



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:45 pm GMT

PDB ID : 1WZ2
Title : The crystal structure of Leucyl-tRNA synthetase and tRNA(leucine) complex
Authors : Fukunaga, R.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-02-21
Resolution : 3.21 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

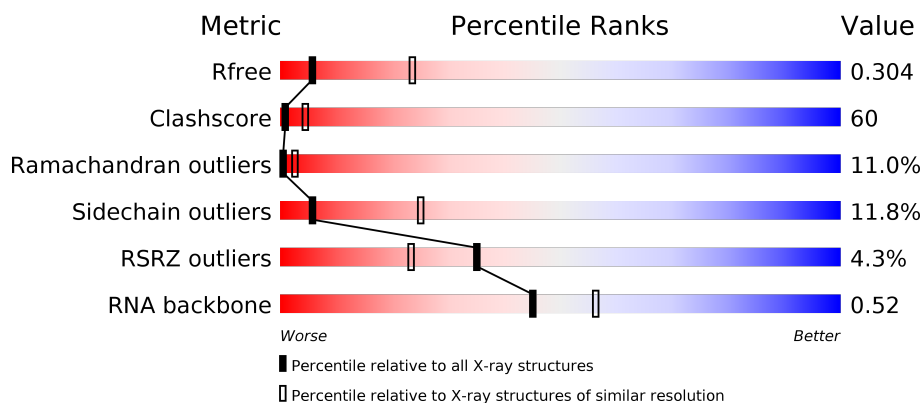
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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}	111664	1145 (3.24-3.20)
Clashscore	122126	1266 (3.24-3.20)
Ramachandran outliers	120053	1245 (3.24-3.20)
Sidechain outliers	120020	1244 (3.24-3.20)
RSRZ outliers	108989	1103 (3.24-3.20)
RNA backbone	2636	1117 (3.64-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	C	88	<div> <div>5%</div> <div>27%</div> <div>44%</div> <div>22%</div> <div>7%</div> </div>
1	D	88	<div> <div>8%</div> <div>36%</div> <div>39%</div> <div>22%</div> <div>.</div> </div>
2	A	967	<div> <div>3%</div> <div>21%</div> <div>60%</div> <div>16%</div> <div>..</div> </div>
2	B	967	<div> <div>5%</div> <div>22%</div> <div>61%</div> <div>14%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19578 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 RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	88	Total	C	N	O	P	0	0	0
			1880	836	339	617	88			
1	D	88	Total	C	N	O	P	0	0	0
			1880	836	339	617	88			

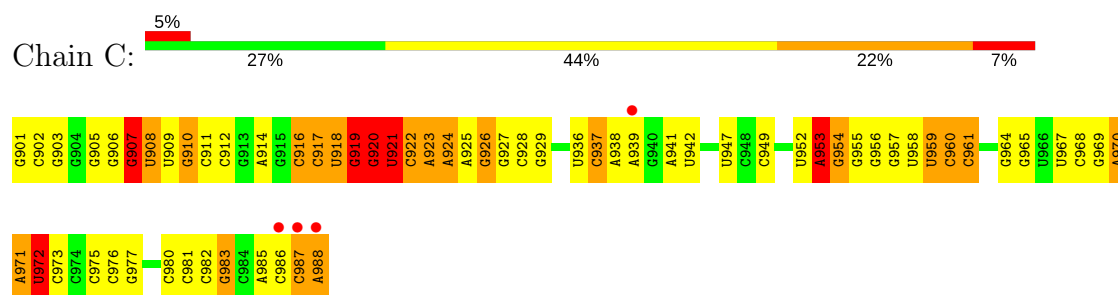
- Molecule 2 is a protein called Leucyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	948	Total	C	N	O	S	0	0	0
			7909	5132	1323	1430	24			
2	B	948	Total	C	N	O	S	0	0	0
			7909	5132	1323	1430	24			

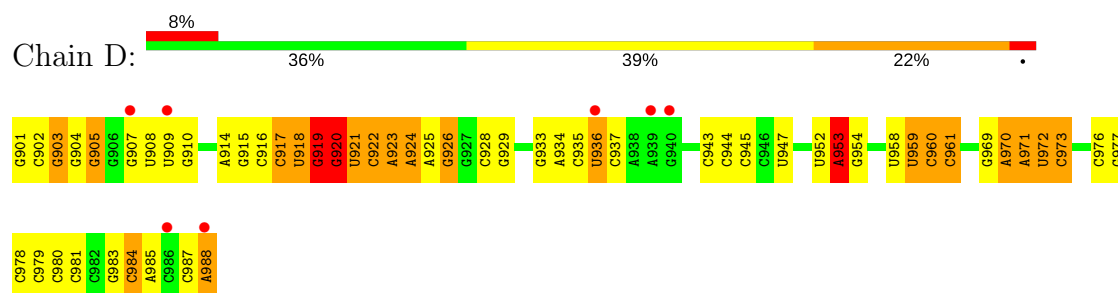
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

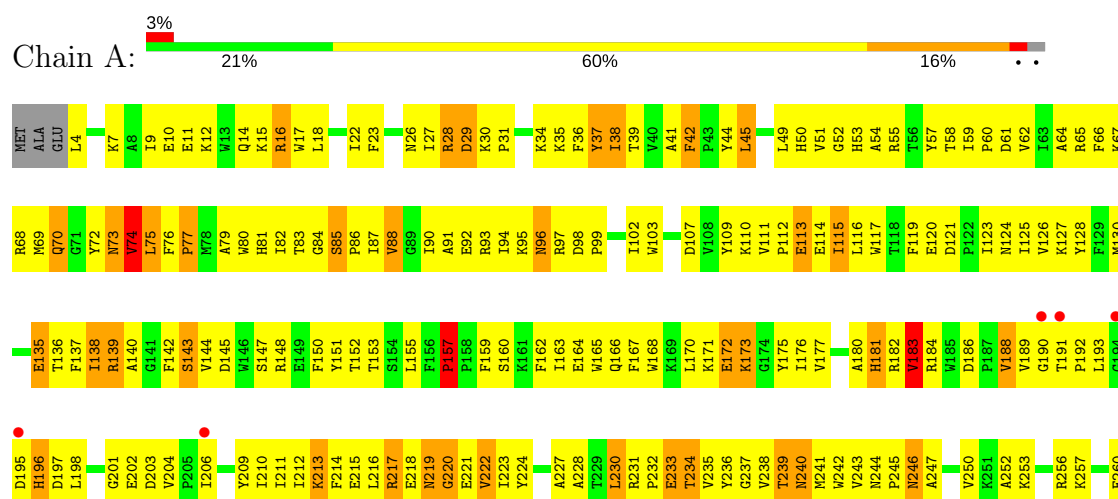
• Molecule 1: tRNA

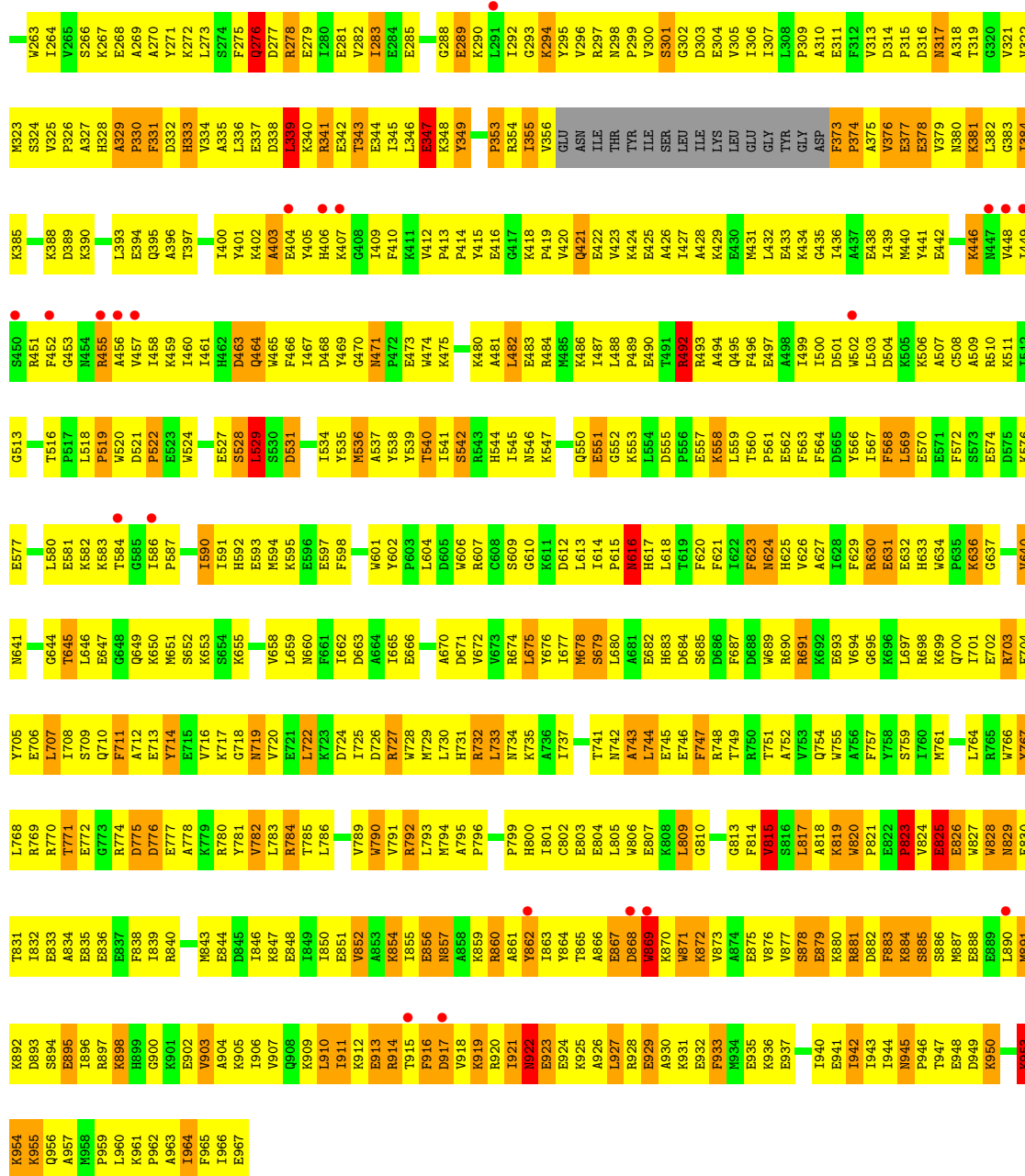


• Molecule 1: tRNA

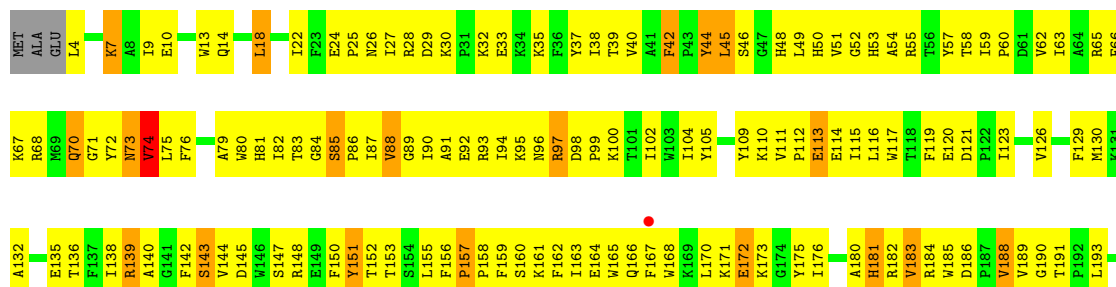
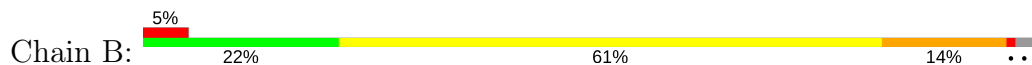


• Molecule 2: Leucyl-tRNA synthetase





• Molecule 2: Leucyl-tRNA synthetase



K954	K955	Q956	A957	M958	P959	L960	K961	G900	K901	E902	V903	A904	K905	I906	V907	H841	H842	H843	H844	H845	H846	K847	H848	H849	H850	H851	H852	H853	K854	H855	H856	H857	H858	K859	H860	A861	H862	H863	H864	T865	A866	E867	D868	K869	K870	H871	K872	G839	E940	E941	I942	I943	I944	N945	P946	D949	K950	G951	G952	K953																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
L890	M891	K892	D893	T894	E895	L896	G897	K900	K901	E902	V903	A904	K905	I906	V907	H841	H842	H843	H844	H845	H846	K847	H848	H849	H850	H851	H852	H853	K854	H855	H856	H857	H858	K859	H860	A861	H862	H863	H864	T865	A866	E867	D868	K869	K870	H871	K872	G839	E940	E941	I942	I943	I944	N945	P946	D949	K950	G951	G952	K953																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
R765	W766	Y767	L768	R769	R770	T771	R774	D775	E776	E777	A778	K779	R780	Y781	W782	L783	R784	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																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
R703	F704	Y705	E706	L707	I708	S709	F710	A711	E712	E713	Y714	K715	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																																																																																																																																																																																																																																																																																																																																																																																																																																																										
D504	K505	K506	K507	C508	A509	R510	K511	L512	L513	L514	G515	L516	F517	L518	P519	W520	K521	P522	E523	W524	L525	V526	E527	S528	L529	S530	D531	S532	T533	E534	Y535	M536	Y537	Y538	Y539	T540	I541	S542	R543	H544	I545	M546	K547	L548	E549	Q550	E551	G552	K553	L554	D555	Q556	E557	K558	L559	T560	P561	E562	F563																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
F564	D565	Y566	I567	F568	L569	E570	S571	K572	E573	L574	L575	F576	E577	L578	E579	L580	E581	K582	K583	T584	E585	L586	P587	L588	I589	H590	H591	H592	E593	M594	K595	E596	E597	F598	E599	Y600	W601	Y602	W603	R604	C605	S606	L607	I608	L609	T610	T611	T612	T613	T614	T615	T616	T617	T618	T619	T620	T621	T622	T623	T624	T625	T626	T627	T628	T629	T630	T631	T632	T633	T634	T635	T636	T637	T638	T639	T640	T641	T642	T643	T644	T645	T646	T647	T648	T649	T650	T651	T652	T653	T654	T655	T656	T657	T658	T659	T660	T661	T662	T663	T664	T665	T666	T667	T668	T669	T670	T671	T672	T673	T674	T675	T676	T677	T678	T679	T680	T681	T682	T683	T684	T685	T686	T687	T688	T689	T690	T691	T692	T693	T694	T695	T696	T697	T698	T699	T700	T701	T702	T703	T704	T705	T706	T707	T708	T709	T710	T711	T712	T713	T714	T715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782	T783	T784	T785	T786	T787	T788	T789	T790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800	T801	T802	T803	T804	T805	T806	T807	T808	T809	T810	T811	T812	T813	T814	T815	T816	T817	T818	T819	T820	T821	T822	T823	T824	T825	T826	T827	T828	T829	T830	T831	T832	T833	T834	T835	T836	T837	T838	T839	T840	T841	T842	T843	T844	T845	T846	T847	T848	T849	T850	T851	T852	T853	T854	T855	T856	T857	T858	T859	T860	T861	T862	T863	T864	T865	T866	T867	T868	T869	T870	T871	T872	T873	T874	T875	T876	T877	T878	T879	T880	T881	T882	T883	T884	T885	T886	T887	T888	T889																																																																																																																																																																																																																																																																																																															
H196	D197	L198	M199	E200	G201	E202	D203	V204	P205	L206	L207	L208	L209	L210	L211	L212	K213	F214	D215	E216	L217	K218	E219	L220	E221	V222	T223	Y224	L225	P226	A227	K228	L229	L230	R231	P232	I233	E234	E235	E236	E237	E238	E239	E240	E241	E242	E243	E244	E245	E246	E247	E248	E249	E250	E251	E252	E253	E254	E255	E256	E257	E258	E259	E260																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
E261	T262	W263	L264	V265	S266	K267	E268	A269	A270	Y271	K272	L273	S274	A275	L276	F277	D278	R279	E280	L281	E282	L283	E284	E285	F286	K287	E288	L289	P290	K291	L292	G293	E294	E295	E296	E297	E298	E299	E300	E301	E302	E303	E304	E305	E306	E307	E308	E309	E310	E311	E312	E313	E314	E315	E316	E317	E318	E319	E320	E321	E322	E323	E324	E325	E326	E327	E328	E329	E330	E331	E332	E333	E334	E335	E336	E337	E338	E339	E340	E341	E342	E343	E344	E345	E346	E347	E348	E349	E350	E351	E352	E353	E354	E355	E356	E357	E358	E359	E360	E361	E362	E363	E364	E365	E366	E367	E368	E369	E370	E371	E372	E373	E374	E375	E376	E377	E378	E379	E380	E381	E382	E383	E384	E385	E386	E387	E388	E389	E390	E391	E392	E393	E394	E395	E396	E397	E398	E399	E400	E401	E402	E403	E404	E405	E406	E407	E408	E409	E410	E411	E412	E413	E414	E415	E416	E417	E418	E419	E420	E421	E422	E423	E424	E425	E426	E427	E428	E429	E430	E431	E432	E433	E434	E435	E436	E437	E438	E439	E440	E441	E442	E443	E444	E445	E446	E447	E448	E449	E450	E451	E452	E453	E454	E455	E456	E457	E458	E459	E460	E461	E462	E463	E464	E465	E466	E467	E468	E469	E470	E471	E472	E473	E474	E475	E476	E477	E478	E479	E480	E481	E482	E483	E484	E485	E486	E487	E488	E489	E490	E491	E492	E493	E494	E495	E496	E497	E498	E499	E500	E501	E502	E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552	E553	E554	E555	E556	E557	E558	E559	E560	E561	E562	E563	E564	E565	E566	E567	E568	E569	E570	E571	E572	E573	E574	E575	E576	E577	E578	E579	E580	E581	E582	E583	E584	E585	E586	E587	E588	E589	E590	E591	E592	E593	E594	E595	E596	E597	E598	E599	E600	E601	E602	E603	E604	E605	E606	E607	E608	E609	E610	E611	E612	E613	E614	E615	E616	E617	E618	E619	E620	E621	E622	E623	E624	E625	E626	E627	E628	E629	E630	E631	E632	E633	E634	E635	E636	E637	E638	E639	E640	E641	E642	E643	E644	E645	E646	E647	E648	E649	E650	E651	E652	E653	E654	E655	E656	E657	E658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.55Å 231.13Å 118.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 3.21 48.69 – 3.21	Depositor EDS
% Data completeness (in resolution range)	90.7 (14.99-3.21) 90.8 (48.69-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.305 0.243 , 0.304	Depositor DCC
R_{free} test set	5012 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19578	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	C	0.55	1/2099 (0.0%)	0.82	7/3270 (0.2%)
1	D	0.52	1/2099 (0.0%)	0.81	3/3270 (0.1%)
2	A	0.59	0/8115	0.76	6/10953 (0.1%)
2	B	0.42	0/8115	0.67	2/10953 (0.0%)
All	All	0.52	2/20428 (0.0%)	0.74	18/28446 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	6
1	D	0	5
2	A	0	2
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	901	G	OP3-P	-7.18	1.52	1.61
1	D	901	G	OP3-P	-7.06	1.52	1.61

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	675	LEU	CA-CB-CG	10.29	138.97	115.30
2	A	815	VAL	CB-CA-C	-8.02	96.17	111.40
1	C	919	G	N9-C1'-C2'	7.77	124.10	114.00
1	D	953	A	N9-C1'-C2'	7.42	123.64	114.00
1	C	907	G	N9-C1'-C2'	7.18	123.33	114.00
1	D	920	G	N9-C1'-C2'	7.04	123.15	114.00
1	C	953	A	N9-C1'-C2'	6.38	122.30	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	972	U	N1-C1'-C2'	5.87	121.63	114.00
1	D	920	G	O4'-C1'-N9	5.84	112.87	108.20
1	C	953	A	C1'-O4'-C4'	-5.72	105.32	109.90
1	C	920	G	N9-C1'-C2'	5.71	121.43	114.00
2	A	927	LEU	CA-CB-CG	5.69	128.38	115.30
1	C	953	A	O4'-C1'-N9	5.62	112.70	108.20
2	B	680	LEU	N-CA-C	5.50	125.84	111.00
2	A	680	LEU	N-CA-C	5.44	125.68	111.00
2	A	74	VAL	N-CA-C	5.33	125.39	111.00
2	A	492	ARG	CG-CD-NE	5.05	122.41	111.80
2	B	74	VAL	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	535	TYR	Sidechain
2	A	767	TYR	Sidechain
1	C	907	G	Sidechain
1	C	919	G	Sidechain
1	C	920	G	Sidechain
1	C	921	U	Sidechain
1	C	926	G	Sidechain
1	C	959	U	Sidechain
1	D	919	G	Sidechain
1	D	920	G	Sidechain
1	D	926	G	Sidechain
1	D	953	A	Sidechain
1	D	959	U	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1880	0	956	88	0
1	D	1880	0	956	65	0
2	A	7909	0	7908	1115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	7909	0	7908	1018	0
All	All	19578	0	17728	2256	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 60.

