



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:17 AM UTC

PDB ID : 2QVW / pdb_00002qvw
Title : Structure of Giardia Dicer refined against twinned data
Authors : Doudna, J.A.; MacRae, I.J.
Deposited on : 2007-08-09
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

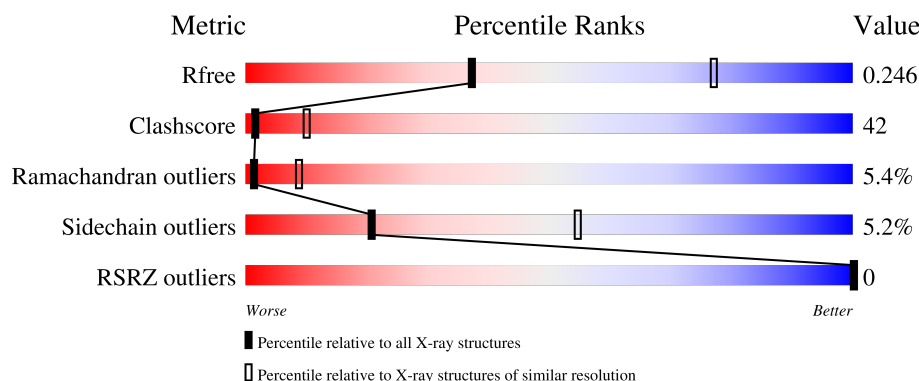
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

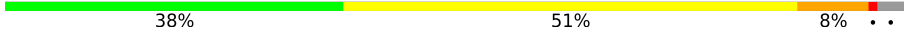
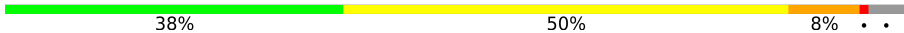
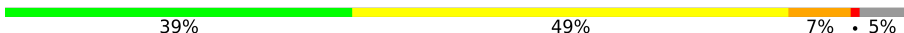
The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	756	 38% 51% 8% . .
1	B	756	 38% 50% 8% . .
1	C	756	 39% 49% 7% . 5%
1	D	756	 38% 49% 8% . 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22372 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 GLP_546_48378_50642.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			5630	3614	957	1029	30			
1	B	726	Total	C	N	O	S	0	0	0
			5590	3589	950	1021	30			
1	C	718	Total	C	N	O	S	0	0	0
			5539	3560	941	1008	30			
1	D	720	Total	C	N	O	S	0	0	0
			5574	3586	942	1016	30			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q7R2M2
A	0	ALA	-	expression tag	UNP Q7R2M2
B	-1	GLY	-	expression tag	UNP Q7R2M2
B	0	ALA	-	expression tag	UNP Q7R2M2
C	-1	GLY	-	expression tag	UNP Q7R2M2
C	0	ALA	-	expression tag	UNP Q7R2M2
D	-1	GLY	-	expression tag	UNP Q7R2M2
D	0	ALA	-	expression tag	UNP Q7R2M2

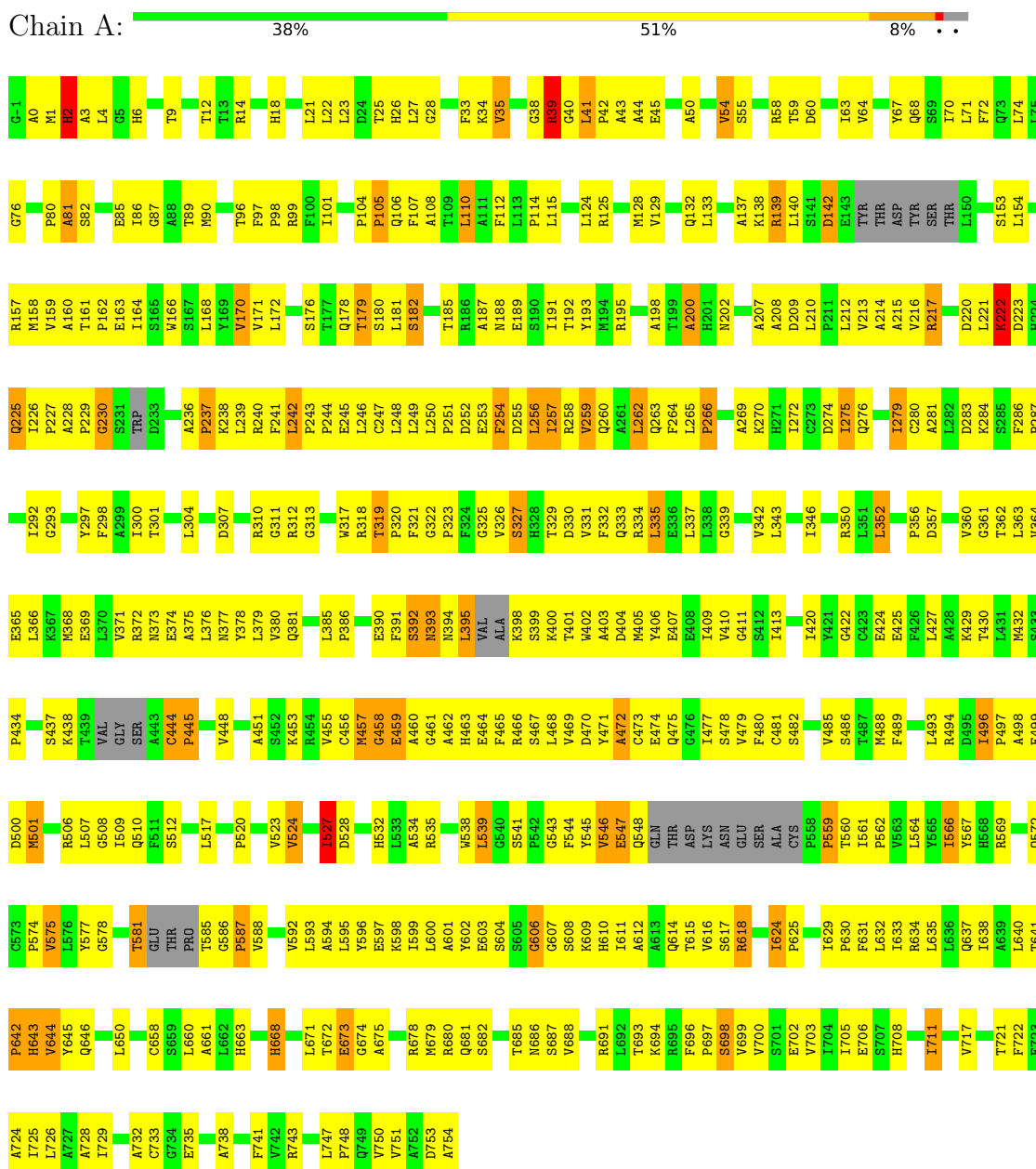
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	Mn	0	0
			12	12		
2	B	9	Total	Mn	0	0
			9	9		
2	C	9	Total	Mn	0	0
			9	9		
2	D	9	Total	Mn	0	0
			9	9		

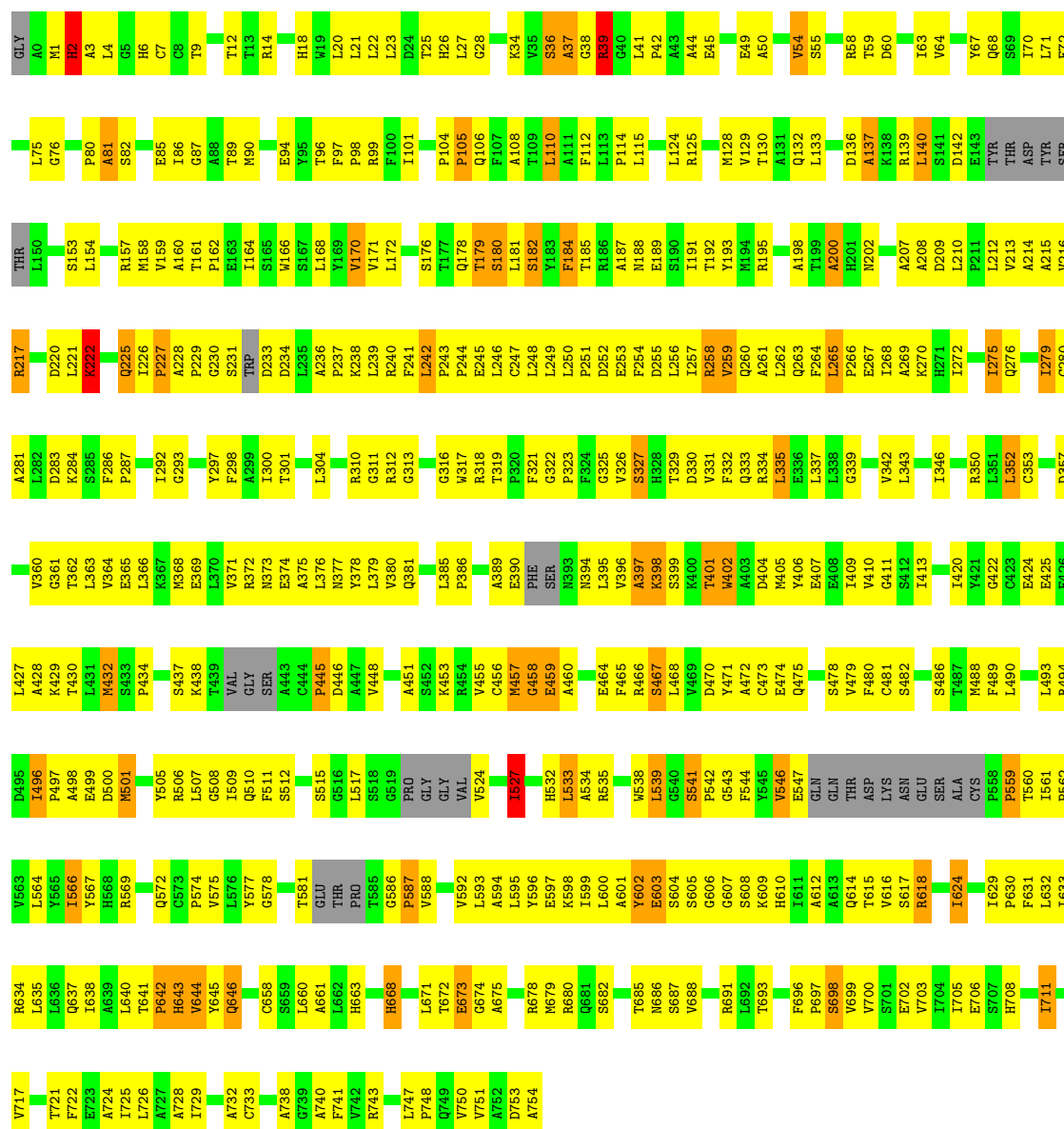
3 Residue-property plots

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

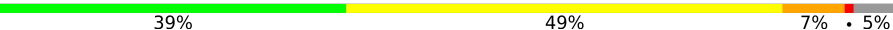
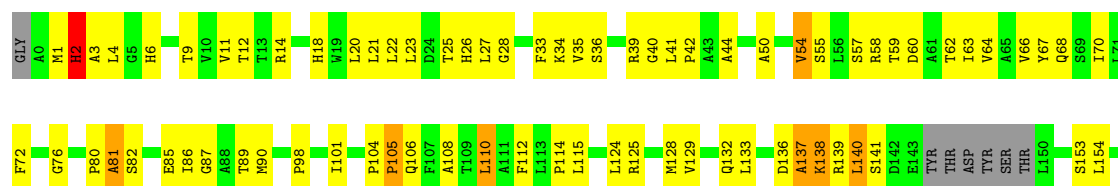
• Molecule 1: GLP_546_48378_50642



• Molecule 1: GLP_546_48378_50642

Chain B:  38% 50% 8% . .

• Molecule 1: GLP_546_48378_50642

Chain C:  39% 49% 7% . 5%



L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715																																																																																																																																																																																																																																																																																													

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.41Å 173.49Å 155.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-3.00) 97.8 (50.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.263 0.216 , 0.246	Depositor DCC
R_{free} test set	3938 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 20.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.478 for l,-k,h	Xtriage
Reported twinning fraction	0.500 for l,-k,h	Depositor
Outliers	0 of 82722 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22372	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/5761	0.99	22/7836 (0.3%)
1	B	0.45	0/5718	0.98	24/7777 (0.3%)
1	C	0.44	0/5666	0.97	27/7704 (0.4%)
1	D	0.45	0/5704	0.98	20/7759 (0.3%)
All	All	0.45	0/22849	0.98	93/31076 (0.3%)

There are no bond length outliers.

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	LEU	CA-C-N	10.32	130.43	120.31
1	A	41	LEU	C-N-CA	10.32	130.43	120.31
1	C	430	THR	N-CA-C	9.07	120.78	111.07
1	A	430	THR	N-CA-C	8.91	120.61	111.07
1	D	430	THR	N-CA-C	8.87	120.56	111.07
1	B	430	THR	N-CA-C	8.72	120.40	111.07
1	C	140	LEU	N-CA-C	-8.41	102.46	112.89
1	A	472	ALA	N-CA-C	-7.62	103.99	113.28
1	D	609	LYS	N-CA-C	-7.59	104.16	113.19
1	B	76	GLY	CA-C-N	7.43	127.60	119.87
1	B	76	GLY	C-N-CA	7.43	127.60	119.87
1	D	541	SER	CA-C-N	7.41	129.10	119.84
1	D	541	SER	C-N-CA	7.41	129.10	119.84
1	C	541	SER	CA-C-N	7.36	129.04	119.84
1	C	541	SER	C-N-CA	7.36	129.04	119.84
1	A	319	THR	CA-C-N	7.26	127.03	119.76
1	A	319	THR	C-N-CA	7.26	127.03	119.76
1	A	76	GLY	CA-C-N	7.26	127.42	119.87
1	A	76	GLY	C-N-CA	7.26	127.42	119.87
1	B	541	SER	CA-C-N	7.20	128.84	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	541	SER	C-N-CA	7.20	128.84	119.84
1	B	319	THR	CA-C-N	7.18	126.94	119.76
1	B	319	THR	C-N-CA	7.18	126.94	119.76
1	A	541	SER	CA-C-N	6.85	128.41	119.84
1	A	541	SER	C-N-CA	6.85	128.41	119.84
1	D	319	THR	CA-C-N	6.81	126.57	119.76
1	D	319	THR	C-N-CA	6.81	126.57	119.76
1	C	76	GLY	CA-C-N	6.70	126.84	119.87
1	C	76	GLY	C-N-CA	6.70	126.84	119.87
1	C	319	THR	CA-C-N	6.70	126.45	119.76
1	C	319	THR	C-N-CA	6.70	126.45	119.76
1	D	76	GLY	CA-C-N	6.61	126.74	119.87
1	D	76	GLY	C-N-CA	6.61	126.74	119.87
1	D	644	VAL	N-CA-C	6.41	117.98	111.00
1	A	392	SER	N-CA-C	-6.21	99.08	108.96
1	C	527	ILE	N-CA-C	-6.15	104.51	110.72
1	B	527	ILE	N-CA-C	-6.14	104.51	110.72
1	B	644	VAL	N-CA-C	6.08	117.62	111.00
1	B	601	ALA	N-CA-C	-6.04	105.41	112.89
1	A	527	ILE	N-CA-C	-6.01	104.88	110.53
1	D	501	MET	N-CA-C	5.97	118.75	111.82
1	A	644	VAL	N-CA-C	5.95	117.48	111.00
1	B	140	LEU	N-CA-C	-5.91	105.16	112.90
1	C	644	VAL	N-CA-C	5.85	117.38	111.00
1	A	501	MET	N-CA-C	5.77	118.52	111.82
1	D	527	ILE	N-CA-C	-5.75	104.91	110.72
1	B	501	MET	N-CA-C	5.74	118.48	111.82
1	B	54	VAL	N-CA-C	5.70	116.62	108.93
1	D	471	TYR	N-CA-C	-5.67	105.13	112.68
1	C	501	MET	N-CA-C	5.65	118.37	111.82
1	B	335	LEU	N-CA-C	-5.64	106.94	113.88
1	D	610	HIS	N-CA-C	-5.56	106.63	113.41
1	C	54	VAL	N-CA-C	5.55	116.42	108.93
1	B	668	HIS	CA-C-N	5.52	125.19	119.56
1	B	668	HIS	C-N-CA	5.52	125.19	119.56
1	B	496	ILE	N-CA-C	5.45	113.32	108.63
1	A	668	HIS	CA-C-N	5.44	125.11	119.56
1	A	668	HIS	C-N-CA	5.44	125.11	119.56
1	A	54	VAL	N-CA-C	5.44	116.27	108.93
1	C	668	HIS	CA-C-N	5.41	125.08	119.56
1	C	668	HIS	C-N-CA	5.41	125.08	119.56
1	A	335	LEU	N-CA-C	-5.39	106.83	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	242	LEU	CA-C-N	5.38	125.92	120.38
1	C	242	LEU	C-N-CA	5.38	125.92	120.38
1	C	185	THR	N-CA-C	5.34	117.09	109.14
1	D	54	VAL	N-CA-C	5.31	116.10	108.93
1	D	185	THR	N-CA-C	5.31	117.06	109.14
1	B	646	GLN	N-CA-C	5.31	117.49	111.02
1	B	265	LEU	N-CA-C	-5.30	106.25	113.57
1	D	646	GLN	N-CA-C	5.25	117.43	111.02
1	B	185	THR	N-CA-C	5.25	116.96	109.14
1	D	496	ILE	N-CA-C	5.24	113.14	108.63
1	C	533	LEU	N-CA-C	-5.24	105.01	111.40
1	C	184	PHE	N-CA-C	-5.22	101.36	109.14
1	A	496	ILE	N-CA-C	5.22	113.12	108.63
1	C	496	ILE	N-CA-C	5.21	113.11	108.63
1	A	185	THR	N-CA-C	5.19	117.08	109.24
1	D	533	LEU	N-CA-C	-5.19	105.06	111.40
1	B	446	ASP	N-CA-C	5.19	119.66	113.23
1	A	266	PRO	N-CA-C	-5.18	106.33	113.53
1	C	250	LEU	CA-C-N	5.17	125.15	120.03
1	C	250	LEU	C-N-CA	5.17	125.15	120.03
1	B	533	LEU	N-CA-C	-5.16	105.10	111.40
1	C	606	GLY	N-CA-C	5.16	118.67	111.19
1	A	600	LEU	N-CA-C	-5.12	106.19	112.90
1	B	399	SER	N-CA-C	5.12	121.70	110.80
1	C	646	GLN	N-CA-C	5.10	117.25	111.02
1	D	355	PHE	CA-C-N	5.05	124.71	119.56
1	D	355	PHE	C-N-CA	5.05	124.71	119.56
1	C	335	LEU	N-CA-C	-5.04	107.27	113.41
1	C	355	PHE	CA-C-N	5.02	124.68	119.56
1	C	355	PHE	C-N-CA	5.02	124.68	119.56
1	B	184	PHE	N-CA-C	-5.01	101.67	109.14

There are no chirality outliers.

There are no planarity outliers.

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	5630	0	5672	468	0
1	B	5590	0	5640	470	0
1	C	5539	0	5592	486	0
1	D	5574	0	5611	477	0
2	A	12	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
2	D	9	0	0	0	0
All	All	22372	0	22515	1889	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 42.

