL:H	3:D:756:GLN:HE22	1.19	0.88
2:C:631:SER:HB2	2:C:635:THR:H	1.36	0.88
2:C:605:LYS:HA	2:C:612:ALA:HB3	1.53	0.88
2:C:32:ALA:HA	2:C:71:TYR:HE1	1.38	0.87
2:C:493:ARG:HH12	3:D:1069:GLU:HA	1.36	0.87
2:C:889:HIS:CE1	3:D:951:ILE:H	1.92	0.87
3:D:1015:TYR:CB	3:D:1019:PRO:HD3	2.05	0.87
2:C:588:VAL:O	2:C:588:VAL:HG12	1.74	0.87
3:D:1043:GLY:HA2	3:D:1057:VAL:HG23	1.54	0.87
2:C:290:LEU:HD11	2:C:298:PHE:HB3	1.56	0.87
2:C:551:GLU:HA	2:C:906:PHE:HE2	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:762:LYS:HD2	2:C:786:LYS:HD2	1.56	0.87
4:E:78:ASN:OD1	4:E:79:LEU:HG	1.73	0.87
2:C:674:VAL:HB	2:C:869:VAL:HG13	1.56	0.87
2:C:1040:LEU:HD12	2:C:1045:ALA:HB3	1.57	0.87
3:D:783:ARG:O	3:D:784:ASP:HB2	1.71	0.87
1:A:79:ILE:HD11	1:A:165:ILE:HD12	1.57	0.87
1:B:211:LEU:O	1:B:215:VAL:HG23	1.74	0.86
2:C:892:LEU:H	2:C:892:LEU:CD2	1.88	0.86
3:D:1466:VAL:O	3:D:1469:GLY:N	2.08	0.86
2:C:15:LEU:HD11	2:C:461:VAL:HG21	1.57	0.86
2:C:396:ASP:OD1	2:C:402:SER:HB3	1.75	0.86
3:D:129:PHE:HA	3:D:454:ALA:CB	2.05	0.86
1:A:79:ILE:HD11	1:A:165:ILE:CD1	2.05	0.86
2:C:1008:ARG:HD3	2:C:1029:GLY:N	1.91	0.86
1:A:59:GLU:HG2	1:A:137:LYS:HE3	1.56	0.86
2:C:115:LEU:CD1	2:C:116:GLY:H	1.89	0.86
3:D:1194:CYS:HB3	3:D:1373:ARG:NH2	1.90	0.86
2:C:1052:MET:O	2:C:1053:LEU:HD13	1.74	0.86
2:C:184:MET:HE3	2:C:191:PHE:HZ	1.40	0.86
2:C:569:VAL:HG13	2:C:569:VAL:O	1.73	0.86
2:C:9:ILE:HG22	2:C:10:ARG:N	1.89	0.85
1:A:131:THR:HG23	2:C:644:ARG:NH2	1.91	0.85
3:D:1043:GLY:HA3	3:D:1057:VAL:H	1.41	0.85
1:A:88:ARG:HB3	1:A:121:GLU:HB2	1.56	0.85
1:B:214:ALA:HA	1:B:217:ILE:HD12	1.55	0.85
2:C:959:PRO:HG2	2:C:960:GLU:H	1.41	0.85
3:D:876:SER:N	3:D:879:ARG:HG3	1.91	0.85
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.59	0.85
3:D:1132:LEU:HD13	3:D:1184:ARG:HH12	1.41	0.85
2:C:642:ARG:HG2	2:C:643:VAL:HG23	1.56	0.85
3:D:113:ALA:HB2	3:D:495:ARG:HH22	1.38	0.85
3:D:855:HIS:H	3:D:855:HIS:CD2	1.93	0.85
2:C:443:THR:HG21	2:C:454:SER:HB2	1.56	0.84
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.12	0.84
2:C:162:ILE:HG13	2:C:171:TRP:CZ3	2.11	0.84
2:C:613:VAL:CG2	2:C:619:ARG:HG2	2.06	0.84
3:D:1280:VAL:HG12	3:D:1281:VAL:CG2	2.08	0.84
2:C:12:VAL:HG12	2:C:13:ILE:N	1.90	0.84
3:D:502:PHE:HE1	3:D:1452:ILE:HG13	1.41	0.84
3:D:772:PRO:HG3	3:D:778:LEU:CB	2.07	0.84
3:D:1147:ARG:HH12	3:D:1190:SER:HB2	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:HE	1:A:159:LYS:CE	1.90	0.84
2:C:852:ILE:HD13	2:C:852:ILE:H	1.37	0.84
2:C:882:LEU:N	2:C:882:LEU:HD23	1.91	0.84
2:C:89:THR:O	2:C:91:GLN:HG3	1.78	0.84
2:C:440:PRO:HB3	2:C:541:SER:HB3	1.58	0.84
2:C:843:HIS:CD2	2:C:884:GLN:HA	2.13	0.84
2:C:278:GLU:HG3	2:C:284:GLY:H	1.43	0.83
2:C:324:ASP:O	2:C:326:ASP:N	2.10	0.83
2:C:1008:ARG:CZ	2:C:1020:PRO:HB3	2.07	0.83
1:B:86:VAL:HG23	1:B:124:ASN:ND2	1.92	0.83
2:C:13:ILE:HG22	2:C:15:LEU:H	1.43	0.83
3:D:879:ARG:NE	3:D:904:VAL:HG22	1.94	0.83
2:C:198:ARG:CG	2:C:228:ALA:HA	2.08	0.83
2:C:333:ILE:HD11	2:C:468:ARG:NE	1.92	0.83
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.59	0.83
2:C:1107:ASN:N	2:C:1108:PRO:HD3	1.93	0.83
3:D:879:ARG:CD	3:D:904:VAL:HG22	2.07	0.83
3:D:1450:ALA:HA	3:D:1455:LYS:HG3	1.61	0.83
2:C:58:ASP:CB	2:C:61:LYS:HG3	2.09	0.83
2:C:672:VAL:HG22	2:C:868:ASP:OD2	1.77	0.83
1:A:131:THR:O	1:A:131:THR:HG22	1.79	0.83
3:D:465:LEU:HD23	3:D:509:PRO:HB3	1.59	0.83
3:D:890:VAL:HG12	3:D:891:GLY:N	1.90	0.83
3:D:908:LYS:HG3	3:D:1027:GLY:CA	2.07	0.83
3:D:1015:TYR:HB3	3:D:1018:ASN:HB2	1.61	0.83
4:E:38:THR:HG22	4:E:40:LEU:H	1.43	0.83
2:C:1051:GLU:HG2	2:C:1056:LYS:HE2	1.58	0.83
3:D:590:PRO:HB3	3:D:599:PRO:HA	1.60	0.83
3:D:1011:PHE:HA	3:D:1014:ASN:O	1.76	0.83
2:C:399:ASN:C	2:C:399:ASN:ND2	2.36	0.83
3:D:511:TRP:O	3:D:512:MET:HG3	1.79	0.83
1:A:143:ARG:NE	1:A:159:LYS:HE2	1.94	0.82
2:C:875:GLY:HA2	2:C:879:ARG:HG3	1.61	0.82
3:D:1003:VAL:O	3:D:1007:VAL:HG12	1.79	0.82
3:D:1107:VAL:HG21	3:D:1215:VAL:HG11	1.61	0.82
3:D:1282:ARG:CG	3:D:1293:PHE:HB2	2.10	0.82
3:D:900:ILE:HG22	3:D:902:MET:N	1.94	0.82
3:D:1154:GLU:HA	3:D:1159:ARG:HA	1.61	0.82
2:C:924:LEU:N	2:C:924:LEU:HD23	1.94	0.82
2:C:1012:PRO:HB3	2:C:1023:GLY:HA3	1.58	0.82
3:D:792:ILE:HG21	3:D:881:LEU:HD23	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LEU:HD11	1:B:28:LEU:HD21	1.59	0.82
3:D:728:LEU:CD2	3:D:745:MET:HE1	2.08	0.82
3:D:1213:ARG:HG3	3:D:1214:PRO:N	1.95	0.82
1:B:103:ALA:HB3	1:B:137:LYS:O	1.80	0.82
3:D:521:PRO:CG	3:D:522:PRO:HD3	2.09	0.82
4:E:48:MET:HG2	4:E:49:ARG:H	1.45	0.82
2:C:110:GLU:H	2:C:369:PRO:HG3	1.44	0.82
3:D:1251:ASP:H	3:D:1269:LYS:NZ	1.76	0.82
3:D:1376:LEU:HD11	3:D:1421:LEU:HD12	1.62	0.82
1:B:98:THR:HG22	1:B:99:LEU:N	1.92	0.82
3:D:1250:THR:HG23	3:D:1269:LYS:HD3	1.61	0.82
2:C:564:MET:SD	2:C:846:LYS:HB3	2.20	0.82
2:C:695:LEU:HD21	2:C:833:LEU:HB3	1.60	0.82
3:D:1403:LEU:HD21	3:D:1415:VAL:H	1.44	0.82
2:C:15:LEU:HD21	2:C:461:VAL:CG2	2.09	0.81
3:D:890:VAL:HG11	3:D:922:LEU:CD1	2.08	0.81
3:D:731:LEU:HD11	3:D:931:LEU:HD12	1.61	0.81
2:C:32:ALA:HA	2:C:71:TYR:CE1	2.14	0.81
3:D:1277:ILE:HD12	3:D:1294:VAL:HG12	1.61	0.81
1:B:151:VAL:HG23	1:B:169:ALA:HB3	1.62	0.81
2:C:256:TYR:C	2:C:260:LEU:HB3	2.06	0.81
2:C:604:VAL:HG11	2:C:619:ARG:NH2	1.94	0.81
2:C:1030:GLN:O	3:D:622:ARG:HA	1.79	0.81
2:C:1005:MET:O	2:C:1005:MET:HG3	1.80	0.81
3:D:1096:ARG:HH11	3:D:1096:ARG:HG3	1.42	0.81
2:C:139:GLN:CD	2:C:334:ARG:HH21	1.88	0.81
2:C:260:LEU:HD23	2:C:261:LEU:N	1.95	0.81
2:C:836:GLY:HA3	2:C:1001:VAL:CG2	2.10	0.81
3:D:1119:SER:HB3	3:D:1185:GLU:HB3	1.62	0.81
2:C:892:LEU:H	2:C:892:LEU:HD22	1.46	0.81
3:D:582:ILE:O	3:D:584:ASN:N	2.14	0.81
2:C:376:ARG:N	2:C:377:PRO:HD2	1.95	0.81
3:D:1037:GLN:HG3	3:D:1042:ARG:HG2	1.63	0.81
3:D:1403:LEU:O	3:D:1407:LEU:HB2	1.81	0.81
1:A:10:VAL:HB	1:A:26:GLU:CG	2.11	0.81
1:A:180:GLN:HE21	2:C:934:PHE:HB3	1.45	0.81
1:B:109:VAL:O	1:B:129:ILE:HB	1.80	0.81
2:C:467:ILE:CG2	2:C:484:VAL:HG21	2.11	0.81
2:C:589:ARG:HH21	2:C:654:LEU:HD12	1.45	0.81
3:D:1459:LEU:HB3	3:D:1465:ASN:HD22	1.46	0.81
2:C:1053:LEU:HD12	3:D:621:LYS:HD2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:882:PHE:HA	3:D:885:ILE:HD12	1.63	0.80
3:D:1258:ARG:CZ	3:D:1262:LEU:HD11	2.11	0.80
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.60	0.80
3:D:969:ARG:HG3	3:D:970:LYS:N	1.95	0.80
2:C:969:LEU:HD11	3:D:952:ASP:H	1.42	0.80
4:E:9:LEU:HA	4:E:12:MET:HE2	1.62	0.80
1:A:158:ILE:HG23	1:A:159:LYS:H	1.45	0.80
1:B:26:GLU:HB3	1:B:27:PRO:CD	2.11	0.80
1:B:41:ARG:HD3	1:B:42:ARG:N	1.96	0.80
2:C:216:ASP:O	2:C:218:VAL:HG23	1.80	0.80
2:C:671:ASN:HA	2:C:993:PHE:HA	1.62	0.80
2:C:889:HIS:HE1	3:D:951:ILE:H	1.26	0.80
3:D:968:ASP:O	3:D:970:LYS:N	2.14	0.80
3:D:1103:HIS:C	3:D:1105:ILE:H	1.89	0.80
2:C:613:VAL:HG12	2:C:614:ARG:N	1.96	0.80
3:D:795:VAL:HG13	3:D:864:VAL:CG2	2.10	0.80
2:C:580:MET:HB2	2:C:584:GLU:OE1	1.81	0.80
2:C:261:LEU:CG	2:C:263:ASP:HB3	2.12	0.80
2:C:572:ILE:O	2:C:573:ARG:HB2	1.81	0.80
2:C:84:ARG:HA	2:C:131:GLY:HA2	1.64	0.80
2:C:108:ILE:HD13	2:C:368:THR:HG22	1.64	0.80
2:C:654:LEU:O	2:C:655:LEU:HB3	1.81	0.80
3:D:881:LEU:O	3:D:885:ILE:HG13	1.82	0.80
1:A:24:VAL:HG12	1:A:25:LEU:O	1.82	0.80
2:C:1005:MET:HB2	3:D:629:SER:HB2	1.63	0.80
3:D:631:ILE:HG21	3:D:745:MET:HE3	1.62	0.80
3:D:1062:ARG:HH11	3:D:1062:ARG:HG3	1.45	0.80
3:D:1086:LEU:HD13	3:D:1238:MET:HB2	1.63	0.80
3:D:1351:GLU:OE1	3:D:1354:LYS:HD2	1.82	0.80
4:E:40:LEU:C	4:E:42:PRO:HD2	2.06	0.80
2:C:9:ILE:HG22	2:C:10:ARG:H	1.47	0.80
3:D:890:VAL:CG1	3:D:922:LEU:HD13	2.11	0.80
3:D:1067:VAL:HG12	3:D:1069:GLU:HB2	1.64	0.80
2:C:149:THR:OG1	2:C:323:ASP:HA	1.82	0.79
2:C:460:ARG:NH1	2:C:464:LEU:HD21	1.97	0.79
2:C:631:SER:HB2	2:C:635:THR:N	1.96	0.79
3:D:772:PRO:HD3	3:D:778:LEU:H	1.47	0.79
3:D:886:VAL:CG1	3:D:900:ILE:HD11	2.12	0.79
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.63	0.79
2:C:147:TYR:O	2:C:322:VAL:HG13	1.83	0.79
3:D:876:SER:H	3:D:879:ARG:CG	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:LEU:HD12	2:C:291:VAL:H	1.45	0.79
3:D:1145:TYR:HD2	3:D:1145:TYR:C	1.90	0.79
3:D:1378:TYR:HE2	3:D:1431:THR:HB	1.45	0.79
2:C:149:THR:HB	2:C:158:TYR:HE1	1.46	0.79
2:C:440:PRO:HG3	2:C:454:SER:H	1.46	0.79
2:C:921:ALA:H	2:C:924:LEU:HD21	1.47	0.79
3:D:860:LEU:C	3:D:862:ASP:N	2.32	0.79
3:D:1459:LEU:CD1	3:D:1470:ARG:HH11	1.96	0.79
2:C:140:ILE:CG2	2:C:333:ILE:HG12	2.12	0.79
2:C:474:VAL:HG13	2:C:529:VAL:O	1.83	0.79
3:D:113:ALA:HB2	3:D:495:ARG:NH2	1.98	0.79
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.64	0.79
1:A:163:ASN:O	1:A:165:ILE:HG23	1.82	0.79
2:C:478:VAL:O	2:C:479:VAL:HG13	1.81	0.79
2:C:613:VAL:HG11	2:C:619:ARG:CG	2.12	0.79
2:C:452:ILE:HG21	5:C:1640:RFP:O11	1.82	0.79
2:C:807:ARG:O	2:C:810:ASP:HB2	1.83	0.79
3:D:721:VAL:HG12	3:D:722:GLU:N	1.98	0.79
2:C:839:LEU:HD12	2:C:994:ILE:CG2	2.12	0.79
3:D:1483:PHE:CZ	4:E:18:ARG:HG3	2.17	0.79
2:C:531:PHE:O	2:C:532:MET:HB2	1.82	0.79
2:C:163:ILE:HG22	2:C:164:PRO:HD2	1.65	0.78
2:C:577:PRO:HG2	2:C:580:MET:HB3	1.65	0.78
3:D:728:LEU:HD22	3:D:745:MET:CE	2.13	0.78
3:D:1207:TYR:HA	3:D:1213:ARG:O	1.82	0.78
2:C:873:PRO:HG2	2:C:874:LEU:H	1.46	0.78
2:C:922:PHE:C	2:C:924:LEU:H	1.89	0.78
3:D:126:VAL:N	3:D:456:MET:HE2	1.98	0.78
2:C:862:PRO:HA	2:C:975:TYR:HE1	1.48	0.78
1:A:222:LEU:HD12	1:B:215:VAL:HG13	1.63	0.78
2:C:690:ILE:HB	2:C:852:ILE:CG2	2.08	0.78
2:C:952:LEU:HD23	2:C:966:LEU:HD11	1.65	0.78
3:D:1160:LEU:HD22	3:D:1164:ARG:NH1	1.98	0.78
3:D:1196:THR:HB	3:D:1199:GLY:O	1.84	0.78
1:B:44:LEU:O	1:B:174:VAL:HG21	1.83	0.78
2:C:225:ALA:O	2:C:229:MET:HG2	1.84	0.78
2:C:401:LEU:HD21	2:C:543:ASN:HB3	1.64	0.78
3:D:1019:PRO:HB2	3:D:1022:VAL:CG2	2.14	0.78
1:B:169:ALA:HB1	1:B:171:PHE:CZ	2.19	0.78
2:C:666:LEU:HD11	2:C:668:LEU:HD21	1.66	0.78
3:D:765:SER:O	3:D:769:LEU:HB2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:947:ILE:O	3:D:947:ILE:HG13	1.83	0.78
3:D:948:THR:O	3:D:1020:LEU:HB2	1.84	0.78
2:C:533:ASP:HB3	2:C:538:GLN:NE2	1.99	0.78
2:C:602:GLU:H	2:C:647:GLN:HA	1.49	0.78
1:A:20:TYR:O	1:A:207:PRO:HG2	1.82	0.78
1:B:195:LEU:CD1	1:B:197:LEU:HD13	2.14	0.78
2:C:460:ARG:HH11	2:C:464:LEU:HD21	1.48	0.78
2:C:597:ALA:HA	2:C:614:ARG:HH11	1.48	0.78
3:D:1211:MET:HE1	4:E:16:LYS:HD2	1.66	0.78
3:D:1280:VAL:CG1	3:D:1281:VAL:HG23	2.11	0.78
3:D:1484:THR:O	3:D:1486:VAL:HG23	1.83	0.78
1:A:23:PHE:CD2	1:A:211:LEU:HD22	2.19	0.77
1:B:47:SER:O	1:B:48:ILE:HG13	1.84	0.77
3:D:905:PRO:O	3:D:906:GLN:HB2	1.84	0.77
3:D:1459:LEU:HD13	3:D:1470:ARG:HH11	1.47	0.77
1:B:94:MET:HE1	1:B:119:ASP:HB2	1.64	0.77
2:C:474:VAL:HG22	2:C:530:GLU:CA	2.14	0.77
3:D:1007:VAL:HG21	3:D:1039:CYS:HB2	1.65	0.77
3:D:544:TYR:O	3:D:548:ILE:HG12	1.85	0.77
3:D:578:VAL:C	3:D:580:ALA:H	1.91	0.77
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.19	0.77
3:D:648:MET:O	3:D:652:LEU:HD23	1.85	0.77
3:D:1205:TYR:HD2	3:D:1215:VAL:HG21	1.49	0.77
2:C:256:TYR:O	2:C:261:LEU:HD22	1.85	0.77
2:C:376:ARG:H	2:C:377:PRO:CD	1.96	0.77
2:C:551:GLU:HA	2:C:906:PHE:CE2	2.18	0.77
2:C:813:VAL:HG12	2:C:815:LEU:HD11	1.64	0.77
3:D:1290:LEU:HB2	3:D:1305:LEU:O	1.85	0.77
1:A:195:LEU:HD23	1:A:196:THR:H	1.49	0.77
2:C:691:SER:HB2	2:C:858:MET:HE2	1.66	0.77
2:C:460:ARG:HD2	2:C:464:LEU:HD22	1.67	0.77
2:C:475:LYS:O	2:C:477:GLY:N	2.18	0.77
2:C:966:LEU:HD11	2:C:986:PRO:HG3	1.66	0.77
3:D:1282:ARG:HG2	3:D:1293:PHE:HB2	1.64	0.77
2:C:159:ILE:CG1	2:C:310:LEU:HD13	2.14	0.77
2:C:333:ILE:CD1	2:C:468:ARG:HE	1.97	0.77
2:C:944:LEU:HD21	2:C:963:LEU:HD22	1.66	0.77
3:D:547:LEU:HD13	3:D:577:ALA:O	1.85	0.77
1:A:109:VAL:HG23	1:A:130:ALA:O	1.85	0.77
2:C:13:ILE:CG2	2:C:15:LEU:H	1.98	0.77
2:C:184:MET:HE2	2:C:196:LEU:HD22	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:493:ARG:NH1	3:D:1069:GLU:HA	2.00	0.77
2:C:1054:THR:HB	2:C:1055:ILE:HD12	1.67	0.77
3:D:731:LEU:CD1	3:D:931:LEU:HD12	2.15	0.77
1:A:173:PRO:O	1:A:202:ASP:HA	1.85	0.76
2:C:257:LEU:HD22	2:C:264:PRO:HG3	1.67	0.76
2:C:274:ARG:HE	2:C:275:TYR:HE1	1.31	0.76
2:C:810:ASP:OD1	2:C:811:PRO:HD2	1.85	0.76
2:C:969:LEU:HD21	3:D:952:ASP:HB2	1.66	0.76
3:D:465:LEU:HD22	3:D:512:MET:SD	2.26	0.76
3:D:822:ALA:HA	3:D:832:ARG:HB3	1.65	0.76
2:C:163:ILE:H	2:C:163:ILE:HD12	1.47	0.76
2:C:890:LEU:O	2:C:890:LEU:HG	1.85	0.76
3:D:855:HIS:H	3:D:855:HIS:HD2	1.30	0.76
1:B:98:THR:CG2	1:B:99:LEU:N	2.48	0.76
2:C:437:ARG:HB3	3:D:1071:PHE:CE1	2.20	0.76
2:C:963:LEU:HD12	2:C:972:VAL:HG22	1.65	0.76
3:D:1043:GLY:CA	3:D:1057:VAL:HG23	2.15	0.76
3:D:1376:LEU:CD1	3:D:1421:LEU:HD12	2.16	0.76
3:D:1481:VAL:O	3:D:1482:ARG:HG3	1.85	0.76
2:C:79:SER:OG	2:C:82:GLU:HB2	1.86	0.76
3:D:767:HIS:CE1	4:E:6:ILE:HG13	2.20	0.76
3:D:795:VAL:H	3:D:862:ASP:CB	1.99	0.76
3:D:1252:ILE:O	3:D:1258:ARG:HB2	1.85	0.76
2:C:181:VAL:HG12	2:C:182:VAL:HG23	1.67	0.76
2:C:398:THR:OG1	2:C:633:GLN:HG3	1.86	0.76
2:C:1016:ILE:HD12	3:D:536:ALA:HA	1.66	0.76
1:A:41:ARG:NE	2:C:860:HIS:NE2	2.34	0.76
2:C:605:LYS:CA	2:C:612:ALA:HB3	2.16	0.76
3:D:1273:VAL:H	3:D:1324:PRO:HG3	1.51	0.76
3:D:1273:VAL:N	3:D:1324:PRO:HG3	2.01	0.76
3:D:1378:TYR:CD1	3:D:1422:MET:HG3	2.20	0.76
1:A:215:VAL:O	1:A:219:LYS:HG3	1.85	0.76
2:C:348:LEU:HD12	2:C:378:LEU:HD11	1.67	0.76
3:D:691:LEU:H	3:D:691:LEU:CD1	1.98	0.76
3:D:806:PHE:HA	3:D:827:ILE:O	1.86	0.76
3:D:1145:TYR:C	3:D:1145:TYR:CD2	2.63	0.76
3:D:1156:LEU:HD12	3:D:1177:ALA:HA	1.68	0.76
2:C:208:VAL:CG1	2:C:218:VAL:HG11	2.12	0.75
2:C:387:SER:O	2:C:388:ARG:HG3	1.85	0.75
3:D:1126:ASP:OD1	3:D:1128:VAL:HB	1.86	0.75
3:D:1443:THR:HG22	3:D:1447:LEU:HD22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:H	1:A:197:LEU:CD2	1.98	0.75
2:C:80:GLN:O	2:C:81:ASP:HB2	1.84	0.75
3:D:506:GLY:O	3:D:507:ASN:HB3	1.86	0.75
3:D:518:PRO:HB3	3:D:544:TYR:CE1	2.21	0.75
3:D:790:TYR:CE2	3:D:906:GLN:HB3	2.22	0.75
3:D:1235:GLN:O	3:D:1236:LEU:HD23	1.87	0.75
1:A:35:THR:HG21	1:B:43:ILE:HD11	1.67	0.75
1:A:72:LYS:CA	2:C:607:ASP:HB3	2.17	0.75
1:B:103:ALA:HB1	1:B:132:LEU:HD11	1.67	0.75
1:B:199:ILE:HG23	1:B:201:THR:HG23	1.68	0.75
2:C:710:ILE:N	2:C:710:ILE:HD12	2.01	0.75
2:C:1053:LEU:CD1	3:D:621:LYS:HD2	2.15	0.75
2:C:440:PRO:HD3	2:C:455:LEU:N	2.02	0.75
3:D:571:LYS:C	3:D:573:MET:H	1.94	0.75
3:D:865:THR:HG22	3:D:866:THR:N	2.01	0.75
1:A:39:PRO:O	1:A:43:ILE:HG12	1.86	0.75
1:B:100:ILE:HG23	1:B:141:GLU:HG2	1.69	0.75
2:C:239:PHE:CE1	2:C:254:LEU:HD23	2.22	0.75
2:C:659:PRO:O	2:C:660:ALA:HB2	1.85	0.75
2:C:748:GLU:HA	2:C:799:ILE:HA	1.66	0.75
3:D:1481:VAL:CG1	4:E:21:VAL:HG21	2.17	0.75
1:B:78:ILE:CG1	1:B:130:ALA:HB2	2.16	0.75
2:C:613:VAL:HG22	2:C:620:LEU:C	2.12	0.75
2:C:730:SER:HA	2:C:734:LEU:HD11	1.67	0.75
3:D:626:SER:HA	3:D:652:LEU:HD11	1.68	0.75
3:D:881:LEU:HG	3:D:885:ILE:HD11	1.68	0.75
3:D:1283:ILE:HG12	3:D:1292:VAL:HG22	1.69	0.75
3:D:1457:ASP:CG	3:D:1459:LEU:HD23	2.11	0.75
2:C:251:ASP:O	2:C:252:LYS:HB3	1.84	0.75
2:C:438:ILE:HD12	2:C:484:VAL:HG22	1.69	0.75
2:C:705:ILE:H	2:C:705:ILE:HD12	1.51	0.75
3:D:855:HIS:O	3:D:857:LEU:N	2.20	0.75
1:B:33:GLY:O	1:B:195:LEU:HD23	1.87	0.75
3:D:100:ALA:HB1	3:D:579:ASP:OD1	1.87	0.75
3:D:968:ASP:O	3:D:971:LEU:N	2.19	0.75
1:B:214:ALA:HA	1:B:217:ILE:CD1	2.17	0.75
2:C:17:PRO:O	2:C:18:LEU:HB2	1.86	0.75
3:D:688:TRP:C	3:D:690:ALA:H	1.94	0.75
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	1.69	0.75
1:B:98:THR:HG23	1:B:142:VAL:O	1.87	0.74
2:C:841:ASN:C	2:C:841:ASN:HD22	1.94	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1069:GLU:HG3	3:D:1072:ILE:HD13	1.69	0.74
3:D:1280:VAL:HG12	3:D:1281:VAL:N	2.02	0.74
3:D:1282:ARG:O	3:D:1283:ILE:HG13	1.87	0.74
1:A:101:LEU:HD12	1:A:102:ARG:N	2.01	0.74
2:C:958:SER:O	2:C:962:GLN:HG3	1.85	0.74
3:D:1092:GLY:HA2	3:D:1096:ARG:NE	2.01	0.74
2:C:168:ARG:NH2	2:C:266:ARG:HG2	2.03	0.74
3:D:115:LEU:C	3:D:117:ASP:H	1.93	0.74
3:D:827:ILE:O	3:D:828:VAL:HG23	1.87	0.74
3:D:1031:ASN:O	3:D:1035:ILE:HG12	1.88	0.74
3:D:1322:GLY:O	3:D:1323:GLN:HB2	1.86	0.74
1:B:178:ALA:HB3	1:B:198:ARG:HE	1.52	0.74
2:C:106:GLY:O	2:C:107:LEU:HD23	1.86	0.74
2:C:260:LEU:HD23	2:C:261:LEU:HB3	1.68	0.74
2:C:571:LEU:HD22	2:C:670:GLN:HG3	1.70	0.74
3:D:1150:ALA:HB2	3:D:1189:ARG:HG2	1.67	0.74
3:D:1459:LEU:HB3	3:D:1465:ASN:ND2	2.01	0.74
2:C:401:LEU:HD21	2:C:543:ASN:CB	2.16	0.74
3:D:675:ARG:HA	3:D:678:GLU:HB2	1.69	0.74
3:D:752:SER:O	3:D:754:PHE:N	2.21	0.74
1:A:89:PHE:O	1:A:119:ASP:HB3	1.86	0.74
1:A:94:MET:CE	1:A:119:ASP:HB2	2.17	0.74
2:C:148:PHE:O	2:C:149:THR:HB	1.87	0.74
2:C:305:PRO:O	2:C:308:ARG:HB3	1.88	0.74
2:C:500:ASN:C	2:C:502:PRO:HD2	2.12	0.74
2:C:861:LEU:CG	2:C:862:PRO:HD2	2.10	0.74
2:C:911:GLU:O	2:C:915:LYS:HG2	1.85	0.74
1:B:25:LEU:HD11	1:B:28:LEU:CD1	2.16	0.74
2:C:290:LEU:HA	2:C:300:ASP:HA	1.68	0.74
2:C:328:LEU:O	2:C:467:ILE:HD13	1.87	0.74
2:C:1030:GLN:HE22	3:D:628:ARG:HD3	1.52	0.74
2:C:256:TYR:O	2:C:260:LEU:HD22	1.87	0.74
3:D:1042:ARG:HG3	3:D:1042:ARG:O	1.87	0.74
3:D:1060:SER:O	3:D:1062:ARG:N	2.19	0.74
3:D:1364:HIS:CG	3:D:1365:ASP:H	2.06	0.74
2:C:710:ILE:CG1	2:C:790:LEU:HD13	2.18	0.74
3:D:795:VAL:HG23	3:D:904:VAL:HG11	1.68	0.74
1:A:6:LEU:C	1:A:8:ALA:H	1.94	0.74
2:C:34:VAL:HG11	2:C:39:ARG:HG2	1.69	0.74
3:D:639:LEU:N	3:D:729:HIS:CD2	2.56	0.74
3:D:1109:GLU:HG3	3:D:1110:ALA:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:262:ALA:HB1	2:C:266:ARG:CD	2.09	0.73
2:C:290:LEU:HD21	2:C:298:PHE:HD2	1.53	0.73
2:C:355:VAL:HG23	2:C:372:LEU:HB3	1.69	0.73
3:D:10:ILE:HG13	3:D:11:ALA:H	1.52	0.73
1:A:165:ILE:O	1:A:165:ILE:HG13	1.87	0.73
1:B:174:VAL:HG12	1:B:201:THR:HG21	1.69	0.73
2:C:492:ASP:H	2:C:532:MET:H	1.36	0.73
2:C:755:LEU:HD12	2:C:790:LEU:CD2	2.18	0.73
2:C:889:HIS:C	2:C:891:GLY:H	1.95	0.73
3:D:519:VAL:HG12	3:D:520:LEU:H	1.50	0.73
3:D:1118:ILE:CD1	3:D:1190:SER:HB3	2.18	0.73
3:D:1251:ASP:C	3:D:1253:THR:H	1.95	0.73
3:D:1275:SER:H	3:D:1322:GLY:HA2	1.52	0.73
2:C:285:LEU:HD23	2:C:286:SER:H	1.53	0.73
2:C:291:VAL:HB	2:C:299:LYS:HG3	1.71	0.73
2:C:613:VAL:HG11	2:C:619:ARG:HG2	1.70	0.73
2:C:727:PRO:HG3	2:C:785:VAL:HG12	1.69	0.73
3:D:1045:MET:HA	3:D:1045:MET:CE	2.18	0.73
4:E:30:LEU:C	4:E:32:ARG:H	1.97	0.73
1:A:83:LYS:HE2	1:A:168:ASP:HB2	1.70	0.73
2:C:256:TYR:O	2:C:260:LEU:HB3	1.88	0.73
3:D:630:VAL:O	3:D:725:SER:HA	1.86	0.73
1:A:184:THR:O	1:A:185:ARG:HD3	1.89	0.73
2:C:285:LEU:HD11	2:C:302:VAL:HG21	1.70	0.73
2:C:391:LEU:HD22	2:C:415:PRO:CD	2.17	0.73
2:C:753:ASP:O	2:C:791:ARG:HA	1.89	0.73
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	1.71	0.73
3:D:1281:VAL:HG12	3:D:1282:ARG:N	2.04	0.73
3:D:1338:ALA:O	3:D:1339:LYS:HB2	1.87	0.73
3:D:1481:VAL:HG11	4:E:21:VAL:HG21	1.69	0.73
2:C:129:ILE:CG2	2:C:387:SER:HB2	2.17	0.73
2:C:629:ALA:O	2:C:630:ARG:HD3	1.88	0.73
2:C:1052:MET:C	2:C:1053:LEU:HD22	2.14	0.73
3:D:1314:LYS:O	3:D:1315:ASP:O	2.07	0.73
3:D:1483:PHE:CE1	4:E:22:VAL:HG23	2.24	0.73
3:D:508:ARG:O	3:D:510:GLU:N	2.21	0.73
2:C:66:LEU:HA	2:C:100:LEU:HA	1.70	0.73
2:C:110:GLU:CB	2:C:369:PRO:HG2	2.19	0.73
2:C:552:HIS:CE1	3:D:1064:GLY:H	2.07	0.73
2:C:553:ASP:OD2	2:C:843:HIS:ND1	2.20	0.73
2:C:1094:ALA:HB1	3:D:603:LEU:HD21	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:790:TYR:CD2	3:D:906:GLN:HB3	2.24	0.73
3:D:879:ARG:HD2	3:D:904:VAL:HG22	1.69	0.73
2:C:363:SER:O	2:C:367:LEU:HG	1.89	0.72
2:C:267:TYR:CD2	2:C:267:TYR:N	2.56	0.72
2:C:795:GLY:O	2:C:797:GLY:N	2.21	0.72
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.18	0.72
3:D:580:ALA:O	3:D:584:ASN:HB2	1.89	0.72
1:A:90:LEU:HB2	1:A:119:ASP:HB3	1.70	0.72
2:C:676:ILE:O	2:C:677:MET:HB3	1.89	0.72
3:D:893:GLU:O	3:D:894:LYS:HB2	1.88	0.72
1:A:12:THR:HB	1:A:24:VAL:HB	1.71	0.72
2:C:597:ALA:HB2	2:C:655:LEU:HD13	1.69	0.72
2:C:277:ALA:HB1	2:C:281:LEU:HD12	1.70	0.72
2:C:559:LEU:HD12	2:C:560:MET:N	2.04	0.72
2:C:775:ARG:O	2:C:780:GLU:N	2.22	0.72
3:D:879:ARG:CZ	3:D:904:VAL:HA	2.19	0.72
1:A:142:VAL:HG22	1:A:142:VAL:O	1.89	0.72
2:C:421:GLU:HG3	2:C:423:ALA:H	1.54	0.72
2:C:801:VAL:CG2	2:C:828:ALA:HB2	2.18	0.72
1:A:143:ARG:O	1:A:144:VAL:HG13	1.89	0.72
2:C:399:ASN:ND2	2:C:401:LEU:N	2.38	0.72
2:C:897:LEU:HD23	2:C:899:GLN:OE1	1.89	0.72
3:D:865:THR:HG22	3:D:866:THR:H	1.53	0.72
3:D:1281:VAL:CG1	3:D:1282:ARG:H	2.01	0.72
3:D:1402:ALA:HB1	3:D:1415:VAL:HG11	1.72	0.72
1:A:41:ARG:HB3	1:A:41:ARG:HH11	1.54	0.72
1:B:55:SER:HA	1:B:166:PRO:HA	1.70	0.72
1:B:202:ASP:C	1:B:204:SER:H	1.98	0.72
2:C:139:GLN:HE22	2:C:416:GLY:HA3	1.53	0.72
2:C:946:ARG:NE	2:C:984:GLU:HB2	2.05	0.72
3:D:1033:GLN:HA	3:D:1036:ARG:HD3	1.72	0.72
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.25	0.72
1:A:42:ARG:HH21	1:B:34:VAL:HB	1.55	0.72
1:A:90:LEU:HD12	1:A:119:ASP:HA	1.69	0.72
3:D:609:GLY:HA2	3:D:615:ARG:CZ	2.19	0.72
3:D:668:PRO:HG2	3:D:672:ALA:CB	2.19	0.72
3:D:1034:GLN:O	3:D:1037:GLN:HB3	1.90	0.72
2:C:1034:GLU:CD	3:D:1096:ARG:HH12	1.98	0.71
3:D:26:VAL:C	3:D:28:LYS:H	1.95	0.71
1:A:162:ILE:HG23	1:A:163:ASN:N	2.05	0.71
2:C:688:ILE:HG23	2:C:871:LEU:HD12	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:877:PRO:HA	2:C:882:LEU:HD21	1.72	0.71
3:D:1094:LEU:HD22	3:D:1256:LEU:HD11	1.72	0.71
1:B:25:LEU:C	1:B:25:LEU:HD12	2.15	0.71
2:C:710:ILE:CD1	2:C:790:LEU:HD22	2.02	0.71
1:A:212:ASN:O	1:A:215:VAL:HG22	1.89	0.71
2:C:80:GLN:HE22	2:C:122:THR:HG23	1.55	0.71
2:C:253:ALA:O	2:C:254:LEU:HB3	1.90	0.71
2:C:261:LEU:C	2:C:263:ASP:H	1.97	0.71
2:C:469:THR:HG22	2:C:483:VAL:HA	1.72	0.71
3:D:1250:THR:HA	3:D:1269:LYS:HZ3	1.55	0.71
3:D:1356:TYR:HB3	3:D:1361:VAL:HB	1.70	0.71
2:C:482:GLU:HA	2:C:486:MET:HE1	1.72	0.71
2:C:674:VAL:HG11	2:C:992:MET:HE3	1.72	0.71
2:C:775:ARG:HA	2:C:780:GLU:CB	2.20	0.71
2:C:1012:PRO:CB	2:C:1023:GLY:HA3	2.21	0.71
3:D:756:GLN:O	3:D:760:ARG:HG2	1.90	0.71
3:D:1443:THR:CG2	3:D:1447:LEU:HD22	2.20	0.71
1:A:10:VAL:H	1:A:26:GLU:HB2	1.55	0.71
1:B:174:VAL:HA	1:B:201:THR:HG22	1.72	0.71
2:C:262:ALA:CB	2:C:266:ARG:HD3	2.08	0.71
2:C:921:ALA:N	2:C:924:LEU:HD21	2.05	0.71
2:C:940:GLU:HG2	2:C:973:VAL:HG21	1.73	0.71
3:D:564:GLU:HG3	3:D:568:ARG:HE	1.55	0.71
3:D:1252:ILE:C	3:D:1254:GLN:H	1.96	0.71
1:B:82:LEU:HD21	1:B:142:VAL:HG21	1.72	0.71
2:C:166:PRO:HB3	2:C:417:GLY:H	1.56	0.71
2:C:399:ASN:HD21	2:C:401:LEU:HB3	1.56	0.71
2:C:523:ILE:O	2:C:525:ALA:N	2.23	0.71
2:C:525:ALA:CB	2:C:526:PRO:HD2	2.20	0.71
2:C:570:PRO:HB3	2:C:659:PRO:O	1.90	0.71
3:D:705:ALA:HB3	3:D:706:PRO:CD	2.21	0.71
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.72	0.71
1:A:75:VAL:HA	1:A:78:ILE:HD12	1.71	0.71
2:C:51:THR:OG1	2:C:348:LEU:HD23	1.91	0.71
2:C:910:THR:HG22	2:C:912:PRO:HD2	1.72	0.71
3:D:691:LEU:HD12	3:D:691:LEU:N	1.98	0.71
3:D:899:LEU:HD13	3:D:899:LEU:N	2.06	0.71
1:A:110:ARG:HB2	1:A:126:ASP:O	1.90	0.71
1:B:213:GLN:O	1:B:217:ILE:HG13	1.90	0.71
2:C:929:ARG:C	2:C:931:GLY:H	1.98	0.71
3:D:688:TRP:O	3:D:690:ALA:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:699:VAL:CB	3:D:716:PHE:O	2.36	0.71
2:C:144:PRO:HA	2:C:162:ILE:CG2	2.21	0.71
2:C:877:PRO:O	2:C:881:ASN:N	2.22	0.71
2:C:939:ARG:HD3	2:C:975:TYR:HE2	1.55	0.71
2:C:1066:ALA:O	2:C:1070:ILE:HD13	1.90	0.71
3:D:486:ARG:HG3	3:D:487:ALA:H	1.55	0.71
3:D:586:ARG:O	3:D:588:GLY:N	2.23	0.71
1:A:47:SER:O	1:A:48:ILE:HG13	1.88	0.70
1:A:112:VAL:O	1:A:114:PHE:N	2.24	0.70
2:C:467:ILE:HG21	2:C:484:VAL:HG21	1.71	0.70
2:C:630:ARG:HA	2:C:705:ILE:HD13	1.73	0.70
3:D:460:ALA:O	3:D:463:GLU:HB3	1.90	0.70
3:D:1311:LEU:HB2	3:D:1323:GLN:OE1	1.91	0.70
1:A:85:LEU:HA	1:A:124:ASN:HD21	1.55	0.70
1:A:106:PRO:O	1:A:107:LYS:HB3	1.91	0.70
1:B:26:GLU:CB	1:B:27:PRO:HD3	2.20	0.70
2:C:196:LEU:O	2:C:200:LEU:HG	1.91	0.70
2:C:564:MET:HG3	2:C:997:LEU:HD11	1.72	0.70
1:A:30:ARG:HD2	1:A:191:ASP:CB	2.19	0.70
3:D:645:PRO:HD2	3:D:648:MET:SD	2.30	0.70
3:D:658:LEU:HA	3:D:661:MET:HE3	1.73	0.70
3:D:899:LEU:HD11	3:D:921:ARG:HD2	1.73	0.70
3:D:1402:ALA:CB	3:D:1415:VAL:HG11	2.22	0.70
2:C:801:VAL:HG21	2:C:828:ALA:HB2	1.74	0.70
2:C:922:PHE:HA	2:C:925:TYR:HB3	1.73	0.70
2:C:943:VAL:HG21	2:C:973:VAL:HG13	1.73	0.70
3:D:502:PHE:HE2	3:D:509:PRO:HG3	1.56	0.70
3:D:1281:VAL:HG12	3:D:1282:ARG:H	1.55	0.70
3:D:1432:LYS:HG3	3:D:1433:SER:H	1.55	0.70
2:C:90:TYR:CE2	2:C:120:LEU:HB2	2.27	0.70
3:D:590:PRO:O	3:D:600:LEU:HD11	1.92	0.70
3:D:1273:VAL:CG2	3:D:1324:PRO:HG3	2.18	0.70
1:A:30:ARG:NH1	1:A:191:ASP:HB2	2.06	0.70
2:C:148:PHE:CZ	2:C:309:TYR:HD2	2.10	0.70
2:C:197:LEU:HD22	2:C:202:TYR:HD1	1.54	0.70
2:C:1099:VAL:HG22	3:D:10:ILE:HD12	1.73	0.70
2:C:142:ARG:HG2	2:C:147:TYR:CZ	2.26	0.70
2:C:874:LEU:HD13	3:D:787:LEU:HD22	1.73	0.70
3:D:890:VAL:CG1	3:D:891:GLY:H	1.97	0.70
3:D:890:VAL:HG13	3:D:926:LYS:HE2	1.74	0.70
3:D:1104:GLU:HG2	3:D:1104:GLU:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1265:ALA:O	3:D:1266:ARG:HG3	1.91	0.70
1:A:66:SER:HB2	1:A:75:VAL:HG21	1.72	0.70
1:B:25:LEU:HD11	1:B:28:LEU:CD2	2.22	0.70
3:D:1211:MET:CE	4:E:16:LYS:HD2	2.21	0.70
3:D:1431:THR:O	3:D:1432:LYS:HG2	1.92	0.70
2:C:291:VAL:HG11	2:C:299:LYS:HE2	1.74	0.70
2:C:674:VAL:HG22	2:C:675:ALA:N	2.07	0.70
4:E:26:ARG:NE	4:E:67:GLU:OE2	2.25	0.70
2:C:588:VAL:HG23	2:C:666:LEU:HB2	1.74	0.69
3:D:657:LEU:O	3:D:660:LYS:N	2.24	0.69
3:D:1019:PRO:CB	3:D:1022:VAL:HG23	2.19	0.69
3:D:1403:LEU:HG	3:D:1415:VAL:HB	1.73	0.69
1:B:25:LEU:HD11	1:B:28:LEU:CG	2.23	0.69
1:B:199:ILE:HG23	1:B:201:THR:CG2	2.22	0.69
2:C:177:GLU:HG2	2:C:181:VAL:H	1.55	0.69
2:C:498:GLN:H	2:C:502:PRO:HD3	1.56	0.69
2:C:862:PRO:HA	2:C:975:TYR:CE1	2.27	0.69
2:C:950:LEU:O	3:D:1018:ASN:OD1	2.10	0.69
3:D:587:ARG:HG2	3:D:588:GLY:N	2.07	0.69
3:D:836:VAL:HG11	3:D:858:LEU:HG	1.72	0.69
3:D:916:TYR:C	3:D:916:TYR:CD2	2.71	0.69
2:C:312:ALA:HB1	2:C:318:PRO:CG	2.22	0.69
2:C:391:LEU:HD22	2:C:415:PRO:HD2	1.74	0.69
2:C:536:PRO:HB3	3:D:1068:LEU:HD11	1.75	0.69
3:D:1107:VAL:HG21	3:D:1215:VAL:CG1	2.21	0.69
3:D:1202:GLN:O	3:D:1203:LYS:HB2	1.92	0.69
1:A:206:THR:HB	1:A:209:GLU:HG3	1.75	0.69
2:C:360:VAL:O	2:C:361:MET:C	2.35	0.69
2:C:666:LEU:HD11	2:C:668:LEU:CD2	2.22	0.69
2:C:910:THR:C	2:C:912:PRO:HD2	2.17	0.69
2:C:1052:MET:HE3	2:C:1056:LYS:HZ1	1.56	0.69
3:D:657:LEU:O	3:D:658:LEU:C	2.35	0.69
1:A:109:VAL:O	1:A:129:ILE:HB	1.93	0.69
2:C:142:ARG:HA	2:C:330:ASN:O	1.91	0.69
2:C:299:LYS:HG3	2:C:299:LYS:O	1.91	0.69
3:D:701:LEU:HD12	3:D:715:ALA:HB2	1.75	0.69
3:D:978:TYR:C	3:D:980:MET:H	2.01	0.69
3:D:1108:ARG:O	3:D:1109:GLU:HG2	1.92	0.69
2:C:352:ALA:O	2:C:355:VAL:HG12	1.92	0.69
3:D:552:ASN:HA	3:D:555:LYS:CB	2.22	0.69
3:D:1145:TYR:HD2	3:D:1146:GLY:N	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:PHE:HB2	1:B:197:LEU:HD12	1.73	0.69
3:D:1270:ALA:CB	3:D:1328:GLY:HA3	2.22	0.69
2:C:126:SER:HB3	2:C:135:VAL:HG13	1.73	0.69
2:C:726:ILE:HD12	2:C:726:ILE:N	2.07	0.69
2:C:796:GLU:HG2	3:D:681:ARG:HH12	1.57	0.69
2:C:1052:MET:HG2	3:D:623:VAL:HG22	1.75	0.69
3:D:42(U):UNK:O	3:D:43(U):UNK:O	2.10	0.69
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.72	0.69
3:D:1144:LEU:O	3:D:1147:ARG:HG2	1.92	0.69
4:E:59:ASN:ND2	4:E:61:VAL:HG23	2.08	0.69
1:B:59:GLU:O	1:B:60:ASP:HB2	1.93	0.69
2:C:42:VAL:N	2:C:46:ALA:HB2	2.08	0.69
2:C:333:ILE:HG21	2:C:460:ARG:HH22	1.58	0.69
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.74	0.69
2:C:683:ASN:HB2	2:C:872:ASN:HB2	1.74	0.69
2:C:1005:MET:HA	3:D:628:ARG:O	1.92	0.69
3:D:968:ASP:O	3:D:969:ARG:C	2.36	0.69
3:D:1147:ARG:HB3	3:D:1188:VAL:HG22	1.74	0.69
2:C:469:THR:HB	2:C:482:GLU:O	1.93	0.69
3:D:493:ARG:O	3:D:496:LEU:HB3	1.93	0.69
3:D:808:THR:N	3:D:809:PRO:HD3	2.08	0.69
3:D:886:VAL:HG11	3:D:900:ILE:CD1	2.18	0.69
3:D:1201:CYS:SG	3:D:1202:GLN:N	2.65	0.69
4:E:50:THR:O	4:E:52:GLU:N	2.26	0.69
1:A:72:LYS:HG3	2:C:607:ASP:OD1	1.92	0.68
1:B:44:LEU:HG	1:B:199:ILE:HD11	1.74	0.68
2:C:613:VAL:HG21	2:C:619:ARG:CG	2.17	0.68
3:D:1104:GLU:HB2	3:D:1461:GLY:HA2	1.75	0.68
1:A:105:GLY:N	1:A:136:GLY:HA3	2.07	0.68
2:C:211:LEU:HD22	2:C:304:LEU:HD12	1.75	0.68
2:C:837:ASP:OD2	2:C:837:ASP:N	2.24	0.68
3:D:1014:ASN:O	3:D:1015:TYR:CG	2.47	0.68
3:D:1105:ILE:HD11	3:D:1374:GLN:NE2	2.07	0.68
3:D:1160:LEU:HD22	3:D:1164:ARG:HH12	1.58	0.68
2:C:54:ILE:HD11	2:C:356:ARG:HB2	1.75	0.68
2:C:64:LEU:HD11	2:C:367:LEU:HD12	1.73	0.68
2:C:545:ASN:HB3	2:C:583:LEU:HD12	1.75	0.68
2:C:569:VAL:HG12	2:C:996:LYS:O	1.94	0.68
3:D:765:SER:HB2	3:D:769:LEU:HD12	1.76	0.68
2:C:139:GLN:NE2	2:C:334:ARG:HH21	1.91	0.68
2:C:759:THR:HB	2:C:785:VAL:CG1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:881:ASN:N	2:C:881:ASN:ND2	2.42	0.68
3:D:1062:ARG:HG3	3:D:1062:ARG:NH1	2.08	0.68
2:C:22:GLN:HE21	2:C:336:VAL:CG2	2.06	0.68
2:C:401:LEU:HD13	2:C:587:VAL:HG11	1.74	0.68
2:C:502:PRO:O	2:C:507:ARG:NH2	2.26	0.68
2:C:613:VAL:HG12	2:C:614:ARG:H	1.58	0.68
2:C:660:ALA:O	2:C:667:ALA:N	2.24	0.68
2:C:816:LYS:HD2	2:C:817:PRO:HD2	1.74	0.68
3:D:750:PRO:HG2	3:D:756:GLN:OE1	1.93	0.68
1:A:175:ARG:HB2	1:A:201:THR:HB	1.76	0.68
2:C:142:ARG:NE	2:C:324:ASP:HA	2.08	0.68
2:C:852:ILE:N	2:C:852:ILE:CD1	2.57	0.68
2:C:939:ARG:HD3	2:C:975:TYR:CE2	2.29	0.68
3:D:456:MET:HG2	3:D:457:GLY:N	2.08	0.68
2:C:193:LEU:HD13	2:C:193:LEU:O	1.94	0.68
2:C:313:LEU:HD13	2:C:319:GLY:O	1.94	0.68
2:C:770:GLU:O	2:C:774:LEU:HG	1.94	0.68
2:C:1089:VAL:O	2:C:1093:GLN:HG3	1.94	0.68
3:D:112:ILE:O	3:D:114:THR:N	2.26	0.68
3:D:836:VAL:HG11	3:D:858:LEU:CG	2.22	0.68
3:D:859:ASP:O	3:D:860:LEU:HB3	1.94	0.68
3:D:976:GLN:C	3:D:978:TYR:H	2.02	0.68
1:B:147:GLY:HA3	1:B:171:PHE:CD1	2.29	0.68
2:C:54:ILE:HG12	2:C:355:VAL:HG13	1.76	0.68
2:C:99:GLN:CB	2:C:109:LYS:HG2	2.22	0.68
2:C:475:LYS:C	2:C:477:GLY:H	2.02	0.68
2:C:580:MET:HB2	2:C:584:GLU:CD	2.19	0.68
2:C:836:GLY:HA3	2:C:1001:VAL:HG21	1.76	0.68
2:C:924:LEU:O	2:C:928:LYS:HG3	1.94	0.68
4:E:81:PRO:HG3	4:E:84:ARG:HD2	1.76	0.68
1:A:157:GLY:HA3	1:A:166:PRO:HB3	1.76	0.68
1:B:66:SER:OG	1:B:67:THR:N	2.19	0.68
2:C:204:GLN:HG3	2:C:205:GLU:HG2	1.75	0.68
2:C:1054:THR:O	2:C:1056:LYS:N	2.27	0.68
3:D:662:GLU:HB2	3:D:670:VAL:HG22	1.75	0.68
3:D:770:LEU:H	3:D:770:LEU:HD12	1.59	0.68
3:D:789:LEU:HD13	3:D:882:PHE:HE1	1.58	0.68
1:B:49:PRO:HB3	1:B:146:ARG:NH2	2.10	0.68
2:C:145:GLY:O	2:C:146:VAL:HG23	1.93	0.68
2:C:147:TYR:O	2:C:148:PHE:HB2	1.93	0.68
3:D:1103:HIS:C	3:D:1105:ILE:N	2.50	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:VAL:O	1:B:164:ALA:O	2.12	0.67
2:C:410:ILE:HG12	2:C:468:ARG:HH21	1.58	0.67
2:C:635:THR:O	2:C:636:ALA:HB3	1.94	0.67
2:C:754:ILE:CD1	2:C:791:ARG:HE	2.07	0.67
2:C:755:LEU:HD23	2:C:792:VAL:CG2	2.24	0.67
3:D:509:PRO:HA	3:D:511:TRP:NE1	2.09	0.67
3:D:721:VAL:CG1	3:D:722:GLU:H	2.06	0.67
3:D:1123:PHE:CE2	3:D:1184:ARG:HG2	2.29	0.67
4:E:14:ASP:CG	4:E:15:SER:N	2.51	0.67
1:A:86:VAL:HG12	1:A:124:ASN:CG	2.18	0.67
2:C:285:LEU:HD11	2:C:302:VAL:CG2	2.24	0.67
2:C:729:LEU:HB2	2:C:787:ASP:OD2	1.93	0.67
3:D:502:PHE:CE1	3:D:1452:ILE:HG13	2.28	0.67
3:D:678:GLU:C	3:D:680:GLN:H	2.02	0.67
3:D:709:HIS:HD2	3:D:711:LEU:HB2	1.59	0.67
3:D:1106:VAL:O	3:D:1108:ARG:HG3	1.94	0.67
4:E:29:GLN:N	4:E:32:ARG:HG2	2.10	0.67
1:B:16:GLN:HB3	1:B:19:HIS:O	1.93	0.67
1:B:26:GLU:O	1:B:28:LEU:HG	1.95	0.67
2:C:35:PRO:O	2:C:37:GLU:N	2.27	0.67
2:C:328:LEU:O	2:C:467:ILE:HG21	1.94	0.67
2:C:903:SER:HB2	2:C:909:ALA:HB2	1.77	0.67
3:D:578:VAL:O	3:D:582:ILE:HG13	1.94	0.67
3:D:957:PRO:HB2	3:D:959:GLU:HG2	1.76	0.67
3:D:1033:GLN:O	3:D:1036:ARG:HG2	1.94	0.67
3:D:1153:VAL:HG12	3:D:1153:VAL:O	1.95	0.67
3:D:1207:TYR:HA	3:D:1214:PRO:HA	1.76	0.67
1:B:72:LYS:N	1:B:131:THR:O	2.27	0.67
2:C:257:LEU:O	2:C:259:GLY:N	2.28	0.67
2:C:285:LEU:CD2	2:C:286:SER:H	2.06	0.67
2:C:605:LYS:HD3	2:C:607:ASP:HA	1.76	0.67
2:C:674:VAL:CG2	2:C:675:ALA:N	2.57	0.67
2:C:677:MET:HE1	2:C:983:PHE:CE1	2.30	0.67
2:C:892:LEU:HD23	2:C:893:ALA:H	1.60	0.67
3:D:551:ASN:O	3:D:555:LYS:HB2	1.93	0.67
3:D:639:LEU:H	3:D:729:HIS:HD2	1.38	0.67
3:D:1327:ARG:NH1	3:D:1327:ARG:HB3	2.10	0.67
2:C:246:ASP:HB3	2:C:247:PRO:CD	2.25	0.67
2:C:423:ALA:HA	2:C:427:VAL:HG21	1.77	0.67
2:C:159:ILE:O	2:C:173:ASP:HA	1.93	0.67
2:C:324:ASP:C	2:C:326:ASP:H	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:440:PRO:HD3	2:C:455:LEU:CA	2.24	0.67
2:C:579:VAL:HG21	2:C:887:GLU:HG3	1.75	0.67
3:D:612:GLY:O	3:D:614:PHE:N	2.27	0.67
4:E:48:MET:HG2	4:E:49:ARG:N	2.10	0.67
2:C:164:PRO:HD3	2:C:267:TYR:CD2	2.30	0.67
2:C:673:LEU:O	2:C:868:ASP:HB2	1.95	0.67
3:D:465:LEU:HD22	3:D:512:MET:CE	2.25	0.67
3:D:553:ARG:O	3:D:554:LEU:HD23	1.95	0.67
3:D:699:VAL:HG22	3:D:756:GLN:NE2	2.10	0.67
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.30	0.67
3:D:947:ILE:HD12	3:D:1020:LEU:HB3	1.77	0.67
3:D:1125:MET:HB2	3:D:1132:LEU:HD23	1.75	0.67
4:E:82:GLU:O	4:E:85:LEU:HB3	1.95	0.67
1:B:76:VAL:HB	3:D:872:ARG:HH22	1.58	0.67
2:C:640:ARG:HH11	2:C:640:ARG:HG3	1.60	0.67
3:D:906:GLN:OE1	3:D:906:GLN:N	2.28	0.67
3:D:1043:GLY:O	3:D:1056:PRO:HA	1.95	0.67
3:D:1103:HIS:HB2	3:D:1462:LEU:HD12	1.77	0.67
1:A:44:LEU:HD13	1:A:199:ILE:HG13	1.75	0.67
1:A:180:GLN:HG3	2:C:934:PHE:CD2	2.30	0.67
1:B:30:ARG:HA	1:B:193:ASP:OD1	1.95	0.67
3:D:557:LEU:HD11	3:D:563:PRO:HD2	1.77	0.67
3:D:891:GLY:N	3:D:926:LYS:HZ1	1.92	0.67
1:A:194:LYS:O	1:A:196:THR:HG22	1.94	0.67
1:A:197:LEU:HD23	1:A:197:LEU:N	2.08	0.67
2:C:605:LYS:HA	2:C:612:ALA:CB	2.24	0.67
3:D:100:ALA:CB	3:D:575:GLN:HG3	2.25	0.67
3:D:795:VAL:HG13	3:D:864:VAL:HG22	1.77	0.67
3:D:952:ASP:C	3:D:954:ALA:H	2.03	0.67
3:D:1136:LYS:O	3:D:1138:SER:N	2.28	0.67
4:E:29:GLN:CA	4:E:32:ARG:HG2	2.25	0.67
2:C:882:LEU:N	2:C:882:LEU:CD2	2.59	0.66
3:D:705:ALA:CB	3:D:706:PRO:CD	2.73	0.66
3:D:760:ARG:HH12	4:E:59:ASN:HD21	1.42	0.66
2:C:629:ALA:C	2:C:630:ARG:HD3	2.21	0.66
3:D:777:PRO:HG2	3:D:912:LYS:HG3	1.76	0.66
3:D:947:ILE:HB	3:D:1020:LEU:HD22	1.76	0.66
4:E:25:LYS:HA	4:E:28:GLN:HB3	1.77	0.66
2:C:438:ILE:CD1	2:C:484:VAL:HG22	2.25	0.66
2:C:559:LEU:HD12	2:C:559:LEU:C	2.21	0.66
2:C:676:ILE:CG2	2:C:873:PRO:HB3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:103:TRP:O	3:D:104:PHE:CB	2.43	0.66
3:D:510:GLU:O	3:D:512:MET:N	2.28	0.66
1:A:62:LEU:HD13	2:C:745:ILE:HB	1.78	0.66
2:C:266:ARG:NE	2:C:268:ASP:HB3	2.10	0.66
2:C:323:ASP:O	2:C:325:ILE:N	2.24	0.66
2:C:440:PRO:HG3	2:C:454:SER:N	2.10	0.66
2:C:755:LEU:CD1	2:C:790:LEU:HD23	2.23	0.66
2:C:876:VAL:HB	2:C:877:PRO:CD	2.25	0.66
2:C:1018:GLN:OE1	2:C:1018:GLN:HA	1.95	0.66
3:D:566:ILE:C	3:D:570:GLU:HG3	2.21	0.66
3:D:728:LEU:HD13	3:D:745:MET:HE1	1.77	0.66
3:D:764:LEU:HG	3:D:766:ALA:H	1.60	0.66
3:D:1304:LYS:HD3	3:D:1304:LYS:N	2.10	0.66
1:A:195:LEU:HD23	1:A:196:THR:N	2.11	0.66
1:B:25:LEU:CD1	1:B:28:LEU:HD21	2.25	0.66
2:C:148:PHE:O	2:C:149:THR:CB	2.42	0.66
2:C:710:ILE:HG12	2:C:790:LEU:HB2	1.77	0.66
3:D:91:ALA:O	3:D:517:VAL:HG13	1.96	0.66
3:D:108:VAL:N	3:D:511:TRP:HH2	1.94	0.66
3:D:849:ALA:O	3:D:853:VAL:HG23	1.95	0.66
3:D:1141:GLU:HA	3:D:1171:VAL:CG1	2.22	0.66
1:A:41:ARG:HG2	1:A:177:VAL:CG1	2.25	0.66
1:B:106:PRO:CA	1:B:133:GLU:HA	2.24	0.66
2:C:184:MET:HE3	2:C:191:PHE:CZ	2.26	0.66
2:C:712:ALA:HB2	2:C:722:ILE:HD12	1.78	0.66
3:D:1486:VAL:HG21	4:E:25:LYS:NZ	2.11	0.66
1:A:31:GLY:H	1:A:193:ASP:CG	2.03	0.66
1:A:86:VAL:HG21	1:A:203:GLY:C	2.20	0.66
2:C:881:ASN:N	2:C:881:ASN:HD22	1.92	0.66
2:C:922:PHE:C	2:C:924:LEU:N	2.49	0.66
3:D:546:ARG:HH12	3:D:589:SER:HB2	1.59	0.66
3:D:879:ARG:NH2	3:D:905:PRO:HD2	2.11	0.66
3:D:904:VAL:HG12	3:D:906:GLN:OE1	1.95	0.66
3:D:1236:LEU:HD11	3:D:1356:TYR:CE2	2.22	0.66
3:D:1396:GLU:O	3:D:1400:VAL:HG23	1.95	0.66
1:A:211:LEU:O	1:A:215:VAL:HG13	1.95	0.66
1:A:217:ILE:HG22	1:A:221:HIS:CD2	2.31	0.66
2:C:323:ASP:C	2:C:325:ILE:N	2.47	0.66
2:C:862:PRO:HG3	2:C:925:TYR:OH	1.96	0.66
2:C:892:LEU:CD2	2:C:892:LEU:N	2.54	0.66
2:C:953:VAL:HG11	2:C:962:GLN:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:839:LEU:HD12	2:C:994:ILE:HG22	1.77	0.66
3:D:91:ALA:HB3	3:D:518:PRO:HG2	1.76	0.66
3:D:1142:SER:O	3:D:1365:ASP:HB2	1.95	0.66
2:C:502:PRO:HB2	2:C:507:ARG:HH12	1.59	0.66
3:D:631:ILE:HD13	3:D:745:MET:HE2	1.78	0.66
3:D:772:PRO:HG3	3:D:778:LEU:CD2	2.26	0.66
3:D:908:LYS:HG3	3:D:1027:GLY:HA3	1.77	0.66
2:C:163:ILE:HG23	2:C:265:LYS:NZ	2.11	0.65
2:C:626:ARG:NE	2:C:637:PHE:HZ	1.94	0.65
4:E:40:LEU:HB3	4:E:44:GLU:O	1.96	0.65
1:B:30:ARG:HG3	1:B:30:ARG:O	1.95	0.65
2:C:327:HIS:C	2:C:329:GLY:H	2.03	0.65
2:C:336:VAL:HA	2:C:339:LEU:HD12	1.78	0.65
2:C:958:SER:HB2	2:C:959:PRO:HD2	1.78	0.65
3:D:772:PRO:HD3	3:D:778:LEU:N	2.11	0.65
3:D:1112:CYS:SG	3:D:1113:GLY:N	2.69	0.65
3:D:1273:VAL:HG23	3:D:1324:PRO:CG	2.19	0.65
2:C:721:ARG:O	2:C:758:ARG:HB2	1.95	0.65
3:D:90:MET:N	3:D:520:LEU:HD21	2.10	0.65
3:D:91:ALA:HB3	3:D:518:PRO:HD2	1.78	0.65
3:D:857:LEU:O	3:D:858:LEU:C	2.39	0.65
1:B:86:VAL:HG23	1:B:124:ASN:CG	2.22	0.65
1:B:150:TYR:CE1	1:B:170:ILE:HG22	2.31	0.65
2:C:613:VAL:CG1	2:C:620:LEU:H	2.05	0.65
2:C:648:ARG:HG2	2:C:648:ARG:HH11	1.61	0.65
2:C:943:VAL:O	2:C:946:ARG:N	2.28	0.65
2:C:1045:ALA:HB1	2:C:1048:THR:CB	2.23	0.65
2:C:1113:GLU:C	2:C:1115:LEU:H	2.02	0.65
3:D:638:LYS:C	3:D:639:LEU:O	2.38	0.65
3:D:681:ARG:O	3:D:682:ASP:HB2	1.97	0.65
3:D:1069:GLU:O	3:D:1072:ILE:N	2.28	0.65
1:A:162:ILE:HG12	1:A:163:ASN:OD1	1.95	0.65
1:B:58:ILE:HG23	1:B:140:MET:HG2	1.77	0.65
1:B:174:VAL:HG12	1:B:201:THR:CG2	2.26	0.65
2:C:142:ARG:HH12	2:C:171:TRP:HH2	1.45	0.65
2:C:159:ILE:HG12	2:C:310:LEU:HD13	1.76	0.65
2:C:410:ILE:HG12	2:C:468:ARG:NH2	2.11	0.65
2:C:576:ALA:H	2:C:662:GLU:HG2	1.62	0.65
2:C:1034:GLU:HB3	3:D:618:LEU:O	1.96	0.65
3:D:754:PHE:O	3:D:758:GLU:HG2	1.96	0.65
3:D:789:LEU:HD11	3:D:934:LEU:HD22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:HG22	1:B:218:LEU:HD13	1.77	0.65
1:B:94:MET:CE	1:B:94:MET:HB2	2.27	0.65
2:C:796:GLU:HG2	3:D:681:ARG:HH22	1.62	0.65
2:C:857:ASP:O	2:C:858:MET:HB2	1.95	0.65
2:C:1020:PRO:HD2	3:D:622:ARG:O	1.96	0.65
3:D:792:ILE:O	3:D:792:ILE:HG22	1.95	0.65
3:D:860:LEU:HA	3:D:877:PRO:CG	2.21	0.65
2:C:404:LEU:HD23	2:C:587:VAL:HG13	1.79	0.65
2:C:467:ILE:HG22	2:C:484:VAL:HG21	1.77	0.65
2:C:564:MET:CG	2:C:997:LEU:HD11	2.26	0.65
2:C:575:GLN:O	2:C:667:ALA:HB1	1.96	0.65
2:C:604:VAL:HG11	2:C:619:ARG:HH22	1.61	0.65
2:C:1008:ARG:HB2	2:C:1028:GLY:HA3	1.77	0.65
1:A:213:GLN:O	1:A:216:ALA:HB3	1.97	0.65
2:C:519:GLY:C	2:C:521:PRO:HD3	2.22	0.65
2:C:730:SER:O	2:C:731:GLU:C	2.40	0.65
2:C:813:VAL:CG1	2:C:815:LEU:HD11	2.26	0.65
2:C:953:VAL:CG2	2:C:966:LEU:HD13	2.27	0.65
3:D:129:PHE:CA	3:D:454:ALA:HB1	2.15	0.65
3:D:932:ASP:O	3:D:933:ALA:C	2.40	0.65
3:D:1019:PRO:C	3:D:1021:TYR:N	2.48	0.65
2:C:439:CYS:SG	2:C:440:PRO:HD2	2.37	0.65
2:C:631:SER:OG	2:C:635:THR:HG22	1.97	0.65
3:D:1017:PHE:HA	3:D:1023:MET:SD	2.37	0.65
1:A:41:ARG:HH11	1:A:41:ARG:C	2.04	0.65
2:C:94:LEU:O	2:C:115:LEU:HB3	1.97	0.65
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.79	0.65
2:C:495:THR:HG22	2:C:496:ILE:H	1.61	0.65
2:C:688:ILE:CG2	2:C:871:LEU:HD12	2.27	0.65
2:C:813:VAL:HG12	2:C:815:LEU:CD1	2.27	0.65
2:C:1008:ARG:CD	2:C:1029:GLY:H	2.02	0.65
3:D:670:VAL:O	3:D:673:ALA:HB3	1.97	0.65
3:D:877:PRO:O	3:D:880:ILE:HB	1.95	0.65
2:C:184:MET:HB3	2:C:191:PHE:CZ	2.32	0.64
2:C:1063:ARG:O	2:C:1066:ALA:HB3	1.97	0.64
4:E:14:ASP:CG	4:E:15:SER:H	2.05	0.64
1:A:23:PHE:HZ	1:A:207:PRO:HB2	1.63	0.64
2:C:163:ILE:HG21	2:C:169:GLY:HA3	1.79	0.64
2:C:605:LYS:CG	2:C:607:ASP:H	2.10	0.64
2:C:573:ARG:HH11	2:C:573:ARG:HG3	1.62	0.64
2:C:721:ARG:C	2:C:758:ARG:HB2	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:854:ALA:O	3:D:855:HIS:C	2.41	0.64
3:D:1093:TYR:HE2	3:D:1097:LYS:NZ	1.96	0.64
3:D:1277:ILE:HG22	3:D:1279:GLY:H	1.62	0.64
3:D:1364:HIS:O	3:D:1365:ASP:HB3	1.97	0.64
2:C:839:LEU:HD23	2:C:849:VAL:HG22	1.80	0.64
3:D:1118:ILE:N	3:D:1118:ILE:HD12	2.11	0.64
3:D:1136:LYS:HE3	3:D:1139:ASP:OD1	1.96	0.64
3:D:1348:LEU:O	3:D:1352:ILE:HG13	1.97	0.64
3:D:1457:ASP:OD1	3:D:1459:LEU:HD23	1.96	0.64
1:A:57:TYR:C	1:A:57:TYR:CD2	2.74	0.64
2:C:564:MET:HE1	2:C:846:LYS:CG	2.26	0.64
2:C:1019:GLN:HB3	2:C:1057:SER:OG	1.96	0.64
2:C:1113:GLU:O	2:C:1115:LEU:HD23	1.98	0.64
3:D:578:VAL:HG12	3:D:582:ILE:HD11	1.79	0.64
3:D:641:GLN:HB3	3:D:719:VAL:HG21	1.79	0.64
3:D:1093:TYR:HE2	3:D:1097:LYS:HZ2	1.45	0.64
2:C:34:VAL:CG1	2:C:38:LYS:HG3	2.27	0.64
2:C:151:ASP:H	2:C:157:ARG:HA	1.63	0.64
2:C:331:ARG:O	2:C:467:ILE:HG12	1.96	0.64
3:D:764:LEU:HD23	3:D:767:HIS:NE2	2.12	0.64
3:D:793:THR:HG22	3:D:879:ARG:HH22	1.61	0.64
3:D:1282:ARG:CB	3:D:1293:PHE:HB2	2.26	0.64
3:D:1381:VAL:HG12	3:D:1382:THR:H	1.62	0.64
2:C:304:LEU:N	2:C:305:PRO:CD	2.61	0.64
2:C:589:ARG:NH2	2:C:654:LEU:HA	2.13	0.64
2:C:768:SER:HB2	2:C:769:PRO:HD2	1.79	0.64
2:C:859:PRO:O	2:C:867:VAL:HG23	1.98	0.64
3:D:612:GLY:C	3:D:614:PHE:H	2.05	0.64
3:D:996:TRP:HA	3:D:999:THR:HG22	1.78	0.64
3:D:1037:GLN:HG3	3:D:1042:ARG:CG	2.26	0.64
3:D:1323:GLN:N	3:D:1324:PRO:CD	2.61	0.64
2:C:12:VAL:HG21	2:C:479:VAL:HG11	1.79	0.64
2:C:256:TYR:CA	2:C:260:LEU:HD13	2.28	0.64
3:D:886:VAL:HG21	3:D:914:LEU:HD11	1.79	0.64
3:D:916:TYR:C	3:D:918:ALA:H	2.05	0.64
3:D:1086:LEU:O	3:D:1089:ALA:HB3	1.98	0.64
3:D:1142:SER:O	3:D:1364:HIS:HD2	1.80	0.64
2:C:527:GLU:O	2:C:528:GLU:C	2.41	0.64
2:C:946:ARG:HH11	2:C:946:ARG:HG2	1.63	0.64
4:E:59:ASN:HD22	4:E:62:THR:HG1	1.46	0.64
3:D:626:SER:HB2	3:D:748:HIS:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1378:TYR:CE2	3:D:1431:THR:HB	2.30	0.64
3:D:1431:THR:C	3:D:1432:LYS:HG2	2.23	0.64
3:D:1433:SER:HB3	3:D:1464:GLU:OE2	1.98	0.64
4:E:59:ASN:HD21	4:E:61:VAL:HG23	1.63	0.64
1:B:14:THR:CB	1:B:22:GLU:HB3	2.27	0.63
3:D:606:ILE:H	3:D:606:ILE:HD12	1.63	0.63
3:D:840:LYS:CB	3:D:846:PRO:HA	2.28	0.63
3:D:961:GLN:O	3:D:962:ARG:C	2.40	0.63
3:D:1326:THR:O	3:D:1327:ARG:HB3	1.97	0.63
3:D:1484:THR:HG21	4:E:79:LEU:HB2	1.79	0.63
4:E:47:LYS:HD3	4:E:54:LEU:HD23	1.80	0.63
1:A:88:ARG:HB2	1:A:123:MET:SD	2.38	0.63
1:A:101:LEU:HD12	1:A:101:LEU:C	2.22	0.63
1:B:23:PHE:HD1	1:B:211:LEU:HD22	1.63	0.63
1:B:76:VAL:HB	3:D:872:ARG:NH2	2.13	0.63
2:C:831:ARG:HH12	2:C:1002:GLU:HB2	1.63	0.63
3:D:1280:VAL:HG12	3:D:1281:VAL:H	1.63	0.63
1:A:115:THR:HG23	1:A:115:THR:O	1.98	0.63
2:C:66:LEU:HD11	2:C:98:LEU:CB	2.27	0.63
2:C:1087:VAL:HG12	2:C:1091:GLU:OE2	1.97	0.63
3:D:496:LEU:HD12	3:D:500:ARG:HG2	1.81	0.63
3:D:723:GLY:O	3:D:724:GLN:HB2	1.98	0.63
3:D:965:GLU:O	3:D:968:ASP:HB2	1.97	0.63
3:D:969:ARG:HG3	3:D:970:LYS:H	1.60	0.63
3:D:1035:ILE:C	3:D:1037:GLN:H	2.05	0.63
3:D:1096:ARG:HG3	3:D:1096:ARG:NH1	2.10	0.63
2:C:303:PHE:H	2:C:305:PRO:HD2	1.63	0.63
3:D:580:ALA:HB2	3:D:587:ARG:HH22	1.63	0.63
3:D:769:LEU:HD22	3:D:779:ALA:HB2	1.80	0.63
3:D:788:GLY:O	3:D:792:ILE:HD13	1.97	0.63
3:D:1043:GLY:HA2	3:D:1057:VAL:CG2	2.28	0.63
3:D:1282:ARG:HB3	3:D:1293:PHE:HB2	1.80	0.63
2:C:38:LYS:O	2:C:39:ARG:HB2	1.98	0.63
2:C:66:LEU:CA	2:C:100:LEU:HA	2.28	0.63
2:C:129:ILE:CD1	2:C:386:PHE:HB3	2.29	0.63
2:C:408:ARG:NH2	2:C:456:ALA:O	2.28	0.63
2:C:602:GLU:O	2:C:603:VAL:HG13	1.99	0.63
2:C:1089:VAL:HG13	2:C:1099:VAL:HB	1.80	0.63
1:A:131:THR:CG2	2:C:644:ARG:HE	2.12	0.63
2:C:87:ASP:OD2	2:C:824:ARG:NH2	2.31	0.63
2:C:202:TYR:CE1	2:C:304:LEU:HB3	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:LEU:O	2:C:404:LEU:HB3	1.99	0.63
2:C:501:THR:O	2:C:502:PRO:C	2.42	0.63
2:C:588:VAL:O	2:C:588:VAL:CG1	2.46	0.63
2:C:685:GLU:OE1	2:C:685:GLU:HA	1.99	0.63
2:C:874:LEU:O	2:C:876:VAL:HG23	1.98	0.63
3:D:89:ARG:O	3:D:520:LEU:HD11	1.97	0.63
3:D:643:GLY:HA2	3:D:721:VAL:HG21	1.80	0.63
3:D:880:ILE:O	3:D:883:ALA:HB3	1.98	0.63
3:D:972:ARG:O	3:D:976:GLN:HB2	1.99	0.63
3:D:1403:LEU:HD12	3:D:1417:TRP:HZ3	1.64	0.63
1:B:87:VAL:HG12	1:B:88:ARG:N	2.14	0.63
1:B:94:MET:HB2	1:B:94:MET:HE2	1.80	0.63
1:B:174:VAL:HA	1:B:201:THR:CB	2.28	0.63
3:D:1139:ASP:O	3:D:1143:GLY:N	2.32	0.63
3:D:1304:LYS:HD3	3:D:1304:LYS:H	1.61	0.63
1:A:46:SER:OG	2:C:856:GLU:HG2	1.98	0.63
1:B:88:ARG:HD3	1:B:123:MET:HE1	1.79	0.63
1:B:90:LEU:HB2	1:B:119:ASP:HA	1.80	0.63
2:C:26:TYR:O	2:C:30:LEU:N	2.29	0.63
2:C:419:THR:O	2:C:420:ARG:C	2.42	0.63
2:C:492:ASP:O	2:C:532:MET:HA	1.98	0.63
2:C:987:ILE:HD11	3:D:946:GLY:C	2.23	0.63
3:D:35(U):UNK:O	3:D:36(U):UNK:CB	2.47	0.63
3:D:456:MET:HG2	3:D:457:GLY:H	1.64	0.63
3:D:519:VAL:HG12	3:D:520:LEU:N	2.13	0.63
3:D:679:ARG:O	3:D:681:ARG:N	2.32	0.63
2:C:202:TYR:HB3	2:C:207:LEU:HD13	1.80	0.63
2:C:257:LEU:CD2	2:C:264:PRO:HG3	2.29	0.63
2:C:268:ASP:O	2:C:270:GLY:N	2.31	0.63
2:C:525:ALA:O	2:C:526:PRO:C	2.40	0.63
2:C:816:LYS:HD2	2:C:817:PRO:CD	2.28	0.63
3:D:898:GLU:C	3:D:899:LEU:HD13	2.24	0.63
3:D:908:LYS:HD3	3:D:909:ASN:HB2	1.81	0.63
3:D:1154:GLU:O	3:D:1155:ALA:HB2	1.98	0.63
3:D:1236:LEU:HD12	3:D:1256:LEU:HD13	1.81	0.63
3:D:1324:PRO:HG2	3:D:1325:LEU:N	2.14	0.63
1:A:217:ILE:HG22	1:A:221:HIS:NE2	2.14	0.62
1:B:98:THR:CG2	1:B:99:LEU:H	2.12	0.62
1:B:115:THR:O	1:B:117:SER:N	2.32	0.62
2:C:110:GLU:HB2	2:C:369:PRO:HG2	1.80	0.62
2:C:787:ASP:O	2:C:787:ASP:OD1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:66:LEU:HD11	2:C:98:LEU:HB3	1.80	0.62
2:C:676:ILE:O	2:C:677:MET:CB	2.47	0.62
2:C:722:ILE:HA	2:C:758:ARG:CB	2.29	0.62
2:C:1107:ASN:N	2:C:1108:PRO:CD	2.62	0.62
3:D:502:PHE:CE2	3:D:509:PRO:HG3	2.33	0.62
3:D:704:ARG:NH1	3:D:743:ASP:CG	2.53	0.62
2:C:348:LEU:C	2:C:350:ARG:H	2.06	0.62
2:C:603:VAL:HG21	2:C:646:GLY:H	1.65	0.62
2:C:1012:PRO:HB3	2:C:1023:GLY:CA	2.29	0.62
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.81	0.62
3:D:767:HIS:HE1	4:E:2:ALA:HB1	1.64	0.62
3:D:1014:ASN:C	3:D:1015:TYR:CG	2.76	0.62
3:D:1059:SER:O	3:D:1060:SER:C	2.38	0.62
3:D:1083:ASP:O	3:D:1086:LEU:HB2	1.99	0.62
2:C:208:VAL:HG12	2:C:209:ARG:HG3	1.80	0.62
3:D:554:LEU:O	3:D:558:LEU:HD12	1.99	0.62
3:D:770:LEU:H	3:D:770:LEU:CD1	2.11	0.62