All (2256) 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)
2:A:866:ALA:N	2:A:955:LYS:HZ3	1.39	1.18
2:A:30:LYS:HB2	2:A:73:ASN:HD22	1.11	1.13
2:A:170:LEU:HB3	2:A:176:ILE:HD11	1.23	1.09
2:A:616:ASN:HD22	2:A:617:HIS:N	1.51	1.08
2:A:68:ARG:HH22	2:A:143:SER:HB3	1.15	1.07
2:A:924:GLU:HB3	2:A:928:ARG:HH21	1.12	1.07
2:B:920:ARG:HA	2:B:920:ARG:HE	1.12	1.06
2:B:26:ASN:HB3	2:B:28:ARG:NH2	1.70	1.06
2:A:480:LYS:HE2	2:A:484:ARG:HH22	1.17	1.05
2:A:921:ILE:HD12	2:A:928:ARG:HH12	1.20	1.05
2:A:922:ASN:HD22	2:A:923:GLU:N	1.53	1.05
2:B:703:ARG:HB2	2:B:703:ARG:HH11	1.18	1.05
2:A:724:ASP:HA	2:A:727:ARG:HG3	1.33	1.04
2:A:771:THR:HG21	2:A:774:ARG:HH11	1.18	1.04
2:B:198:LEU:HB2	2:B:202:GLU:HG2	1.40	1.02
2:A:924:GLU:HB3	2:A:928:ARG:NH2	1.75	1.02
2:B:733:LEU:HD11	2:B:789:VAL:HG11	1.41	1.02
2:B:866:ALA:H	2:B:955:LYS:NZ	1.58	1.01
2:A:616:ASN:ND2	2:A:617:HIS:H	1.57	1.01
2:B:558:LYS:HB3	2:B:584:THR:HA	1.43	1.01
2:B:860:ARG:NH1	2:B:943:ILE:H	1.59	1.01
2:B:650:LYS:HE2	2:B:651:MET:H	1.22	1.00
2:A:529:LEU:H	2:A:529:LEU:HD12	1.27	1.00
2:A:163:ILE:HD12	2:A:531:ASP:HB2	1.40	1.00
2:A:722:LEU:HD22	2:A:722:LEU:H	1.22	1.00
2:A:87:ILE:HG13	2:A:88:VAL:H	1.24	0.99
2:B:703:ARG:NH1	2:B:703:ARG:HB2	1.77	0.99
2:A:188:VAL:HG23	2:A:189:VAL:H	1.28	0.99
1:D:904:G:H2'	1:D:905:G:H5''	1.45	0.98
2:A:848:GLU:O	2:A:852:VAL:HG23	1.63	0.98
2:B:227:ALA:HA	2:B:321:VAL:HG23	1.45	0.98
2:A:567:ILE:HA	2:A:595:LYS:HD2	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:916:C:H5'	1:C:917:C:C5	1.99	0.97
2:A:227:ALA:HA	2:A:321:VAL:HG23	1.46	0.97
2:A:426:ALA:HA	2:A:429:LYS:HE2	1.45	0.97
2:A:690:ARG:NH1	2:A:693:GLU:HG3	1.79	0.96
2:A:922:ASN:C	2:A:922:ASN:HD22	1.68	0.96
2:A:68:ARG:NH2	2:A:143:SER:HB3	1.79	0.96
2:A:890:LEU:HD12	2:A:906:ILE:HD11	1.48	0.96
2:A:345:ILE:HG12	2:A:346:LEU:H	1.29	0.95
1:C:986:C:H4'	1:C:987:C:H5''	1.47	0.95
2:B:88:VAL:HG21	2:B:513:GLY:HA2	1.48	0.95
2:A:68:ARG:HH22	2:A:143:SER:CB	1.80	0.95
2:A:558:LYS:HB3	2:A:584:THR:HA	1.48	0.94
2:B:860:ARG:HH11	2:B:943:ILE:N	1.66	0.94
2:A:792:ARG:HG3	2:A:792:ARG:HH21	1.30	0.94
2:A:660:ASN:HB2	2:A:663:ASP:HB3	1.50	0.93
2:A:741:THR:HG1	2:A:820:TRP:HZ3	1.04	0.93
2:B:866:ALA:H	2:B:955:LYS:HZ3	1.01	0.93
2:A:860:ARG:NH1	2:A:861:ALA:HA	1.84	0.93
2:A:771:THR:HG21	2:A:774:ARG:NH1	1.82	0.93
2:B:429:LYS:O	2:B:433:GLU:HG2	1.67	0.92
2:A:182:ARG:HD2	2:A:206:ILE:HG21	1.49	0.92
2:A:28:ARG:HE	2:A:28:ARG:H	1.01	0.92
2:A:139:ARG:HG3	2:A:139:ARG:HH11	1.34	0.92
2:A:860:ARG:NH1	2:A:943:ILE:H	1.66	0.92
2:A:866:ALA:H	2:A:955:LYS:HZ3	0.98	0.92
2:B:784:ARG:HH22	2:B:810:GLY:H	1.15	0.92
2:A:770:ARG:HD2	2:A:933:PHE:CE2	2.06	0.91
2:B:927:LEU:HD12	2:B:944:ILE:HD12	1.50	0.91
2:B:82:ILE:HG21	2:B:126:VAL:HG13	1.50	0.91
2:A:480:LYS:HE2	2:A:484:ARG:NH2	1.84	0.91
2:A:866:ALA:H	2:A:955:LYS:NZ	1.69	0.91
2:B:49:LEU:HD12	2:B:49:LEU:H	1.34	0.91
2:B:233:GLU:HA	2:B:427:ILE:HD12	1.51	0.91
2:B:734:ASN:HD21	2:B:824:VAL:H	1.12	0.91
2:B:355:ILE:HG22	2:B:356:VAL:H	1.36	0.91
2:A:210:ILE:HD11	2:A:232:PRO:HG3	1.54	0.90
2:B:860:ARG:HH11	2:B:943:ILE:H	0.99	0.90
2:B:26:ASN:HB3	2:B:28:ARG:HH22	1.34	0.90
2:B:167:PHE:HA	2:B:170:LEU:HD12	1.55	0.89
2:B:826:GLU:C	2:B:828:TRP:H	1.70	0.89
2:A:567:ILE:HG22	2:A:595:LYS:HB2	1.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:198:LEU:HB2	2:A:202:GLU:HG2	1.52	0.89
2:A:49:LEU:HD12	2:A:49:LEU:H	1.35	0.89
2:B:920:ARG:HA	2:B:920:ARG:NE	1.85	0.89
2:A:771:THR:CG2	2:A:774:ARG:HH11	1.86	0.89
2:A:496:PHE:CE1	2:A:614:ILE:HG12	2.08	0.89
2:A:230:LEU:H	2:A:230:LEU:HD23	1.37	0.88
2:A:730:LEU:HB3	2:A:827:TRP:NE1	1.88	0.88
2:A:826:GLU:C	2:A:828:TRP:H	1.70	0.88
2:B:870:LYS:HE3	2:B:905:LYS:HE3	1.55	0.88
2:A:111:VAL:HG22	2:A:128:TYR:HE2	1.39	0.88
2:A:343:THR:HG23	2:A:344:GLU:H	1.37	0.88
1:D:983:G:H2'	1:D:984:C:H5''	1.53	0.88
2:B:83:THR:HG22	2:B:515:GLY:HA2	1.56	0.88
2:B:675:LEU:HD23	2:B:697:LEU:HD21	1.54	0.87
2:B:567:ILE:HG22	2:B:595:LYS:HB2	1.55	0.87
1:D:922:C:H4'	1:D:923:A:O5'	1.72	0.87
2:A:489:PRO:HG3	2:A:684:ASP:OD2	1.75	0.87
2:B:555:ASP:HB3	2:B:558:LYS:HG2	1.55	0.87
2:A:471:ASN:OD1	2:A:473:GLU:HG2	1.73	0.87
2:B:714:TYR:H	2:B:714:TYR:HD2	1.21	0.87
2:A:219:ASN:ND2	2:A:220:GLY:H	1.72	0.87
2:B:188:VAL:HG23	2:B:189:VAL:H	1.40	0.87
2:A:921:ILE:HB	2:A:928:ARG:HH22	1.40	0.87
2:A:211:ILE:HG22	2:A:228:ALA:HB2	1.57	0.86
1:C:902:C:H2'	1:C:903:G:O4'	1.74	0.86
2:A:482:LEU:HD23	2:A:482:LEU:O	1.75	0.86
2:B:44:TYR:HE1	2:B:87:ILE:HD11	1.39	0.86
2:A:496:PHE:HE1	2:A:614:ILE:HG12	1.40	0.86
2:B:351:ILE:HD12	2:B:351:ILE:H	1.39	0.86
2:A:836:GLU:O	2:A:840:ARG:HG3	1.74	0.86
2:A:204:VAL:HG21	2:A:448:VAL:CG2	2.05	0.86
2:B:342:GLU:HG2	2:B:343:THR:H	1.40	0.86
2:B:882:ASP:CG	2:B:883:PHE:H	1.79	0.85
2:A:829:ASN:OD1	2:A:832:ILE:HG13	1.77	0.85
2:B:587:PRO:HB2	2:B:590:ILE:HG12	1.56	0.85
2:B:182:ARG:HD2	2:B:206:ILE:HG21	1.59	0.84
2:B:413:PRO:HB2	2:B:414:PRO:HD3	1.57	0.84
2:A:819:LYS:H	2:A:819:LYS:HE3	1.43	0.84
2:A:803:GLU:HA	2:A:815:VAL:CG2	2.07	0.84
2:B:446:LYS:HD2	2:B:446:LYS:N	1.92	0.84
1:C:928:C:H2'	1:C:929:G:C8	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:ARG:HD2	2:B:707:LEU:HD11	1.60	0.84
2:A:145:ASP:OD1	2:A:147:SER:HB3	1.78	0.83
1:C:928:C:H2'	1:C:929:G:H8	1.42	0.83
2:A:731:HIS:HE1	2:A:833:GLU:OE1	1.60	0.83
2:B:705:TYR:CE2	2:B:805:LEU:HD21	2.13	0.83
2:B:866:ALA:N	2:B:955:LYS:HZ3	1.76	0.83
2:A:671:ASP:OD2	2:A:800:HIS:HB2	1.78	0.83
2:B:4:LEU:HD23	2:B:4:LEU:O	1.79	0.83
2:A:966:ILE:O	2:A:967:GLU:HB2	1.79	0.83
2:B:186:ASP:HB2	2:B:193:LEU:HD11	1.59	0.83
2:A:770:ARG:HD2	2:A:933:PHE:HE2	1.41	0.83
2:B:86:PRO:O	2:B:90:ILE:HG12	1.78	0.83
2:A:732:ARG:HH11	2:A:735:LYS:HD3	1.45	0.82
2:A:28:ARG:H	2:A:28:ARG:NE	1.76	0.82
2:B:935:GLU:OE1	2:B:941:GLU:HA	1.80	0.82
2:A:59:ILE:HG12	2:A:678:MET:HE1	1.60	0.82
1:D:923:A:H4'	1:D:924:A:O5'	1.79	0.82
2:A:51:VAL:O	2:A:54:ALA:HB3	1.80	0.82
2:B:13:TRP:CE2	2:B:803:GLU:HB3	2.15	0.82
2:A:238:VAL:HG11	2:A:298:ASN:HD22	1.45	0.81
2:A:345:ILE:HG12	2:A:346:LEU:N	1.94	0.81
2:A:384:ILE:HG22	2:A:385:LYS:H	1.45	0.81
2:A:859:LYS:HB3	2:A:941:GLU:HB3	1.63	0.81
2:A:355:ILE:HG22	2:A:356:VAL:H	1.45	0.81
2:B:230:LEU:H	2:B:230:LEU:HD23	1.45	0.81
1:C:922:C:H4'	1:C:923:A:O5'	1.78	0.81
2:A:722:LEU:N	2:A:722:LEU:HD22	1.95	0.81
2:B:340:LYS:NZ	2:B:341:ARG:HH12	1.79	0.81
2:B:860:ARG:HB3	2:B:966:ILE:HG22	1.61	0.81
2:A:895:GLU:OE1	2:A:898:LYS:HD2	1.81	0.81
2:A:690:ARG:HH11	2:A:693:GLU:HG3	1.45	0.80
2:B:268:GLU:HG3	2:B:316:ASP:HA	1.63	0.80
2:B:641:ASN:HA	2:B:683:HIS:O	1.80	0.80
2:B:170:LEU:HB2	2:B:176:ILE:HD11	1.62	0.80
2:A:660:ASN:HB2	2:A:663:ASP:CB	2.10	0.80
2:B:186:ASP:HB3	2:B:191:THR:HG23	1.61	0.80
2:A:412:VAL:HG23	2:A:414:PRO:HD2	1.64	0.80
2:B:384:ILE:HG22	2:B:385:LYS:H	1.47	0.80
1:C:986:C:N3	2:A:506:LYS:HG2	1.97	0.80
2:A:73:ASN:O	2:A:601:TRP:HH2	1.64	0.80
2:A:39:THR:HG23	2:A:604:LEU:HD11	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:931:LYS:O	2:A:935:GLU:HG3	1.80	0.79
2:B:860:ARG:HE	2:B:942:ILE:HA	1.48	0.79
1:D:904:G:C2'	1:D:905:G:H5''	2.11	0.79
2:B:863:ILE:HB	2:B:953:LYS:HD3	1.64	0.79
1:C:911:C:H2'	1:C:912:C:H6	1.47	0.79
2:B:157:PRO:HB2	2:B:158:PRO:HD3	1.65	0.79
2:A:170:LEU:CB	2:A:176:ILE:HD11	2.11	0.79
2:A:732:ARG:NH1	2:A:735:LYS:HD3	1.98	0.79
2:A:82:ILE:HG13	2:A:153:THR:HG23	1.63	0.79
2:A:922:ASN:ND2	2:A:923:GLU:N	2.30	0.79
2:B:116:LEU:HD12	2:B:119:PHE:CD2	2.17	0.79
2:B:547:LYS:HE2	2:B:547:LYS:HA	1.63	0.79
2:B:919:LYS:O	2:B:922:ASN:HB2	1.82	0.79
2:A:297:ARG:HG2	2:A:304:GLU:HG2	1.63	0.79
2:A:487:ILE:HG22	2:A:489:PRO:O	1.82	0.79
2:B:297:ARG:HG2	2:B:304:GLU:HG2	1.63	0.79
2:B:826:GLU:C	2:B:828:TRP:N	2.34	0.79
1:D:902:C:H3'	1:D:903:G:H5''	1.64	0.79
2:A:867:GLU:H	2:A:867:GLU:CD	1.86	0.78
2:A:924:GLU:CB	2:A:928:ARG:HH21	1.94	0.78
2:A:186:ASP:HB3	2:A:191:THR:HG23	1.65	0.78
2:B:343:THR:HG23	2:B:344:GLU:H	1.47	0.78
2:B:345:ILE:HG12	2:B:346:LEU:H	1.47	0.78
2:B:464:GLN:HA	2:B:524:TRP:CH2	2.18	0.78
2:A:204:VAL:HG21	2:A:448:VAL:HG22	1.66	0.78
2:B:51:VAL:O	2:B:54:ALA:HB3	1.84	0.78
2:B:722:LEU:CD2	2:B:722:LEU:H	1.97	0.78
2:B:949:ASP:HB2	2:B:954:LYS:HE2	1.64	0.78
1:C:986:C:H4'	1:C:987:C:C5'	2.14	0.78
2:A:348:LYS:HB3	2:A:348:LYS:NZ	1.99	0.78
2:A:871:TRP:CZ3	2:A:918:VAL:HG13	2.18	0.78
2:A:826:GLU:C	2:A:828:TRP:N	2.34	0.78
2:B:471:ASN:ND2	2:B:473:GLU:HG2	1.99	0.78
2:B:55:ARG:O	2:B:59:ILE:HG13	1.83	0.78
2:A:393:LEU:HD12	2:A:396:ALA:HB3	1.66	0.78
2:A:482:LEU:HD12	2:A:500:ILE:HD11	1.66	0.78
2:A:87:ILE:HG13	2:A:88:VAL:N	1.98	0.78
2:B:333:HIS:HA	2:B:336:LEU:HB2	1.66	0.78
2:B:45:LEU:HD11	2:B:80:TRP:HB3	1.64	0.78
2:A:482:LEU:HD11	2:A:496:PHE:HB3	1.66	0.77
2:A:650:LYS:HD2	2:A:651:MET:H	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:540:THR:HG23	2:B:541:ILE:HG23	1.64	0.77
2:B:731:HIS:CD2	2:B:829:ASN:H	2.02	0.77
2:B:801:ILE:O	2:B:805:LEU:HG	1.84	0.77
2:A:529:LEU:CD1	2:A:529:LEU:H	1.96	0.77
2:A:209:TYR:HE1	2:A:317:ASN:HD21	1.30	0.77
2:A:860:ARG:HB3	2:A:966:ILE:HG22	1.64	0.77
1:C:985:A:H61	2:A:504:ASP:HB2	1.47	0.77
2:A:871:TRP:CD1	2:A:959:PRO:HG3	2.18	0.77
2:A:242:TRP:HH2	2:A:332:ASP:HA	1.50	0.77
1:C:986:C:N3	2:A:507:ALA:N	2.32	0.77
2:B:446:LYS:HD2	2:B:446:LYS:H	1.47	0.77
2:B:834:ALA:HA	2:B:837:GLU:OE2	1.83	0.77
2:A:819:LYS:H	2:A:819:LYS:CE	1.97	0.77
2:A:722:LEU:H	2:A:722:LEU:CD2	1.98	0.77
2:B:150:PHE:HD1	2:B:151:TYR:O	1.68	0.77
2:B:866:ALA:N	2:B:955:LYS:NZ	2.31	0.77
2:A:919:LYS:HD2	2:A:960:LEU:CD1	2.16	0.76
2:A:770:ARG:NH1	2:A:933:PHE:HD2	1.81	0.76
2:B:845:ASP:O	2:B:849:ILE:HG13	1.84	0.76
2:B:880:LYS:HG3	2:B:885:SER:HB2	1.67	0.76
2:A:198:LEU:HB2	2:A:202:GLU:CG	2.14	0.76
2:B:631:GLU:HA	2:B:634:TRP:CE2	2.20	0.76
2:A:27:ILE:N	2:A:28:ARG:HH21	1.83	0.76
2:B:914:ARG:HH21	2:B:915:THR:HG23	1.51	0.76
2:A:28:ARG:HE	2:A:28:ARG:N	1.81	0.76
2:A:488:LEU:HD12	2:A:606:TRP:CH2	2.21	0.76
2:A:88:VAL:HG21	2:A:513:GLY:HA2	1.66	0.76
2:A:731:HIS:CE1	2:A:833:GLU:OE1	2.39	0.76
2:A:928:ARG:O	2:A:930:ALA:N	2.18	0.76
2:B:82:ILE:HG21	2:B:126:VAL:CG1	2.16	0.76
2:B:887:MET:SD	2:B:906:ILE:HD12	2.26	0.76
2:B:931:LYS:O	2:B:935:GLU:HG3	1.86	0.76
2:B:165:TRP:CD1	2:B:561:PRO:HA	2.21	0.75
1:D:929:G:H1	1:D:947:U:H3	1.35	0.75
2:A:238:VAL:CG1	2:A:298:ASN:HD22	1.98	0.75
2:A:949:ASP:HB2	2:A:954:LYS:HE2	1.69	0.75
2:A:641:ASN:HA	2:A:683:HIS:O	1.85	0.75
2:B:767:TYR:HE2	2:B:783:LEU:HD11	1.49	0.75
2:B:678:MET:HB3	2:B:749:THR:HB	1.68	0.75