All (1889) 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:465:PHE:HE2	1:B:533:LEU:HD21	1.23	1.03
1:C:597:GLU:HA	1:C:600:LEU:HD12	1.40	1.02
1:C:114:PRO:HA	1:C:258:ARG:HH12	1.21	1.01
1:B:99:ARG:HH12	1:B:390:GLU:C	1.70	0.98
1:C:465:PHE:HE1	1:C:502:LEU:HB2	1.29	0.97
1:B:373:ASN:HD21	1:B:401:THR:HG21	1.26	0.97
1:D:110:LEU:HD13	1:D:272:ILE:HD12	1.44	0.96
1:A:432:MET:HE2	1:A:534:ALA:HB1	1.47	0.95
1:A:373:ASN:HD21	1:A:401:THR:HG21	1.32	0.94
1:B:466:ARG:NE	1:B:498:ALA:HB2	1.81	0.93
1:C:115:LEU:H	1:C:258:ARG:HH22	0.94	0.93
1:A:39:ARG:HD2	1:A:317:TRP:CZ2	2.06	0.91
1:A:220:ASP:HB3	1:A:238:LYS:HD3	1.53	0.91
1:B:432:MET:HE2	1:B:534:ALA:HB1	1.52	0.91
1:A:104:PRO:HB3	1:A:280:CYS:SG	2.10	0.90
1:C:158:MET:HE3	1:C:256:LEU:HB2	1.54	0.89
1:B:466:ARG:HH21	1:B:498:ALA:H	1.18	0.89
1:C:138:LYS:O	1:C:139:ARG:HD2	1.73	0.87
1:D:432:MET:HE2	1:D:534:ALA:HB1	1.54	0.87
1:D:258:ARG:HH11	1:D:258:ARG:HA	1.40	0.87
1:C:110:LEU:HD13	1:C:272:ILE:HD12	1.57	0.87
1:C:115:LEU:H	1:C:258:ARG:NH2	1.73	0.86
1:A:743:ARG:HA	1:A:747:LEU:HB2	1.59	0.85
1:C:432:MET:HE2	1:C:534:ALA:HB1	1.56	0.85
1:C:178:GLN:HE21	1:C:212:LEU:HD12	1.41	0.84
1:D:178:GLN:HE21	1:D:212:LEU:HD12	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:PRO:HB3	1:D:280:CYS:SG	2.17	0.84
1:D:279:ILE:O	1:D:283:ASP:HB2	1.77	0.84
1:B:377:ASN:HD21	1:B:395:LEU:HD21	1.42	0.84
1:C:743:ARG:HA	1:C:747:LEU:HB2	1.57	0.84
1:B:178:GLN:HE21	1:B:212:LEU:HD12	1.43	0.83
1:C:233:ASP:HB3	1:C:236:ALA:HB2	1.60	0.83
1:B:743:ARG:HA	1:B:747:LEU:HB2	1.61	0.83
1:D:743:ARG:HA	1:D:747:LEU:HB2	1.58	0.83
1:B:279:ILE:O	1:B:283:ASP:HB2	1.80	0.82
1:C:279:ILE:O	1:C:283:ASP:HB2	1.79	0.82
1:A:279:ILE:O	1:A:283:ASP:HB2	1.78	0.82
1:C:381:GLN:NE2	1:C:402:TRP:HD1	1.77	0.81
1:C:508:GLY:HA3	1:C:532:HIS:O	1.79	0.81
1:D:1:MET:HG3	1:D:55:SER:HB3	1.61	0.81
1:C:104:PRO:HB3	1:C:280:CYS:SG	2.21	0.81
1:B:220:ASP:HB3	1:B:238:LYS:HD3	1.61	0.81
1:C:350:ARG:HD3	1:C:538:TRP:O	1.81	0.81
1:A:99:ARG:HH11	1:A:390:GLU:CD	1.89	0.80
1:B:36:SER:O	1:B:38:GLY:N	2.15	0.80
1:C:543:GLY:HA3	1:C:561:ILE:O	1.82	0.80
1:A:178:GLN:HE21	1:A:212:LEU:HD12	1.43	0.80
1:C:465:PHE:HA	1:C:468:LEU:HD12	1.64	0.79
1:D:543:GLY:HA3	1:D:561:ILE:O	1.82	0.79
1:A:39:ARG:HD2	1:A:317:TRP:CE2	2.17	0.79
1:D:508:GLY:HA3	1:D:532:HIS:O	1.82	0.79
1:C:305:ARG:HD2	1:C:390:GLU:HB3	1.64	0.79
1:D:333:GLN:NE2	1:D:672:THR:HB	1.98	0.79
1:D:747:LEU:O	1:D:750:VAL:HG12	1.83	0.79
1:D:362:THR:O	1:D:366:LEU:HG	1.83	0.79
1:A:110:LEU:HD13	1:A:272:ILE:HD12	1.64	0.78
1:B:85:GLU:O	1:B:89:THR:HG23	1.83	0.78
1:B:362:THR:O	1:B:366:LEU:HG	1.83	0.78
1:C:85:GLU:O	1:C:89:THR:HG23	1.83	0.78
1:A:609:LYS:HD3	1:A:641:THR:HG22	1.65	0.78
1:C:138:LYS:C	1:C:139:ARG:HD2	2.08	0.78
1:C:362:THR:O	1:C:366:LEU:HG	1.83	0.78
1:D:3:ALA:HB3	1:D:54:VAL:O	1.82	0.78
1:A:85:GLU:O	1:A:89:THR:HG23	1.84	0.78
1:C:747:LEU:O	1:C:750:VAL:HG12	1.85	0.77
1:A:596:TYR:O	1:A:599:ILE:HG22	1.85	0.77
1:D:180:SER:HB2	1:D:208:ALA:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:THR:O	1:A:366:LEU:HG	1.84	0.77
1:B:747:LEU:O	1:B:750:VAL:HG12	1.84	0.77
1:A:399:SER:HA	1:B:395:LEU:HD12	1.66	0.77
1:D:38:GLY:H	1:D:41:LEU:HD12	1.49	0.77
1:D:172:LEU:HD12	1:D:239:LEU:HD13	1.67	0.77
1:C:471:TYR:O	1:C:475:GLN:HB2	1.85	0.77
1:B:465:PHE:HA	1:B:468:LEU:HD12	1.66	0.76
1:D:147:TYR:CG	1:D:150:LEU:HB2	2.20	0.76
1:B:432:MET:HE1	1:B:538:TRP:HB2	1.68	0.76
1:C:205:LEU:HB3	1:C:245:GLU:OE2	1.86	0.76
1:D:139:ARG:NH1	1:D:162:PRO:HG3	2.00	0.76
1:A:508:GLY:HA3	1:A:532:HIS:O	1.85	0.76
1:D:337:LEU:HD22	1:D:673:GLU:HA	1.67	0.76
1:D:369:GLU:HG2	1:D:485:VAL:HG23	1.66	0.76
1:A:3:ALA:HB3	1:A:54:VAL:O	1.85	0.76
1:B:115:LEU:H	1:B:258:ARG:HH22	1.33	0.76
1:C:21:LEU:HD21	1:C:272:ILE:HD11	1.66	0.76
1:C:159:VAL:HG23	1:C:248:LEU:O	1.85	0.76
1:D:352:LEU:HD11	1:D:650:LEU:HD23	1.67	0.76
1:A:392:SER:O	1:A:394:ASN:N	2.17	0.76
1:C:596:TYR:O	1:C:599:ILE:HG22	1.85	0.76
1:D:1:MET:HG3	1:D:55:SER:CB	2.15	0.76
1:D:160:ALA:HB2	1:D:168:LEU:HD23	1.68	0.76
1:A:310:ARG:HH22	1:A:392:SER:HB3	1.49	0.76
1:B:3:ALA:HB3	1:B:54:VAL:O	1.86	0.76
1:B:300:ILE:HG23	1:B:304:LEU:HD12	1.68	0.76
1:A:747:LEU:O	1:A:750:VAL:HG12	1.85	0.75
1:B:160:ALA:HB2	1:B:168:LEU:HD23	1.66	0.75
1:C:465:PHE:CE1	1:C:502:LEU:HB2	2.19	0.75
1:D:300:ILE:HG23	1:D:304:LEU:HD12	1.69	0.75
1:A:300:ILE:HG23	1:A:304:LEU:HD12	1.68	0.75
1:C:160:ALA:HB2	1:C:168:LEU:HD23	1.67	0.75
1:C:705:ILE:HG12	1:C:711:ILE:HD11	1.69	0.75
1:C:180:SER:HB2	1:C:208:ALA:O	1.87	0.75
1:D:635:LEU:HD12	1:D:732:ALA:HB2	1.68	0.75
1:A:635:LEU:HD12	1:A:732:ALA:HB2	1.66	0.74
1:D:596:TYR:O	1:D:599:ILE:HG22	1.87	0.74
1:A:160:ALA:HB2	1:A:168:LEU:HD23	1.69	0.74
1:B:508:GLY:HA3	1:B:532:HIS:O	1.87	0.74
1:C:255:ASP:O	1:C:259:VAL:HG23	1.86	0.74
1:D:343:LEU:HD13	1:D:427:LEU:HD21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:TYR:O	1:B:599:ILE:HG22	1.88	0.74
1:C:115:LEU:N	1:C:258:ARG:HH22	1.78	0.74
1:C:635:LEU:HD12	1:C:732:ALA:HB2	1.69	0.74
1:D:180:SER:HA	1:D:212:LEU:HD21	1.70	0.74
1:A:180:SER:HA	1:A:212:LEU:HD21	1.70	0.74
1:A:180:SER:HB2	1:A:208:ALA:O	1.88	0.74
1:C:180:SER:HA	1:C:212:LEU:HD21	1.70	0.74
1:B:466:ARG:CZ	1:B:498:ALA:HB2	2.17	0.74
1:B:180:SER:HB2	1:B:208:ALA:O	1.87	0.74
1:A:379:LEU:HD21	1:A:481:CYS:HB3	1.70	0.73
1:B:465:PHE:CE2	1:B:533:LEU:HD21	2.15	0.73
1:B:139:ARG:HG3	1:B:247:CYS:O	1.88	0.73
1:D:259:VAL:O	1:D:262:LEU:HB3	1.89	0.73
1:C:432:MET:HE1	1:C:538:TRP:HB2	1.69	0.73
1:B:346:ILE:HG21	1:B:427:LEU:HD13	1.71	0.73
1:B:350:ARG:HD3	1:B:538:TRP:O	1.88	0.73
1:B:139:ARG:HG2	1:B:245:GLU:O	1.87	0.73
1:A:158:MET:HG3	1:A:259:VAL:HG21	1.70	0.73
1:B:39:ARG:HG3	1:B:317:TRP:CZ2	2.24	0.73
1:C:634:ARG:O	1:C:638:ILE:HG13	1.88	0.72
1:D:432:MET:HE1	1:D:538:TRP:HB2	1.71	0.72
1:A:432:MET:HA	1:A:479:VAL:O	1.90	0.72
1:B:178:GLN:HB2	1:B:182:SER:OG	1.89	0.72
1:B:180:SER:HA	1:B:212:LEU:HD21	1.70	0.72
1:B:394:ASN:OD1	1:B:396:VAL:HG12	1.88	0.72
1:B:561:ILE:H	1:B:561:ILE:HD12	1.54	0.72
1:A:634:ARG:O	1:A:638:ILE:HG13	1.90	0.72
1:A:352:LEU:HD12	1:A:363:LEU:HD13	1.70	0.72
1:B:264:PHE:O	1:B:268:ILE:HG13	1.90	0.72
1:B:635:LEU:HD12	1:B:732:ALA:HB2	1.71	0.72
1:C:235:LEU:C	1:C:237:PRO:HD2	2.14	0.72
1:D:609:LYS:NZ	1:D:641:THR:HG21	2.05	0.72
1:C:14:ARG:NH2	1:C:224:HIS:O	2.22	0.72
1:A:310:ARG:NH1	1:A:310:ARG:HB2	2.05	0.72
1:D:342:VAL:HG12	1:D:658:CYS:SG	2.29	0.72
1:A:561:ILE:HD12	1:A:561:ILE:H	1.53	0.72
1:C:14:ARG:HD2	1:C:260:GLN:OE1	1.89	0.72
1:C:114:PRO:CA	1:C:258:ARG:HH12	2.01	0.72
1:B:602:TYR:HD2	1:B:634:ARG:NH1	1.86	0.71
1:C:133:LEU:O	1:C:137:ALA:N	2.23	0.71
1:D:705:ILE:HG12	1:D:711:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:ILE:HG12	1:A:711:ILE:HD11	1.72	0.71
1:A:228:ALA:O	1:A:230:GLY:N	2.23	0.71
1:A:624:ILE:HD13	1:A:624:ILE:H	1.55	0.71
1:C:178:GLN:HB2	1:C:182:SER:OG	1.90	0.71
1:C:310:ARG:NH1	1:C:310:ARG:HB2	2.05	0.71
1:D:624:ILE:H	1:D:624:ILE:HD13	1.54	0.71
1:B:705:ILE:HG12	1:B:711:ILE:HD11	1.73	0.71
1:D:448:VAL:HG13	1:D:468:LEU:HD23	1.72	0.71
1:A:41:LEU:HD12	1:A:41:LEU:O	1.90	0.71
1:A:98:PRO:HA	1:A:101:ILE:HD11	1.73	0.71
1:D:498:ALA:HA	1:D:501:MET:HE3	1.72	0.71
1:D:561:ILE:H	1:D:561:ILE:HD12	1.55	0.71
1:B:437:SER:HB3	1:B:478:SER:O	1.90	0.71
1:C:466:ARG:NH2	1:C:498:ALA:H	1.89	0.71
1:D:236:ALA:N	1:D:237:PRO:HD2	2.06	0.71
1:C:98:PRO:HA	1:C:101:ILE:HD11	1.73	0.70
1:A:520:PRO:HD2	1:D:698:SER:OG	1.92	0.70
1:B:98:PRO:HA	1:B:101:ILE:HD11	1.73	0.70
1:B:634:ARG:O	1:B:638:ILE:HG13	1.90	0.70
1:D:178:GLN:HB2	1:D:182:SER:OG	1.91	0.70
1:D:463:HIS:O	1:D:466:ARG:HB3	1.91	0.70
1:C:596:TYR:O	1:C:600:LEU:HG	1.90	0.70
1:C:597:GLU:HA	1:C:600:LEU:CD1	2.19	0.70
1:D:98:PRO:HA	1:D:101:ILE:HD11	1.73	0.70
1:B:21:LEU:HD21	1:B:272:ILE:HD11	1.72	0.70
1:D:37:ALA:HB2	1:D:43:ALA:HB2	1.72	0.70
1:D:85:GLU:O	1:D:89:THR:HG23	1.91	0.70
1:D:310:ARG:NH1	1:D:310:ARG:HB2	2.07	0.70
1:A:67:TYR:OH	1:A:114:PRO:HG3	1.92	0.70
1:B:129:VAL:O	1:B:133:LEU:HG	1.90	0.70
1:D:602:TYR:O	1:D:634:ARG:NH1	2.25	0.69
1:C:300:ILE:HG23	1:C:304:LEU:HD12	1.73	0.69
1:A:337:LEU:HD22	1:A:673:GLU:HA	1.74	0.69
1:B:498:ALA:HA	1:B:501:MET:HE3	1.74	0.69
1:A:137:ALA:CB	1:A:248:LEU:HD21	2.22	0.69
1:B:352:LEU:HD12	1:B:363:LEU:HD13	1.73	0.69
1:D:158:MET:HE1	1:D:170:VAL:HB	1.75	0.69
1:C:158:MET:HG3	1:C:259:VAL:HG21	1.74	0.69
1:B:466:ARG:NH2	1:B:498:ALA:H	1.89	0.69
1:C:343:LEU:HD13	1:C:427:LEU:HD21	1.75	0.69
1:C:624:ILE:HD13	1:C:624:ILE:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:ALA:HA	1:A:501:MET:HE3	1.74	0.69
1:C:158:MET:HE1	1:C:170:VAL:HB	1.75	0.69
1:D:352:LEU:HD12	1:D:363:LEU:HD13	1.75	0.69
1:B:310:ARG:NH1	1:B:310:ARG:HB2	2.07	0.69
1:C:129:VAL:O	1:C:133:LEU:HG	1.93	0.69
1:D:172:LEU:HD12	1:D:239:LEU:CD1	2.23	0.69
1:D:172:LEU:HB2	1:D:214:ALA:O	1.92	0.69
1:A:610:HIS:CD2	1:A:614:GLN:HE21	2.11	0.68
1:B:618:ARG:HB2	1:B:618:ARG:HH11	1.57	0.68
1:B:624:ILE:H	1:B:624:ILE:HD13	1.57	0.68
1:C:561:ILE:H	1:C:561:ILE:HD12	1.58	0.68
1:D:634:ARG:O	1:D:638:ILE:HG13	1.93	0.68
1:B:110:LEU:HD13	1:B:272:ILE:HD12	1.74	0.68
1:D:159:VAL:HG23	1:D:248:LEU:C	2.19	0.68
1:A:138:LYS:HD3	1:A:142:ASP:HB3	1.73	0.68
1:C:36:SER:HB3	1:C:317:TRP:HB3	1.76	0.68
1:A:369:GLU:HG3	1:A:482:SER:OG	1.93	0.68
1:C:125:ARG:HG2	1:C:125:ARG:HH11	1.58	0.68
1:C:180:SER:O	1:C:193:TYR:HB2	1.93	0.68
1:C:284:LYS:HD2	1:C:284:LYS:H	1.58	0.68
1:C:158:MET:HE3	1:C:256:LEU:CB	2.23	0.68
1:D:609:LYS:HE3	1:D:637:GLN:HB3	1.74	0.68
1:A:178:GLN:HB2	1:A:182:SER:OG	1.93	0.68
1:B:333:GLN:HE21	1:B:673:GLU:HB3	1.58	0.68
1:C:198:ALA:O	1:C:202:ASN:HA	1.94	0.68
1:A:548:GLN:HA	1:A:548:GLN:HE21	1.57	0.68
1:B:139:ARG:HH21	1:B:162:PRO:HG3	1.58	0.68
1:A:307:ASP:HB3	1:A:391:PHE:HB2	1.75	0.68
1:C:420:ILE:O	1:C:424:GLU:HG3	1.94	0.68
1:D:602:TYR:CE1	1:D:603:GLU:HG2	2.28	0.68
1:C:67:TYR:OH	1:C:114:PRO:HG3	1.94	0.68
1:A:543:GLY:HA3	1:A:561:ILE:O	1.94	0.67
1:D:615:THR:HA	1:D:618:ARG:HH12	1.59	0.67
1:A:129:VAL:O	1:A:133:LEU:HG	1.94	0.67
1:A:618:ARG:HH11	1:A:618:ARG:HB2	1.58	0.67
1:D:139:ARG:HH12	1:D:162:PRO:HG3	1.54	0.67
1:B:377:ASN:HD21	1:B:395:LEU:CD2	2.05	0.67
1:C:114:PRO:HA	1:C:258:ARG:NH1	2.02	0.67
1:C:618:ARG:HB2	1:C:618:ARG:HH11	1.60	0.67
1:C:498:ALA:HA	1:C:501:MET:HE3	1.75	0.67
1:B:284:LYS:H	1:B:284:LYS:HD2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:SER:HB3	1:D:478:SER:O	1.95	0.67
1:A:284:LYS:H	1:A:284:LYS:HD2	1.60	0.67
1:A:339:GLY:HA3	1:A:407:GLU:O	1.95	0.67
1:B:236:ALA:N	1:B:237:PRO:HD2	2.10	0.67
1:C:193:TYR:CE2	1:C:241:PHE:HB2	2.30	0.67
1:A:523:VAL:HG11	1:D:618:ARG:HB2	1.77	0.67
1:B:39:ARG:HD2	1:B:39:ARG:N	2.09	0.67
1:C:159:VAL:HG23	1:C:248:LEU:C	2.20	0.67
1:C:260:GLN:O	1:C:263:GLN:HG2	1.95	0.67
1:D:180:SER:O	1:D:193:TYR:HB2	1.95	0.67
1:D:608:SER:HA	1:D:611:ILE:HG12	1.77	0.67
1:B:373:ASN:ND2	1:B:401:THR:HG21	2.07	0.66
1:C:3:ALA:HB3	1:C:54:VAL:O	1.94	0.66
1:A:420:ILE:O	1:A:424:GLU:HG3	1.95	0.66
1:C:381:GLN:NE2	1:C:402:TRP:CD1	2.61	0.66
1:B:679:MET:O	1:B:750:VAL:HG23	1.96	0.66
1:C:333:GLN:NE2	1:C:672:THR:HB	2.10	0.66
1:C:687:SER:O	1:C:691:ARG:HG3	1.95	0.66
1:D:527:ILE:H	1:D:527:ILE:HD12	1.59	0.66
1:A:527:ILE:H	1:A:527:ILE:HD12	1.61	0.66
1:B:527:ILE:H	1:B:527:ILE:HD12	1.60	0.66
1:D:213:VAL:O	1:D:241:PHE:HA	1.95	0.66
1:C:337:LEU:HD22	1:C:673:GLU:HA	1.76	0.66
1:C:305:ARG:CD	1:C:390:GLU:HG2	2.25	0.66
1:D:60:ASP:CG	1:D:124:LEU:HD13	2.21	0.66
1:D:129:VAL:O	1:D:133:LEU:HG	1.95	0.66
1:B:180:SER:O	1:B:193:TYR:HB2	1.95	0.66
1:C:615:THR:HA	1:C:618:ARG:HH12	1.59	0.66
1:D:198:ALA:O	1:D:202:ASN:HA	1.95	0.66
1:D:610:HIS:CD2	1:D:614:GLN:HE21	2.13	0.66
1:B:172:LEU:HB2	1:B:214:ALA:O	1.96	0.66
1:D:67:TYR:OH	1:D:114:PRO:HG3	1.94	0.66
1:C:332:PHE:CZ	1:C:400:LYS:HE2	2.31	0.66
1:B:90:MET:CE	1:B:318:ARG:HH22	2.09	0.65
1:B:610:HIS:CD2	1:B:614:GLN:HE21	2.14	0.65
1:D:409:ILE:O	1:D:413:ILE:HG12	1.97	0.65
1:B:228:ALA:O	1:B:230:GLY:N	2.30	0.65
1:C:39:ARG:O	1:C:41:LEU:N	2.29	0.65
1:D:138:LYS:HD3	1:D:142:ASP:HB3	1.77	0.65
1:D:172:LEU:HD11	1:D:216:VAL:HG23	1.78	0.65
1:A:717:VAL:O	1:A:721:THR:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:610:HIS:CD2	1:C:614:GLN:HE21	2.13	0.65
1:D:14:ARG:HD3	1:D:257:ILE:HD13	1.76	0.65
1:B:420:ILE:O	1:B:424:GLU:HG3	1.95	0.65
1:C:172:LEU:HB2	1:C:214:ALA:O	1.97	0.65
1:A:158:MET:HE1	1:A:170:VAL:HB	1.78	0.65
1:A:180:SER:O	1:A:193:TYR:HB2	1.97	0.65
1:B:1:MET:HG3	1:B:55:SER:HB3	1.77	0.65
1:C:527:ILE:HD12	1:C:527:ILE:H	1.62	0.65
1:D:251:PRO:HG2	1:D:254:PHE:CD1	2.31	0.65
1:B:255:ASP:OD1	1:B:258:ARG:HB2	1.95	0.65
1:D:679:MET:O	1:D:750:VAL:HG23	1.97	0.65
1:A:629:ILE:O	1:A:633:ILE:HG12	1.96	0.65
1:B:615:THR:HA	1:B:618:ARG:HH12	1.62	0.65
1:A:469:VAL:O	1:A:473:CYS:HB2	1.96	0.65
1:D:125:ARG:HH11	1:D:125:ARG:HG2	1.62	0.65
1:A:642:PRO:O	1:A:644:VAL:N	2.30	0.65
1:A:1:MET:HG3	1:A:55:SER:HB3	1.80	0.64
1:A:226:ILE:N	1:A:226:ILE:HD12	2.12	0.64
1:A:523:VAL:C	1:A:524:VAL:HG23	2.20	0.64
1:B:140:LEU:HD21	1:B:249:LEU:HB2	1.77	0.64
1:B:629:ILE:O	1:B:633:ILE:HG12	1.97	0.64
1:C:44:ALA:HB3	1:C:264:PHE:CE2	2.31	0.64
1:C:115:LEU:O	1:C:258:ARG:NH2	2.29	0.64
1:C:137:ALA:CB	1:C:248:LEU:HD21	2.26	0.64
1:A:4:LEU:HD22	1:A:25:THR:O	1.97	0.64
1:A:60:ASP:O	1:A:64:VAL:HG23	1.97	0.64
1:B:225:GLN:NE2	1:B:225:GLN:H	1.95	0.64
1:B:458:GLY:C	1:B:460:ALA:H	2.06	0.64
1:C:466:ARG:NE	1:C:498:ALA:HB2	2.10	0.64
1:A:310:ARG:HB2	1:A:310:ARG:HH11	1.62	0.64
1:A:343:LEU:HD13	1:A:427:LEU:HD21	1.79	0.64
1:A:432:MET:HE1	1:A:538:TRP:HB2	1.77	0.64
1:B:157:ARG:HE	1:B:249:LEU:HD21	1.62	0.64
1:B:198:ALA:O	1:B:202:ASN:HA	1.97	0.64
1:B:225:GLN:H	1:B:225:GLN:CD	2.05	0.64
1:A:140:LEU:HB2	1:A:244:PRO:O	1.96	0.64
1:A:352:LEU:HD11	1:A:650:LEU:HD23	1.78	0.64
1:C:172:LEU:HD11	1:C:216:VAL:HG23	1.78	0.64
1:D:1:MET:HE2	1:D:55:SER:HB3	1.78	0.64
1:D:1:MET:HA	1:D:56:LEU:H	1.63	0.64
1:A:198:ALA:O	1:A:202:ASN:HA	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:MET:HE1	1:B:170:VAL:HB	1.78	0.64
1:C:352:LEU:HD12	1:C:363:LEU:HD13	1.78	0.64
1:A:444:CYS:SG	1:A:448:VAL:HB	2.36	0.64
1:C:381:GLN:HE21	1:C:402:TRP:HD1	1.43	0.64
1:D:140:LEU:HB3	1:D:144:TYR:HE2	1.63	0.64
1:A:458:GLY:C	1:A:460:ALA:H	2.06	0.64
1:B:139:ARG:NH2	1:B:162:PRO:HG3	2.13	0.64
1:C:82:SER:O	1:C:86:ILE:HG13	1.97	0.64
1:D:226:ILE:N	1:D:226:ILE:HD12	2.13	0.64
1:D:284:LYS:H	1:D:284:LYS:HD2	1.62	0.64
1:B:67:TYR:OH	1:B:114:PRO:HG3	1.97	0.64
1:D:420:ILE:O	1:D:424:GLU:HG3	1.96	0.64
1:A:256:LEU:O	1:A:257:ILE:C	2.41	0.64
1:C:39:ARG:C	1:C:41:LEU:H	2.06	0.64
1:D:4:LEU:HD22	1:D:25:THR:O	1.98	0.64
1:D:191:ILE:HG23	1:D:195:ARG:HD3	1.79	0.64
1:A:125:ARG:HG2	1:A:125:ARG:HH11	1.63	0.64
1:A:561:ILE:HD12	1:A:561:ILE:N	2.13	0.64
1:B:373:ASN:HD21	1:B:401:THR:CG2	2.08	0.64
1:B:409:ILE:O	1:B:413:ILE:HG12	1.98	0.64
1:D:637:GLN:O	1:D:641:THR:HG23	1.98	0.64
1:A:402:TRP:CH2	1:B:396:VAL:HG23	2.34	0.63
1:A:494:ARG:HG2	1:A:494:ARG:NH1	2.13	0.63
1:A:615:THR:HA	1:A:618:ARG:HH12	1.62	0.63
1:B:4:LEU:HD22	1:B:25:THR:O	1.98	0.63
1:C:4:LEU:HD22	1:C:25:THR:O	1.99	0.63
1:C:458:GLY:C	1:C:460:ALA:H	2.05	0.63
1:D:386:PRO:O	1:D:389:ALA:HB3	1.98	0.63
1:B:125:ARG:HG2	1:B:125:ARG:HH11	1.62	0.63
1:C:114:PRO:HB3	1:C:258:ARG:NH1	2.12	0.63
1:C:310:ARG:HB2	1:C:310:ARG:HH11	1.63	0.63
1:D:458:GLY:C	1:D:460:ALA:H	2.06	0.63
1:C:717:VAL:O	1:C:721:THR:HG23	1.99	0.63
1:A:679:MET:O	1:A:750:VAL:HG23	1.98	0.63
1:B:191:ILE:HG23	1:B:195:ARG:HD3	1.81	0.63
1:C:1:MET:HG3	1:C:55:SER:HB3	1.80	0.63
1:C:191:ILE:HG23	1:C:195:ARG:HD3	1.79	0.63
1:A:158:MET:HE3	1:A:256:LEU:HB2	1.80	0.63
1:B:226:ILE:HD12	1:B:226:ILE:N	2.13	0.63
1:B:310:ARG:HB2	1:B:310:ARG:HH11	1.64	0.63
1:B:561:ILE:HD12	1:B:561:ILE:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:ALA:N	1:D:237:PRO:CD	2.62	0.63
1:B:687:SER:O	1:B:691:ARG:HG3	1.98	0.63
1:C:41:LEU:HD13	1:C:264:PHE:CE2	2.33	0.63
1:D:225:GLN:H	1:D:225:GLN:CD	2.07	0.63
1:A:307:ASP:OD1	1:A:391:PHE:HA	1.97	0.63
1:A:432:MET:HE3	1:A:480:PHE:CZ	2.33	0.63
1:B:265:LEU:N	1:B:266:PRO:CD	2.62	0.63
1:C:256:LEU:O	1:C:259:VAL:N	2.29	0.63
1:A:137:ALA:HB1	1:A:248:LEU:HD21	1.78	0.63
1:A:243:PRO:HD2	1:A:246:LEU:HD12	1.81	0.63
1:A:310:ARG:NH2	1:A:392:SER:HB3	2.14	0.63
1:D:687:SER:O	1:D:691:ARG:HG3	1.98	0.63
1:A:82:SER:O	1:A:86:ILE:HG13	1.99	0.62
1:C:226:ILE:HD12	1:C:226:ILE:N	2.14	0.62
1:D:494:ARG:HG2	1:D:494:ARG:HH11	1.64	0.62
1:A:472:ALA:HA	1:A:477:ILE:HD12	1.81	0.62
1:C:187:ALA:O	1:C:188:ASN:HB2	1.99	0.62
1:B:60:ASP:O	1:B:64:VAL:HG23	1.99	0.62
1:B:94:GLU:HG2	1:B:316:GLY:CA	2.29	0.62
1:A:494:ARG:HG2	1:A:494:ARG:HH11	1.64	0.62
1:A:678:ARG:NH2	1:A:753:ASP:OD1	2.33	0.62
1:D:251:PRO:HG2	1:D:254:PHE:CE1	2.35	0.62
1:A:395:LEU:N	1:A:395:LEU:HD23	2.15	0.62
1:B:159:VAL:HG23	1:B:248:LEU:C	2.23	0.62
1:B:434:PRO:HA	1:B:527:ILE:CG2	2.28	0.62
1:D:225:GLN:H	1:D:225:GLN:NE2	1.97	0.62
1:A:705:ILE:HG23	1:A:711:ILE:HD11	1.82	0.62
1:B:717:VAL:O	1:B:721:THR:HG23	1.98	0.62
1:D:243:PRO:HD2	1:D:246:LEU:HD12	1.82	0.62
1:D:260:GLN:O	1:D:264:PHE:HE1	1.83	0.62
1:D:618:ARG:HB2	1:D:618:ARG:HH11	1.64	0.62
1:A:38:GLY:HA3	1:A:317:TRP:CZ3	2.35	0.62
1:A:172:LEU:HD11	1:A:216:VAL:HG23	1.82	0.62
1:B:434:PRO:HA	1:B:527:ILE:HG22	1.81	0.62
1:C:305:ARG:NE	1:C:390:GLU:HG2	2.15	0.62
1:C:473:CYS:C	1:C:475:GLN:H	2.08	0.62
1:C:679:MET:O	1:C:750:VAL:HG23	2.00	0.62
1:A:172:LEU:HB2	1:A:214:ALA:O	2.00	0.62
1:B:187:ALA:O	1:B:188:ASN:HB2	2.00	0.62
1:C:60:ASP:O	1:C:64:VAL:HG23	2.00	0.62
1:C:372:ARG:HD2	1:C:374:GLU:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:747:LEU:HB3	1:C:748:PRO:HD3	1.81	0.62
1:A:60:ASP:CG	1:A:124:LEU:HD13	2.24	0.62
1:B:104:PRO:HB3	1:B:280:CYS:SG	2.40	0.62
1:C:346:ILE:HG21	1:C:427:LEU:HD13	1.80	0.62
1:C:629:ILE:O	1:C:633:ILE:HG12	1.99	0.62
1:A:225:GLN:NE2	1:A:225:GLN:H	1.98	0.61
1:B:394:ASN:O	1:B:395:LEU:HB2	1.98	0.61
1:D:494:ARG:HG2	1:D:494:ARG:NH1	2.14	0.61
1:A:405:MET:O	1:A:409:ILE:HD13	1.99	0.61
1:C:361:GLY:O	1:C:365:GLU:HG3	2.00	0.61
1:C:699:VAL:O	1:C:703:VAL:HG23	2.00	0.61
1:D:642:PRO:O	1:D:644:VAL:N	2.33	0.61
1:A:687:SER:O	1:A:691:ARG:HG3	2.01	0.61
1:B:60:ASP:CG	1:B:124:LEU:HD13	2.25	0.61
1:B:721:THR:O	1:B:725:ILE:HG12	2.01	0.61
1:D:147:TYR:HB3	1:D:150:LEU:HD22	1.82	0.61
1:A:191:ILE:HG23	1:A:195:ARG:HD3	1.83	0.61
1:C:642:PRO:O	1:C:644:VAL:N	2.33	0.61
1:A:71:LEU:HD22	1:A:262:LEU:HD13	1.81	0.61
1:A:747:LEU:HB3	1:A:748:PRO:HD3	1.81	0.61
1:C:178:GLN:HE21	1:C:212:LEU:CD1	2.14	0.61
1:B:139:ARG:HH21	1:B:162:PRO:CG	2.13	0.61
1:B:243:PRO:HD2	1:B:246:LEU:HD12	1.82	0.61
1:D:629:ILE:O	1:D:633:ILE:HG12	2.01	0.61
1:B:154:LEU:HA	1:B:157:ARG:HD3	1.83	0.61
1:C:262:LEU:HB3	1:C:263:GLN:NE2	2.16	0.61
1:D:717:VAL:O	1:D:721:THR:HG23	2.00	0.61
1:A:310:ARG:O	1:A:312:ARG:HG2	2.01	0.61
1:B:705:ILE:HG23	1:B:711:ILE:HD11	1.81	0.61
1:A:217:ARG:HB3	1:A:220:ASP:OD2	2.01	0.61
1:A:225:GLN:H	1:A:225:GLN:CD	2.07	0.61
1:B:432:MET:HA	1:B:479:VAL:O	2.01	0.61
1:C:60:ASP:CG	1:C:124:LEU:HD13	2.25	0.61
1:D:60:ASP:O	1:D:64:VAL:HG23	2.01	0.61
1:B:140:LEU:C	1:B:142:ASP:H	2.09	0.60
1:D:136:ASP:O	1:D:137:ALA:C	2.44	0.60
1:D:310:ARG:HB2	1:D:310:ARG:HH11	1.64	0.60
1:D:693:THR:OG1	1:D:722:PHE:HB2	2.01	0.60
1:A:489:PHE:CZ	1:A:534:ALA:HA	2.36	0.60
1:B:172:LEU:HD11	1:B:216:VAL:HG23	1.81	0.60
1:D:369:GLU:HG3	1:D:482:SER:CB	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:ILE:HD12	1:D:561:ILE:N	2.16	0.60
1:D:699:VAL:O	1:D:703:VAL:HG23	2.00	0.60
1:A:33:PHE:CD2	1:A:318:ARG:HB2	2.36	0.60
1:A:115:LEU:O	1:A:258:ARG:NH2	2.34	0.60
1:A:535:ARG:O	1:A:539:LEU:HD12	2.01	0.60
1:B:217:ARG:HB3	1:B:220:ASP:OD2	2.00	0.60
1:B:372:ARG:HD2	1:B:374:GLU:OE1	2.02	0.60
1:A:346:ILE:HG21	1:A:427:LEU:HD13	1.81	0.60
1:B:564:LEU:HB3	1:B:592:VAL:HG11	1.83	0.60
1:B:437:SER:HB3	1:B:478:SER:H	1.65	0.60
1:C:605:SER:HB3	1:C:634:ARG:HH12	1.66	0.60
1:D:37:ALA:HB2	1:D:43:ALA:CA	2.31	0.60
1:D:41:LEU:HD12	1:D:41:LEU:O	2.00	0.60
1:D:235:LEU:C	1:D:237:PRO:HD2	2.26	0.60
1:A:12:THR:HG22	1:A:44:ALA:HB2	1.82	0.60
1:A:564:LEU:HB3	1:A:592:VAL:HG11	1.84	0.60
1:D:154:LEU:HA	1:D:157:ARG:HD3	1.84	0.60
1:D:292:ILE:HD12	1:D:292:ILE:C	2.26	0.60
1:D:342:VAL:HA	1:D:658:CYS:SG	2.42	0.60
1:D:567:TYR:HA	1:D:572:GLN:HE22	1.66	0.60
1:D:609:LYS:HZ3	1:D:641:THR:HG21	1.64	0.60
1:C:409:ILE:O	1:C:413:ILE:HG12	2.01	0.60
1:C:564:LEU:HB3	1:C:592:VAL:HG11	1.82	0.60
1:D:145:THR:C	1:D:147:TYR:H	2.08	0.60
1:D:310:ARG:O	1:D:312:ARG:HG2	2.02	0.60
1:D:369:GLU:CG	1:D:485:VAL:HG23	2.30	0.60
1:D:405:MET:O	1:D:409:ILE:HD13	2.02	0.60
1:B:535:ARG:O	1:B:539:LEU:HD12	2.01	0.60
1:B:699:VAL:O	1:B:703:VAL:HG23	2.02	0.60
1:D:80:PRO:O	1:D:82:SER:N	2.35	0.60
1:D:678:ARG:NH2	1:D:753:ASP:OD1	2.34	0.60
1:A:350:ARG:HD3	1:A:538:TRP:O	2.02	0.60