3:D:1062:ARG:C	3:D:1062:ARG:HD3	2.25	0.62
1:A:28:LEU:HD12	1:A:195:LEU:HB2	1.81	0.62
1:A:173:PRO:O	1:A:203:GLY:N	2.31	0.62
2:C:100:LEU:HD11	2:C:369:PRO:HD3	1.81	0.62
2:C:911:GLU:HA	2:C:914:ILE:HD12	1.81	0.62
2:C:1001:VAL:O	2:C:1004:LYS:N	2.27	0.62
3:D:688:TRP:HA	3:D:688:TRP:CE3	2.34	0.62
4:E:29:GLN:HE21	4:E:89:MET:HE2	1.64	0.62
1:B:76:VAL:O	1:B:80:LEU:HG	1.98	0.62
2:C:595:LEU:HD21	2:C:623:HIS:HB3	1.82	0.62
2:C:946:ARG:NE	3:D:861:GLN:HE22	1.89	0.62
2:C:1038:TRP:CD1	3:D:1099:VAL:HG11	2.34	0.62
3:D:558:LEU:CD2	3:D:567:ILE:HG13	2.30	0.62
3:D:631:ILE:CD1	3:D:745:MET:HE2	2.29	0.62
3:D:1291:SER:HA	3:D:1303:TYR:O	1.99	0.62
3:D:1462:LEU:HD23	3:D:1473:PRO:HG2	1.80	0.62
1:B:53:VAL:HG11	1:B:82:LEU:HG	1.82	0.62
1:B:174:VAL:HA	1:B:201:THR:CG2	2.29	0.62
2:C:502:PRO:HB2	2:C:507:ARG:NH1	2.14	0.62
3:D:3(U):UNK:O	3:D:39(U):UNK:O	2.16	0.62
3:D:639:LEU:HD23	3:D:729:HIS:CD2	2.35	0.62
3:D:793:THR:CG2	3:D:879:ARG:HH22	2.12	0.62
3:D:795:VAL:HG12	3:D:796:ARG:N	2.15	0.62
3:D:1204:CYS:C	3:D:1206:GLY:H	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:CD	1:B:123:MET:HE1	2.29	0.62
2:C:349:ALA:C	2:C:350:ARG:HG3	2.23	0.62
2:C:635:THR:HG22	2:C:636:ALA:N	2.14	0.62
3:D:1075:HIS:O	3:D:1077:ALA:N	2.32	0.62
3:D:1084:THR:C	3:D:1086:LEU:H	2.07	0.62
3:D:1266:ARG:O	3:D:1268:PRO:HD3	2.00	0.62
1:B:49:PRO:HD2	1:B:213:GLN:NE2	2.15	0.62
1:B:80:LEU:O	1:B:83:LYS:HB2	2.00	0.62
2:C:168:ARG:HH21	2:C:266:ARG:HG2	1.64	0.62
3:D:637:LEU:O	3:D:638:LYS:O	2.17	0.62
3:D:903:ASP:OD1	3:D:903:ASP:O	2.18	0.62
2:C:379:GLU:O	2:C:380:ALA:HB3	1.99	0.62
3:D:793:THR:CG2	3:D:879:ARG:HH12	2.13	0.62
3:D:863:THR:N	3:D:876:SER:OG	2.33	0.62
3:D:1059:SER:O	3:D:1061:PHE:N	2.33	0.62
3:D:1304:LYS:O	3:D:1304:LYS:HG2	2.00	0.62
3:D:1403:LEU:CD2	3:D:1415:VAL:H	2.11	0.62
1:A:110:ARG:HD3	1:A:113:ASP:OD2	2.00	0.61
1:A:224:TYR:CD1	1:B:9:PRO:HD2	2.35	0.61
2:C:22:GLN:HE21	2:C:336:VAL:HG21	1.64	0.61
2:C:22:GLN:O	2:C:24:GLU:N	2.32	0.61
3:D:10:ILE:HG21	3:D:1450:ALA:HB1	1.82	0.61
3:D:757:ALA:HB2	4:E:61:VAL:CG1	2.30	0.61
3:D:1263:PHE:CE2	3:D:1352:ILE:HD13	2.35	0.61
1:A:35:THR:HG21	1:B:43:ILE:CD1	2.30	0.61
2:C:159:ILE:HG21	2:C:306:THR:CG2	2.30	0.61
2:C:438:ILE:HG23	2:C:470:PRO:HB3	1.81	0.61
2:C:613:VAL:CG1	2:C:614:ARG:N	2.64	0.61
2:C:946:ARG:NE	3:D:861:GLN:NE2	2.43	0.61
3:D:1262:LEU:HD21	3:D:1351:GLU:HG3	1.81	0.61
3:D:1264:GLU:HG2	3:D:1266:ARG:NH2	2.15	0.61
1:B:188:GLN:CG	3:D:688:TRP:HD1	2.13	0.61
2:C:14:PRO:O	2:C:15:LEU:HB3	1.99	0.61
2:C:325:ILE:C	2:C:327:HIS:H	2.07	0.61
2:C:686:ASP:OD2	3:D:739:ASP:OD2	2.18	0.61
3:D:518:PRO:CB	3:D:544:TYR:CE1	2.82	0.61
3:D:770:LEU:HD12	3:D:770:LEU:N	2.15	0.61
3:D:891:GLY:N	3:D:926:LYS:NZ	2.47	0.61
3:D:921:ARG:O	3:D:922:LEU:HD23	2.00	0.61
3:D:1103:HIS:O	3:D:1104:GLU:HB3	2.01	0.61
3:D:1270:ALA:HB3	3:D:1328:GLY:HA3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1333:HIS:CE1	3:D:1421:LEU:HB3	2.35	0.61
1:A:142:VAL:O	1:A:143:ARG:O	2.18	0.61
2:C:493:ARG:HH12	3:D:1069:GLU:CD	2.08	0.61
2:C:614:ARG:O	2:C:616:GLU:N	2.30	0.61
3:D:633:VAL:HG22	3:D:634:GLY:N	2.15	0.61
3:D:638:LYS:HA	3:D:729:HIS:CG	2.35	0.61
3:D:699:VAL:HG12	3:D:717:GLN:CG	2.30	0.61
3:D:934:LEU:O	3:D:935:LYS:C	2.44	0.61
1:A:169:ALA:O	1:A:170:ILE:HD13	2.01	0.61
2:C:184:MET:HB3	2:C:191:PHE:CE1	2.36	0.61
2:C:348:LEU:CD1	2:C:378:LEU:HD11	2.30	0.61
2:C:588:VAL:CG2	2:C:666:LEU:HB2	2.29	0.61
2:C:605:LYS:HA	2:C:612:ALA:H	1.65	0.61
2:C:729:LEU:O	2:C:731:GLU:N	2.33	0.61
3:D:790:TYR:CE1	3:D:1023:MET:HE3	2.36	0.61
3:D:1036:ARG:O	3:D:1040:GLY:O	2.18	0.61
3:D:1150:ALA:HB2	3:D:1189:ARG:CG	2.29	0.61
1:A:10:VAL:HB	1:A:26:GLU:HG3	1.82	0.61
1:B:125:PRO:HG2	1:B:126:ASP:H	1.65	0.61
2:C:9:ILE:CG2	2:C:10:ARG:N	2.61	0.61
2:C:342:ASP:O	2:C:345:ARG:HB2	2.01	0.61
2:C:466:PHE:CE1	2:C:467:ILE:HD12	2.35	0.61
2:C:1005:MET:HB2	3:D:629:SER:CB	2.29	0.61
3:D:760:ARG:NH1	4:E:59:ASN:HD21	1.98	0.61
3:D:792:ILE:N	3:D:792:ILE:HD12	2.16	0.61
2:C:491:GLU:O	2:C:509:ALA:HB1	2.01	0.61
2:C:1101:THR:O	2:C:1110:ASP:N	2.33	0.61
3:D:88:TYR:C	3:D:520:LEU:HD13	2.25	0.61
3:D:607:LEU:O	3:D:608:SER:HB2	2.00	0.61
2:C:1067:TYR:CG	2:C:1067:TYR:O	2.54	0.61
3:D:509:PRO:HA	3:D:511:TRP:HE1	1.64	0.61
3:D:590:PRO:HA	3:D:600:LEU:HG	1.82	0.61
3:D:985:ASP:O	3:D:988:ARG:HB3	2.00	0.61
3:D:1278:ASP:HA	3:D:1317:ASP:O	2.01	0.61
2:C:1054:THR:C	2:C:1056:LYS:H	2.08	0.61
3:D:1379:VAL:O	3:D:1393:GLN:HA	2.01	0.61
1:A:159:LYS:C	1:A:161:ARG:H	2.09	0.61
1:A:175:ARG:O	1:A:176:ARG:HB2	2.01	0.61
1:A:180:GLN:HE21	2:C:934:PHE:CB	2.12	0.61
1:B:26:GLU:HG3	1:B:194:LYS:CD	2.22	0.61
2:C:482:GLU:HA	2:C:486:MET:CE	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:552:HIS:CE1	3:D:1064:GLY:N	2.69	0.61
2:C:1052:MET:HE3	2:C:1056:LYS:NZ	2.16	0.61
3:D:115:LEU:C	3:D:117:ASP:N	2.59	0.61
3:D:545:ARG:HG3	3:D:546:ARG:N	2.15	0.61
3:D:1475:GLY:C	3:D:1477:GLY:N	2.59	0.61
2:C:8:ARG:HH11	2:C:495:THR:HG23	1.65	0.60
2:C:328:LEU:C	2:C:467:ILE:HD13	2.26	0.60
2:C:569:VAL:O	2:C:569:VAL:CG1	2.44	0.60
2:C:963:LEU:CD1	2:C:972:VAL:HG22	2.30	0.60
3:D:916:TYR:HD2	3:D:917:GLN:N	1.99	0.60
3:D:1192:LEU:HD13	3:D:1345:GLU:OE1	2.01	0.60
3:D:1356:TYR:HD1	3:D:1363:LEU:HD21	1.65	0.60
3:D:1485:GLN:CB	4:E:22:VAL:HG22	2.31	0.60
1:A:198:ARG:O	1:A:199:ILE:C	2.44	0.60
1:B:143:ARG:HD2	1:B:159:LYS:CG	2.31	0.60
2:C:475:LYS:CB	2:C:527:GLU:H	2.14	0.60
2:C:491:GLU:HG3	2:C:510:THR:HB	1.81	0.60
2:C:589:ARG:NH1	2:C:596:TYR:HB3	2.16	0.60
2:C:598:GLU:OE2	2:C:614:ARG:NH2	2.33	0.60
3:D:1324:PRO:HG2	3:D:1325:LEU:H	1.67	0.60
1:B:42:ARG:HG3	1:B:42:ARG:HH11	1.65	0.60
2:C:342:ASP:O	2:C:346:VAL:HG23	2.01	0.60
2:C:588:VAL:HG11	2:C:661:SER:HB3	1.81	0.60
2:C:729:LEU:HB3	2:C:734:LEU:HD21	1.83	0.60
2:C:1055:ILE:H	2:C:1055:ILE:CD1	2.02	0.60
3:D:948:THR:H	3:D:1020:LEU:HD13	1.66	0.60
3:D:1079:LYS:C	3:D:1081:GLY:H	2.07	0.60
3:D:1251:ASP:H	3:D:1269:LYS:HZ2	1.49	0.60
1:B:148:VAL:HG23	1:B:149:GLY:N	2.16	0.60
2:C:165:LEU:HD13	2:C:342:ASP:OD2	2.01	0.60
2:C:841:ASN:C	2:C:841:ASN:ND2	2.59	0.60
2:C:944:LEU:C	2:C:946:ARG:H	2.07	0.60
3:D:100:ALA:HB2	3:D:575:GLN:HG3	1.83	0.60
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.02	0.60
3:D:1272:ALA:CB	3:D:1325:LEU:HA	2.31	0.60
3:D:1346:ARG:HH12	3:D:1349:VAL:HG11	1.66	0.60
3:D:1364:HIS:CD2	3:D:1365:ASP:H	2.19	0.60
4:E:29:GLN:HA	4:E:32:ARG:HG2	1.84	0.60
1:B:51:THR:HG21	1:B:87:VAL:O	2.01	0.60
2:C:317:VAL:H	2:C:318:PRO:HD2	1.66	0.60
2:C:706:GLU:HG3	2:C:707:ARG:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:875:GLY:HA3	2:C:879:ARG:HD2	1.84	0.60
3:D:10:ILE:HG13	3:D:11:ALA:N	2.17	0.60
3:D:609:GLY:HA2	3:D:615:ARG:NH2	2.15	0.60
3:D:659:LYS:C	3:D:659:LYS:HD3	2.27	0.60
3:D:902:MET:O	3:D:902:MET:HE3	2.01	0.60
3:D:904:VAL:HG12	3:D:906:GLN:CD	2.26	0.60
3:D:1236:LEU:CB	3:D:1256:LEU:HB2	2.27	0.60
3:D:1251:ASP:H	3:D:1269:LYS:HZ3	1.49	0.60
1:A:30:ARG:HH11	1:A:191:ASP:HB2	1.66	0.60
2:C:110:GLU:HB2	2:C:369:PRO:CG	2.32	0.60
2:C:391:LEU:HD22	2:C:415:PRO:HD3	1.82	0.60
2:C:636:ALA:HB2	2:C:705:ILE:HD11	1.82	0.60
2:C:665:PHE:O	2:C:666:LEU:C	2.44	0.60
3:D:1059:SER:C	3:D:1061:PHE:N	2.56	0.60
1:A:16:GLN:HG3	1:A:20:TYR:HB2	1.83	0.60
2:C:152:PRO:HD2	2:C:158:TYR:CE2	2.35	0.60
2:C:440:PRO:CG	2:C:454:SER:H	2.15	0.60
2:C:460:ARG:HD2	2:C:464:LEU:CD2	2.30	0.60
2:C:1033:GLY:O	2:C:1035:MET:N	2.35	0.60
3:D:88:TYR:O	3:D:520:LEU:HD13	2.01	0.60
3:D:566:ILE:HG22	3:D:566:ILE:O	2.01	0.60
3:D:663:GLU:C	3:D:665:ALA:H	2.09	0.60
3:D:969:ARG:CG	3:D:970:LYS:N	2.62	0.60
3:D:1194:CYS:SG	3:D:1201:CYS:HB2	2.41	0.60
3:D:1372:VAL:HG22	3:D:1375:MET:HE3	1.82	0.60
3:D:1394:VAL:HG12	3:D:1395:LEU:N	2.15	0.60
4:E:30:LEU:O	4:E:32:ARG:N	2.31	0.60
2:C:572:ILE:O	2:C:573:ARG:CB	2.49	0.60
2:C:743:VAL:HG11	2:C:800:VAL:HG21	1.83	0.60
3:D:91:ALA:HB3	3:D:518:PRO:CG	2.31	0.60
3:D:807:ALA:C	3:D:809:PRO:HD3	2.27	0.60
3:D:1402:ALA:C	3:D:1404:ASN:H	2.10	0.60
1:A:44:LEU:O	1:A:174:VAL:HG21	2.01	0.60
2:C:253:ALA:CA	2:C:256:TYR:HB2	2.22	0.60
2:C:613:VAL:HG11	2:C:619:ARG:HA	1.83	0.60
2:C:712:ALA:HB1	2:C:720:GLU:O	2.02	0.60
2:C:815:LEU:HD12	2:C:815:LEU:N	2.16	0.60
2:C:1005:MET:HE1	3:D:648:MET:HB3	1.84	0.60
2:C:1054:THR:CB	2:C:1055:ILE:HD12	2.32	0.60
3:D:587:ARG:HG2	3:D:588:GLY:H	1.66	0.60
3:D:901:GLN:CB	3:D:905:PRO:HG3	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:969:ARG:CG	3:D:970:LYS:H	2.14	0.60
2:C:77:PRO:HD3	2:C:92:ALA:HA	1.83	0.60
2:C:261:LEU:O	2:C:263:ASP:N	2.35	0.60
2:C:423:ALA:HA	2:C:427:VAL:CG2	2.32	0.60
2:C:759:THR:HB	2:C:785:VAL:HG13	1.83	0.60
2:C:881:ASN:ND2	3:D:1034:GLN:CD	2.60	0.60
3:D:637:LEU:CB	3:D:641:GLN:HG3	2.32	0.60
3:D:1192:LEU:HD13	3:D:1345:GLU:HB3	1.83	0.60
3:D:1219:GLU:O	3:D:1221:VAL:N	2.33	0.60
3:D:1475:GLY:C	3:D:1477:GLY:H	2.08	0.60
1:A:158:ILE:HD11	1:A:161:ARG:NE	2.06	0.59
2:C:8:ARG:NH1	2:C:495:THR:HG23	2.17	0.59
2:C:80:GLN:NE2	2:C:122:THR:HG23	2.17	0.59
2:C:313:LEU:HD13	2:C:319:GLY:C	2.27	0.59
3:D:1382:THR:HG21	3:D:1418:LYS:CE	2.29	0.59
3:D:1479:ASP:C	3:D:1481:VAL:H	2.07	0.59
2:C:1054:THR:CG2	2:C:1055:ILE:HD12	2.32	0.59
2:C:1085:PHE:CE1	3:D:1468:LEU:HD13	2.36	0.59
3:D:638:LYS:HA	3:D:729:HIS:CD2	2.37	0.59
3:D:1435:LEU:HD21	3:D:1468:LEU:HD21	1.85	0.59
3:D:1435:LEU:O	3:D:1438:ALA:HB3	2.02	0.59
1:A:30:ARG:CD	1:A:191:ASP:HB3	2.23	0.59
1:B:37:GLY:HA3	1:B:195:LEU:HD21	1.82	0.59
1:B:175:ARG:O	1:B:176:ARG:HB2	2.01	0.59
2:C:149:THR:HG23	2:C:150:PRO:HD2	1.84	0.59
3:D:21:TRP:O	3:D:23:TYR:N	2.35	0.59
3:D:1275:SER:H	3:D:1322:GLY:CA	2.14	0.59
1:A:100:ILE:HG22	1:A:101:LEU:N	2.17	0.59
2:C:31:GLN:O	2:C:33:ASP:N	2.36	0.59
2:C:89:THR:HG23	2:C:129:ILE:HA	1.84	0.59
2:C:850:ALA:HA	3:D:632:VAL:HG11	1.84	0.59
3:D:24(U):UNK:O	3:D:25(U):UNK:CB	2.50	0.59
3:D:767:HIS:CE1	4:E:2:ALA:HB1	2.38	0.59
3:D:860:LEU:O	3:D:862:ASP:N	2.34	0.59
1:A:162:ILE:HG23	1:A:163:ASN:H	1.67	0.59
2:C:257:LEU:O	2:C:258:PHE:C	2.46	0.59
2:C:369:PRO:O	2:C:370:ALA:HB3	2.02	0.59
2:C:539:VAL:O	2:C:539:VAL:HG12	2.02	0.59
2:C:780:GLU:O	2:C:781:LYS:C	2.46	0.59
2:C:981:GLU:HB3	2:C:982:PRO:HD2	1.85	0.59
3:D:466:LYS:O	3:D:468:LEU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:747:VAL:O	3:D:747:VAL:HG22	2.01	0.59
3:D:1014:ASN:O	3:D:1015:TYR:CD2	2.54	0.59
4:E:68:LEU:CD1	4:E:73:LEU:HD12	2.32	0.59
2:C:9:ILE:N	2:C:9:ILE:HD12	2.18	0.59
2:C:679:PHE:O	2:C:681:GLY:N	2.35	0.59
2:C:861:LEU:HG	2:C:862:PRO:CD	2.16	0.59
3:D:701:LEU:HD12	3:D:715:ALA:CB	2.33	0.59
3:D:964:LEU:O	3:D:966:GLU:N	2.33	0.59
3:D:1222:GLY:O	3:D:1225:ALA:HB3	2.02	0.59
3:D:1364:HIS:CG	3:D:1365:ASP:N	2.69	0.59
3:D:1407:LEU:C	3:D:1409:ALA:H	2.10	0.59
1:B:79:ILE:HG23	1:B:167:VAL:HG12	1.85	0.59
2:C:480:THR:HG23	2:C:480:THR:O	2.03	0.59
2:C:564:MET:SD	2:C:840:ALA:CB	2.87	0.59
2:C:577:PRO:HA	2:C:671:ASN:HD22	1.67	0.59
2:C:769:PRO:O	2:C:771:GLU:N	2.34	0.59
2:C:1034:GLU:HA	2:C:1037:VAL:CG2	2.33	0.59
3:D:518:PRO:HB3	3:D:544:TYR:CZ	2.38	0.59
3:D:542:ASP:O	3:D:543:LEU:C	2.45	0.59
3:D:719:VAL:O	3:D:721:VAL:HG23	2.02	0.59
3:D:850:LEU:HA	3:D:853:VAL:HB	1.85	0.59
3:D:978:TYR:CG	3:D:988:ARG:HD2	2.37	0.59
3:D:1017:PHE:HA	3:D:1023:MET:CE	2.33	0.59
3:D:1107:VAL:HG13	3:D:1202:GLN:HA	1.84	0.59
3:D:1109:GLU:HG3	3:D:1110:ALA:H	1.67	0.59
1:B:42:ARG:HG3	1:B:42:ARG:NH1	2.18	0.59
1:B:214:ALA:HA	1:B:217:ILE:CG1	2.32	0.59
1:B:223:ASN:O	1:B:225:PHE:N	2.36	0.59
2:C:11:GLU:OE1	2:C:473:ARG:HG3	2.03	0.59
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.85	0.59
2:C:439:CYS:HB2	2:C:468:ARG:NH1	2.17	0.59
2:C:882:LEU:HD11	2:C:884:GLN:HE21	1.67	0.59
2:C:950:LEU:HB3	3:D:1018:ASN:OD1	2.03	0.59
3:D:26:VAL:C	3:D:28:LYS:N	2.60	0.59
3:D:795:VAL:HG21	3:D:904:VAL:HG21	1.85	0.59
1:B:199:ILE:O	1:B:199:ILE:HG22	2.03	0.59
2:C:574:ALA:C	2:C:575:GLN:HG3	2.28	0.59
2:C:972:VAL:O	2:C:974:LEU:N	2.35	0.59
3:D:7(U):UNK:O	3:D:35(U):UNK:N	2.36	0.59
3:D:590:PRO:CB	3:D:599:PRO:HA	2.33	0.59
3:D:927:THR:HG22	3:D:931:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1271:LYS:O	3:D:1272:ALA:C	2.46	0.59
1:A:104:GLU:C	1:A:136:GLY:HA3	2.27	0.59
1:B:149:GLY:HA2	1:B:172:SER:OG	2.03	0.59
2:C:181:VAL:HG21	2:C:220:GLY:HA3	1.85	0.59
2:C:368:THR:HB	2:C:369:PRO:HD2	1.85	0.59
2:C:461:VAL:O	2:C:462:ASP:CB	2.51	0.59
2:C:467:ILE:O	2:C:469:THR:HG23	2.03	0.59
2:C:613:VAL:CG1	2:C:614:ARG:H	2.16	0.59
2:C:1021:LEU:HG	3:D:622:ARG:HD2	1.84	0.59
2:C:1103:ASP:HB2	2:C:1108:PRO:CB	2.30	0.59
3:D:1147:ARG:CB	3:D:1188:VAL:HG21	2.32	0.59
4:E:86:GLN:O	4:E:89:MET:HB2	2.03	0.59
1:A:185:ARG:HH21	1:A:194:LYS:HE3	1.68	0.58
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.38	0.58
2:C:162:ILE:CG2	2:C:163:ILE:N	2.66	0.58
2:C:440:PRO:HG3	2:C:454:SER:HB3	1.85	0.58
2:C:755:LEU:O	2:C:755:LEU:HD13	2.03	0.58
2:C:882:LEU:HD23	2:C:882:LEU:H	1.68	0.58
2:C:989:VAL:HG12	2:C:990:GLY:N	2.16	0.58
3:D:762:GLN:NE2	4:E:20:THR:HG21	2.18	0.58
3:D:948:THR:N	3:D:1020:LEU:HD13	2.18	0.58
2:C:164:PRO:HG2	2:C:168:ARG:HG2	1.84	0.58
2:C:831:ARG:O	2:C:832:LYS:C	2.46	0.58
2:C:839:LEU:O	2:C:995:MET:O	2.21	0.58
2:C:958:SER:C	2:C:962:GLN:HE21	2.10	0.58
3:D:879:ARG:HG2	3:D:879:ARG:HH11	1.68	0.58
3:D:1273:VAL:N	3:D:1324:PRO:CG	2.67	0.58
1:B:14:THR:OG1	1:B:22:GLU:HB3	2.03	0.58
1:B:80:LEU:HD13	3:D:839:LEU:CB	2.33	0.58
1:B:101:LEU:HD13	1:B:114:PHE:HA	1.85	0.58
2:C:110:GLU:H	2:C:369:PRO:CG	2.16	0.58
2:C:266:ARG:C	2:C:268:ASP:H	2.11	0.58
2:C:483:VAL:O	2:C:486:MET:N	2.36	0.58
2:C:603:VAL:CG2	2:C:646:GLY:H	2.16	0.58
2:C:841:ASN:ND2	2:C:845:ASN:H	2.00	0.58
3:D:701:LEU:HD11	3:D:759:ALA:HB1	1.85	0.58
3:D:757:ALA:HB2	4:E:61:VAL:HG11	1.86	0.58
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.38	0.58
1:A:224:TYR:CE1	1:B:9:PRO:HD2	2.39	0.58
2:C:11:GLU:OE2	2:C:473:ARG:NE	2.36	0.58
2:C:636:ALA:CB	2:C:705:ILE:HD11	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:850:ALA:HA	3:D:632:VAL:CG1	2.34	0.58
2:C:885:ILE:O	2:C:887:GLU:N	2.37	0.58
3:D:1125:MET:HG2	3:D:1126:ASP:N	2.19	0.58
3:D:1200:VAL:HA	3:D:1373:ARG:HH12	1.69	0.58
2:C:483:VAL:O	2:C:486:MET:HB2	2.03	0.58
2:C:945:ALA:O	2:C:949:LYS:HG3	2.03	0.58
2:C:1098:ASP:OD1	2:C:1100:GLN:HG3	2.02	0.58
3:D:129:PHE:O	3:D:130:ASN:CB	2.50	0.58
3:D:599:PRO:O	3:D:600:LEU:HD23	2.04	0.58
3:D:723:GLY:C	3:D:724:GLN:HE21	2.12	0.58
3:D:798:GLU:HG3	3:D:821:VAL:CB	2.32	0.58
3:D:907:GLU:HB3	3:D:911:LEU:HD22	1.86	0.58
3:D:948:THR:H	3:D:1020:LEU:CD1	2.16	0.58
3:D:1353:GLN:HE21	3:D:1368:ILE:CD1	2.07	0.58
2:C:328:LEU:C	2:C:484:VAL:HG11	2.28	0.58
3:D:699:VAL:HA	3:D:717:GLN:HA	1.84	0.58
3:D:876:SER:O	3:D:877:PRO:C	2.46	0.58
3:D:1479:ASP:C	3:D:1481:VAL:N	2.61	0.58
1:A:131:THR:HG23	2:C:644:ARG:HE	1.68	0.58
1:A:138:LEU:O	1:A:139:TYR:C	2.47	0.58
2:C:198:ARG:NH1	2:C:231:PRO:HD3	2.19	0.58
2:C:312:ALA:HB1	2:C:318:PRO:HG3	1.85	0.58
2:C:493:ARG:NH1	3:D:1069:GLU:CD	2.62	0.58
2:C:613:VAL:CG1	2:C:619:ARG:HG2	2.33	0.58
2:C:901:TYR:C	2:C:902:ILE:HD12	2.29	0.58
2:C:1100:GLN:O	3:D:8:VAL:O	2.22	0.58
3:D:551:ASN:HA	3:D:574:LEU:HD13	1.84	0.58
3:D:582:ILE:HG22	3:D:583:ASP:H	1.68	0.58
1:A:90:LEU:HB2	1:A:119:ASP:CB	2.34	0.58
1:A:143:ARG:HD3	1:A:145:ASP:OD1	2.04	0.58
1:A:158:ILE:HG13	1:A:161:ARG:HG2	1.86	0.58
1:A:181:VAL:O	1:A:181:VAL:HG12	2.04	0.58
1:B:36:LEU:O	1:B:39:PRO:HD2	2.03	0.58
1:B:55:SER:OG	1:B:157:GLY:HA3	2.03	0.58
2:C:395:LYS:HG3	2:C:397:GLU:HG3	1.85	0.58
2:C:566:THR:C	2:C:568:ALA:H	2.12	0.58
2:C:949:LYS:C	2:C:951:GLY:H	2.11	0.58
3:D:117:ASP:C	3:D:119:SER:H	2.10	0.58
3:D:642:CYS:SG	3:D:702:LEU:HD23	2.43	0.58
3:D:790:TYR:HE1	3:D:1023:MET:HE3	1.68	0.58
3:D:959:GLU:O	3:D:963:TYR:CD1	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HH12	2:C:932:GLU:HB3	1.68	0.58
2:C:386:PHE:O	2:C:392:SER:OG	2.15	0.58
2:C:487:THR:O	2:C:489:SER:N	2.37	0.58
2:C:684:PHE:CD2	2:C:685:GLU:HG2	2.39	0.58
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.18	0.58
3:D:1008:PHE:CE1	3:D:1035:ILE:HG13	2.28	0.58
3:D:1194:CYS:HB3	3:D:1373:ARG:HH22	1.66	0.58
3:D:1281:VAL:HA	3:D:1314:LYS:HA	1.85	0.58
3:D:1452:ILE:HG22	3:D:1453:ALA:N	2.19	0.58
3:D:1486:VAL:O	4:E:79:LEU:HD12	2.04	0.58
2:C:128:ILE:HD12	2:C:128:ILE:N	2.19	0.58
2:C:758:ARG:HH11	2:C:758:ARG:HG3	1.68	0.58
2:C:1082:PRO:HG2	2:C:1085:PHE:CB	2.34	0.58
2:C:1103:ASP:O	2:C:1104:GLU:C	2.47	0.58
3:D:1234:THR:HG22	3:D:1234:THR:O	2.04	0.58
3:D:1261:GLU:OE1	3:D:1268:PRO:HB3	2.02	0.58
1:A:124:ASN:O	1:A:125:PRO:O	2.22	0.57
2:C:118:LEU:HD23	2:C:118:LEU:C	2.28	0.57
2:C:281:LEU:HD21	2:C:306:THR:OG1	2.04	0.57
2:C:579:VAL:CG2	2:C:887:GLU:HG3	2.34	0.57
2:C:635:THR:O	2:C:636:ALA:CB	2.51	0.57
3:D:789:LEU:HD13	3:D:882:PHE:CE1	2.39	0.57
3:D:794:GLN:O	3:D:795:VAL:HB	2.03	0.57
3:D:1031:ASN:OD1	3:D:1033:GLN:HG2	2.04	0.57
4:E:68:LEU:HD13	4:E:73:LEU:HD12	1.84	0.57
2:C:136:ILE:CG2	2:C:336:VAL:HG13	2.33	0.57
2:C:137:VAL:CG1	2:C:411:SER:HB2	2.34	0.57
2:C:695:LEU:O	2:C:698:ASP:N	2.35	0.57
2:C:889:HIS:C	2:C:891:GLY:N	2.60	0.57
2:C:926:PHE:CE1	2:C:929:ARG:HD2	2.39	0.57
2:C:946:ARG:O	2:C:950:LEU:HG	2.04	0.57
3:D:910:SER:O	3:D:911:LEU:C	2.46	0.57
3:D:959:GLU:O	3:D:963:TYR:HD1	1.87	0.57
1:A:106:PRO:O	1:A:107:LYS:CB	2.52	0.57
2:C:26:TYR:CE2	2:C:30:LEU:HD22	2.39	0.57
2:C:399:ASN:ND2	2:C:401:LEU:H	2.01	0.57
2:C:551:GLU:HG3	2:C:906:PHE:CD2	2.39	0.57
2:C:742:ILE:HG23	2:C:756:VAL:HG22	1.86	0.57
3:D:578:VAL:C	3:D:580:ALA:N	2.62	0.57
3:D:969:ARG:HG3	3:D:970:LYS:HG3	1.85	0.57
3:D:1076:GLY:O	3:D:1079:LYS:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1103:HIS:H	3:D:1222:GLY:HA3	1.70	0.57
3:D:1109:GLU:O	3:D:1217:ILE:HD11	2.03	0.57
1:A:71:VAL:HG13	1:A:132:LEU:HB3	1.85	0.57
1:A:222:LEU:HD12	1:B:215:VAL:CG1	2.33	0.57
1:B:73:GLU:N	1:B:73:GLU:OE2	2.38	0.57
2:C:64:LEU:CD1	2:C:367:LEU:HD12	2.34	0.57
2:C:157:ARG:HG3	2:C:313:LEU:HG	1.85	0.57
2:C:466:PHE:CD1	2:C:467:ILE:HG13	2.39	0.57
2:C:478:VAL:C	2:C:479:VAL:HG22	2.29	0.57
2:C:568:ALA:O	2:C:569:VAL:HB	2.03	0.57
3:D:772:PRO:CD	3:D:778:LEU:HB2	2.34	0.57
1:A:74:ASP:C	1:A:74:ASP:OD1	2.46	0.57
1:A:186:LEU:O	1:A:187:GLY:C	2.46	0.57
1:A:228:PRO:HA	1:B:11:PHE:O	2.05	0.57
1:B:95:ALA:O	1:B:96:SER:HB3	2.05	0.57
2:C:34:VAL:HG11	2:C:38:LYS:HG3	1.86	0.57
3:D:639:LEU:HD23	3:D:729:HIS:HD2	1.68	0.57
3:D:829:VAL:O	3:D:830:ALA:HB3	2.05	0.57
3:D:965:GLU:C	3:D:968:ASP:H	2.13	0.57
3:D:1275:SER:N	3:D:1322:GLY:HA2	2.18	0.57
3:D:1280:VAL:HG13	3:D:1315:ASP:CA	2.18	0.57
3:D:1280:VAL:CG1	3:D:1281:VAL:N	2.68	0.57
3:D:1353:GLN:HB3	3:D:1357:ARG:CD	2.34	0.57
4:E:25:LYS:HZ3	4:E:29:GLN:CD	2.12	0.57
4:E:38:THR:HG22	4:E:39:VAL:N	2.20	0.57
1:A:162:ILE:HG12	1:A:163:ASN:CG	2.30	0.57
1:B:19:HIS:HB3	1:B:201:THR:O	2.04	0.57
2:C:3:ILE:CG2	2:C:902:ILE:HD13	2.35	0.57
2:C:142:ARG:CD	2:C:324:ASP:HA	2.34	0.57
2:C:662:GLU:O	2:C:663:GLU:HB2	2.04	0.57
3:D:758:GLU:O	3:D:762:GLN:HG3	2.04	0.57
3:D:1365:ASP:C	3:D:1366:LYS:HG3	2.29	0.57
3:D:1430:SER:O	3:D:1431:THR:HB	2.05	0.57
4:E:17:TYR:O	4:E:21:VAL:HG23	2.05	0.57
1:A:56:VAL:HB	1:A:142:VAL:HB	1.86	0.57
2:C:137:VAL:HG21	2:C:393:GLN:CD	2.29	0.57
2:C:202:TYR:CD1	2:C:304:LEU:HD13	2.39	0.57
2:C:374:ASN:O	2:C:376:ARG:N	2.38	0.57
2:C:600:ASP:C	2:C:648:ARG:HB2	2.28	0.57
2:C:747:ALA:O	2:C:749:VAL:HG23	2.05	0.57
2:C:760:SER:O	2:C:785:VAL:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:558:LEU:HD21	3:D:567:ILE:HG13	1.86	0.57
3:D:890:VAL:HG11	3:D:922:LEU:HD11	1.87	0.57
4:E:79:LEU:O	4:E:81:PRO:HD2	2.04	0.57
1:A:41:ARG:HG2	1:A:177:VAL:HB	1.85	0.57
1:A:225:PHE:CZ	1:B:25:LEU:HD23	2.40	0.57
1:B:25:LEU:CD1	1:B:28:LEU:HD11	2.29	0.57
2:C:149:THR:HB	2:C:158:TYR:CE1	2.34	0.57
2:C:162:ILE:HG22	2:C:163:ILE:N	2.20	0.57
2:C:211:LEU:HD22	2:C:304:LEU:CD1	2.34	0.57
2:C:232:GLU:C	2:C:234:ALA:N	2.61	0.57
2:C:369:PRO:C	2:C:371:LYS:H	2.12	0.57
2:C:410:ILE:HG21	2:C:468:ARG:NH2	2.19	0.57
2:C:1052:MET:HE2	3:D:623:VAL:HG11	1.87	0.57
3:D:1014:ASN:O	3:D:1015:TYR:CB	2.53	0.57
3:D:1486:VAL:HG21	4:E:25:LYS:HZ1	1.69	0.57
2:C:51:THR:HG1	2:C:348:LEU:HD23	1.70	0.57
2:C:260:LEU:HD12	2:C:292:ARG:CB	2.35	0.57
2:C:988:VAL:HG12	3:D:948:THR:OG1	2.04	0.57
3:D:480:GLU:HA	3:D:493:ARG:NH1	2.19	0.57
3:D:853:VAL:HG21	3:D:877:PRO:CB	2.35	0.57
3:D:1312:LEU:O	3:D:1313:VAL:CB	2.53	0.57
1:B:26:GLU:CB	1:B:27:PRO:CD	2.79	0.57
1:B:101:LEU:HD23	1:B:140:MET:HE3	1.85	0.57
1:B:129:ILE:O	1:B:130:ALA:HB2	2.04	0.57
2:C:12:VAL:O	2:C:13:ILE:HD12	2.05	0.57
2:C:545:ASN:CB	2:C:583:LEU:HD12	2.35	0.57
2:C:659:PRO:O	2:C:660:ALA:CB	2.52	0.57
3:D:69:GLU:O	3:D:70:ALA:HB3	2.05	0.57
3:D:626:SER:HA	3:D:652:LEU:CD1	2.35	0.57
3:D:1023:MET:SD	3:D:1023:MET:N	2.77	0.57
3:D:1250:THR:HG21	3:D:1270:ALA:HB2	1.86	0.57
4:E:3:GLU:HB3	4:E:4:PRO:CD	2.35	0.57
1:A:72:LYS:N	2:C:607:ASP:HB3	2.20	0.56
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.85	0.56
1:B:150:TYR:CD1	1:B:170:ILE:HG22	2.40	0.56
2:C:468:ARG:O	2:C:469:THR:O	2.23	0.56
2:C:597:ALA:HA	2:C:614:ARG:NH1	2.19	0.56
2:C:728:HIS:CD2	2:C:783:ARG:HH11	2.22	0.56
2:C:843:HIS:HD2	2:C:884:GLN:HA	1.66	0.56
2:C:874:LEU:CD2	3:D:784:ASP:HA	2.35	0.56
2:C:892:LEU:HD23	2:C:892:LEU:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1077:PRO:O	2:C:1079:PRO:HD3	2.05	0.56
3:D:691:LEU:C	3:D:693:GLU:N	2.63	0.56
3:D:777:PRO:CG	3:D:912:LYS:HG3	2.34	0.56
3:D:1277:ILE:HG22	3:D:1278:ASP:N	2.20	0.56
3:D:1379:VAL:HG22	3:D:1394:VAL:O	2.04	0.56
1:B:53:VAL:HG12	1:B:167:VAL:HG21	1.86	0.56
1:B:72:LYS:HB3	1:B:131:THR:HB	1.87	0.56
2:C:100:LEU:HD21	2:C:368:THR:CA	2.36	0.56
2:C:129:ILE:HD12	2:C:386:PHE:HB3	1.85	0.56
2:C:142:ARG:HE	2:C:324:ASP:HA	1.69	0.56
2:C:163:ILE:CG2	2:C:164:PRO:HD2	2.34	0.56
2:C:317:VAL:N	2:C:318:PRO:HD2	2.20	0.56
2:C:568:ALA:O	2:C:569:VAL:CB	2.53	0.56
2:C:1055:ILE:CG2	2:C:1066:ALA:HB2	2.34	0.56
3:D:461:ILE:HG22	3:D:465:LEU:CD1	2.35	0.56
3:D:580:ALA:HB2	3:D:587:ARG:NH2	2.21	0.56
3:D:702:LEU:HD12	3:D:745:MET:SD	2.45	0.56
3:D:957:PRO:HG3	3:D:1007:VAL:HB	1.87	0.56
3:D:1221:VAL:O	3:D:1222:GLY:C	2.46	0.56
1:A:52:ALA:HB3	1:A:171:PHE:CE1	2.39	0.56
1:A:178:ALA:O	1:A:179:PHE:HB3	2.04	0.56
1:B:74:ASP:O	1:B:75:VAL:C	2.48	0.56
1:B:77:GLU:OE1	1:B:77:GLU:HA	2.05	0.56
1:B:100:ILE:HA	1:B:141:GLU:HA	1.86	0.56
1:B:126:ASP:O	1:B:127:LEU:HB3	2.05	0.56
2:C:159:ILE:HD11	2:C:310:LEU:CB	2.29	0.56
2:C:169:GLY:HA2	2:C:264:PRO:O	2.06	0.56
2:C:640:ARG:HG3	2:C:640:ARG:NH1	2.20	0.56
2:C:726:ILE:H	2:C:726:ILE:CD1	2.14	0.56
2:C:735:ARG:HA	2:C:737:LEU:O	2.04	0.56
2:C:873:PRO:HG2	2:C:874:LEU:N	2.18	0.56
2:C:881:ASN:CG	3:D:1034:GLN:CD	2.73	0.56
2:C:989:VAL:CG1	2:C:990:GLY:N	2.68	0.56
3:D:88:TYR:O	3:D:89:ARG:CB	2.53	0.56
3:D:91:ALA:CB	3:D:518:PRO:HG2	2.36	0.56
3:D:571:LYS:C	3:D:573:MET:N	2.62	0.56
3:D:599:PRO:C	3:D:600:LEU:HD23	2.30	0.56
3:D:809:PRO:C	3:D:811:GLU:N	2.62	0.56
3:D:811:GLU:CA	3:D:814:ALA:HB3	2.24	0.56
3:D:1154:GLU:CB	3:D:1159:ARG:HG2	2.25	0.56
3:D:1381:VAL:HG12	3:D:1382:THR:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:OE2	1:A:185:ARG:CZ	2.53	0.56
1:A:99:LEU:O	1:A:100:ILE:HD13	2.06	0.56
2:C:100:LEU:HD21	2:C:368:THR:HA	1.87	0.56
2:C:873:PRO:CG	2:C:874:LEU:H	2.18	0.56
2:C:940:GLU:HA	2:C:973:VAL:HG21	1.87	0.56
3:D:20(U):UNK:O	3:D:21(U):UNK:CB	2.53	0.56
3:D:863:THR:C	3:D:864:VAL:HG23	2.30	0.56
3:D:864:VAL:H	3:D:876:SER:HG	1.50	0.56
3:D:898:GLU:OE1	3:D:921:ARG:NH1	2.38	0.56
3:D:1208:ASP:HA	3:D:1215:VAL:HG22	1.87	0.56
3:D:1376:LEU:HD11	3:D:1421:LEU:CD1	2.32	0.56
3:D:1463:LYS:O	3:D:1467:ILE:HG13	2.05	0.56
3:D:1483:PHE:HE2	4:E:18:ARG:NE	2.03	0.56
1:A:199:ILE:HG22	1:A:199:ILE:O	2.05	0.56
2:C:443:THR:N	2:C:444:PRO:CD	2.69	0.56
2:C:456:ALA:HB3	2:C:459:ALA:CB	2.24	0.56
2:C:918:LEU:HD13	2:C:968:ASP:HA	1.87	0.56
2:C:1076:VAL:HG21	3:D:753:SER:HB3	1.88	0.56
2:C:1087:VAL:HG12	2:C:1087:VAL:O	2.06	0.56
3:D:87:ARG:CB	3:D:522:PRO:HG2	2.36	0.56
3:D:616:GLN:O	3:D:617:ASN:HB2	2.04	0.56
1:A:185:ARG:NH2	1:A:194:LYS:HE3	2.20	0.56
1:B:188:GLN:HG2	3:D:688:TRP:CD1	2.40	0.56
2:C:151:ASP:HB2	2:C:156:GLY:O	2.04	0.56
2:C:314:THR:O	2:C:315:ALA:CB	2.53	0.56
2:C:601:GLY:HA3	2:C:647:GLN:C	2.31	0.56
2:C:681:GLY:HA2	3:D:939:PHE:CE2	2.40	0.56
2:C:873:PRO:O	2:C:874:LEU:C	2.47	0.56
2:C:950:LEU:O	2:C:951:GLY:C	2.49	0.56
3:D:502:PHE:CD1	3:D:1452:ILE:HG23	2.40	0.56
3:D:1266:ARG:O	3:D:1268:PRO:CD	2.54	0.56
4:E:30:LEU:C	4:E:32:ARG:N	2.64	0.56
1:A:157:GLY:CA	1:A:166:PRO:HB3	2.35	0.56
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.41	0.56
1:B:94:MET:SD	1:B:97:THR:HG22	2.45	0.56
2:C:100:LEU:CD1	2:C:108:ILE:HB	2.35	0.56
2:C:260:LEU:CD2	2:C:261:LEU:HB3	2.34	0.56
2:C:337:GLY:O	2:C:341:ALA:HB2	2.06	0.56
2:C:605:LYS:HG3	2:C:611:ILE:HA	1.88	0.56
2:C:693:GLU:OE1	2:C:693:GLU:HA	2.06	0.56
3:D:554:LEU:HD11	3:D:571:LYS:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:795:VAL:N	3:D:862:ASP:CB	2.67	0.56
3:D:978:TYR:C	3:D:980:MET:N	2.59	0.56
3:D:1030:GLY:O	3:D:1031:ASN:HB3	2.06	0.56
3:D:1194:CYS:HB3	3:D:1373:ARG:HH21	1.70	0.56
3:D:1381:VAL:HB	3:D:1390:LEU:O	2.06	0.56
4:E:10:PHE:CE2	4:E:16:LYS:HG3	2.41	0.56
1:A:41:ARG:HH21	2:C:860:HIS:CD2	2.24	0.56
1:B:78:ILE:HA	1:B:81:ASN:HD22	1.71	0.56
2:C:31:GLN:HG2	2:C:39:ARG:HD2	1.86	0.56
2:C:144:PRO:HA	2:C:162:ILE:HG21	1.87	0.56
2:C:440:PRO:HG2	2:C:453:THR:OG1	2.06	0.56
2:C:498:GLN:H	2:C:502:PRO:CD	2.18	0.56
2:C:1008:ARG:NE	2:C:1010:THR:O	2.39	0.56
3:D:612:GLY:C	3:D:614:PHE:N	2.63	0.56
3:D:897:GLN:HE21	3:D:897:GLN:HA	1.71	0.56
3:D:1330:ILE:O	3:D:1331:ASP:C	2.49	0.56
1:B:118:ALA:C	1:B:120:VAL:H	2.13	0.56
2:C:183:THR:HG21	2:C:190:LYS:HG3	1.88	0.56
2:C:233:GLU:O	2:C:237:ARG:HG2	2.06	0.56
2:C:263:ASP:OD2	2:C:264:PRO:HD3	2.05	0.56
2:C:352:ALA:CA	2:C:355:VAL:HG12	2.32	0.56
2:C:395:LYS:CE	2:C:403:SER:HB2	2.35	0.56
2:C:565:GLN:CG	2:C:995:MET:HE1	2.17	0.56
2:C:750:LYS:HE3	3:D:680:GLN:HE22	1.71	0.56
2:C:1008:ARG:HH12	2:C:1021:LEU:N	2.04	0.56
3:D:1280:VAL:CG1	3:D:1281:VAL:H	2.18	0.56
3:D:1353:GLN:HB3	3:D:1357:ARG:HD2	1.87	0.56
3:D:1450:ALA:CA	3:D:1455:LYS:HG3	2.33	0.56
1:B:103:ALA:HB1	1:B:132:LEU:CD1	2.36	0.56
2:C:166:PRO:CB	2:C:417:GLY:H	2.19	0.56
2:C:203:ASP:N	2:C:207:LEU:HB2	2.21	0.56
2:C:430:VAL:O	2:C:431:HIS:C	2.49	0.56
2:C:731:GLU:O	2:C:733:ALA:N	2.38	0.56
3:D:699:VAL:HG12	3:D:717:GLN:HG2	1.87	0.56
3:D:808:THR:N	3:D:809:PRO:CD	2.69	0.56
3:D:971:LEU:O	3:D:974:ILE:N	2.36	0.56
3:D:1015:TYR:CB	3:D:1018:ASN:HB2	2.34	0.56
3:D:1031:ASN:HD21	3:D:1034:GLN:HB2	1.71	0.56
3:D:1252:ILE:C	3:D:1254:GLN:N	2.64	0.56
1:A:121:GLU:O	1:A:123:MET:N	2.31	0.55
1:A:143:ARG:HG3	1:A:159:LYS:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:VAL:HG21	2:C:218:VAL:HG13	1.87	0.55
2:C:343:GLN:HG2	2:C:385:PHE:CB	2.36	0.55
2:C:567:GLN:O	2:C:997:LEU:HA	2.06	0.55
2:C:605:LYS:CD	2:C:607:ASP:HA	2.35	0.55
2:C:867:VAL:HG12	2:C:868:ASP:H	1.70	0.55
3:D:99:ALA:HB3	3:D:458:ALA:HB1	1.87	0.55
3:D:552:ASN:C	3:D:554:LEU:H	2.13	0.55
3:D:603:LEU:HA	3:D:606:ILE:HD13	1.87	0.55
3:D:936:TYR:O	3:D:940:THR:HG22	2.05	0.55
3:D:1437:ALA:HA	3:D:1440:PHE:HD1	1.71	0.55
3:D:1483:PHE:HE1	4:E:22:VAL:HG23	1.72	0.55
1:A:131:THR:HG23	2:C:644:ARG:CZ	2.37	0.55
1:B:94:MET:CE	1:B:94:MET:CB	2.84	0.55
2:C:21:ILE:O	2:C:25:SER:HB2	2.06	0.55
2:C:31:GLN:HG2	2:C:39:ARG:CD	2.35	0.55
2:C:263:ASP:CG	2:C:264:PRO:HD3	2.31	0.55
2:C:360:VAL:HG12	2:C:361:MET:N	2.20	0.55
2:C:501:THR:N	2:C:502:PRO:HD2	2.20	0.55
2:C:580:MET:O	2:C:581:THR:HB	2.07	0.55
2:C:595:LEU:HG	2:C:655:LEU:CD2	2.37	0.55
2:C:755:LEU:HD13	2:C:755:LEU:C	2.31	0.55
2:C:845:ASN:ND2	2:C:884:GLN:OE1	2.36	0.55
3:D:25(U):UNK:HA	3:D:40(U):UNK:O	2.06	0.55
3:D:1008:PHE:CD2	3:D:1008:PHE:O	2.59	0.55
3:D:1109:GLU:CG	3:D:1110:ALA:N	2.68	0.55
3:D:1335:LEU:HD23	3:D:1344:VAL:HG22	1.88	0.55
2:C:549:PHE:HE1	2:C:579:VAL:HG11	1.71	0.55
2:C:603:VAL:HG21	2:C:645:VAL:HA	1.87	0.55
2:C:755:LEU:HB3	2:C:790:LEU:HD23	1.86	0.55
2:C:831:ARG:O	2:C:832:LYS:O	2.25	0.55
2:C:943:VAL:O	2:C:944:LEU:C	2.49	0.55
2:C:950:LEU:C	3:D:1018:ASN:HD21	2.14	0.55
3:D:857:LEU:CD1	3:D:858:LEU:H	2.14	0.55
3:D:865:THR:CG2	3:D:866:THR:N	2.69	0.55
3:D:1141:GLU:CA	3:D:1171:VAL:HG11	2.27	0.55
3:D:1429:LEU:HD12	3:D:1429:LEU:O	2.07	0.55
1:A:198:ARG:NH1	2:C:934:PHE:CE1	2.74	0.55
2:C:30:LEU:O	2:C:32:ALA:N	2.40	0.55
2:C:163:ILE:HG23	2:C:265:LYS:HZ1	1.72	0.55
2:C:177:GLU:CG	2:C:181:VAL:H	2.19	0.55
2:C:304:LEU:HD23	2:C:305:PRO:CD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:355:VAL:HG13	2:C:356:ARG:N	2.21	0.55
2:C:796:GLU:HA	3:D:681:ARG:HH22	1.72	0.55
2:C:837:ASP:H	2:C:1001:VAL:HG23	1.71	0.55
3:D:100:ALA:HA	3:D:575:GLN:OE1	2.06	0.55
3:D:502:PHE:CD2	3:D:507:ASN:ND2	2.73	0.55
3:D:657:LEU:HG	3:D:661:MET:HE2	1.89	0.55
3:D:675:ARG:HA	3:D:678:GLU:CB	2.37	0.55
3:D:865:THR:CG2	3:D:866:THR:H	2.18	0.55
3:D:907:GLU:CG	3:D:911:LEU:HD13	2.37	0.55
3:D:1457:ASP:C	3:D:1459:LEU:H	2.14	0.55
3:D:1490:ARG:C	3:D:1492:LEU:H	2.15	0.55
1:A:16:GLN:HG3	1:A:20:TYR:CB	2.36	0.55
1:A:131:THR:O	1:A:131:THR:CG2	2.52	0.55
1:B:101:LEU:CD2	1:B:140:MET:HE3	2.37	0.55
1:B:173:PRO:HG3	1:B:204:SER:OG	2.06	0.55
2:C:142:ARG:HG2	2:C:147:TYR:OH	2.07	0.55
2:C:754:ILE:HD13	2:C:791:ARG:HE	1.71	0.55
2:C:1009:SER:HB2	3:D:651:GLU:O	2.07	0.55
3:D:681:ARG:O	3:D:682:ASP:CB	2.55	0.55
3:D:728:LEU:HD13	3:D:745:MET:CE	2.36	0.55
3:D:772:PRO:HG2	3:D:772:PRO:O	2.06	0.55
2:C:15:LEU:HD21	2:C:461:VAL:HG21	1.86	0.55
2:C:35:PRO:C	2:C:37:GLU:H	2.12	0.55
2:C:803:ARG:HB3	2:C:825:VAL:HG22	1.88	0.55
2:C:852:ILE:O	2:C:852:ILE:HG12	2.06	0.55
2:C:1073:GLY:HA2	3:D:659:LYS:HE3	1.88	0.55
3:D:648:MET:CE	3:D:747:VAL:HG11	2.36	0.55
3:D:793:THR:HG21	3:D:907:GLU:OE1	2.06	0.55
3:D:1069:GLU:HG3	3:D:1072:ILE:CD1	2.35	0.55
3:D:1083:ASP:O	3:D:1086:LEU:N	2.37	0.55
3:D:1276:GLU:CD	3:D:1301:LYS:HE2	2.32	0.55
3:D:1283:ILE:HD12	3:D:1312:LEU:HA	1.89	0.55
3:D:1324:PRO:CG	3:D:1325:LEU:H	2.20	0.55
3:D:1459:LEU:CD1	3:D:1470:ARG:NH1	2.69	0.55
3:D:1471:LEU:HG	3:D:1471:LEU:O	2.06	0.55
1:A:6:LEU:C	1:A:8:ALA:N	2.62	0.55
1:A:15:THR:OG1	1:A:16:GLN:N	2.32	0.55
1:B:58:ILE:O	1:B:59:GLU:C	2.49	0.55
2:C:254:LEU:C	2:C:256:TYR:H	2.12	0.55
2:C:1020:PRO:O	2:C:1021:LEU:HG	2.06	0.55
2:C:1054:THR:C	2:C:1056:LYS:N	2.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:824:ASN:O	3:D:825:ALA:C	2.50	0.55
1:A:34:VAL:O	1:A:35:THR:C	2.48	0.55
1:B:12:THR:HB	1:B:24:VAL:HB	1.88	0.55
2:C:44:ILE:H	2:C:44:ILE:HD12	1.71	0.55
2:C:327:HIS:O	2:C:329:GLY:N	2.36	0.55
2:C:479:VAL:O	2:C:480:THR:O	2.25	0.55
2:C:688:ILE:HG22	2:C:869:VAL:HG23	1.89	0.55
2:C:816:LYS:HG3	2:C:819:VAL:HG23	1.89	0.55
2:C:1012:PRO:CG	2:C:1023:GLY:HA3	2.37	0.55
3:D:30(U):UNK:O	3:D:31(U):UNK:CB	2.55	0.55
3:D:616:GLN:O	3:D:617:ASN:CB	2.54	0.55
3:D:965:GLU:O	3:D:968:ASP:N	2.40	0.55
3:D:1449:GLU:O	3:D:1450:ALA:C	2.50	0.55
1:A:56:VAL:O	1:A:165:ILE:HG12	2.07	0.55
1:A:122:ILE:O	1:A:122:ILE:HG22	2.06	0.55
1:B:104:GLU:O	1:B:136:GLY:HA3	2.06	0.55
1:B:143:ARG:HG2	1:B:144:VAL:N	2.21	0.55
2:C:407:LYS:C	2:C:409:ARG:H	2.13	0.55
2:C:601:GLY:O	2:C:602:GLU:CB	2.54	0.55
2:C:613:VAL:HG11	2:C:619:ARG:HG3	1.87	0.55
2:C:676:ILE:HG21	2:C:873:PRO:HB3	1.87	0.55
2:C:831:ARG:HG2	2:C:1002:GLU:OE2	2.06	0.55
2:C:839:LEU:O	2:C:840:ALA:O	2.25	0.55
2:C:924:LEU:N	2:C:924:LEU:CD2	2.66	0.55
2:C:1005:MET:HG2	3:D:724:GLN:HG3	1.88	0.55
2:C:1106:ASP:C	2:C:1108:PRO:HD3	2.32	0.55
3:D:1281:VAL:HG13	3:D:1314:LYS:CB	2.36	0.55
3:D:1402:ALA:O	3:D:1406:ARG:HB2	2.06	0.55
1:A:95:ALA:O	1:A:96:SER:HB3	2.06	0.55
1:B:62:LEU:HD23	1:B:163:ASN:OD1	2.07	0.55
1:B:78:ILE:HG13	1:B:129:ILE:O	2.07	0.55
2:C:291:VAL:O	2:C:299:LYS:N	2.38	0.55
2:C:552:HIS:CE1	3:D:1064:GLY:HA2	2.42	0.55
2:C:672:VAL:HG22	2:C:673:LEU:H	1.71	0.55
2:C:700:TYR:HB2	2:C:833:LEU:HD22	1.89	0.55
3:D:666:PHE:O	3:D:667:ALA:HB3	2.06	0.55
3:D:669:ASN:O	3:D:672:ALA:HB3	2.06	0.55
3:D:970:LYS:HA	3:D:973:GLN:HB2	1.87	0.55
3:D:1065:LEU:C	3:D:1067:VAL:H	2.15	0.55
3:D:1148:VAL:HG23	3:D:1165:TYR:CD2	2.42	0.55
3:D:1436:SER:HB3	3:D:1464:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLY:O	1:A:158:ILE:C	2.50	0.54
1:B:100:ILE:HA	1:B:140:MET:O	2.06	0.54
1:B:151:VAL:HG23	1:B:169:ALA:CB	2.32	0.54
2:C:5:ARG:HH22	2:C:10:ARG:NH1	2.05	0.54
2:C:163:ILE:HD12	2:C:163:ILE:N	2.20	0.54
2:C:200:LEU:HD22	2:C:290:LEU:HD13	1.88	0.54
2:C:203:ASP:O	2:C:204:GLN:O	2.25	0.54
2:C:352:ALA:O	2:C:353:ARG:C	2.50	0.54
2:C:440:PRO:HG3	2:C:454:SER:CB	2.36	0.54
2:C:472:ARG:HG2	2:C:472:ARG:HH11	1.73	0.54
2:C:495:THR:HG22	2:C:496:ILE:N	2.21	0.54
3:D:660:LYS:O	3:D:664:LYS:HB2	2.06	0.54
3:D:762:GLN:O	3:D:768:ASN:HB2	2.07	0.54
3:D:1051:GLU:O	3:D:1052:THR:C	2.50	0.54
3:D:1142:SER:O	3:D:1364:HIS:CD2	2.59	0.54
3:D:1324:PRO:CG	3:D:1325:LEU:N	2.70	0.54
3:D:1434:TRP:CD1	3:D:1447:LEU:HD12	2.43	0.54
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.89	0.54
1:A:72:LYS:HA	2:C:607:ASP:CB	2.32	0.54
2:C:17:PRO:HD2	2:C:20:GLU:CB	2.23	0.54
2:C:202:TYR:HE1	2:C:304:LEU:HB3	1.73	0.54
2:C:261:LEU:C	2:C:263:ASP:N	2.64	0.54
2:C:291:VAL:HB	2:C:299:LYS:CG	2.37	0.54
2:C:410:ILE:HB	2:C:453:THR:HG23	1.89	0.54
2:C:1111:VAL:O	2:C:1111:VAL:HG12	2.07	0.54
3:D:104:PHE:O	3:D:511:TRP:HZ3	1.90	0.54
3:D:564:GLU:CG	3:D:568:ARG:HE	2.20	0.54
4:E:38:THR:HG22	4:E:40:LEU:N	2.18	0.54
1:A:26:GLU:CB	1:A:27:PRO:CD	2.72	0.54
1:B:147:GLY:HA3	1:B:171:PHE:CG	2.43	0.54
1:B:170:ILE:HD12	1:B:170:ILE:O	2.07	0.54
1:B:173:PRO:O	1:B:201:THR:HB	2.07	0.54
2:C:101:ILE:HG22	2:C:102:HIS:H	1.72	0.54
2:C:439:CYS:HB2	2:C:468:ARG:HH11	1.72	0.54
2:C:845:ASN:HD22	2:C:884:GLN:CD	2.15	0.54
2:C:1052:MET:HG2	3:D:623:VAL:CG2	2.37	0.54
3:D:91:ALA:HB3	3:D:518:PRO:CD	2.36	0.54
3:D:110:SER:C	3:D:112:ILE:H	2.15	0.54
3:D:461:ILE:HG22	3:D:465:LEU:HD13	1.89	0.54
3:D:629:SER:HB3	3:D:726:ILE:HD12	1.88	0.54
3:D:699:VAL:CA	3:D:716:PHE:O	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:905:PRO:O	3:D:906:GLN:CB	2.54	0.54
3:D:936:TYR:C	3:D:936:TYR:CD2	2.86	0.54
3:D:952:ASP:O	3:D:954:ALA:N	2.41	0.54
3:D:1105:ILE:HG23	3:D:1200:VAL:CB	2.37	0.54
3:D:1444:THR:O	3:D:1448:THR:N	2.35	0.54
1:B:73:GLU:OE1	1:B:128:HIS:CE1	2.60	0.54
2:C:202:TYR:C	2:C:203:ASP:CG	2.75	0.54
2:C:470:PRO:HG3	2:C:472:ARG:NH2	2.23	0.54
2:C:492:ASP:HA	2:C:509:ALA:CB	2.37	0.54
2:C:929:ARG:C	2:C:931:GLY:N	2.66	0.54
2:C:1038:TRP:HE1	3:D:1463:LYS:HE3	1.73	0.54
3:D:573:MET:HA	3:D:576:GLU:HB2	1.88	0.54
3:D:897:GLN:HA	3:D:897:GLN:NE2	2.22	0.54
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.89	0.54
3:D:1118:ILE:HD11	3:D:1193:THR:HG22	1.90	0.54
3:D:1236:LEU:CD1	3:D:1259:VAL:HG21	2.37	0.54
4:E:42:PRO:HG2	4:E:44:GLU:HG2	1.89	0.54
1:A:162:ILE:HG23	1:A:163:ASN:ND2	2.22	0.54
2:C:159:ILE:HG21	2:C:306:THR:HG23	1.88	0.54
2:C:238:LEU:O	2:C:241:LEU:HB2	2.07	0.54
2:C:328:LEU:CB	2:C:484:VAL:HG11	2.38	0.54
2:C:691:SER:O	2:C:692:GLU:C	2.49	0.54
2:C:692:GLU:OE1	2:C:696:LYS:HE3	2.07	0.54
2:C:727:PRO:C	2:C:729:LEU:H	2.14	0.54
2:C:881:ASN:OD1	3:D:1034:GLN:NE2	2.40	0.54
2:C:1052:MET:HG3	2:C:1056:LYS:HE3	1.89	0.54
3:D:772:PRO:CB	3:D:778:LEU:HB2	2.36	0.54
3:D:911:LEU:O	3:D:915:VAL:HG23	2.08	0.54
3:D:953:ASP:OD1	3:D:1020:LEU:HG	2.06	0.54
3:D:1148:VAL:O	3:D:1148:VAL:HG12	2.08	0.54
1:B:118:ALA:O	1:B:120:VAL:N	2.41	0.54
1:B:143:ARG:HD2	1:B:159:LYS:HG2	1.90	0.54
3:D:480:GLU:O	3:D:493:ARG:NH2	2.39	0.54
4:E:26:ARG:NH2	4:E:30:LEU:CD1	2.70	0.54
1:A:9:PRO:HG3	1:B:224:TYR:CG	2.43	0.54
1:A:128:HIS:CE1	1:A:131:THR:OG1	2.61	0.54
1:B:188:GLN:CG	3:D:688:TRP:CD1	2.91	0.54
2:C:603:VAL:O	2:C:604:VAL:HG23	2.07	0.54
2:C:908:GLY:O	2:C:909:ALA:HB3	2.07	0.54
3:D:969:ARG:NH2	3:D:970:LYS:HE3	2.22	0.54
3:D:1069:GLU:O	3:D:1071:PHE:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1331:ASP:O	3:D:1333:HIS:N	2.40	0.54
1:A:91:ASP:OD1	1:A:94:MET:HE3	2.07	0.54
1:A:157:GLY:N	1:A:166:PRO:HB3	2.23	0.54
1:A:175:ARG:O	1:A:176:ARG:CB	2.56	0.54
2:C:231:PRO:O	2:C:233:GLU:N	2.40	0.54
2:C:745:ILE:HD12	2:C:802:GLY:HA2	1.90	0.54
3:D:654:LYS:O	3:D:657:LEU:HB3	2.08	0.54
3:D:703:ASN:OD1	3:D:704:ARG:N	2.41	0.54
3:D:957:PRO:CD	3:D:1007:VAL:HB	2.38	0.54
3:D:1031:ASN:ND2	3:D:1034:GLN:HB2	2.23	0.54
1:B:47:SER:O	1:B:48:ILE:CG1	2.55	0.54
1:B:76:VAL:HA	1:B:79:ILE:HB	1.90	0.54
2:C:148:PHE:HE2	2:C:310:LEU:HA	1.73	0.54
2:C:289:THR:O	2:C:290:LEU:O	2.26	0.54
2:C:676:ILE:C	3:D:948:THR:HG22	2.32	0.54
2:C:1001:VAL:HG11	3:D:724:GLN:CB	2.32	0.54
3:D:28:LYS:CB	3:D:548:ILE:HG23	2.38	0.54
3:D:497:GLU:HG2	3:D:1389:LEU:HD21	1.88	0.54
1:A:83:LYS:CE	1:A:168:ASP:HB2	2.38	0.54
1:B:46:SER:O	1:B:47:SER:C	2.50	0.54
1:B:220:GLU:O	1:B:223:ASN:HB2	2.08	0.54
1:B:221:HIS:HA	1:B:224:TYR:CE1	2.43	0.54
2:C:31:GLN:HG2	2:C:39:ARG:NE	2.23	0.54
2:C:115:LEU:HA	2:C:375:SER:OG	2.08	0.54
2:C:198:ARG:HD3	2:C:198:ARG:C	2.32	0.54
2:C:198:ARG:HG3	2:C:228:ALA:HA	1.89	0.54
2:C:586:ARG:O	2:C:588:VAL:N	2.40	0.54
2:C:722:ILE:HA	2:C:758:ARG:HB2	1.90	0.54
2:C:1115:LEU:HD23	2:C:1115:LEU:N	2.23	0.54
3:D:82:ARG:O	3:D:84:ILE:N	2.41	0.54
3:D:117:ASP:C	3:D:119:SER:N	2.65	0.54
3:D:558:LEU:HD11	3:D:567:ILE:HD11	1.90	0.54
3:D:760:ARG:HH12	4:E:59:ASN:ND2	2.06	0.54
3:D:832:ARG:O	3:D:832:ARG:HG2	2.07	0.54
3:D:1213:ARG:HG3	3:D:1214:PRO:CD	2.38	0.54
1:B:177:VAL:HG13	1:B:199:ILE:HD12	1.90	0.53
2:C:421:GLU:O	2:C:422:ARG:C	2.50	0.53
2:C:559:LEU:C	2:C:559:LEU:CD1	2.80	0.53
2:C:640:ARG:HG3	2:C:641:PRO:HD2	1.89	0.53
2:C:915:LYS:O	2:C:919:ALA:N	2.41	0.53
3:D:149:LYS:O	3:D:151:GLN:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:732:VAL:O	3:D:733:CYS:C	2.49	0.53
3:D:1009:ASN:OD1	3:D:1009:ASN:O	2.25	0.53
3:D:1264:GLU:O	3:D:1265:ALA:HB3	2.08	0.53
3:D:1425:THR:C	3:D:1427:SER:H	2.15	0.53
2:C:520:GLU:N	2:C:521:PRO:HD3	2.22	0.53
2:C:555:ALA:O	2:C:558:ALA:HB3	2.08	0.53
2:C:959:PRO:HG2	2:C:960:GLU:N	2.18	0.53
3:D:879:ARG:HE	3:D:904:VAL:H	1.56	0.53
1:A:22:GLU:HA	1:A:198:ARG:HA	1.89	0.53
1:B:53:VAL:HG23	1:B:85:LEU:HD23	1.90	0.53
2:C:13:ILE:HG23	2:C:14:PRO:CD	2.38	0.53
2:C:163:ILE:HG21	2:C:169:GLY:C	2.33	0.53
2:C:363:SER:OG	2:C:364:PRO:HD2	2.08	0.53
2:C:466:PHE:HD1	2:C:467:ILE:CG1	2.22	0.53
2:C:487:THR:O	2:C:488:ALA:C	2.51	0.53
2:C:598:GLU:N	2:C:614:ARG:NH1	2.56	0.53
2:C:854:PRO:HB2	2:C:856:GLU:HG3	1.91	0.53
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.43	0.53
3:D:8:VAL:HG12	3:D:1434:TRP:HH2	1.72	0.53
3:D:702:LEU:O	3:D:713:ILE:O	2.26	0.53
3:D:882:PHE:HA	3:D:885:ILE:CD1	2.35	0.53
3:D:951:ILE:HG22	3:D:952:ASP:N	2.23	0.53
3:D:1156:LEU:CD1	3:D:1177:ALA:HA	2.38	0.53
3:D:1281:VAL:HG22	3:D:1315:ASP:H	1.73	0.53
3:D:1363:LEU:O	3:D:1364:HIS:HB2	2.08	0.53
3:D:1409:ALA:O	3:D:1413:VAL:N	2.40	0.53
3:D:1465:ASN:HD21	3:D:1470:ARG:NH1	2.06	0.53
1:B:71:VAL:HA	1:B:132:LEU:HA	1.91	0.53
1:B:124:ASN:OD1	1:B:124:ASN:N	2.41	0.53
2:C:243:ARG:HG3	2:C:244:PRO:HA	1.89	0.53
2:C:399:ASN:ND2	2:C:402:SER:H	2.06	0.53
2:C:479:VAL:O	2:C:480:THR:C	2.52	0.53
2:C:613:VAL:HG22	2:C:620:LEU:N	2.24	0.53
2:C:801:VAL:HG23	2:C:828:ALA:HB2	1.88	0.53
2:C:882:LEU:HD11	2:C:884:GLN:NE2	2.23	0.53
3:D:989:TYR:CZ	3:D:993:ILE:HG13	2.44	0.53
3:D:1043:GLY:CA	3:D:1057:VAL:H	2.17	0.53
3:D:1224:VAL:O	3:D:1224:VAL:HG12	2.08	0.53
3:D:1420:LEU:HD12	3:D:1421:LEU:H	1.72	0.53
3:D:1434:TRP:HD1	3:D:1447:LEU:HD12	1.74	0.53
3:D:1459:LEU:HD12	3:D:1470:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:41:GLU:N	4:E:42:PRO:HD2	2.23	0.53
1:B:109:VAL:HG21	1:B:138:LEU:HD23	1.91	0.53
2:C:100:LEU:HD23	2:C:372:LEU:HD12	1.90	0.53
2:C:466:PHE:HD1	2:C:467:ILE:HG13	1.72	0.53
2:C:580:MET:O	2:C:581:THR:O	2.27	0.53
2:C:628:TYR:O	2:C:629:ALA:O	2.26	0.53
2:C:672:VAL:O	2:C:991:GLN:HA	2.08	0.53
2:C:900:ARG:C	2:C:901:TYR:CD1	2.86	0.53
2:C:1076:VAL:HG21	3:D:753:SER:CB	2.38	0.53
3:D:715:ALA:O	3:D:764:LEU:HD12	2.07	0.53
3:D:916:TYR:CD2	3:D:917:GLN:N	2.76	0.53
3:D:949:ILE:O	3:D:949:ILE:HG22	2.08	0.53
3:D:1041:MET:HG2	3:D:1042:ARG:N	2.24	0.53
1:A:31:GLY:N	1:A:193:ASP:OD2	2.37	0.53
1:B:33:GLY:HA3	1:B:181:VAL:HG21	1.90	0.53
2:C:102:HIS:HD2	2:C:106:GLY:HA3	1.72	0.53
2:C:376:ARG:N	2:C:377:PRO:CD	2.62	0.53
2:C:440:PRO:HG3	2:C:454:SER:CA	2.38	0.53
2:C:449:ILE:O	2:C:451:LEU:N	2.41	0.53
2:C:839:LEU:O	2:C:994:ILE:HG22	2.08	0.53
2:C:892:LEU:HD23	2:C:893:ALA:N	2.22	0.53
3:D:552:ASN:C	3:D:555:LYS:H	2.16	0.53
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.39	0.53
3:D:792:ILE:HG12	3:D:941:LEU:HG	1.91	0.53
3:D:879:ARG:NE	3:D:904:VAL:H	2.06	0.53
3:D:935:LYS:O	3:D:936:TYR:C	2.52	0.53
3:D:1223:VAL:C	3:D:1225:ALA:H	2.16	0.53
3:D:1311:LEU:H	3:D:1311:LEU:HD12	1.73	0.53
3:D:1393:GLN:HE21	3:D:1420:LEU:HD21	1.74	0.53
1:A:131:THR:HG23	2:C:644:ARG:NE	2.23	0.53
2:C:324:ASP:C	2:C:326:ASP:N	2.66	0.53
2:C:443:THR:H	2:C:444:PRO:CD	2.21	0.53
2:C:589:ARG:HH12	2:C:596:TYR:CB	2.22	0.53
2:C:718:GLY:HA3	2:C:761:PHE:CG	2.43	0.53
2:C:1019:GLN:HB2	3:D:622:ARG:HB2	1.91	0.53
3:D:89:ARG:O	3:D:520:LEU:HD21	2.07	0.53
3:D:542:ASP:O	3:D:544:TYR:N	2.42	0.53
3:D:634:GLY:O	3:D:636:GLN:N	2.42	0.53
3:D:876:SER:CA	3:D:879:ARG:HG3	2.38	0.53
3:D:1231:GLU:HB3	3:D:1232:PRO:CD	2.32	0.53
4:E:63:TRP:O	4:E:66:LYS:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HH12	2:C:932:GLU:CD	2.17	0.53
1:B:207:PRO:O	1:B:210:ALA:N	2.42	0.53
2:C:144:PRO:HA	2:C:162:ILE:HG22	1.89	0.53
2:C:240:THR:O	2:C:240:THR:HG22	2.09	0.53
2:C:476:ASN:O	2:C:477:GLY:C	2.51	0.53
2:C:759:THR:HB	2:C:785:VAL:HG11	1.89	0.53
2:C:841:ASN:HD21	2:C:845:ASN:H	1.55	0.53
2:C:987:ILE:HD11	3:D:946:GLY:CA	2.38	0.53
3:D:563:PRO:O	3:D:565:ILE:N	2.42	0.53
3:D:707:THR:C	3:D:708:LEU:HG	2.34	0.53
3:D:1129:THR:O	3:D:1130:ARG:C	2.52	0.53
1:A:133:GLU:C	1:A:135:GLY:H	2.16	0.53
2:C:87:ASP:CG	2:C:824:ARG:HH22	2.16	0.53
2:C:111:ASP:O	2:C:113:VAL:N	2.34	0.53
2:C:218:VAL:O	2:C:221:LEU:N	2.42	0.53
2:C:336:VAL:O	2:C:339:LEU:N	2.41	0.53
2:C:552:HIS:CE1	3:D:1064:GLY:CA	2.92	0.53
2:C:811:PRO:O	2:C:813:VAL:N	2.41	0.53
2:C:840:ALA:HB2	2:C:846:LYS:HA	1.91	0.53
3:D:468:LEU:O	3:D:471:GLU:HG2	2.09	0.53
3:D:1402:ALA:O	3:D:1404:ASN:N	2.42	0.53
1:A:41:ARG:HH11	1:A:41:ARG:CB	2.21	0.53
1:A:41:ARG:HE	2:C:860:HIS:CE1	2.26	0.53
1:A:52:ALA:HB3	1:A:171:PHE:CD1	2.44	0.53
1:A:121:GLU:C	1:A:123:MET:H	2.16	0.53
1:A:128:HIS:C	1:A:128:HIS:CD2	2.86	0.53
1:A:225:PHE:HE1	1:B:36:LEU:HD13	1.73	0.53
1:B:53:VAL:CG2	1:B:85:LEU:HD23	2.40	0.53
1:B:58:ILE:HA	1:B:139:TYR:O	2.09	0.53
1:B:174:VAL:HA	1:B:201:THR:HB	1.90	0.53
2:C:17:PRO:O	2:C:18:LEU:CB	2.56	0.53
2:C:257:LEU:O	2:C:260:LEU:N	2.41	0.53
2:C:290:LEU:HD12	2:C:291:VAL:N	2.21	0.53
2:C:308:ARG:O	2:C:310:LEU:N	2.42	0.53
2:C:564:MET:CE	2:C:846:LYS:HB3	2.39	0.53
2:C:577:PRO:HG2	2:C:580:MET:CB	2.38	0.53
2:C:745:ILE:C	2:C:747:ALA:H	2.16	0.53
2:C:892:LEU:C	2:C:894:GLY:H	2.17	0.53
2:C:1017:THR:O	2:C:1018:GLN:CB	2.48	0.53
2:C:1023:GLY:C	2:C:1024:LYS:HG3	2.34	0.53
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:696:HIS:CD2	4:E:48:MET:HE2	2.44	0.53
3:D:811:GLU:HA	3:D:814:ALA:CB	2.24	0.53
3:D:971:LEU:O	3:D:974:ILE:HG22	2.09	0.53
3:D:1015:TYR:HA	3:D:1018:ASN:HD22	1.74	0.53
3:D:1260:ILE:HG22	3:D:1261:GLU:N	2.23	0.53
1:A:26:GLU:OE2	1:A:185:ARG:NH2	2.42	0.52
1:B:14:THR:HB	1:B:22:GLU:HB3	1.90	0.52
1:B:179:PHE:CB	1:B:197:LEU:HD12	2.39	0.52
2:C:163:ILE:HG21	2:C:169:GLY:CA	2.39	0.52
2:C:880:MET:C	2:C:881:ASN:ND2	2.67	0.52
2:C:921:ALA:HA	2:C:924:LEU:HG	1.92	0.52
3:D:509:PRO:HA	3:D:511:TRP:CD1	2.44	0.52
3:D:542:ASP:O	3:D:545:ARG:N	2.41	0.52
3:D:638:LYS:CB	3:D:932:ASP:OD1	2.57	0.52
3:D:705:ALA:HB3	3:D:706:PRO:HD2	1.91	0.52
3:D:1033:GLN:HG3	3:D:1034:GLN:N	2.24	0.52
3:D:1043:GLY:O	3:D:1057:VAL:HG23	2.08	0.52
3:D:1192:LEU:CD2	3:D:1369:GLU:HB3	2.39	0.52
4:E:3:GLU:HG3	4:E:6:ILE:HD11	1.91	0.52
1:B:79:ILE:HG23	1:B:167:VAL:CG1	2.40	0.52
1:B:203:GLY:O	1:B:204:SER:CB	2.58	0.52
2:C:501:THR:N	2:C:502:PRO:CD	2.73	0.52
2:C:507:ARG:O	2:C:518:ARG:HA	2.09	0.52
2:C:552:HIS:NE2	2:C:886:LEU:HD12	2.24	0.52
3:D:502:PHE:HE1	3:D:1452:ILE:CG1	2.17	0.52
3:D:890:VAL:HG13	3:D:922:LEU:HD13	1.90	0.52
3:D:1082:ALA:O	3:D:1085:ALA:HB3	2.09	0.52
3:D:1119:SER:HA	3:D:1186:VAL:O	2.09	0.52
3:D:1216:SER:OG	4:E:16:LYS:N	2.42	0.52
3:D:1223:VAL:O	3:D:1227:GLU:HG3	2.10	0.52
3:D:1439:SER:OG	3:D:1467:ILE:HD11	2.09	0.52
4:E:25:LYS:O	4:E:25:LYS:HD3	2.08	0.52
1:A:112:VAL:C	1:A:114:PHE:H	2.17	0.52
2:C:874:LEU:O	2:C:876:VAL:N	2.42	0.52
3:D:569:ASN:O	3:D:572:ARG:HG2	2.10	0.52
3:D:764:LEU:HD21	3:D:766:ALA:HB3	1.92	0.52
3:D:1274:ILE:HD11	3:D:1334:GLN:NE2	2.24	0.52
4:E:25:LYS:O	4:E:28:GLN:C	2.52	0.52
1:A:76:VAL:HG21	2:C:628:TYR:OH	2.09	0.52
1:A:101:LEU:O	1:A:139:TYR:HA	2.09	0.52
1:B:164:ALA:O	1:B:165:ILE:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:PHE:CD2	2:C:98:LEU:HD22	2.43	0.52
2:C:603:VAL:O	2:C:604:VAL:CB	2.58	0.52
2:C:642:ARG:O	2:C:643:VAL:HB	2.09	0.52
2:C:831:ARG:NH1	2:C:1002:GLU:CD	2.67	0.52
2:C:922:PHE:CD2	2:C:964:LYS:HG3	2.45	0.52
2:C:953:VAL:HG23	2:C:966:LEU:HD13	1.91	0.52
2:C:1045:ALA:CB	2:C:1048:THR:HB	2.28	0.52
2:C:1059:ASP:CG	2:C:1083:GLU:HB2	2.35	0.52
3:D:494:LYS:O	3:D:497:GLU:HB2	2.08	0.52
3:D:495:ARG:O	3:D:499:VAL:N	2.28	0.52
3:D:885:ILE:HG12	3:D:937:TYR:CE2	2.44	0.52
3:D:1202:GLN:O	3:D:1203:LYS:CB	2.57	0.52
3:D:1251:ASP:O	3:D:1253:THR:N	2.40	0.52
4:E:9:LEU:HD23	4:E:69:LEU:HD13	1.90	0.52
1:A:9:PRO:HA	1:A:27:PRO:HD2	1.91	0.52
1:A:16:GLN:HA	1:A:16:GLN:HE21	1.75	0.52
1:B:81:ASN:O	1:B:82:LEU:C	2.51	0.52
1:B:199:ILE:HG22	1:B:207:PRO:HB3	1.90	0.52
2:C:72:ARG:HH11	2:C:112:GLU:CD	2.17	0.52
2:C:146:VAL:HG22	2:C:161:SER:HA	1.91	0.52
2:C:325:ILE:C	2:C:327:HIS:N	2.66	0.52