2:A:492:ARG:CG	2:A:492:ARG:HH11	1.99	0.75
2:A:17:TRP:CH2	2:A:800:HIS:HD2	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:957:ALA:HB2	2:A:963:ALA:HB2	1.67	0.75
2:B:846:ILE:HG12	2:B:964:ILE:CD1	2.16	0.75
2:A:139:ARG:NH1	2:A:139:ARG:HG3	1.95	0.74
2:A:624:ASN:HD22	2:A:624:ASN:H	1.35	0.74
2:B:211:ILE:HG22	2:B:228:ALA:HB2	1.68	0.74
2:A:213:LYS:HD2	2:A:435:GLY:O	1.87	0.74
2:B:631:GLU:HA	2:B:634:TRP:NE1	2.01	0.74
2:A:551:GLU:O	2:A:553:LYS:HG2	1.86	0.74
2:B:681:ALA:HA	2:B:750:ARG:HG3	1.68	0.74
2:B:89:GLY:O	2:B:93:ARG:HG3	1.87	0.74
2:A:755:TRP:O	2:A:759:SER:HB3	1.87	0.74
2:A:645:THR:HG22	2:A:650:LYS:HA	1.68	0.74
1:C:908:U:H5'	1:C:961:C:OP2	1.88	0.74
1:D:902:C:C3'	1:D:903:G:H5''	2.17	0.74
2:A:354:ARG:HD2	2:A:376:VAL:CG1	2.17	0.74
2:A:432:LEU:HD11	2:A:439:ILE:HG13	1.70	0.74
2:B:836:GLU:O	2:B:840:ARG:HG3	1.87	0.74
2:A:230:LEU:H	2:A:230:LEU:CD2	2.01	0.73
2:A:30:LYS:HB2	2:A:73:ASN:ND2	1.96	0.73
2:A:882:ASP:CG	2:A:883:PHE:H	1.92	0.73
2:B:26:ASN:CB	2:B:28:ARG:HH22	2.01	0.73
2:B:928:ARG:O	2:B:930:ALA:N	2.21	0.73
2:A:566:TYR:HA	2:A:570:GLU:HB2	1.70	0.73
2:A:766:TRP:CH2	2:A:770:ARG:HD3	2.23	0.73
2:B:703:ARG:HH11	2:B:703:ARG:CB	2.00	0.73
2:B:859:LYS:HB3	2:B:941:GLU:HB3	1.69	0.73
2:A:345:ILE:HG23	2:A:346:LEU:HD13	1.71	0.73
2:B:198:LEU:CB	2:B:202:GLU:HG2	2.19	0.73
2:B:544:HIS:O	2:B:548:LEU:HG	1.87	0.73
2:B:857:ASN:ND2	2:B:967:GLU:HG2	2.03	0.73
2:B:867:GLU:CD	2:B:867:GLU:H	1.92	0.73
2:B:957:ALA:HB2	2:B:963:ALA:HB2	1.67	0.73
2:A:413:PRO:HB2	2:A:414:PRO:HD3	1.70	0.73
2:A:537:ALA:O	2:A:540:THR:HG22	1.88	0.73
2:A:691:ARG:O	2:A:694:VAL:HG12	1.88	0.73
1:C:982:C:H2'	1:C:983:G:C8	2.24	0.73
2:A:233:GLU:HB3	2:A:423:VAL:HG23	1.68	0.73
2:A:42:PHE:CD1	2:A:81:HIS:HB2	2.24	0.73
2:A:792:ARG:HG3	2:A:792:ARG:NH2	2.04	0.73
2:A:832:ILE:HA	2:A:835:GLU:HG3	1.71	0.73
2:A:17:TRP:CH2	2:A:800:HIS:CD2	2.76	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:373:PHE:CD1	2:A:374:PRO:HD3	2.24	0.73
2:A:250:VAL:HG12	2:A:285:GLU:HA	1.70	0.72
2:A:342:GLU:HG2	2:A:343:THR:H	1.54	0.72
2:A:558:LYS:HD2	2:A:583:LYS:O	1.89	0.72
2:A:860:ARG:NH2	2:A:862:TYR:HB3	2.04	0.72
2:B:734:ASN:HD21	2:B:824:VAL:N	1.86	0.72
2:B:803:GLU:OE2	2:B:815:VAL:N	2.23	0.72
2:B:925:LYS:HA	2:B:928:ARG:HG2	1.68	0.72
2:A:771:THR:HG22	2:A:774:ARG:HD3	1.70	0.72
2:B:695:GLY:O	2:B:698:ARG:HB3	1.90	0.72
2:B:848:GLU:O	2:B:852:VAL:HG23	1.89	0.72
2:A:488:LEU:HD12	2:A:606:TRP:CZ3	2.24	0.72
2:A:239:THR:CG2	2:A:326:PRO:HD2	2.20	0.72
2:B:757:PHE:HD1	2:B:794:MET:SD	2.12	0.72
2:B:480:LYS:HA	2:B:483:GLU:OE1	1.89	0.72
2:B:167:PHE:HA	2:B:170:LEU:CD1	2.19	0.72
2:B:467:ILE:HG13	2:B:508:CYS:SG	2.30	0.72
2:A:863:ILE:HB	2:A:953:LYS:HD3	1.70	0.71
2:A:119:PHE:CD1	2:A:125:ILE:HG12	2.24	0.71
2:A:342:GLU:HG2	2:A:343:THR:N	2.04	0.71
2:A:690:ARG:HD3	2:A:693:GLU:OE2	1.89	0.71
2:B:32:LYS:HG2	2:B:600:TYR:CD1	2.25	0.71
2:A:860:ARG:HH22	2:A:862:TYR:N	1.87	0.71
2:A:922:ASN:C	2:A:922:ASN:ND2	2.34	0.71
2:B:784:ARG:NH2	2:B:810:GLY:H	1.88	0.71
2:B:22:ILE:HG13	2:B:817:LEU:HD21	1.73	0.71
2:B:957:ALA:HB2	2:B:963:ALA:CB	2.21	0.71
2:A:219:ASN:HD22	2:A:220:GLY:H	1.37	0.71
2:A:731:HIS:CD2	2:A:829:ASN:H	2.08	0.71
2:A:770:ARG:NH1	2:A:933:PHE:CD2	2.59	0.71
2:A:957:ALA:HB2	2:A:963:ALA:CB	2.20	0.71
2:A:67:LYS:HD3	2:A:70:GLN:HE21	1.54	0.71
2:A:734:ASN:OD1	2:A:823:PRO:HA	1.91	0.71
2:B:30:LYS:HE3	2:B:71:GLY:O	1.90	0.71
2:B:890:LEU:HD12	2:B:906:ILE:HD11	1.73	0.71
2:A:730:LEU:HB3	2:A:827:TRP:HE1	1.54	0.70
2:A:198:LEU:HD22	2:A:202:GLU:HA	1.73	0.70
2:A:631:GLU:HA	2:A:634:TRP:CE2	2.26	0.70
2:B:282:VAL:HG12	2:B:283:ILE:N	2.07	0.70
2:A:419:PRO:HG2	2:A:422:GLU:HG3	1.71	0.70
2:A:276:GLN:HA	2:A:460:ILE:HD13	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:857:ASN:O	2:A:940:ILE:HD11	1.90	0.70
2:B:471:ASN:HD21	2:B:473:GLU:HG2	1.55	0.70
2:B:826:GLU:O	2:B:827:TRP:HB3	1.91	0.70
2:A:824:VAL:HG11	2:A:827:TRP:HE3	1.56	0.70
2:B:487:ILE:HG22	2:B:489:PRO:O	1.91	0.70
1:C:970:A:H4'	1:C:971:A:OP1	1.91	0.70
2:A:613:LEU:O	2:A:618:LEU:HB2	1.91	0.70
2:A:140:ALA:HB2	2:A:665:ILE:HD11	1.72	0.70
2:A:204:VAL:HG21	2:A:448:VAL:HG21	1.74	0.70
2:A:333:HIS:HA	2:A:336:LEU:HB2	1.73	0.70
2:A:795:ALA:HB3	2:A:796:PRO:HD3	1.72	0.70
2:A:826:GLU:O	2:A:827:TRP:HB3	1.90	0.70
2:A:12:LYS:NZ	2:A:16:ARG:HH12	1.90	0.70
2:B:803:GLU:OE2	2:B:815:VAL:HG12	1.91	0.70
2:A:866:ALA:N	2:A:955:LYS:NZ	2.27	0.69
2:A:919:LYS:O	2:A:922:ASN:HB2	1.92	0.69
2:B:297:ARG:NH2	2:B:297:ARG:HB3	2.07	0.69
2:B:927:LEU:CD1	2:B:944:ILE:HD12	2.23	0.69
1:C:920:G:H5''	1:C:921:U:H5	1.57	0.69
2:A:339:LEU:HD22	2:A:340:LYS:N	2.08	0.69
2:A:374:PRO:HG2	2:A:379:VAL:HG21	1.74	0.69
2:B:660:ASN:HB2	2:B:663:ASP:CB	2.22	0.69
2:B:690:ARG:HB3	2:B:690:ARG:NH1	2.06	0.69
2:B:95:LYS:C	2:B:97:ARG:H	1.96	0.69
2:A:22:ILE:HG23	2:A:23:PHE:CD1	2.27	0.69
2:A:165:TRP:HD1	2:A:561:PRO:HA	1.58	0.69
2:B:741:THR:HG1	2:B:820:TRP:HZ3	1.41	0.69
2:A:91:ALA:O	2:A:94:ILE:HG13	1.91	0.69
2:B:400:ILE:HD12	2:B:401:TYR:N	2.06	0.69
2:B:770:ARG:HD2	2:B:933:PHE:CE2	2.27	0.69
1:C:923:A:H4'	1:C:924:A:O5'	1.91	0.69
2:A:577:GLU:OE2	2:A:592:HIS:HB2	1.92	0.69
2:B:675:LEU:CD2	2:B:697:LEU:HD21	2.22	0.69
2:B:675:LEU:HD22	2:B:701:ILE:HD11	1.74	0.69
2:B:7:LYS:NZ	2:B:7:LYS:HB2	2.07	0.69
2:A:449:ILE:N	2:A:449:ILE:HD12	2.08	0.69
2:A:163:ILE:CD1	2:A:531:ASP:HB2	2.22	0.69
2:A:863:ILE:HG22	2:A:953:LYS:HG2	1.74	0.69
2:B:35:LYS:HB2	2:B:601:TRP:CZ3	2.28	0.69
2:A:221:GLU:HA	2:A:221:GLU:OE2	1.93	0.69
2:A:45:LEU:HD11	2:A:80:TRP:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:10:GLU:O	2:A:14:GLN:HG3	1.93	0.69
2:A:480:LYS:CE	2:A:484:ARG:HH22	1.99	0.68
2:B:920:ARG:C	2:B:922:ASN:H	1.97	0.68
2:A:730:LEU:HB3	2:A:827:TRP:CD1	2.28	0.68
2:B:341:ARG:HD3	2:B:341:ARG:N	2.07	0.68
2:A:920:ARG:C	2:A:922:ASN:H	1.96	0.68
2:A:95:LYS:C	2:A:97:ARG:H	1.96	0.68
2:B:14:GLN:O	2:B:18:LEU:HB2	1.93	0.68
2:B:566:TYR:HA	2:B:570:GLU:HB3	1.75	0.68
2:B:882:ASP:CG	2:B:883:PHE:N	2.47	0.68
2:A:198:LEU:CB	2:A:202:GLU:HG2	2.23	0.68
2:A:239:THR:HG23	2:A:326:PRO:HD2	1.74	0.68
2:A:62:VAL:HG21	2:A:678:MET:HE3	1.75	0.68
2:A:30:LYS:CB	2:A:73:ASN:HD22	1.98	0.68
2:B:650:LYS:HE2	2:B:651:MET:N	2.03	0.68
2:B:65:ARG:HA	2:B:68:ARG:NH1	2.08	0.68
2:B:871:TRP:NE1	2:B:959:PRO:HB3	2.09	0.68
2:A:629:PHE:O	2:A:631:GLU:N	2.25	0.68
2:B:116:LEU:HD12	2:B:119:PHE:HD2	1.59	0.68
2:B:276:GLN:O	2:B:460:ILE:HD12	1.92	0.68
2:B:767:TYR:CE2	2:B:783:LEU:HD11	2.27	0.68
2:A:717:LYS:HD3	2:A:717:LYS:O	1.94	0.68
2:B:28:ARG:HG3	2:B:28:ARG:HH11	1.59	0.68
2:B:678:MET:HE3	2:B:749:THR:HG21	1.74	0.68
2:A:652:SER:OG	2:A:655:LYS:HB2	1.94	0.68
2:A:722:LEU:N	2:A:722:LEU:CD2	2.55	0.68
2:A:82:ILE:HG21	2:A:126:VAL:HG13	1.74	0.68
2:B:770:ARG:HA	2:B:933:PHE:HE2	1.58	0.68
2:B:198:LEU:HD12	2:B:198:LEU:H	1.59	0.68
2:B:26:ASN:HB2	2:B:29:ASP:OD2	1.93	0.68
2:B:734:ASN:ND2	2:B:823:PRO:HA	2.07	0.68
1:C:988:A:H5''	2:A:528:SER:OG	1.94	0.68
2:A:803:GLU:CD	2:A:815:VAL:HG23	2.14	0.68
2:B:237:GLY:O	2:B:325:VAL:HG13	1.94	0.68
2:B:300:VAL:HG13	2:B:301:SER:H	1.59	0.68
1:C:929:G:H1	1:C:947:U:H3	1.42	0.68
2:A:75:LEU:HD12	2:A:75:LEU:C	2.14	0.67
2:B:185:TRP:CZ2	2:B:190:GLY:HA2	2.29	0.67
2:B:345:ILE:HG12	2:B:346:LEU:N	2.09	0.67
1:D:920:G:H5''	1:D:921:U:H5	1.59	0.67
2:B:555:ASP:HB3	2:B:558:LYS:CG	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:GLU:O	2:B:95:LYS:HB3	1.94	0.67
2:A:423:VAL:C	2:A:425:GLU:H	1.95	0.67
2:B:795:ALA:HB3	2:B:796:PRO:HD3	1.77	0.67
2:A:919:LYS:H	2:A:919:LYS:CE	2.07	0.67
2:B:26:ASN:CB	2:B:28:ARG:NH2	2.55	0.67
2:A:404:GLU:O	2:A:420:VAL:HG21	1.95	0.67
2:A:872:LYS:O	2:A:876:VAL:HG23	1.94	0.67
2:B:423:VAL:C	2:B:425:GLU:H	1.97	0.67
1:D:977:G:H2'	1:D:978:C:C6	2.30	0.67
2:A:242:TRP:CH2	2:A:332:ASP:HA	2.29	0.67
2:B:614:ILE:N	2:B:615:PRO:HD2	2.09	0.67
2:A:139:ARG:NH2	2:A:666:GLU:OE1	2.27	0.67
2:A:870:LYS:HE2	2:A:905:LYS:HE3	1.77	0.67
2:A:428:ALA:O	2:A:432:LEU:HD23	1.95	0.66
1:C:916:C:H4'	1:C:916:C:OP1	1.93	0.66
2:A:891:MET:SD	2:A:897:ARG:HG3	2.35	0.66
2:B:57:TYR:O	2:B:60:PRO:HG2	1.95	0.66
2:B:741:THR:OG1	2:B:820:TRP:HZ3	1.78	0.66
2:A:529:LEU:N	2:A:529:LEU:HD12	2.06	0.66
2:A:536:MET:SD	2:A:607:ARG:NH1	2.69	0.66
2:A:717:LYS:HD3	2:A:717:LYS:C	2.15	0.66
2:A:682:GLU:OE1	2:A:748:ARG:HB3	1.95	0.66
2:B:326:PRO:HA	2:B:332:ASP:HB2	1.77	0.66
2:B:136:THR:HG22	2:B:661:PHE:HD2	1.60	0.66
2:A:266:SER:HB2	2:A:269:ALA:HB2	1.78	0.66
2:A:488:LEU:HD22	2:A:683:HIS:CE1	2.31	0.66
2:B:935:GLU:HG2	2:B:942:ILE:HD13	1.78	0.66
2:A:703:ARG:HG3	2:A:707:LEU:HD12	1.78	0.66
2:B:871:TRP:CZ3	2:B:918:VAL:HG13	2.30	0.66
2:B:793:LEU:CD2	2:B:821:PRO:HG2	2.25	0.66
2:B:921:ILE:HB	2:B:928:ARG:NH2	2.09	0.66
2:A:188:VAL:HG23	2:A:189:VAL:N	2.06	0.66
2:A:434:LYS:HB3	2:A:436:ILE:HG12	1.77	0.66
2:A:921:ILE:HD12	2:A:928:ARG:NH1	2.03	0.66
2:B:171:LYS:HG2	2:B:176:ILE:HD12	1.78	0.66
2:B:459:LYS:NZ	2:B:461:ILE:HD13	2.11	0.66
2:B:690:ARG:HB3	2:B:690:ARG:CZ	2.25	0.66
2:A:198:LEU:HB2	2:A:202:GLU:CD	2.15	0.66
2:A:947:THR:HG23	2:A:948:GLU:N	2.11	0.66
2:B:256:ARG:HG3	2:B:257:LYS:H	1.61	0.66
2:A:784:ARG:HH22	2:A:810:GLY:H	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:ARG:HG3	2:B:139:ARG:HH11	1.60	0.65
2:A:860:ARG:NH1	2:A:943:ILE:N	2.41	0.65
2:B:197:ASP:HB3	2:B:451:ARG:HB2	1.78	0.65
2:B:650:LYS:CE	2:B:651:MET:H	2.05	0.65
1:D:983:G:C2'	1:D:984:C:H5''	2.25	0.65
2:A:83:THR:HG23	2:A:152:THR:HB	1.78	0.65
2:B:198:LEU:HB2	2:B:202:GLU:CG	2.20	0.65
2:B:537:ALA:HB2	2:B:602:TYR:CZ	2.31	0.65
2:A:354:ARG:HD2	2:A:376:VAL:HG12	1.78	0.65
2:A:914:ARG:NH2	2:A:915:THR:HG23	2.11	0.65
2:A:82:ILE:HG21	2:A:126:VAL:CG1	2.26	0.65
2:A:730:LEU:HD22	2:A:827:TRP:CZ2	2.31	0.65
2:A:210:ILE:CD1	2:A:232:PRO:HG3	2.24	0.65
2:A:297:ARG:HG2	2:A:304:GLU:CG	2.25	0.65
2:A:590:ILE:O	2:A:594:MET:HG3	1.97	0.65
2:A:109:TYR:OH	2:A:653:LYS:HE2	1.96	0.65
2:A:647:GLU:OE2	2:A:690:ARG:HA	1.97	0.65
2:A:767:TYR:HE2	2:A:783:LEU:CD1	2.09	0.65
2:A:86:PRO:O	2:A:90:ILE:HG13	1.95	0.65
2:A:914:ARG:HH21	2:A:915:THR:HG23	1.62	0.65
2:B:50:HIS:CE1	2:B:52:GLY:HA3	2.31	0.65
2:B:616:ASN:ND2	2:B:617:HIS:H	1.93	0.65
1:C:967:U:H2'	1:C:969:G:N7	2.11	0.65
2:A:233:GLU:HA	2:A:427:ILE:HD12	1.77	0.65
2:A:4:LEU:O	2:A:4:LEU:HD23	1.97	0.65
2:B:540:THR:CG2	2:B:541:ILE:HG23	2.25	0.65
2:B:87:ILE:HD13	2:B:126:VAL:CG2	2.27	0.65
2:B:909:LYS:NZ	2:B:914:ARG:O	2.29	0.65
2:A:197:ASP:HB3	2:A:451:ARG:HB2	1.78	0.64
2:A:650:LYS:HD2	2:A:651:MET:N	2.11	0.64