1:A:368:MET:O	1:A:372:ARG:HB2	2.02	0.60
1:B:361:GLY:O	1:B:365:GLU:HG3	2.02	0.60
1:C:235:LEU:C	1:C:237:PRO:CD	2.75	0.60
1:C:259:VAL:O	1:C:263:GLN:NE2	2.35	0.60
1:C:284:LYS:HD2	1:C:284:LYS:N	2.17	0.60
1:C:561:ILE:HD12	1:C:561:ILE:N	2.17	0.60
1:C:705:ILE:HG23	1:C:711:ILE:HD11	1.83	0.60
1:D:221:LEU:O	1:D:222:LYS:C	2.45	0.60
1:D:327:SER:O	1:D:331:VAL:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:MET:CE	1:A:256:LEU:HD13	2.32	0.59
1:A:409:ILE:O	1:A:413:ILE:HG12	2.02	0.59
1:B:642:PRO:O	1:B:644:VAL:N	2.35	0.59
1:C:36:SER:HB2	1:C:312:ARG:O	2.03	0.59
1:C:139:ARG:HG3	1:C:247:CYS:O	2.02	0.59
1:C:140:LEU:HD23	1:C:249:LEU:HB2	1.84	0.59
1:C:161:THR:OG1	1:C:164:ILE:HB	2.01	0.59
1:D:217:ARG:HB3	1:D:220:ASP:OD2	2.00	0.59
1:D:747:LEU:HB3	1:D:748:PRO:HD3	1.84	0.59
1:A:567:TYR:HA	1:A:572:GLN:HE22	1.68	0.59
1:C:693:THR:OG1	1:C:722:PHE:HB2	2.02	0.59
1:C:612:ALA:O	1:C:616:VAL:HG23	2.02	0.59
1:D:187:ALA:O	1:D:188:ASN:HB2	2.02	0.59
1:D:261:ALA:O	1:D:264:PHE:HD1	1.84	0.59
1:A:432:MET:HE2	1:A:534:ALA:CB	2.28	0.59
1:A:34:LYS:HB3	1:A:45:GLU:HG3	1.82	0.59
1:B:693:THR:OG1	1:B:722:PHE:HB2	2.03	0.59
1:C:21:LEU:HD11	1:C:110:LEU:HB2	1.84	0.59
1:C:171:VAL:HA	1:C:215:ALA:HB2	1.84	0.59
1:C:262:LEU:C	1:C:264:PHE:H	2.10	0.59
1:A:420:ILE:HD13	1:A:569:ARG:NH2	2.17	0.59
1:A:523:VAL:HB	1:A:528:ASP:OD2	2.02	0.59
1:B:71:LEU:HD22	1:B:262:LEU:CD1	2.33	0.59
1:B:494:ARG:NH1	1:B:494:ARG:HG2	2.17	0.59
1:C:225:GLN:CD	1:C:225:GLN:H	2.08	0.59
1:B:448:VAL:HG13	1:B:468:LEU:HD23	1.84	0.59
1:C:14:ARG:HH12	1:C:223:ASP:HA	1.67	0.59
1:C:154:LEU:HA	1:C:157:ARG:HD3	1.83	0.59
1:D:82:SER:O	1:D:86:ILE:HG13	2.02	0.59
1:B:559:PRO:CG	1:B:599:ILE:HG13	2.33	0.59
1:B:599:ILE:HG21	1:B:631:PHE:CE1	2.38	0.59
1:B:637:GLN:O	1:B:641:THR:HG23	2.02	0.59
1:A:187:ALA:O	1:A:188:ASN:HB2	2.03	0.59
1:B:136:ASP:O	1:B:137:ALA:C	2.46	0.59
1:B:333:GLN:NE2	1:B:672:THR:HB	2.18	0.59
1:B:497:PRO:HG2	1:B:500:ASP:OD2	2.03	0.59
1:C:327:SER:O	1:C:331:VAL:HG23	2.02	0.59
1:D:141:SER:C	1:D:143:GLU:H	2.11	0.59
1:D:144:TYR:CE2	1:D:244:PRO:HB3	2.38	0.59
1:D:548:GLN:HA	1:D:548:GLN:HE21	1.67	0.59
1:B:94:GLU:HG2	1:B:316:GLY:HA3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:PRO:O	1:B:699:VAL:N	2.36	0.59
1:C:225:GLN:H	1:C:225:GLN:NE2	2.00	0.59
1:C:391:PHE:O	1:C:392:SER:HB3	2.03	0.59
1:C:605:SER:CB	1:C:634:ARG:HH12	2.16	0.59
1:D:171:VAL:HA	1:D:215:ALA:HB2	1.84	0.59
1:D:612:ALA:HB2	1:D:703:VAL:HG21	1.85	0.59
1:D:705:ILE:HG23	1:D:711:ILE:HD11	1.85	0.59
1:B:473:CYS:HA	1:B:490:LEU:HD13	1.84	0.58
1:C:217:ARG:HB3	1:C:220:ASP:OD2	2.02	0.58
1:C:494:ARG:HG2	1:C:494:ARG:NH1	2.17	0.58
1:D:608:SER:C	1:D:610:HIS:H	2.11	0.58
1:A:80:PRO:O	1:A:82:SER:N	2.35	0.58
1:A:266:PRO:O	1:A:270:LYS:HG3	2.04	0.58
1:A:535:ARG:HG3	1:A:535:ARG:HH11	1.69	0.58
1:B:310:ARG:O	1:B:312:ARG:HG2	2.03	0.58
1:C:310:ARG:O	1:C:312:ARG:HG2	2.03	0.58
1:D:457:MET:O	1:D:459:GLU:N	2.36	0.58
1:D:564:LEU:HB3	1:D:592:VAL:HG11	1.84	0.58
1:A:159:VAL:HG23	1:A:248:LEU:C	2.28	0.58
1:A:372:ARG:HD2	1:A:374:GLU:OE1	2.02	0.58
1:B:292:ILE:C	1:B:292:ILE:HD12	2.28	0.58
1:D:401:THR:HG22	1:D:402:TRP:N	2.17	0.58
1:A:221:LEU:O	1:A:222:LYS:C	2.47	0.58
1:A:253:GLU:O	1:A:255:ASP:N	2.35	0.58
1:A:373:ASN:ND2	1:A:401:THR:HG21	2.13	0.58
1:A:457:MET:O	1:A:459:GLU:N	2.36	0.58
1:B:82:SER:O	1:B:86:ILE:HG13	2.03	0.58
1:B:678:ARG:NH2	1:B:753:ASP:OD1	2.35	0.58
1:C:193:TYR:HE2	1:C:241:PHE:HB2	1.66	0.58
1:A:292:ILE:C	1:A:292:ILE:HD12	2.28	0.58
1:A:445:PRO:HG2	1:A:448:VAL:HG23	1.85	0.58
1:B:159:VAL:HG23	1:B:248:LEU:O	2.02	0.58
1:C:335:LEU:O	1:C:411:GLY:HA3	2.03	0.58
1:C:463:HIS:O	1:C:464:GLU:C	2.46	0.58
1:C:535:ARG:O	1:C:539:LEU:HD12	2.03	0.58
1:A:693:THR:OG1	1:A:722:PHE:HB2	2.04	0.58
1:A:699:VAL:O	1:A:703:VAL:HG23	2.02	0.58
1:B:256:LEU:O	1:B:257:ILE:C	2.47	0.58
1:B:327:SER:O	1:B:331:VAL:HG23	2.03	0.58
1:C:159:VAL:HA	1:C:250:LEU:HG	1.86	0.58
1:D:137:ALA:HB2	1:D:251:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:ARG:HG3	1:D:247:CYS:O	2.03	0.58
1:D:612:ALA:O	1:D:616:VAL:HG23	2.03	0.58
1:D:721:THR:O	1:D:725:ILE:HG12	2.01	0.58
1:B:284:LYS:HD2	1:B:284:LYS:N	2.18	0.58
1:C:137:ALA:HB3	1:C:248:LEU:HD21	1.84	0.58
1:C:292:ILE:C	1:C:292:ILE:HD12	2.28	0.58
1:C:432:MET:HE3	1:C:480:PHE:CZ	2.39	0.58
1:D:472:ALA:CB	1:D:477:ILE:HD12	2.33	0.58
1:A:154:LEU:HA	1:A:157:ARG:HD3	1.84	0.58
1:A:456:CYS:SG	1:A:524:VAL:HA	2.44	0.58
1:A:523:VAL:HG13	1:D:619:SER:OG	2.03	0.58
1:B:213:VAL:O	1:B:241:PHE:HA	2.04	0.58
1:B:321:PHE:CD2	1:B:325:GLY:HA2	2.39	0.58
1:C:310:ARG:O	1:C:312:ARG:N	2.37	0.58
1:C:494:ARG:HG2	1:C:494:ARG:HH11	1.68	0.58
1:C:497:PRO:HG2	1:C:500:ASP:OD2	2.04	0.58
1:B:343:LEU:HD13	1:B:427:LEU:HD21	1.85	0.58
1:B:360:VAL:O	1:B:364:VAL:HG23	2.04	0.58
1:C:114:PRO:O	1:C:115:LEU:HD23	2.03	0.58
1:C:327:SER:OG	1:C:329:THR:HB	2.04	0.58
1:C:612:ALA:HB2	1:C:703:VAL:HG21	1.85	0.58
1:D:310:ARG:O	1:D:312:ARG:N	2.37	0.58
1:D:527:ILE:HD12	1:D:527:ILE:N	2.19	0.58
1:A:721:THR:O	1:A:725:ILE:HG12	2.03	0.58
1:B:337:LEU:HD22	1:B:673:GLU:HA	1.84	0.58
1:C:21:LEU:HD13	1:C:112:PHE:CE1	2.38	0.58
1:C:80:PRO:O	1:C:82:SER:N	2.35	0.58
1:C:405:MET:O	1:C:409:ILE:HD13	2.04	0.58
1:D:255:ASP:O	1:D:256:LEU:C	2.46	0.58
1:D:361:GLY:O	1:D:365:GLU:HG3	2.03	0.58
1:A:401:THR:HG22	1:A:403:ALA:N	2.19	0.57
1:C:221:LEU:O	1:C:222:LYS:C	2.45	0.57
1:A:327:SER:OG	1:A:329:THR:HB	2.04	0.57
1:A:376:LEU:O	1:A:380:VAL:HG23	2.04	0.57
1:B:599:ILE:HG21	1:B:631:PHE:HE1	1.69	0.57
1:C:125:ARG:HG2	1:C:125:ARG:NH1	2.18	0.57
1:C:243:PRO:HD2	1:C:246:LEU:HD12	1.85	0.57
1:C:564:LEU:HD23	1:C:592:VAL:HG12	1.85	0.57
1:D:161:THR:OG1	1:D:164:ILE:HB	2.04	0.57
1:A:298:PHE:CZ	1:A:331:VAL:HG21	2.40	0.57
1:A:310:ARG:O	1:A:312:ARG:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LEU:HD22	1:B:262:LEU:HD13	1.86	0.57
1:B:112:PHE:CG	1:B:265:LEU:HD22	2.40	0.57
1:C:675:ALA:O	1:C:679:MET:HG3	2.04	0.57
1:D:4:LEU:HD21	1:D:26:HIS:ND1	2.20	0.57
1:D:372:ARG:HD2	1:D:374:GLU:OE1	2.04	0.57
1:A:497:PRO:HG2	1:A:500:ASP:OD2	2.04	0.57
1:A:637:GLN:O	1:A:641:THR:HG23	2.05	0.57
1:B:221:LEU:O	1:B:222:LYS:C	2.47	0.57
1:C:567:TYR:HA	1:C:572:GLN:HE22	1.69	0.57
1:D:37:ALA:HB2	1:D:43:ALA:CB	2.35	0.57
1:A:161:THR:OG1	1:A:164:ILE:HB	2.04	0.57
1:A:284:LYS:HD2	1:A:284:LYS:N	2.18	0.57
1:A:392:SER:C	1:A:394:ASN:H	2.10	0.57
1:B:747:LEU:HB3	1:B:748:PRO:HD3	1.85	0.57
1:C:236:ALA:C	1:C:238:LYS:H	2.13	0.57
1:D:227:PRO:HG3	1:D:234:ASP:OD2	2.05	0.57
1:D:637:GLN:HA	1:D:640:LEU:HD12	1.85	0.57
1:A:507:LEU:HD22	1:A:588:VAL:HG21	1.85	0.57
1:B:251:PRO:HG2	1:B:254:PHE:CD1	2.40	0.57
1:B:261:ALA:C	1:B:263:GLN:H	2.13	0.57
1:D:178:GLN:HE21	1:D:212:LEU:CD1	2.14	0.57
1:D:497:PRO:HG2	1:D:500:ASP:OD2	2.04	0.57
1:A:470:ASP:O	1:A:474:GLU:HG2	2.04	0.57
1:B:310:ARG:O	1:B:312:ARG:N	2.38	0.57
1:C:140:LEU:HD12	1:C:213:VAL:HG21	1.87	0.57
1:A:112:PHE:CD2	1:A:265:LEU:HD13	2.40	0.57
1:C:33:PHE:CD2	1:C:318:ARG:HB2	2.40	0.57
1:C:321:PHE:CD2	1:C:325:GLY:HA2	2.40	0.57
1:C:462:ALA:O	1:C:465:PHE:N	2.36	0.57
1:C:721:THR:O	1:C:725:ILE:HG12	2.05	0.57
1:D:34:LYS:HB3	1:D:45:GLU:HG3	1.85	0.57
1:B:612:ALA:O	1:B:616:VAL:HG23	2.04	0.57
1:A:99:ARG:NH1	1:A:390:GLU:CD	2.60	0.56
1:B:494:ARG:HG2	1:B:494:ARG:HH11	1.69	0.56
1:C:527:ILE:HD12	1:C:527:ILE:N	2.20	0.56
1:D:37:ALA:HB2	1:D:43:ALA:N	2.20	0.56
1:A:327:SER:O	1:A:331:VAL:HG23	2.05	0.56
1:A:603:GLU:CD	1:A:603:GLU:N	2.62	0.56
1:B:236:ALA:N	1:B:237:PRO:CD	2.68	0.56
1:C:637:GLN:O	1:C:641:THR:HG23	2.05	0.56
1:C:678:ARG:NH2	1:C:753:ASP:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:THR:HG22	1:D:487:THR:HG21	1.87	0.56
1:C:708:HIS:HB3	1:C:711:ILE:HG21	1.87	0.56
1:D:145:THR:O	1:D:147:TYR:N	2.38	0.56
1:A:4:LEU:HD21	1:A:26:HIS:ND1	2.20	0.56
1:A:97:PHE:HZ	1:A:301:THR:HA	1.71	0.56
1:A:612:ALA:HB2	1:A:703:VAL:HG21	1.87	0.56
1:B:14:ARG:HB2	1:B:257:ILE:HD12	1.87	0.56
1:B:112:PHE:CE2	1:B:265:LEU:HB3	2.41	0.56
1:B:172:LEU:HD12	1:B:239:LEU:HD13	1.87	0.56
1:C:437:SER:HB3	1:C:478:SER:O	2.06	0.56
1:D:462:ALA:HA	1:D:498:ALA:HB1	1.86	0.56
1:A:321:PHE:CD2	1:A:325:GLY:HA2	2.41	0.56
1:B:242:LEU:N	1:B:242:LEU:HD23	2.20	0.56
1:B:258:ARG:C	1:B:260:GLN:H	2.13	0.56
1:B:711:ILE:HD12	1:B:711:ILE:O	2.06	0.56
1:D:327:SER:OG	1:D:329:THR:HB	2.05	0.56
1:D:369:GLU:CG	1:D:482:SER:OG	2.54	0.56
1:A:512:SER:HA	1:A:517:LEU:HD11	1.88	0.56
1:B:527:ILE:HD12	1:B:527:ILE:N	2.19	0.56
1:B:680:ARG:HH11	1:B:680:ARG:HG3	1.71	0.56
1:D:262:LEU:HD12	1:D:262:LEU:O	2.05	0.56
1:D:725:ILE:HG22	1:D:729:ILE:HD11	1.88	0.56
1:B:339:GLY:HA3	1:B:407:GLU:O	2.06	0.56
1:C:432:MET:HA	1:C:479:VAL:O	2.06	0.56
1:C:547:GLU:HG2	1:C:548:GLN:N	2.21	0.56
1:D:23:LEU:CD2	1:D:110:LEU:HB3	2.36	0.56
1:D:512:SER:HA	1:D:517:LEU:HD11	1.88	0.56
1:A:624:ILE:H	1:A:624:ILE:CD1	2.19	0.56
1:B:80:PRO:O	1:B:82:SER:N	2.38	0.56
1:C:432:MET:HE3	1:C:480:PHE:CE2	2.40	0.56
1:D:251:PRO:O	1:D:252:ASP:C	2.48	0.56
1:D:369:GLU:HG3	1:D:482:SER:HB2	1.87	0.56
1:B:178:GLN:HE21	1:B:212:LEU:CD1	2.16	0.55
1:B:457:MET:O	1:B:459:GLU:N	2.38	0.55
1:B:612:ALA:HB2	1:B:703:VAL:HG21	1.87	0.55
1:D:143:GLU:O	1:D:146:ASP:N	2.39	0.55
1:D:376:LEU:O	1:D:380:VAL:HG23	2.06	0.55
1:A:464:GLU:O	1:A:468:LEU:HG	2.06	0.55
1:B:191:ILE:HG22	1:B:192:THR:N	2.21	0.55
1:B:394:ASN:HD21	1:B:396:VAL:HB	1.71	0.55
1:C:489:PHE:CZ	1:C:534:ALA:HA	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:608:SER:C	1:D:610:HIS:N	2.62	0.55
1:D:711:ILE:HD12	1:D:711:ILE:O	2.05	0.55
1:A:361:GLY:O	1:A:365:GLU:HG3	2.07	0.55
1:B:603:GLU:HA	1:B:634:ARG:HH22	1.70	0.55
1:B:738:ALA:O	1:B:741:PHE:HB3	2.06	0.55
1:C:637:GLN:HA	1:C:640:LEU:HD12	1.87	0.55
1:D:342:VAL:HG23	1:D:343:LEU:N	2.20	0.55
1:D:360:VAL:O	1:D:364:VAL:HG23	2.06	0.55
1:A:23:LEU:HD21	1:A:272:ILE:HD13	1.89	0.55
1:A:207:ALA:HB1	1:A:210:LEU:HG	1.88	0.55
1:B:171:VAL:HA	1:B:215:ALA:HB2	1.87	0.55
1:D:708:HIS:HB3	1:D:711:ILE:HG21	1.89	0.55
1:D:21:LEU:HD13	1:D:112:PHE:CE1	2.41	0.55
1:D:207:ALA:HB1	1:D:210:LEU:HG	1.87	0.55
1:A:527:ILE:HD12	1:A:527:ILE:N	2.22	0.55
1:B:342:VAL:HG12	1:B:658:CYS:SG	2.46	0.55
1:C:457:MET:O	1:C:459:GLU:N	2.38	0.55
1:C:725:ILE:HG22	1:C:729:ILE:HD11	1.89	0.55
1:D:242:LEU:N	1:D:242:LEU:HD23	2.21	0.55
1:D:284:LYS:HD2	1:D:284:LYS:N	2.20	0.55
1:D:471:TYR:CZ	1:D:475:GLN:HG3	2.42	0.55
1:D:663:HIS:CD2	1:D:743:ARG:HB3	2.41	0.55
1:A:171:VAL:HA	1:A:215:ALA:HB2	1.88	0.55
1:A:298:PHE:HZ	1:A:331:VAL:HG21	1.72	0.55
1:A:725:ILE:HG22	1:A:729:ILE:HD11	1.89	0.55
1:B:4:LEU:HD21	1:B:26:HIS:ND1	2.22	0.55
1:B:114:PRO:O	1:B:115:LEU:HD23	2.06	0.55
1:B:708:HIS:HB3	1:B:711:ILE:HG21	1.88	0.55
1:B:725:ILE:HG22	1:B:729:ILE:HD11	1.89	0.55
1:C:298:PHE:CZ	1:C:331:VAL:HG21	2.42	0.55
1:C:342:VAL:HG23	1:C:343:LEU:N	2.21	0.55
1:C:697:PRO:O	1:C:699:VAL:N	2.39	0.55
1:D:114:PRO:O	1:D:115:LEU:HD23	2.07	0.55
1:D:375:ALA:O	1:D:378:TYR:HB3	2.06	0.55
1:A:462:ALA:HB1	1:A:498:ALA:HB3	1.88	0.55
1:B:90:MET:HE3	1:B:318:ARG:HH22	1.71	0.55
1:B:564:LEU:HD23	1:B:592:VAL:HG12	1.88	0.55
1:C:42:PRO:HB3	1:C:223:ASP:HB3	1.88	0.55
1:D:110:LEU:HD13	1:D:272:ILE:CD1	2.29	0.55
1:A:178:GLN:HE21	1:A:212:LEU:CD1	2.15	0.55
1:B:489:PHE:CZ	1:B:534:ALA:HA	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:GLY:HA3	1:B:561:ILE:O	2.06	0.55
1:B:562:PRO:HB3	1:B:595:LEU:HB2	1.89	0.55
1:C:306:LEU:HD22	1:C:400:LYS:NZ	2.22	0.55
1:C:360:VAL:O	1:C:364:VAL:HG23	2.07	0.55
1:A:437:SER:HB3	1:A:478:SER:O	2.07	0.55
1:B:425:GLU:HG2	1:B:429:LYS:HE3	1.89	0.55
1:D:191:ILE:HG22	1:D:192:THR:N	2.22	0.55
1:D:350:ARG:HD3	1:D:538:TRP:O	2.05	0.55
1:A:637:GLN:HA	1:A:640:LEU:HD12	1.89	0.54
1:B:161:THR:OG1	1:B:164:ILE:HB	2.06	0.54
1:B:179:THR:HG22	1:B:181:LEU:H	1.72	0.54
1:B:327:SER:OG	1:B:329:THR:HB	2.06	0.54
1:B:637:GLN:HA	1:B:640:LEU:HD12	1.89	0.54
1:B:680:ARG:HG3	1:B:680:ARG:NH1	2.21	0.54
1:C:305:ARG:HD2	1:C:390:GLU:CB	2.37	0.54
1:D:369:GLU:HG3	1:D:482:SER:OG	2.07	0.54
1:A:711:ILE:HD12	1:A:711:ILE:O	2.06	0.54
1:B:428:ALA:HB3	1:B:511:PHE:CZ	2.42	0.54
1:D:147:TYR:HB3	1:D:150:LEU:HB2	1.90	0.54
1:D:675:ALA:O	1:D:679:MET:HG3	2.07	0.54
1:A:738:ALA:O	1:A:741:PHE:HB3	2.07	0.54
1:B:14:ARG:HD3	1:B:257:ILE:HD13	1.90	0.54
1:B:258:ARG:C	1:B:260:GLN:N	2.65	0.54
1:B:333:GLN:HE21	1:B:673:GLU:CB	2.21	0.54
1:C:164:ILE:O	1:C:164:ILE:HG22	2.07	0.54
1:C:191:ILE:HG22	1:C:192:THR:N	2.22	0.54
1:C:375:ALA:O	1:C:378:TYR:HB3	2.07	0.54
1:C:663:HIS:CD2	1:C:743:ARG:HB3	2.42	0.54
1:D:335:LEU:O	1:D:411:GLY:HA3	2.08	0.54
1:D:564:LEU:C	1:D:566:ILE:H	2.15	0.54
1:A:21:LEU:HD21	1:A:272:ILE:HD11	1.88	0.54
1:A:265:LEU:N	1:A:266:PRO:CD	2.70	0.54
1:B:20:LEU:HB2	1:B:115:LEU:HD11	1.90	0.54
1:B:567:TYR:HA	1:B:572:GLN:HE22	1.71	0.54
1:B:663:HIS:CD2	1:B:743:ARG:HB3	2.43	0.54
1:C:265:LEU:HB2	1:C:266:PRO:HD3	1.89	0.54
1:C:545:TYR:HD1	1:C:560:THR:HG1	1.50	0.54
1:D:128:MET:O	1:D:132:GLN:HG3	2.07	0.54
1:A:697:PRO:O	1:A:699:VAL:N	2.40	0.54
1:C:23:LEU:HD21	1:C:272:ILE:HD13	1.89	0.54
1:C:105:PRO:HG2	1:C:106:GLN:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:PHE:HZ	1:C:331:VAL:HG21	1.73	0.54
1:C:624:ILE:H	1:C:624:ILE:CD1	2.21	0.54
1:D:170:VAL:HG11	1:D:221:LEU:HD22	1.87	0.54
1:D:564:LEU:HD23	1:D:592:VAL:HG12	1.88	0.54
1:C:158:MET:HG3	1:C:259:VAL:CG2	2.37	0.54
1:C:546:VAL:HB	1:C:644:VAL:HG13	1.89	0.54
1:C:596:TYR:CE2	1:C:600:LEU:HD11	2.42	0.54
1:D:489:PHE:CZ	1:D:534:ALA:HA	2.42	0.54
1:A:708:HIS:HB3	1:A:711:ILE:HG21	1.90	0.54
1:B:230:GLY:HA2	1:B:233:ASP:OD2	2.07	0.54
1:B:376:LEU:O	1:B:380:VAL:HG23	2.08	0.54
1:C:451:ALA:O	1:C:455:VAL:HG23	2.08	0.54
1:D:401:THR:H	1:D:404:ASP:CG	2.15	0.54
1:A:125:ARG:HG2	1:A:125:ARG:NH1	2.23	0.54
1:A:159:VAL:HG21	1:A:247:CYS:HB3	1.90	0.54
1:A:164:ILE:HG22	1:A:164:ILE:O	2.08	0.54
1:A:172:LEU:HD12	1:A:239:LEU:HD13	1.89	0.54
1:A:342:VAL:HG23	1:A:343:LEU:N	2.23	0.54
1:B:266:PRO:O	1:B:270:LYS:HG3	2.08	0.54
1:B:600:LEU:HD21	1:B:631:PHE:HA	1.89	0.54
1:C:4:LEU:HD21	1:C:26:HIS:ND1	2.22	0.54
1:D:321:PHE:CD2	1:D:325:GLY:HA2	2.42	0.54
1:A:564:LEU:HD23	1:A:592:VAL:HG12	1.88	0.54
1:A:680:ARG:HG3	1:A:680:ARG:HH11	1.73	0.54
1:B:125:ARG:HG2	1:B:125:ARG:NH1	2.22	0.54
1:B:207:ALA:HB1	1:B:210:LEU:HG	1.89	0.54
1:B:456:CYS:SG	1:B:524:VAL:HG13	2.47	0.54
1:C:242:LEU:HD23	1:C:242:LEU:N	2.23	0.54
1:C:332:PHE:C	1:C:332:PHE:CD2	2.86	0.54
1:C:535:ARG:HH11	1:C:535:ARG:HG3	1.73	0.54
1:C:12:THR:HG22	1:C:44:ALA:HB2	1.89	0.54
1:C:353:CYS:HB3	1:C:541:SER:HB2	1.90	0.54
1:C:497:PRO:HB2	1:C:499:GLU:OE2	2.07	0.54
1:B:23:LEU:HD21	1:B:272:ILE:HD13	1.90	0.53
1:B:172:LEU:HD12	1:B:239:LEU:CD1	2.38	0.53
1:B:512:SER:HA	1:B:517:LEU:HD11	1.89	0.53
1:C:160:ALA:HB2	1:C:168:LEU:CD2	2.37	0.53
1:C:207:ALA:HB1	1:C:210:LEU:HG	1.89	0.53
1:A:342:VAL:HG12	1:A:658:CYS:SG	2.48	0.53
1:A:369:GLU:CG	1:A:482:SER:OG	2.55	0.53
1:A:375:ALA:O	1:A:378:TYR:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:TYR:O	1:A:634:ARG:NH2	2.41	0.53
1:C:140:LEU:CD2	1:C:249:LEU:HD12	2.37	0.53
1:D:220:ASP:HB3	1:D:238:LYS:HD3	1.90	0.53
1:A:332:PHE:C	1:A:332:PHE:CD2	2.86	0.53
1:B:342:VAL:O	1:B:346:ILE:HG12	2.08	0.53
1:C:339:GLY:HA3	1:C:407:GLU:O	2.08	0.53
1:C:376:LEU:O	1:C:380:VAL:HG23	2.08	0.53
1:C:390:GLU:O	1:C:391:PHE:HB3	2.07	0.53
1:D:125:ARG:HG2	1:D:125:ARG:NH1	2.23	0.53
1:D:461:GLY:H	1:D:464:GLU:CD	2.16	0.53
1:A:342:VAL:O	1:A:346:ILE:HG12	2.07	0.53
1:A:594:ALA:O	1:A:598:LYS:HG3	2.09	0.53
1:A:612:ALA:O	1:A:616:VAL:HG23	2.08	0.53
1:B:405:MET:O	1:B:409:ILE:HD13	2.07	0.53
1:C:391:PHE:CE2	1:C:402:TRP:HH2	2.27	0.53
1:C:446:ASP:O	1:C:447:ALA:C	2.51	0.53
1:C:453:LYS:O	1:C:457:MET:HE3	2.09	0.53
1:A:548:GLN:HA	1:A:548:GLN:NE2	2.23	0.53
1:A:725:ILE:O	1:A:728:ALA:N	2.41	0.53
1:B:298:PHE:CZ	1:B:331:VAL:HG21	2.43	0.53
1:C:562:PRO:HB3	1:C:595:LEU:HB2	1.89	0.53
1:D:546:VAL:HB	1:D:644:VAL:HG13	1.91	0.53
1:A:160:ALA:HB2	1:A:168:LEU:CD2	2.39	0.53
1:B:39:ARG:NH2	1:B:267:GLU:OE2	2.41	0.53
1:B:375:ALA:O	1:B:378:TYR:HB3	2.08	0.53
1:C:425:GLU:HG2	1:C:429:LYS:HE3	1.90	0.53
1:D:262:LEU:HA	1:D:265:LEU:HD12	1.89	0.53
1:A:172:LEU:HD12	1:A:239:LEU:CD1	2.39	0.53
1:A:437:SER:HB3	1:A:478:SER:H	1.74	0.53
1:A:680:ARG:HG3	1:A:680:ARG:NH1	2.23	0.53
1:B:170:VAL:HG11	1:B:221:LEU:HD22	1.91	0.53
1:B:497:PRO:HB2	1:B:499:GLU:OE2	2.09	0.53
1:C:512:SER:HA	1:C:517:LEU:HD11	1.90	0.53
1:D:697:PRO:O	1:D:699:VAL:N	2.41	0.53
1:A:675:ALA:O	1:A:679:MET:HG3	2.08	0.53
1:C:42:PRO:HD3	1:C:222:LYS:O	2.08	0.53
1:C:402:TRP:CE3	1:C:405:MET:CE	2.92	0.53
1:D:298:PHE:CZ	1:D:331:VAL:HG21	2.44	0.53
1:A:663:HIS:CD2	1:A:743:ARG:HB3	2.43	0.53
1:B:456:CYS:HB2	1:B:457:MET:HE3	1.91	0.53
1:D:753:ASP:O	1:D:754:ALA:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:C	1:A:566:ILE:H	2.17	0.52
1:A:753:ASP:O	1:A:754:ALA:C	2.52	0.52
1:D:290:GLY:HA3	1:D:417:PRO:HG2	1.90	0.52
1:D:332:PHE:CD2	1:D:332:PHE:C	2.87	0.52
1:D:469:VAL:C	1:D:471:TYR:H	2.16	0.52
1:A:360:VAL:O	1:A:364:VAL:HG23	2.09	0.52
1:A:369:GLU:HG3	1:A:482:SER:CB	2.40	0.52
1:A:497:PRO:HB2	1:A:499:GLU:OE2	2.09	0.52
1:A:523:VAL:HG21	1:D:618:ARG:NH1	2.24	0.52
1:C:72:PHE:CG	1:C:81:ALA:HA	2.44	0.52
1:C:170:VAL:O	1:C:215:ALA:HB1	2.09	0.52
1:C:401:THR:H	1:C:404:ASP:CG	2.17	0.52
1:C:614:GLN:O	1:C:617:SER:HB3	2.09	0.52
1:D:451:ALA:O	1:D:455:VAL:HG23	2.08	0.52
1:D:456:CYS:HB2	1:D:457:MET:HE3	1.90	0.52
1:D:535:ARG:O	1:D:539:LEU:HD12	2.09	0.52
1:B:353:CYS:HB3	1:B:541:SER:HB2	1.91	0.52
1:C:170:VAL:HG11	1:C:221:LEU:HD22	1.91	0.52
1:C:456:CYS:HB2	1:C:457:MET:HE3	1.90	0.52
1:C:629:ILE:N	1:C:630:PRO:HD2	2.24	0.52
1:C:738:ALA:O	1:C:741:PHE:HB3	2.09	0.52
1:A:179:THR:HG22	1:A:181:LEU:H	1.73	0.52
1:D:145:THR:C	1:D:147:TYR:N	2.67	0.52
1:D:147:TYR:CB	1:D:150:LEU:HB2	2.39	0.52
1:D:172:LEU:CD1	1:D:239:LEU:HD13	2.39	0.52
1:D:425:GLU:HG2	1:D:429:LYS:HE3	1.91	0.52
1:A:191:ILE:HG22	1:A:192:THR:N	2.24	0.52
1:A:248:LEU:C	1:A:248:LEU:HD23	2.35	0.52
1:A:562:PRO:HB3	1:A:595:LEU:HB2	1.90	0.52
1:B:4:LEU:CD2	1:B:26:HIS:HA	2.40	0.52
1:B:160:ALA:HB2	1:B:168:LEU:CD2	2.37	0.52
1:B:248:LEU:C	1:B:248:LEU:HD23	2.35	0.52
1:B:546:VAL:O	1:B:547:GLU:C	2.51	0.52
1:C:564:LEU:C	1:C:566:ILE:H	2.17	0.52
1:C:682:SER:HB2	1:C:751:VAL:HG12	1.91	0.52
1:D:602:TYR:O	1:D:603:GLU:C	2.53	0.52
1:A:599:ILE:HG21	1:A:631:PHE:HE1	1.75	0.52
1:A:643:HIS:O	1:A:646:GLN:HG2	2.09	0.52
1:B:99:ARG:NH1	1:B:390:GLU:O	2.42	0.52
1:B:298:PHE:HZ	1:B:331:VAL:HG21	1.75	0.52
1:C:36:SER:HB3	1:C:317:TRP:HE3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ALA:CB	1:C:168:LEU:HD23	2.39	0.52
1:A:259:VAL:O	1:A:262:LEU:HB3	2.09	0.52
1:A:432:MET:HE3	1:A:480:PHE:CE2	2.45	0.52
1:A:466:ARG:O	1:A:470:ASP:OD1	2.28	0.52
1:B:594:ALA:O	1:B:598:LYS:HG3	2.10	0.52
1:B:682:SER:HB2	1:B:751:VAL:HG12	1.92	0.52
1:D:20:LEU:HD23	1:D:122:LEU:HD13	1.92	0.52
1:D:227:PRO:CB	1:D:233:ASP:N	2.73	0.52
1:D:298:PHE:HZ	1:D:331:VAL:HG21	1.75	0.52
1:D:356:PRO:O	1:D:647:LYS:NZ	2.43	0.52
1:D:562:PRO:HB3	1:D:595:LEU:HB2	1.91	0.52
1:A:260:GLN:HA	1:A:263:GLN:HG2	1.92	0.52
1:A:379:LEU:HD21	1:A:481:CYS:CB	2.38	0.52
1:B:164:ILE:O	1:B:164:ILE:HG22	2.09	0.52
1:C:307:ASP:OD1	1:C:391:PHE:HA	2.10	0.52
1:C:466:ARG:NH1	1:C:501:MET:HE1	2.25	0.52
1:D:38:GLY:N	1:D:41:LEU:HD12	2.24	0.52
1:D:264:PHE:N	1:D:264:PHE:CD1	2.77	0.52
1:D:594:ALA:O	1:D:598:LYS:HG3	2.10	0.52
1:D:624:ILE:H	1:D:624:ILE:CD1	2.20	0.52
1:A:35:VAL:O	1:A:43:ALA:HA	2.10	0.52
1:A:300:ILE:CG2	1:A:304:LEU:HD12	2.39	0.52
1:A:462:ALA:HA	1:A:498:ALA:HB1	1.91	0.52
1:A:729:ILE:N	1:A:729:ILE:HD12	2.25	0.52
1:B:139:ARG:N	1:B:142:ASP:OD2	2.42	0.52
1:C:42:PRO:CB	1:C:223:ASP:HB3	2.40	0.52
1:D:160:ALA:HB2	1:D:168:LEU:CD2	2.39	0.52
1:A:606:GLY:HA2	1:A:610:HIS:CB	2.39	0.51
1:B:38:GLY:HA3	1:B:41:LEU:HD11	1.90	0.51
1:B:332:PHE:C	1:B:332:PHE:CD2	2.88	0.51
1:C:342:VAL:O	1:C:346:ILE:HG12	2.10	0.51
1:D:72:PHE:CG	1:D:81:ALA:HA	2.45	0.51
1:D:101:ILE:HG23	1:D:277:ASN:HD21	1.76	0.51
1:D:300:ILE:CG2	1:D:304:LEU:HD12	2.38	0.51
1:D:368:MET:O	1:D:372:ARG:HB2	2.09	0.51
1:D:738:ALA:O	1:D:741:PHE:HB3	2.10	0.51
1:A:242:LEU:N	1:A:242:LEU:HD23	2.25	0.51
1:A:395:LEU:O	1:A:398:LYS:N	2.43	0.51
1:B:251:PRO:HG2	1:B:254:PHE:HD1	1.75	0.51
1:C:18:HIS:O	1:C:258:ARG:NH2	2.43	0.51
1:C:112:PHE:CD2	1:C:265:LEU:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:ILE:O	1:C:728:ALA:N	2.43	0.51
1:A:157:ARG:HH21	1:A:249:LEU:HD21	1.75	0.51
1:A:425:GLU:HG2	1:A:429:LYS:HE3	1.92	0.51
1:B:624:ILE:H	1:B:624:ILE:CD1	2.21	0.51
1:C:236:ALA:N	1:C:237:PRO:CD	2.73	0.51
1:C:357:ASP:OD1	1:D:716:LYS:NZ	2.38	0.51
1:C:594:ALA:O	1:C:598:LYS:HG3	2.10	0.51
1:A:451:ALA:O	1:A:455:VAL:HG23	2.10	0.51
1:B:90:MET:HE1	1:B:318:ARG:NH2	2.25	0.51
1:B:602:TYR:C	1:B:634:ARG:NH2	2.68	0.51
1:C:128:MET:O	1:C:129:VAL:C	2.53	0.51