2:C:552:HIS:ND1	3:D:1064:GLY:HA2	2.25	0.52
2:C:626:ARG:NE	2:C:637:PHE:CZ	2.76	0.52
2:C:820:ARG:O	2:C:821:GLU:O	2.27	0.52
2:C:959:PRO:CG	2:C:960:GLU:H	2.18	0.52
3:D:21:TRP:C	3:D:23:TYR:H	2.18	0.52
3:D:927:THR:O	3:D:931:LEU:HD23	2.09	0.52
3:D:1399:ASP:OD2	3:D:1417:TRP:HB3	2.10	0.52
1:B:148:VAL:HG23	1:B:149:GLY:H	1.74	0.52
2:C:445:GLU:HG3	5:C:1640:RFP:H303	1.90	0.52
2:C:568:ALA:O	2:C:569:VAL:HG12	2.10	0.52
3:D:564:GLU:O	3:D:565:ILE:C	2.53	0.52
3:D:783:ARG:O	3:D:784:ASP:CB	2.49	0.52
3:D:1292:VAL:HG23	3:D:1305:LEU:HD23	1.91	0.52
3:D:1336:LEU:HD13	3:D:1340:GLY:C	2.35	0.52
3:D:1437:ALA:HA	3:D:1440:PHE:CD1	2.45	0.52
1:A:56:VAL:HG13	1:A:167:VAL:CG2	2.40	0.52
1:B:59:GLU:O	1:B:60:ASP:CB	2.58	0.52
1:B:118:ALA:C	1:B:120:VAL:N	2.68	0.52
1:B:119:ASP:C	1:B:120:VAL:HG23	2.35	0.52
1:B:132:LEU:N	1:B:132:LEU:CD2	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:141:HIS:HE1	2:C:334:ARG:HG3	1.75	0.52
2:C:613:VAL:HG22	2:C:621:VAL:N	2.24	0.52
2:C:671:ASN:HB3	2:C:993:PHE:HB2	1.92	0.52
2:C:911:GLU:N	2:C:912:PRO:HD2	2.25	0.52
3:D:774:SER:HA	3:D:1209:LEU:HD21	1.92	0.52
3:D:1110:ALA:O	3:D:1112:CYS:N	2.42	0.52
3:D:1155:ALA:O	3:D:1156:LEU:C	2.53	0.52
3:D:1462:LEU:HD23	3:D:1473:PRO:CG	2.40	0.52
1:A:53:VAL:HG21	1:A:82:LEU:O	2.09	0.52
1:A:105:GLY:HA2	1:A:136:GLY:H	1.75	0.52
1:A:134:GLU:CB	2:C:606:VAL:HG23	2.40	0.52
1:A:195:LEU:C	1:A:196:THR:HG22	2.34	0.52
1:B:38:ASN:HB3	1:B:39:PRO:CD	2.35	0.52
2:C:713:ARG:HB2	2:C:720:GLU:OE1	2.09	0.52
3:D:545:ARG:CG	3:D:546:ARG:N	2.72	0.52
3:D:699:VAL:HG12	3:D:717:GLN:HG3	1.92	0.52
3:D:885:ILE:HD13	3:D:937:TYR:HD2	1.75	0.52
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.89	0.52
3:D:1304:LYS:H	3:D:1304:LYS:CD	2.23	0.52
3:D:1365:ASP:O	3:D:1366:LYS:HB2	2.09	0.52
1:A:28:LEU:CD1	1:A:195:LEU:HB2	2.40	0.52
1:A:152:PRO:C	1:A:154:GLU:H	2.18	0.52
2:C:84:ARG:HA	2:C:131:GLY:CA	2.38	0.52
2:C:327:HIS:C	2:C:329:GLY:N	2.68	0.52
3:D:759:ALA:HA	3:D:763:MET:HG2	1.92	0.52
3:D:968:ASP:O	3:D:971:LEU:HB2	2.09	0.52
3:D:1365:ASP:O	3:D:1366:LYS:CB	2.58	0.52
1:A:122:ILE:O	1:A:124:ASN:N	2.43	0.52
1:A:124:ASN:ND2	1:A:127:LEU:HD22	2.25	0.52
1:A:222:LEU:O	1:A:225:PHE:HD1	1.92	0.52
1:B:113:ASP:O	1:B:114:PHE:C	2.53	0.52
2:C:16:PRO:HB3	2:C:586:ARG:HH21	1.75	0.52
2:C:52:PHE:O	2:C:52:PHE:HD1	1.93	0.52
2:C:65:VAL:HB	2:C:101:ILE:HG12	1.91	0.52
2:C:215:GLY:O	2:C:217:LEU:HG	2.10	0.52
2:C:613:VAL:HG21	2:C:619:ARG:HE	1.75	0.52
2:C:875:GLY:O	2:C:876:VAL:C	2.53	0.52
3:D:518:PRO:HA	3:D:544:TYR:OH	2.09	0.52
3:D:1335:LEU:HD23	3:D:1344:VAL:CG2	2.40	0.52
3:D:1486:VAL:O	4:E:79:LEU:CD1	2.58	0.52
1:A:108:GLU:HG2	2:C:644:ARG:NH2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:216:ASP:C	2:C:218:VAL:N	2.67	0.51
2:C:325:ILE:O	2:C:327:HIS:N	2.43	0.51
2:C:399:ASN:OD1	2:C:668:LEU:HD22	2.11	0.51
2:C:554:ASP:O	2:C:555:ALA:C	2.53	0.51
2:C:586:ARG:O	2:C:589:ARG:N	2.43	0.51
2:C:845:ASN:HD21	2:C:876:VAL:HG11	1.75	0.51
3:D:149:LYS:C	3:D:151:GLN:N	2.68	0.51
3:D:823:LEU:O	3:D:824:ASN:CB	2.58	0.51
3:D:1237:THR:O	3:D:1257:PRO:HD3	2.11	0.51
3:D:1443:THR:O	3:D:1447:LEU:HB2	2.09	0.51
1:A:59:GLU:HG2	1:A:137:LYS:CE	2.34	0.51
1:A:125:PRO:O	1:A:127:LEU:N	2.43	0.51
2:C:73:ILE:HG22	2:C:74:GLY:N	2.26	0.51
2:C:78:PHE:HB3	2:C:82:GLU:CD	2.36	0.51
2:C:610:ARG:HA	2:C:623:HIS:O	2.11	0.51
2:C:662:GLU:O	2:C:662:GLU:HG3	2.10	0.51
2:C:690:ILE:O	2:C:852:ILE:HA	2.10	0.51
3:D:643:GLY:HA3	3:D:727:GLN:N	2.16	0.51
3:D:962:ARG:O	3:D:966:GLU:HG3	2.10	0.51
1:A:34:VAL:C	1:A:36:LEU:N	2.67	0.51
1:B:56:VAL:HG13	1:B:142:VAL:HB	1.92	0.51
2:C:184:MET:CG	2:C:193:LEU:HD23	2.40	0.51
2:C:603:VAL:O	2:C:604:VAL:HB	2.11	0.51
2:C:747:ALA:O	2:C:748:GLU:C	2.52	0.51
3:D:552:ASN:C	3:D:554:LEU:N	2.66	0.51
3:D:553:ARG:C	3:D:554:LEU:HD23	2.36	0.51
3:D:617:ASN:OD1	3:D:621:LYS:HE3	2.11	0.51
3:D:1377:LYS:HG2	3:D:1378:TYR:CE1	2.45	0.51
3:D:1403:LEU:HD12	3:D:1417:TRP:CZ3	2.43	0.51
1:B:38:ASN:ND2	1:B:41:ARG:HD2	2.25	0.51
2:C:163:ILE:CB	2:C:164:PRO:HD2	2.41	0.51
2:C:236:VAL:HG13	2:C:248:PRO:O	2.10	0.51
2:C:283:VAL:CG1	2:C:284:GLY:N	2.73	0.51
2:C:358:ARG:O	2:C:359:MET:C	2.53	0.51
2:C:577:PRO:HB3	2:C:993:PHE:CE2	2.44	0.51
2:C:874:LEU:HD21	3:D:784:ASP:N	2.25	0.51
3:D:104:PHE:O	3:D:511:TRP:CZ3	2.62	0.51
3:D:639:LEU:O	3:D:641:GLN:N	2.41	0.51
3:D:916:TYR:O	3:D:918:ALA:N	2.43	0.51
3:D:1094:LEU:O	3:D:1095:THR:C	2.53	0.51
3:D:1475:GLY:O	3:D:1477:GLY:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.92	0.51
1:A:225:PHE:CE2	1:B:25:LEU:HD23	2.46	0.51
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.91	0.51
2:C:13:ILE:HG23	2:C:14:PRO:HD2	1.91	0.51
2:C:193:LEU:HD11	2:C:307:LEU:HD22	1.93	0.51
2:C:243:ARG:CG	2:C:244:PRO:HA	2.41	0.51
2:C:270:GLY:O	2:C:274:ARG:HG2	2.09	0.51
2:C:937:ASP:OD1	2:C:939:ARG:HD2	2.11	0.51
3:D:729:HIS:O	3:D:731:LEU:N	2.44	0.51
3:D:808:THR:HG22	3:D:808:THR:O	2.09	0.51
4:E:55:TYR:O	4:E:56:ASP:C	2.54	0.51
1:B:188:GLN:NE2	1:B:188:GLN:C	2.69	0.51
2:C:8:ARG:O	2:C:494:TYR:OH	2.27	0.51
2:C:15:LEU:HD21	2:C:461:VAL:CB	2.41	0.51
2:C:44:ILE:HD11	2:C:340:MET:HE1	1.93	0.51
2:C:308:ARG:C	2:C:310:LEU:H	2.19	0.51
2:C:443:THR:H	2:C:444:PRO:HD3	1.76	0.51
2:C:460:ARG:HG3	2:C:461:VAL:N	2.26	0.51
2:C:548:PRO:HG3	2:C:842:ARG:NH2	2.25	0.51
2:C:631:SER:OG	2:C:636:ALA:N	2.31	0.51
2:C:699:PHE:O	2:C:701:THR:N	2.43	0.51
2:C:713:ARG:HH12	2:C:816:LYS:HG2	1.74	0.51
2:C:1034:GLU:O	2:C:1037:VAL:N	2.43	0.51
3:D:75:ARG:C	3:D:77:ALA:H	2.19	0.51
3:D:486:ARG:CG	3:D:487:ALA:H	2.22	0.51
3:D:560:GLN:O	3:D:561:GLY:C	2.54	0.51
3:D:752:SER:O	3:D:753:SER:C	2.54	0.51
3:D:1016:PRO:O	3:D:1023:MET:HE1	2.10	0.51
3:D:1038:LEU:O	3:D:1060:SER:O	2.28	0.51
3:D:1397:LYS:HD2	3:D:1400:VAL:HB	1.92	0.51
1:A:196:THR:O	1:A:196:THR:OG1	2.26	0.51
2:C:282:GLY:O	2:C:283:VAL:CB	2.59	0.51
2:C:310:LEU:O	2:C:313:LEU:HB3	2.10	0.51
2:C:672:VAL:HG22	2:C:868:ASP:CG	2.36	0.51
2:C:874:LEU:CD2	3:D:784:ASP:CA	2.88	0.51
2:C:976:ASP:O	2:C:978:ARG:N	2.44	0.51
3:D:468:LEU:C	3:D:470:LEU:N	2.67	0.51
3:D:678:GLU:C	3:D:680:GLN:N	2.69	0.51
3:D:999:THR:HG23	3:D:1000:THR:N	2.26	0.51
3:D:1088:THR:O	3:D:1091:SER:HB3	2.10	0.51
3:D:1110:ALA:HA	3:D:1202:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1166:LEU:HD22	3:D:1166:LEU:H	1.75	0.51
1:B:205:VAL:HG12	1:B:206:THR:N	2.26	0.51
1:B:211:LEU:C	1:B:215:VAL:HG23	2.33	0.51
2:C:758:ARG:HG3	2:C:758:ARG:NH1	2.25	0.51
2:C:1034:GLU:OE2	3:D:1096:ARG:NH1	2.44	0.51
3:D:542:ASP:O	3:D:545:ARG:HG2	2.10	0.51
3:D:654:LYS:O	3:D:655:PRO:C	2.51	0.51
3:D:879:ARG:CZ	3:D:904:VAL:CA	2.88	0.51
3:D:1065:LEU:C	3:D:1067:VAL:N	2.67	0.51
3:D:1089:ALA:C	3:D:1091:SER:H	2.19	0.51
4:E:41:GLU:N	4:E:42:PRO:CD	2.74	0.51
1:A:105:GLY:O	1:A:133:GLU:HA	2.10	0.51
1:A:158:ILE:HG13	1:A:161:ARG:CG	2.41	0.51
2:C:333:ILE:HG21	2:C:460:ARG:NH2	2.26	0.51
2:C:401:LEU:HD21	2:C:543:ASN:HB2	1.92	0.51
2:C:676:ILE:HG22	2:C:677:MET:N	2.25	0.51
2:C:729:LEU:HD21	2:C:754:ILE:CD1	2.40	0.51
2:C:925:TYR:OH	2:C:972:VAL:HG21	2.11	0.51
2:C:981:GLU:HB3	2:C:982:PRO:CD	2.41	0.51
2:C:1101:THR:HB	2:C:1110:ASP:CB	2.41	0.51
3:D:98:PRO:CB	3:D:571:LYS:HZ3	2.24	0.51
3:D:489:ARG:O	3:D:493:ARG:HG2	2.11	0.51
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.92	0.51
3:D:645:PRO:HB3	3:D:724:GLN:H	1.76	0.51
3:D:658:LEU:HA	3:D:661:MET:CE	2.39	0.51
3:D:709:HIS:HA	3:D:1227:GLU:CD	2.36	0.51
3:D:1150:ALA:O	3:D:1151:ARG:HB2	2.10	0.51
3:D:1228:SER:O	3:D:1232:PRO:HD2	2.11	0.51
1:A:72:LYS:O	1:A:73:GLU:O	2.29	0.51
1:B:64:GLU:HA	1:B:75:VAL:HG11	1.93	0.51
1:B:97:THR:HG21	1:B:120:VAL:CG2	2.30	0.51
2:C:115:LEU:CG	2:C:116:GLY:H	2.24	0.51
2:C:428:ARG:O	2:C:429:ASP:CB	2.59	0.51
2:C:564:MET:HG3	2:C:997:LEU:CD1	2.39	0.51
2:C:735:ARG:C	2:C:737:LEU:N	2.66	0.51
2:C:796:GLU:CG	3:D:681:ARG:HH22	2.24	0.51
2:C:1008:ARG:O	3:D:652:LEU:HD13	2.11	0.51
2:C:1059:ASP:HA	2:C:1083:GLU:CB	2.41	0.51
3:D:905:PRO:HG2	3:D:906:GLN:N	2.26	0.51
3:D:1277:ILE:CG2	3:D:1279:GLY:H	2.24	0.51
4:E:17:TYR:N	4:E:17:TYR:CD1	2.77	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HD3	2:C:977:GLY:O	2.12	0.50
1:B:114:PHE:O	1:B:116:PRO:N	2.44	0.50
2:C:139:GLN:NE2	2:C:334:ARG:NH2	2.59	0.50
2:C:183:THR:CG2	2:C:190:LYS:HG3	2.40	0.50
2:C:201:GLY:O	2:C:203:ASP:OD2	2.29	0.50
2:C:354:GLY:O	2:C:357:GLU:HB3	2.11	0.50
2:C:434:HIS:C	2:C:436:GLY:N	2.69	0.50
2:C:637:PHE:HB2	2:C:659:PRO:CB	2.41	0.50
3:D:521:PRO:N	3:D:522:PRO:CD	2.73	0.50
3:D:538:SER:O	3:D:539:ASP:C	2.55	0.50
3:D:729:HIS:HE1	3:D:935:LYS:HD3	1.75	0.50
3:D:795:VAL:HG12	3:D:796:ARG:H	1.75	0.50
3:D:1105:ILE:HG21	3:D:1370:ILE:HG23	1.92	0.50
3:D:1107:VAL:HG12	3:D:1217:ILE:HD13	1.92	0.50
3:D:1353:GLN:O	3:D:1356:TYR:N	2.43	0.50
3:D:1483:PHE:CE2	4:E:18:ARG:NE	2.79	0.50
4:E:77:GLU:OE1	4:E:77:GLU:HA	2.11	0.50
1:A:6:LEU:O	1:A:8:ALA:N	2.45	0.50
1:A:125:PRO:O	1:A:126:ASP:C	2.52	0.50
2:C:148:PHE:HE2	2:C:310:LEU:CA	2.23	0.50
2:C:203:ASP:O	2:C:204:GLN:C	2.55	0.50
2:C:377:PRO:O	2:C:379:GLU:O	2.27	0.50
2:C:743:VAL:HG13	2:C:744:ARG:N	2.26	0.50
2:C:796:GLU:HG2	3:D:681:ARG:NH1	2.25	0.50
3:D:153:LEU:C	3:D:155:ASP:H	2.19	0.50
3:D:690:ALA:O	3:D:694:VAL:HG23	2.11	0.50
3:D:968:ASP:HA	3:D:971:LEU:HB2	1.94	0.50
4:E:28:GLN:O	4:E:28:GLN:HG2	2.11	0.50
4:E:48:MET:O	4:E:49:ARG:HG3	2.12	0.50
2:C:15:LEU:HD22	2:C:471:TYR:OH	2.11	0.50
2:C:66:LEU:HD11	2:C:98:LEU:HB2	1.94	0.50
2:C:137:VAL:HG12	2:C:411:SER:HB2	1.93	0.50
2:C:415:PRO:O	2:C:416:GLY:O	2.29	0.50
2:C:1082:PRO:HG2	2:C:1085:PHE:HB3	1.93	0.50
3:D:859:ASP:C	3:D:861:GLN:H	2.19	0.50
3:D:1273:VAL:H	3:D:1324:PRO:CG	2.22	0.50
3:D:1459:LEU:HD12	3:D:1470:ARG:HH11	1.76	0.50
4:E:27:ALA:HB1	4:E:60:ALA:CB	2.41	0.50
1:A:56:VAL:HG13	1:A:167:VAL:HG23	1.94	0.50
1:A:126:ASP:O	1:A:127:LEU:C	2.54	0.50
1:B:57:TYR:C	1:B:57:TYR:CD2	2.88	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:HG23	1:B:140:MET:CG	2.42	0.50
1:B:68:ILE:N	1:B:68:ILE:HD12	2.27	0.50
2:C:118:LEU:HD23	2:C:119:PRO:O	2.10	0.50
2:C:186:VAL:HG11	2:C:258:PHE:CD2	2.47	0.50
2:C:348:LEU:HA	2:C:351:LEU:HB3	1.93	0.50
2:C:492:ASP:H	2:C:532:MET:N	2.08	0.50
2:C:492:ASP:N	2:C:532:MET:H	2.05	0.50
2:C:613:VAL:CB	2:C:619:ARG:HG2	2.41	0.50
2:C:692:GLU:O	2:C:693:GLU:C	2.53	0.50
3:D:492:ALA:O	3:D:495:ARG:HB2	2.11	0.50
3:D:908:LYS:HG3	3:D:1027:GLY:HA2	1.90	0.50
3:D:1008:PHE:HE1	3:D:1035:ILE:CG1	2.18	0.50
3:D:1118:ILE:CD1	3:D:1190:SER:H	2.24	0.50
3:D:1322:GLY:O	3:D:1323:GLN:CB	2.58	0.50
1:B:49:PRO:HD2	1:B:213:GLN:HE21	1.76	0.50
1:B:144:VAL:HG12	1:B:145:ASP:H	1.76	0.50
1:B:199:ILE:O	1:B:199:ILE:CG2	2.59	0.50
2:C:7:GLY:O	2:C:8:ARG:HG3	2.12	0.50
2:C:8:ARG:C	2:C:494:TYR:OH	2.55	0.50
2:C:282:GLY:O	2:C:283:VAL:HB	2.10	0.50
2:C:321:GLU:O	2:C:322:VAL:C	2.54	0.50
2:C:393:GLN:HE22	5:C:1640:RFP:C8	2.25	0.50
2:C:502:PRO:O	2:C:507:ARG:CZ	2.59	0.50
2:C:1038:TRP:CD1	3:D:1463:LYS:HZ1	2.30	0.50
2:C:1108:PRO:O	2:C:1109:VAL:C	2.55	0.50
3:D:506:GLY:O	3:D:507:ASN:CB	2.59	0.50
3:D:570:GLU:O	3:D:573:MET:HE3	2.11	0.50
3:D:795:VAL:HA	3:D:862:ASP:CB	2.41	0.50
3:D:879:ARG:NH2	3:D:904:VAL:CA	2.63	0.50
3:D:989:TYR:C	3:D:991:GLN:H	2.18	0.50
3:D:1118:ILE:HD11	3:D:1190:SER:H	1.76	0.50
3:D:1363:LEU:O	3:D:1363:LEU:HD23	2.11	0.50
3:D:1381:VAL:O	3:D:1382:THR:HG23	2.11	0.50
1:A:218:LEU:O	1:A:222:LEU:HD23	2.12	0.50
1:B:40:LEU:O	1:B:44:LEU:HB2	2.11	0.50
1:B:151:VAL:CG2	1:B:169:ALA:HB3	2.36	0.50
2:C:65:VAL:HB	2:C:101:ILE:CG1	2.42	0.50
2:C:218:VAL:O	2:C:219:GLN:C	2.54	0.50
2:C:342:ASP:N	2:C:345:ARG:HH11	2.10	0.50
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.37	0.50
2:C:545:ASN:C	2:C:547:ILE:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:733:ALA:O	2:C:734:LEU:C	2.55	0.50
2:C:902:ILE:O	2:C:902:ILE:HG22	2.10	0.50
3:D:853:VAL:HG11	3:D:860:LEU:HB2	1.93	0.50
3:D:885:ILE:CD1	3:D:937:TYR:HD2	2.24	0.50
3:D:1004:THR:HG22	3:D:1005:GLN:N	2.27	0.50
3:D:1007:VAL:HG13	3:D:1008:PHE:N	2.26	0.50
3:D:1170:ASP:C	3:D:1172:HIS:N	2.70	0.50
3:D:1347:TYR:CZ	3:D:1351:GLU:HG2	2.46	0.50
1:A:67:THR:O	1:A:69:PRO:HD3	2.12	0.50
1:A:108:GLU:HG3	2:C:644:ARG:HH22	1.77	0.50
1:A:121:GLU:C	1:A:123:MET:N	2.70	0.50
1:B:23:PHE:CD1	1:B:211:LEU:HD22	2.47	0.50
2:C:148:PHE:CE2	2:C:310:LEU:HA	2.47	0.50
2:C:220:GLY:HA2	2:C:223:ASP:OD2	2.10	0.50
2:C:277:ALA:O	2:C:281:LEU:N	2.36	0.50
2:C:662:GLU:O	2:C:663:GLU:CB	2.58	0.50
2:C:710:ILE:HG21	2:C:758:ARG:HD2	1.92	0.50
2:C:755:LEU:HD23	2:C:792:VAL:HG23	1.92	0.50
2:C:798:GLY:O	2:C:827:VAL:HG13	2.12	0.50
3:D:653:PHE:O	3:D:654:LYS:C	2.55	0.50
3:D:1250:THR:HG23	3:D:1269:LYS:CD	2.39	0.50
3:D:1347:TYR:OH	3:D:1351:GLU:HG2	2.11	0.50
3:D:1436:SER:CB	3:D:1464:GLU:HG2	2.41	0.50
1:A:41:ARG:HB3	1:A:41:ARG:CZ	2.40	0.50
1:B:106:PRO:HA	1:B:132:LEU:O	2.12	0.50
2:C:42:VAL:H	2:C:46:ALA:HB2	1.77	0.50
2:C:180:GLY:O	2:C:181:VAL:HB	2.12	0.50
2:C:250:LYS:HG3	2:C:250:LYS:O	2.12	0.50
2:C:705:ILE:HG23	2:C:828:ALA:HA	1.94	0.50
2:C:722:ILE:O	2:C:722:ILE:HG22	2.12	0.50
3:D:1434:TRP:HB2	3:D:1450:ALA:HB2	1.94	0.50
3:D:1465:ASN:OD1	3:D:1470:ARG:HB3	2.11	0.50
1:A:111:ALA:O	1:A:112:VAL:C	2.53	0.50
1:A:158:ILE:HG12	1:A:159:LYS:N	2.27	0.50
1:B:4:SER:O	1:B:5:LYS:CB	2.59	0.50
2:C:159:ILE:HG13	2:C:310:LEU:HD13	1.89	0.50
2:C:354:GLY:O	2:C:358:ARG:HG2	2.12	0.50
2:C:434:HIS:O	2:C:436:GLY:N	2.45	0.50
2:C:635:THR:CG2	2:C:636:ALA:N	2.74	0.50
2:C:704:HIS:ND1	2:C:831:ARG:HD2	2.26	0.50
2:C:712:ALA:HB3	2:C:820:ARG:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:768:SER:O	2:C:769:PRO:O	2.30	0.50
3:D:1205:TYR:CD1	3:D:1366:LYS:HD2	2.47	0.50
3:D:1236:LEU:HD13	3:D:1259:VAL:HG21	1.92	0.50
1:A:127:LEU:HG	1:A:129:ILE:HD11	1.94	0.49
1:A:178:ALA:HB2	2:C:864:GLY:HA3	1.94	0.49
1:A:188:GLN:O	1:A:189:ARG:HB3	2.12	0.49
1:B:15:THR:C	1:B:17:GLY:H	2.18	0.49
2:C:9:ILE:CG2	2:C:10:ARG:H	2.13	0.49
2:C:33:ASP:O	2:C:33:ASP:CG	2.55	0.49
2:C:222:LEU:O	2:C:225:ALA:N	2.43	0.49
2:C:257:LEU:HB2	2:C:258:PHE:HD1	1.77	0.49
2:C:755:LEU:HD11	2:C:825:VAL:HB	1.94	0.49
2:C:1043:TYR:CE2	3:D:710:ARG:HD3	2.47	0.49
2:C:1113:GLU:C	2:C:1115:LEU:N	2.69	0.49
3:D:10:ILE:HG21	3:D:1450:ALA:CB	2.42	0.49
3:D:21:TRP:C	3:D:23:TYR:N	2.70	0.49
3:D:691:LEU:C	3:D:693:GLU:H	2.19	0.49
3:D:935:LYS:HG3	3:D:939:PHE:HE1	1.77	0.49
3:D:1035:ILE:C	3:D:1037:GLN:N	2.68	0.49
3:D:1085:ALA:C	3:D:1087:ARG:H	2.19	0.49
3:D:1290:LEU:O	3:D:1291:SER:C	2.54	0.49
3:D:1352:ILE:O	3:D:1353:GLN:C	2.55	0.49
3:D:1403:LEU:HD21	3:D:1415:VAL:N	2.20	0.49
1:A:41:ARG:HH11	1:A:42:ARG:N	2.10	0.49
1:A:108:GLU:CG	2:C:644:ARG:NH2	2.75	0.49
2:C:551:GLU:HG2	2:C:906:PHE:HA	1.94	0.49
2:C:712:ALA:HB2	2:C:722:ILE:CD1	2.41	0.49
2:C:1054:THR:HG22	2:C:1055:ILE:N	2.27	0.49
3:D:40(U):UNK:O	3:D:41(U):UNK:O	2.30	0.49
3:D:502:PHE:HD1	3:D:1452:ILE:HG23	1.77	0.49
3:D:1060:SER:C	3:D:1062:ARG:N	2.69	0.49
3:D:1319:VAL:O	3:D:1320:GLU:C	2.54	0.49
3:D:1353:GLN:NE2	3:D:1368:ILE:HD11	2.08	0.49
1:A:77:GLU:O	1:A:80:LEU:N	2.45	0.49
1:A:88:ARG:HD3	1:A:121:GLU:CD	2.37	0.49
1:A:198:ARG:HH22	2:C:932:GLU:CD	2.17	0.49
1:B:132:LEU:HD23	1:B:132:LEU:H	1.77	0.49
2:C:181:VAL:CG1	2:C:182:VAL:HG23	2.40	0.49
2:C:226:VAL:HG23	2:C:227:LEU:N	2.27	0.49
2:C:474:VAL:HG22	2:C:530:GLU:CB	2.43	0.49
2:C:483:VAL:O	2:C:485:TYR:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:571:LEU:CD2	2:C:670:GLN:HG3	2.40	0.49
2:C:747:ALA:O	2:C:800:VAL:HG23	2.12	0.49
3:D:9(U):UNK:O	3:D:10(U):UNK:CB	2.60	0.49
3:D:679:ARG:C	3:D:680:GLN:HG2	2.38	0.49
3:D:935:LYS:HG3	3:D:939:PHE:CE1	2.48	0.49
3:D:1266:ARG:C	3:D:1268:PRO:HD3	2.37	0.49
3:D:1321:ALA:O	3:D:1324:PRO:HD2	2.12	0.49
1:A:150:TYR:HB2	2:C:696:LYS:HE2	1.93	0.49
2:C:263:ASP:CB	2:C:264:PRO:HD3	2.42	0.49
2:C:598:GLU:HG3	2:C:614:ARG:NH2	2.28	0.49
2:C:872:ASN:HD21	2:C:874:LEU:HB3	1.77	0.49
3:D:149:LYS:C	3:D:151:GLN:H	2.19	0.49
3:D:633:VAL:HA	3:D:740:PHE:CZ	2.47	0.49
3:D:684:LYS:HE2	3:D:685:ASP:OD2	2.12	0.49
3:D:924:MET:O	3:D:925:GLU:C	2.54	0.49
3:D:973:GLN:O	3:D:977:ALA:HB2	2.13	0.49
3:D:996:TRP:HA	3:D:999:THR:CG2	2.42	0.49
4:E:9:LEU:C	4:E:11:GLY:H	2.20	0.49
1:A:111:ALA:HB2	1:A:127:LEU:HB3	1.93	0.49
2:C:23:VAL:C	2:C:25:SER:H	2.19	0.49
2:C:45:GLN:O	2:C:48:PHE:HB2	2.12	0.49
2:C:164:PRO:HD3	2:C:267:TYR:CE2	2.48	0.49
2:C:328:LEU:O	2:C:484:VAL:HG11	2.12	0.49
3:D:728:LEU:CD1	3:D:745:MET:HE1	2.40	0.49
3:D:1327:ARG:CB	3:D:1327:ARG:HH11	2.25	0.49
3:D:1331:ASP:O	3:D:1334:GLN:N	2.28	0.49
3:D:1343:ALA:O	3:D:1344:VAL:C	2.55	0.49
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.95	0.49
1:A:167:VAL:HG12	1:A:168:ASP:N	2.27	0.49
1:B:14:THR:HG22	1:B:14:THR:O	2.12	0.49
1:B:133:GLU:C	1:B:135:GLY:H	2.21	0.49
2:C:910:THR:CG2	2:C:912:PRO:HD2	2.40	0.49
3:D:663:GLU:C	3:D:665:ALA:N	2.69	0.49
3:D:687:VAL:O	3:D:690:ALA:CB	2.60	0.49
3:D:739:ASP:O	3:D:741:ASP:N	2.46	0.49
3:D:764:LEU:HB3	3:D:767:HIS:CD2	2.48	0.49
3:D:864:VAL:HG12	3:D:874:GLU:O	2.13	0.49
3:D:879:ARG:HH22	3:D:905:PRO:HD2	1.78	0.49
3:D:1017:PHE:O	3:D:1019:PRO:N	2.46	0.49
3:D:1208:ASP:OD2	3:D:1211:MET:HE2	2.12	0.49
1:A:77:GLU:OE2	2:C:640:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:HB3	3:D:839:LEU:CB	2.42	0.49
2:C:12:VAL:HG21	2:C:479:VAL:CG1	2.43	0.49
2:C:89:THR:HG23	2:C:129:ILE:HG23	1.94	0.49
2:C:100:LEU:CD1	2:C:369:PRO:HD3	2.42	0.49
2:C:142:ARG:HG2	2:C:147:TYR:CE1	2.47	0.49
2:C:344:PHE:HE2	2:C:378:LEU:HD23	1.77	0.49
2:C:584:GLU:C	2:C:586:ARG:H	2.19	0.49
2:C:636:ALA:HB2	2:C:705:ILE:CD1	2.42	0.49
2:C:969:LEU:CD2	3:D:952:ASP:HB2	2.40	0.49
2:C:1053:LEU:HD13	3:D:621:LYS:HD2	1.94	0.49
3:D:97:THR:O	3:D:571:LYS:HE3	2.13	0.49
3:D:1156:LEU:HB3	3:D:1173:PHE:HE1	1.77	0.49
3:D:1429:LEU:HD13	3:D:1440:PHE:CD2	2.47	0.49
1:A:41:ARG:HG2	1:A:177:VAL:CB	2.43	0.49
1:A:41:ARG:NH2	2:C:860:HIS:CD2	2.81	0.49
1:A:160:ASP:O	1:A:161:ARG:C	2.55	0.49
2:C:44:ILE:HG22	2:C:45:GLN:N	2.27	0.49
2:C:149:THR:HG23	2:C:323:ASP:CB	2.42	0.49
2:C:173:ASP:HB3	2:C:185:LYS:HE3	1.95	0.49
2:C:544:THR:O	2:C:545:ASN:C	2.54	0.49
2:C:875:GLY:HA2	2:C:879:ARG:CG	2.39	0.49
2:C:889:HIS:HE1	3:D:951:ILE:N	2.03	0.49
2:C:1030:GLN:NE2	3:D:628:ARG:HD3	2.25	0.49
3:D:583:ASP:O	3:D:585:GLY:N	2.46	0.49
3:D:688:TRP:C	3:D:690:ALA:N	2.60	0.49
3:D:960:LYS:O	3:D:961:GLN:C	2.56	0.49
3:D:1034:GLN:HE22	3:D:1037:GLN:NE2	2.11	0.49
3:D:1083:ASP:C	3:D:1085:ALA:N	2.69	0.49
3:D:1324:PRO:CD	3:D:1325:LEU:H	2.25	0.49
3:D:1394:VAL:CG1	3:D:1395:LEU:N	2.75	0.49
1:A:9:PRO:HB2	1:A:25:LEU:HD13	1.93	0.49
1:A:15:THR:HG22	1:B:230:ALA:CB	2.34	0.49
1:A:43:ILE:O	1:A:44:LEU:C	2.56	0.49
1:B:29:GLU:O	1:B:30:ARG:C	2.55	0.49
1:B:57:TYR:CD2	1:B:58:ILE:N	2.81	0.49
2:C:286:SER:O	2:C:288:ARG:N	2.46	0.49
2:C:551:GLU:O	3:D:1065:LEU:HB3	2.13	0.49
2:C:691:SER:O	2:C:693:GLU:N	2.45	0.49
2:C:705:ILE:HD12	2:C:705:ILE:N	2.26	0.49
2:C:803:ARG:H	2:C:803:ARG:HD2	1.78	0.49
3:D:22:SER:C	3:D:24:GLY:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:794:GLN:OE1	3:D:794:GLN:HA	2.12	0.49
3:D:809:PRO:C	3:D:811:GLU:H	2.19	0.49
3:D:1171:VAL:O	3:D:1171:VAL:HG12	2.12	0.49
3:D:1353:GLN:O	3:D:1354:LYS:C	2.55	0.49
4:E:63:TRP:O	4:E:64:ALA:C	2.56	0.49
1:A:16:GLN:OE1	1:A:19:HIS:HE1	1.96	0.49
1:A:164:ALA:O	1:A:165:ILE:C	2.56	0.49
1:B:143:ARG:CG	1:B:144:VAL:N	2.76	0.49
2:C:129:ILE:HG22	2:C:130:ASN:ND2	2.28	0.49
2:C:159:ILE:HG21	2:C:306:THR:HG21	1.95	0.49
2:C:215:GLY:O	2:C:216:ASP:C	2.54	0.49
2:C:340:MET:SD	2:C:340:MET:C	2.96	0.49
2:C:556:ASN:O	2:C:559:LEU:HG	2.12	0.49
2:C:737:LEU:O	2:C:738:ASP:C	2.53	0.49
2:C:745:ILE:HG22	2:C:746:GLY:N	2.28	0.49
2:C:1020:PRO:HD3	2:C:1057:SER:HA	1.94	0.49
2:C:1091:GLU:OE1	3:D:613:ARG:HG3	2.13	0.49
3:D:482:LYS:HE2	3:D:488:ARG:HB3	1.95	0.49
3:D:552:ASN:O	3:D:555:LYS:N	2.44	0.49
3:D:709:HIS:HA	3:D:1227:GLU:HB3	1.95	0.49
3:D:1027:GLY:O	3:D:1028:ALA:HB2	2.13	0.49
3:D:1272:ALA:HB1	3:D:1325:LEU:HA	1.95	0.49
1:A:10:VAL:HB	1:A:26:GLU:HG2	1.90	0.48
1:B:77:GLU:O	1:B:81:ASN:ND2	2.46	0.48
2:C:115:LEU:HD13	2:C:375:SER:OG	2.13	0.48
2:C:256:TYR:CG	2:C:260:LEU:HD13	2.48	0.48
2:C:307:LEU:O	2:C:310:LEU:HB3	2.13	0.48
2:C:473:ARG:HE	2:C:476:ASN:HA	1.77	0.48
2:C:569:VAL:O	2:C:571:LEU:HD12	2.13	0.48
2:C:845:ASN:O	2:C:845:ASN:OD1	2.30	0.48
2:C:1021:LEU:O	2:C:1022:GLY:C	2.56	0.48
3:D:468:LEU:C	3:D:470:LEU:H	2.21	0.48
3:D:664:LYS:O	3:D:665:ALA:HB3	2.13	0.48
3:D:1071:PHE:CE2	3:D:1075:HIS:NE2	2.78	0.48
3:D:1164:ARG:HG2	3:D:1165:TYR:N	2.28	0.48
3:D:1483:PHE:HZ	4:E:18:ARG:HG3	1.76	0.48
4:E:79:LEU:O	4:E:81:PRO:CD	2.61	0.48
1:A:162:ILE:CG2	1:A:163:ASN:N	2.73	0.48
1:A:195:LEU:CD2	1:A:196:THR:N	2.76	0.48
1:A:198:ARG:NH1	2:C:934:PHE:HE1	2.11	0.48
2:C:342:ASP:HA	2:C:345:ARG:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:465:GLY:O	2:C:466:PHE:HB3	2.13	0.48
2:C:489:SER:O	2:C:490:GLU:CB	2.61	0.48
2:C:836:GLY:O	2:C:837:ASP:O	2.31	0.48
2:C:983:PHE:O	2:C:984:GLU:C	2.55	0.48
3:D:88:TYR:C	3:D:520:LEU:CD1	2.85	0.48
3:D:92:HIS:O	3:D:93:ILE:C	2.57	0.48
3:D:680:GLN:C	3:D:681:ARG:HG3	2.38	0.48
3:D:1117:TYR:C	3:D:1118:ILE:HD12	2.38	0.48
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.76	0.48
1:A:62:LEU:CD1	2:C:745:ILE:HB	2.43	0.48
1:A:200:TRP:CD1	1:A:201:THR:H	2.31	0.48
1:B:26:GLU:O	1:B:27:PRO:C	2.53	0.48
2:C:520:GLU:C	2:C:522:VAL:N	2.69	0.48
2:C:725:ASP:OD1	2:C:725:ASP:O	2.31	0.48
2:C:773:LEU:O	2:C:774:LEU:C	2.56	0.48
2:C:839:LEU:HD23	2:C:849:VAL:CG2	2.42	0.48
2:C:872:ASN:HD21	2:C:874:LEU:CB	2.26	0.48
2:C:946:ARG:HG2	2:C:946:ARG:NH1	2.29	0.48
3:D:28:LYS:O	3:D:548:ILE:HG21	2.13	0.48
3:D:462:GLN:O	3:D:463:GLU:C	2.56	0.48
3:D:626:SER:OG	3:D:748:HIS:N	2.46	0.48
3:D:961:GLN:O	3:D:964:LEU:O	2.30	0.48
3:D:1008:PHE:O	3:D:1008:PHE:HD2	1.96	0.48
3:D:1231:GLU:C	3:D:1233:GLY:N	2.67	0.48
3:D:1274:ILE:O	3:D:1275:SER:C	2.57	0.48
2:C:134:ARG:HB3	2:C:393:GLN:O	2.14	0.48
3:D:669:ASN:OD1	3:D:670:VAL:N	2.47	0.48
3:D:853:VAL:HG13	3:D:858:LEU:O	2.13	0.48
3:D:875:THR:HG21	3:D:902:MET:HE2	1.94	0.48
3:D:1102:ALA:O	3:D:1103:HIS:O	2.31	0.48
3:D:1467:ILE:C	3:D:1469:GLY:H	2.20	0.48
3:D:1476:THR:HG22	4:E:21:VAL:CG2	2.43	0.48
1:A:80:LEU:HD11	2:C:572:ILE:HG21	1.96	0.48
1:A:152:PRO:O	1:A:154:GLU:N	2.44	0.48
1:A:158:ILE:HG23	1:A:159:LYS:N	2.22	0.48
1:B:128:HIS:O	1:B:129:ILE:HB	2.13	0.48
1:B:185:ARG:CB	1:B:190:THR:HA	2.43	0.48
2:C:142:ARG:HD2	2:C:324:ASP:HA	1.95	0.48
2:C:278:GLU:HG3	2:C:284:GLY:N	2.22	0.48
2:C:304:LEU:H	2:C:305:PRO:CD	2.26	0.48
2:C:493:ARG:NH1	3:D:1069:GLU:OE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:674:VAL:CG2	2:C:675:ALA:H	2.26	0.48
2:C:800:VAL:O	2:C:800:VAL:HG12	2.12	0.48
2:C:816:LYS:HB3	2:C:819:VAL:HG21	1.96	0.48
2:C:836:GLY:C	2:C:837:ASP:OD2	2.55	0.48
2:C:1052:MET:HE1	3:D:748:HIS:HB3	1.94	0.48
2:C:1059:ASP:HA	2:C:1083:GLU:OE1	2.13	0.48
3:D:646:LYS:HB3	3:D:720:LEU:HD23	1.96	0.48
3:D:699:VAL:N	3:D:756:GLN:HE22	1.99	0.48
3:D:1278:ASP:HA	3:D:1318:TYR:CA	2.36	0.48
3:D:1311:LEU:O	3:D:1323:GLN:OE1	2.30	0.48
3:D:1316:GLY:O	3:D:1317:ASP:CB	2.61	0.48
1:B:44:LEU:HG	1:B:199:ILE:CD1	2.40	0.48
1:B:44:LEU:CD2	1:B:199:ILE:HD11	2.44	0.48
1:B:157:GLY:HA3	1:B:166:PRO:HB3	1.95	0.48
1:B:184:THR:HG21	1:B:194:LYS:HD3	1.96	0.48
2:C:208:VAL:HG21	2:C:218:VAL:CG1	2.43	0.48
2:C:255:ALA:O	2:C:298:PHE:HE2	1.97	0.48
2:C:573:ARG:O	2:C:670:GLN:HG2	2.13	0.48
2:C:574:ALA:O	2:C:575:GLN:HG3	2.14	0.48
2:C:648:ARG:O	2:C:653:ASP:HB2	2.14	0.48
2:C:699:PHE:C	2:C:701:THR:H	2.22	0.48
2:C:705:ILE:HA	2:C:827:VAL:O	2.13	0.48
2:C:860:HIS:HD2	2:C:977:GLY:HA3	1.77	0.48
2:C:948:GLU:HA	2:C:953:VAL:H	1.77	0.48
3:D:669:ASN:OD1	3:D:671:LYS:HG2	2.13	0.48
3:D:793:THR:HG22	3:D:879:ARG:HH12	1.77	0.48
3:D:1231:GLU:C	3:D:1233:GLY:H	2.21	0.48
3:D:1341:PRO:HD2	3:D:1342:GLU:OE1	2.14	0.48
4:E:9:LEU:C	4:E:11:GLY:N	2.72	0.48
2:C:95:TYR:HB3	2:C:114:PHE:HA	1.95	0.48
2:C:172:ILE:HD13	2:C:184:MET:SD	2.54	0.48
2:C:466:PHE:CD1	2:C:467:ILE:CG1	2.96	0.48
2:C:1109:VAL:O	2:C:1109:VAL:HG13	2.13	0.48
3:D:590:PRO:C	3:D:600:LEU:HD21	2.39	0.48
3:D:687:VAL:O	3:D:688:TRP:C	2.56	0.48
3:D:795:VAL:CG2	3:D:904:VAL:HG21	2.44	0.48
3:D:905:PRO:C	3:D:906:GLN:CD	2.81	0.48
3:D:1045:MET:HG2	3:D:1073:SER:HB3	1.94	0.48
3:D:1105:ILE:CG2	3:D:1200:VAL:CB	2.92	0.48
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.14	0.48
3:D:1235:GLN:C	3:D:1236:LEU:HD23	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1253:THR:CA	3:D:1258:ARG:HD2	2.36	0.48
3:D:1434:TRP:HZ3	3:D:1457:ASP:H	1.62	0.48
4:E:8:LYS:CE	4:E:69:LEU:HD21	2.43	0.48
1:A:131:THR:CG2	2:C:644:ARG:HH21	2.11	0.48
1:B:203:GLY:O	1:B:204:SER:HB3	2.14	0.48
2:C:14:PRO:HA	2:C:458:TYR:CE1	2.49	0.48
2:C:91:GLN:HA	2:C:119:PRO:HA	1.96	0.48
2:C:186:VAL:O	2:C:187:ASN:C	2.57	0.48
2:C:427:VAL:O	2:C:430:VAL:HB	2.14	0.48
2:C:761:PHE:O	2:C:762:LYS:O	2.31	0.48
2:C:953:VAL:HG11	2:C:962:GLN:CB	2.42	0.48
2:C:1020:PRO:O	2:C:1021:LEU:CB	2.62	0.48
2:C:1106:ASP:N	2:C:1108:PRO:HD3	2.29	0.48
3:D:8:VAL:CG1	3:D:1434:TRP:HH2	2.27	0.48
3:D:631:ILE:HD13	3:D:745:MET:CE	2.44	0.48
3:D:647:ARG:HD2	3:D:647:ARG:HA	1.63	0.48
3:D:716:PHE:CE2	3:D:765:SER:HB3	2.48	0.48
3:D:1336:LEU:HA	3:D:1340:GLY:O	2.14	0.48
3:D:1393:GLN:HE21	3:D:1420:LEU:CD2	2.27	0.48
1:B:25:LEU:HD12	1:B:26:GLU:N	2.28	0.48
1:B:31:GLY:O	1:B:35:THR:OG1	2.31	0.48
2:C:13:ILE:HG13	2:C:14:PRO:HD2	1.96	0.48
2:C:44:ILE:H	2:C:44:ILE:CD1	2.26	0.48
2:C:254:LEU:O	2:C:257:LEU:HD12	2.14	0.48
2:C:328:LEU:HD23	2:C:468:ARG:HD2	1.95	0.48
2:C:724:ARG:C	2:C:726:ILE:HD12	2.38	0.48
3:D:124:GLU:HA	3:D:456:MET:SD	2.54	0.48
3:D:632:VAL:HG12	3:D:633:VAL:O	2.13	0.48
3:D:836:VAL:HG11	3:D:858:LEU:CD1	2.44	0.48
3:D:905:PRO:HG2	3:D:906:GLN:H	1.78	0.48
3:D:1103:HIS:H	3:D:1222:GLY:CA	2.27	0.48
3:D:1238:MET:HG3	3:D:1238:MET:O	2.13	0.48
3:D:1331:ASP:C	3:D:1333:HIS:N	2.70	0.48
3:D:1443:THR:O	3:D:1444:THR:C	2.57	0.48
1:A:43:ILE:CD1	1:B:32:PHE:CE1	2.97	0.48
2:C:74:GLY:O	2:C:76:PRO:N	2.47	0.48
2:C:156:GLY:O	2:C:157:ARG:O	2.32	0.48
2:C:520:GLU:O	2:C:521:PRO:C	2.55	0.48
2:C:613:VAL:CG1	2:C:619:ARG:HA	2.44	0.48
3:D:500:ARG:O	3:D:504:ASP:HB2	2.14	0.48
3:D:724:GLN:O	3:D:725:SER:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:848:GLU:HA	3:D:851:LEU:HB3	1.96	0.48
3:D:1015:TYR:HB3	3:D:1018:ASN:CB	2.40	0.48
3:D:1071:PHE:HA	3:D:1074:SER:HB3	1.96	0.48
3:D:1076:GLY:HA2	3:D:1079:LYS:HE2	1.96	0.48
3:D:1086:LEU:HD12	3:D:1089:ALA:CB	2.44	0.48
3:D:1101:VAL:HG21	3:D:1424:VAL:CG2	2.24	0.48
1:A:13:ALA:O	1:A:15:THR:N	2.46	0.47
1:A:72:LYS:HB3	1:A:73:GLU:OE2	2.14	0.47
2:C:173:ASP:CB	2:C:185:LYS:HE3	2.44	0.47
2:C:495:THR:O	2:C:496:ILE:CB	2.61	0.47
2:C:831:ARG:HH12	2:C:1002:GLU:CB	2.27	0.47
2:C:1103:ASP:O	2:C:1106:ASP:N	2.44	0.47
3:D:690:ALA:O	3:D:694:VAL:N	2.47	0.47
3:D:716:PHE:CE2	3:D:765:SER:CB	2.97	0.47
3:D:815:ALA:O	3:D:817:GLU:N	2.47	0.47
3:D:879:ARG:HG2	3:D:879:ARG:NH1	2.29	0.47
3:D:916:TYR:C	3:D:918:ALA:N	2.72	0.47
3:D:1140:ILE:HD13	3:D:1175:ILE:HG12	1.95	0.47
3:D:1274:ILE:H	3:D:1274:ILE:HD12	1.77	0.47
3:D:1344:VAL:O	3:D:1348:LEU:N	2.44	0.47
4:E:8:LYS:NZ	4:E:69:LEU:HD21	2.29	0.47
1:A:221:HIS:O	1:A:222:LEU:C	2.57	0.47
1:A:225:PHE:CE1	1:B:36:LEU:HD13	2.50	0.47
2:C:6:PHE:HD2	2:C:909:ALA:H	1.61	0.47
2:C:21:ILE:HD11	2:C:455:LEU:HD21	1.97	0.47
2:C:73:ILE:HD12	2:C:94:LEU:HD13	1.96	0.47
2:C:328:LEU:HD21	2:C:468:ARG:NH1	2.29	0.47
2:C:399:ASN:HD21	2:C:401:LEU:N	2.10	0.47
2:C:589:ARG:NH2	2:C:654:LEU:HD12	2.23	0.47
2:C:679:PHE:N	2:C:683:ASN:OD1	2.43	0.47
2:C:967:PHE:C	2:C:969:LEU:H	2.22	0.47
2:C:1008:ARG:HH12	2:C:1021:LEU:H	1.61	0.47
2:C:1082:PRO:HG2	2:C:1085:PHE:HB2	1.96	0.47
3:D:643:GLY:O	3:D:644:LEU:HB2	2.13	0.47
3:D:800:LYS:CB	3:D:821:VAL:H	2.26	0.47
3:D:1384:PRO:HG3	3:D:1389:LEU:O	2.14	0.47
4:E:26:ARG:HH22	4:E:37:ASN:HB3	1.77	0.47
1:B:132:LEU:CD2	1:B:132:LEU:H	2.27	0.47
2:C:7:GLY:HA2	2:C:907:ASP:OD1	2.14	0.47
2:C:13:ILE:HG22	2:C:15:LEU:N	2.21	0.47
2:C:14:PRO:HA	2:C:458:TYR:CD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:631:SER:C	2:C:634:GLY:H	2.23	0.47
2:C:790:LEU:O	2:C:791:ARG:O	2.32	0.47
2:C:831:ARG:NH1	2:C:1002:GLU:OE2	2.48	0.47
2:C:993:PHE:CD1	2:C:993:PHE:O	2.67	0.47
3:D:472:LYS:O	3:D:473:LEU:C	2.58	0.47
3:D:575:GLN:NE2	3:D:579:ASP:OD2	2.47	0.47
3:D:1481:VAL:O	3:D:1482:ARG:CG	2.60	0.47
1:A:10:VAL:O	1:A:12:THR:N	2.43	0.47
1:B:44:LEU:HG	1:B:199:ILE:CG1	2.44	0.47
2:C:83:CYS:SG	2:C:88:LEU:HB2	2.55	0.47
2:C:261:LEU:O	2:C:264:PRO:HD2	2.14	0.47
2:C:274:ARG:CG	2:C:275:TYR:N	2.78	0.47
2:C:405:ARG:HD2	2:C:543:ASN:ND2	2.29	0.47
2:C:601:GLY:HA3	2:C:648:ARG:N	2.30	0.47
2:C:657:ASP:OD1	2:C:663:GLU:HA	2.14	0.47
3:D:654:LYS:O	3:D:657:LEU:N	2.47	0.47
3:D:936:TYR:C	3:D:936:TYR:HD2	2.22	0.47
3:D:1053:PHE:CD1	3:D:1072:ILE:HG23	2.49	0.47
3:D:1274:ILE:HA	3:D:1322:GLY:N	2.30	0.47
1:A:18:ASP:O	1:A:19:HIS:HB3	2.15	0.47
1:A:79:ILE:CD1	1:A:165:ILE:HD12	2.38	0.47
1:A:88:ARG:CB	1:A:121:GLU:HB2	2.38	0.47
1:A:108:GLU:CG	2:C:644:ARG:HH22	2.27	0.47
1:B:87:VAL:CG1	1:B:88:ARG:N	2.77	0.47
1:B:219:LYS:O	1:B:222:LEU:HB2	2.14	0.47
2:C:23:VAL:HG12	2:C:24:GLU:N	2.30	0.47
2:C:46:ALA:O	2:C:50:GLU:N	2.31	0.47
2:C:159:ILE:CD1	2:C:310:LEU:HB2	2.34	0.47
2:C:195:LEU:HD13	2:C:227:LEU:CD1	2.31	0.47
2:C:333:ILE:CG2	2:C:460:ARG:HH22	2.25	0.47
2:C:408:ARG:NH1	2:C:455:LEU:HD23	2.29	0.47
2:C:425:PHE:O	2:C:426:ASP:CB	2.62	0.47
2:C:449:ILE:HG22	2:C:450:GLY:N	2.29	0.47
2:C:637:PHE:HE1	2:C:1639:GLN:HE21	1.61	0.47
2:C:768:SER:CB	2:C:769:PRO:HD2	2.42	0.47
2:C:778:PHE:N	2:C:778:PHE:CD1	2.82	0.47
2:C:966:LEU:CD1	2:C:986:PRO:HG3	2.40	0.47
2:C:985:GLY:O	2:C:986:PRO:O	2.32	0.47
2:C:1036:GLU:O	2:C:1039:ALA:HB3	2.14	0.47
2:C:1095:LEU:CD1	3:D:603:LEU:HD23	2.35	0.47
3:D:836:VAL:CG1	3:D:858:LEU:HD11	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1069:GLU:O	3:D:1070:TYR:C	2.58	0.47
3:D:1069:GLU:C	3:D:1071:PHE:N	2.70	0.47
3:D:1156:LEU:H	3:D:1182:GLU:CD	2.21	0.47
3:D:1277:ILE:HG22	3:D:1279:GLY:N	2.27	0.47
4:E:8:LYS:HB3	4:E:69:LEU:HD11	1.96	0.47
1:A:35:THR:HG21	1:B:43:ILE:CG1	2.45	0.47
1:A:41:ARG:HH12	1:A:42:ARG:HG2	1.80	0.47
1:B:111:ALA:O	1:B:114:PHE:CD1	2.68	0.47
1:B:181:VAL:O	1:B:181:VAL:HG13	2.14	0.47
2:C:74:GLY:O	2:C:75:ASP:C	2.57	0.47
2:C:501:THR:O	2:C:501:THR:HG22	2.14	0.47
2:C:518:ARG:C	2:C:520:GLU:N	2.70	0.47
2:C:686:ASP:CG	3:D:739:ASP:OD2	2.57	0.47
2:C:1007:ALA:HB1	3:D:652:LEU:CD2	2.44	0.47
3:D:464:LEU:O	3:D:468:LEU:CB	2.63	0.47
3:D:497:GLU:HG2	3:D:1389:LEU:HD11	1.96	0.47
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.44	0.47
3:D:859:ASP:OD1	3:D:861:GLN:NE2	2.48	0.47
3:D:897:GLN:HE21	3:D:897:GLN:CA	2.27	0.47
3:D:899:LEU:HD22	3:D:899:LEU:H	1.79	0.47
3:D:1071:PHE:O	3:D:1074:SER:N	2.46	0.47
3:D:1142:SER:C	3:D:1364:HIS:HD2	2.22	0.47
1:B:26:GLU:OE1	1:B:27:PRO:HD3	2.15	0.47
2:C:11:GLU:CD	2:C:473:ARG:NE	2.73	0.47
2:C:15:LEU:HD21	2:C:461:VAL:HB	1.96	0.47
2:C:30:LEU:HD12	2:C:44:ILE:HG12	1.97	0.47
2:C:78:PHE:HB3	2:C:82:GLU:OE2	2.15	0.47
2:C:193:LEU:HD13	2:C:193:LEU:C	2.39	0.47
2:C:224:GLU:C	2:C:226:VAL:N	2.70	0.47
2:C:395:LYS:HG2	2:C:397:GLU:CD	2.40	0.47
2:C:397:GLU:OE2	2:C:632:ASN:ND2	2.47	0.47
2:C:460:ARG:HB2	2:C:468:ARG:HA	1.97	0.47
2:C:547:ILE:HG23	2:C:843:HIS:CE1	2.50	0.47
2:C:749:VAL:HG23	2:C:800:VAL:HG23	1.96	0.47
2:C:1034:GLU:OE2	3:D:1096:ARG:NH2	2.47	0.47
2:C:1067:TYR:O	2:C:1071:ILE:HD13	2.15	0.47
2:C:1073:GLY:CA	3:D:659:LYS:HE3	2.44	0.47
3:D:586:ARG:C	3:D:587:ARG:HD3	2.40	0.47
3:D:602:SER:O	3:D:606:ILE:HD12	2.15	0.47
3:D:708:LEU:O	3:D:709:HIS:O	2.33	0.47
3:D:937:TYR:O	3:D:938:GLY:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:962:ARG:O	3:D:966:GLU:CG	2.63	0.47
3:D:1071:PHE:O	3:D:1072:ILE:C	2.56	0.47
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.13	0.47
3:D:1132:LEU:CD1	3:D:1184:ARG:HH12	2.20	0.47
3:D:1136:LYS:CG	3:D:1139:ASP:OD2	2.62	0.47
3:D:1329:ALA:O	3:D:1330:ILE:C	2.57	0.47
3:D:1336:LEU:CD1	3:D:1340:GLY:C	2.88	0.47
3:D:1427:SER:C	3:D:1429:LEU:N	2.72	0.47
3:D:1465:ASN:O	3:D:1470:ARG:HB2	2.15	0.47
2:C:97:ARG:HG2	2:C:112:GLU:H	1.79	0.47
2:C:198:ARG:CZ	2:C:203:ASP:OD2	2.63	0.47
2:C:208:VAL:HG12	2:C:209:ARG:N	2.29	0.47
2:C:254:LEU:C	2:C:254:LEU:HD12	2.39	0.47
2:C:586:ARG:O	2:C:587:VAL:C	2.58	0.47
2:C:693:GLU:O	2:C:694:LEU:C	2.57	0.47
2:C:745:ILE:C	2:C:747:ALA:N	2.71	0.47
2:C:774:LEU:O	2:C:778:PHE:N	2.47	0.47
2:C:944:LEU:HD11	2:C:963:LEU:CD2	2.45	0.47
2:C:985:GLY:O	2:C:986:PRO:C	2.57	0.47
2:C:987:ILE:O	2:C:987:ILE:HG22	2.14	0.47
2:C:1034:GLU:O	2:C:1037:VAL:HB	2.15	0.47
2:C:1056:LYS:O	3:D:624:ASP:HB2	2.14	0.47
3:D:537:THR:O	3:D:537:THR:HG22	2.15	0.47
3:D:687:VAL:O	3:D:690:ALA:HB3	2.15	0.47
3:D:734:GLU:O	3:D:735:ALA:C	2.57	0.47
3:D:764:LEU:CD2	3:D:766:ALA:HB3	2.45	0.47
3:D:947:ILE:CA	3:D:1020:LEU:HD13	2.43	0.47
3:D:1005:GLN:O	3:D:1009:ASN:HB3	2.15	0.47
3:D:1311:LEU:HD12	3:D:1311:LEU:N	2.30	0.47
3:D:1466:VAL:O	3:D:1467:ILE:C	2.57	0.47
1:A:199:ILE:HD12	1:A:199:ILE:N	2.30	0.47
1:A:223:ASN:O	1:A:225:PHE:N	2.48	0.47
1:B:32:PHE:HA	1:B:35:THR:OG1	2.15	0.47
2:C:26:TYR:HE2	2:C:30:LEU:HD22	1.80	0.47
2:C:208:VAL:O	2:C:209:ARG:HB2	2.14	0.47
2:C:252:LYS:HE3	2:C:298:PHE:HE1	1.80	0.47
2:C:730:SER:O	2:C:731:GLU:O	2.33	0.47
2:C:794:PRO:HG2	2:C:1027:PHE:HB2	1.97	0.47
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.94	0.47
2:C:890:LEU:HD11	2:C:917:LEU:HD13	1.97	0.47
2:C:1055:ILE:HD12	2:C:1055:ILE:N	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1091:GLU:OE1	3:D:606:ILE:HG22	2.15	0.47
3:D:120:ALA:HB1	3:D:126:VAL:CB	2.45	0.47
3:D:638:LYS:O	3:D:639:LEU:C	2.55	0.47
3:D:793:THR:HA	3:D:879:ARG:HH12	1.80	0.47
3:D:999:THR:O	3:D:1000:THR:C	2.58	0.47
3:D:1134:LEU:N	3:D:1134:LEU:HD23	2.29	0.47
3:D:1327:ARG:NH1	3:D:1327:ARG:CB	2.76	0.47
1:A:222:LEU:CD1	1:B:215:VAL:HG13	2.40	0.47
1:B:11:PHE:HA	1:B:25:LEU:HA	1.96	0.47
1:B:30:ARG:CZ	2:C:854:PRO:HB3	2.45	0.47
2:C:20:GLU:OE2	2:C:461:VAL:HG23	2.15	0.47
2:C:78:PHE:HD2	2:C:82:GLU:OE2	1.98	0.47
2:C:101:ILE:HG22	2:C:102:HIS:N	2.29	0.47
2:C:175:GLU:O	2:C:182:VAL:HA	2.15	0.47
2:C:257:LEU:C	2:C:259:GLY:N	2.72	0.47
2:C:304:LEU:HD23	2:C:305:PRO:N	2.30	0.47
2:C:314:THR:O	2:C:315:ALA:HB3	2.15	0.47
2:C:706:GLU:O	2:C:826:PHE:HA	2.15	0.47
2:C:862:PRO:HG2	2:C:863:ASP:H	1.80	0.47
2:C:892:LEU:C	2:C:894:GLY:N	2.73	0.47
3:D:99:ALA:O	3:D:575:GLN:HB2	2.14	0.47
3:D:507:ASN:O	3:D:508:ARG:HG2	2.15	0.47
3:D:937:TYR:O	3:D:941:LEU:HB2	2.14	0.47
3:D:984:THR:O	3:D:985:ASP:C	2.59	0.47
3:D:1081:GLY:HA2	3:D:1084:THR:HG23	1.97	0.47
3:D:1205:TYR:O	3:D:1206:GLY:O	2.32	0.47
3:D:1236:LEU:HB3	3:D:1256:LEU:N	2.30	0.47
3:D:1471:LEU:O	3:D:1472:ILE:C	2.57	0.47
4:E:13:VAL:HG21	4:E:19:LEU:CB	2.45	0.47
1:A:134:GLU:HB3	2:C:606:VAL:HG23	1.96	0.46
1:A:199:ILE:HG21	1:A:207:PRO:HA	1.97	0.46
1:B:24:VAL:HG12	1:B:24:VAL:O	2.13	0.46
2:C:115:LEU:HA	2:C:375:SER:CB	2.45	0.46
2:C:127:PHE:N	2:C:127:PHE:CD1	2.83	0.46
2:C:149:THR:CB	2:C:158:TYR:HE1	2.22	0.46
2:C:595:LEU:HG	2:C:655:LEU:HD23	1.97	0.46
2:C:674:VAL:HG23	2:C:869:VAL:O	2.15	0.46
2:C:796:GLU:HG2	3:D:681:ARG:NH2	2.28	0.46
2:C:846:LYS:HD2	2:C:846:LYS:O	2.16	0.46
2:C:890:LEU:HD11	2:C:901:TYR:CE2	2.50	0.46
2:C:897:LEU:O	2:C:898:GLY:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:789:LEU:CD1	3:D:934:LEU:HD22	2.44	0.46
3:D:1075:HIS:H	3:D:1075:HIS:CD2	2.33	0.46
3:D:1101:VAL:CG2	3:D:1424:VAL:HG22	2.24	0.46
3:D:1251:ASP:O	3:D:1252:ILE:HB	2.15	0.46
3:D:1340:GLY:HA3	3:D:1342:GLU:OE1	2.15	0.46
1:A:32:PHE:O	1:A:33:GLY:C	2.57	0.46
1:A:70:GLY:HA2	2:C:606:VAL:HG22	1.97	0.46
1:A:198:ARG:HH12	2:C:932:GLU:CB	2.27	0.46
2:C:34:VAL:O	2:C:35:PRO:C	2.58	0.46
2:C:65:VAL:HB	2:C:101:ILE:HB	1.97	0.46
2:C:166:PRO:HB3	2:C:417:GLY:N	2.27	0.46
2:C:202:TYR:O	2:C:203:ASP:CG	2.58	0.46
2:C:215:GLY:O	2:C:216:ASP:O	2.34	0.46
2:C:613:VAL:HG13	2:C:620:LEU:N	2.15	0.46
2:C:728:HIS:CD2	2:C:783:ARG:NH1	2.83	0.46
2:C:928:LYS:O	2:C:931:GLY:N	2.48	0.46
4:E:86:GLN:HA	4:E:89:MET:HG2	1.97	0.46
1:B:15:THR:C	1:B:17:GLY:N	2.74	0.46
1:B:41:ARG:HD3	1:B:41:ARG:C	2.40	0.46
1:B:222:LEU:O	1:B:223:ASN:C	2.57	0.46
2:C:308:ARG:C	2:C:310:LEU:N	2.68	0.46
2:C:545:ASN:HA	2:C:905:VAL:HG21	1.98	0.46
2:C:609:THR:O	2:C:609:THR:HG23	2.14	0.46
2:C:728:HIS:C	2:C:730:SER:N	2.73	0.46
2:C:1099:VAL:HG22	3:D:10:ILE:CD1	2.42	0.46
2:C:1105:LYS:C	2:C:1108:PRO:HD3	2.40	0.46
3:D:149:LYS:O	3:D:152:LEU:N	2.48	0.46
3:D:631:ILE:HD11	3:D:743:ASP:CB	2.45	0.46
3:D:638:LYS:CB	3:D:729:HIS:NE2	2.78	0.46
3:D:794:GLN:HB3	3:D:1017:PHE:CZ	2.49	0.46
3:D:952:ASP:C	3:D:954:ALA:N	2.71	0.46
3:D:1339:LYS:HD2	3:D:1339:LYS:HA	1.58	0.46
2:C:100:LEU:HD23	2:C:372:LEU:CD1	2.45	0.46
2:C:437:ARG:HG3	2:C:437:ARG:O	2.14	0.46
2:C:461:VAL:O	2:C:481:GLU:HG2	2.16	0.46
2:C:575:GLN:C	2:C:667:ALA:HB1	2.39	0.46
2:C:605:LYS:HD2	2:C:607:ASP:CG	2.40	0.46
2:C:727:PRO:O	2:C:729:LEU:N	2.48	0.46
2:C:1108:PRO:O	2:C:1109:VAL:O	2.33	0.46
3:D:552:ASN:O	3:D:556:LYS:N	2.49	0.46
3:D:645:PRO:O	3:D:646:LYS:C	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:660:LYS:O	3:D:664:LYS:N	2.42	0.46
3:D:695:ILE:HG23	3:D:718:PRO:HD2	1.96	0.46
3:D:696:HIS:CG	4:E:48:MET:HE2	2.51	0.46
3:D:701:LEU:CD1	3:D:715:ALA:HB2	2.44	0.46
3:D:773:ALA:O	3:D:774:SER:CB	2.64	0.46
3:D:855:HIS:CD2	3:D:855:HIS:N	2.66	0.46
3:D:1110:ALA:O	3:D:1111:ASP:C	2.58	0.46
3:D:1273:VAL:O	3:D:1322:GLY:HA3	2.15	0.46
4:E:15:SER:O	4:E:17:TYR:N	2.49	0.46
4:E:78:ASN:O	4:E:79:LEU:HB2	2.15	0.46
1:A:30:ARG:HH11	1:A:192:LEU:HD23	1.80	0.46
2:C:186:VAL:HG11	2:C:258:PHE:HD2	1.79	0.46
2:C:258:PHE:CD1	2:C:258:PHE:N	2.83	0.46
2:C:460:ARG:CA	2:C:468:ARG:O	2.63	0.46
2:C:494:TYR:O	2:C:495:THR:CB	2.62	0.46
2:C:549:PHE:HA	2:C:551:GLU:OE1	2.15	0.46
2:C:641:PRO:HA	2:C:656:ALA:HA	1.96	0.46
2:C:684:PHE:O	2:C:686:ASP:N	2.49	0.46
2:C:1001:VAL:O	2:C:1002:GLU:C	2.58	0.46
3:D:99:ALA:HB3	3:D:458:ALA:CB	2.45	0.46
3:D:772:PRO:CB	3:D:778:LEU:HD23	2.46	0.46
3:D:887:GLY:C	3:D:889:ALA:H	2.23	0.46
3:D:1114:THR:CB	3:D:1189:ARG:HH11	2.27	0.46
3:D:1156:LEU:HB3	3:D:1173:PHE:CE1	2.50	0.46
1:A:105:GLY:HA2	1:A:136:GLY:N	2.30	0.46
1:B:101:LEU:HD23	1:B:140:MET:CE	2.45	0.46
1:B:144:VAL:HG12	1:B:145:ASP:N	2.30	0.46
2:C:30:LEU:O	2:C:31:GLN:C	2.58	0.46
2:C:122:THR:HG22	2:C:123:GLU:N	2.30	0.46
2:C:351:LEU:HA	2:C:377:PRO:HG3	1.98	0.46
2:C:358:ARG:HB2	2:C:372:LEU:CD2	2.45	0.46
2:C:395:LYS:CG	2:C:397:GLU:HG3	2.44	0.46
2:C:1639:GLN:HG2	2:C:658:GLY:HA2	1.97	0.46
2:C:756:VAL:O	2:C:790:LEU:N	2.48	0.46
2:C:805:ARG:NE	2:C:821:GLU:OE2	2.38	0.46
2:C:946:ARG:CD	2:C:984:GLU:HB2	2.45	0.46
3:D:23:TYR:O	3:D:24:GLY:C	2.58	0.46
3:D:31(U):UNK:O	3:D:32(U):UNK:CB	2.62	0.46
3:D:467:GLU:O	3:D:468:LEU:O	2.34	0.46
3:D:700:VAL:N	3:D:716:PHE:O	2.48	0.46
3:D:988:ARG:O	3:D:989:TYR:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1067:VAL:C	3:D:1069:GLU:N	2.74	0.46
3:D:1109:GLU:O	3:D:1202:GLN:CB	2.64	0.46
3:D:1435:LEU:CD2	3:D:1457:ASP:OD2	2.64	0.46
3:D:1472:ILE:O	3:D:1477:GLY:HA3	2.15	0.46
1:A:30:ARG:NH1	1:A:192:LEU:CD2	2.79	0.46
1:A:194:LYS:O	1:A:194:LYS:HG2	2.16	0.46
1:A:198:ARG:NH2	2:C:932:GLU:OE1	2.32	0.46
1:B:22:GLU:O	1:B:23:PHE:HD2	1.98	0.46
2:C:43:GLY:O	2:C:44:ILE:C	2.58	0.46
2:C:66:LEU:N	2:C:100:LEU:HA	2.30	0.46
2:C:143:SER:O	2:C:147:TYR:OH	2.27	0.46
2:C:218:VAL:C	2:C:220:GLY:N	2.73	0.46
2:C:340:MET:SD	2:C:340:MET:O	2.73	0.46
2:C:525:ALA:O	2:C:527:GLU:N	2.48	0.46
2:C:575:GLN:HA	2:C:662:GLU:CD	2.40	0.46
2:C:682:TYR:CE1	2:C:851:LYS:HD2	2.51	0.46
2:C:813:VAL:HG12	2:C:815:LEU:CG	2.46	0.46
2:C:816:LYS:O	2:C:819:VAL:HB	2.15	0.46
2:C:912:PRO:O	2:C:915:LYS:HB2	2.16	0.46
2:C:969:LEU:HD11	3:D:952:ASP:N	2.22	0.46
2:C:1014:SER:O	2:C:1018:GLN:OE1	2.34	0.46
2:C:1038:TRP:CH2	3:D:1096:ARG:HA	2.50	0.46
2:C:1049:LEU:C	2:C:1051:GLU:H	2.24	0.46
2:C:1055:ILE:HG22	2:C:1055:ILE:O	2.16	0.46
2:C:1059:ASP:HA	2:C:1083:GLU:CG	2.46	0.46
3:D:28:LYS:O	3:D:30:GLU:N	2.49	0.46
3:D:98:PRO:CB	3:D:574:LEU:HD23	2.46	0.46
3:D:23(U):UNK:CB	3:D:43(U):UNK:N	2.79	0.46
3:D:548:ILE:O	3:D:552:ASN:ND2	2.49	0.46
3:D:760:ARG:NH2	4:E:3:GLU:OE2	2.38	0.46
3:D:794:GLN:OE1	3:D:906:GLN:NE2	2.49	0.46
3:D:937:TYR:N	3:D:937:TYR:HD1	2.14	0.46
3:D:1166:LEU:HB2	3:D:1170:ASP:HB2	1.96	0.46
3:D:1377:LYS:HE2	3:D:1378:TYR:CZ	2.51	0.46
1:A:74:ASP:OD1	1:A:76:VAL:HG23	2.16	0.46
1:A:184:THR:O	1:A:184:THR:HG23	2.15	0.46
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.31	0.46
2:C:12:VAL:CG1	2:C:13:ILE:H	1.96	0.46
2:C:252:LYS:HE3	2:C:298:PHE:CE1	2.51	0.46
2:C:425:PHE:O	2:C:426:ASP:HB3	2.14	0.46
2:C:462:ASP:O	2:C:464:LEU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:672:VAL:HG13	2:C:673:LEU:N	2.31	0.46
2:C:679:PHE:C	2:C:681:GLY:N	2.73	0.46
2:C:787:ASP:O	2:C:789:SER:N	2.49	0.46
3:D:75:ARG:O	3:D:77:ALA:N	2.49	0.46
3:D:82:ARG:C	3:D:84:ILE:H	2.24	0.46
3:D:6(U):UNK:CB	3:D:36(U):UNK:HA	2.46	0.46
3:D:968:ASP:HA	3:D:971:LEU:HD12	1.96	0.46
3:D:1055:VAL:O	3:D:1055:VAL:HG12	2.13	0.46
3:D:1057:VAL:HG12	3:D:1067:VAL:HG21	1.98	0.46
3:D:1277:ILE:O	3:D:1317:ASP:O	2.33	0.46
3:D:1441:GLN:O	3:D:1442:ASN:HB3	2.16	0.46
3:D:1449:GLU:O	3:D:1452:ILE:N	2.49	0.46
3:D:1489:GLN:CB	4:E:72:ARG:HD2	2.46	0.46
4:E:26:ARG:NH2	4:E:30:LEU:HD12	2.30	0.46
4:E:26:ARG:HH22	4:E:37:ASN:CB	2.29	0.46
1:A:164:ALA:O	1:A:165:ILE:HG12	2.15	0.46
1:B:26:GLU:CG	1:B:27:PRO:HD3	2.45	0.46
1:B:64:GLU:O	1:B:75:VAL:HG21	2.16	0.46
1:B:99:LEU:HD13	1:B:114:PHE:CD2	2.51	0.46
2:C:197:LEU:HD22	2:C:202:TYR:CD1	2.43	0.46
2:C:514:VAL:C	2:C:516:ARG:H	2.23	0.46
2:C:777:ILE:C	2:C:779:GLY:H	2.23	0.46
3:D:472:LYS:C	3:D:474:GLU:N	2.71	0.46
3:D:520:LEU:HB3	3:D:521:PRO:HD2	1.97	0.46
3:D:558:LEU:C	3:D:560:GLN:N	2.73	0.46
3:D:642:CYS:SG	3:D:702:LEU:CD2	3.04	0.46
3:D:836:VAL:HB	3:D:858:LEU:HD21	1.98	0.46
3:D:1485:GLN:HA	4:E:75:PHE:HA	1.98	0.46
4:E:26:ARG:HH21	4:E:30:LEU:CD1	2.29	0.46
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.98	0.46
2:C:94:LEU:HD21	2:C:344:PHE:HZ	1.81	0.46
2:C:162:ILE:HD12	2:C:162:ILE:N	2.31	0.46
2:C:415:PRO:O	2:C:416:GLY:C	2.58	0.46
2:C:474:VAL:O	2:C:474:VAL:HG12	2.16	0.46
2:C:570:PRO:CG	2:C:635:THR:HG23	2.46	0.46
2:C:599:GLU:O	2:C:600:ASP:O	2.33	0.46
2:C:640:ARG:O	2:C:657:ASP:N	2.49	0.46
2:C:679:PHE:HE2	2:C:978:ARG:NH2	2.14	0.46
2:C:684:PHE:O	2:C:685:GLU:HB2	2.16	0.46
2:C:769:PRO:C	2:C:771:GLU:N	2.74	0.46
3:D:690:ALA:O	3:D:693:GLU:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:709:HIS:CE1	3:D:1231:GLU:HG3	2.51	0.46
3:D:901:GLN:O	3:D:905:PRO:HD3	2.16	0.46
3:D:957:PRO:CG	3:D:1007:VAL:HB	2.45	0.46
3:D:1170:ASP:C	3:D:1172:HIS:H	2.24	0.46
3:D:1278:ASP:CA	3:D:1317:ASP:O	2.64	0.46
3:D:1321:ALA:C	3:D:1323:GLN:N	2.74	0.46
3:D:1347:TYR:CE1	3:D:1351:GLU:HB2	2.51	0.46
3:D:1485:GLN:CB	4:E:75:PHE:HB3	2.46	0.46
1:A:175:ARG:HB2	1:A:201:THR:CB	2.46	0.45
1:B:43:ILE:HD12	1:B:218:LEU:HB2	1.97	0.45
1:B:213:GLN:O	1:B:216:ALA:HB3	2.16	0.45
2:C:157:ARG:NH1	2:C:321:GLU:HG2	2.31	0.45
2:C:172:ILE:CG2	2:C:173:ASP:N	2.79	0.45
2:C:253:ALA:C	2:C:255:ALA:H	2.24	0.45
2:C:306:THR:O	2:C:310:LEU:N	2.49	0.45
2:C:589:ARG:NH1	2:C:596:TYR:CB	2.79	0.45
2:C:695:LEU:O	2:C:696:LYS:C	2.59	0.45
2:C:976:ASP:C	2:C:978:ARG:H	2.23	0.45
2:C:1099:VAL:O	2:C:1099:VAL:HG12	2.16	0.45
3:D:508:ARG:HB2	3:D:510:GLU:OE2	2.15	0.45
3:D:700:VAL:CG2	3:D:718:PRO:HG3	2.46	0.45
3:D:710:ARG:C	3:D:712:GLY:H	2.24	0.45
3:D:791:TYR:CE1	3:D:1023:MET:HG3	2.51	0.45
3:D:836:VAL:HG11	3:D:858:LEU:HD11	1.98	0.45
3:D:937:TYR:N	3:D:937:TYR:CD1	2.84	0.45
3:D:1007:VAL:HG13	3:D:1008:PHE:H	1.81	0.45
3:D:1007:VAL:C	3:D:1009:ASN:H	2.24	0.45
3:D:1017:PHE:O	3:D:1018:ASN:C	2.58	0.45
3:D:1165:TYR:CE2	3:D:1214:PRO:HB3	2.51	0.45
3:D:1346:ARG:NH1	3:D:1369:GLU:OE2	2.50	0.45
3:D:1382:THR:O	3:D:1383:ASP:C	2.58	0.45
3:D:1454:GLY:O	3:D:1455:LYS:HB2	2.15	0.45
3:D:1475:GLY:HA2	4:E:17:TYR:CE2	2.51	0.45
1:A:24:VAL:HG22	1:A:196:THR:HB	1.98	0.45
1:A:212:ASN:O	1:A:213:GLN:C	2.59	0.45
2:C:6:PHE:CD2	2:C:909:ALA:HA	2.52	0.45
2:C:289:THR:HG23	2:C:302:VAL:O	2.16	0.45
2:C:352:ALA:C	2:C:355:VAL:HG12	2.41	0.45
2:C:540:PHE:CE1	2:C:906:PHE:HE1	2.34	0.45
2:C:574:ALA:O	2:C:575:GLN:O	2.34	0.45
2:C:880:MET:O	2:C:881:ASN:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:937:ASP:O	2:C:939:ARG:N	2.48	0.45
2:C:1004:LYS:O	2:C:1005:MET:HB3	2.15	0.45
3:D:638:LYS:CB	3:D:729:HIS:CE1	2.99	0.45
3:D:762:GLN:HE21	4:E:20:THR:CB	2.28	0.45
3:D:1066:THR:C	3:D:1068:LEU:N	2.71	0.45
3:D:1148:VAL:HG22	3:D:1163:GLY:O	2.17	0.45
3:D:1302:GLU:C	3:D:1303:TYR:CD1	2.94	0.45
3:D:1333:HIS:HE1	3:D:1421:LEU:HB3	1.80	0.45
1:B:110:ARG:C	1:B:112:VAL:H	2.23	0.45
2:C:137:VAL:HG11	2:C:411:SER:HB2	1.97	0.45
2:C:257:LEU:HA	2:C:261:LEU:CD2	2.45	0.45
2:C:351:LEU:HG	2:C:352:ALA:N	2.31	0.45
2:C:380:ALA:O	2:C:384:GLU:CB	2.64	0.45
2:C:521:PRO:O	2:C:522:VAL:C	2.58	0.45
2:C:653:ASP:O	2:C:653:ASP:CG	2.60	0.45
2:C:654:LEU:HG	2:C:655:LEU:N	2.32	0.45
2:C:959:PRO:O	2:C:962:GLN:N	2.50	0.45
3:D:78:VAL:N	3:D:81:THR:O	2.43	0.45
3:D:632:VAL:HG12	3:D:633:VAL:N	2.30	0.45
3:D:729:HIS:ND1	3:D:730:PRO:HD2	2.30	0.45
3:D:772:PRO:HG3	3:D:778:LEU:HD23	1.99	0.45
3:D:1462:LEU:CD2	3:D:1473:PRO:HG2	2.46	0.45
1:A:17:GLY:O	1:A:18:ASP:HB2	2.16	0.45
1:A:50:GLY:HA3	1:A:171:PHE:O	2.15	0.45
1:B:171:PHE:O	1:B:172:SER:OG	2.33	0.45
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.98	0.45
2:C:152:PRO:O	2:C:153:ALA:O	2.35	0.45
2:C:222:LEU:O	2:C:223:ASP:C	2.60	0.45
2:C:520:GLU:N	2:C:521:PRO:CD	2.80	0.45
2:C:574:ALA:HB1	2:C:667:ALA:O	2.17	0.45
2:C:584:GLU:C	2:C:586:ARG:N	2.74	0.45