2:B:300:VAL:HG13	2:B:301:SER:N	2.12	0.64
2:B:39:THR:HG22	2:B:40:VAL:H	1.60	0.64
2:B:924:GLU:O	2:B:928:ARG:N	2.28	0.64
2:B:924:GLU:HB3	2:B:928:ARG:HH21	1.62	0.64
2:B:922:ASN:HD22	2:B:923:GLU:N	1.96	0.64
2:A:345:ILE:CG1	2:A:346:LEU:H	2.06	0.64
2:B:198:LEU:HD22	2:B:202:GLU:HA	1.78	0.64
2:B:27:ILE:HG13	2:B:28:ARG:N	2.13	0.64
2:B:724:ASP:HA	2:B:727:ARG:HG3	1.79	0.64
2:B:880:LYS:CG	2:B:885:SER:HB2	2.28	0.64
2:A:139:ARG:CG	2:A:139:ARG:HH11	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:467:ILE:HG13	2:A:508:CYS:HB3	1.80	0.64
2:B:33:GLU:CD	2:B:33:GLU:H	2.00	0.64
2:B:563:PHE:CD1	2:B:584:THR:HG21	2.33	0.64
2:B:632:GLU:HG3	2:B:633:HIS:ND1	2.13	0.64
2:B:958:MET:CE	2:B:959:PRO:HD2	2.27	0.64
2:A:313:VAL:HG12	2:A:322:VAL:HG21	1.78	0.64
2:A:890:LEU:CD1	2:A:906:ILE:HD11	2.27	0.64
2:B:289:GLU:O	2:B:292:ILE:HB	1.98	0.64
2:B:570:GLU:OE1	2:B:576:LYS:HE2	1.98	0.64
2:B:729:MET:HE3	2:B:763:ASP:O	1.97	0.64
2:A:492:ARG:HG2	2:A:492:ARG:HH11	1.63	0.64
1:C:920:G:H5''	1:C:921:U:C5	2.33	0.64
1:D:977:G:H2'	1:D:978:C:H6	1.62	0.64
2:A:871:TRP:HH2	2:A:919:LYS:HE3	1.61	0.64
2:B:660:ASN:HB2	2:B:663:ASP:HB3	1.80	0.64
2:A:212:ILE:HD13	2:A:235:VAL:CG1	2.27	0.64
2:A:475:LYS:NZ	2:A:503:LEU:O	2.31	0.64
2:B:860:ARG:HB3	2:B:966:ILE:HA	1.78	0.64
1:D:943:C:H2'	1:D:944:C:C6	2.33	0.64
2:A:136:THR:HG23	2:A:662:ILE:HB	1.80	0.64
2:B:864:TYR:HH	2:B:871:TRP:HZ2	1.45	0.64
2:A:49:LEU:HD12	2:A:49:LEU:N	2.10	0.63
2:A:92:GLU:O	2:A:95:LYS:HB3	1.99	0.63
2:B:73:ASN:O	2:B:601:TRP:HH2	1.81	0.63
2:A:342:GLU:CG	2:A:343:THR:H	2.11	0.63
2:A:924:GLU:O	2:A:928:ARG:N	2.28	0.63
2:B:373:PHE:N	2:B:374:PRO:HD2	2.14	0.63
2:B:213:LYS:HD2	2:B:435:GLY:O	1.99	0.63
2:B:256:ARG:HH11	2:B:278:ARG:HG3	1.63	0.63
2:A:343:THR:HG23	2:A:344:GLU:N	2.12	0.63
2:A:272:LYS:HE3	2:A:442:GLU:OE1	1.98	0.63
2:A:924:GLU:CD	2:A:927:LEU:HD13	2.19	0.63
2:B:755:TRP:O	2:B:759:SER:HB3	1.99	0.63
2:A:616:ASN:ND2	2:A:617:HIS:N	2.24	0.63
2:B:10:GLU:O	2:B:14:GLN:HG3	1.97	0.63
2:A:724:ASP:HA	2:A:727:ARG:CG	2.19	0.63
2:A:85:SER:H	2:A:86:PRO:CD	2.12	0.63
2:B:139:ARG:HG3	2:B:139:ARG:NH1	2.13	0.63
2:B:681:ALA:CA	2:B:750:ARG:HG3	2.28	0.63
2:B:428:ALA:O	2:B:432:LEU:HD23	1.98	0.63
2:B:495:GLN:HE21	2:B:614:ILE:HG21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ILE:HD13	2:B:126:VAL:HG22	1.79	0.63
2:A:282:VAL:HG12	2:A:283:ILE:H	1.64	0.63
2:A:631:GLU:HA	2:A:634:TRP:NE1	2.14	0.63
2:A:728:TRP:HE3	2:A:729:MET:N	1.97	0.63
2:A:924:GLU:O	2:A:927:LEU:HB3	1.99	0.63
2:B:45:LEU:HD11	2:B:80:TRP:CB	2.29	0.63
2:B:826:GLU:N	2:B:826:GLU:CD	2.52	0.63
2:A:268:GLU:N	2:A:268:GLU:OE1	2.26	0.62
2:A:544:HIS:H	2:A:544:HIS:CD2	2.15	0.62
2:B:332:ASP:O	2:B:333:HIS:HB2	1.99	0.62
2:B:894:SER:C	2:B:896:ILE:H	2.03	0.62
2:A:180:ALA:O	2:A:181:HIS:HB2	1.99	0.62
2:B:216:LEU:HD11	2:B:294:LYS:HB3	1.80	0.62
2:B:26:ASN:HB2	2:B:29:ASP:CG	2.19	0.62
2:B:764:LEU:HD13	2:B:786:LEU:HD13	1.80	0.62
1:C:918:U:H5''	1:C:919:G:OP1	1.98	0.62
2:A:235:VAL:HB	2:A:300:VAL:HG11	1.79	0.62
2:B:51:VAL:HG11	2:B:689:TRP:CE3	2.33	0.62
2:A:126:VAL:HG12	2:A:126:VAL:O	1.99	0.62
2:A:41:ALA:HA	2:A:607:ARG:NH2	2.15	0.62
2:A:724:ASP:CA	2:A:727:ARG:HG3	2.20	0.62
2:A:730:LEU:CB	2:A:827:TRP:HE1	2.12	0.62
2:A:733:LEU:O	2:A:737:ILE:HG13	1.99	0.62
1:C:911:C:H2'	1:C:912:C:C6	2.33	0.62
2:A:168:TRP:CH2	2:A:520:TRP:HB3	2.34	0.62
2:A:306:ILE:HG12	2:A:307:ILE:N	2.14	0.62
2:A:540:THR:OG1	2:A:598:PHE:HA	2.00	0.62
2:A:894:SER:C	2:A:896:ILE:H	2.02	0.62
2:A:94:ILE:HD12	2:A:95:LYS:N	2.14	0.62
2:A:7:LYS:NZ	2:A:7:LYS:HB2	2.15	0.62
2:B:218:GLU:CD	2:B:219:ASN:HD22	2.03	0.62
2:B:181:HIS:ND1	2:B:464:GLN:HG2	2.14	0.62
2:B:531:ASP:OD2	2:B:532:SER:N	2.32	0.62
2:A:213:LYS:HB2	2:A:224:TYR:CD2	2.35	0.62
2:A:933:PHE:C	2:A:933:PHE:CD1	2.72	0.62
2:B:126:VAL:O	2:B:126:VAL:HG12	1.99	0.62
2:B:212:ILE:HD13	2:B:235:VAL:HG12	1.82	0.62
2:B:277:ASP:O	2:B:278:ARG:HG3	1.99	0.62
2:B:68:ARG:NH2	2:B:143:SER:HB3	2.14	0.62
2:B:85:SER:H	2:B:86:PRO:HD3	1.64	0.62
2:A:186:ASP:HB2	2:A:193:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:702:GLU:O	2:A:706:GLU:HG3	2.00	0.62
2:B:234:THR:HG22	2:B:325:VAL:HG11	1.80	0.62
1:C:914:A:H1'	1:C:925:A:C6	2.35	0.62
2:A:709:SER:O	2:A:712:ALA:HB3	1.99	0.62
2:A:776:ASP:OD2	2:A:778:ALA:HB3	1.99	0.62
2:A:860:ARG:HH11	2:A:943:ILE:H	1.48	0.62
2:B:140:ALA:O	2:B:674:ARG:NH1	2.31	0.62
2:B:709:SER:O	2:B:712:ALA:HB3	2.00	0.62
2:A:906:ILE:O	2:A:910:LEU:HB2	2.00	0.61
2:B:49:LEU:HD12	2:B:49:LEU:N	2.13	0.61
2:B:793:LEU:HD21	2:B:821:PRO:HG2	1.81	0.61
1:D:970:A:H2'	1:D:972:U:OP2	2.00	0.61
2:A:297:ARG:CB	2:A:297:ARG:NH2	2.63	0.61
2:B:745:GLU:OE2	2:B:745:GLU:HA	1.99	0.61
2:A:102:ILE:HD12	2:A:103:TRP:N	2.15	0.61
2:A:11:GLU:O	2:A:15:LYS:HG3	2.00	0.61
1:C:986:C:C2	2:A:507:ALA:HB3	2.36	0.61
2:B:264:ILE:HG21	2:B:291:LEU:HD21	1.81	0.61
2:B:44:TYR:CE1	2:B:87:ILE:HD11	2.30	0.61
2:A:326:PRO:HA	2:A:332:ASP:HB2	1.81	0.61
2:A:803:GLU:HA	2:A:815:VAL:HG23	1.82	0.61
2:B:401:TYR:O	2:B:405:TYR:HB2	2.00	0.61
2:B:44:TYR:OH	2:B:87:ILE:HG13	2.00	0.61
2:B:920:ARG:CA	2:B:920:ARG:HE	2.01	0.61
2:A:82:ILE:H	2:A:152:THR:HG1	1.45	0.61
2:A:864:TYR:CZ	2:A:922:ASN:OD1	2.53	0.61
2:B:345:ILE:CG1	2:B:346:LEU:H	2.13	0.61
2:B:723:LYS:HG3	2:B:724:ASP:H	1.66	0.61
2:B:91:ALA:O	2:B:94:ILE:HG13	1.99	0.61
2:A:297:ARG:NH2	2:A:297:ARG:HB3	2.15	0.61
2:A:26:ASN:O	2:A:29:ASP:HB2	2.01	0.61
2:A:924:GLU:OE2	2:A:927:LEU:HD13	2.01	0.61
2:A:857:ASN:ND2	2:A:967:GLU:HG2	2.16	0.61
2:B:879:GLU:O	2:B:880:LYS:HD2	2.00	0.61
2:A:618:LEU:O	2:A:621:PHE:HB3	2.00	0.61
2:B:277:ASP:OD1	2:B:462:HIS:NE2	2.33	0.61
2:B:890:LEU:CD1	2:B:906:ILE:HD11	2.31	0.61
2:A:893:ASP:OD1	2:A:894:SER:O	2.19	0.61
2:A:919:LYS:HD2	2:A:960:LEU:HD11	1.82	0.61
2:B:145:ASP:OD1	2:B:147:SER:HB3	1.99	0.61
2:B:914:ARG:NE	2:B:915:THR:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:ARG:H	2:B:28:ARG:NH1	1.98	0.61
2:A:866:ALA:CA	2:A:955:LYS:HZ3	2.11	0.61
2:B:770:ARG:HA	2:B:933:PHE:CE2	2.35	0.61
1:D:970:A:H4'	1:D:971:A:OP1	2.01	0.61
2:A:94:ILE:HD11	2:A:120:GLU:N	2.15	0.60
2:A:492:ARG:HD2	2:A:614:ILE:CD1	2.30	0.60
2:A:123:ILE:O	2:A:127:LYS:HB2	2.00	0.60
2:A:241:MET:HB2	2:A:307:ILE:HA	1.81	0.60
2:A:567:ILE:O	2:A:568:PHE:CG	2.54	0.60
2:A:803:GLU:OE2	2:A:814:PHE:HB3	2.01	0.60
2:B:448:VAL:HG12	2:B:456:ALA:HB3	1.82	0.60
2:B:730:LEU:HB3	2:B:827:TRP:NE1	2.16	0.60
2:A:427:ILE:O	2:A:431:MET:HG3	2.00	0.60
2:A:45:LEU:HD11	2:A:80:TRP:CB	2.31	0.60
2:A:860:ARG:NE	2:A:860:ARG:O	2.35	0.60
2:A:381:LYS:HB3	2:A:382:LEU:HD12	1.83	0.60
2:A:594:MET:O	2:A:597:GLU:HB2	2.01	0.60
2:B:748:ARG:HB3	2:B:748:ARG:HH11	1.67	0.60
2:A:210:ILE:HG22	2:A:439:ILE:HG12	1.83	0.60
2:A:234:THR:HG22	2:A:325:VAL:HG11	1.83	0.60
2:A:461:ILE:CG2	2:A:464:GLN:HB2	2.32	0.60
2:B:166:GLN:O	2:B:170:LEU:HG	2.01	0.60
2:B:186:ASP:HB3	2:B:191:THR:CG2	2.32	0.60
1:C:976:C:O2'	1:C:977:G:H5'	2.01	0.60
2:A:12:LYS:HZ3	2:A:16:ARG:HH12	1.50	0.60
2:A:266:SER:HB2	2:A:269:ALA:CB	2.32	0.60
1:C:953:A:H5'	1:C:954:G:OP1	2.02	0.60
2:A:919:LYS:H	2:A:919:LYS:HE3	1.66	0.60
2:A:919:LYS:NZ	2:A:960:LEU:HD11	2.16	0.60
2:B:266:SER:HB3	2:B:269:ALA:HB2	1.83	0.60
2:B:32:LYS:HG2	2:B:600:TYR:HD1	1.65	0.60
2:B:85:SER:H	2:B:86:PRO:CD	2.14	0.60
2:A:412:VAL:CG2	2:A:414:PRO:HD2	2.32	0.60
2:B:781:TYR:CE2	2:B:785:THR:HG21	2.37	0.60
2:B:781:TYR:O	2:B:785:THR:HG23	2.02	0.60
1:D:979:C:H2'	1:D:980:C:C6	2.37	0.60
2:A:560:THR:HB	2:A:561:PRO:HD2	1.84	0.60
2:A:767:TYR:CZ	2:A:782:VAL:HG11	2.37	0.60
2:B:282:VAL:HG12	2:B:283:ILE:H	1.66	0.60
2:B:79:ALA:HB1	2:B:150:PHE:O	2.01	0.60
2:A:857:ASN:OD1	2:A:967:GLU:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:725:ILE:HG21	2:B:771:THR:CG2	2.31	0.59
2:A:17:TRP:HH2	2:A:800:HIS:CD2	2.20	0.59
2:A:297:ARG:HB2	2:A:297:ARG:HH21	1.67	0.59
2:A:354:ARG:HD2	2:A:376:VAL:HG13	1.82	0.59
2:A:915:THR:OG1	2:A:916:PHE:N	2.31	0.59
2:B:540:THR:OG1	2:B:598:PHE:HA	2.01	0.59
2:B:569:LEU:HA	2:B:630:ARG:HD3	1.85	0.59
2:B:746:GLU:HB2	2:B:748:ARG:HD2	1.84	0.59
2:A:678:MET:HB3	2:A:749:THR:HB	1.84	0.59
2:A:895:GLU:OE1	2:A:898:LYS:CD	2.50	0.59
2:A:960:LEU:HD22	2:A:960:LEU:N	2.17	0.59
2:A:711:PHE:HA	2:A:714:TYR:CD2	2.38	0.59
2:A:914:ARG:NE	2:A:915:THR:O	2.35	0.59
2:B:339:LEU:HD22	2:B:340:LYS:N	2.17	0.59
2:B:475:LYS:HG2	2:B:479:ARG:NH2	2.18	0.59
2:B:935:GLU:OE1	2:B:942:ILE:N	2.34	0.59
2:A:182:ARG:O	2:A:183:VAL:HB	2.02	0.59
2:A:75:LEU:HD23	2:A:601:TRP:CD2	2.37	0.59
2:A:79:ALA:HB1	2:A:150:PHE:O	2.01	0.59
2:A:824:VAL:HG11	2:A:827:TRP:CE3	2.37	0.59
2:A:860:ARG:CB	2:A:966:ILE:HG22	2.33	0.59
2:B:100:LYS:HE2	2:B:104:ILE:HD11	1.83	0.59
2:B:241:MET:HB2	2:B:307:ILE:HA	1.84	0.59
2:B:711:PHE:CD1	2:B:783:LEU:HB3	2.38	0.59
2:A:152:THR:HG22	2:A:159:PHE:HE1	1.67	0.59
2:A:560:THR:O	2:A:563:PHE:HB3	2.03	0.59
2:A:819:LYS:HD2	2:A:819:LYS:N	2.17	0.59
2:A:921:ILE:HB	2:A:928:ARG:NH2	2.16	0.59
2:B:112:PRO:O	2:B:114:GLU:N	2.36	0.59
2:B:594:MET:O	2:B:597:GLU:HB2	2.02	0.59
2:B:618:LEU:O	2:B:621:PHE:HB3	2.03	0.59
1:C:986:C:C2	2:A:506:LYS:HG2	2.37	0.59
2:A:242:TRP:CE3	2:A:324:SER:HB2	2.38	0.59
2:A:401:TYR:O	2:A:405:TYR:HB2	2.03	0.59
2:B:94:ILE:HD12	2:B:95:LYS:N	2.18	0.59
1:D:916:C:O2'	1:D:972:U:H4'	2.03	0.59
2:A:231:ARG:HB3	2:A:233:GLU:OE2	2.02	0.59
2:B:233:GLU:HB3	2:B:423:VAL:HG23	1.84	0.59
2:B:250:VAL:O	2:B:264:ILE:HA	2.02	0.59
2:B:227:ALA:CA	2:B:321:VAL:HG23	2.26	0.59
2:A:211:ILE:CG2	2:A:228:ALA:HB2	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:297:ARG:CB	2:A:297:ARG:HH21	2.16	0.59
2:B:404:GLU:HA	2:B:407:LYS:O	2.03	0.59
2:B:50:HIS:H	2:B:53:HIS:CD2	2.21	0.59
2:B:921:ILE:HD12	2:B:928:ARG:HH22	1.68	0.59
2:B:943:ILE:HG22	2:B:946:PRO:HG3	1.84	0.59
2:B:966:ILE:O	2:B:967:GLU:HB2	2.03	0.59
2:A:250:VAL:O	2:A:264:ILE:HA	2.04	0.58
2:A:378:GLU:HA	2:A:378:GLU:OE2	2.02	0.58
2:A:393:LEU:HG	2:A:397:THR:OG1	2.03	0.58
2:A:547:LYS:O	2:A:550:GLN:HB3	2.03	0.58
2:A:66:PHE:CD1	2:A:744:LEU:HD12	2.37	0.58
2:A:847:LYS:O	2:A:851:GLU:HG3	2.03	0.58
2:A:882:ASP:CG	2:A:883:PHE:N	2.56	0.58
2:B:355:ILE:HG22	2:B:356:VAL:N	2.12	0.58
2:B:641:ASN:HD22	2:B:641:ASN:C	2.06	0.58
2:B:722:LEU:H	2:B:722:LEU:HD23	1.68	0.58
2:A:75:LEU:HD12	2:A:77:PRO:HD3	1.85	0.58
2:A:966:ILE:O	2:A:967:GLU:CB	2.50	0.58
2:B:105:TYR:O	2:B:111:VAL:HG23	2.03	0.58
2:B:49:LEU:CD1	2:B:49:LEU:H	2.12	0.58
1:D:904:G:C3'	1:D:905:G:H5''	2.33	0.58
2:A:216:LEU:HG	2:A:216:LEU:O	2.03	0.58
2:A:263:TRP:HH2	2:A:438:GLU:OE1	1.86	0.58