1:D:128:MET:O	1:D:129:VAL:C	2.54	0.51
1:D:172:LEU:HD11	1:D:216:VAL:CG2	2.40	0.51
1:D:390:GLU:O	1:D:391:PHE:HB3	2.10	0.51
1:B:1:MET:HG3	1:B:55:SER:CB	2.40	0.51
1:B:72:PHE:CG	1:B:81:ALA:HA	2.46	0.51
1:B:258:ARG:O	1:B:260:GLN:N	2.44	0.51
1:B:453:LYS:O	1:B:457:MET:HE3	2.10	0.51
1:B:507:LEU:HD22	1:B:588:VAL:HG21	1.92	0.51
1:A:587:PRO:HG2	1:A:588:VAL:H	1.76	0.51
1:C:212:LEU:HD13	1:C:241:PHE:HB3	1.92	0.51
1:D:170:VAL:O	1:D:215:ALA:HB1	2.11	0.51
1:D:401:THR:HG22	1:D:402:TRP:H	1.76	0.51
1:A:4:LEU:CD2	1:A:26:HIS:HA	2.41	0.51
1:A:698:SER:O	1:A:702:GLU:HG3	2.11	0.51
1:B:39:ARG:H	1:B:39:ARG:CD	2.23	0.51
1:B:39:ARG:HH22	1:B:267:GLU:CD	2.19	0.51
1:B:559:PRO:HG3	1:B:599:ILE:HG13	1.92	0.51
1:D:463:HIS:HA	1:D:466:ARG:HB3	1.91	0.51
1:D:535:ARG:HG3	1:D:535:ARG:HH11	1.75	0.51
1:D:614:GLN:O	1:D:617:SER:HB3	2.11	0.51
1:A:41:LEU:HD13	1:A:264:PHE:CE2	2.46	0.51
1:D:587:PRO:HG2	1:D:588:VAL:H	1.76	0.51
1:A:434:PRO:HA	1:A:527:ILE:HG22	1.92	0.51
1:A:456:CYS:HB2	1:A:457:MET:HE3	1.93	0.51
1:B:368:MET:O	1:B:372:ARG:HB2	2.11	0.51
1:C:366:LEU:O	1:C:369:GLU:HB3	2.10	0.51
1:D:248:LEU:C	1:D:248:LEU:HD23	2.36	0.51
1:D:373:ASN:HD21	1:D:401:THR:HG21	1.75	0.51
1:A:614:GLN:O	1:A:617:SER:HB3	2.11	0.51
1:B:90:MET:HE1	1:B:318:ARG:HH22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE2	1:C:55:SER:HB3	1.93	0.51
1:D:456:CYS:HB2	1:D:457:MET:CE	2.41	0.51
1:B:614:GLN:O	1:B:617:SER:HB3	2.11	0.50
1:C:179:THR:HG22	1:C:181:LEU:H	1.75	0.50
1:C:434:PRO:HA	1:C:527:ILE:CG2	2.41	0.50
1:C:446:ASP:HA	1:C:449:THR:HB	1.92	0.50
1:D:497:PRO:HB2	1:D:499:GLU:OE2	2.11	0.50
1:D:725:ILE:HG22	1:D:729:ILE:CD1	2.42	0.50
1:A:213:VAL:O	1:A:241:PHE:HA	2.11	0.50
1:B:564:LEU:C	1:B:566:ILE:H	2.18	0.50
1:D:36:SER:HB3	1:D:317:TRP:HE3	1.75	0.50
1:D:99:ARG:NH1	1:D:390:GLU:OE2	2.44	0.50
1:D:366:LEU:O	1:D:369:GLU:HB3	2.10	0.50
1:B:105:PRO:HG2	1:B:106:GLN:H	1.76	0.50
1:B:429:LYS:O	1:B:432:MET:O	2.29	0.50
1:B:517:LEU:C	1:B:517:LEU:HD12	2.36	0.50
1:B:574:PRO:O	1:B:575:VAL:C	2.54	0.50
1:C:248:LEU:C	1:C:248:LEU:HD23	2.36	0.50
1:D:4:LEU:CD2	1:D:26:HIS:HA	2.42	0.50
1:A:455:VAL:HG21	1:A:468:LEU:CD1	2.42	0.50
1:B:39:ARG:HD2	1:B:39:ARG:H	1.75	0.50
1:B:342:VAL:HG23	1:B:343:LEU:N	2.27	0.50
1:B:629:ILE:N	1:B:630:PRO:HD2	2.27	0.50
1:D:179:THR:HG22	1:D:181:LEU:H	1.76	0.50
1:B:377:ASN:ND2	1:B:395:LEU:HD11	2.26	0.50
1:C:172:LEU:HD11	1:C:216:VAL:CG2	2.39	0.50
1:D:144:TYR:OH	1:D:213:VAL:HG22	2.11	0.50
1:D:432:MET:HE2	1:D:534:ALA:CB	2.33	0.50
1:A:1:MET:HG3	1:A:55:SER:CB	2.41	0.50
1:A:21:LEU:HD11	1:A:110:LEU:HB2	1.93	0.50
1:A:682:SER:HB2	1:A:751:VAL:HG12	1.93	0.50
1:B:602:TYR:O	1:B:603:GLU:HB2	2.11	0.50
1:D:105:PRO:HG2	1:D:106:GLN:H	1.77	0.50
1:D:609:LYS:NZ	1:D:641:THR:CG2	2.74	0.50
1:D:632:LEU:HD22	1:D:733:CYS:SG	2.52	0.50
1:A:72:PHE:CG	1:A:81:ALA:HA	2.47	0.50
1:A:96:THR:HG21	1:A:301:THR:HG23	1.94	0.50
1:B:160:ALA:CB	1:B:168:LEU:HD23	2.38	0.50
1:B:603:GLU:CA	1:B:634:ARG:HH22	2.24	0.50
1:C:41:LEU:HD13	1:C:264:PHE:CZ	2.47	0.50
1:C:327:SER:HG	1:C:329:THR:HB	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:TYR:CD2	1:D:150:LEU:HB2	2.47	0.50
1:D:446:ASP:O	1:D:447:ALA:C	2.55	0.50
1:D:463:HIS:HA	1:D:466:ARG:CB	2.42	0.50
1:A:105:PRO:HG2	1:A:106:GLN:H	1.76	0.50
1:A:251:PRO:O	1:A:252:ASP:C	2.55	0.50
1:A:381:GLN:HE21	1:A:402:TRP:CD1	2.29	0.50
1:A:434:PRO:HA	1:A:527:ILE:CG2	2.42	0.50
1:A:569:ARG:NE	1:A:735:GLU:OE1	2.44	0.50
1:B:685:THR:OG1	1:B:688:VAL:HG23	2.12	0.50
1:C:350:ARG:HD2	1:C:539:LEU:HA	1.94	0.50
1:C:454:ARG:HE	1:C:464:GLU:CD	2.20	0.50
1:D:60:ASP:HA	1:D:63:ILE:HD12	1.93	0.50
1:D:227:PRO:HB2	1:D:233:ASP:N	2.26	0.50
1:D:261:ALA:O	1:D:264:PHE:CD1	2.62	0.50
1:D:574:PRO:O	1:D:575:VAL:C	2.55	0.50
1:A:172:LEU:HD11	1:A:216:VAL:CG2	2.42	0.50
1:A:255:ASP:O	1:A:258:ARG:HB2	2.12	0.50
1:B:94:GLU:HG2	1:B:316:GLY:HA2	1.92	0.50
1:B:172:LEU:HD11	1:B:216:VAL:CG2	2.42	0.50
1:B:179:THR:HG23	1:B:180:SER:N	2.26	0.50
1:B:602:TYR:C	1:B:634:ARG:HH22	2.20	0.50
1:B:603:GLU:CA	1:B:634:ARG:HH12	2.23	0.50
1:B:753:ASP:O	1:B:754:ALA:C	2.55	0.50
1:C:4:LEU:CD2	1:C:26:HIS:HA	2.42	0.50
1:C:385:LEU:N	1:C:386:PRO:CD	2.75	0.50
1:A:453:LYS:O	1:A:457:MET:HE3	2.12	0.49
1:A:561:ILE:H	1:A:561:ILE:CD1	2.24	0.49
1:A:593:LEU:O	1:A:597:GLU:HG3	2.12	0.49
1:B:170:VAL:O	1:B:215:ALA:HB1	2.12	0.49
1:B:377:ASN:ND2	1:B:395:LEU:HD21	2.21	0.49
1:B:486:SER:O	1:B:489:PHE:HB3	2.12	0.49
1:B:559:PRO:HG2	1:B:599:ILE:HG13	1.93	0.49
1:C:114:PRO:CB	1:C:258:ARG:NH1	2.75	0.49
1:C:368:MET:O	1:C:372:ARG:HB2	2.12	0.49
1:C:456:CYS:HB2	1:C:457:MET:CE	2.42	0.49
1:C:643:HIS:O	1:C:646:GLN:HG2	2.11	0.49
1:C:711:ILE:O	1:C:711:ILE:HD12	2.11	0.49
1:D:402:TRP:CE3	1:D:402:TRP:HA	2.47	0.49
1:A:574:PRO:O	1:A:575:VAL:C	2.55	0.49
1:A:708:HIS:O	1:A:711:ILE:HG13	2.12	0.49
1:B:39:ARG:NH1	1:B:41:LEU:HD21	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:SER:HG	1:B:329:THR:HB	1.76	0.49
1:B:396:VAL:HG13	1:B:396:VAL:O	2.11	0.49
1:B:459:GLU:HG2	1:B:459:GLU:O	2.12	0.49
1:C:333:GLN:HE21	1:C:673:GLU:HB3	1.76	0.49
1:C:574:PRO:O	1:C:575:VAL:C	2.55	0.49
1:D:259:VAL:O	1:D:262:LEU:N	2.39	0.49
1:A:34:LYS:HA	1:A:45:GLU:HA	1.93	0.49
1:A:366:LEU:O	1:A:369:GLU:HB3	2.12	0.49
1:B:451:ALA:O	1:B:455:VAL:HG23	2.11	0.49
1:C:14:ARG:NH1	1:C:223:ASP:HA	2.26	0.49
1:C:21:LEU:HD12	1:C:22:LEU:N	2.26	0.49
1:C:434:PRO:HA	1:C:527:ILE:HG22	1.94	0.49
1:C:456:CYS:SG	1:C:524:VAL:HG13	2.52	0.49
1:C:473:CYS:C	1:C:475:GLN:N	2.70	0.49
1:D:160:ALA:CB	1:D:168:LEU:HD23	2.40	0.49
1:A:87:GLY:O	1:A:90:MET:HG3	2.13	0.49
1:A:310:ARG:NH2	1:A:392:SER:CB	2.75	0.49
1:A:369:GLU:HG2	1:A:485:VAL:HG23	1.93	0.49
1:A:604:SER:N	1:A:634:ARG:HH12	2.10	0.49
1:B:663:HIS:NE2	1:B:743:ARG:HB3	2.27	0.49
1:D:164:ILE:HG22	1:D:164:ILE:O	2.11	0.49
1:D:261:ALA:HA	1:D:264:PHE:CE1	2.47	0.49
1:D:377:ASN:O	1:D:381:GLN:HG2	2.13	0.49
1:A:128:MET:O	1:A:129:VAL:C	2.55	0.49
1:C:306:LEU:HB3	1:C:400:LYS:HZ3	1.78	0.49
1:C:353:CYS:HB3	1:C:541:SER:CB	2.41	0.49
1:C:465:PHE:O	1:C:468:LEU:N	2.46	0.49
1:D:629:ILE:N	1:D:630:PRO:HD2	2.28	0.49
1:A:170:VAL:HG11	1:A:221:LEU:HD22	1.93	0.49
1:A:179:THR:HG23	1:A:180:SER:N	2.27	0.49
1:B:292:ILE:HD12	1:B:292:ILE:O	2.13	0.49
1:B:401:THR:O	1:B:404:ASP:CG	2.55	0.49
1:B:535:ARG:HH11	1:B:535:ARG:HG3	1.77	0.49
1:B:703:VAL:O	1:B:706:GLU:HB3	2.13	0.49
1:C:517:LEU:C	1:C:517:LEU:HD12	2.38	0.49
1:C:708:HIS:O	1:C:711:ILE:HG13	2.13	0.49
1:C:753:ASP:O	1:C:754:ALA:C	2.55	0.49
1:D:256:LEU:O	1:D:257:ILE:C	2.56	0.49
1:D:643:HIS:O	1:D:646:GLN:HG2	2.13	0.49
1:A:399:SER:CA	1:B:395:LEU:HD12	2.40	0.49
1:A:406:TYR:O	1:A:410:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:VAL:O	1:A:524:VAL:HG23	2.13	0.49
1:C:172:LEU:HD12	1:C:239:LEU:HD13	1.93	0.49
1:C:698:SER:O	1:C:702:GLU:HG3	2.13	0.49
1:C:725:ILE:HG22	1:C:729:ILE:CD1	2.43	0.49
1:D:90:MET:CE	1:D:318:ARG:HH22	2.26	0.49
1:D:110:LEU:HD23	1:D:110:LEU:N	2.28	0.49
1:D:327:SER:HG	1:D:329:THR:HB	1.77	0.49
1:D:457:MET:C	1:D:459:GLU:H	2.20	0.49
1:D:725:ILE:O	1:D:728:ALA:N	2.44	0.49
1:B:110:LEU:HD11	1:B:269:ALA:HA	1.95	0.49
1:B:115:LEU:N	1:B:258:ARG:HH22	2.07	0.49
1:B:261:ALA:C	1:B:263:GLN:N	2.69	0.49
1:B:333:GLN:HG2	1:B:673:GLU:HB2	1.95	0.49
1:B:643:HIS:O	1:B:646:GLN:HG2	2.12	0.49
1:C:136:ASP:O	1:C:138:LYS:HG3	2.13	0.49
1:C:459:GLU:O	1:C:459:GLU:HG2	2.12	0.49
1:C:721:THR:O	1:C:724:ALA:HB3	2.13	0.49
1:D:38:GLY:H	1:D:41:LEU:CD1	2.23	0.49
1:D:336:GLU:HG3	1:D:407:GLU:HB2	1.95	0.49
1:D:472:ALA:HA	1:D:477:ILE:HD12	1.94	0.49
1:D:682:SER:HB2	1:D:751:VAL:HG12	1.94	0.49
1:B:39:ARG:HG3	1:B:317:TRP:CE2	2.47	0.49
1:B:432:MET:HE3	1:B:480:PHE:CZ	2.48	0.49
1:C:205:LEU:HD22	1:C:245:GLU:CD	2.38	0.49
1:C:352:LEU:HD11	1:C:650:LEU:HD23	1.95	0.49
1:D:36:SER:HB2	1:D:312:ARG:O	2.13	0.49
1:D:90:MET:HE3	1:D:318:ARG:HH22	1.77	0.49
1:D:698:SER:O	1:D:702:GLU:HG3	2.13	0.49
1:A:110:LEU:HD11	1:A:269:ALA:HA	1.95	0.49
1:A:624:ILE:HD13	1:A:624:ILE:N	2.26	0.49
1:B:546:VAL:HB	1:B:644:VAL:HG13	1.94	0.49
1:C:179:THR:HG23	1:C:180:SER:N	2.27	0.49
1:C:466:ARG:NH2	1:C:498:ALA:N	2.59	0.49
1:C:473:CYS:HA	1:C:490:LEU:HD13	1.95	0.49
1:C:729:ILE:HD12	1:C:729:ILE:N	2.28	0.49
1:D:138:LYS:CD	1:D:142:ASP:HB3	2.42	0.49
1:D:453:LYS:O	1:D:457:MET:HE3	2.12	0.49
1:D:517:LEU:C	1:D:517:LEU:HD12	2.38	0.49
1:D:624:ILE:HD13	1:D:624:ILE:N	2.27	0.49
1:A:1:MET:HE2	1:A:55:SER:HB3	1.95	0.48
1:A:455:VAL:HG21	1:A:468:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:TYR:O	1:A:475:GLN:HB2	2.13	0.48
1:B:1:MET:HE2	1:B:55:SER:HB3	1.94	0.48
1:B:128:MET:O	1:B:132:GLN:HG3	2.13	0.48
1:C:480:PHE:C	1:C:482:SER:H	2.20	0.48
1:C:703:VAL:O	1:C:706:GLU:HB3	2.13	0.48
1:D:140:LEU:HB3	1:D:144:TYR:CE2	2.46	0.48
1:D:465:PHE:O	1:D:466:ARG:C	2.55	0.48
1:D:609:LYS:HZ2	1:D:641:THR:HG21	1.77	0.48
1:D:696:PHE:HB3	1:D:700:VAL:HG21	1.95	0.48
1:A:114:PRO:O	1:A:115:LEU:HD23	2.13	0.48
1:B:21:LEU:HD12	1:B:22:LEU:N	2.28	0.48
1:B:725:ILE:HG22	1:B:729:ILE:CD1	2.43	0.48
1:C:39:ARG:C	1:C:41:LEU:N	2.71	0.48
1:C:220:ASP:HB3	1:C:238:LYS:HD3	1.94	0.48
1:C:708:HIS:HB3	1:C:711:ILE:CG2	2.43	0.48
1:D:30:LEU:O	1:D:48:PHE:HB2	2.13	0.48
1:A:390:GLU:OE1	1:A:390:GLU:HA	2.13	0.48
1:A:599:ILE:HG21	1:A:631:PHE:CE1	2.47	0.48
1:A:609:LYS:CD	1:A:641:THR:HG22	2.41	0.48
1:B:685:THR:HG1	1:B:688:VAL:HG23	1.78	0.48
1:C:256:LEU:C	1:C:256:LEU:HD12	2.37	0.48
1:C:465:PHE:O	1:C:466:ARG:C	2.56	0.48
1:B:675:ALA:O	1:B:679:MET:HG3	2.14	0.48
1:C:460:ALA:HA	1:C:464:GLU:HG2	1.94	0.48
1:C:663:HIS:NE2	1:C:743:ARG:HB3	2.27	0.48
1:D:179:THR:HG23	1:D:180:SER:N	2.27	0.48
1:D:599:ILE:HG21	1:D:631:PHE:HE1	1.78	0.48
1:A:461:GLY:H	1:A:464:GLU:CD	2.21	0.48
1:B:99:ARG:NH2	1:B:390:GLU:O	2.46	0.48
1:B:698:SER:O	1:B:699:VAL:C	2.57	0.48
1:C:546:VAL:O	1:C:547:GLU:O	2.31	0.48
1:D:271:HIS:O	1:D:275:ILE:HG13	2.13	0.48
1:D:663:HIS:NE2	1:D:743:ARG:HB3	2.28	0.48
1:A:255:ASP:O	1:A:256:LEU:C	2.57	0.48
1:A:459:GLU:O	1:A:459:GLU:HG2	2.12	0.48
1:B:323:PRO:O	1:B:326:VAL:HG23	2.13	0.48
1:B:561:ILE:H	1:B:561:ILE:CD1	2.25	0.48
1:C:346:ILE:HD12	1:C:424:GLU:HG2	1.95	0.48
1:D:159:VAL:HG23	1:D:248:LEU:O	2.13	0.48
1:A:6:HIS:HB2	1:A:21:LEU:HB3	1.96	0.48
1:A:601:ALA:O	1:A:603:GLU:OE2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ARG:HH11	1:C:310:ARG:CB	2.27	0.48
1:D:39:ARG:O	1:D:40:GLY:C	2.55	0.48
1:D:680:ARG:HG3	1:D:680:ARG:NH1	2.29	0.48
1:B:12:THR:HG22	1:B:44:ALA:HB2	1.94	0.48
1:B:472:ALA:O	1:B:475:GLN:N	2.41	0.48
1:A:356:PRO:CB	1:A:544:PHE:HA	2.44	0.48
1:A:629:ILE:N	1:A:630:PRO:HD2	2.29	0.48
1:B:110:LEU:N	1:B:110:LEU:HD23	2.29	0.48
1:B:725:ILE:O	1:B:728:ALA:N	2.47	0.48
1:C:168:LEU:HD13	1:C:259:VAL:CG1	2.42	0.48
1:C:238:LYS:O	1:C:240:ARG:HG3	2.14	0.48
1:C:342:VAL:HG12	1:C:658:CYS:SG	2.54	0.48
1:D:459:GLU:HG2	1:D:459:GLU:O	2.13	0.48
1:D:548:GLN:O	1:D:643:HIS:HB3	2.14	0.48
1:A:377:ASN:O	1:A:381:GLN:HG2	2.13	0.48
1:B:157:ARG:HH21	1:B:249:LEU:HD21	1.77	0.48
1:B:353:CYS:HB3	1:B:541:SER:CB	2.44	0.48
1:B:366:LEU:O	1:B:369:GLU:HB3	2.14	0.48
1:B:420:ILE:HD13	1:B:569:ARG:NH2	2.28	0.48
1:B:708:HIS:O	1:B:711:ILE:HG13	2.13	0.48
1:C:377:ASN:O	1:C:381:GLN:HG2	2.13	0.48
1:C:473:CYS:O	1:C:475:GLN:N	2.47	0.48
1:C:624:ILE:HD13	1:C:624:ILE:N	2.28	0.48
1:C:680:ARG:HG3	1:C:680:ARG:NH1	2.29	0.48
1:D:39:ARG:C	1:D:41:LEU:N	2.66	0.48
1:D:708:HIS:HB3	1:D:711:ILE:CG2	2.44	0.48
1:A:67:TYR:CZ	1:A:114:PRO:HG3	2.48	0.47
1:A:480:PHE:C	1:A:482:SER:H	2.21	0.47
1:B:480:PHE:C	1:B:482:SER:H	2.22	0.47
1:B:729:ILE:N	1:B:729:ILE:HD12	2.28	0.47
1:C:306:LEU:HB2	1:C:391:PHE:HB3	1.95	0.47
1:D:39:ARG:HE	1:D:41:LEU:HD21	1.79	0.47
1:D:67:TYR:CZ	1:D:114:PRO:HG3	2.49	0.47
1:D:463:HIS:O	1:D:464:GLU:C	2.56	0.47
1:D:635:LEU:HA	1:D:638:ILE:HD12	1.96	0.47
1:B:377:ASN:O	1:B:381:GLN:HG2	2.13	0.47
1:B:708:HIS:HB3	1:B:711:ILE:CG2	2.44	0.47
1:C:535:ARG:O	1:C:538:TRP:HB3	2.14	0.47
1:D:260:GLN:O	1:D:264:PHE:CE1	2.66	0.47
1:A:128:MET:O	1:A:132:GLN:HG3	2.13	0.47
1:B:457:MET:C	1:B:459:GLU:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:LEU:O	1:B:661:ALA:C	2.57	0.47
1:C:254:PHE:O	1:C:255:ASP:O	2.32	0.47
1:C:698:SER:O	1:C:699:VAL:C	2.56	0.47
1:D:323:PRO:O	1:D:326:VAL:HG23	2.14	0.47
1:A:249:LEU:HD23	1:A:250:LEU:O	2.14	0.47
1:A:310:ARG:HH11	1:A:310:ARG:CB	2.27	0.47
1:B:96:THR:HG21	1:B:301:THR:HG23	1.96	0.47
1:C:34:LYS:HZ3	1:C:319:THR:HB	1.78	0.47
1:C:87:GLY:O	1:C:90:MET:HG3	2.15	0.47
1:C:139:ARG:HB3	1:C:141:SER:H	1.79	0.47
1:D:67:TYR:O	1:D:70:ILE:HB	2.15	0.47
1:D:471:TYR:CE1	1:D:475:GLN:HG3	2.49	0.47
1:A:395:LEU:HD23	1:A:395:LEU:H	1.76	0.47
1:A:517:LEU:C	1:A:517:LEU:HD12	2.39	0.47
1:B:632:LEU:HD22	1:B:733:CYS:SG	2.54	0.47
1:C:67:TYR:CZ	1:C:114:PRO:HG3	2.48	0.47
1:C:307:ASP:CG	1:C:391:PHE:HA	2.39	0.47
1:C:406:TYR:O	1:C:410:VAL:HG23	2.15	0.47
1:D:140:LEU:HD21	1:D:249:LEU:HD12	1.95	0.47
1:D:342:VAL:O	1:D:346:ILE:HG12	2.13	0.47
1:A:369:GLU:CG	1:A:485:VAL:HG23	2.45	0.47
1:A:395:LEU:N	1:A:395:LEU:CD2	2.78	0.47
1:A:535:ARG:HG3	1:A:535:ARG:NH1	2.29	0.47
1:B:21:LEU:HD13	1:B:112:PHE:CE1	2.49	0.47
1:B:128:MET:O	1:B:129:VAL:C	2.57	0.47
1:B:593:LEU:O	1:B:597:GLU:HG3	2.15	0.47
1:C:249:LEU:HD23	1:C:250:LEU:O	2.15	0.47
1:D:292:ILE:HD12	1:D:292:ILE:O	2.14	0.47
1:D:593:LEU:O	1:D:597:GLU:HG3	2.15	0.47
1:D:609:LYS:HD3	1:D:641:THR:HG22	1.95	0.47
1:A:41:LEU:HD23	1:A:263:GLN:HB3	1.95	0.47
1:A:176:SER:C	1:A:178:GLN:N	2.70	0.47
1:A:445:PRO:HG2	1:A:448:VAL:CG2	2.44	0.47
1:A:486:SER:O	1:A:489:PHE:HB3	2.14	0.47
1:B:259:VAL:O	1:B:259:VAL:HG12	2.15	0.47
1:B:371:VAL:O	1:B:371:VAL:HG12	2.15	0.47
1:C:114:PRO:CA	1:C:258:ARG:NH1	2.69	0.47
1:C:429:LYS:O	1:C:432:MET:O	2.33	0.47
1:C:457:MET:C	1:C:459:GLU:H	2.22	0.47
1:C:462:ALA:O	1:C:465:PHE:HB2	2.15	0.47
1:D:406:TYR:O	1:D:410:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:ILE:H	1:D:527:ILE:CD1	2.27	0.47
1:D:596:TYR:CE2	1:D:600:LEU:HD11	2.49	0.47
1:D:703:VAL:O	1:D:706:GLU:HB3	2.14	0.47
1:D:729:ILE:N	1:D:729:ILE:HD12	2.30	0.47
1:A:0:ALA:O	1:A:1:MET:C	2.55	0.47
1:A:160:ALA:CB	1:A:168:LEU:HD23	2.40	0.47
1:A:457:MET:C	1:A:459:GLU:H	2.21	0.47
1:A:546:VAL:O	1:A:547:GLU:O	2.33	0.47
1:A:721:THR:O	1:A:724:ALA:HB3	2.14	0.47
1:C:176:SER:C	1:C:178:GLN:N	2.71	0.47
1:C:486:SER:O	1:C:489:PHE:HB3	2.14	0.47
1:C:587:PRO:HG2	1:C:588:VAL:H	1.79	0.47
1:D:87:GLY:O	1:D:90:MET:HG3	2.14	0.47
1:A:472:ALA:CB	1:A:477:ILE:HD12	2.45	0.47
1:B:4:LEU:HD12	1:B:4:LEU:N	2.29	0.47
1:B:406:TYR:O	1:B:410:VAL:HG23	2.15	0.47
1:C:6:HIS:HB2	1:C:21:LEU:HB3	1.97	0.47
1:C:381:GLN:HE22	1:C:402:TRP:CD1	2.31	0.47
1:D:259:VAL:O	1:D:260:GLN:C	2.56	0.47
1:D:385:LEU:N	1:D:386:PRO:CD	2.78	0.47
1:D:668:HIS:CB	1:D:671:LEU:HD12	2.45	0.47
1:A:385:LEU:N	1:A:386:PRO:CD	2.78	0.47
1:A:399:SER:HA	1:B:395:LEU:CD1	2.39	0.47
1:B:38:GLY:HA3	1:B:41:LEU:CD1	2.45	0.47
1:B:157:ARG:NE	1:B:249:LEU:HD21	2.26	0.47
1:B:381:GLN:NE2	1:B:402:TRP:HD1	2.13	0.47
1:B:456:CYS:HB2	1:B:457:MET:CE	2.45	0.47
1:B:721:THR:O	1:B:724:ALA:HB3	2.15	0.47
1:C:461:GLY:O	1:C:462:ALA:O	2.33	0.47
1:A:137:ALA:HB1	1:A:248:LEU:CD2	2.45	0.46
1:A:139:ARG:CG	1:A:245:GLU:O	2.63	0.46
1:A:725:ILE:HG22	1:A:729:ILE:CD1	2.45	0.46
1:B:176:SER:C	1:B:178:GLN:N	2.70	0.46
1:B:624:ILE:HD13	1:B:624:ILE:N	2.28	0.46
1:B:698:SER:O	1:B:702:GLU:HG3	2.14	0.46
1:C:35:VAL:HG12	1:C:318:ARG:HB3	1.98	0.46
1:C:696:PHE:HB3	1:C:700:VAL:HG21	1.96	0.46
1:D:6:HIS:HB2	1:D:21:LEU:HB3	1.97	0.46
1:D:609:LYS:CE	1:D:637:GLN:HB3	2.42	0.46
1:A:429:LYS:O	1:A:432:MET:O	2.33	0.46
1:A:698:SER:O	1:A:699:VAL:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:LYS:O	1:D:240:ARG:HG3	2.14	0.46
1:D:458:GLY:C	1:D:460:ALA:N	2.72	0.46
1:A:38:GLY:O	1:A:41:LEU:O	2.33	0.46
1:A:110:LEU:HD23	1:A:110:LEU:N	2.30	0.46
1:A:179:THR:HG21	1:A:209:ASP:HA	1.97	0.46
1:A:480:PHE:C	1:A:482:SER:N	2.73	0.46
1:A:535:ARG:O	1:A:538:TRP:HB3	2.14	0.46
1:A:632:LEU:HD22	1:A:733:CYS:SG	2.55	0.46
1:B:238:LYS:O	1:B:240:ARG:HG3	2.14	0.46
1:B:465:PHE:HZ	1:B:505:TYR:CG	2.33	0.46
1:C:4:LEU:N	1:C:4:LEU:HD12	2.30	0.46
1:C:300:ILE:CG2	1:C:304:LEU:HD12	2.43	0.46
1:C:386:PRO:HB3	1:C:402:TRP:NE1	2.31	0.46
1:C:480:PHE:C	1:C:482:SER:N	2.72	0.46
1:C:597:GLU:O	1:C:600:LEU:HB2	2.16	0.46
1:D:176:SER:C	1:D:178:GLN:N	2.69	0.46
1:A:34:LYS:CB	1:A:45:GLU:HG3	2.46	0.46
1:A:323:PRO:O	1:A:326:VAL:HG23	2.16	0.46
1:A:402:TRP:CE3	1:A:405:MET:CE	2.98	0.46
1:B:300:ILE:CG2	1:B:304:LEU:HD12	2.40	0.46
1:B:587:PRO:HG2	1:B:588:VAL:H	1.79	0.46
1:C:599:ILE:HG21	1:C:631:PHE:HE1	1.80	0.46
1:D:20:LEU:HB2	1:D:115:LEU:HD11	1.96	0.46
1:D:432:MET:HE3	1:D:480:PHE:CZ	2.51	0.46
1:A:587:PRO:HG2	1:A:588:VAL:N	2.30	0.46
1:B:6:HIS:HB2	1:B:21:LEU:HB3	1.96	0.46
1:C:82:SER:HB3	1:C:85:GLU:HB3	1.98	0.46
1:C:153:SER:O	1:C:157:ARG:HD2	2.15	0.46
1:C:465:PHE:CZ	1:C:502:LEU:HD13	2.50	0.46
1:D:33:PHE:CD2	1:D:318:ARG:HB2	2.51	0.46
1:A:90:MET:CE	1:A:318:ARG:HH22	2.29	0.46
1:A:96:THR:CG2	1:A:301:THR:HG23	2.45	0.46
1:A:494:ARG:HH11	1:A:494:ARG:CG	2.29	0.46
1:A:708:HIS:HB3	1:A:711:ILE:CG2	2.46	0.46
1:B:59:THR:O	1:B:63:ILE:HG13	2.16	0.46
1:D:21:LEU:HD12	1:D:22:LEU:N	2.31	0.46
1:D:142:ASP:O	1:D:143:GLU:HG3	2.16	0.46
1:D:680:ARG:HG3	1:D:680:ARG:HH11	1.80	0.46
1:A:4:LEU:N	1:A:4:LEU:HD12	2.31	0.46
1:A:280:CYS:SG	1:A:280:CYS:O	2.74	0.46
1:A:335:LEU:O	1:A:411:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:CYS:HB2	1:A:457:MET:CE	2.45	0.46
1:A:663:HIS:NE2	1:A:743:ARG:HB3	2.30	0.46
1:B:39:ARG:N	1:B:39:ARG:CD	2.75	0.46
1:D:142:ASP:C	1:D:143:GLU:HG3	2.40	0.46
1:D:153:SER:O	1:D:157:ARG:HD2	2.16	0.46
1:D:352:LEU:CD1	1:D:363:LEU:HD13	2.45	0.46
1:D:546:VAL:O	1:D:547:GLU:O	2.33	0.46
1:A:401:THR:HB	1:A:404:ASP:OD2	2.15	0.46
1:C:161:THR:CB	1:C:164:ILE:HB	2.46	0.46
1:D:265:LEU:N	1:D:266:PRO:CD	2.79	0.46
1:D:708:HIS:O	1:D:711:ILE:HG13	2.15	0.46
1:A:685:THR:OG1	1:A:688:VAL:HG23	2.15	0.46
1:B:39:ARG:NH2	1:B:267:GLU:CD	2.74	0.46
1:B:480:PHE:C	1:B:482:SER:N	2.73	0.46
1:B:493:LEU:HD23	1:B:496:ILE:HD12	1.98	0.46
1:C:262:LEU:C	1:C:264:PHE:N	2.73	0.46
1:C:564:LEU:C	1:C:564:LEU:HD12	2.41	0.46
1:C:685:THR:OG1	1:C:688:VAL:HG23	2.16	0.46
1:D:708:HIS:CB	1:D:711:ILE:HG21	2.46	0.46
1:B:7:CYS:HB2	1:B:49:GLU:HG3	1.96	0.46
1:B:607:GLY:C	1:B:609:LYS:H	2.24	0.46
1:C:90:MET:CE	1:C:318:ARG:HH22	2.28	0.46
1:C:254:PHE:C	1:C:255:ASP:O	2.58	0.46
1:D:480:PHE:C	1:D:482:SER:H	2.23	0.46
1:D:494:ARG:HH11	1:D:494:ARG:CG	2.29	0.46
1:D:564:LEU:C	1:D:566:ILE:N	2.73	0.46
1:A:189:GLU:OE2	1:A:191:ILE:HD11	2.16	0.45
1:A:292:ILE:HD12	1:A:292:ILE:O	2.15	0.45
1:A:458:GLY:O	1:A:460:ALA:N	2.49	0.45
1:C:466:ARG:NH1	1:C:501:MET:CE	2.80	0.45
1:D:189:GLU:OE2	1:D:191:ILE:HD11	2.16	0.45
1:D:685:THR:OG1	1:D:688:VAL:HG23	2.17	0.45
1:D:698:SER:O	1:D:699:VAL:C	2.59	0.45
1:A:170:VAL:O	1:A:215:ALA:HB1	2.15	0.45
1:A:371:VAL:HG12	1:A:371:VAL:O	2.15	0.45
1:A:604:SER:HB3	1:A:634:ARG:NH1	2.32	0.45
1:C:632:LEU:HD22	1:C:733:CYS:SG	2.57	0.45
1:C:680:ARG:HG3	1:C:680:ARG:HH11	1.81	0.45
1:D:9:THR:HG23	1:D:18:HIS:CE1	2.51	0.45
1:D:39:ARG:O	1:D:41:LEU:N	2.49	0.45
1:D:330:ASP:O	1:D:334:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:PRO:O	1:C:326:VAL:HG23	2.16	0.45
1:C:593:LEU:O	1:C:597:GLU:HG3	2.17	0.45
1:D:4:LEU:HD12	1:D:4:LEU:N	2.32	0.45
1:D:235:LEU:HD23	1:D:235:LEU:HA	1.75	0.45
1:D:332:PHE:CD1	1:D:408:GLU:HG3	2.51	0.45
1:D:339:GLY:HA3	1:D:407:GLU:O	2.16	0.45
1:D:480:PHE:C	1:D:482:SER:N	2.74	0.45
1:D:535:ARG:O	1:D:538:TRP:HB3	2.15	0.45
1:B:67:TYR:CZ	1:B:114:PRO:HG3	2.51	0.45
1:B:154:LEU:HD22	1:B:249:LEU:CD1	2.47	0.45
1:B:465:PHE:CZ	1:B:505:TYR:HB2	2.52	0.45
1:C:110:LEU:N	1:C:110:LEU:HD23	2.32	0.45
1:D:371:VAL:O	1:D:371:VAL:HG12	2.16	0.45
1:D:381:GLN:NE2	1:D:402:TRP:HD1	2.15	0.45
1:A:524:VAL:O	1:A:524:VAL:HG12	2.16	0.45
1:B:96:THR:CG2	1:B:301:THR:HG23	2.47	0.45
1:B:287:PRO:HG2	1:B:409:ILE:HG12	1.99	0.45
1:B:385:LEU:N	1:B:386:PRO:CD	2.79	0.45
1:B:535:ARG:O	1:B:538:TRP:HB3	2.17	0.45
1:B:635:LEU:HA	1:B:638:ILE:HD12	1.97	0.45
1:C:1:MET:O	1:C:2:HIS:C	2.60	0.45
1:C:22:LEU:O	1:C:110:LEU:HA	2.16	0.45
1:C:279:ILE:HD11	1:C:293:GLY:O	2.17	0.45
1:D:334:ARG:NH2	1:D:669:PRO:HA	2.32	0.45
1:D:429:LYS:O	1:D:432:MET:O	2.34	0.45
1:D:506:ARG:O	1:D:510:GLN:HB2	2.16	0.45
1:D:682:SER:CB	1:D:751:VAL:HG12	2.47	0.45
1:A:258:ARG:O	1:A:259:VAL:C	2.60	0.45
1:A:703:VAL:O	1:A:706:GLU:HB3	2.17	0.45
1:B:153:SER:O	1:B:157:ARG:HD2	2.16	0.45
1:B:708:HIS:CB	1:B:711:ILE:HG21	2.46	0.45
1:C:137:ALA:HB1	1:C:248:LEU:HD21	1.98	0.45
1:C:154:LEU:HD22	1:C:249:LEU:HD11	1.98	0.45
1:C:708:HIS:CB	1:C:711:ILE:HG21	2.45	0.45
1:D:1:MET:O	1:D:2:HIS:C	2.60	0.45
1:A:158:MET:HE1	1:A:256:LEU:HD13	1.98	0.45
1:A:608:SER:O	1:A:611:ILE:N	2.50	0.45
1:A:682:SER:CB	1:A:751:VAL:HG12	2.47	0.45