2:C:681:GLY:CA	3:D:939:PHE:CE2	2.99	0.45
2:C:762:LYS:HD2	2:C:786:LYS:CD	2.38	0.45
2:C:881:ASN:HB2	3:D:1061:PHE:CE2	2.52	0.45
2:C:926:PHE:HE1	2:C:929:ARG:NH1	2.14	0.45
2:C:935:GLY:O	2:C:936:VAL:C	2.60	0.45
2:C:969:LEU:HD13	3:D:952:ASP:CG	2.41	0.45
2:C:1112:PHE:C	2:C:1114:GLY:H	2.25	0.45
3:D:678:GLU:O	3:D:680:GLN:N	2.45	0.45
3:D:770:LEU:CD1	3:D:770:LEU:N	2.77	0.45
3:D:845:ASN:O	3:D:847:ASP:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:963:TYR:HE2	3:D:1002:LYS:HB3	1.81	0.45
3:D:1044:LEU:HD12	3:D:1044:LEU:HA	1.73	0.45
3:D:1065:LEU:HD12	3:D:1067:VAL:HG23	1.98	0.45
3:D:1075:HIS:CD2	3:D:1075:HIS:N	2.85	0.45
3:D:1237:THR:HG22	3:D:1239:ARG:H	1.81	0.45
3:D:1251:ASP:C	3:D:1253:THR:N	2.62	0.45
4:E:62:THR:O	4:E:63:TRP:C	2.58	0.45
4:E:63:TRP:O	4:E:67:GLU:N	2.41	0.45
1:A:74:ASP:HB2	2:C:627:ARG:NH2	2.31	0.45
1:B:173:PRO:HA	1:B:203:GLY:HA3	1.99	0.45
1:B:202:ASP:C	1:B:204:SER:N	2.64	0.45
1:B:223:ASN:O	1:B:224:TYR:C	2.60	0.45
2:C:64:LEU:HA	2:C:101:ILE:O	2.16	0.45
2:C:553:ASP:HA	2:C:882:LEU:HA	1.98	0.45
2:C:588:VAL:CG2	2:C:666:LEU:HD13	2.46	0.45
2:C:848:VAL:HG12	3:D:740:PHE:O	2.16	0.45
3:D:92:HIS:O	3:D:94:GLU:N	2.50	0.45
3:D:601:ARG:HD2	3:D:605:ASP:OD2	2.16	0.45
3:D:631:ILE:HD11	3:D:743:ASP:HB2	1.97	0.45
3:D:655:PRO:O	3:D:656:PHE:C	2.58	0.45
3:D:706:PRO:HG2	3:D:706:PRO:O	2.15	0.45
3:D:764:LEU:HG	3:D:766:ALA:N	2.29	0.45
3:D:1051:GLU:O	3:D:1052:THR:O	2.35	0.45
3:D:1066:THR:O	3:D:1067:VAL:C	2.59	0.45
3:D:1086:LEU:HD13	3:D:1238:MET:CB	2.38	0.45
3:D:1118:ILE:HD11	3:D:1193:THR:CG2	2.46	0.45
3:D:1130:ARG:HG2	3:D:1130:ARG:NH1	2.32	0.45
3:D:1140:ILE:O	3:D:1144:LEU:N	2.49	0.45
3:D:1271:LYS:O	3:D:1273:VAL:N	2.49	0.45
3:D:1283:ILE:CD1	3:D:1312:LEU:HA	2.47	0.45
1:A:30:ARG:NH1	1:A:192:LEU:HD23	2.32	0.45
1:A:42:ARG:NH2	1:B:34:VAL:HB	2.26	0.45
1:A:122:ILE:O	1:A:123:MET:C	2.60	0.45
1:A:126:ASP:OD1	1:A:126:ASP:N	2.49	0.45
1:B:12:THR:O	1:B:24:VAL:N	2.50	0.45
1:B:22:GLU:C	1:B:23:PHE:CD2	2.95	0.45
2:C:32:ALA:HB2	2:C:73:ILE:HD13	1.99	0.45
2:C:78:PHE:N	2:C:78:PHE:CD1	2.83	0.45
2:C:216:ASP:C	2:C:218:VAL:H	2.24	0.45
2:C:304:LEU:H	2:C:305:PRO:HD3	1.82	0.45
2:C:374:ASN:O	2:C:376:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:406:HIS:ND1	2:C:406:HIS:O	2.50	0.45
2:C:462:ASP:O	2:C:463:ALA:C	2.59	0.45
2:C:630:ARG:HA	2:C:705:ILE:CD1	2.45	0.45
2:C:935:GLY:O	2:C:936:VAL:O	2.33	0.45
3:D:91:ALA:CB	3:D:518:PRO:CG	2.95	0.45
3:D:469:ASP:C	3:D:471:GLU:N	2.72	0.45
3:D:666:PHE:CZ	3:D:676:MET:SD	3.10	0.45
3:D:767:HIS:C	3:D:769:LEU:H	2.24	0.45
3:D:958:GLU:C	3:D:960:LYS:H	2.23	0.45
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.32	0.45
3:D:1268:PRO:HB2	3:D:1269:LYS:H	1.67	0.45
3:D:1425:THR:C	3:D:1427:SER:N	2.75	0.45
4:E:77:GLU:HG3	4:E:77:GLU:O	2.17	0.45
1:A:179:PHE:O	1:A:179:PHE:CD1	2.69	0.45
1:A:189:ARG:O	1:A:191:ASP:N	2.50	0.45
1:A:198:ARG:NH1	2:C:932:GLU:HB3	2.31	0.45
1:B:36:LEU:O	1:B:40:LEU:HD23	2.17	0.45
2:C:115:LEU:HD13	2:C:375:SER:CB	2.47	0.45
2:C:378:LEU:HD12	2:C:378:LEU:N	2.31	0.45
2:C:552:HIS:O	2:C:553:ASP:C	2.59	0.45
2:C:758:ARG:O	2:C:788:THR:O	2.35	0.45
2:C:877:PRO:HG2	3:D:949:ILE:HD12	1.98	0.45
2:C:905:VAL:O	2:C:906:PHE:HB2	2.17	0.45
2:C:940:GLU:HA	2:C:973:VAL:CG2	2.45	0.45
2:C:949:LYS:C	2:C:951:GLY:N	2.74	0.45
3:D:106:LYS:O	3:D:109:PRO:N	2.50	0.45
3:D:609:GLY:O	3:D:611:GLN:N	2.50	0.45
3:D:860:LEU:HD12	3:D:878:GLY:CA	2.47	0.45
3:D:876:SER:O	3:D:878:GLY:N	2.50	0.45
3:D:1076:GLY:HA2	3:D:1079:LYS:HG2	1.97	0.45
3:D:1167:SER:C	3:D:1169:GLU:N	2.73	0.45
3:D:1192:LEU:HG	3:D:1369:GLU:HB3	1.99	0.45
1:A:157:GLY:O	1:A:164:ALA:HB1	2.17	0.45
1:A:157:GLY:H	1:A:166:PRO:HB3	1.80	0.45
1:A:173:PRO:O	1:A:202:ASP:CA	2.62	0.45
1:B:44:LEU:CG	1:B:199:ILE:HD11	2.43	0.45
2:C:282:GLY:O	2:C:283:VAL:HG23	2.17	0.45
2:C:299:LYS:O	2:C:299:LYS:CG	2.64	0.45
2:C:410:ILE:HG21	2:C:468:ARG:HH22	1.81	0.45
2:C:576:ALA:HB1	2:C:577:PRO:HD2	1.99	0.45
2:C:670:GLN:OE1	2:C:699:PHE:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:764:GLU:N	2:C:764:GLU:CD	2.75	0.45
2:C:1035:MET:HB3	3:D:707:THR:HB	1.98	0.45
2:C:1078:GLU:CD	4:E:32:ARG:HH12	2.25	0.45
3:D:77:ALA:C	3:D:79:GLU:H	2.25	0.45
3:D:695:ILE:HD13	3:D:718:PRO:HB2	1.98	0.45
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.98	0.45
3:D:957:PRO:HG3	3:D:1007:VAL:CA	2.47	0.45
3:D:1456:LYS:O	3:D:1457:ASP:C	2.58	0.45
1:A:23:PHE:CZ	1:A:207:PRO:HB2	2.49	0.45
1:A:38:ASN:O	1:A:39:PRO:C	2.60	0.45
1:A:195:LEU:HD22	1:A:197:LEU:HD22	1.99	0.45
1:B:118:ALA:O	1:B:119:ASP:CG	2.60	0.45
2:C:31:GLN:O	2:C:32:ALA:C	2.60	0.45
2:C:202:TYR:CE1	2:C:304:LEU:HD13	2.52	0.45
2:C:246:ASP:O	2:C:248:PRO:HD3	2.17	0.45
2:C:545:ASN:O	2:C:547:ILE:N	2.49	0.45
2:C:854:PRO:C	2:C:856:GLU:N	2.74	0.45
2:C:884:GLN:HG3	2:C:885:ILE:HD12	1.98	0.45
3:D:511:TRP:CD1	3:D:511:TRP:N	2.84	0.45
3:D:710:ARG:NH1	3:D:768:ASN:HD21	2.15	0.45
3:D:901:GLN:O	3:D:902:MET:C	2.60	0.45
3:D:924:MET:N	4:E:7:ASP:OD2	2.50	0.45
3:D:1011:PHE:C	3:D:1013:GLU:N	2.73	0.45
3:D:1197:ARG:O	3:D:1198:TYR:C	2.60	0.45
3:D:1204:CYS:C	3:D:1206:GLY:N	2.71	0.45
1:A:225:PHE:CD2	1:B:11:PHE:CE1	3.05	0.45
1:B:188:GLN:HG2	3:D:688:TRP:HD1	1.77	0.45
2:C:143:SER:OG	2:C:330:ASN:HA	2.17	0.45
2:C:150:PRO:HD3	2:C:321:GLU:HB3	1.98	0.45
2:C:163:ILE:CG2	2:C:169:GLY:HA3	2.45	0.45
2:C:405:ARG:NH1	2:C:566:THR:OG1	2.48	0.45
2:C:491:GLU:HA	2:C:531:PHE:CA	2.21	0.45
2:C:491:GLU:O	2:C:510:THR:N	2.43	0.45
2:C:531:PHE:O	2:C:532:MET:CB	2.60	0.45
2:C:537:LYS:O	2:C:540:PHE:N	2.48	0.45
2:C:563:ASN:O	2:C:564:MET:C	2.60	0.45
2:C:674:VAL:HG21	2:C:871:LEU:HB2	1.99	0.45
2:C:778:PHE:O	2:C:780:GLU:N	2.50	0.45
2:C:840:ALA:CB	2:C:846:LYS:HA	2.47	0.45
2:C:944:LEU:O	2:C:946:ARG:N	2.50	0.45
3:D:778:LEU:HD12	3:D:778:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:907:GLU:HG3	3:D:911:LEU:HD13	1.97	0.45
3:D:924:MET:O	3:D:927:THR:N	2.49	0.45
3:D:983:LEU:HD23	3:D:983:LEU:HA	1.73	0.45
3:D:989:TYR:C	3:D:991:GLN:N	2.75	0.45
3:D:1083:ASP:O	3:D:1086:LEU:CB	2.62	0.45
3:D:1283:ILE:HD13	3:D:1312:LEU:CD2	2.47	0.45
3:D:1311:LEU:H	3:D:1311:LEU:CD1	2.29	0.45
3:D:1369:GLU:O	3:D:1370:ILE:C	2.60	0.45
3:D:1435:LEU:HD21	3:D:1468:LEU:CD2	2.47	0.45
3:D:1463:LYS:HA	3:D:1466:VAL:HB	1.99	0.45
1:A:94:MET:HE1	1:A:119:ASP:HB2	1.96	0.44
1:A:178:ALA:HB2	2:C:863:ASP:O	2.17	0.44
1:B:19:HIS:HA	1:B:207:PRO:HG3	1.98	0.44
1:B:80:LEU:HD22	3:D:839:LEU:CB	2.48	0.44
2:C:292:ARG:C	2:C:294:GLU:N	2.74	0.44
2:C:874:LEU:HD12	2:C:874:LEU:HA	1.66	0.44
2:C:1008:ARG:HH22	2:C:1020:PRO:HA	1.82	0.44
2:C:1105:LYS:C	2:C:1107:ASN:H	2.24	0.44
3:D:638:LYS:O	3:D:639:LEU:O	2.34	0.44
3:D:905:PRO:CG	3:D:906:GLN:N	2.80	0.44
3:D:1084:THR:C	3:D:1086:LEU:N	2.69	0.44
3:D:1478:SER:O	3:D:1481:VAL:N	2.45	0.44
1:B:99:LEU:O	1:B:141:GLU:HA	2.17	0.44
1:B:111:ALA:HA	1:B:114:PHE:CE1	2.52	0.44
2:C:30:LEU:HD13	2:C:118:LEU:HD11	1.98	0.44
2:C:45:GLN:O	2:C:46:ALA:C	2.60	0.44
2:C:378:LEU:O	2:C:382:LEU:HB2	2.17	0.44
2:C:520:GLU:O	2:C:522:VAL:N	2.49	0.44
2:C:588:VAL:HG21	2:C:666:LEU:HA	1.99	0.44
2:C:641:PRO:HA	2:C:656:ALA:CB	2.47	0.44
2:C:677:MET:H	2:C:873:PRO:HD3	1.82	0.44
2:C:728:HIS:C	2:C:730:SER:H	2.24	0.44
2:C:897:LEU:O	2:C:899:GLN:HG3	2.17	0.44
2:C:1104:GLU:HA	3:D:6:ARG:HG3	1.99	0.44
3:D:890:VAL:HG13	3:D:926:LYS:CE	2.45	0.44
3:D:1007:VAL:HG11	3:D:1040:GLY:HA3	2.00	0.44
3:D:1043:GLY:C	3:D:1057:VAL:HG23	2.42	0.44
3:D:1094:LEU:HA	3:D:1094:LEU:HD12	1.63	0.44
3:D:1238:MET:O	3:D:1238:MET:HE3	2.18	0.44
3:D:1344:VAL:HG11	3:D:1421:LEU:HD11	1.99	0.44
4:E:13:VAL:HB	4:E:18:ARG:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:HIS:C	1:A:20:TYR:O	2.59	0.44
1:A:111:ALA:N	1:A:129:ILE:HG12	2.31	0.44
2:C:182:VAL:HG12	2:C:193:LEU:CB	2.48	0.44
2:C:440:PRO:HD3	2:C:455:LEU:HA	1.96	0.44
2:C:493:ARG:NH2	3:D:1069:GLU:OE2	2.50	0.44
2:C:856:GLU:C	2:C:857:ASP:O	2.59	0.44
2:C:1045:ALA:O	2:C:1046:ALA:C	2.61	0.44
3:D:84:ILE:O	3:D:85:VAL:CB	2.65	0.44
3:D:792:ILE:N	3:D:792:ILE:CD1	2.79	0.44
3:D:948:THR:O	3:D:1020:LEU:CB	2.58	0.44
3:D:1067:VAL:C	3:D:1069:GLU:H	2.25	0.44
3:D:1400:VAL:O	3:D:1400:VAL:HG12	2.17	0.44
4:E:4:PRO:CG	4:E:66:LYS:HE2	2.47	0.44
1:A:26:GLU:HB3	1:A:27:PRO:HD2	1.88	0.44
1:A:74:ASP:OD2	2:C:627:ARG:NH2	2.50	0.44
1:A:185:ARG:NH2	1:A:194:LYS:CE	2.80	0.44
1:B:36:LEU:O	1:B:37:GLY:C	2.60	0.44
1:B:112:VAL:O	1:B:113:ASP:C	2.60	0.44
2:C:103:LYS:HD3	2:C:103:LYS:HA	1.85	0.44
2:C:394:PHE:HB2	5:C:1640:RFP:O8	2.18	0.44
2:C:407:LYS:C	2:C:409:ARG:N	2.75	0.44
2:C:413:LEU:HD11	2:C:448:ASN:OD1	2.17	0.44
2:C:722:ILE:HD13	2:C:821:GLU:OE1	2.17	0.44
2:C:729:LEU:CB	2:C:734:LEU:HD21	2.48	0.44
2:C:754:ILE:HD13	2:C:791:ARG:NE	2.33	0.44
2:C:1070:ILE:N	2:C:1070:ILE:HD12	2.32	0.44
2:C:1112:PHE:C	2:C:1114:GLY:N	2.73	0.44
3:D:43(U):UNK:O	3:D:44(U):UNK:CB	2.66	0.44
3:D:490:ALA:O	3:D:491:LYS:C	2.60	0.44
3:D:947:ILE:HA	3:D:1020:LEU:HD13	1.99	0.44
3:D:1133:ARG:HG3	3:D:1134:LEU:N	2.31	0.44
3:D:1172:HIS:O	3:D:1173:PHE:C	2.61	0.44
3:D:1306:PRO:O	3:D:1307:LYS:C	2.61	0.44
1:A:82:LEU:HD23	1:A:129:ILE:HD12	1.98	0.44
1:A:224:TYR:C	1:A:226:ALA:H	2.25	0.44
1:B:169:ALA:HB1	1:B:171:PHE:CE1	2.52	0.44
2:C:8:ARG:HB3	2:C:494:TYR:OH	2.18	0.44
2:C:9:ILE:O	2:C:10:ARG:HB3	2.18	0.44
2:C:15:LEU:HD21	2:C:461:VAL:HG23	1.94	0.44
2:C:73:ILE:CD1	2:C:94:LEU:HD13	2.48	0.44
2:C:79:SER:O	2:C:82:GLU:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:MET:HA	2:C:126:SER:O	2.17	0.44
2:C:143:SER:O	2:C:144:PRO:C	2.61	0.44
2:C:202:TYR:CB	2:C:207:LEU:HD13	2.47	0.44
2:C:267:TYR:HD1	2:C:273:GLY:HA3	1.81	0.44
2:C:328:LEU:HB3	2:C:467:ILE:HG21	1.98	0.44
2:C:341:ALA:O	2:C:344:PHE:N	2.45	0.44
2:C:445:GLU:HG3	5:C:1640:RFP:C30	2.47	0.44
2:C:605:LYS:HA	2:C:612:ALA:N	2.30	0.44
2:C:648:ARG:HH11	2:C:648:ARG:CG	2.27	0.44
2:C:669:GLY:HA3	2:C:995:MET:HA	1.98	0.44
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.52	0.44
3:D:98:PRO:O	3:D:514:LEU:HD13	2.18	0.44
3:D:106:LYS:O	3:D:107:ASP:C	2.60	0.44
3:D:633:VAL:CG2	3:D:634:GLY:N	2.80	0.44
3:D:853:VAL:HG21	3:D:877:PRO:HB3	1.99	0.44
3:D:864:VAL:CG1	3:D:874:GLU:O	2.66	0.44
3:D:984:THR:O	3:D:988:ARG:N	2.48	0.44
3:D:1011:PHE:C	3:D:1013:GLU:H	2.25	0.44
3:D:1047:LYS:CA	3:D:1053:PHE:CE1	2.92	0.44
3:D:1461:GLY:N	3:D:1464:GLU:OE1	2.47	0.44
4:E:22:VAL:HG21	4:E:75:PHE:CD2	2.52	0.44
1:A:109:VAL:O	1:A:110:ARG:C	2.61	0.44
1:A:221:HIS:HA	1:A:224:TYR:CE2	2.52	0.44
2:C:46:ALA:O	2:C:47:ALA:C	2.61	0.44
2:C:416:GLY:C	2:C:419:THR:OG1	2.61	0.44
2:C:527:GLU:O	2:C:529:VAL:N	2.50	0.44
2:C:569:VAL:HA	2:C:570:PRO:HD2	1.77	0.44
2:C:605:LYS:CG	2:C:606:VAL:H	2.30	0.44
2:C:606:VAL:O	2:C:607:ASP:HB2	2.18	0.44
2:C:713:ARG:HH12	2:C:816:LYS:CG	2.31	0.44
2:C:895:TYR:HD2	2:C:896:PHE:CE1	2.36	0.44
3:D:629:SER:HB3	3:D:726:ILE:CD1	2.47	0.44
3:D:641:GLN:HB3	3:D:719:VAL:CG2	2.46	0.44
3:D:776:GLU:HB3	3:D:777:PRO:HD2	1.98	0.44
3:D:879:ARG:NH1	3:D:904:VAL:HG13	2.32	0.44
3:D:911:LEU:HD12	3:D:911:LEU:HA	1.85	0.44
3:D:976:GLN:C	3:D:978:TYR:N	2.71	0.44
3:D:1069:GLU:HG3	3:D:1072:ILE:CG1	2.48	0.44
3:D:1093:TYR:HE2	3:D:1097:LYS:CE	2.31	0.44
3:D:1207:TYR:C	3:D:1215:VAL:HG23	2.43	0.44
3:D:1304:LYS:N	3:D:1304:LYS:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASP:O	1:A:19:HIS:CB	2.66	0.44
1:A:201:THR:HG22	1:A:202:ASP:N	2.31	0.44
1:A:225:PHE:HD2	1:B:11:PHE:CE1	2.36	0.44
1:B:52:ALA:O	1:B:53:VAL:C	2.61	0.44
1:B:160:ASP:O	1:B:162:ILE:N	2.50	0.44
2:C:12:VAL:CG1	2:C:13:ILE:N	2.62	0.44
2:C:141:HIS:CE1	2:C:334:ARG:HG3	2.52	0.44
2:C:236:VAL:CG2	2:C:250:LYS:HA	2.47	0.44
2:C:399:ASN:HD21	2:C:401:LEU:CB	2.27	0.44
2:C:488:ALA:O	2:C:490:GLU:N	2.51	0.44
2:C:584:GLU:H	2:C:584:GLU:HG3	1.31	0.44
2:C:613:VAL:H	2:C:621:VAL:HA	1.83	0.44
2:C:628:TYR:HE2	2:C:703:ILE:HD13	1.81	0.44
2:C:688:ILE:CG2	2:C:869:VAL:HG23	2.48	0.44
2:C:705:ILE:HA	2:C:828:ALA:HA	2.00	0.44
2:C:714:ASP:O	2:C:715:THR:O	2.35	0.44
2:C:778:PHE:O	2:C:779:GLY:C	2.61	0.44
2:C:835:VAL:HG13	2:C:850:ALA:O	2.18	0.44
3:D:143:ASP:O	3:D:145:VAL:N	2.51	0.44
3:D:772:PRO:CG	3:D:778:LEU:HD23	2.47	0.44
3:D:791:TYR:HE1	3:D:1023:MET:HG3	1.82	0.44
3:D:906:GLN:O	3:D:907:GLU:HB2	2.18	0.44
3:D:1047:LYS:HA	3:D:1053:PHE:CZ	2.49	0.44
3:D:1068:LEU:C	3:D:1070:TYR:N	2.70	0.44
3:D:1114:THR:HA	3:D:1189:ARG:HH11	1.83	0.44
3:D:1125:MET:HG2	3:D:1126:ASP:H	1.81	0.44
3:D:1231:GLU:O	3:D:1233:GLY:N	2.51	0.44
3:D:1427:SER:C	3:D:1429:LEU:H	2.25	0.44
1:A:86:VAL:HG13	1:A:123:MET:HB3	1.99	0.44
1:B:188:GLN:NE2	1:B:188:GLN:O	2.50	0.44
2:C:598:GLU:HB3	2:C:599:GLU:H	1.59	0.44
2:C:925:TYR:CE2	2:C:972:VAL:HG21	2.53	0.44
2:C:944:LEU:C	2:C:946:ARG:N	2.71	0.44
2:C:1015:LEU:C	2:C:1015:LEU:HD12	2.43	0.44
3:D:688:TRP:HA	3:D:688:TRP:HE3	1.82	0.44
3:D:1017:PHE:HA	3:D:1023:MET:HE1	2.00	0.44
3:D:1236:LEU:HD12	3:D:1256:LEU:CD1	2.47	0.44
1:B:210:ALA:O	1:B:211:LEU:C	2.61	0.44
2:C:11:GLU:OE1	2:C:473:ARG:CD	2.66	0.44
2:C:11:GLU:OE1	2:C:473:ARG:CG	2.66	0.44
2:C:79:SER:O	2:C:80:GLN:C	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:172:ILE:HG22	2:C:173:ASP:N	2.32	0.44
2:C:278:GLU:HA	2:C:283:VAL:HA	1.99	0.44
2:C:539:VAL:C	2:C:540:PHE:CD1	2.96	0.44
2:C:881:ASN:CG	3:D:1034:GLN:NE2	2.76	0.44
2:C:1038:TRP:CZ2	3:D:1096:ARG:HA	2.52	0.44
2:C:1088:LEU:HD23	3:D:1468:LEU:CD2	2.48	0.44
3:D:628:ARG:O	3:D:629:SER:HB2	2.18	0.44
3:D:674:ARG:C	3:D:674:ARG:HD3	2.42	0.44
3:D:896:ALA:HA	3:D:899:LEU:HD22	2.00	0.44
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.45	0.44
3:D:1141:GLU:CD	3:D:1168:LEU:CD1	2.90	0.44
3:D:1151:ARG:O	3:D:1152:GLU:C	2.61	0.44
3:D:1220:ALA:O	3:D:1224:VAL:HG23	2.18	0.44
3:D:1252:ILE:HG21	3:D:1261:GLU:OE1	2.18	0.44
4:E:3:GLU:HB3	4:E:4:PRO:HD2	1.99	0.44
1:A:100:ILE:HG22	1:A:101:LEU:H	1.82	0.43
1:B:59:GLU:OE1	1:B:60:ASP:N	2.50	0.43
1:B:95:ALA:O	1:B:96:SER:CB	2.60	0.43
2:C:64:LEU:N	2:C:101:ILE:O	2.51	0.43
2:C:100:LEU:HD11	2:C:369:PRO:CD	2.46	0.43
2:C:104:ASP:OD1	2:C:104:ASP:N	2.50	0.43
2:C:343:GLN:HG2	2:C:385:PHE:HB2	2.00	0.43
2:C:710:ILE:N	2:C:710:ILE:CD1	2.74	0.43
2:C:738:ASP:HA	2:C:743:VAL:HA	2.00	0.43
2:C:771:GLU:O	2:C:772:ARG:C	2.61	0.43
2:C:794:PRO:HG2	2:C:1027:PHE:CB	2.48	0.43
2:C:881:ASN:HB2	3:D:1061:PHE:HE2	1.81	0.43
2:C:976:ASP:C	2:C:978:ARG:N	2.76	0.43
2:C:992:MET:HE3	2:C:992:MET:HB2	1.92	0.43
3:D:564:GLU:HG3	3:D:568:ARG:NE	2.29	0.43
3:D:606:ILE:HD12	3:D:606:ILE:N	2.28	0.43
3:D:658:LEU:O	3:D:661:MET:N	2.51	0.43
1:A:41:ARG:NH1	1:A:42:ARG:N	2.66	0.43
1:B:151:VAL:O	1:B:169:ALA:N	2.46	0.43
2:C:54:ILE:HG13	2:C:55:GLU:O	2.18	0.43
2:C:95:TYR:CD1	2:C:112:GLU:OE1	2.71	0.43
2:C:233:GLU:CD	2:C:237:ARG:HE	2.25	0.43
2:C:251:ASP:C	2:C:253:ALA:H	2.26	0.43
2:C:443:THR:O	2:C:444:PRO:O	2.36	0.43
2:C:626:ARG:CZ	2:C:637:PHE:CZ	3.00	0.43
2:C:760:SER:OG	2:C:762:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1042:ALA:CB	3:D:1227:GLU:OE1	2.66	0.43
5:C:1640:RFP:N1	5:C:1640:RFP:N2	2.65	0.43
3:D:564:GLU:O	3:D:567:ILE:HG22	2.19	0.43
3:D:851:LEU:HD12	3:D:851:LEU:O	2.18	0.43
3:D:899:LEU:O	3:D:900:ILE:CG1	2.53	0.43
3:D:905:PRO:CG	3:D:906:GLN:H	2.31	0.43
3:D:931:LEU:HD13	3:D:931:LEU:HA	1.84	0.43
3:D:969:ARG:CZ	3:D:970:LYS:HE3	2.47	0.43
3:D:1011:PHE:CE2	3:D:1022:VAL:CG1	3.01	0.43
3:D:1192:LEU:HD21	3:D:1369:GLU:HA	2.00	0.43
1:A:184:THR:C	1:A:185:ARG:HD3	2.43	0.43
1:B:187:GLY:O	1:B:188:GLN:C	2.60	0.43
2:C:85:GLU:O	2:C:806:LEU:HD11	2.18	0.43
2:C:291:VAL:HB	2:C:299:LYS:O	2.19	0.43
2:C:297:GLU:C	2:C:298:PHE:HD1	2.25	0.43
2:C:348:LEU:C	2:C:350:ARG:N	2.71	0.43
2:C:380:ALA:O	2:C:384:GLU:N	2.38	0.43
2:C:602:GLU:C	2:C:603:VAL:HG22	2.43	0.43
2:C:605:LYS:HG2	2:C:606:VAL:N	2.33	0.43
2:C:1034:GLU:HG3	2:C:1035:MET:N	2.33	0.43
3:D:513:ILE:CG2	3:D:514:LEU:N	2.81	0.43
3:D:770:LEU:HD23	3:D:927:THR:CG2	2.49	0.43
3:D:805:ALA:O	3:D:806:PHE:CB	2.66	0.43
3:D:808:THR:O	3:D:809:PRO:O	2.36	0.43
3:D:816:TYR:HA	3:D:832:ARG:NH2	2.33	0.43
3:D:899:LEU:N	3:D:899:LEU:CD1	2.78	0.43
3:D:1071:PHE:O	3:D:1075:HIS:HD2	2.01	0.43
3:D:1253:THR:HG21	3:D:1327:ARG:HG2	2.00	0.43
3:D:1261:GLU:OE2	3:D:1268:PRO:HB3	2.18	0.43
4:E:40:LEU:HA	4:E:44:GLU:HG3	2.00	0.43
1:A:76:VAL:O	1:A:77:GLU:C	2.62	0.43
1:A:165:ILE:O	1:A:165:ILE:CG1	2.60	0.43
1:A:222:LEU:HD21	1:B:218:LEU:HD23	2.00	0.43
1:B:11:PHE:HZ	1:B:211:LEU:HD21	1.83	0.43
2:C:73:ILE:HD12	2:C:73:ILE:N	2.32	0.43
2:C:203:ASP:H	2:C:207:LEU:HB2	1.83	0.43
2:C:761:PHE:O	2:C:762:LYS:C	2.62	0.43
2:C:768:SER:C	2:C:769:PRO:O	2.61	0.43
3:D:785:ILE:HD13	3:D:935:LYS:HA	2.00	0.43
3:D:1292:VAL:CG2	3:D:1305:LEU:HD23	2.49	0.43
1:A:74:ASP:O	1:A:75:VAL:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:O	1:A:218:LEU:HD12	2.18	0.43
1:B:214:ALA:HA	1:B:217:ILE:HG13	1.99	0.43
2:C:56:GLU:N	2:C:56:GLU:CD	2.76	0.43
2:C:67:ASP:N	2:C:67:ASP:OD1	2.50	0.43
2:C:220:GLY:C	2:C:222:LEU:H	2.26	0.43
2:C:236:VAL:CG1	2:C:248:PRO:O	2.67	0.43
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.97	0.43
2:C:596:TYR:O	2:C:596:TYR:CD1	2.71	0.43
2:C:972:VAL:O	2:C:973:VAL:C	2.61	0.43
2:C:1035:MET:HB2	2:C:1036:GLU:OE2	2.17	0.43
3:D:100:ALA:HA	3:D:575:GLN:CD	2.43	0.43
3:D:567:ILE:CA	3:D:570:GLU:HB2	2.49	0.43
3:D:935:LYS:HG2	3:D:939:PHE:HD1	1.83	0.43
3:D:1011:PHE:O	3:D:1013:GLU:N	2.51	0.43
3:D:1175:ILE:O	3:D:1179:GLU:HG3	2.18	0.43
3:D:1407:LEU:C	3:D:1409:ALA:N	2.75	0.43
3:D:1464:GLU:C	3:D:1466:VAL:N	2.75	0.43
4:E:12:MET:HE1	4:E:68:LEU:HG	2.01	0.43
1:B:119:ASP:C	1:B:120:VAL:CG2	2.91	0.43
1:B:133:GLU:HG2	1:B:134:GLU:N	2.33	0.43
2:C:306:THR:HG22	2:C:307:LEU:N	2.34	0.43
2:C:398:THR:O	2:C:635:THR:HG21	2.19	0.43
2:C:428:ARG:O	2:C:429:ASP:HB2	2.18	0.43
2:C:491:GLU:CA	2:C:531:PHE:HA	2.21	0.43
2:C:539:VAL:HB	2:C:540:PHE:CD1	2.53	0.43
2:C:568:ALA:O	2:C:569:VAL:CG1	2.66	0.43
2:C:595:LEU:HD21	2:C:623:HIS:CB	2.47	0.43
2:C:697:ARG:O	2:C:698:ASP:C	2.61	0.43
2:C:795:GLY:C	2:C:797:GLY:H	2.27	0.43
3:D:669:ASN:O	3:D:672:ALA:N	2.50	0.43
3:D:700:VAL:HG13	3:D:748:HIS:O	2.18	0.43
3:D:906:GLN:N	3:D:906:GLN:CD	2.77	0.43
3:D:908:LYS:HG3	3:D:1027:GLY:C	2.43	0.43
3:D:1057:VAL:HG13	3:D:1067:VAL:HG11	2.01	0.43
3:D:1102:ALA:C	3:D:1103:HIS:O	2.59	0.43
3:D:1250:THR:HG22	3:D:1251:ASP:O	2.18	0.43
3:D:1306:PRO:O	3:D:1308:ASP:N	2.52	0.43
3:D:1323:GLN:H	3:D:1324:PRO:HD2	1.83	0.43
1:A:28:LEU:O	1:A:192:LEU:HB3	2.19	0.43
1:B:118:ALA:C	1:B:119:ASP:OD1	2.62	0.43
1:B:188:GLN:HG3	3:D:688:TRP:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:99:GLN:OE1	2:C:109:LYS:HE3	2.18	0.43
2:C:369:PRO:C	2:C:371:LYS:N	2.76	0.43
2:C:399:ASN:ND2	2:C:399:ASN:O	2.44	0.43
2:C:467:ILE:HG22	2:C:484:VAL:CG2	2.48	0.43
2:C:606:VAL:HG22	2:C:606:VAL:O	2.19	0.43
2:C:750:LYS:HG2	2:C:753:ASP:CG	2.43	0.43
2:C:754:ILE:O	2:C:754:ILE:HG22	2.18	0.43
3:D:465:LEU:HD22	3:D:512:MET:HE1	2.00	0.43
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.54	0.43
3:D:806:PHE:N	3:D:827:ILE:HA	2.17	0.43
3:D:836:VAL:CB	3:D:858:LEU:HD21	2.49	0.43
3:D:853:VAL:O	3:D:854:ALA:O	2.35	0.43
3:D:885:ILE:HG12	3:D:937:TYR:CD2	2.54	0.43
3:D:1059:SER:C	3:D:1061:PHE:H	2.24	0.43
3:D:1258:ARG:HG3	3:D:1258:ARG:NH1	2.33	0.43
3:D:1349:VAL:O	3:D:1350:ASP:C	2.62	0.43
3:D:1480:PHE:HE2	4:E:15:SER:HB2	1.82	0.43
3:D:1481:VAL:HG12	4:E:21:VAL:HG21	1.98	0.43
1:A:71:VAL:HG22	1:A:132:LEU:HB3	2.00	0.43
1:B:61:VAL:O	1:B:62:LEU:O	2.36	0.43
1:B:177:VAL:HG13	1:B:199:ILE:CD1	2.49	0.43
2:C:15:LEU:CD1	2:C:461:VAL:HG21	2.37	0.43
2:C:26:TYR:CZ	2:C:340:MET:HE2	2.53	0.43
2:C:35:PRO:C	2:C:37:GLU:N	2.73	0.43
2:C:84:ARG:HE	2:C:128:ILE:HG12	1.84	0.43
2:C:89:THR:HA	2:C:130:ASN:H	1.84	0.43
2:C:163:ILE:CG2	2:C:265:LYS:HD2	2.48	0.43
2:C:413:LEU:CD2	2:C:451:LEU:HD13	2.44	0.43
2:C:769:PRO:HG2	2:C:770:GLU:HG3	2.00	0.43
2:C:788:THR:O	2:C:788:THR:HG23	2.19	0.43
2:C:1095:LEU:O	2:C:1096:ALA:HB3	2.18	0.43
3:D:110:SER:O	3:D:112:ILE:N	2.48	0.43
3:D:491:LYS:HE2	3:D:495:ARG:HH21	1.84	0.43
3:D:550:ARG:C	3:D:552:ASN:N	2.76	0.43
3:D:1103:HIS:O	3:D:1105:ILE:HG12	2.19	0.43
3:D:1331:ASP:C	3:D:1333:HIS:H	2.27	0.43
4:E:38:THR:HG23	4:E:63:TRP:CZ3	2.53	0.43
1:A:19:HIS:O	1:A:20:TYR:C	2.61	0.43
1:A:122:ILE:C	1:A:124:ASN:N	2.75	0.43
1:B:70:GLY:O	1:B:132:LEU:HB2	2.18	0.43
1:B:173:PRO:HA	1:B:203:GLY:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:VAL:O	1:B:174:VAL:HG23	2.19	0.43
2:C:5:ARG:NH2	2:C:10:ARG:NH1	2.66	0.43
2:C:110:GLU:HB2	2:C:369:PRO:HB2	2.00	0.43
2:C:218:VAL:O	2:C:220:GLY:N	2.52	0.43
2:C:254:LEU:O	2:C:254:LEU:HD12	2.19	0.43
2:C:260:LEU:HD23	2:C:261:LEU:CB	2.45	0.43
2:C:336:VAL:O	2:C:337:GLY:C	2.62	0.43
2:C:397:GLU:HB2	2:C:632:ASN:HD22	1.83	0.43
2:C:536:PRO:O	2:C:537:LYS:C	2.61	0.43
2:C:586:ARG:C	2:C:588:VAL:N	2.76	0.43
2:C:648:ARG:CG	2:C:648:ARG:NH1	2.81	0.43
2:C:714:ASP:O	2:C:715:THR:C	2.62	0.43
2:C:730:SER:CA	2:C:734:LEU:HD11	2.44	0.43
2:C:796:GLU:HA	3:D:681:ARG:NH2	2.33	0.43
2:C:923:ASN:C	2:C:924:LEU:HD23	2.43	0.43
2:C:974:LEU:HD23	2:C:987:ILE:HG21	2.01	0.43
3:D:15:PRO:O	3:D:19:ARG:HG3	2.19	0.43
3:D:483:HIS:N	3:D:484:PRO:CD	2.54	0.43
3:D:711:LEU:HD21	3:D:768:ASN:O	2.19	0.43
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.54	0.43
3:D:1079:LYS:C	3:D:1081:GLY:N	2.73	0.43
4:E:28:GLN:O	4:E:29:GLN:HB2	2.19	0.43
1:A:110:ARG:O	1:A:111:ALA:C	2.61	0.43
1:B:40:LEU:O	1:B:44:LEU:HD22	2.18	0.43
1:B:41:ARG:HA	1:B:177:VAL:HG11	2.01	0.43
2:C:148:PHE:HA	2:C:159:ILE:HA	2.01	0.43
2:C:182:VAL:HG11	2:C:307:LEU:HD11	2.01	0.43
2:C:205:GLU:OE2	2:C:209:ARG:HD2	2.19	0.43
2:C:424:GLY:O	2:C:427:VAL:HG23	2.18	0.43
2:C:575:GLN:C	2:C:576:ALA:O	2.61	0.43
2:C:625:LEU:O	2:C:626:ARG:C	2.62	0.43
2:C:710:ILE:HD12	2:C:710:ILE:H	1.83	0.43
2:C:954:SER:H	2:C:965:GLU:CD	2.26	0.43
3:D:658:LEU:O	3:D:659:LYS:C	2.62	0.43
3:D:759:ALA:HA	3:D:763:MET:CG	2.47	0.43
3:D:793:THR:CA	3:D:879:ARG:HH12	2.31	0.43
3:D:901:GLN:O	3:D:903:ASP:N	2.52	0.43
3:D:971:LEU:C	3:D:973:GLN:N	2.75	0.43
3:D:1114:THR:CB	3:D:1189:ARG:NH1	2.82	0.43
3:D:1122:LEU:CD1	3:D:1186:VAL:HG23	2.49	0.43
3:D:1154:GLU:O	3:D:1155:ALA:CB	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HG	1:A:127:LEU:O	2.19	0.42
1:A:162:ILE:CG2	1:A:163:ASN:H	2.30	0.42
2:C:63:GLY:O	2:C:64:LEU:HB2	2.19	0.42
2:C:211:LEU:HG	2:C:212:SER:N	2.33	0.42
2:C:221:LEU:O	2:C:221:LEU:HG	2.18	0.42
2:C:310:LEU:O	2:C:313:LEU:N	2.44	0.42
2:C:442:GLU:OE1	2:C:558:ALA:HB3	2.18	0.42
2:C:549:PHE:CE2	2:C:886:LEU:HB3	2.54	0.42
2:C:679:PHE:O	2:C:680:ASP:C	2.61	0.42
2:C:754:ILE:CD1	2:C:791:ARG:NE	2.80	0.42
2:C:953:VAL:HG12	2:C:954:SER:N	2.33	0.42
2:C:1112:PHE:O	2:C:1114:GLY:N	2.52	0.42
3:D:498:VAL:O	3:D:501:ALA:HB3	2.19	0.42
3:D:694:VAL:O	3:D:696:HIS:N	2.52	0.42
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.52	0.42
3:D:770:LEU:HD23	3:D:927:THR:HG21	2.00	0.42
3:D:772:PRO:CD	3:D:778:LEU:N	2.81	0.42
3:D:957:PRO:HD3	3:D:1007:VAL:HG23	2.01	0.42
3:D:1286:GLY:O	3:D:1287:GLU:C	2.61	0.42
4:E:13:VAL:HG11	4:E:19:LEU:N	2.34	0.42
1:A:36:LEU:O	1:A:40:LEU:HG	2.19	0.42
1:A:118:ALA:O	1:A:120:VAL:N	2.48	0.42
1:B:5:LYS:O	1:B:6:LEU:C	2.61	0.42
1:B:34:VAL:O	1:B:36:LEU:N	2.52	0.42
1:B:76:VAL:O	1:B:79:ILE:HB	2.19	0.42
2:C:79:SER:OG	2:C:82:GLU:CB	2.64	0.42
2:C:164:PRO:CG	2:C:168:ARG:HG2	2.49	0.42
2:C:341:ALA:CB	2:C:345:ARG:HH12	2.32	0.42
2:C:421:GLU:C	2:C:423:ALA:N	2.77	0.42
2:C:676:ILE:HD12	2:C:676:ILE:N	2.33	0.42
2:C:739:GLU:O	2:C:739:GLU:HG3	2.19	0.42
2:C:922:PHE:O	2:C:926:PHE:N	2.51	0.42
2:C:1069:ALA:O	2:C:1075:ASP:O	2.37	0.42
3:D:707:THR:HG23	3:D:712:GLY:HA3	2.00	0.42
3:D:752:SER:O	3:D:755:ALA:N	2.47	0.42
3:D:930:LEU:HD12	3:D:934:LEU:HG	2.01	0.42
3:D:1062:ARG:C	3:D:1062:ARG:CD	2.90	0.42
3:D:1149:LEU:HD23	3:D:1188:VAL:HG23	2.00	0.42
3:D:1151:ARG:HA	3:D:1162:GLU:HG3	2.01	0.42
3:D:1179:GLU:C	3:D:1181:GLY:N	2.74	0.42
3:D:1252:ILE:HD12	3:D:1269:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1275:SER:O	3:D:1319:VAL:HA	2.19	0.42
3:D:1303:TYR:O	3:D:1305:LEU:N	2.52	0.42
3:D:1462:LEU:C	3:D:1464:GLU:H	2.26	0.42
1:A:41:ARG:NE	2:C:860:HIS:CE1	2.85	0.42
1:A:86:VAL:HG13	1:A:86:VAL:O	2.18	0.42
1:B:183:ASP:HA	1:B:192:LEU:O	2.19	0.42
2:C:342:ASP:CA	2:C:345:ARG:HH11	2.32	0.42
2:C:349:ALA:O	2:C:350:ARG:HG3	2.20	0.42
2:C:515:ALA:CB	3:D:1069:GLU:OE2	2.67	0.42
2:C:518:ARG:O	2:C:519:GLY:C	2.62	0.42
2:C:526:PRO:O	2:C:527:GLU:C	2.62	0.42
2:C:574:ALA:O	2:C:669:GLY:O	2.37	0.42
2:C:748:GLU:C	2:C:748:GLU:CD	2.87	0.42
2:C:816:LYS:HA	2:C:817:PRO:HD2	1.88	0.42
2:C:1059:ASP:HA	2:C:1083:GLU:HB2	2.01	0.42
2:C:1071:ILE:HD11	3:D:655:PRO:HB3	2.00	0.42
3:D:540:LEU:HD11	3:D:603:LEU:HD13	2.00	0.42
3:D:583:ASP:OD1	3:D:604:THR:OG1	2.26	0.42
3:D:584:ASN:HB2	3:D:602:SER:HB3	2.01	0.42
3:D:795:VAL:CA	3:D:862:ASP:CB	2.97	0.42
3:D:907:GLU:O	3:D:908:LYS:CB	2.67	0.42
3:D:1004:THR:OG1	3:D:1036:ARG:HB2	2.19	0.42
3:D:1030:GLY:O	3:D:1031:ASN:CB	2.67	0.42
3:D:1194:CYS:SG	3:D:1201:CYS:CB	3.06	0.42
3:D:1326:THR:O	3:D:1327:ARG:CB	2.65	0.42
3:D:1327:ARG:HG3	3:D:1327:ARG:O	2.19	0.42
1:A:41:ARG:HG2	1:A:177:VAL:HG12	1.99	0.42
1:A:63:HIS:HA	1:A:165:ILE:HG22	2.01	0.42
1:B:29:GLU:OE1	1:B:189:ARG:NH1	2.52	0.42
1:B:101:LEU:N	1:B:140:MET:O	2.52	0.42
1:B:109:VAL:HG23	1:B:132:LEU:HD22	2.01	0.42
2:C:32:ALA:C	2:C:34:VAL:H	2.27	0.42
2:C:122:THR:HG22	2:C:123:GLU:H	1.83	0.42
2:C:268:ASP:HB2	2:C:269:LEU:H	1.54	0.42
2:C:342:ASP:HA	2:C:345:ARG:HH11	1.83	0.42
2:C:385:PHE:O	2:C:386:PHE:C	2.62	0.42
2:C:517:ARG:CG	2:C:518:ARG:N	2.82	0.42
2:C:547:ILE:HD12	2:C:550:LEU:HD13	2.00	0.42
2:C:603:VAL:O	2:C:604:VAL:CG2	2.66	0.42
2:C:676:ILE:HD12	2:C:676:ILE:H	1.84	0.42
2:C:959:PRO:O	2:C:960:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:632:VAL:CG1	3:D:633:VAL:N	2.81	0.42
3:D:907:GLU:HB3	3:D:911:LEU:CD2	2.48	0.42
3:D:1114:THR:CA	3:D:1189:ARG:HH11	2.32	0.42
4:E:26:ARG:NH2	4:E:30:LEU:HD13	2.35	0.42
4:E:64:ALA:O	4:E:68:LEU:N	2.52	0.42
1:A:13:ALA:O	1:B:230:ALA:CB	2.68	0.42
1:A:143:ARG:NH1	1:A:145:ASP:OD1	2.52	0.42
1:B:32:PHE:C	1:B:34:VAL:N	2.72	0.42
1:B:73:GLU:HG3	1:B:77:GLU:HG2	2.01	0.42
1:B:202:ASP:O	1:B:204:SER:N	2.52	0.42
2:C:9:ILE:O	2:C:10:ARG:CB	2.68	0.42
2:C:72:ARG:NE	2:C:95:TYR:HE1	2.17	0.42
2:C:113:VAL:O	2:C:114:PHE:C	2.62	0.42
2:C:261:LEU:CD1	2:C:263:ASP:HB3	2.47	0.42
2:C:418:LEU:HG	2:C:418:LEU:O	2.19	0.42
2:C:534:VAL:N	2:C:538:GLN:HE22	2.17	0.42
2:C:549:PHE:CD1	2:C:886:LEU:O	2.71	0.42
2:C:727:PRO:C	2:C:729:LEU:N	2.77	0.42
2:C:923:ASN:N	2:C:924:LEU:HD23	2.35	0.42
3:D:558:LEU:HD21	3:D:567:ILE:CD1	2.49	0.42
3:D:568:ARG:C	3:D:570:GLU:H	2.27	0.42
3:D:609:GLY:HA2	3:D:615:ARG:NE	2.34	0.42
3:D:722:GLU:HB3	3:D:723:GLY:H	1.48	0.42
3:D:819:GLY:O	3:D:820:GLU:C	2.62	0.42
3:D:884:ARG:O	3:D:887:GLY:N	2.52	0.42
3:D:1258:ARG:HG3	3:D:1258:ARG:HH11	1.84	0.42
3:D:1324:PRO:O	3:D:1325:LEU:C	2.62	0.42
3:D:1378:TYR:CD1	3:D:1378:TYR:N	2.88	0.42
3:D:1476:THR:HG22	4:E:21:VAL:HG23	2.00	0.42
1:B:57:TYR:O	1:B:140:MET:HA	2.20	0.42
1:B:206:THR:OG1	1:B:209:GLU:HG3	2.20	0.42
1:B:207:PRO:O	1:B:208:LEU:C	2.63	0.42
2:C:34:VAL:O	2:C:34:VAL:HG12	2.19	0.42
2:C:124:ASP:OD1	2:C:407:LYS:NZ	2.39	0.42
2:C:266:ARG:O	2:C:266:ARG:HG3	2.18	0.42
2:C:446:GLY:C	2:C:448:ASN:H	2.26	0.42
2:C:561:GLY:O	2:C:562:SER:C	2.61	0.42
2:C:573:ARG:HH11	2:C:573:ARG:CG	2.29	0.42
2:C:613:VAL:CG2	2:C:619:ARG:HE	2.31	0.42
2:C:710:ILE:CG1	2:C:790:LEU:HB2	2.48	0.42
2:C:755:LEU:CD1	2:C:756:VAL:HG23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:839:LEU:O	2:C:840:ALA:C	2.62	0.42
2:C:950:LEU:O	3:D:1018:ASN:CG	2.62	0.42
2:C:1051:GLU:OE2	3:D:751:LEU:HB3	2.19	0.42
3:D:713:ILE:HG22	3:D:714:GLN:N	2.35	0.42
3:D:887:GLY:C	3:D:889:ALA:N	2.77	0.42
3:D:935:LYS:HG2	3:D:939:PHE:CD1	2.54	0.42
3:D:1024:ALA:O	3:D:1025:GLN:C	2.61	0.42
3:D:1201:CYS:SG	3:D:1204:CYS:HB2	2.60	0.42
4:E:6:ILE:HG22	4:E:10:PHE:CD1	2.54	0.42
4:E:38:THR:CG2	4:E:40:LEU:H	2.24	0.42
1:A:90:LEU:HD21	1:A:121:GLU:OE2	2.20	0.42
1:A:115:THR:O	1:A:115:THR:CG2	2.67	0.42
1:A:159:LYS:C	1:A:161:ARG:N	2.76	0.42
1:B:129:ILE:O	1:B:130:ALA:CB	2.68	0.42
2:C:194:VAL:HG22	2:C:221:LEU:HD12	2.02	0.42
2:C:208:VAL:HG13	2:C:212:SER:OG	2.20	0.42
2:C:402:SER:O	2:C:403:SER:C	2.63	0.42
2:C:533:ASP:C	2:C:538:GLN:NE2	2.78	0.42
2:C:561:GLY:HA3	2:C:842:ARG:O	2.20	0.42
2:C:592:LEU:HA	2:C:592:LEU:HD23	1.80	0.42
2:C:603:VAL:HB	2:C:604:VAL:H	1.61	0.42
2:C:677:MET:HE1	2:C:983:PHE:CD1	2.54	0.42
2:C:750:LYS:HE2	2:C:753:ASP:OD2	2.18	0.42
2:C:772:ARG:HH11	2:C:776:SER:HB3	1.84	0.42
2:C:1038:TRP:O	2:C:1039:ALA:C	2.62	0.42
2:C:1055:ILE:HD11	2:C:1079:PRO:CG	2.49	0.42
2:C:1067:TYR:CE1	2:C:1071:ILE:HD11	2.55	0.42
3:D:22:SER:C	3:D:24:GLY:N	2.75	0.42
3:D:75:ARG:C	3:D:77:ALA:N	2.77	0.42
3:D:497:GLU:CG	3:D:1389:LEU:HD21	2.50	0.42
3:D:654:LYS:HB3	3:D:655:PRO:CD	2.45	0.42
3:D:729:HIS:CE1	3:D:935:LYS:HD3	2.54	0.42
3:D:795:VAL:CG1	3:D:796:ARG:N	2.83	0.42
3:D:795:VAL:CG1	3:D:864:VAL:CG2	2.92	0.42
3:D:876:SER:O	3:D:879:ARG:N	2.53	0.42
3:D:905:PRO:CD	3:D:906:GLN:H	2.32	0.42
3:D:953:ASP:OD1	3:D:1020:LEU:CB	2.68	0.42
3:D:953:ASP:OD1	3:D:1020:LEU:CG	2.66	0.42
3:D:1068:LEU:C	3:D:1070:TYR:H	2.20	0.42
3:D:1266:ARG:C	3:D:1268:PRO:CD	2.93	0.42
4:E:26:ARG:NH2	4:E:67:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:80:VAL:CB	4:E:81:PRO:CD	2.97	0.42
1:A:56:VAL:CG1	1:A:167:VAL:HG21	2.50	0.42
1:B:100:ILE:HG22	1:B:101:LEU:N	2.35	0.42
1:B:209:GLU:O	1:B:210:ALA:C	2.61	0.42
2:C:32:ALA:O	2:C:34:VAL:N	2.52	0.42
2:C:247:PRO:C	2:C:249:LYS:H	2.28	0.42
2:C:342:ASP:N	2:C:345:ARG:NH1	2.68	0.42
2:C:420:ARG:HD3	2:C:420:ARG:H	1.84	0.42
2:C:446:GLY:C	2:C:448:ASN:N	2.78	0.42
2:C:810:ASP:CG	2:C:811:PRO:HD2	2.42	0.42
2:C:1106:ASP:C	2:C:1108:PRO:CD	2.92	0.42
3:D:106:LYS:O	3:D:110:SER:N	2.53	0.42
3:D:496:LEU:O	3:D:500:ARG:HB2	2.19	0.42
3:D:550:ARG:C	3:D:552:ASN:H	2.26	0.42
3:D:876:SER:O	3:D:879:ARG:HG3	2.20	0.42
3:D:1145:TYR:CD2	3:D:1146:GLY:N	2.80	0.42
3:D:1276:GLU:HG3	3:D:1303:TYR:OH	2.20	0.42
3:D:1402:ALA:C	3:D:1404:ASN:N	2.74	0.42
3:D:1417:TRP:CD1	3:D:1417:TRP:C	2.97	0.42
1:A:25:LEU:HB3	1:A:26:GLU:H	1.61	0.42
1:B:14:THR:O	1:B:15:THR:C	2.61	0.42
1:B:21:GLY:O	1:B:23:PHE:CD2	2.73	0.42
1:B:159:LYS:O	1:B:161:ARG:N	2.40	0.42
2:C:21:ILE:HD11	2:C:455:LEU:CD2	2.50	0.42
2:C:355:VAL:O	2:C:356:ARG:C	2.62	0.42
2:C:433:THR:HG21	3:D:1075:HIS:CD2	2.55	0.42
2:C:471:TYR:O	2:C:472:ARG:HG2	2.20	0.42
2:C:597:ALA:CA	2:C:614:ARG:HH11	2.26	0.42
2:C:874:LEU:CD1	3:D:787:LEU:HD22	2.47	0.42
2:C:885:ILE:HD12	2:C:885:ILE:N	2.34	0.42
2:C:892:LEU:HA	2:C:895:TYR:CB	2.50	0.42
2:C:1025:ALA:HB1	2:C:1026:GLN:NE2	2.35	0.42
3:D:69:GLU:O	3:D:70:ALA:CB	2.68	0.42
3:D:151:GLN:O	3:D:154:THR:N	2.53	0.42
3:D:661:MET:O	3:D:662:GLU:C	2.63	0.42
3:D:732:VAL:HG22	3:D:769:LEU:HD11	2.01	0.42
3:D:879:ARG:CZ	3:D:904:VAL:HG22	2.48	0.42
3:D:964:LEU:O	3:D:965:GLU:HB3	2.20	0.42
3:D:1075:HIS:O	3:D:1076:GLY:C	2.63	0.42
3:D:1094:LEU:O	3:D:1097:LYS:N	2.53	0.42
1:A:27:PRO:HG2	1:A:27:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLY:C	1:B:71:VAL:HG23	2.45	0.42
1:B:138:LEU:HD11	1:B:140:MET:HE2	2.01	0.42
2:C:56:GLU:OE1	2:C:64:LEU:O	2.38	0.42
2:C:148:PHE:CE1	2:C:309:TYR:HD2	2.38	0.42
2:C:252:LYS:HG2	2:C:256:TYR:HD1	1.83	0.42
2:C:278:GLU:O	2:C:283:VAL:HG22	2.19	0.42
2:C:332:ARG:NH1	2:C:465:GLY:O	2.53	0.42
2:C:358:ARG:HB2	2:C:372:LEU:HD23	2.00	0.42
2:C:421:GLU:O	2:C:423:ALA:N	2.53	0.42
2:C:539:VAL:HB	2:C:540:PHE:CE1	2.54	0.42
2:C:937:ASP:OD1	2:C:939:ARG:CD	2.68	0.42
3:D:638:LYS:CA	3:D:729:HIS:CD2	3.03	0.42
3:D:710:ARG:HG3	3:D:711:LEU:N	2.35	0.42
3:D:874:GLU:O	3:D:875:THR:O	2.38	0.42
3:D:920:LEU:N	3:D:920:LEU:CD2	2.83	0.42
3:D:1108:ARG:O	3:D:1109:GLU:CG	2.65	0.42
3:D:1294:VAL:O	3:D:1301:LYS:N	2.53	0.42
4:E:54:LEU:O	4:E:55:TYR:CB	2.67	0.42
1:A:143:ARG:NH1	1:A:145:ASP:CG	2.77	0.41
2:C:140:ILE:HD12	2:C:331:ARG:HD2	2.02	0.41
2:C:197:LEU:HD23	2:C:197:LEU:HA	1.92	0.41
2:C:200:LEU:HD21	2:C:290:LEU:HD22	2.02	0.41
2:C:552:HIS:CD2	2:C:886:LEU:HD12	2.55	0.41
2:C:674:VAL:HG11	2:C:992:MET:HB2	2.02	0.41
2:C:734:LEU:O	2:C:737:LEU:O	2.38	0.41
2:C:873:PRO:CG	2:C:874:LEU:N	2.78	0.41
3:D:9:ARG:HA	3:D:1456:LYS:HA	2.02	0.41
3:D:974:ILE:CG2	3:D:975:GLU:N	2.83	0.41
3:D:1130:ARG:HG2	3:D:1130:ARG:HH11	1.85	0.41
3:D:1402:ALA:HB3	3:D:1415:VAL:HG11	2.01	0.41
3:D:1468:LEU:C	3:D:1470:ARG:N	2.78	0.41
1:B:51:THR:HA	1:B:145:ASP:O	2.19	0.41
1:B:109:VAL:HG23	1:B:132:LEU:CD2	2.49	0.41
2:C:137:VAL:CG2	2:C:406:HIS:HE1	2.33	0.41
2:C:167:LYS:O	2:C:168:ARG:HB2	2.19	0.41
2:C:224:GLU:O	2:C:227:LEU:N	2.46	0.41
2:C:355:VAL:CG1	2:C:356:ARG:N	2.83	0.41
2:C:481:GLU:H	2:C:481:GLU:CD	2.19	0.41
2:C:560:MET:O	2:C:564:MET:HB2	2.20	0.41
2:C:614:ARG:CZ	2:C:623:HIS:HE1	2.33	0.41
2:C:704:HIS:HD1	2:C:831:ARG:HD2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:808:ARG:C	2:C:810:ASP:H	2.27	0.41
2:C:839:LEU:HD13	2:C:839:LEU:HA	1.76	0.41
2:C:924:LEU:HD23	2:C:924:LEU:H	1.75	0.41
2:C:1020:PRO:O	2:C:1021:LEU:CG	2.68	0.41
3:D:12:LEU:HD12	3:D:12:LEU:HA	1.79	0.41
3:D:471:GLU:O	3:D:471:GLU:HG3	2.20	0.41
3:D:496:LEU:CD1	3:D:500:ARG:HG2	2.48	0.41
3:D:566:ILE:O	3:D:570:GLU:HG3	2.20	0.41
3:D:620:GLY:O	3:D:621:LYS:HG3	2.20	0.41
3:D:962:ARG:O	3:D:966:GLU:HB2	2.19	0.41
3:D:964:LEU:HD21	3:D:1041:MET:HE3	2.02	0.41
3:D:1094:LEU:HB3	3:D:1095:THR:H	1.77	0.41
3:D:1436:SER:OG	3:D:1464:GLU:HG2	2.20	0.41
4:E:26:ARG:HA	4:E:26:ARG:HD2	1.79	0.41
4:E:83:ASP:C	4:E:85:LEU:H	2.27	0.41
1:A:79:ILE:HG23	1:A:167:VAL:CG2	2.50	0.41
1:A:133:GLU:C	1:A:135:GLY:N	2.77	0.41
2:C:83:CYS:HB3	2:C:88:LEU:O	2.21	0.41
2:C:334:ARG:HA	2:C:338:GLU:OE2	2.20	0.41
2:C:542:LEU:HA	2:C:545:ASN:HD22	1.85	0.41
2:C:564:MET:HB2	2:C:564:MET:HE3	1.70	0.41
2:C:623:HIS:HA	2:C:624:PRO:HD3	1.89	0.41
2:C:633:GLN:CD	2:C:633:GLN:N	2.76	0.41
2:C:1023:GLY:O	2:C:1024:LYS:HG3	2.21	0.41
3:D:85:VAL:O	3:D:86:ARG:C	2.63	0.41
3:D:97:THR:O	3:D:571:LYS:CE	2.68	0.41
3:D:597:GLU:HG2	3:D:598:ARG:N	2.36	0.41
3:D:876:SER:H	3:D:879:ARG:CD	2.33	0.41
3:D:963:TYR:CE2	3:D:1002:LYS:HB3	2.55	0.41
3:D:1199:GLY:O	3:D:1200:VAL:C	2.63	0.41
3:D:1331:ASP:O	3:D:1334:GLN:HB2	2.20	0.41
1:A:200:TRP:O	1:A:201:THR:O	2.38	0.41
2:C:248:PRO:O	2:C:249:LYS:C	2.63	0.41
2:C:333:ILE:O	2:C:333:ILE:HG22	2.19	0.41
2:C:442:GLU:HG3	2:C:442:GLU:O	2.20	0.41
2:C:511:ASP:OD1	2:C:516:ARG:HB2	2.20	0.41
2:C:591:SER:C	2:C:593:ALA:N	2.76	0.41
2:C:717:LEU:O	2:C:761:PHE:CB	2.68	0.41
2:C:758:ARG:HD3	2:C:788:THR:O	2.20	0.41
2:C:822:VAL:O	2:C:822:VAL:HG12	2.19	0.41
2:C:947:ALA:O	2:C:950:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1034:GLU:HG3	2:C:1035:MET:H	1.86	0.41
3:D:805:ALA:HB1	3:D:809:PRO:HD2	2.03	0.41
3:D:855:HIS:O	3:D:856:GLY:C	2.63	0.41
3:D:965:GLU:O	3:D:968:ASP:CB	2.67	0.41
3:D:999:THR:O	3:D:1002:LYS:N	2.53	0.41
3:D:1065:LEU:HD12	3:D:1067:VAL:CG2	2.50	0.41
3:D:1192:LEU:CD1	3:D:1345:GLU:HB3	2.49	0.41
3:D:1348:LEU:HD12	3:D:1348:LEU:HA	1.71	0.41
3:D:1403:LEU:CG	3:D:1415:VAL:HB	2.46	0.41
3:D:1431:THR:HG23	3:D:1432:LYS:HG2	2.03	0.41
1:A:71:VAL:HA	1:A:132:LEU:HA	2.01	0.41
1:B:122:ILE:HD12	1:B:122:ILE:N	2.35	0.41
2:C:83:CYS:C	2:C:85:GLU:N	2.77	0.41
2:C:115:LEU:HD11	2:C:378:LEU:HD22	2.01	0.41
2:C:198:ARG:HG2	2:C:228:ALA:CA	2.37	0.41
2:C:368:THR:O	2:C:371:LYS:HB2	2.21	0.41
2:C:574:ALA:C	2:C:575:GLN:CG	2.93	0.41
2:C:588:VAL:HG21	2:C:666:LEU:HD13	2.02	0.41
2:C:657:ASP:HB3	2:C:658:GLY:H	1.46	0.41
2:C:773:LEU:O	2:C:777:ILE:HG13	2.20	0.41
2:C:806:LEU:O	2:C:821:GLU:HA	2.20	0.41
2:C:889:HIS:O	2:C:891:GLY:N	2.53	0.41
2:C:918:LEU:HD13	2:C:968:ASP:CA	2.51	0.41
2:C:1014:SER:O	2:C:1018:GLN:HA	2.20	0.41
2:C:1085:PHE:CE1	3:D:1468:LEU:HD22	2.55	0.41
3:D:99:ALA:HB1	3:D:512:MET:O	2.20	0.41
3:D:570:GLU:OE1	3:D:573:MET:HE1	2.21	0.41
3:D:694:VAL:C	3:D:696:HIS:N	2.73	0.41
3:D:710:ARG:NH2	3:D:1219:GLU:OE2	2.51	0.41
3:D:767:HIS:O	3:D:769:LEU:N	2.49	0.41
3:D:794:GLN:O	3:D:795:VAL:CB	2.65	0.41
3:D:795:VAL:CG2	3:D:904:VAL:HG11	2.45	0.41
3:D:809:PRO:O	3:D:811:GLU:N	2.53	0.41
3:D:868:TYR:HA	3:D:871:ARG:O	2.20	0.41
3:D:891:GLY:H	3:D:926:LYS:NZ	2.17	0.41
3:D:1101:VAL:HG22	3:D:1424:VAL:O	2.20	0.41
3:D:1258:ARG:C	3:D:1260:ILE:N	2.75	0.41
3:D:1282:ARG:HG2	3:D:1293:PHE:CB	2.44	0.41
3:D:1394:VAL:HG11	3:D:1398:TRP:HE3	1.84	0.41
1:A:104:GLU:C	1:A:136:GLY:CA	2.94	0.41
1:B:128:HIS:HE1	1:B:131:THR:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:29:ALA:O	2:C:44:ILE:HD13	2.20	0.41
2:C:498:GLN:CB	2:C:503:LEU:H	2.34	0.41
2:C:648:ARG:NH1	2:C:653:ASP:HB3	2.35	0.41
2:C:837:ASP:C	2:C:848:VAL:HG23	2.46	0.41
3:D:558:LEU:C	3:D:560:GLN:H	2.29	0.41
3:D:904:VAL:HG12	3:D:906:GLN:NE2	2.36	0.41
3:D:904:VAL:C	3:D:906:GLN:OE1	2.63	0.41
3:D:956:ILE:HD11	3:D:1062:ARG:HB3	2.01	0.41
3:D:1113:GLY:O	3:D:1114:THR:O	2.38	0.41
3:D:1478:SER:C	3:D:1480:PHE:N	2.78	0.41
4:E:47:LYS:CD	4:E:54:LEU:HD23	2.48	0.41
1:A:171:PHE:O	1:A:172:SER:C	2.63	0.41
1:A:178:ALA:HB2	2:C:863:ASP:C	2.45	0.41
1:B:174:VAL:CA	1:B:201:THR:HG22	2.48	0.41
2:C:147:TYR:O	2:C:148:PHE:CB	2.66	0.41
2:C:162:ILE:HG13	2:C:171:TRP:HZ3	1.77	0.41
2:C:197:LEU:O	2:C:198:ARG:C	2.62	0.41
2:C:202:TYR:O	2:C:203:ASP:OD2	2.39	0.41
2:C:216:ASP:O	2:C:218:VAL:N	2.54	0.41
2:C:239:PHE:C	2:C:241:LEU:H	2.26	0.41
2:C:460:ARG:N	2:C:468:ARG:O	2.54	0.41
2:C:550:LEU:HD23	2:C:905:VAL:CG1	2.51	0.41
2:C:931:GLY:C	2:C:933:GLY:N	2.75	0.41
2:C:1051:GLU:OE2	3:D:752:SER:OG	2.34	0.41
3:D:497:GLU:O	3:D:501:ALA:HB2	2.21	0.41
3:D:521:PRO:CD	3:D:522:PRO:HD3	2.51	0.41
3:D:575:GLN:O	3:D:578:VAL:N	2.53	0.41
3:D:590:PRO:HA	3:D:600:LEU:CG	2.50	0.41
3:D:626:SER:CB	3:D:748:HIS:HA	2.50	0.41
3:D:697:GLY:O	3:D:760:ARG:NH1	2.53	0.41
3:D:850:LEU:O	3:D:853:VAL:HB	2.20	0.41
3:D:1136:LYS:HE3	3:D:1139:ASP:CG	2.46	0.41
3:D:1462:LEU:C	3:D:1464:GLU:N	2.79	0.41
3:D:1486:VAL:HG21	4:E:25:LYS:CE	2.50	0.41
4:E:32:ARG:HG3	4:E:33:HIS:N	2.32	0.41
4:E:38:THR:HG22	4:E:39:VAL:H	1.84	0.41
1:A:14:THR:O	1:A:14:THR:HG22	2.21	0.41
1:B:88:ARG:HD2	1:B:123:MET:HE1	2.01	0.41
1:B:205:VAL:HG13	1:B:209:GLU:OE1	2.20	0.41
2:C:80:GLN:OE1	2:C:122:THR:HG23	2.21	0.41
2:C:100:LEU:HD21	2:C:368:THR:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:471:TYR:HB3	2:C:534:VAL:HG21	2.03	0.41
2:C:614:ARG:NH1	2:C:623:HIS:HE1	2.19	0.41
2:C:892:LEU:HA	2:C:895:TYR:HB2	2.03	0.41
2:C:943:VAL:O	2:C:946:ARG:HB3	2.19	0.41
2:C:959:PRO:HA	2:C:962:GLN:NE2	2.36	0.41
2:C:969:LEU:CD1	3:D:952:ASP:H	2.24	0.41
3:D:511:TRP:CD1	3:D:511:TRP:H	2.39	0.41
3:D:659:LYS:O	3:D:662:GLU:HB3	2.20	0.41
3:D:1011:PHE:CE2	3:D:1022:VAL:HG11	2.55	0.41
3:D:1141:GLU:OE1	3:D:1168:LEU:HD11	2.20	0.41
3:D:1277:ILE:C	3:D:1279:GLY:H	2.24	0.41
1:A:13:ALA:O	1:A:14:THR:C	2.63	0.41
1:A:43:ILE:O	1:A:46:SER:N	2.54	0.41
1:A:169:ALA:C	1:A:170:ILE:HD13	2.45	0.41
1:A:220:GLU:HA	1:A:223:ASN:HD22	1.85	0.41
1:B:40:LEU:O	1:B:44:LEU:N	2.42	0.41
1:B:110:ARG:C	1:B:112:VAL:N	2.77	0.41
1:B:127:LEU:O	1:B:129:ILE:HG12	2.20	0.41
1:B:173:PRO:C	1:B:201:THR:HB	2.46	0.41
1:B:205:VAL:CG1	1:B:206:THR:N	2.84	0.41
2:C:13:ILE:HG23	2:C:14:PRO:N	2.36	0.41
2:C:34:VAL:HG13	2:C:38:LYS:HG3	2.00	0.41
2:C:53:PRO:O	2:C:54:ILE:C	2.63	0.41
2:C:137:VAL:HG23	2:C:393:GLN:HG3	2.03	0.41
2:C:149:THR:CG2	2:C:150:PRO:HD2	2.50	0.41
2:C:313:LEU:HA	2:C:319:GLY:HA2	2.03	0.41
2:C:361:MET:O	2:C:362:GLY:O	2.39	0.41
2:C:427:VAL:HG12	2:C:428:ARG:N	2.35	0.41
2:C:432:ARG:CZ	3:D:1048:PRO:O	2.68	0.41
2:C:445:GLU:HB3	2:C:446:GLY:H	1.67	0.41
2:C:566:THR:C	2:C:568:ALA:N	2.78	0.41
2:C:598:GLU:HG3	2:C:614:ARG:CZ	2.51	0.41
2:C:611:ILE:HD11	2:C:641:PRO:CB	2.51	0.41
2:C:769:PRO:O	2:C:770:GLU:HB2	2.21	0.41
2:C:816:LYS:HD2	2:C:817:PRO:HG2	2.03	0.41
2:C:841:ASN:ND2	2:C:842:ARG:N	2.69	0.41
2:C:1052:MET:CE	3:D:748:HIS:HB3	2.50	0.41
3:D:701:LEU:HG	3:D:763:MET:CE	2.50	0.41
3:D:776:GLU:H	3:D:776:GLU:HG2	1.47	0.41
3:D:816:TYR:HA	3:D:832:ARG:HH22	1.86	0.41
3:D:879:ARG:CG	3:D:879:ARG:NH1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:930:LEU:HD12	3:D:930:LEU:O	2.21	0.41
3:D:989:TYR:O	3:D:991:GLN:N	2.53	0.41
3:D:1088:THR:O	3:D:1089:ALA:C	2.63	0.41
3:D:1093:TYR:CE2	3:D:1097:LYS:HD2	2.56	0.41
3:D:1132:LEU:HD13	3:D:1184:ARG:NH1	2.20	0.41
3:D:1137:ARG:N	3:D:1137:ARG:HD2	2.35	0.41
3:D:1151:ARG:N	3:D:1162:GLU:HG3	2.35	0.41
3:D:1227:GLU:O	3:D:1228:SER:C	2.63	0.41
3:D:1455:LYS:O	3:D:1456:LYS:HG2	2.21	0.41
3:D:1468:LEU:C	3:D:1470:ARG:H	2.29	0.41
4:E:26:ARG:CZ	4:E:67:GLU:OE2	2.68	0.41
4:E:75:PHE:CD1	4:E:75:PHE:N	2.89	0.41
1:B:16:GLN:CB	1:B:20:TYR:HB3	2.51	0.41
2:C:152:PRO:HD2	2:C:158:TYR:HE2	1.84	0.41
2:C:440:PRO:CD	2:C:455:LEU:N	2.80	0.41
2:C:705:ILE:CD1	2:C:705:ILE:N	2.84	0.41
2:C:750:LYS:HG2	2:C:753:ASP:OD1	2.21	0.41
3:D:709:HIS:O	3:D:710:ARG:C	2.63	0.41
3:D:782:SER:HA	3:D:786:ILE:HD11	2.03	0.41
3:D:1107:VAL:HG23	3:D:1221:VAL:HG23	2.03	0.41
3:D:1323:GLN:H	3:D:1324:PRO:CD	2.32	0.41
1:A:88:ARG:O	1:A:89:PHE:HD1	2.05	0.40
1:B:32:PHE:HA	1:B:35:THR:CB	2.51	0.40
1:B:49:PRO:HB3	1:B:146:ARG:HH21	1.84	0.40
2:C:25:SER:O	2:C:28:LYS:HG2	2.20	0.40
2:C:151:ASP:N	2:C:157:ARG:HA	2.32	0.40
2:C:162:ILE:N	2:C:162:ILE:CD1	2.84	0.40
2:C:247:PRO:C	2:C:249:LYS:N	2.78	0.40
2:C:566:THR:O	2:C:568:ALA:N	2.53	0.40
2:C:629:ALA:C	2:C:630:ARG:CD	2.91	0.40
2:C:692:GLU:O	2:C:695:LEU:N	2.54	0.40
2:C:811:PRO:O	2:C:812:GLY:C	2.64	0.40
2:C:836:GLY:C	2:C:848:VAL:HG22	2.46	0.40
2:C:1091:GLU:CD	3:D:613:ARG:HG3	2.46	0.40
3:D:675:ARG:CZ	3:D:675:ARG:HB2	2.50	0.40
3:D:829:VAL:O	3:D:830:ALA:CB	2.69	0.40
3:D:1145:TYR:HA	3:D:1171:VAL:HG21	2.02	0.40
3:D:1445:HIS:O	3:D:1446:VAL:C	2.63	0.40
4:E:18:ARG:O	4:E:19:LEU:C	2.64	0.40
1:A:187:GLY:HA3	1:A:192:LEU:HD11	2.03	0.40
2:C:102:HIS:HB3	2:C:103:LYS:H	1.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:LEU:CD1	2:C:116:GLY:N	2.65	0.40
2:C:412:ALA:C	2:C:414:GLY:H	2.29	0.40
2:C:653:ASP:O	2:C:654:LEU:C	2.64	0.40
2:C:734:LEU:H	2:C:734:LEU:HG	1.68	0.40
2:C:881:ASN:ND2	3:D:1034:GLN:CG	2.85	0.40
2:C:881:ASN:OD1	3:D:1034:GLN:CD	2.64	0.40
2:C:916:GLU:C	2:C:918:LEU:N	2.78	0.40
2:C:1008:ARG:NH2	2:C:1020:PRO:CB	2.83	0.40
2:C:1070:ILE:C	2:C:1072:LYS:N	2.77	0.40
3:D:557:LEU:O	3:D:558:LEU:HG	2.21	0.40
3:D:709:HIS:CA	3:D:1227:GLU:HB3	2.51	0.40
3:D:963:TYR:C	3:D:964:LEU:O	2.62	0.40
3:D:1329:ALA:O	3:D:1330:ILE:O	2.39	0.40
4:E:15:SER:O	4:E:18:ARG:N	2.30	0.40
1:A:12:THR:HG22	1:A:13:ALA:N	2.36	0.40
1:A:127:LEU:O	1:A:129:ILE:HG12	2.20	0.40
1:A:185:ARG:HH21	1:A:194:LYS:CE	2.32	0.40
2:C:66:LEU:HB2	2:C:100:LEU:HB3	2.02	0.40
2:C:182:VAL:CG1	2:C:307:LEU:HD11	2.51	0.40
2:C:342:ASP:OD1	2:C:345:ARG:HD2	2.21	0.40
2:C:439:CYS:CB	2:C:468:ARG:NH1	2.84	0.40
2:C:498:GLN:CB	2:C:502:PRO:HA	2.52	0.40
2:C:550:LEU:O	2:C:551:GLU:C	2.64	0.40
2:C:840:ALA:CA	2:C:846:LYS:HA	2.52	0.40
2:C:1068:GLN:C	2:C:1070:ILE:N	2.78	0.40
3:D:660:LYS:NZ	4:E:58:PRO:HG2	2.36	0.40
3:D:733:CYS:O	3:D:737:ASN:N	2.47	0.40
3:D:1083:ASP:C	3:D:1085:ALA:H	2.27	0.40
3:D:1107:VAL:CG2	3:D:1215:VAL:HG11	2.43	0.40
3:D:1356:TYR:O	3:D:1357:ARG:C	2.63	0.40
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.84	0.40
1:A:13:ALA:O	1:B:230:ALA:HB2	2.22	0.40
1:A:127:LEU:O	1:A:128:HIS:C	2.65	0.40
1:A:147:GLY:HA3	1:A:171:PHE:CZ	2.56	0.40
1:A:178:ALA:HB2	2:C:864:GLY:CA	2.51	0.40
1:A:191:ASP:O	1:A:192:LEU:O	2.39	0.40
1:B:65:PHE:O	1:B:65:PHE:HD1	2.05	0.40
1:B:91:ASP:HA	1:B:92:PRO:HD3	1.96	0.40
1:B:99:LEU:HB3	1:B:114:PHE:HD2	1.86	0.40
2:C:26:TYR:HB2	2:C:121:MET:HE3	2.02	0.40
2:C:207:LEU:HG	2:C:208:VAL:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:336:VAL:O	2:C:338:GLU:N	2.55	0.40
2:C:533:ASP:O	2:C:535:SER:N	2.54	0.40
2:C:564:MET:O	2:C:565:GLN:C	2.65	0.40
2:C:729:LEU:CD1	2:C:791:ARG:NH2	2.85	0.40
2:C:750:LYS:CE	2:C:753:ASP:OD2	2.70	0.40
2:C:860:HIS:HD2	2:C:977:GLY:CA	2.34	0.40
2:C:875:GLY:CA	2:C:879:ARG:HD2	2.50	0.40
2:C:895:TYR:CD1	2:C:991:GLN:NE2	2.89	0.40
2:C:916:GLU:O	2:C:919:ALA:N	2.55	0.40
2:C:969:LEU:HD13	3:D:952:ASP:OD1	2.21	0.40
3:D:776:GLU:HB3	3:D:912:LYS:HE2	2.02	0.40
3:D:948:THR:HB	3:D:949:ILE:H	1.68	0.40
3:D:971:LEU:C	3:D:974:ILE:H	2.28	0.40
3:D:1153:VAL:HG11	3:D:1174:LEU:HD21	2.03	0.40
3:D:1457:ASP:OD1	3:D:1459:LEU:N	2.52	0.40
3:D:1466:VAL:O	3:D:1469:GLY:CA	2.70	0.40
4:E:81:PRO:CG	4:E:84:ARG:HD2	2.49	0.40
1:A:41:ARG:HD3	1:A:177:VAL:O	2.22	0.40
1:A:223:ASN:O	1:A:224:TYR:C	2.64	0.40
1:B:175:ARG:O	1:B:176:ARG:CB	2.69	0.40
1:B:178:ALA:CB	1:B:198:ARG:HE	2.28	0.40
2:C:9:ILE:HD13	2:C:494:TYR:CE1	2.57	0.40
2:C:473:ARG:C	2:C:474:VAL:HG23	2.47	0.40
2:C:535:SER:HA	2:C:536:PRO:HD3	1.91	0.40
2:C:580:MET:HB2	2:C:584:GLU:OE2	2.21	0.40
2:C:611:ILE:O	2:C:611:ILE:HG22	2.21	0.40
2:C:880:MET:O	2:C:881:ASN:C	2.63	0.40
2:C:1049:LEU:C	2:C:1051:GLU:N	2.78	0.40
2:C:1107:ASN:OD1	2:C:1107:ASN:O	2.40	0.40
3:D:121:THR:CB	3:D:461:ILE:HD11	2.51	0.40
3:D:571:LYS:O	3:D:573:MET:N	2.53	0.40
3:D:625:TYR:O	3:D:652:LEU:HD12	2.22	0.40
3:D:885:ILE:HD13	3:D:937:TYR:CD2	2.55	0.40
3:D:1004:THR:C	3:D:1006:ALA:N	2.78	0.40
3:D:1192:LEU:HD21	3:D:1369:GLU:CA	2.52	0.40
3:D:1232:PRO:HB3	3:D:1361:VAL:CG1	2.51	0.40
3:D:1431:THR:O	3:D:1432:LYS:CG	2.68	0.40
4:E:38:THR:CG2	4:E:63:TRP:HZ3	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/314 (71%)	111 (50%)	61 (28%)	50 (22%)	0	0
1	B	228/314 (73%)	123 (54%)	62 (27%)	43 (19%)	0	0
2	C	1111/1118 (99%)	591 (53%)	277 (25%)	243 (22%)	0	0
3	D	1126/1264 (89%)	588 (52%)	291 (26%)	247 (22%)	0	0
4	E	96/99 (97%)	50 (52%)	24 (25%)	22 (23%)	0	0
All	All	2783/3109 (90%)	1463 (53%)	715 (26%)	605 (22%)	0	0