2:A:819:LYS:CD	2:A:819:LYS:N	2.66	0.58
2:A:860:ARG:HH11	2:A:943:ILE:N	2.01	0.58
2:A:860:ARG:HH22	2:A:862:TYR:HB3	1.68	0.58
2:A:920:ARG:O	2:A:922:ASN:N	2.36	0.58
2:B:733:LEU:HD13	2:B:737:ILE:HG13	1.85	0.58
2:B:857:ASN:O	2:B:940:ILE:HD11	2.03	0.58
2:A:27:ILE:H	2:A:28:ARG:NH2	2.01	0.58
2:A:235:VAL:HA	2:A:323:MET:HE3	1.85	0.58
2:A:541:ILE:HB	2:A:594:MET:HE2	1.86	0.58
2:A:729:MET:SD	2:A:764:LEU:HA	2.44	0.58
2:B:901:LYS:O	2:B:901:LYS:HD3	2.03	0.58
2:A:410:PHE:O	2:A:416:GLU:HB3	2.03	0.58
2:A:944:ILE:HG22	2:A:945:ASN:N	2.18	0.58
2:B:180:ALA:O	2:B:181:HIS:HB2	2.04	0.58
2:B:429:LYS:NZ	2:B:429:LYS:HB3	2.19	0.58
2:B:660:ASN:HB2	2:B:663:ASP:HB2	1.86	0.58
2:B:342:GLU:HG2	2:B:343:THR:N	2.15	0.58
2:B:60:PRO:HB2	2:B:76:PHE:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:804:GLU:O	2:B:807:GLU:HB3	2.03	0.58
2:B:238:VAL:HA	2:B:325:VAL:HG22	1.85	0.58
2:B:50:HIS:HE1	2:B:52:GLY:HA3	1.68	0.58
2:A:239:THR:O	2:A:240:ASN:HB3	2.03	0.58
2:A:566:TYR:O	2:A:595:LYS:HD2	2.04	0.58
2:A:710:GLN:O	2:A:712:ALA:N	2.37	0.58
2:B:495:GLN:O	2:B:499:ILE:HG12	2.04	0.58
2:B:652:SER:OG	2:B:655:LYS:HB2	2.04	0.58
2:B:713:GLU:HA	2:B:713:GLU:OE2	2.04	0.58
2:B:682:GLU:OE1	2:B:748:ARG:HB3	2.03	0.58
2:A:167:PHE:O	2:A:170:LEU:HB2	2.04	0.58
2:A:482:LEU:HD23	2:A:482:LEU:C	2.24	0.58
2:A:862:TYR:C	2:A:862:TYR:CD2	2.77	0.58
2:B:211:ILE:HG12	2:B:438:GLU:O	2.03	0.58
2:B:377:GLU:OE2	2:B:380:ASN:HB2	2.04	0.58
2:B:410:PHE:O	2:B:416:GLU:HB3	2.04	0.58
2:B:835:GLU:OE1	2:B:921:ILE:HG13	2.03	0.58
2:A:860:ARG:NE	2:A:860:ARG:C	2.57	0.57
2:A:871:TRP:HZ3	2:A:918:VAL:HG22	1.69	0.57
2:B:467:ILE:HG13	2:B:508:CYS:HB3	1.85	0.57
2:B:860:ARG:O	2:B:860:ARG:CZ	2.52	0.57
1:C:937:C:O5'	1:C:937:C:H6	1.87	0.57
2:A:112:PRO:O	2:A:114:GLU:N	2.37	0.57
2:A:355:ILE:HG23	2:A:412:VAL:CG1	2.34	0.57
2:B:459:LYS:HZ3	2:B:461:ILE:HD13	1.70	0.57
2:B:629:PHE:O	2:B:631:GLU:N	2.29	0.57
2:A:145:ASP:OD1	2:A:145:ASP:C	2.43	0.57
2:A:404:GLU:HA	2:A:407:LYS:O	2.05	0.57
2:A:614:ILE:N	2:A:615:PRO:HD2	2.19	0.57
2:A:646:LEU:O	2:A:647:GLU:HB2	2.04	0.57
2:B:563:PHE:CE1	2:B:584:THR:HG21	2.39	0.57
2:B:727:ARG:HH11	2:B:727:ARG:HG2	1.69	0.57
2:B:831:THR:O	2:B:835:GLU:HG3	2.05	0.57
1:D:943:C:H2'	1:D:944:C:H6	1.66	0.57
2:A:42:PHE:HD1	2:A:42:PHE:O	1.87	0.57
2:B:784:ARG:O	2:B:784:ARG:HD3	2.05	0.57
2:A:348:LYS:HB3	2:A:348:LYS:HZ3	1.70	0.57
2:A:541:ILE:HB	2:A:594:MET:CE	2.34	0.57
2:B:631:GLU:HA	2:B:634:TRP:CD1	2.40	0.57
2:A:757:PHE:HD1	2:A:794:MET:SD	2.27	0.57
2:A:860:ARG:CB	2:A:966:ILE:HA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:LEU:HD12	2:B:119:PHE:CE2	2.40	0.57
2:B:541:ILE:O	2:B:545:ILE:HG12	2.05	0.57
2:B:793:LEU:CD2	2:B:821:PRO:CG	2.82	0.57
2:A:331:PHE:O	2:A:334:VAL:HG23	2.04	0.57
2:A:559:LEU:HD22	2:A:563:PHE:CE2	2.40	0.57
2:A:770:ARG:HD2	2:A:933:PHE:CD2	2.39	0.57
2:B:32:LYS:O	2:B:35:LYS:HG3	2.04	0.57
2:B:410:PHE:CE2	2:B:423:VAL:HG11	2.40	0.57
2:B:846:ILE:HG12	2:B:964:ILE:HD13	1.86	0.57
2:A:253:LYS:HD3	2:A:260:GLU:OE1	2.04	0.57
2:A:233:GLU:HA	2:A:427:ILE:CD1	2.34	0.57
2:A:551:GLU:O	2:A:553:LYS:N	2.37	0.57
2:A:804:GLU:O	2:A:807:GLU:HB3	2.05	0.57
2:B:242:TRP:CH2	2:B:332:ASP:HA	2.40	0.57
2:B:624:ASN:HD22	2:B:624:ASN:H	1.51	0.57
1:D:928:C:OP1	2:B:696:LYS:HE3	2.04	0.57
2:B:697:LEU:O	2:B:701:ILE:HG12	2.05	0.57
2:B:928:ARG:C	2:B:930:ALA:H	2.09	0.57
2:A:171:LYS:HE2	2:A:520:TRP:CE2	2.40	0.57
2:A:745:GLU:HA	2:A:745:GLU:OE2	2.05	0.57
2:B:151:TYR:CD1	2:B:156:PHE:HB2	2.40	0.57
2:A:83:THR:HG22	2:A:153:THR:HG22	1.87	0.56
2:A:256:ARG:HH11	2:A:278:ARG:HD3	1.70	0.56
2:A:920:ARG:C	2:A:922:ASN:N	2.58	0.56
2:B:239:THR:O	2:B:240:ASN:HB3	2.04	0.56
2:B:662:ILE:HG23	2:B:663:ASP:H	1.70	0.56
2:A:840:ARG:O	2:A:844:GLU:HG3	2.04	0.56
2:B:212:ILE:HD13	2:B:235:VAL:CG1	2.35	0.56
2:B:161:LYS:HD2	2:B:559:LEU:O	2.05	0.56
2:B:57:TYR:C	2:B:60:PRO:HD2	2.26	0.56
2:B:705:TYR:CD2	2:B:805:LEU:HD21	2.40	0.56
2:B:870:LYS:HE2	2:B:957:ALA:O	2.05	0.56
2:A:196:HIS:CD2	2:A:197:ASP:H	2.22	0.56
2:A:864:TYR:HD2	2:A:962:PRO:HB3	1.70	0.56
2:A:93:ARG:HG2	2:A:451:ARG:NH2	2.21	0.56
2:B:135:GLU:O	2:B:138:ILE:HG22	2.06	0.56
2:B:609:SER:O	2:B:640:VAL:HA	2.05	0.56
2:B:867:GLU:CD	2:B:867:GLU:N	2.57	0.56
2:B:918:VAL:HG11	2:B:920:ARG:HD2	1.87	0.56
2:B:95:LYS:C	2:B:97:ARG:N	2.58	0.56
2:A:877:VAL:HG22	2:A:906:ILE:HG23	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:ASP:O	2:B:390:LYS:HD3	2.05	0.56
2:B:432:LEU:HD11	2:B:439:ILE:HG13	1.87	0.56
2:A:93:ARG:HD3	2:A:451:ARG:NH2	2.20	0.56
2:A:481:ALA:O	2:A:484:ARG:N	2.34	0.56
2:B:165:TRP:HD1	2:B:561:PRO:HA	1.70	0.56
2:B:44:TYR:HE1	2:B:87:ILE:CD1	2.16	0.56
2:B:743:ALA:HB2	2:B:751:THR:HG22	1.87	0.56
2:B:725:ILE:HD13	2:B:770:ARG:NH2	2.21	0.56
2:B:884:LYS:O	2:B:887:MET:N	2.38	0.56
2:A:325:VAL:N	2:A:332:ASP:OD2	2.39	0.56
2:A:662:ILE:HG23	2:A:663:ASP:N	2.19	0.56
2:A:928:ARG:C	2:A:930:ALA:H	2.08	0.56
2:B:53:HIS:O	2:B:57:TYR:HD2	1.89	0.56
2:B:852:VAL:HG12	2:B:852:VAL:O	2.06	0.56
2:B:920:ARG:O	2:B:922:ASN:N	2.37	0.56
2:A:16:ARG:CG	2:A:16:ARG:HH11	2.19	0.56
2:A:384:ILE:HG22	2:A:385:LYS:N	2.18	0.56
2:A:45:LEU:HD21	2:A:80:TRP:HB3	1.87	0.56
2:A:825:GLU:HG2	2:A:826:GLU:HG2	1.87	0.56
2:B:272:LYS:HE2	2:B:442:GLU:OE1	2.05	0.56
2:B:236:TYR:CE2	2:B:414:PRO:HG2	2.41	0.56
2:B:742:ASN:HD22	2:B:742:ASN:N	2.03	0.56
2:B:708:ILE:HB	2:B:805:LEU:HD13	1.87	0.56
2:B:98:ASP:O	2:B:102:ILE:HG23	2.06	0.56
1:D:979:C:H2'	1:D:980:C:H6	1.71	0.56
2:A:27:ILE:N	2:A:28:ARG:NH2	2.53	0.56
2:A:771:THR:CG2	2:A:774:ARG:HD3	2.35	0.56
2:A:831:THR:O	2:A:835:GLU:HG3	2.06	0.56
2:A:884:LYS:O	2:A:887:MET:N	2.38	0.56
2:A:95:LYS:C	2:A:97:ARG:N	2.58	0.56
2:B:374:PRO:HG3	2:B:379:VAL:HG21	1.88	0.56
2:B:475:LYS:O	2:B:475:LYS:HG2	2.06	0.56
2:B:779:LYS:O	2:B:783:LEU:HD13	2.04	0.56
2:B:797:PHE:CD2	2:B:797:PHE:N	2.73	0.56
2:A:355:ILE:HD12	2:A:412:VAL:HG11	1.88	0.56
2:A:706:GLU:O	2:A:709:SER:HB2	2.06	0.56
2:A:953:LYS:NZ	2:A:953:LYS:HB3	2.19	0.56
2:A:212:ILE:HD13	2:A:235:VAL:HG12	1.88	0.56
2:A:67:LYS:CE	2:A:70:GLN:NE2	2.69	0.56
2:A:690:ARG:HH12	2:A:693:GLU:HG3	1.70	0.56
2:A:860:ARG:HH22	2:A:862:TYR:CB	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:767:TYR:HE2	2:B:783:LEU:CD1	2.19	0.56
2:A:82:ILE:HG13	2:A:153:THR:CG2	2.33	0.56
2:A:708:ILE:HD12	2:A:791:VAL:HG23	1.87	0.56
2:A:866:ALA:HB3	2:A:955:LYS:NZ	2.21	0.56
2:B:551:GLU:O	2:B:553:LYS:N	2.39	0.56
2:B:744:LEU:HD23	2:B:752:ALA:HB2	1.87	0.56
2:B:935:GLU:CD	2:B:942:ILE:H	2.09	0.56
1:C:905:G:H2'	1:C:906:G:O4'	2.06	0.56
2:A:468:ASP:C	2:A:470:GLY:H	2.08	0.55
2:A:675:LEU:HD12	2:A:697:LEU:HD21	1.88	0.55
2:A:728:TRP:O	2:A:731:HIS:N	2.38	0.55
2:A:863:ILE:HG13	2:A:945:ASN:OD1	2.05	0.55
2:B:613:LEU:O	2:B:618:LEU:HB2	2.06	0.55
2:B:746:GLU:O	2:B:748:ARG:HG3	2.06	0.55
2:B:868:ASP:O	2:B:870:LYS:N	2.39	0.55
2:A:112:PRO:HG2	2:A:115:ILE:HD12	1.87	0.55
2:A:331:PHE:HD1	2:A:334:VAL:HG21	1.72	0.55
2:B:167:PHE:O	2:B:170:LEU:HB2	2.06	0.55
2:B:727:ARG:HG2	2:B:727:ARG:NH1	2.21	0.55
2:A:198:LEU:H	2:A:198:LEU:HD12	1.70	0.55
2:A:631:GLU:HA	2:A:634:TRP:CD1	2.42	0.55
2:A:933:PHE:HD1	2:A:933:PHE:C	2.08	0.55
2:B:468:ASP:C	2:B:470:GLY:H	2.09	0.55
2:B:555:ASP:OD2	2:B:558:LYS:HE2	2.07	0.55
2:B:636:LYS:HB3	2:B:636:LYS:HZ2	1.71	0.55
2:B:920:ARG:C	2:B:922:ASN:N	2.60	0.55
1:C:920:G:OP1	1:C:920:G:H4'	2.06	0.55
2:A:349:TYR:H	2:A:349:TYR:HD1	1.55	0.55
2:A:84:GLY:O	2:A:513:GLY:HA3	2.07	0.55
2:A:644:GLY:O	2:A:650:LYS:NZ	2.38	0.55
2:A:767:TYR:HE2	2:A:783:LEU:HD13	1.70	0.55
2:A:859:LYS:CB	2:A:941:GLU:HB3	2.33	0.55
1:D:980:C:O2'	1:D:981:C:H5'	2.06	0.55
2:A:868:ASP:O	2:A:870:LYS:N	2.40	0.55
2:B:878:SER:CB	2:B:915:THR:HG22	2.36	0.55
2:A:297:ARG:HG2	2:A:304:GLU:CD	2.27	0.55
2:A:488:LEU:HA	2:A:489:PRO:C	2.27	0.55
2:B:314:ASP:HB3	2:B:317:ASN:HB3	1.88	0.55
2:B:835:GLU:O	2:B:838:PHE:HB3	2.07	0.55
2:B:847:LYS:O	2:B:851:GLU:HG3	2.06	0.55
2:A:142:PHE:C	2:A:144:VAL:H	2.11	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:884:LYS:O	2:A:886:SER:N	2.40	0.55
2:B:142:PHE:C	2:B:144:VAL:H	2.10	0.55
2:B:235:VAL:HB	2:B:300:VAL:HG11	1.88	0.55
2:B:860:ARG:C	2:B:860:ARG:CZ	2.75	0.55
2:B:884:LYS:HG2	2:B:888:GLU:OE1	2.07	0.55
2:A:469:TYR:HB3	2:A:503:LEU:HD23	1.89	0.55
2:A:567:ILE:HA	2:A:595:LYS:CD	2.28	0.55
2:A:66:PHE:CE2	2:A:70:GLN:NE2	2.69	0.55
2:B:508:CYS:O	2:B:509:ALA:HB2	2.06	0.55
2:A:555:ASP:OD2	2:A:558:LYS:HG2	2.07	0.55
2:A:733:LEU:HD11	2:A:789:VAL:HG21	1.89	0.55
2:B:489:PRO:HG3	2:B:684:ASP:OD2	2.06	0.55
2:B:537:ALA:O	2:B:540:THR:HG22	2.07	0.55
2:A:342:GLU:CG	2:A:343:THR:N	2.68	0.54
2:A:58:THR:O	2:A:62:VAL:HG23	2.07	0.54
2:A:714:TYR:CD1	2:A:780:ARG:HG2	2.42	0.54
2:A:766:TRP:CH2	2:A:836:GLU:OE1	2.60	0.54
2:B:139:ARG:CG	2:B:139:ARG:HH11	2.19	0.54
2:B:471:ASN:CG	2:B:473:GLU:HG2	2.28	0.54
2:B:84:GLY:O	2:B:513:GLY:HA3	2.07	0.54
2:B:864:TYR:HD2	2:B:962:PRO:HB3	1.72	0.54
2:A:152:THR:HG22	2:A:159:PHE:CE1	2.43	0.54
2:B:219:ASN:OD1	2:B:220:GLY:N	2.41	0.54
2:B:136:THR:HG22	2:B:661:PHE:CD2	2.41	0.54
1:D:933:G:O2'	1:D:934:A:H5'	2.07	0.54
2:A:388:LYS:HD3	2:A:389:ASP:N	2.21	0.54
2:A:480:LYS:CE	2:A:484:ARG:NH2	2.64	0.54
2:A:784:ARG:CZ	2:A:809:LEU:HD23	2.37	0.54
2:B:432:LEU:HD13	2:B:437:ALA:O	2.06	0.54
2:A:27:ILE:H	2:A:28:ARG:HH21	1.54	0.54
2:A:49:LEU:CD1	2:A:49:LEU:H	2.13	0.54
2:A:75:LEU:HD12	2:A:76:PHE:N	2.22	0.54
2:A:922:ASN:HD22	2:A:923:GLU:CA	2.18	0.54
2:B:536:MET:SD	2:B:536:MET:N	2.81	0.54
2:B:728:TRP:O	2:B:731:HIS:N	2.38	0.54
2:B:753:VAL:HG23	2:B:797:PHE:CE1	2.42	0.54
1:C:986:C:C5	2:A:181:HIS:NE2	2.72	0.54
2:A:282:VAL:HG12	2:A:283:ILE:N	2.22	0.54
2:A:623:PHE:O	2:A:626:VAL:HG22	2.08	0.54
2:A:67:LYS:HE2	2:A:70:GLN:NE2	2.23	0.54
2:A:964:ILE:HD12	2:A:965:PHE:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:LYS:HB3	2:B:175:TYR:CE2	2.43	0.54
2:B:298:ASN:HD22	2:B:299:PRO:HD2	1.71	0.54
2:B:730:LEU:HD22	2:B:827:TRP:CZ2	2.42	0.54
2:A:98:ASP:O	2:A:102:ILE:HG23	2.07	0.54
2:A:343:THR:HG23	2:A:344:GLU:HG2	1.89	0.54
2:A:377:GLU:O	2:A:378:GLU:HB2	2.07	0.54
2:A:734:ASN:OD1	2:A:823:PRO:CA	2.56	0.54
2:B:206:ILE:HG22	2:B:206:ILE:O	2.08	0.54
2:B:275:PHE:O	2:B:277:ASP:N	2.39	0.54
2:B:567:ILE:O	2:B:568:PHE:CG	2.60	0.54
2:B:729:MET:HG3	2:B:729:MET:O	2.07	0.54
2:B:757:PHE:CD1	2:B:794:MET:SD	2.99	0.54
2:A:51:VAL:HG23	2:A:52:GLY:N	2.23	0.54
2:A:560:THR:HB	2:A:561:PRO:CD	2.38	0.54
2:A:75:LEU:HD23	2:A:601:TRP:CG	2.42	0.54
2:A:724:ASP:HB2	2:A:929:GLU:OE2	2.07	0.54