1:B:178:GLN:NE2	1:B:212:LEU:HD12	2.23	0.45
1:B:243:PRO:HA	1:B:244:PRO:HD3	1.89	0.45
1:B:429:LYS:HE2	1:B:515:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:LEU:C	1:B:564:LEU:HD12	2.42	0.45
1:C:90:MET:HE3	1:C:318:ARG:HH22	1.82	0.45
1:D:469:VAL:C	1:D:471:TYR:N	2.75	0.45
1:A:74:LEU:HD11	1:A:254:PHE:CE2	2.52	0.45
1:A:645:TYR:C	1:A:645:TYR:CD1	2.94	0.45
1:B:524:VAL:O	1:B:524:VAL:HG12	2.17	0.45
1:C:601:ALA:O	1:C:634:ARG:NH2	2.49	0.45
1:A:21:LEU:HD12	1:A:22:LEU:N	2.32	0.45
1:A:258:ARG:HD3	1:A:258:ARG:HA	1.78	0.45
1:B:1:MET:O	1:B:2:HIS:C	2.59	0.45
1:B:352:LEU:CD1	1:B:363:LEU:HD13	2.44	0.45
1:B:542:PRO:HA	1:B:592:VAL:HG22	1.98	0.45
1:B:696:PHE:HB3	1:B:700:VAL:HG21	1.99	0.45
1:C:222:LYS:O	1:C:260:GLN:NE2	2.50	0.45
1:C:262:LEU:HB3	1:C:263:GLN:HE21	1.81	0.45
1:C:401:THR:O	1:C:402:TRP:C	2.59	0.45
1:C:682:SER:CB	1:C:751:VAL:HG12	2.47	0.45
1:D:14:ARG:HH12	1:D:223:ASP:HA	1.80	0.45
1:D:21:LEU:HD11	1:D:110:LEU:HB2	1.98	0.45
1:D:286:PHE:O	1:D:287:PRO:C	2.59	0.45
1:D:310:ARG:HH11	1:D:310:ARG:CB	2.29	0.45
1:D:448:VAL:HG13	1:D:468:LEU:CD2	2.43	0.45
1:D:462:ALA:O	1:D:463:HIS:C	2.60	0.45
1:A:1:MET:O	1:A:2:HIS:C	2.60	0.45
1:A:330:ASP:O	1:A:334:ARG:HG2	2.17	0.45
1:C:330:ASP:O	1:C:334:ARG:HG2	2.17	0.45
1:C:535:ARG:HG3	1:C:535:ARG:NH1	2.32	0.45
1:C:635:LEU:HA	1:C:638:ILE:HD12	1.98	0.45
1:D:428:ALA:HB3	1:D:511:PHE:CZ	2.52	0.45
1:A:90:MET:HE3	1:A:318:ARG:HH22	1.82	0.44
1:A:139:ARG:NH2	1:A:163:GLU:OE2	2.49	0.44
1:A:368:MET:HG3	1:B:368:MET:HG3	1.99	0.44
1:B:90:MET:CE	1:B:318:ARG:NH2	2.79	0.44
1:B:256:LEU:C	1:B:258:ARG:N	2.74	0.44
1:B:330:ASP:O	1:B:334:ARG:HG2	2.16	0.44
1:B:458:GLY:O	1:B:460:ALA:N	2.50	0.44
1:C:179:THR:HG21	1:C:209:ASP:HA	1.98	0.44
1:C:292:ILE:HD12	1:C:292:ILE:O	2.16	0.44
1:C:472:ALA:CB	1:C:477:ILE:HD12	2.46	0.44
1:D:178:GLN:NE2	1:D:212:LEU:HD12	2.22	0.44
1:D:524:VAL:O	1:D:524:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:574:PRO:HA	1:D:578:GLY:H	1.83	0.44
1:D:587:PRO:HG2	1:D:588:VAL:N	2.32	0.44
1:A:312:ARG:HG3	1:A:313:GLY:N	2.32	0.44
1:A:413:ILE:HG21	1:A:422:GLY:C	2.42	0.44
1:A:564:LEU:C	1:A:564:LEU:HD12	2.42	0.44
1:B:170:VAL:HG12	1:B:216:VAL:O	2.17	0.44
1:C:462:ALA:O	1:C:463:HIS:C	2.60	0.44
1:C:609:LYS:HD3	1:C:641:THR:HG22	1.99	0.44
1:D:243:PRO:HA	1:D:244:PRO:HD3	1.91	0.44
1:D:402:TRP:HA	1:D:402:TRP:HE3	1.82	0.44
1:A:390:GLU:O	1:A:391:PHE:HB3	2.16	0.44
1:A:391:PHE:CE1	1:A:393:ASN:HA	2.52	0.44
1:B:14:ARG:HD3	1:B:257:ILE:CD1	2.48	0.44
1:B:189:GLU:OE2	1:B:191:ILE:HD11	2.17	0.44
1:C:312:ARG:HG3	1:C:313:GLY:N	2.32	0.44
1:C:566:ILE:HD11	1:C:577:TYR:CE2	2.53	0.44
1:C:705:ILE:HG12	1:C:711:ILE:CD1	2.44	0.44
1:D:312:ARG:HG3	1:D:313:GLY:N	2.33	0.44
1:D:353:CYS:SG	1:D:563:VAL:HG21	2.58	0.44
1:A:238:LYS:O	1:A:240:ARG:HG3	2.17	0.44
1:B:67:TYR:O	1:B:70:ILE:HB	2.18	0.44
1:B:115:LEU:H	1:B:258:ARG:NH2	2.09	0.44
1:C:11:VAL:O	1:C:44:ALA:HB1	2.17	0.44
1:C:322:GLY:O	1:C:323:PRO:C	2.60	0.44
1:C:645:TYR:CD1	1:C:645:TYR:C	2.96	0.44
1:D:159:VAL:HG21	1:D:247:CYS:HB3	1.99	0.44
1:D:322:GLY:O	1:D:323:PRO:C	2.60	0.44
1:A:21:LEU:HD13	1:A:112:PHE:CE1	2.52	0.44
1:A:322:GLY:O	1:A:323:PRO:C	2.60	0.44
1:B:27:LEU:O	1:B:28:GLY:C	2.61	0.44
1:B:312:ARG:HG3	1:B:313:GLY:N	2.31	0.44
1:B:458:GLY:C	1:B:460:ALA:N	2.72	0.44
1:C:1:MET:O	1:C:3:ALA:N	2.51	0.44
1:C:371:VAL:O	1:C:371:VAL:HG12	2.17	0.44
1:C:458:GLY:O	1:C:460:ALA:N	2.50	0.44
1:C:527:ILE:H	1:C:527:ILE:CD1	2.29	0.44
1:D:12:THR:HG22	1:D:44:ALA:HB2	1.98	0.44
1:D:280:CYS:SG	1:D:280:CYS:O	2.75	0.44
1:D:486:SER:O	1:D:489:PHE:HB3	2.18	0.44
1:D:564:LEU:C	1:D:564:LEU:HD12	2.42	0.44
1:D:599:ILE:HG21	1:D:631:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:THR:HG23	1:A:18:HIS:CE1	2.53	0.44
1:A:159:VAL:HG23	1:A:248:LEU:O	2.17	0.44
1:A:259:VAL:O	1:A:262:LEU:N	2.44	0.44
1:A:668:HIS:CB	1:A:671:LEU:HD12	2.48	0.44
1:B:432:MET:HE3	1:B:480:PHE:CE2	2.53	0.44
1:C:189:GLU:OE2	1:C:191:ILE:HD11	2.17	0.44
1:C:642:PRO:HB2	1:C:643:HIS:H	1.63	0.44
1:D:104:PRO:HG2	1:D:107:PHE:CE1	2.52	0.44
1:A:170:VAL:HG12	1:A:216:VAL:O	2.18	0.44
1:B:1:MET:O	1:B:3:ALA:N	2.51	0.44
1:B:36:SER:O	1:B:37:ALA:C	2.61	0.44
1:B:41:LEU:C	1:B:41:LEU:HD12	2.43	0.44
1:B:75:LEU:HD21	1:B:262:LEU:O	2.18	0.44
1:B:527:ILE:H	1:B:527:ILE:CD1	2.28	0.44
1:C:34:LYS:NZ	1:C:319:THR:HB	2.32	0.44
1:C:446:ASP:O	1:C:449:THR:HB	2.18	0.44
1:C:564:LEU:C	1:C:566:ILE:N	2.74	0.44
1:D:33:PHE:N	1:D:321:PHE:CE1	2.85	0.44
1:D:82:SER:HB3	1:D:85:GLU:HB3	1.99	0.44
1:D:170:VAL:HG12	1:D:216:VAL:O	2.18	0.44
1:A:139:ARG:HG3	1:A:245:GLU:O	2.18	0.44
1:A:506:ARG:O	1:A:510:GLN:HB2	2.18	0.44
1:B:132:GLN:O	1:B:133:LEU:C	2.61	0.44
1:C:599:ILE:HG21	1:C:631:PHE:CE1	2.53	0.44
1:C:660:LEU:O	1:C:661:ALA:C	2.61	0.44
1:A:226:ILE:N	1:A:226:ILE:CD1	2.81	0.44
1:A:574:PRO:HA	1:A:578:GLY:H	1.83	0.44
1:B:279:ILE:HD11	1:B:293:GLY:O	2.18	0.44
1:B:498:ALA:HA	1:B:501:MET:CE	2.46	0.44
1:B:564:LEU:C	1:B:566:ILE:N	2.75	0.44
1:C:178:GLN:NE2	1:C:212:LEU:HD12	2.21	0.44
1:A:527:ILE:H	1:A:527:ILE:CD1	2.29	0.43
1:A:587:PRO:CG	1:A:588:VAL:H	2.31	0.43
1:B:21:LEU:HD11	1:B:110:LEU:HB2	1.99	0.43
1:B:140:LEU:C	1:B:142:ASP:N	2.74	0.43
1:B:179:THR:HG21	1:B:209:ASP:HA	2.00	0.43
1:B:264:PHE:N	1:B:264:PHE:CD1	2.86	0.43
1:C:413:ILE:HG21	1:C:422:GLY:C	2.43	0.43
1:C:428:ALA:HB3	1:C:511:PHE:CZ	2.52	0.43
1:C:465:PHE:CE1	1:C:502:LEU:CB	2.98	0.43
1:D:200:ALA:C	1:D:202:ASN:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:O	1:A:3:ALA:N	2.51	0.43
1:A:38:GLY:O	1:A:40:GLY:N	2.51	0.43
1:A:696:PHE:HB3	1:A:700:VAL:HG21	1.99	0.43
1:B:310:ARG:HH11	1:B:310:ARG:CB	2.29	0.43
1:B:445:PRO:HD2	1:B:471:TYR:CE1	2.53	0.43
1:B:618:ARG:HH11	1:B:618:ARG:CB	2.30	0.43
1:B:682:SER:CB	1:B:751:VAL:HG12	2.48	0.43
1:C:132:GLN:O	1:C:133:LEU:C	2.59	0.43
1:A:59:THR:O	1:A:63:ILE:HG13	2.18	0.43
1:B:97:PHE:HZ	1:B:301:THR:HA	1.83	0.43
1:B:249:LEU:HD23	1:B:250:LEU:O	2.18	0.43
1:C:34:LYS:HZ3	1:C:319:THR:CG2	2.31	0.43
1:D:279:ILE:HD11	1:D:293:GLY:O	2.18	0.43
1:D:660:LEU:O	1:D:661:ALA:C	2.59	0.43
1:A:402:TRP:HA	1:A:402:TRP:HE3	1.83	0.43
1:B:41:LEU:HB2	1:B:42:PRO:HD2	1.99	0.43
1:C:27:LEU:O	1:C:28:GLY:C	2.60	0.43
1:C:564:LEU:HD23	1:C:592:VAL:CG1	2.48	0.43
1:A:14:ARG:HH12	1:A:223:ASP:HA	1.83	0.43
1:A:402:TRP:CE3	1:A:402:TRP:HA	2.53	0.43
1:A:564:LEU:C	1:A:566:ILE:N	2.74	0.43
1:A:708:HIS:CB	1:A:711:ILE:HG21	2.47	0.43
1:B:87:GLY:O	1:B:90:MET:HG3	2.19	0.43
1:D:432:MET:HE3	1:D:480:PHE:CE2	2.53	0.43
1:D:645:TYR:C	1:D:645:TYR:CD1	2.97	0.43
1:A:27:LEU:O	1:A:28:GLY:C	2.61	0.43
1:B:322:GLY:O	1:B:323:PRO:C	2.60	0.43
1:B:566:ILE:HD11	1:B:577:TYR:CD2	2.54	0.43
1:B:604:SER:C	1:B:606:GLY:H	2.26	0.43
1:C:264:PHE:O	1:C:268:ILE:HG13	2.18	0.43
1:D:179:THR:HG21	1:D:209:ASP:HA	2.00	0.43
1:D:546:VAL:O	1:D:547:GLU:C	2.62	0.43
1:D:566:ILE:HD11	1:D:577:TYR:CE2	2.54	0.43
1:D:641:THR:O	1:D:642:PRO:O	2.36	0.43
1:A:635:LEU:HA	1:A:638:ILE:HD12	2.01	0.43
1:B:130:THR:HG23	1:B:253:GLU:OE1	2.19	0.43
1:B:280:CYS:SG	1:B:280:CYS:O	2.76	0.43
1:B:413:ILE:HG21	1:B:422:GLY:C	2.44	0.43
1:C:561:ILE:H	1:C:561:ILE:CD1	2.29	0.43
1:D:34:LYS:CB	1:D:45:GLU:HG3	2.48	0.43
1:D:161:THR:CB	1:D:164:ILE:HB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:721:THR:O	1:D:724:ALA:HB3	2.19	0.43
1:A:161:THR:CB	1:A:164:ILE:HB	2.48	0.43
1:A:265:LEU:H	1:A:266:PRO:CD	2.31	0.43
1:A:275:ILE:HG23	1:A:297:TYR:HB2	1.99	0.43
1:A:333:GLN:NE2	1:A:672:THR:HB	2.34	0.43
1:A:432:MET:HE1	1:A:534:ALA:O	2.19	0.43
1:A:566:ILE:HD11	1:A:577:TYR:CD2	2.54	0.43
1:A:674:GLY:O	1:A:675:ALA:C	2.61	0.43
1:C:27:LEU:HA	1:C:293:GLY:HA3	2.00	0.43
1:C:235:LEU:O	1:C:237:PRO:HD2	2.18	0.43
1:C:326:VAL:HG12	1:C:330:ASP:HB2	2.01	0.43
1:C:432:MET:HE2	1:C:534:ALA:CB	2.40	0.43
1:D:1:MET:CE	1:D:55:SER:HB3	2.48	0.43
1:D:27:LEU:O	1:D:28:GLY:C	2.60	0.43
1:D:472:ALA:HB1	1:D:477:ILE:HB	2.00	0.43
1:A:178:GLN:NE2	1:A:212:LEU:HD12	2.23	0.43
1:A:307:ASP:CG	1:A:391:PHE:HA	2.44	0.43
1:A:470:ASP:O	1:A:474:GLU:N	2.51	0.43
1:A:523:VAL:HB	1:A:528:ASP:CG	2.43	0.43
1:B:228:ALA:HB3	1:B:231:SER:HB3	2.01	0.43
1:B:566:ILE:HD11	1:B:577:TYR:CE2	2.54	0.43
1:D:59:THR:O	1:D:63:ILE:HG13	2.19	0.43
1:D:141:SER:C	1:D:143:GLU:N	2.75	0.43
1:D:237:PRO:O	1:D:238:LYS:HG3	2.19	0.43
1:D:249:LEU:HD23	1:D:250:LEU:O	2.19	0.43
1:D:535:ARG:HG3	1:D:535:ARG:NH1	2.34	0.43
1:A:60:ASP:HB3	1:A:124:LEU:HD13	2.00	0.43
1:A:279:ILE:HD11	1:A:293:GLY:O	2.19	0.43
1:A:402:TRP:O	1:A:403:ALA:C	2.61	0.43
1:A:470:ASP:C	1:A:473:CYS:H	2.27	0.43
1:B:178:GLN:NE2	1:B:193:TYR:OH	2.49	0.43
1:B:668:HIS:CB	1:B:671:LEU:HD12	2.49	0.43
1:C:60:ASP:HA	1:C:63:ILE:HD12	1.99	0.43
1:C:140:LEU:CD1	1:C:213:VAL:HG21	2.48	0.43
1:D:564:LEU:HD23	1:D:592:VAL:CG1	2.49	0.43
1:A:137:ALA:HB3	1:A:248:LEU:HD21	1.99	0.42
1:A:352:LEU:CD1	1:A:363:LEU:HD13	2.43	0.42
1:A:685:THR:HG1	1:A:688:VAL:HG23	1.84	0.42
1:B:506:ARG:O	1:B:510:GLN:HB2	2.19	0.42
1:B:559:PRO:HB2	1:B:560:THR:H	1.69	0.42
1:D:143:GLU:O	1:D:146:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:MET:HE1	1:D:256:LEU:HD13	2.01	0.42
1:D:346:ILE:HG21	1:D:427:LEU:HD13	2.00	0.42
1:D:460:ALA:HA	1:D:464:GLU:OE2	2.18	0.42
1:A:462:ALA:HB1	1:A:498:ALA:CB	2.47	0.42
1:A:566:ILE:HD11	1:A:577:TYR:CE2	2.54	0.42
1:B:254:PHE:CD1	1:B:254:PHE:N	2.86	0.42
1:B:256:LEU:O	1:B:258:ARG:N	2.53	0.42
1:B:381:GLN:HE21	1:B:402:TRP:HD1	1.66	0.42
1:C:205:LEU:HA	1:C:245:GLU:OE1	2.18	0.42
1:C:280:CYS:SG	1:C:280:CYS:O	2.76	0.42
1:C:465:PHE:HZ	1:C:502:LEU:HD13	1.84	0.42
1:C:611:ILE:O	1:C:615:THR:HG23	2.19	0.42
1:C:624:ILE:HB	1:C:625:PRO:HD2	2.01	0.42
1:D:261:ALA:HA	1:D:264:PHE:CD1	2.54	0.42
1:D:566:ILE:HD11	1:D:577:TYR:CD2	2.54	0.42
1:D:668:HIS:HB3	1:D:671:LEU:HD12	2.00	0.42
1:A:326:VAL:HG12	1:A:330:ASP:HB2	2.01	0.42
1:B:230:GLY:HA2	1:B:233:ASP:CG	2.44	0.42
1:B:379:LEU:HD21	1:B:481:CYS:HB3	2.01	0.42
1:B:494:ARG:HH11	1:B:494:ARG:CG	2.33	0.42
1:C:33:PHE:HD2	1:C:318:ARG:HB2	1.84	0.42
1:C:41:LEU:HD12	1:C:42:PRO:O	2.20	0.42
1:C:350:ARG:CD	1:C:539:LEU:HA	2.50	0.42
1:C:402:TRP:CE3	1:C:402:TRP:HA	2.55	0.42
1:D:1:MET:O	1:D:3:ALA:N	2.52	0.42
1:D:14:ARG:HD3	1:D:257:ILE:CD1	2.47	0.42
1:D:97:PHE:HZ	1:D:301:THR:HA	1.84	0.42
1:D:158:MET:CE	1:D:256:LEU:HD13	2.49	0.42
1:A:67:TYR:O	1:A:70:ILE:HB	2.19	0.42
1:A:327:SER:HG	1:A:329:THR:HB	1.82	0.42
1:A:725:ILE:O	1:A:726:LEU:C	2.62	0.42
1:A:747:LEU:N	1:A:748:PRO:CD	2.82	0.42
1:B:603:GLU:N	1:B:634:ARG:HH22	2.17	0.42
1:C:36:SER:CB	1:C:317:TRP:HE3	2.33	0.42
1:C:170:VAL:HG12	1:C:216:VAL:O	2.19	0.42
1:C:200:ALA:C	1:C:202:ASN:N	2.76	0.42
1:C:494:ARG:HH11	1:C:494:ARG:CG	2.32	0.42
1:C:725:ILE:O	1:C:726:LEU:C	2.63	0.42
1:D:60:ASP:HB3	1:D:124:LEU:HD13	2.01	0.42
1:D:257:ILE:O	1:D:258:ARG:C	2.61	0.42
1:D:464:GLU:O	1:D:465:PHE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:ILE:H	1:D:561:ILE:CD1	2.27	0.42
1:D:587:PRO:CG	1:D:588:VAL:H	2.32	0.42
1:A:236:ALA:N	1:A:237:PRO:HD3	2.34	0.42
1:A:402:TRP:CE3	1:A:405:MET:HE3	2.54	0.42
1:A:493:LEU:HD23	1:A:496:ILE:HD12	2.02	0.42
1:B:191:ILE:CG2	1:B:195:ARG:HD3	2.49	0.42
1:B:200:ALA:C	1:B:202:ASN:N	2.76	0.42
1:B:437:SER:CB	1:B:478:SER:O	2.64	0.42
1:B:686:ASN:O	1:B:687:SER:C	2.62	0.42
1:C:170:VAL:C	1:C:215:ALA:HB1	2.45	0.42
1:C:256:LEU:O	1:C:257:ILE:C	2.62	0.42
1:C:466:ARG:HD3	1:C:466:ARG:HA	1.84	0.42
1:D:609:LYS:CD	1:D:641:THR:HG22	2.49	0.42
1:A:153:SER:O	1:A:157:ARG:HD2	2.19	0.42
1:A:217:ARG:HG2	1:A:217:ARG:NH1	2.34	0.42
1:A:523:VAL:O	1:A:524:VAL:CB	2.66	0.42
1:B:9:THR:HG23	1:B:18:HIS:CE1	2.54	0.42
1:B:326:VAL:HG12	1:B:330:ASP:HB2	2.02	0.42
1:C:286:PHE:O	1:C:287:PRO:C	2.63	0.42
1:C:596:TYR:CD2	1:C:600:LEU:HD11	2.54	0.42
1:D:96:THR:HG21	1:D:301:THR:HG23	2.00	0.42
1:D:226:ILE:N	1:D:226:ILE:CD1	2.82	0.42
1:A:200:ALA:C	1:A:202:ASN:N	2.77	0.42
1:A:381:GLN:NE2	1:A:402:TRP:CD1	2.88	0.42
1:B:82:SER:HB3	1:B:85:GLU:HB3	2.02	0.42
1:B:397:ALA:O	1:B:398:LYS:C	2.63	0.42
1:B:465:PHE:CD2	1:B:501:MET:HB3	2.55	0.42
1:B:638:ILE:HG13	1:B:638:ILE:H	1.60	0.42
1:C:668:HIS:CB	1:C:671:LEU:HD12	2.49	0.42
1:A:275:ILE:O	1:A:276:GLN:C	2.63	0.42
1:B:161:THR:CB	1:B:164:ILE:HB	2.49	0.42
1:B:470:ASP:O	1:B:474:GLU:HG3	2.20	0.42
1:C:62:THR:O	1:C:66:VAL:HG23	2.19	0.42
1:C:242:LEU:HA	1:C:243:PRO:HD3	1.89	0.42
1:C:265:LEU:O	1:C:266:PRO:C	2.63	0.42
1:D:242:LEU:HD12	1:D:247:CYS:SG	2.59	0.42
1:A:252:ASP:O	1:A:253:GLU:C	2.61	0.42
1:A:342:VAL:CG2	1:A:410:VAL:HG12	2.49	0.42
1:A:548:GLN:NE2	1:A:548:GLN:CA	2.83	0.42
1:B:110:LEU:HD11	1:B:269:ALA:CB	2.50	0.42
1:B:574:PRO:HA	1:B:578:GLY:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:TYR:CD1	1:B:645:TYR:C	2.97	0.42
1:C:20:LEU:HB2	1:C:115:LEU:HD11	2.02	0.42
1:C:265:LEU:N	1:C:266:PRO:CD	2.83	0.42
1:C:506:ARG:O	1:C:510:GLN:HB2	2.20	0.42
1:C:566:ILE:HD11	1:C:577:TYR:CD2	2.55	0.42
1:D:90:MET:HE1	1:D:318:ARG:NH2	2.34	0.42
1:D:251:PRO:HG2	1:D:254:PHE:HD1	1.82	0.42
1:D:289:CYS:SG	1:D:291:ARG:HG3	2.60	0.42
1:D:602:TYR:CD1	1:D:603:GLU:HG2	2.55	0.42
1:A:39:ARG:CD	1:A:317:TRP:CE2	2.97	0.42
1:A:374:GLU:H	1:A:374:GLU:CD	2.28	0.42
1:A:392:SER:C	1:A:394:ASN:N	2.74	0.42
1:A:445:PRO:CG	1:A:448:VAL:HG23	2.49	0.42
1:A:660:LEU:O	1:A:661:ALA:C	2.63	0.42
1:B:265:LEU:N	1:B:266:PRO:HD3	2.35	0.42
1:C:401:THR:O	1:C:404:ASP:N	2.43	0.42
1:C:493:LEU:HD23	1:C:496:ILE:HD12	2.01	0.42
1:C:747:LEU:N	1:C:748:PRO:CD	2.83	0.42
1:D:162:PRO:HA	1:D:166:TRP:CD1	2.55	0.42
1:D:458:GLY:O	1:D:460:ALA:N	2.51	0.42
1:A:110:LEU:HD12	1:A:112:PHE:CZ	2.55	0.41
1:A:444:CYS:SG	1:A:445:PRO:HD2	2.60	0.41
1:A:668:HIS:HB3	1:A:671:LEU:HD12	2.01	0.41
1:A:747:LEU:O	1:A:747:LEU:HD23	2.19	0.41
1:B:41:LEU:HD13	1:B:42:PRO:O	2.20	0.41
1:B:226:ILE:N	1:B:226:ILE:CD1	2.82	0.41
1:B:248:LEU:C	1:B:248:LEU:CD2	2.93	0.41
1:B:587:PRO:HG2	1:B:588:VAL:N	2.35	0.41
1:C:466:ARG:HH21	1:C:498:ALA:H	1.65	0.41
1:C:524:VAL:O	1:C:524:VAL:HG12	2.20	0.41
1:C:546:VAL:O	1:C:547:GLU:C	2.63	0.41
1:C:631:PHE:CZ	1:C:635:LEU:HD11	2.55	0.41
1:D:67:TYR:CZ	1:D:114:PRO:CG	3.03	0.41
1:D:141:SER:HB3	1:D:210:LEU:CD1	2.50	0.41
1:D:312:ARG:O	1:D:317:TRP:HA	2.19	0.41
1:D:725:ILE:O	1:D:726:LEU:C	2.63	0.41
1:A:587:PRO:CG	1:A:588:VAL:N	2.83	0.41
1:B:226:ILE:HA	1:B:227:PRO:HD3	1.97	0.41
1:B:725:ILE:O	1:B:726:LEU:C	2.63	0.41
1:C:137:ALA:HB1	1:C:248:LEU:CD2	2.49	0.41
1:D:608:SER:O	1:D:611:ILE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PHE:CZ	1:A:301:THR:HA	2.52	0.41
1:A:139:ARG:O	1:A:140:LEU:C	2.64	0.41
1:B:377:ASN:HD21	1:B:395:LEU:HD11	1.84	0.41
1:C:210:LEU:HB3	1:C:244:PRO:HG2	2.02	0.41
1:D:23:LEU:HD23	1:D:110:LEU:HB3	2.02	0.41
1:D:462:ALA:O	1:D:464:GLU:N	2.52	0.41
1:A:23:LEU:HD21	1:A:272:ILE:CD1	2.49	0.41
1:A:248:LEU:C	1:A:248:LEU:CD2	2.94	0.41
1:A:332:PHE:C	1:A:332:PHE:HD2	2.29	0.41
1:A:747:LEU:HD23	1:A:747:LEU:C	2.46	0.41
1:C:233:ASP:O	1:C:234:ASP:C	2.64	0.41
1:C:685:THR:CG2	1:D:487:THR:HG21	2.50	0.41
1:D:275:ILE:O	1:D:276:GLN:C	2.62	0.41
1:D:305:ARG:HD2	1:D:305:ARG:HA	1.92	0.41
1:B:466:ARG:O	1:B:467:SER:C	2.62	0.41
1:C:248:LEU:C	1:C:248:LEU:CD2	2.94	0.41
1:C:677:THR:O	1:C:681:GLN:HG3	2.21	0.41
1:D:170:VAL:C	1:D:215:ALA:HB1	2.45	0.41
1:D:413:ILE:HG21	1:D:422:GLY:C	2.45	0.41
1:B:162:PRO:HA	1:B:166:TRP:CD1	2.56	0.41
1:B:217:ARG:NH1	1:B:217:ARG:HG2	2.35	0.41
1:B:252:ASP:O	1:B:253:GLU:C	2.63	0.41
1:B:445:PRO:HD2	1:B:471:TYR:CZ	2.56	0.41
1:B:472:ALA:O	1:B:473:CYS:C	2.63	0.41
1:B:747:LEU:N	1:B:748:PRO:CD	2.83	0.41
1:C:332:PHE:CD1	1:C:408:GLU:HG3	2.56	0.41
1:C:333:GLN:HE21	1:C:673:GLU:CB	2.34	0.41
1:D:176:SER:C	1:D:178:GLN:H	2.29	0.41
1:D:178:GLN:HG3	1:D:212:LEU:HD12	2.03	0.41
1:D:342:VAL:CG1	1:D:658:CYS:SG	3.06	0.41
1:A:243:PRO:HA	1:A:244:PRO:HD3	1.90	0.41
1:B:179:THR:HG23	1:B:208:ALA:O	2.21	0.41
1:B:275:ILE:HG23	1:B:297:TYR:HB2	2.02	0.41
1:B:331:VAL:O	1:B:335:LEU:HG	2.21	0.41
1:B:335:LEU:O	1:B:411:GLY:HA3	2.21	0.41
1:C:166:TRP:O	1:C:167:SER:C	2.64	0.41
1:C:227:PRO:HG3	1:C:234:ASP:OD2	2.20	0.41
1:C:332:PHE:C	1:C:332:PHE:HD2	2.28	0.41
1:D:57:SER:O	1:D:58:ARG:C	2.63	0.41
1:D:217:ARG:NH1	1:D:217:ARG:HG2	2.35	0.41
1:A:60:ASP:HA	1:A:63:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:HG23	1:A:208:ALA:O	2.21	0.41
1:A:319:THR:HA	1:A:320:PRO:HD3	1.84	0.41
1:A:463:HIS:CD2	1:A:464:GLU:HG3	2.56	0.41
1:A:686:ASN:O	1:A:687:SER:C	2.63	0.41
1:B:71:LEU:HD22	1:B:262:LEU:HD11	2.02	0.41
1:B:251:PRO:O	1:B:252:ASP:C	2.61	0.41
1:B:257:ILE:O	1:B:260:GLN:HB3	2.21	0.41
1:B:261:ALA:HA	1:B:264:PHE:CD1	2.55	0.41
1:B:275:ILE:O	1:B:276:GLN:C	2.63	0.41
1:C:9:THR:HG23	1:C:18:HIS:CE1	2.56	0.41
1:C:23:LEU:CD2	1:C:110:LEU:HB3	2.51	0.41
1:C:275:ILE:O	1:C:276:GLN:C	2.63	0.41
1:C:379:LEU:HD21	1:C:481:CYS:HB3	2.02	0.41
1:C:674:GLY:O	1:C:675:ALA:C	2.61	0.41
1:D:200:ALA:C	1:D:202:ASN:H	2.29	0.41
1:D:381:GLN:NE2	1:D:402:TRP:CD1	2.89	0.41
1:D:456:CYS:SG	1:D:524:VAL:HG13	2.60	0.41
1:A:138:LYS:HD3	1:A:142:ASP:CB	2.45	0.41
1:A:274:ASP:O	1:A:275:ILE:C	2.64	0.41
1:A:455:VAL:HA	1:A:460:ALA:CB	2.51	0.41
1:A:465:PHE:O	1:A:468:LEU:HB2	2.20	0.41
1:A:469:VAL:O	1:A:473:CYS:N	2.53	0.41
1:A:546:VAL:HB	1:A:644:VAL:HG13	2.03	0.41
1:A:680:ARG:HG3	1:A:681:GLN:N	2.35	0.41
1:A:750:VAL:O	1:A:750:VAL:HG13	2.20	0.41
1:B:34:LYS:HG3	1:B:321:PHE:CD1	2.55	0.41
1:B:140:LEU:CD2	1:B:249:LEU:HB2	2.47	0.41
1:B:286:PHE:O	1:B:287:PRO:C	2.61	0.41
1:B:544:PHE:O	1:B:560:THR:HG23	2.21	0.41
1:B:668:HIS:HB3	1:B:671:LEU:HD12	2.03	0.41
1:C:67:TYR:O	1:C:70:ILE:HB	2.21	0.41
1:C:136:ASP:O	1:C:138:LYS:N	2.54	0.41
1:C:380:VAL:HG21	1:C:402:TRP:O	2.21	0.41
1:C:455:VAL:HG21	1:C:468:LEU:HD11	2.03	0.41
1:C:455:VAL:HA	1:C:460:ALA:HB3	2.03	0.41
1:C:463:HIS:HA	1:C:466:ARG:HB2	2.02	0.41
1:C:574:PRO:HA	1:C:578:GLY:H	1.85	0.41
1:C:587:PRO:HG2	1:C:588:VAL:N	2.35	0.41
1:D:221:LEU:O	1:D:223:ASP:N	2.54	0.41
1:D:374:GLU:CD	1:D:374:GLU:H	2.29	0.41
1:D:461:GLY:O	1:D:462:ALA:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:O	1:A:266:PRO:C	2.63	0.41
1:A:286:PHE:O	1:A:287:PRO:C	2.63	0.41
1:A:624:ILE:HB	1:A:625:PRO:HD2	2.03	0.41
1:B:4:LEU:HD21	1:B:26:HIS:HA	2.02	0.41
1:B:99:ARG:NH1	1:B:390:GLU:C	2.55	0.41
1:B:460:ALA:HA	1:B:464:GLU:HG2	2.02	0.41
1:B:674:GLY:O	1:B:675:ALA:C	2.62	0.41
1:C:67:TYR:CZ	1:C:114:PRO:CG	3.04	0.41
1:C:191:ILE:CG2	1:C:195:ARG:HD3	2.48	0.41
1:C:352:LEU:CD1	1:C:363:LEU:HD13	2.50	0.41
1:C:455:VAL:HA	1:C:460:ALA:CB	2.51	0.41
1:D:248:LEU:C	1:D:248:LEU:CD2	2.94	0.41
1:D:747:LEU:N	1:D:748:PRO:CD	2.84	0.41
1:A:104:PRO:HG2	1:A:107:PHE:CE1	2.56	0.40
1:A:132:GLN:O	1:A:133:LEU:C	2.64	0.40
1:A:258:ARG:O	1:A:259:VAL:O	2.38	0.40
1:B:39:ARG:HH12	1:B:41:LEU:HD21	1.86	0.40
1:B:377:ASN:CG	1:B:395:LEU:HD11	2.46	0.40
1:B:434:PRO:CA	1:B:527:ILE:HG22	2.49	0.40
1:C:115:LEU:N	1:C:258:ARG:NH2	2.50	0.40
1:C:128:MET:O	1:C:132:GLN:HG3	2.21	0.40
1:D:60:ASP:CB	1:D:124:LEU:HD13	2.52	0.40
1:D:147:TYR:CD2	1:D:147:TYR:C	2.98	0.40
1:D:631:PHE:CE2	1:D:635:LEU:HD11	2.56	0.40
1:A:259:VAL:O	1:A:260:GLN:C	2.64	0.40
1:A:312:ARG:O	1:A:317:TRP:HA	2.22	0.40
1:B:455:VAL:HA	1:B:460:ALA:CB	2.51	0.40
1:C:235:LEU:HD23	1:C:235:LEU:HA	1.88	0.40
1:C:609:LYS:CD	1:C:641:THR:HG22	2.52	0.40
1:D:498:ALA:HA	1:D:501:MET:CE	2.47	0.40
1:A:67:TYR:CZ	1:A:114:PRO:CG	3.04	0.40
1:A:162:PRO:HA	1:A:166:TRP:CD1	2.56	0.40
1:A:581:THR:O	1:A:585:THR:HG22	2.21	0.40
1:B:394:ASN:ND2	1:B:396:VAL:HB	2.34	0.40
1:B:642:PRO:HB2	1:B:643:HIS:H	1.64	0.40
1:B:740:ALA:HA	1:B:743:ARG:HG2	2.04	0.40
1:C:57:SER:O	1:C:59:THR:N	2.54	0.40
1:C:470:ASP:O	1:C:471:TYR:C	2.65	0.40
1:D:17:SER:OG	1:D:258:ARG:NH1	2.54	0.40
1:D:107:PHE:O	1:D:108:ALA:C	2.64	0.40
1:D:150:LEU:HD12	1:D:153:SER:OG	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LYS:HA	1:B:45:GLU:HA	2.03	0.40
1:B:157:ARG:NH2	1:B:249:LEU:HD21	2.36	0.40
1:B:170:VAL:C	1:B:215:ALA:HB1	2.46	0.40
1:C:36:SER:HB3	1:C:317:TRP:CE3	2.55	0.40
1:C:543:GLY:CA	1:C:561:ILE:O	2.63	0.40
1:C:587:PRO:CG	1:C:588:VAL:H	2.35	0.40
1:D:12:THR:O	1:D:13:THR:C	2.65	0.40
1:D:90:MET:CE	1:D:318:ARG:NH2	2.85	0.40
1:D:609:LYS:HZ2	1:D:641:THR:CG2	2.32	0.40
1:A:82:SER:HB3	1:A:85:GLU:HB3	2.04	0.40
1:A:368:MET:O	1:A:372:ARG:CB	2.68	0.40
1:A:545:TYR:HD1	1:A:560:THR:HG1	1.65	0.40
1:A:694:LYS:C	1:A:696:PHE:H	2.29	0.40
1:B:184:PHE:CD1	1:B:184:PHE:C	2.99	0.40
1:C:12:THR:OG1	1:C:14:ARG:HG3	2.22	0.40
1:C:200:ALA:C	1:C:202:ASN:H	2.30	0.40
1:C:210:LEU:HA	1:C:211:PRO:HD3	1.92	0.40
1:C:342:VAL:CG2	1:C:410:VAL:HG12	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	718/756 (95%)	593 (83%)	87 (12%)	38 (5%)	1	9
1	B	710/756 (94%)	580 (82%)	91 (13%)	39 (6%)	1	8
1	C	700/756 (93%)	578 (83%)	87 (12%)	35 (5%)	1	10
1	D	702/756 (93%)	578 (82%)	82 (12%)	42 (6%)	1	7
All	All	2830/3024 (94%)	2329 (82%)	347 (12%)	154 (5%)	1	9