All (605) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	19	HIS
1	A	26	GLU
1	A	59	GLU
1	A	73	GLU
1	A	92	PRO
1	A	105	GLY
1	A	107	LYS
1	A	113	ASP
1	A	125	PRO
1	A	143	ARG
1	A	144	VAL
1	A	153	ALA
1	A	158	ILE
1	A	162	ILE
1	A	176	ARG
1	A	187	GLY
1	A	192	LEU
1	A	201	THR
1	B	4	SER
1	B	5	LYS

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Mol	Chain	Res	Type
1	B	6	LEU
1	B	26	GLU
1	B	60	ASP
1	B	62	LEU
1	B	63	HIS
1	B	75	VAL
1	B	96	SER
1	B	126	ASP
1	B	138	LEU
1	B	156	HIS
1	B	158	ILE
1	B	160	ASP
1	B	161	ARG
1	B	176	ARG
1	B	204	SER
1	B	224	TYR
2	C	31	GLN
2	C	32	ALA
2	C	33	ASP
2	C	36	PRO
2	C	44	ILE
2	C	77	PRO
2	C	153	ALA
2	C	157	ARG
2	C	204	GLN
2	C	216	ASP
2	C	258	PHE
2	C	261	LEU
2	C	268	ASP
2	C	269	LEU
2	C	276	LYS
2	C	283	VAL
2	C	287	GLY
2	C	290	LEU
2	C	295	ASP
2	C	325	ILE
2	C	360	VAL
2	C	361	MET
2	C	375	SER
2	C	388	ARG
2	C	402	SER
2	C	416	GLY