2:B:48:HIS:HB2	2:B:109:TYR:HD1	1.73	0.54
2:B:213:LYS:HB3	2:B:213:LYS:NZ	2.21	0.54
2:B:226:PRO:HG3	2:B:263:TRP:CE3	2.43	0.54
2:B:343:THR:HG23	2:B:344:GLU:N	2.21	0.54
2:B:413:PRO:CB	2:B:414:PRO:HD3	2.33	0.54
2:B:50:HIS:ND1	2:B:52:GLY:N	2.56	0.54
1:D:914:A:H4'	2:B:750:ARG:HH22	1.72	0.54
1:D:960:C:O2'	1:D:961:C:OP2	2.16	0.54
2:A:67:LYS:CD	2:A:70:GLN:HE21	2.18	0.54
2:B:45:LEU:HD13	2:B:130:MET:CB	2.38	0.54
2:B:347:GLU:OE1	2:B:348:LYS:N	2.39	0.54
2:B:467:ILE:HG13	2:B:508:CYS:CB	2.37	0.54
2:B:475:LYS:HA	2:B:623:PHE:HE1	1.72	0.54
2:A:388:LYS:HD3	2:A:389:ASP:HB2	1.89	0.54
2:A:860:ARG:NH2	2:A:862:TYR:N	2.56	0.54
2:A:923:GLU:CD	2:A:923:GLU:N	2.61	0.54
2:B:188:VAL:HG23	2:B:189:VAL:N	2.16	0.54
2:B:393:LEU:HD12	2:B:396:ALA:HB3	1.88	0.54
2:B:51:VAL:HG23	2:B:659:LEU:HB3	1.89	0.54
2:B:776:ASP:OD2	2:B:778:ALA:HB3	2.08	0.54
2:B:838:PHE:O	2:B:842:VAL:HG23	2.07	0.54
2:A:150:PHE:HD1	2:A:151:TYR:O	1.91	0.54
2:A:420:VAL:HG12	2:A:424:LYS:NZ	2.23	0.54
2:A:420:VAL:C	2:A:422:GLU:H	2.12	0.54
2:A:495:GLN:HG2	2:A:614:ILE:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:609:SER:O	2:A:640:VAL:HA	2.08	0.54
2:A:62:VAL:HG21	2:A:678:MET:CE	2.38	0.54
2:A:824:VAL:CG1	2:A:827:TRP:HE3	2.20	0.54
2:A:867:GLU:N	2:A:867:GLU:CD	2.58	0.54
2:B:243:VAL:HG12	2:B:321:VAL:HG12	1.90	0.54
1:C:955:G:OP1	2:A:961:LYS:NZ	2.39	0.54
2:A:15:LYS:NZ	2:A:15:LYS:HB3	2.23	0.53
2:A:216:LEU:HB2	2:A:296:VAL:HG12	1.91	0.53
2:A:508:CYS:O	2:A:509:ALA:HB2	2.07	0.53
2:A:953:LYS:HB3	2:A:953:LYS:HZ3	1.72	0.53
2:B:55:ARG:HD2	2:B:687:PHE:CE1	2.44	0.53
2:B:710:GLN:O	2:B:712:ALA:N	2.41	0.53
2:B:871:TRP:CD1	2:B:959:PRO:HB3	2.42	0.53
1:C:985:A:H2'	1:C:986:C:C4	2.43	0.53
2:A:12:LYS:NZ	2:A:16:ARG:NH1	2.55	0.53
2:A:193:LEU:HG	2:A:197:ASP:HB2	1.90	0.53
2:B:616:ASN:HA	2:B:620:PHE:CE1	2.44	0.53
2:B:725:ILE:HD13	2:B:770:ARG:HH21	1.72	0.53
2:B:733:LEU:CD1	2:B:789:VAL:HG11	2.28	0.53
2:A:263:TRP:CH2	2:A:438:GLU:OE1	2.62	0.53
2:A:233:GLU:HB3	2:A:423:VAL:CG2	2.36	0.53
2:A:555:ASP:OD2	2:A:558:LYS:HE2	2.09	0.53
2:A:730:LEU:O	2:A:827:TRP:NE1	2.42	0.53
2:B:182:ARG:O	2:B:183:VAL:HB	2.07	0.53
2:B:235:VAL:HG23	2:B:236:TYR:N	2.23	0.53
2:B:240:ASN:HA	2:B:305:VAL:HB	1.90	0.53
2:B:729:MET:HA	2:B:729:MET:HE2	1.90	0.53
2:B:66:PHE:CG	2:B:744:LEU:HD12	2.43	0.53
2:B:855:ILE:O	2:B:856:GLU:HB2	2.07	0.53
2:A:39:THR:HG23	2:A:604:LEU:CD1	2.36	0.53
2:A:826:GLU:O	2:A:828:TRP:N	2.40	0.53
2:A:860:ARG:HB3	2:A:966:ILE:HA	1.90	0.53
2:B:166:GLN:NE2	2:B:534:ILE:HG12	2.23	0.53
2:B:42:PHE:O	2:B:42:PHE:HD1	1.91	0.53
2:B:475:LYS:O	2:B:479:ARG:NH1	2.41	0.53
2:B:966:ILE:O	2:B:967:GLU:CB	2.57	0.53
2:A:242:TRP:CD1	2:A:310:ALA:HB2	2.44	0.53
2:A:336:LEU:O	2:A:338:ASP:N	2.42	0.53
2:A:459:LYS:HG2	2:A:460:ILE:N	2.22	0.53
2:A:923:GLU:H	2:A:923:GLU:CD	2.11	0.53
2:B:461:ILE:CG2	2:B:464:GLN:HB2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:256:ARG:NH1	2:A:278:ARG:HD3	2.24	0.53
2:A:733:LEU:HD11	2:A:789:VAL:CB	2.38	0.53
2:A:884:LYS:NZ	2:A:884:LYS:HB2	2.23	0.53
2:B:253:LYS:NZ	2:B:283:ILE:HD11	2.23	0.53
2:B:340:LYS:HZ2	2:B:341:ARG:HH12	1.55	0.53
2:B:488:LEU:HA	2:B:489:PRO:C	2.29	0.53
2:B:681:ALA:N	2:B:750:ARG:HG3	2.23	0.53
2:B:797:PHE:HD2	2:B:797:PHE:H	1.56	0.53
2:B:336:LEU:O	2:B:338:ASP:N	2.42	0.53
2:B:39:THR:HG22	2:B:40:VAL:N	2.23	0.53
2:B:620:PHE:CD1	2:B:620:PHE:N	2.76	0.53
2:B:79:ALA:HB2	2:B:539:TYR:HE2	1.73	0.53
2:A:173:LYS:HD3	2:A:175:TYR:CE2	2.44	0.53
2:A:198:LEU:HD13	2:A:202:GLU:OE1	2.09	0.53
2:A:887:MET:HE2	2:A:891:MET:HG2	1.90	0.53
2:B:171:LYS:HD2	2:B:520:TRP:CZ3	2.44	0.53
2:B:384:ILE:HG22	2:B:385:LYS:N	2.20	0.53
2:B:395:GLN:HG3	2:B:396:ALA:N	2.24	0.53
2:B:66:PHE:CE2	2:B:744:LEU:HB3	2.44	0.53
2:B:884:LYS:O	2:B:886:SER:N	2.41	0.53
2:B:860:ARG:NE	2:B:942:ILE:HA	2.20	0.53
1:C:985:A:H2'	1:C:986:C:C5	2.44	0.53
2:A:235:VAL:HA	2:A:323:MET:CE	2.38	0.53
2:A:51:VAL:HG13	2:A:659:LEU:HB3	1.90	0.53
2:A:676:TYR:HB2	2:A:697:LEU:HD23	1.91	0.53
2:A:751:THR:O	2:A:752:ALA:C	2.48	0.53
2:B:44:TYR:CD1	2:B:44:TYR:C	2.82	0.53
2:B:751:THR:O	2:B:752:ALA:C	2.47	0.53
2:B:860:ARG:HA	2:B:966:ILE:HA	1.90	0.53
1:C:988:A:C5'	2:A:528:SER:OG	2.57	0.53
2:A:150:PHE:CE2	2:A:538:TYR:HD2	2.27	0.53
2:B:54:ALA:HB1	2:B:661:PHE:CE1	2.44	0.53
1:D:902:C:C2'	1:D:903:G:H5''	2.38	0.53
2:A:17:TRP:CZ3	2:A:800:HIS:CD2	2.97	0.52
2:A:136:THR:CG2	2:A:662:ILE:HB	2.39	0.52
2:B:687:PHE:C	2:B:687:PHE:CD2	2.82	0.52
2:A:241:MET:HG3	2:A:296:VAL:HG21	1.90	0.52
2:A:528:SER:OG	2:A:529:LEU:HD12	2.09	0.52
2:A:716:VAL:O	2:A:716:VAL:HG12	2.09	0.52
2:A:801:ILE:O	2:A:805:LEU:HG	2.10	0.52
2:A:766:TRP:CZ3	2:A:836:GLU:OE1	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:LEU:O	2:B:737:ILE:HG13	2.09	0.52
2:B:781:TYR:CZ	2:B:785:THR:HG21	2.44	0.52
2:B:761:MET:SD	2:B:790:TRP:HH2	2.32	0.52
2:A:662:ILE:HG23	2:A:663:ASP:H	1.74	0.52
2:A:826:GLU:OE2	2:A:826:GLU:N	2.42	0.52
2:B:703:ARG:HD2	2:B:707:LEU:CD1	2.37	0.52
2:B:782:VAL:HG12	2:B:783:LEU:HD12	1.91	0.52
2:A:188:VAL:CG2	2:A:189:VAL:H	2.07	0.52
2:B:297:ARG:NH2	2:B:297:ARG:CB	2.72	0.52
2:B:420:VAL:C	2:B:422:GLU:H	2.12	0.52
2:B:624:ASN:HD22	2:B:624:ASN:N	2.08	0.52
2:B:625:HIS:CD2	2:B:635:PRO:HD3	2.44	0.52
2:B:486:LYS:H	2:B:637:GLY:HA2	1.74	0.52
2:B:720:VAL:HG12	2:B:777:GLU:HG2	1.91	0.52
2:B:82:ILE:HG13	2:B:153:THR:HG23	1.91	0.52
2:B:83:THR:HG23	2:B:152:THR:HB	1.91	0.52
1:D:988:A:C8	2:B:529:LEU:HD21	2.44	0.52
2:A:292:ILE:HD13	2:A:307:ILE:HG22	1.91	0.52
2:A:482:LEU:CD1	2:A:500:ILE:HD11	2.38	0.52
2:B:223:ILE:HD11	2:B:264:ILE:HG13	1.92	0.52
2:B:661:PHE:CE2	2:B:665:ILE:HD11	2.44	0.52
2:B:722:LEU:H	2:B:722:LEU:HD22	1.71	0.52
2:B:723:LYS:HG3	2:B:724:ASP:N	2.24	0.52
2:A:14:GLN:O	2:A:18:LEU:HB2	2.08	0.52
2:A:234:THR:O	2:A:325:VAL:HG21	2.10	0.52
2:A:752:ALA:O	2:A:755:TRP:N	2.43	0.52
2:A:860:ARG:O	2:A:860:ARG:CZ	2.58	0.52
2:B:100:LYS:O	2:B:104:ILE:HG13	2.10	0.52
2:B:356:VAL:HG21	2:B:411:LYS:HB2	1.91	0.52
2:B:764:LEU:O	2:B:768:LEU:HG	2.08	0.52
2:A:342:GLU:N	2:A:342:GLU:OE2	2.41	0.52
2:A:355:ILE:HG22	2:A:356:VAL:N	2.21	0.52
2:B:803:GLU:HG2	2:B:815:VAL:HG12	1.92	0.52
2:A:323:MET:HG3	2:A:323:MET:O	2.08	0.52
2:B:671:ASP:OD1	2:B:799:PRO:HD2	2.10	0.52
2:B:826:GLU:O	2:B:828:TRP:N	2.42	0.52
2:A:37:TYR:HD2	2:A:38:ILE:H	1.58	0.52
2:B:241:MET:HG3	2:B:296:VAL:HG21	1.91	0.52
2:B:345:ILE:CG1	2:B:346:LEU:N	2.73	0.52
2:B:676:TYR:O	2:B:679:SER:HB3	2.10	0.52
2:A:480:LYS:HG2	2:A:484:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:GLU:CD	2:B:147:SER:HB2	2.30	0.52
2:B:233:GLU:OE2	2:B:234:THR:N	2.42	0.52
2:B:232:PRO:HD2	2:B:424:LYS:HG3	1.92	0.52
2:B:433:GLU:HA	2:B:433:GLU:OE2	2.10	0.52
2:B:558:LYS:O	2:B:584:THR:HG22	2.10	0.52
2:A:177:VAL:HG23	2:A:466:PHE:HB2	1.92	0.51
2:A:864:TYR:CG	2:A:865:THR:N	2.77	0.51
2:B:266:SER:HB3	2:B:269:ALA:CB	2.41	0.51
2:B:44:TYR:C	2:B:44:TYR:HD1	2.14	0.51
2:B:956:GLN:HG2	2:B:956:GLN:O	2.09	0.51
2:A:326:PRO:HA	2:A:332:ASP:CB	2.40	0.51
2:A:373:PHE:HD1	2:A:374:PRO:HD3	1.68	0.51
2:A:496:PHE:HE1	2:A:614:ILE:CG1	2.18	0.51
2:A:486:LYS:H	2:A:637:GLY:HA2	1.75	0.51
2:A:860:ARG:CZ	2:A:861:ALA:HA	2.39	0.51
2:A:44:TYR:OH	2:A:87:ILE:HG12	2.09	0.51
2:B:273:LEU:HA	2:B:276:GLN:HG3	1.92	0.51
2:B:35:LYS:HB2	2:B:601:TRP:HZ3	1.75	0.51
2:B:834:ALA:O	2:B:837:GLU:OE2	2.29	0.51
2:B:915:THR:O	2:B:916:PHE:HD2	1.93	0.51
2:A:36:PHE:O	2:A:36:PHE:CD2	2.64	0.51
2:A:555:ASP:HB3	2:A:558:LYS:HG2	1.93	0.51
2:A:65:ARG:O	2:A:68:ARG:N	2.44	0.51
2:A:672:VAL:HG21	2:A:698:ARG:HG3	1.93	0.51
2:A:789:VAL:O	2:A:790:TRP:C	2.49	0.51
2:B:427:ILE:HG22	2:B:431:MET:SD	2.50	0.51
2:B:679:SER:O	2:B:750:ARG:HG2	2.10	0.51
2:B:863:ILE:HG22	2:B:953:LYS:HG2	1.92	0.51
2:A:102:ILE:HD12	2:A:102:ILE:C	2.30	0.51
2:A:148:ARG:NH1	2:A:597:GLU:OE1	2.43	0.51
2:B:235:VAL:HG23	2:B:236:TYR:H	1.76	0.51
2:B:62:VAL:HG21	2:B:678:MET:CE	2.39	0.51
2:A:488:LEU:HD22	2:A:683:HIS:HE1	1.75	0.51
2:A:722:LEU:HD23	2:A:722:LEU:O	2.10	0.51
2:B:789:VAL:O	2:B:790:TRP:C	2.49	0.51
2:B:913:GLU:O	2:B:914:ARG:O	2.29	0.51
2:B:946:PRO:HG2	2:B:953:LYS:HE2	1.92	0.51
2:A:268:GLU:O	2:A:271:TYR:HB3	2.11	0.51
2:A:306:ILE:CG1	2:A:307:ILE:N	2.74	0.51
2:A:423:VAL:C	2:A:425:GLU:N	2.64	0.51
2:A:53:HIS:O	2:A:57:TYR:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:630:ARG:O	2:A:632:GLU:N	2.38	0.51
2:B:297:ARG:CB	2:B:297:ARG:HH21	2.24	0.51
2:B:391:GLU:HG3	2:B:394:GLU:HB2	1.93	0.51
2:B:67:LYS:HE3	2:B:72:TYR:CE1	2.45	0.51
2:B:717:LYS:O	2:B:717:LYS:HD3	2.11	0.51
2:B:678:MET:CE	2:B:749:THR:HG21	2.40	0.51
2:B:44:TYR:OH	2:B:86:PRO:HD2	2.11	0.51
2:A:480:LYS:HA	2:A:483:GLU:OE1	2.11	0.51
2:A:803:GLU:OE1	2:A:815:VAL:HG23	2.11	0.51
2:B:547:LYS:O	2:B:550:GLN:HB3	2.10	0.51
2:B:636:LYS:HB3	2:B:636:LYS:NZ	2.25	0.51
2:B:870:LYS:O	2:B:872:LYS:N	2.43	0.51
2:A:268:GLU:H	2:A:268:GLU:CD	2.12	0.51
2:A:51:VAL:O	2:A:54:ALA:CB	2.56	0.51
2:A:860:ARG:CZ	2:A:861:ALA:CA	2.89	0.51
2:A:913:GLU:O	2:A:914:ARG:O	2.29	0.51
2:B:45:LEU:HD13	2:B:130:MET:HA	1.92	0.51
2:B:793:LEU:HD23	2:B:821:PRO:HG3	1.93	0.51
1:C:916:C:O2'	1:C:972:U:H1'	2.10	0.51
1:D:961:C:H2'	1:D:961:C:O2	2.10	0.51
2:A:112:PRO:CG	2:A:115:ILE:HD12	2.41	0.51
2:A:168:TRP:NE1	2:A:519:PRO:HB2	2.25	0.51
2:A:239:THR:HG21	2:A:326:PRO:HD2	1.92	0.51
2:A:690:ARG:HH11	2:A:693:GLU:CG	2.20	0.51
2:A:838:PHE:HE2	2:A:922:ASN:ND2	2.09	0.51
2:A:93:ARG:HG3	2:A:93:ARG:HH11	1.74	0.51
2:A:95:LYS:O	2:A:97:ARG:N	2.44	0.51
2:B:630:ARG:O	2:B:632:GLU:N	2.41	0.51
2:B:742:ASN:O	2:B:743:ALA:C	2.49	0.51
1:C:949:C:C2	1:C:957:G:N2	2.79	0.51
2:A:819:LYS:H	2:A:819:LYS:CD	2.24	0.51
2:A:873:VAL:CG1	2:A:906:ILE:HG12	2.40	0.51
2:A:871:TRP:NE1	2:A:959:PRO:HB3	2.26	0.51
2:B:200:GLU:HG2	2:B:201:GLY:N	2.26	0.51
2:B:860:ARG:CB	2:B:966:ILE:HA	2.41	0.51
2:A:332:ASP:O	2:A:333:HIS:HB2	2.11	0.50
2:A:490:GLU:OE1	2:A:493:ARG:HB2	2.11	0.50
2:A:751:THR:O	2:A:754:GLN:N	2.43	0.50
2:A:919:LYS:HD2	2:A:960:LEU:HD13	1.93	0.50
2:B:915:THR:OG1	2:B:916:PHE:N	2.44	0.50
1:D:902:C:H2'	1:D:903:G:H5''	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:217:ARG:HH21	2:A:222:VAL:CG1	2.24	0.50
2:A:269:ALA:O	2:A:273:LEU:HD12	2.10	0.50
2:A:880:LYS:HG3	2:A:886:SER:HA	1.92	0.50
2:A:950:LYS:H	2:A:953:LYS:NZ	2.10	0.50
2:B:160:SER:O	2:B:164:GLU:HG3	2.11	0.50
2:B:51:VAL:CG2	2:B:659:LEU:HB3	2.41	0.50
2:B:743:ALA:HB2	2:B:751:THR:CG2	2.41	0.50
2:A:135:GLU:O	2:A:138:ILE:HG22	2.11	0.50
2:A:676:TYR:HA	2:A:697:LEU:CD2	2.41	0.50
2:A:793:LEU:HD23	2:A:821:PRO:CG	2.41	0.50