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	39	ARG
1	A	81	ALA
1	A	182	SER
1	A	222	LYS
1	A	259	VAL
1	A	393	ASN
1	A	524	VAL
1	A	547	GLU
1	A	642	PRO
1	A	643	HIS
1	A	698	SER
1	B	2	HIS
1	B	37	ALA
1	B	182	SER
1	B	222	LYS
1	B	234	ASP
1	B	398	LYS
1	B	642	PRO
1	B	643	HIS
1	B	698	SER
1	C	2	HIS
1	C	81	ALA
1	C	138	LYS
1	C	182	SER
1	C	222	LYS
1	C	255	ASP
1	C	462	ALA
1	C	547	GLU
1	C	642	PRO
1	C	643	HIS
1	C	698	SER
1	D	2	HIS
1	D	39	ARG
1	D	81	ALA
1	D	182	SER
1	D	222	LYS
1	D	256	LEU
1	D	445	PRO
1	D	462	ALA
1	D	463	HIS
1	D	547	GLU
1	D	642	PRO

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Mol	Chain	Res	Type
1	D	643	HIS
1	D	698	SER
1	A	229	PRO
1	A	275	ILE
1	A	281	ALA
1	A	311	GLY
1	A	458	GLY
1	A	586	GLY
1	A	606	GLY
1	B	39	ARG
1	B	81	ALA
1	B	275	ILE
1	B	311	GLY
1	B	458	GLY
1	B	586	GLY
1	B	602	TYR
1	B	603	GLU
1	B	605	SER
1	C	40	GLY
1	C	275	ILE
1	C	281	ALA
1	C	311	GLY
1	C	391	PHE
1	C	458	GLY
1	C	474	GLU
1	C	586	GLY
1	D	50	ALA
1	D	146	ASP
1	D	252	ASP
1	D	253	GLU
1	D	257	ILE
1	D	275	ILE
1	D	311	GLY
1	D	447	ALA
1	D	458	GLY
1	D	586	GLY
1	A	50	ALA
1	A	58	ARG
1	A	200	ALA
1	A	237	PRO
1	A	459	GLU
1	A	559	PRO