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Mol	Chain	Res	Type
2	C	426	ASP
2	C	427	VAL
2	C	432	ARG
2	C	449	ILE
2	C	450	GLY
2	C	460	ARG
2	C	461	VAL
2	C	462	ASP
2	C	467	ILE
2	C	468	ARG
2	C	469	THR
2	C	476	ASN
2	C	477	GLY
2	C	479	VAL
2	C	480	THR
2	C	484	VAL
2	C	488	ALA
2	C	489	SER
2	C	495	THR
2	C	496	ILE
2	C	502	PRO
2	C	517	ARG
2	C	526	PRO
2	C	528	GLU
2	C	568	ALA
2	C	569	VAL
2	C	573	ARG
2	C	575	GLN
2	C	600	ASP
2	C	602	GLU
2	C	603	VAL
2	C	604	VAL
2	C	606	VAL
2	C	613	VAL
2	C	615	TYR
2	C	629	ALA
2	C	636	ALA
2	C	654	LEU
2	C	660	ALA
2	C	677	MET
2	C	680	ASP
2	C	700	TYR

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Mol	Chain	Res	Type
2	C	715	THR
2	C	730	SER
2	C	734	LEU
2	C	762	LYS
2	C	788	THR
2	C	791	ARG
2	C	796	GLU
2	C	811	PRO
2	C	821	GLU
2	C	832	LYS
2	C	837	ASP
2	C	840	ALA
2	C	876	VAL
2	C	881	ASN
2	C	887	GLU
2	C	936	VAL
2	C	943	VAL
2	C	973	VAL
2	C	992	MET
2	C	993	PHE
2	C	1001	VAL
2	C	1018	GLN
2	C	1021	LEU
2	C	1022	GLY
2	C	1034	GLU
2	C	1055	ILE
2	C	1080	SER
2	C	1104	GLU
2	C	1109	VAL
3	D	28	LYS
3	D	83	SER
3	D	84	ILE
3	D	85	VAL
3	D	86	ARG
3	D	93	ILE
3	D	98	PRO
3	D	104	PHE
3	D	112	ILE
3	D	113	ALA
3	D	127	LEU
3	D	130	ASN
3	D	133	ILE