2:B:210:ILE:C	2:B:210:ILE:HD12	2.31	0.50
2:B:148:ARG:HB3	2:B:542:SER:HB3	1.93	0.50
2:B:540:THR:HG21	2:B:598:PHE:HD1	1.76	0.50
2:B:51:VAL:CG2	2:B:659:LEU:HD23	2.40	0.50
2:B:51:VAL:HG21	2:B:659:LEU:HD23	1.92	0.50
2:B:730:LEU:HB3	2:B:827:TRP:CD1	2.46	0.50
2:A:172:GLU:OE1	2:A:172:GLU:N	2.45	0.50
2:A:240:ASN:O	2:A:324:SER:HB3	2.11	0.50
2:A:275:PHE:O	2:A:277:ASP:N	2.39	0.50
2:A:41:ALA:HA	2:A:607:ARG:HH22	1.75	0.50
2:A:884:LYS:HG3	2:A:888:GLU:HG3	1.93	0.50
2:A:871:TRP:CD2	2:A:920:ARG:NH2	2.78	0.50
2:B:94:ILE:HD11	2:B:120:GLU:N	2.27	0.50
2:B:242:TRP:HH2	2:B:332:ASP:HA	1.75	0.50
2:B:395:GLN:O	2:B:399:THR:HG23	2.10	0.50
2:B:910:LEU:C	2:B:910:LEU:HD13	2.32	0.50
1:C:941:A:O3'	2:A:699:LYS:NZ	2.32	0.50
2:A:235:VAL:HG23	2:A:236:TYR:N	2.26	0.50
2:A:354:ARG:HE	2:A:375:ALA:C	2.13	0.50
2:A:381:LYS:C	2:A:381:LYS:NZ	2.64	0.50
2:B:495:GLN:HG2	2:B:614:ILE:HG21	1.92	0.50
2:B:782:VAL:HG12	2:B:783:LEU:N	2.26	0.50
2:A:413:PRO:CB	2:A:414:PRO:HD3	2.42	0.50
2:A:61:ASP:OD1	2:A:143:SER:N	2.25	0.50
2:A:72:TYR:O	2:A:74:VAL:HG23	2.11	0.50
2:B:244:ASN:HB2	2:B:313:VAL:HG23	1.94	0.50
2:B:327:ALA:HB2	2:B:353:PRO:O	2.12	0.50
2:A:231:ARG:HB3	2:A:233:GLU:CD	2.32	0.50
2:A:389:ASP:O	2:A:390:LYS:HD3	2.12	0.50
2:A:235:VAL:HG11	2:A:431:MET:CE	2.42	0.50
2:A:781:TYR:O	2:A:785:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:817:LEU:HD23	2:A:817:LEU:N	2.27	0.50
2:A:862:TYR:OH	2:A:926:ALA:HB1	2.11	0.50
2:A:863:ILE:CB	2:A:953:LYS:HD3	2.41	0.50
2:A:98:ASP:OD2	2:A:99:PRO:HD2	2.11	0.50
2:B:196:HIS:CD2	2:B:197:ASP:H	2.30	0.50
2:B:482:LEU:HD11	2:B:496:PHE:HB3	1.94	0.50
2:B:587:PRO:HB2	2:B:590:ILE:CG1	2.35	0.50
2:A:235:VAL:HG23	2:A:236:TYR:H	1.76	0.50
2:A:300:VAL:HG13	2:A:301:SER:N	2.27	0.50
2:A:425:GLU:O	2:A:429:LYS:HD3	2.11	0.50
2:A:569:LEU:HD12	2:A:569:LEU:N	2.26	0.50
2:A:931:LYS:HE2	2:A:942:ILE:HG22	1.92	0.50
2:A:947:THR:HG23	2:A:948:GLU:H	1.77	0.50
2:A:860:ARG:HA	2:A:966:ILE:HA	1.93	0.50
2:A:252:ALA:HB2	2:A:282:VAL:HA	1.94	0.50
2:A:292:ILE:HG13	2:A:309:PRO:HB3	1.94	0.50
2:A:382:LEU:C	2:A:384:ILE:H	2.15	0.50
2:A:232:PRO:HD2	2:A:424:LYS:HG3	1.93	0.50
2:A:474:TRP:NE1	2:A:627:ALA:HB2	2.27	0.50
2:A:855:ILE:HG23	2:A:855:ILE:O	2.10	0.50
2:B:866:ALA:HB3	2:B:869:TRP:CD1	2.47	0.50
1:C:909:U:H5''	1:C:910:G:OP2	2.12	0.50
2:A:393:LEU:C	2:A:395:GLN:H	2.15	0.49
2:A:568:PHE:HD1	2:A:598:PHE:CE2	2.30	0.49
2:A:79:ALA:HB2	2:A:539:TYR:HE2	1.76	0.49
2:A:85:SER:H	2:A:86:PRO:HD3	1.78	0.49
2:B:268:GLU:OE2	2:B:315:PRO:HB2	2.11	0.49
2:B:330:PRO:CD	2:B:400:ILE:HG12	2.42	0.49
2:B:49:LEU:HA	2:B:53:HIS:HD2	1.77	0.49
2:B:871:TRP:CE3	2:B:920:ARG:NH1	2.80	0.49
2:B:921:ILE:HD12	2:B:928:ARG:NH2	2.27	0.49
1:C:916:C:C5'	1:C:917:C:C5	2.86	0.49
2:A:45:LEU:HD13	2:A:130:MET:HB2	1.94	0.49
2:A:142:PHE:O	2:A:144:VAL:N	2.45	0.49
2:A:870:LYS:O	2:A:872:LYS:N	2.44	0.49
2:A:924:GLU:OE1	2:A:927:LEU:HD22	2.13	0.49
2:B:175:TYR:CE1	2:B:474:TRP:HB2	2.47	0.49
2:B:185:TRP:CD1	2:B:186:ASP:N	2.81	0.49
2:B:587:PRO:O	2:B:591:ILE:HG12	2.12	0.49
2:B:966:ILE:O	2:B:966:ILE:HG13	2.12	0.49
2:A:111:VAL:HG22	2:A:128:TYR:CE2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:41:ALA:HB2	2:A:607:ARG:HH21	1.76	0.49
2:A:697:LEU:O	2:A:701:ILE:HG12	2.12	0.49
2:A:878:SER:CB	2:A:915:THR:HG22	2.42	0.49
2:B:196:HIS:HD2	2:B:197:ASP:H	1.58	0.49
2:B:282:VAL:CG1	2:B:283:ILE:N	2.72	0.49
2:B:662:ILE:HG23	2:B:663:ASP:N	2.25	0.49
2:A:616:ASN:HB2	2:A:620:PHE:CE2	2.47	0.49
2:A:717:LYS:HD2	2:A:777:GLU:OE2	2.12	0.49
2:A:894:SER:C	2:A:896:ILE:N	2.65	0.49
2:B:297:ARG:CZ	2:B:297:ARG:HB3	2.41	0.49
2:B:354:ARG:HD2	2:B:376:VAL:HG12	1.95	0.49
2:B:42:PHE:O	2:B:42:PHE:CD1	2.65	0.49
2:B:455:ARG:HG2	2:B:455:ARG:HH11	1.78	0.49
2:B:746:GLU:OE1	2:B:748:ARG:HD2	2.13	0.49
2:B:846:ILE:HD12	2:B:938:LEU:HD21	1.94	0.49
2:B:907:VAL:O	2:B:910:LEU:HB3	2.12	0.49
2:B:95:LYS:O	2:B:97:ARG:N	2.45	0.49
2:A:467:ILE:HG21	2:A:469:TYR:CZ	2.47	0.49
2:A:691:ARG:CG	2:A:691:ARG:HH11	2.26	0.49
2:B:185:TRP:HZ2	2:B:190:GLY:HA2	1.75	0.49
2:B:273:LEU:HB3	2:B:280:ILE:HD11	1.94	0.49
2:B:423:VAL:C	2:B:425:GLU:N	2.66	0.49
1:C:958:U:H6	1:C:958:U:H3'	1.78	0.49
2:A:218:GLU:HG3	2:A:219:ASN:N	2.28	0.49
2:B:488:LEU:HD12	2:B:606:TRP:CZ3	2.46	0.49
2:B:79:ALA:O	2:B:80:TRP:CE3	2.65	0.49
2:B:741:THR:HA	2:B:820:TRP:CH2	2.47	0.49
2:B:724:ASP:HB2	2:B:929:GLU:OE2	2.11	0.49
2:A:214:PHE:CE2	2:A:298:ASN:HA	2.48	0.49
2:A:240:ASN:HA	2:A:305:VAL:HB	1.93	0.49
2:A:66:PHE:CZ	2:A:70:GLN:OE1	2.66	0.49
2:A:730:LEU:HD22	2:A:827:TRP:HZ2	1.78	0.49
2:A:947:THR:CG2	2:A:948:GLU:N	2.75	0.49
2:B:298:ASN:HD22	2:B:299:PRO:CD	2.25	0.49
2:B:889:GLU:O	2:B:889:GLU:HG3	2.11	0.49
2:A:184:ARG:NH1	2:A:195:ASP:OD2	2.46	0.49
2:A:184:ARG:NH2	2:A:202:GLU:O	2.45	0.49
2:A:691:ARG:HG2	2:A:691:ARG:NH1	2.26	0.49
2:A:871:TRP:CZ3	2:A:918:VAL:HA	2.47	0.49
2:B:151:TYR:CE1	2:B:156:PHE:HD1	2.30	0.49
2:B:163:ILE:O	2:B:166:GLN:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:LEU:C	2:B:395:GLN:H	2.16	0.49
2:B:474:TRP:CZ2	2:B:623:PHE:HB3	2.47	0.49
2:B:22:ILE:CG1	2:B:817:LEU:HD21	2.42	0.49
1:C:910:G:C6	1:C:911:C:N4	2.81	0.49
1:C:941:A:H2'	1:C:942:U:C6	2.48	0.49
2:A:227:ALA:CA	2:A:321:VAL:HG23	2.31	0.49
2:A:826:GLU:CD	2:A:826:GLU:N	2.63	0.49
2:B:172:GLU:N	2:B:172:GLU:OE1	2.46	0.49
2:B:212:ILE:HD13	2:B:431:MET:HE1	1.94	0.49
2:B:213:LYS:HZ2	2:B:213:LYS:HB3	1.77	0.49
2:B:540:THR:HG21	2:B:598:PHE:HB2	1.93	0.49
2:B:751:THR:O	2:B:754:GLN:N	2.45	0.49
2:B:860:ARG:HH22	2:B:861:ALA:C	2.16	0.49
2:B:922:ASN:O	2:B:925:LYS:N	2.44	0.49
1:D:935:C:H5'	1:D:936:U:H5''	1.95	0.49
2:A:196:HIS:CD2	2:A:197:ASP:N	2.81	0.49
2:A:237:GLY:C	2:A:325:VAL:HG22	2.33	0.49
2:A:311:GLU:HG2	2:A:389:ASP:OD2	2.12	0.49
2:A:840:ARG:O	2:A:843:MET:HB2	2.12	0.49
2:B:37:TYR:HD2	2:B:38:ILE:H	1.60	0.49
2:B:45:LEU:HD13	2:B:130:MET:HB2	1.95	0.49
2:B:760:ILE:HD12	2:B:790:TRP:CD1	2.48	0.49
2:B:868:ASP:O	2:B:869:TRP:C	2.52	0.49
2:A:355:ILE:HD12	2:A:412:VAL:CG1	2.43	0.48
2:A:570:GLU:O	2:A:595:LYS:HE2	2.13	0.48
2:A:782:VAL:HG12	2:A:783:LEU:N	2.28	0.48
2:A:836:GLU:HA	2:A:839:ILE:HD11	1.94	0.48
2:B:166:GLN:CG	2:B:534:ILE:HD11	2.43	0.48
2:B:256:ARG:CZ	2:B:277:ASP:OD2	2.61	0.48
2:B:65:ARG:O	2:B:68:ARG:N	2.46	0.48
2:B:676:TYR:CZ	2:B:680:LEU:HD11	2.48	0.48
2:B:728:TRP:C	2:B:730:LEU:N	2.67	0.48
2:B:834:ALA:O	2:B:837:GLU:CD	2.52	0.48
2:A:65:ARG:HG2	2:A:143:SER:OG	2.13	0.48
2:A:165:TRP:CD1	2:A:561:PRO:HA	2.44	0.48
2:A:880:LYS:HG3	2:A:886:SER:HB3	1.95	0.48
2:A:933:PHE:HD1	2:A:933:PHE:O	1.95	0.48
2:B:282:VAL:CG1	2:B:283:ILE:H	2.25	0.48
2:B:375:ALA:O	2:B:377:GLU:N	2.40	0.48
2:B:389:ASP:C	2:B:390:LYS:HD3	2.33	0.48
2:B:67:LYS:HD2	2:B:70:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:953:A:O2'	2:B:849:ILE:HG23	2.12	0.48
2:A:126:VAL:CG1	2:A:126:VAL:O	2.60	0.48
2:A:289:GLU:O	2:A:292:ILE:HB	2.13	0.48
2:A:242:TRP:HZ3	2:A:332:ASP:CG	2.17	0.48
2:A:388:LYS:CD	2:A:389:ASP:HB2	2.42	0.48
2:A:467:ILE:HG13	2:A:508:CYS:CB	2.43	0.48
2:A:488:LEU:CD1	2:A:606:TRP:CH2	2.92	0.48
2:A:931:LYS:HE2	2:A:942:ILE:O	2.13	0.48
2:B:275:PHE:C	2:B:277:ASP:H	2.17	0.48
2:B:35:LYS:HD2	2:B:35:LYS:C	2.34	0.48
2:B:382:LEU:C	2:B:384:ILE:H	2.16	0.48
2:B:496:PHE:CE1	2:B:614:ILE:HG23	2.49	0.48
2:B:614:ILE:N	2:B:615:PRO:CD	2.75	0.48
2:B:741:THR:O	2:B:745:GLU:HG2	2.13	0.48
2:A:170:LEU:O	2:A:176:ILE:HG12	2.13	0.48
2:A:227:ALA:HA	2:A:321:VAL:O	2.12	0.48
2:A:256:ARG:HG3	2:A:257:LYS:H	1.78	0.48
2:A:42:PHE:CD1	2:A:42:PHE:O	2.66	0.48
2:A:501:ASP:O	2:A:503:LEU:N	2.39	0.48
2:A:725:ILE:CD1	2:A:770:ARG:HE	2.26	0.48
2:A:784:ARG:HH22	2:A:810:GLY:N	2.11	0.48
2:A:871:TRP:C	2:A:875:GLU:OE2	2.52	0.48
2:B:256:ARG:HG3	2:B:257:LYS:N	2.28	0.48
2:B:340:LYS:HB3	2:B:341:ARG:HH11	1.77	0.48
2:B:351:ILE:CD1	2:B:351:ILE:H	2.16	0.48
2:B:429:LYS:O	2:B:433:GLU:CG	2.52	0.48
2:B:505:LYS:HD2	2:B:505:LYS:H	1.78	0.48
2:B:601:TRP:HA	2:B:601:TRP:CE3	2.48	0.48
2:B:677:ILE:HG22	2:B:678:MET:N	2.28	0.48
2:B:775:ASP:C	2:B:775:ASP:OD1	2.51	0.48
2:B:79:ALA:N	2:B:539:TYR:OH	2.46	0.48
2:B:42:PHE:CD1	2:B:81:HIS:HB2	2.49	0.48
1:C:954:G:N2	2:A:961:LYS:HG3	2.29	0.48
2:A:631:GLU:C	2:A:633:HIS:H	2.16	0.48
2:A:742:ASN:O	2:A:743:ALA:C	2.51	0.48
2:A:725:ILE:HD13	2:A:770:ARG:HE	1.78	0.48
2:A:855:ILE:HG13	2:A:856:GLU:HG2	1.95	0.48
2:A:964:ILE:HD11	2:A:966:ILE:HG23	1.96	0.48
2:B:327:ALA:HB1	2:B:354:ARG:CB	2.44	0.48
2:B:37:TYR:CD2	2:B:38:ILE:N	2.82	0.48
2:B:501:ASP:O	2:B:503:LEU:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:ILE:HG23	2:B:623:PHE:CZ	2.49	0.48
2:B:752:ALA:O	2:B:755:TRP:N	2.46	0.48
2:B:894:SER:C	2:B:896:ILE:N	2.66	0.48
1:C:916:C:H2'	1:C:972:U:O3'	2.12	0.48
2:A:162:PHE:HA	2:A:564:PHE:CE2	2.49	0.48
2:A:198:LEU:HD22	2:A:202:GLU:CA	2.43	0.48
2:A:41:ALA:CA	2:A:607:ARG:NH2	2.77	0.48
2:A:705:TYR:CD2	2:A:805:LEU:HD11	2.48	0.48
2:B:126:VAL:O	2:B:126:VAL:CG1	2.61	0.48
2:B:354:ARG:HD2	2:B:376:VAL:CG1	2.42	0.48
2:B:377:GLU:O	2:B:378:GLU:HB2	2.13	0.48
2:B:464:GLN:NE2	2:B:507:ALA:HB1	2.28	0.48
2:B:732:ARG:HH11	2:B:732:ARG:HB3	1.77	0.48
1:D:917:C:O5'	1:D:917:C:H6	1.96	0.48
2:A:449:ILE:N	2:A:449:ILE:CD1	2.75	0.48
2:A:892:LYS:O	2:A:892:LYS:HG2	2.13	0.48
2:B:471:ASN:C	2:B:471:ASN:ND2	2.66	0.48
2:A:860:ARG:CZ	2:A:860:ARG:C	2.82	0.48
2:A:868:ASP:O	2:A:869:TRP:C	2.52	0.48
2:B:48:HIS:HB2	2:B:109:TYR:CD1	2.48	0.48
2:B:171:LYS:CG	2:B:176:ILE:HD12	2.42	0.48
2:B:345:ILE:O	2:B:346:LEU:HB2	2.13	0.48
2:B:356:VAL:HB	2:B:409:ILE:O	2.14	0.48
2:B:423:VAL:HA	2:B:426:ALA:HB3	1.95	0.48
2:B:623:PHE:O	2:B:624:ASN:C	2.52	0.48
1:C:920:G:H1'	1:C:969:G:H21	1.78	0.48
1:D:958:U:O5'	1:D:958:U:H6	1.97	0.48
1:C:941:A:H4'	2:A:699:LYS:NZ	2.29	0.48
2:A:792:ARG:CG	2:A:792:ARG:HH21	2.15	0.48
2:A:860:ARG:NH2	2:A:861:ALA:C	2.67	0.48
2:B:112:PRO:O	2:B:113:GLU:C	2.52	0.48
2:B:420:VAL:HG12	2:B:424:LYS:NZ	2.28	0.48
2:B:198:LEU:HD23	2:B:448:VAL:HG13	1.95	0.48
2:B:560:THR:HB	2:B:561:PRO:HD2	1.95	0.48
2:B:53:HIS:O	2:B:57:TYR:CD2	2.67	0.48
2:B:732:ARG:HB3	2:B:732:ARG:NH1	2.29	0.48
2:B:894:SER:O	2:B:896:ILE:N	2.47	0.48
1:D:970:A:O2'	1:D:971:A:O5'	2.32	0.48
2:A:953:LYS:NZ	2:A:953:LYS:CB	2.76	0.48
2:A:956:GLN:HG2	2:A:956:GLN:O	2.14	0.48
2:B:710:GLN:O	2:B:713:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:188:VAL:HG23	2:A:190:GLY:H	1.79	0.47
2:A:419:PRO:O	2:A:422:GLU:HB2	2.14	0.47
2:A:55:ARG:O	2:A:59:ILE:HG13	2.14	0.47
2:A:846:ILE:O	2:A:850:ILE:HG13	2.14	0.47