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Mol	Chain	Res	Type
1	A	587	PRO
1	A	607	GLY
1	B	36	SER
1	B	58	ARG
1	B	108	ALA
1	B	137	ALA
1	B	200	ALA
1	B	229	PRO
1	B	258	ARG
1	B	281	ALA
1	B	397	ALA
1	B	445	PRO
1	B	459	GLU
1	B	559	PRO
1	B	587	PRO
1	C	50	ALA
1	C	58	ARG
1	C	108	ALA
1	C	200	ALA
1	C	459	GLU
1	C	587	PRO
1	D	58	ARG
1	D	108	ALA
1	D	137	ALA
1	D	200	ALA
1	D	258	ARG
1	D	281	ALA
1	D	459	GLU
1	D	464	GLU
1	D	587	PRO
1	A	105	PRO
1	A	108	ALA
1	A	230	GLY
1	A	254	PHE
1	B	50	ALA
1	B	259	VAL
1	B	389	ALA
1	C	473	CYS
1	D	212	LEU
1	D	259	VAL
1	A	673	GLU
1	B	105	PRO

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Mol	Chain	Res	Type
1	B	673	GLU
1	C	105	PRO
1	C	137	ALA
1	C	236	ALA
1	C	257	ILE
1	C	673	GLU
1	D	105	PRO
1	D	238	LYS
1	D	673	GLU
1	A	256	LEU
1	A	257	ILE
1	B	180	SER
1	B	227	PRO
1	C	212	LEU
1	D	82	SER
1	A	227	PRO
1	A	445	PRO
1	C	227	PRO
1	D	227	PRO
1	B	279	ILE
1	D	38	GLY
1	C	279	ILE
1	C	469	VAL
1	A	279	ILE
1	A	575	VAL
1	D	279	ILE
1	D	575	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	611/632 (97%)	576 (94%)	35 (6%)	18	52
1	B	607/632 (96%)	577 (95%)	30 (5%)	22	56
1	C	602/632 (95%)	574 (95%)	28 (5%)	23	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	605/632 (96%)	571 (94%)	34 (6%)	19	52
All	All	2425/2528 (96%)	2298 (95%)	127 (5%)	21	55