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Mol	Chain	Res	Type
3	D	137	PRO
3	D	143	ASP
3	D	467	GLU
3	D	468	LEU
3	D	483	HIS
3	D	509	PRO
3	D	511	TRP
3	D	512	MET
3	D	513	ILE
3	D	515	GLU
3	D	539	ASP
3	D	564	GLU
3	D	583	ASP
3	D	584	ASN
3	D	587	ARG
3	D	610	LYS
3	D	638	LYS
3	D	657	LEU
3	D	658	LEU
3	D	680	GLN
3	D	682	ASP
3	D	689	ASP
3	D	705	ALA
3	D	709	HIS
3	D	722	GLU
3	D	725	SER
3	D	740	PHE
3	D	748	HIS
3	D	753	SER
3	D	774	SER
3	D	783	ARG
3	D	795	VAL
3	D	824	ASN
3	D	827	ILE
3	D	828	VAL
3	D	835	SER
3	D	838	ARG
3	D	839	LEU
3	D	854	ALA
3	D	856	GLY
3	D	869	LEU
3	D	875	THR

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Mol	Chain	Res	Type
3	D	892	ASP
3	D	902	MET
3	D	908	LYS
3	D	969	ARG
3	D	1015	TYR
3	D	1018	ASN
3	D	1028	ALA
3	D	1052	THR
3	D	1075	HIS
3	D	1076	GLY
3	D	1089	ALA
3	D	1111	ASP
3	D	1112	CYS
3	D	1114	THR
3	D	1137	ARG
3	D	1197	ARG
3	D	1203	LYS
3	D	1206	GLY
3	D	1268	PRO
3	D	1270	ALA
3	D	1271	LYS
3	D	1279	GLY
3	D	1281	VAL
3	D	1282	ARG
3	D	1307	LYS
3	D	1312	LEU
3	D	1313	VAL
3	D	1315	ASP
3	D	1317	ASP
3	D	1320	GLU
3	D	1322	GLY
3	D	1323	GLN
3	D	1325	LEU
3	D	1339	LYS
3	D	1364	HIS
3	D	1392	GLY
3	D	1403	LEU
3	D	1442	ASN
3	D	1472	ILE
3	D	1482	ARG
4	E	29	GLN
4	E	31	LEU