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	35	VAL
1	A	39	ARG
1	A	42	PRO
1	A	68	GLN
1	A	110	LEU
1	A	139	ARG
1	A	142	ASP
1	A	170	VAL
1	A	179	THR
1	A	217	ARG
1	A	222	LYS
1	A	225	GLN
1	A	242	LEU
1	A	262	LEU
1	A	327	SER
1	A	352	LEU
1	A	357	ASP
1	A	395	LEU
1	A	400	LYS
1	A	438	LYS
1	A	444	CYS
1	A	457	MET
1	A	467	SER
1	A	488	MET
1	A	509	ILE
1	A	527	ILE
1	A	539	LEU
1	A	546	VAL
1	A	559	PRO
1	A	566	ILE
1	A	581	THR
1	A	618	ARG
1	A	624	ILE
1	A	711	ILE
1	B	2	HIS

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Mol	Chain	Res	Type
1	B	39	ARG
1	B	68	GLN
1	B	110	LEU
1	B	170	VAL
1	B	179	THR
1	B	217	ARG
1	B	222	LYS
1	B	225	GLN
1	B	242	LEU
1	B	327	SER
1	B	352	LEU
1	B	357	ASP
1	B	401	THR
1	B	402	TRP
1	B	432	MET
1	B	438	LYS
1	B	457	MET
1	B	467	SER
1	B	488	MET
1	B	509	ILE
1	B	527	ILE
1	B	539	LEU
1	B	546	VAL
1	B	566	ILE
1	B	581	THR
1	B	608	SER
1	B	618	ARG
1	B	624	ILE
1	B	711	ILE
1	C	2	HIS
1	C	68	GLN
1	C	110	LEU
1	C	170	VAL
1	C	179	THR
1	C	217	ARG
1	C	222	LYS
1	C	225	GLN
1	C	242	LEU
1	C	327	SER
1	C	352	LEU
1	C	357	ASP
1	C	402	TRP

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Mol	Chain	Res	Type
1	C	438	LYS
1	C	444	CYS
1	C	457	MET
1	C	464	GLU
1	C	488	MET
1	C	509	ILE
1	C	527	ILE
1	C	539	LEU
1	C	546	VAL
1	C	566	ILE
1	C	581	THR
1	C	618	ARG
1	C	624	ILE
1	C	711	ILE
1	C	730	LEU
1	D	2	HIS
1	D	34	LYS
1	D	35	VAL
1	D	68	GLN
1	D	110	LEU
1	D	139	ARG
1	D	141	SER
1	D	145	THR
1	D	170	VAL
1	D	179	THR
1	D	217	ARG
1	D	222	LYS
1	D	225	GLN
1	D	242	LEU
1	D	252	ASP
1	D	258	ARG
1	D	264	PHE
1	D	327	SER
1	D	352	LEU
1	D	402	TRP
1	D	438	LYS
1	D	457	MET
1	D	463	HIS
1	D	488	MET
1	D	509	ILE
1	D	527	ILE
1	D	539	LEU

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Mol	Chain	Res	Type
1	D	546	VAL
1	D	566	ILE
1	D	581	THR
1	D	618	ARG
1	D	624	ILE
1	D	711	ILE
1	D	730	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	132	GLN
1	A	178	GLN
1	A	202	ASN
1	A	225	GLN
1	A	263	GLN
1	A	333	GLN
1	A	373	ASN
1	A	463	HIS
1	A	548	GLN
1	A	572	GLN
1	A	610	HIS
1	A	614	GLN
1	A	637	GLN
1	A	665	HIS
1	B	68	GLN
1	B	178	GLN
1	B	202	ASN
1	B	204	HIS
1	B	225	GLN
1	B	333	GLN
1	B	373	ASN
1	B	377	ASN
1	B	381	GLN
1	B	393	ASN
1	B	568	HIS
1	B	572	GLN
1	B	610	HIS
1	B	614	GLN
1	B	665	HIS
1	B	745	HIS

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Mol	Chain	Res	Type
1	C	68	GLN
1	C	178	GLN
1	C	224	HIS
1	C	225	GLN
1	C	333	GLN
1	C	373	ASN
1	C	548	GLN
1	C	572	GLN
1	C	610	HIS
1	C	614	GLN
1	C	637	GLN
1	C	665	HIS
1	D	6	HIS
1	D	132	GLN
1	D	178	GLN
1	D	202	ASN
1	D	225	GLN
1	D	271	HIS
1	D	333	GLN
1	D	373	ASN
1	D	475	GLN
1	D	548	GLN
1	D	572	GLN
1	D	610	HIS
1	D	614	GLN
1	D	665	HIS
1	D	745	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 39 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	732/756 (96%)	-1.71	0 100 100	19, 36, 65, 92	1 (0%)
1	B	726/756 (96%)	-1.69	0 100 100	21, 36, 67, 93	1 (0%)
1	C	718/756 (94%)	-1.68	0 100 100	18, 36, 66, 92	1 (0%)
1	D	720/756 (95%)	-1.70	0 100 100	20, 36, 65, 92	1 (0%)
All	All	2896/3024 (95%)	-1.70	0 100 100	18, 36, 66, 93	4 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	A	761	1/1	0.96	0.09	63,63,63,63	0
2	MN	C	758	1/1	0.96	0.09	85,85,85,85	0
2	MN	D	762	1/1	0.96	0.06	114,114,114,114	0
2	MN	C	763	1/1	0.97	0.05	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	C	759	1/1	0.98	0.05	113,113,113,113	0
2	MN	C	760	1/1	0.98	0.13	92,92,92,92	0
2	MN	D	763	1/1	0.98	0.06	86,86,86,86	0
2	MN	B	758	1/1	0.99	0.07	97,97,97,97	0
2	MN	B	759	1/1	0.99	0.10	49,49,49,49	0
2	MN	B	760	1/1	0.99	0.02	49,49,49,49	0
2	MN	B	761	1/1	0.99	0.07	72,72,72,72	0
2	MN	B	762	1/1	0.99	0.05	61,61,61,61	0
2	MN	C	757	1/1	0.99	0.05	100,100,100,100	0
2	MN	A	759	1/1	0.99	0.10	49,49,49,49	0
2	MN	A	757	1/1	0.99	0.05	77,77,77,77	0
2	MN	A	763	1/1	0.99	0.04	65,65,65,65	0
2	MN	C	761	1/1	0.99	0.07	78,78,78,78	0
2	MN	C	762	1/1	0.99	0.08	93,93,93,93	0
2	MN	A	764	1/1	0.99	0.02	96,96,96,96	0
2	MN	D	755	1/1	0.99	0.04	39,39,39,39	0
2	MN	D	757	1/1	0.99	0.04	70,70,70,70	0
2	MN	D	758	1/1	0.99	0.03	99,99,99,99	0
2	MN	D	759	1/1	0.99	0.08	107,107,107,107	0
2	MN	D	761	1/1	0.99	0.05	82,82,82,82	0
2	MN	A	766	1/1	0.99	0.06	76,76,76,76	0
2	MN	B	757	1/1	0.99	0.12	79,79,79,79	0
2	MN	A	762	1/1	1.00	0.03	50,50,50,50	0
2	MN	A	758	1/1	1.00	0.02	68,68,68,68	0
2	MN	A	756	1/1	1.00	0.01	20,20,20,20	0
2	MN	A	765	1/1	1.00	0.02	83,83,83,83	0
2	MN	A	760	1/1	1.00	0.08	34,34,34,34	0
2	MN	D	756	1/1	1.00	0.01	34,34,34,34	0
2	MN	B	763	1/1	1.00	0.03	48,48,48,48	0
2	MN	C	755	1/1	1.00	0.02	48,48,48,48	0
2	MN	C	756	1/1	1.00	0.01	39,39,39,39	0
2	MN	D	760	1/1	1.00	0.04	107,107,107,107	0
2	MN	B	755	1/1	1.00	0.03	38,38,38,38	0
2	MN	B	756	1/1	1.00	0.02	25,25,25,25	0
2	MN	A	755	1/1	1.00	0.03	32,32,32,32	0

6.5 Other polymers

There are no such residues in this entry.