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Mol	Chain	Res	Type
4	E	34	ARG
4	E	35	PHE
4	E	43	GLU
4	E	51	LEU
4	E	55	TYR
4	E	80	VAL
4	E	94	PRO
1	A	14	THR
1	A	30	ARG
1	A	90	LEU
1	A	96	SER
1	A	123	MET
1	A	139	TYR
1	A	161	ARG
1	A	182	GLU
1	A	190	THR
1	A	200	TRP
1	A	224	TYR
1	B	35	THR
1	B	47	SER
1	B	105	GLY
1	B	107	LYS
1	B	116	PRO
1	B	119	ASP
1	B	120	VAL
1	B	130	ALA
1	B	152	PRO
1	B	195	LEU
1	B	196	THR
2	C	10	ARG
2	C	23	VAL
2	C	42	VAL
2	C	59	LYS
2	C	90	TYR
2	C	148	PHE
2	C	155	PRO
2	C	168	ARG
2	C	262	ALA
2	C	303	PHE
2	C	309	TYR
2	C	315	ALA
2	C	319	GLY

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Mol	Chain	Res	Type
2	C	320	HIS
2	C	322	VAL
2	C	362	GLY
2	C	435	TYR
2	C	444	PRO
2	C	474	VAL
2	C	482	GLU
2	C	524	VAL
2	C	529	VAL
2	C	534	VAL
2	C	546	LEU
2	C	567	GLN
2	C	581	THR
2	C	587	VAL
2	C	643	VAL
2	C	657	ASP
2	C	663	GLU
2	C	713	ARG
2	C	728	HIS
2	C	731	GLU
2	C	769	PRO
2	C	777	ILE
2	C	779	GLY
2	C	812	GLY
2	C	874	LEU
2	C	886	LEU
2	C	922	PHE
2	C	938	LYS
2	C	945	ALA
2	C	969	LEU
2	C	970	GLY
2	C	975	TYR
2	C	977	GLY
2	C	1002	GLU
2	C	1025	ALA
2	C	1059	ASP
2	C	1074	GLU
2	C	1110	ASP
3	D	9	ARG
3	D	22	SER
3	D	29	PRO
3	D	72	VAL

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Mol	Chain	Res	Type
3	D	76	CYS
3	D	78	VAL
3	D	87	ARG
3	D	89	ARG
3	D	95	LEU
3	D	111	LYS
3	D	126	VAL
3	D	144	ALA
3	D	150	ARG
3	D	453	ASP
3	D	561	GLY
3	D	567	ILE
3	D	590	PRO
3	D	613	ARG
3	D	617	ASN
3	D	643	GLY
3	D	668	PRO
3	D	730	PRO
3	D	733	CYS
3	D	747	VAL
3	D	773	ALA
3	D	784	ASP
3	D	799	LYS
3	D	806	PHE
3	D	822	ALA
3	D	825	ALA
3	D	855	HIS
3	D	858	LEU
3	D	917	GLN
3	D	935	LYS
3	D	946	GLY
3	D	983	LEU
3	D	995	LEU
3	D	1070	TYR
3	D	1103	HIS
3	D	1109	GLU
3	D	1130	ARG
3	D	1151	ARG
3	D	1155	ALA
3	D	1156	LEU
3	D	1200	VAL
3	D	1220	ALA

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Mol	Chain	Res	Type
3	D	1272	ALA
3	D	1291	SER
3	D	1304	LYS
3	D	1316	GLY
3	D	1324	PRO
3	D	1330	ILE
3	D	1354	LYS
3	D	1366	LYS
3	D	1367	HIS
3	D	1408	ILE
3	D	1470	ARG
4	E	16	LYS
4	E	70	THR
1	A	20	TYR
1	A	48	ILE
1	A	112	VAL
1	A	160	ASP
1	A	199	ILE
1	B	90	LEU
1	B	207	PRO
2	C	55	GLU
2	C	75	ASP
2	C	103	LYS
2	C	156	GLY
2	C	203	ASP
2	C	210	GLU
2	C	264	PRO
2	C	328	LEU
2	C	420	ARG
2	C	457	ALA
2	C	463	ALA
2	C	512	ARG
2	C	527	GLU
2	C	531	PHE
2	C	551	GLU
2	C	555	ALA
2	C	610	ARG
2	C	692	GLU
2	C	732	ALA
2	C	738	ASP
2	C	857	ASP
2	C	873	PRO

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Mol	Chain	Res	Type
2	C	875	GLY
2	C	966	LEU
2	C	986	PRO
2	C	998	TYR
2	C	1043	TYR
2	C	1061	GLU
2	C	1072	LYS
2	C	1105	LYS
2	C	1112	PHE
2	C	1113	GLU
3	D	11	ALA
3	D	125	GLN
3	D	486	ARG
3	D	507	ASN
3	D	543	LEU
3	D	652	LEU
3	D	711	LEU
3	D	714	GLN
3	D	734	GLU
3	D	768	ASN
3	D	793	THR
3	D	809	PRO
3	D	816	TYR
3	D	840	LYS
3	D	862	ASP
3	D	893	GLU
3	D	905	PRO
3	D	953	ASP
3	D	959	GLU
3	D	968	ASP
3	D	990	ASP
3	D	1090	ASP
3	D	1152	GLU
3	D	1251	ASP
3	D	1252	ILE
3	D	1283	ILE
3	D	1309	ALA
3	D	1319	VAL
3	D	1426	LYS
3	D	1452	ILE
3	D	1488	ASP
4	E	30	LEU

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Mol	Chain	Res	Type
1	A	67	THR
1	A	119	ASP
1	A	126	ASP
1	A	128	HIS
1	A	152	PRO
1	B	15	THR
1	B	202	ASP
2	C	9	ILE
2	C	51	THR
2	C	58	ASP
2	C	66	LEU
2	C	105	THR
2	C	149	THR
2	C	181	VAL
2	C	187	ASN
2	C	232	GLU
2	C	324	ASP
2	C	326	ASP
2	C	380	ALA
2	C	425	PHE
2	C	431	HIS
2	C	499	ALA
2	C	626	ARG
2	C	685	GLU
2	C	699	PHE
2	C	781	LYS
2	C	890	LEU
2	C	894	GLY
2	C	1012	PRO
2	C	1044	GLY
3	D	522	PRO
3	D	599	PRO
3	D	629	SER
3	D	639	LEU
3	D	679	ARG
3	D	685	ASP
3	D	695	ILE
3	D	737	ASN
3	D	805	ALA
3	D	823	LEU
3	D	829	VAL
3	D	830	ALA

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Mol	Chain	Res	Type
3	D	904	VAL
3	D	906	GLN
3	D	907	GLU
3	D	961	GLN
3	D	1009	ASN
3	D	1031	ASN
3	D	1036	ARG
3	D	1060	SER
3	D	1061	PHE
3	D	1138	SER
3	D	1161	GLU
3	D	1207	TYR
3	D	1327	ARG
3	D	1344	VAL
4	E	2	ALA
4	E	12	MET
4	E	49	ARG
4	E	56	ASP
4	E	95	THR
1	A	64	GLU
1	A	111	ALA
1	A	118	ALA
1	A	122	ILE
1	A	134	GLU
1	A	189	ARG
1	A	196	THR
1	B	37	GLY
1	B	159	LYS
2	C	12	VAL
2	C	15	LEU
2	C	39	ARG
2	C	46	ALA
2	C	112	GLU
2	C	182	VAL
2	C	617	ASP
2	C	656	ALA
2	C	716	LYS
2	C	793	PRO
2	C	858	MET
2	C	877	PRO
2	C	898	GLY
2	C	921	ALA

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Mol	Chain	Res	Type
2	C	1077	PRO
3	D	94	GLU
3	D	132	TYR
3	D	134	VAL
3	D	145	VAL
3	D	540	LEU
3	D	558	LEU
3	D	572	ARG
3	D	582	ILE
3	D	644	LEU
3	D	654	LYS
3	D	673	ALA
3	D	861	GLN
3	D	894	LYS
3	D	1008	PHE
3	D	1321	ALA
3	D	1453	ALA
3	D	1476	THR
4	E	71	GLY
4	E	72	ARG
4	E	93	TYR
1	B	42	ARG
1	B	115	THR
1	B	128	HIS
1	B	134	GLU
2	C	35	PRO
2	C	376	ARG
2	C	856	GLU
2	C	1000	MET
2	C	1010	THR
2	C	1107	ASN
3	D	542	ASP
3	D	609	GLY
3	D	640	HIS
3	D	667	ALA
3	D	1332	PRO
3	D	1396	GLU
4	E	62	THR
1	A	109	VAL
1	A	203	GLY
2	C	113	VAL
2	C	164	PRO

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Mol	Chain	Res	Type
2	C	166	PRO
2	C	337	GLY
2	C	478	VAL
2	C	520	GLU
2	C	982	PRO
2	C	1011	GLY
3	D	771	SER
3	D	864	VAL
3	D	1043	GLY
3	D	1081	GLY
3	D	1381	VAL
1	B	24	VAL
1	B	125	PRO
1	B	136	GLY
2	C	54	ILE
2	C	144	PRO
2	C	819	VAL
3	D	1064	GLY
2	C	470	PRO
2	C	972	VAL
3	D	719	VAL
3	D	900	ILE
3	D	1267	ARG
2	C	535	SER
2	C	951	GLY
2	C	959	PRO
2	C	1079	PRO
3	D	136	ASP
3	D	1050	GLY
3	D	1222	GLY
4	E	41	GLU
1	A	136	GLY
1	B	71	VAL
2	C	443	THR
2	C	931	GLY
3	D	634	GLY
3	D	845	ASN
3	D	890	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/271 (70%)	159 (84%)	30 (16%)	2	12
1	B	190/271 (70%)	166 (87%)	24 (13%)	4	18
2	C	870/935 (93%)	754 (87%)	116 (13%)	4	17
3	D	782/1035 (76%)	661 (84%)	121 (16%)	2	12
4	E	67/88 (76%)	60 (90%)	7 (10%)	7	25
All	All	2098/2600 (81%)	1800 (86%)	298 (14%)	3	14

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	25	LEU
1	A	26	GLU
1	A	27	PRO
1	A	30	ARG
1	A	41	ARG
1	A	48	ILE
1	A	56	VAL
1	A	57	TYR
1	A	63	HIS
1	A	67	THR
1	A	69	PRO
1	A	74	ASP
1	A	77	GLU
1	A	91	ASP
1	A	97	THR
1	A	101	LEU
1	A	109	VAL
1	A	123	MET
1	A	126	ASP
1	A	142	VAL
1	A	143	ARG
1	A	144	VAL

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Mol	Chain	Res	Type
1	A	192	LEU
1	A	195	LEU
1	A	196	THR
1	A	197	LEU
1	A	200	TRP
1	A	213	GLN
1	A	222	LEU
1	B	25	LEU
1	B	38	ASN
1	B	44	LEU
1	B	48	ILE
1	B	51	THR
1	B	56	VAL
1	B	75	VAL
1	B	78	ILE
1	B	79	ILE
1	B	86	VAL
1	B	89	PHE
1	B	90	LEU
1	B	94	MET
1	B	123	MET
1	B	132	LEU
1	B	151	VAL
1	B	167	VAL
1	B	171	PHE
1	B	183	ASP
1	B	188	GLN
1	B	194	LYS
1	B	195	LEU
1	B	197	LEU
1	B	199	ILE
2	C	9	ILE
2	C	13	ILE
2	C	34	VAL
2	C	36	PRO
2	C	52	PHE
2	C	56	GLU
2	C	67	ASP
2	C	70	GLU
2	C	75	ASP
2	C	95	TYR
2	C	100	LEU

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Mol	Chain	Res	Type
2	C	104	ASP
2	C	115	LEU
2	C	126	SER
2	C	129	ILE
2	C	135	VAL
2	C	138	SER
2	C	142	ARG
2	C	147	TYR
2	C	157	ARG
2	C	158	TYR
2	C	163	ILE
2	C	176	VAL
2	C	177	GLU
2	C	182	VAL
2	C	184	MET
2	C	194	VAL
2	C	198	ARG
2	C	203	ASP
2	C	214	TYR
2	C	217	LEU
2	C	232	GLU
2	C	254	LEU
2	C	258	PHE
2	C	261	LEU
2	C	263	ASP
2	C	267	TYR
2	C	283	VAL
2	C	285	LEU
2	C	303	PHE
2	C	304	LEU
2	C	306	THR
2	C	335	THR
2	C	351	LEU
2	C	393	GLN
2	C	399	ASN
2	C	407	LYS
2	C	410	ILE
2	C	425	PHE
2	C	433	THR
2	C	434	HIS
2	C	435	TYR
2	C	438	ILE

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Mol	Chain	Res	Type
2	C	445	GLU
2	C	461	VAL
2	C	479	VAL
2	C	502	PRO
2	C	508	ILE
2	C	526	PRO
2	C	534	VAL
2	C	559	LEU
2	C	575	GLN
2	C	579	VAL
2	C	603	VAL
2	C	611	ILE
2	C	630	ARG
2	C	633	GLN
2	C	635	THR
2	C	637	PHE
2	C	672	VAL
2	C	673	LEU
2	C	674	VAL
2	C	683	ASN
2	C	686	ASP
2	C	688	ILE
2	C	691	SER
2	C	698	ASP
2	C	699	PHE
2	C	705	ILE
2	C	710	ILE
2	C	722	ILE
2	C	723	THR
2	C	726	ILE
2	C	739	GLU
2	C	743	VAL
2	C	755	LEU
2	C	758	ARG
2	C	810	ASP
2	C	813	VAL
2	C	815	LEU
2	C	837	ASP
2	C	839	LEU
2	C	841	ASN
2	C	846	LYS
2	C	852	ILE

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Mol	Chain	Res	Type
2	C	859	PRO
2	C	860	HIS
2	C	866	PRO
2	C	869	VAL
2	C	871	LEU
2	C	881	ASN
2	C	882	LEU
2	C	888	THR
2	C	892	LEU
2	C	924	LEU
2	C	981	GLU
2	C	988	VAL
2	C	1005	MET
2	C	1012	PRO
2	C	1013	TYR
2	C	1018	GLN
2	C	1019	GLN
2	C	1027	PHE
2	C	1031	ARG
2	C	1043	TYR
2	C	1115	LEU
3	D	5	VAL
3	D	21	TRP
3	D	469	ASP
3	D	502	PHE
3	D	509	PRO
3	D	567	ILE
3	D	576	GLU
3	D	607	LEU
3	D	619	LEU
3	D	639	LEU
3	D	640	HIS
3	D	651	GLU
3	D	678	GLU
3	D	685	ASP
3	D	688	TRP
3	D	691	LEU
3	D	701	LEU
3	D	702	LEU
3	D	722	GLU
3	D	724	GLN
3	D	752	SER

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Mol	Chain	Res	Type
3	D	762	GLN
3	D	769	LEU
3	D	772	PRO
3	D	776	GLU
3	D	778	LEU
3	D	791	TYR
3	D	792	ILE
3	D	794	GLN
3	D	796	ARG
3	D	798	GLU
3	D	834	THR
3	D	836	VAL
3	D	851	LEU
3	D	855	HIS
3	D	857	LEU
3	D	860	LEU
3	D	864	VAL
3	D	876	SER
3	D	879	ARG
3	D	886	VAL
3	D	899	LEU
3	D	904	VAL
3	D	906	GLN
3	D	911	LEU
3	D	914	LEU
3	D	920	LEU
3	D	925	GLU
3	D	931	LEU
3	D	941	LEU
3	D	947	ILE
3	D	951	ILE
3	D	953	ASP
3	D	955	VAL
3	D	964	LEU
3	D	971	LEU
3	D	974	ILE
3	D	984	THR
3	D	998	GLU
3	D	1009	ASN
3	D	1031	ASN
3	D	1038	LEU
3	D	1041	MET

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Mol	Chain	Res	Type
3	D	1042	ARG
3	D	1045	MET
3	D	1052	THR
3	D	1055	VAL
3	D	1057	VAL
3	D	1061	PHE
3	D	1062	ARG
3	D	1068	LEU
3	D	1078	ARG
3	D	1093	TYR
3	D	1103	HIS
3	D	1104	GLU
3	D	1118	ILE
3	D	1119	SER
3	D	1126	ASP
3	D	1130	ARG
3	D	1134	LEU
3	D	1137	ARG
3	D	1142	SER
3	D	1145	TYR
3	D	1148	VAL
3	D	1154	GLU
3	D	1161	GLU
3	D	1162	GLU
3	D	1166	LEU
3	D	1182	GLU
3	D	1188	VAL
3	D	1190	SER
3	D	1192	LEU
3	D	1194	CYS
3	D	1196	THR
3	D	1207	TYR
3	D	1210	SER
3	D	1213	ARG
3	D	1231	GLU
3	D	1250	THR
3	D	1260	ILE
3	D	1273	VAL
3	D	1274	ILE
3	D	1278	ASP
3	D	1281	VAL
3	D	1315	ASP

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Mol	Chain	Res	Type
3	D	1327	ARG
3	D	1332	PRO
3	D	1348	LEU
3	D	1372	VAL
3	D	1373	ARG
3	D	1376	LEU
3	D	1381	VAL
3	D	1390	LEU
3	D	1399	ASP
3	D	1424	VAL
3	D	1434	TRP
3	D	1447	LEU
3	D	1465	ASN
3	D	1466	VAL
3	D	1476	THR
3	D	1483	PHE
4	E	23	VAL
4	E	31	LEU
4	E	32	ARG
4	E	61	VAL
4	E	75	PHE
4	E	78	ASN
4	E	92	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	63	HIS
1	A	128	HIS
1	A	156	HIS
1	A	180	GLN
1	A	212	ASN
1	A	223	ASN
1	A	227	ASN
1	B	38	ASN
1	B	81	ASN
1	B	188	GLN
1	B	213	GLN
1	B	223	ASN
2	C	22	GLN
2	C	102	HIS

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Mol	Chain	Res	Type
2	C	141	HIS
2	C	320	HIS
2	C	327	HIS
2	C	343	GLN
2	C	399	ASN
2	C	538	GLN
2	C	545	ASN
2	C	623	HIS
2	C	632	ASN
2	C	1639	GLN
2	C	671	ASN
2	C	834	GLN
2	C	841	ASN
2	C	845	ASN
2	C	860	HIS
2	C	872	ASN
2	C	881	ASN
2	C	884	GLN
2	C	889	HIS
2	C	962	GLN
2	C	991	GLN
2	C	1026	GLN
2	C	1030	GLN
2	C	1107	ASN
3	D	507	ASN
3	D	551	ASN
3	D	552	ASN
3	D	636	GLN
3	D	640	HIS
3	D	709	HIS
3	D	724	GLN
3	D	727	GLN
3	D	729	HIS
3	D	756	GLN
3	D	762	GLN
3	D	767	HIS
3	D	855	HIS
3	D	861	GLN
3	D	897	GLN
3	D	909	ASN
3	D	1018	ASN
3	D	1034	GLN

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Mol	Chain	Res	Type
3	D	1333	HIS
3	D	1364	HIS
3	D	1374	GLN
3	D	1393	GLN
3	D	1445	HIS
3	D	1465	ASN
4	E	33	HIS
4	E	59	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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	RFP	C	1640	-	63,63,63	1.28	8 (12%)	94,94,94	0.96	4 (4%)

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
5	RFP	C	1640	-	-	15/60/85/85	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1640	RFP	O5-C29	3.51	1.48	1.39
5	C	1640	RFP	O4-C11	3.37	1.27	1.21
5	C	1640	RFP	C5-C10	3.14	1.49	1.42
5	C	1640	RFP	C8-C9	2.99	1.51	1.43
5	C	1640	RFP	C39-N4	2.66	1.52	1.46
5	C	1640	RFP	C2-C1	2.15	1.43	1.38
5	C	1640	RFP	O2-C8	-2.06	1.28	1.35
5	C	1640	RFP	O6-C27	2.01	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1640	RFP	C5-C10-C9	-2.60	115.41	119.77
5	C	1640	RFP	C34-C26-C25	-2.41	107.15	111.40
5	C	1640	RFP	C24-C23-C22	2.14	118.97	115.41
5	C	1640	RFP	O12-C4-C10	2.08	124.19	119.17

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1640	RFP	C17-C18-C19-C20
5	C	1640	RFP	C26-C27-C28-C29
5	C	1640	RFP	O6-C27-C28-C29
5	C	1640	RFP	C32-C22-C23-C24
5	C	1640	RFP	C21-C22-C23-C24
5	C	1640	RFP	C32-C22-C23-O9
5	C	1640	RFP	C43-N2-N3-C40
5	C	1640	RFP	C21-C22-C23-O9
5	C	1640	RFP	C3-C2-N1-C15
5	C	1640	RFP	C43-N2-N3-C41
5	C	1640	RFP	C28-C29-O5-C12
5	C	1640	RFP	C33-C24-C25-C26
5	C	1640	RFP	C23-C24-C25-C26
5	C	1640	RFP	C18-C19-C20-C31

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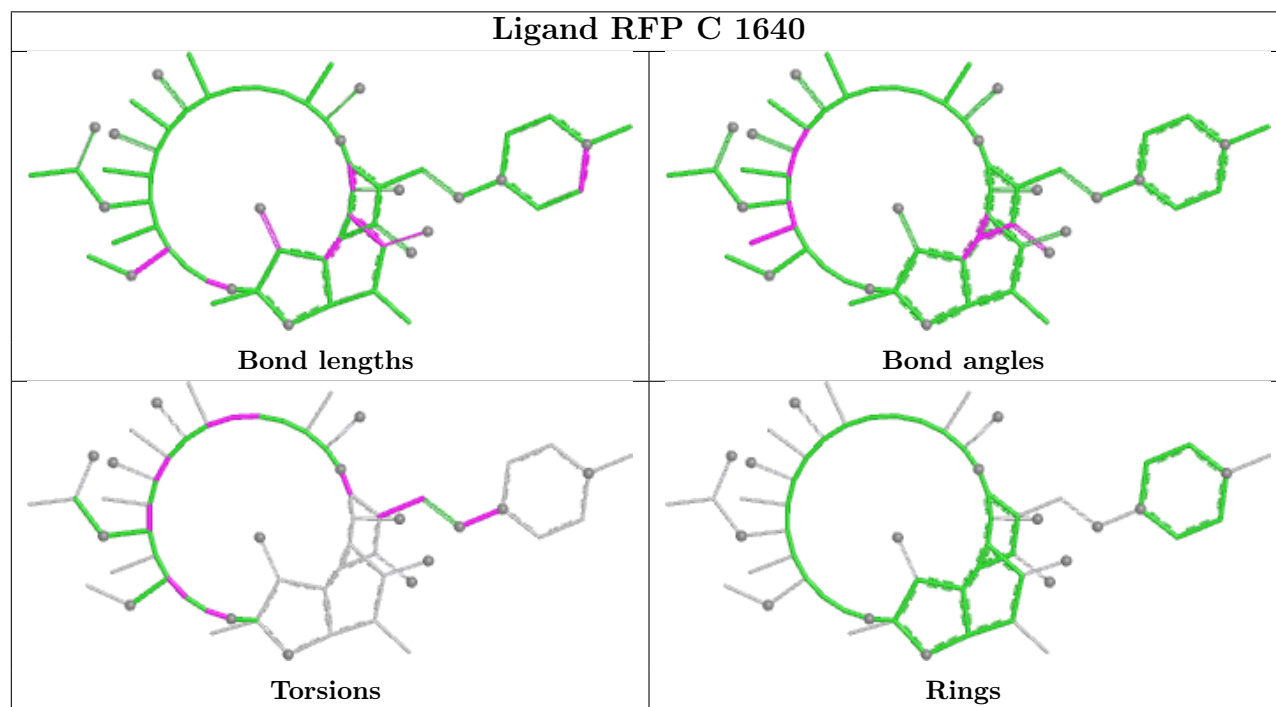
Mol	Chain	Res	Type	Atoms
5	C	1640	RFP	C4-C3-C43-N2

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1640	RFP	6	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	155:ASP	C	2(U):UNK	N	54.72
1	D	46(U):UNK	C	452:ILE	N	47.08
1	D	10(U):UNK	C	20(U):UNK	N	15.58
1	D	1270:ALA	C	1271:LYS	N	1.06

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.