2:A:877:VAL:C	2:A:879:GLU:H	2.16	0.47
2:B:276:GLN:O	2:B:277:ASP:HB3	2.14	0.47
2:B:568:PHE:C	2:B:569:LEU:HD12	2.34	0.47
2:B:793:LEU:HD23	2:B:821:PRO:CG	2.44	0.47
2:A:279:GLU:OE1	2:A:281:GLU:OE1	2.32	0.47
2:A:671:ASP:OD1	2:A:799:PRO:HD2	2.13	0.47
2:A:717:LYS:HD2	2:A:718:GLY:O	2.14	0.47
2:A:827:TRP:O	2:A:827:TRP:HD1	1.95	0.47
2:A:770:ARG:CD	2:A:933:PHE:HE2	2.19	0.47
2:B:233:GLU:HA	2:B:427:ILE:CD1	2.33	0.47
2:B:646:LEU:HD12	2:B:689:TRP:HB3	1.96	0.47
2:B:704:PHE:HE1	2:B:790:TRP:CD2	2.31	0.47
1:C:958:U:H3'	1:C:958:U:C6	2.49	0.47
1:D:984:C:H6	1:D:984:C:H5'	1.79	0.47
2:A:112:PRO:O	2:A:113:GLU:C	2.53	0.47
1:C:986:C:H5	2:A:181:HIS:HE2	1.56	0.47
2:A:375:ALA:O	2:A:377:GLU:N	2.40	0.47
2:A:714:TYR:HD1	2:A:780:ARG:CG	2.27	0.47
2:A:746:GLU:O	2:A:748:ARG:HG3	2.14	0.47
2:A:767:TYR:CE2	2:A:782:VAL:HG11	2.49	0.47
2:A:42:PHE:CE1	2:A:81:HIS:HB2	2.48	0.47
2:A:854:LYS:HE2	2:A:967:GLU:CD	2.34	0.47
2:B:340:LYS:CB	2:B:341:ARG:HH11	2.28	0.47
2:B:68:ARG:HB2	2:B:74:VAL:HG11	1.96	0.47
2:B:701:ILE:O	2:B:704:PHE:HB3	2.13	0.47
2:A:145:ASP:OD1	2:A:145:ASP:O	2.32	0.47
2:A:238:VAL:HA	2:A:325:VAL:HG22	1.96	0.47
2:A:37:TYR:HD2	2:A:38:ILE:N	2.12	0.47
2:A:53:HIS:O	2:A:57:TYR:CD2	2.67	0.47
2:A:568:PHE:HB2	2:A:569:LEU:HD12	1.96	0.47
2:A:695:GLY:O	2:A:698:ARG:HB3	2.15	0.47
2:B:326:PRO:HA	2:B:332:ASP:CB	2.44	0.47
2:B:725:ILE:CD1	2:B:770:ARG:HE	2.27	0.47
2:B:734:ASN:HD21	2:B:823:PRO:HA	1.75	0.47
1:C:922:C:H4'	1:C:923:A:C5'	2.44	0.47
2:A:198:LEU:CD2	2:A:202:GLU:HA	2.44	0.47
2:A:609:SER:OG	2:A:610:GLY:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:710:GLN:C	2:A:712:ALA:N	2.68	0.47
2:A:964:ILE:CD1	2:A:966:ILE:HG23	2.45	0.47
2:B:400:ILE:C	2:B:400:ILE:HD12	2.34	0.47
2:B:729:MET:HE3	2:B:763:ASP:C	2.35	0.47
2:A:12:LYS:HZ2	2:A:16:ARG:NH1	2.12	0.47
2:A:267:LYS:O	2:A:270:ALA:HB3	2.14	0.47
2:A:546:ASN:O	2:A:550:GLN:HB2	2.14	0.47
2:A:871:TRP:CH2	2:A:919:LYS:HE3	2.47	0.47
2:A:922:ASN:O	2:A:925:LYS:N	2.47	0.47
2:A:942:ILE:C	2:A:943:ILE:HG13	2.35	0.47
2:A:944:ILE:HG22	2:A:945:ASN:H	1.78	0.47
2:B:277:ASP:O	2:B:277:ASP:CG	2.50	0.47
2:B:45:LEU:HD13	2:B:130:MET:CA	2.45	0.47
2:B:58:THR:HG22	2:B:678:MET:HE1	1.96	0.47
2:B:830:GLU:HG3	2:B:831:THR:N	2.29	0.47
2:B:85:SER:N	2:B:86:PRO:CD	2.77	0.47
2:A:318:ALA:HA	2:A:440:MET:SD	2.55	0.47
2:A:75:LEU:CD1	2:A:77:PRO:HD3	2.44	0.47
2:A:866:ALA:HB3	2:A:955:LYS:HZ1	1.78	0.47
2:B:83:THR:CG2	2:B:153:THR:HG22	2.44	0.47
2:B:216:LEU:CD1	2:B:294:LYS:HB3	2.43	0.47
2:B:256:ARG:CG	2:B:257:LYS:H	2.23	0.47
2:B:393:LEU:HG	2:B:397:THR:OG1	2.14	0.47
2:B:395:GLN:HG3	2:B:396:ALA:H	1.80	0.47
2:B:540:THR:HG21	2:B:598:PHE:CD1	2.50	0.47
2:B:860:ARG:NH1	2:B:861:ALA:HA	2.30	0.47
2:B:862:TYR:HB3	2:B:964:ILE:HB	1.95	0.47
2:A:518:LEU:HD12	2:A:524:TRP:CB	2.44	0.47
2:A:835:GLU:O	2:A:838:PHE:HB3	2.15	0.47
2:A:877:VAL:CG2	2:A:906:ILE:HG23	2.45	0.47
2:A:894:SER:O	2:A:896:ILE:N	2.47	0.47
2:A:99:PRO:O	2:A:102:ILE:HG13	2.14	0.47
2:B:150:PHE:CD1	2:B:151:TYR:O	2.58	0.47
2:B:212:ILE:CD1	2:B:235:VAL:CG1	2.93	0.47
2:B:554:LEU:HD12	2:B:586:ILE:HD11	1.97	0.47
2:B:864:TYR:CG	2:B:865:THR:N	2.82	0.47
2:B:951:GLY:HA3	2:B:965:PHE:CE1	2.49	0.47
2:A:241:MET:HG3	2:A:296:VAL:CG2	2.45	0.47
2:A:348:LYS:HB3	2:A:348:LYS:HZ2	1.77	0.47
2:A:423:VAL:HA	2:A:426:ALA:HB3	1.96	0.47
2:A:558:LYS:HB3	2:A:584:THR:CA	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:728:TRP:C	2:A:730:LEU:N	2.68	0.47
2:A:767:TYR:HE2	2:A:783:LEU:HD11	1.79	0.47
2:A:830:GLU:HG3	2:A:831:THR:N	2.30	0.47
2:B:135:GLU:HA	2:B:138:ILE:HG22	1.97	0.47
2:B:238:VAL:O	2:B:238:VAL:HG13	2.15	0.47
2:B:519:PRO:HG2	2:B:520:TRP:CE3	2.49	0.47
2:B:690:ARG:HB2	2:B:693:GLU:HG3	1.97	0.47
1:C:957:G:O2'	1:C:958:U:H5'	2.15	0.47
1:C:919:G:C6	1:C:969:G:C6	3.03	0.47
2:A:16:ARG:CG	2:A:16:ARG:NH1	2.77	0.47
2:A:314:ASP:HB3	2:A:317:ASN:HB3	1.95	0.47
2:A:327:ALA:HB2	2:A:353:PRO:O	2.15	0.47
2:A:210:ILE:HG22	2:A:439:ILE:HG23	1.97	0.47
2:A:461:ILE:HG21	2:A:464:GLN:HB2	1.97	0.47
2:A:59:ILE:HB	2:A:60:PRO:CD	2.45	0.47
2:A:747:PHE:CD1	2:A:747:PHE:N	2.83	0.47
2:A:825:GLU:OE2	2:A:825:GLU:O	2.33	0.47
2:A:860:ARG:O	2:A:860:ARG:NH1	2.47	0.47
2:A:880:LYS:HG3	2:A:886:SER:CA	2.45	0.47
2:B:402:LYS:O	2:B:405:TYR:HB3	2.15	0.47
2:B:793:LEU:HD21	2:B:821:PRO:CG	2.43	0.47
2:B:958:MET:HE1	2:B:959:PRO:HD2	1.95	0.47
1:D:914:A:H2'	1:D:915:G:O4'	2.15	0.47
2:A:168:TRP:CE2	2:A:519:PRO:HB2	2.49	0.47
2:A:215:GLU:O	2:A:296:VAL:HA	2.15	0.47
2:A:354:ARG:HH11	2:A:354:ARG:HG3	1.80	0.47
2:A:544:HIS:H	2:A:544:HIS:HD2	1.59	0.47
2:A:576:LYS:O	2:A:580:LEU:HD13	2.15	0.47
2:A:800:HIS:O	2:A:802:CYS:N	2.48	0.47
2:A:93:ARG:O	2:A:98:ASP:HB2	2.15	0.47
2:B:167:PHE:HA	2:B:170:LEU:CG	2.44	0.47
2:B:521:ASP:N	2:B:522:PRO:HD3	2.30	0.47
2:B:63:ILE:O	2:B:67:LYS:HG2	2.15	0.47
2:A:243:VAL:HG22	2:A:292:ILE:HD11	1.95	0.46
2:A:275:PHE:C	2:A:277:ASP:H	2.18	0.46
2:A:331:PHE:CD1	2:A:334:VAL:HG21	2.51	0.46
2:A:587:PRO:O	2:A:591:ILE:HG12	2.15	0.46
2:A:75:LEU:HD23	2:A:601:TRP:CE2	2.50	0.46
2:B:164:GLU:O	2:B:165:TRP:C	2.54	0.46
2:B:259:LYS:HE2	2:B:261:GLU:OE1	2.15	0.46
2:B:482:LEU:CD1	2:B:496:PHE:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:980:C:H2'	1:D:981:C:H6	1.79	0.46
2:A:196:HIS:HD2	2:A:197:ASP:H	1.64	0.46
2:A:213:LYS:HB3	2:A:213:LYS:NZ	2.30	0.46
2:A:238:VAL:HG11	2:A:298:ASN:HB2	1.97	0.46
2:A:268:GLU:HG3	2:A:316:ASP:HA	1.97	0.46
2:A:381:LYS:HZ2	2:A:382:LEU:HD12	1.80	0.46
2:A:457:VAL:HG23	2:A:458:ILE:N	2.31	0.46
2:A:544:HIS:O	2:A:547:LYS:HB3	2.14	0.46
2:A:626:VAL:HG12	2:A:634:TRP:CE2	2.50	0.46
2:A:772:GLU:OE1	2:A:936:LYS:HE3	2.15	0.46
2:B:495:GLN:HE21	2:B:614:ILE:CG2	2.27	0.46
2:B:558:LYS:HG3	2:B:584:THR:O	2.14	0.46
2:B:698:ARG:HG3	2:B:698:ARG:HH11	1.80	0.46
2:B:733:LEU:CD1	2:B:737:ILE:HD11	2.45	0.46
2:B:766:TRP:HH2	2:B:836:GLU:OE1	1.97	0.46
2:B:45:LEU:CD1	2:B:80:TRP:HB3	2.40	0.46
1:D:953:A:C2	2:B:966:ILE:HG12	2.50	0.46
2:B:860:ARG:CB	2:B:966:ILE:HG22	2.40	0.46
2:A:150:PHE:CD1	2:A:150:PHE:C	2.88	0.46
2:A:164:GLU:O	2:A:165:TRP:C	2.53	0.46
2:A:42:PHE:CE1	2:A:81:HIS:CG	3.04	0.46
2:A:768:LEU:O	2:A:769:ARG:C	2.53	0.46
2:B:418:LYS:HB3	2:B:419:PRO:HD2	1.97	0.46
2:B:436:ILE:O	2:B:436:ILE:HG22	2.16	0.46
2:B:546:ASN:O	2:B:550:GLN:HB2	2.15	0.46
2:B:616:ASN:HD22	2:B:617:HIS:H	1.60	0.46
2:B:67:LYS:O	2:B:72:TYR:HD1	1.99	0.46
2:B:829:ASN:OD1	2:B:832:ILE:HG13	2.16	0.46
2:B:834:ALA:CA	2:B:837:GLU:OE2	2.60	0.46
2:B:933:PHE:CD1	2:B:933:PHE:C	2.89	0.46
2:A:204:VAL:O	2:A:204:VAL:HG23	2.16	0.46
2:A:297:ARG:HB3	2:A:297:ARG:CZ	2.45	0.46
2:A:355:ILE:HG23	2:A:412:VAL:HG11	1.97	0.46
2:A:412:VAL:HG23	2:A:414:PRO:CD	2.39	0.46
2:A:717:LYS:NZ	2:A:719:ASN:HB2	2.29	0.46
2:A:933:PHE:HE1	2:A:937:GLU:HB2	1.81	0.46
2:B:418:LYS:HG3	2:B:422:GLU:OE2	2.16	0.46
2:A:210:ILE:HD11	2:A:232:PRO:CG	2.37	0.46
2:A:393:LEU:C	2:A:395:GLN:N	2.69	0.46
2:A:455:ARG:HD3	2:A:456:ALA:N	2.30	0.46
2:A:728:TRP:CE3	2:A:729:MET:N	2.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:809:LEU:O	2:A:810:GLY:C	2.54	0.46
2:A:918:VAL:HG11	2:A:920:ARG:HD2	1.97	0.46
2:A:327:ALA:HB1	2:A:354:ARG:CB	2.46	0.46
2:A:50:HIS:H	2:A:53:HIS:CD2	2.34	0.46
2:A:860:ARG:NH1	2:A:861:ALA:CA	2.69	0.46
2:A:911:ILE:O	2:A:911:ILE:HG13	2.15	0.46
2:B:204:VAL:HG11	2:B:443:PHE:HB3	1.97	0.46
2:B:238:VAL:HB	2:B:323:MET:HE1	1.96	0.46
2:B:722:LEU:HG	2:B:727:ARG:NH1	2.31	0.46
1:C:956:G:O2'	1:C:957:G:H5'	2.16	0.46
2:A:356:VAL:HB	2:A:409:ILE:O	2.16	0.46
2:A:678:MET:N	2:A:678:MET:SD	2.88	0.46
2:A:872:LYS:HA	2:A:875:GLU:OE2	2.15	0.46
2:B:789:VAL:O	2:B:791:VAL:N	2.49	0.46
2:B:789:VAL:O	2:B:792:ARG:N	2.49	0.46
2:B:734:ASN:ND2	2:B:824:VAL:H	1.94	0.46
1:D:954:G:O6	2:B:963:ALA:HA	2.16	0.46
2:A:183:VAL:HG13	2:A:184:ARG:O	2.16	0.46
2:A:424:LYS:NZ	2:A:424:LYS:HB2	2.31	0.46
2:A:93:ARG:HG2	2:A:451:ARG:HH21	1.80	0.46
2:A:806:TRP:CB	2:A:815:VAL:HG22	2.45	0.46
2:A:863:ILE:HG22	2:A:953:LYS:CG	2.44	0.46
2:B:459:LYS:HZ2	2:B:461:ILE:CD1	2.29	0.46
2:B:557:GLU:O	2:B:559:LEU:N	2.49	0.46
2:B:631:GLU:C	2:B:633:HIS:H	2.17	0.46
2:B:65:ARG:O	2:B:68:ARG:HB3	2.16	0.46
2:B:717:LYS:C	2:B:717:LYS:HD3	2.36	0.46
2:B:722:LEU:N	2:B:722:LEU:HD23	2.30	0.46
2:B:824:VAL:O	2:B:825:GLU:C	2.53	0.46
2:B:839:ILE:C	2:B:839:ILE:HD12	2.36	0.46
2:B:877:VAL:C	2:B:879:GLU:H	2.18	0.46
2:B:918:VAL:CG1	2:B:920:ARG:HD2	2.46	0.46
2:A:232:PRO:HG2	2:A:428:ALA:HB2	1.98	0.46
2:A:64:ALA:O	2:A:68:ARG:HB2	2.16	0.46
2:A:731:HIS:HD2	2:A:828:TRP:HA	1.80	0.46
2:B:328:HIS:O	2:B:329:ALA:C	2.53	0.46
2:B:476:GLU:HA	2:B:476:GLU:OE1	2.16	0.46
2:B:710:GLN:C	2:B:712:ALA:N	2.69	0.46
2:A:159:PHE:O	2:A:162:PHE:HB3	2.16	0.46
2:A:173:LYS:HB3	2:A:175:TYR:CE2	2.51	0.46
2:A:230:LEU:N	2:A:230:LEU:CD2	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:382:LEU:HD12	2:A:382:LEU:N	2.31	0.46
2:A:395:GLN:HG3	2:A:396:ALA:H	1.81	0.46
2:A:489:PRO:HD3	2:A:683:HIS:HB3	1.98	0.46
2:A:624:ASN:HD22	2:A:624:ASN:N	2.07	0.46
2:A:660:ASN:HB2	2:A:663:ASP:HB2	1.94	0.46
2:B:234:THR:O	2:B:325:VAL:HG21	2.16	0.46
2:B:516:THR:O	2:B:526:ILE:HG13	2.15	0.46
2:B:641:ASN:ND2	2:B:641:ASN:C	2.69	0.46
2:B:70:GLN:HB3	2:B:72:TYR:CD1	2.51	0.46
2:A:183:VAL:O	2:A:184:ARG:C	2.54	0.45
2:A:297:ARG:O	2:A:299:PRO:HD3	2.16	0.45
2:A:393:LEU:O	2:A:395:GLN:N	2.49	0.45
2:A:545:ILE:HG12	2:A:594:MET:HE3	1.98	0.45
2:A:903:VAL:HG12	2:A:906:ILE:HG13	1.97	0.45
2:B:231:ARG:HB3	2:B:233:GLU:OE2	2.17	0.45
2:B:882:ASP:O	2:B:883:PHE:HB3	2.15	0.45
1:C:949:C:C2	1:C:957:G:C2	3.04	0.45
2:A:51:VAL:CG2	2:A:52:GLY:N	2.79	0.45
2:A:741:THR:O	2:A:745:GLU:HG2	2.17	0.45
2:A:855:ILE:O	2:A:856:GLU:HB2	2.15	0.45
2:B:292:ILE:HG13	2:B:309:PRO:HB3	1.98	0.45
2:B:505:LYS:HD2	2:B:505:LYS:N	2.30	0.45
2:B:914:ARG:HE	2:B:915:THR:N	2.13	0.45
2:A:186:ASP:HB3	2:A:191:THR:CG2	2.41	0.45
2:A:23:PHE:CD2	2:A:143:SER:HA	2.51	0.45
2:A:328:HIS:O	2:A:329:ALA:C	2.54	0.45
2:A:166:GLN:HB2	2:A:534:ILE:HD11	1.97	0.45
2:A:950:LYS:HG2	2:A:953:LYS:HZ1	1.82	0.45
2:B:535:TYR:CE1	2:B:536:MET:SD	3.10	0.45
2:B:9:ILE:HD13	2:B:804:GLU:HG2	1.97	0.45
2:B:928:ARG:C	2:B:930:ALA:N	2.69	0.45
1:D:919:G:H1'	1:D:970:A:C2	2.52	0.45
2:A:155:LEU:C	2:A:157:PRO:HD3	2.37	0.45
2:A:211:ILE:HG21	2:A:319:THR:CG2	2.46	0.45
2:A:464:GLN:NE2	2:A:465:TRP:O	2.49	0.45
2:A:61:ASP:OD2	2:A:674:ARG:NH2	2.45	0.45
2:A:742:ASN:O	2:A:744:LEU:N	2.50	0.45
2:B:412:VAL:H	2:B:416:GLU:HG2	1.82	0.45
2:B:485:MET:SD	2:B:635:PRO:HB2	2.57	0.45
2:B:136:THR:CG2	2:B:661:PHE:HD2	2.26	0.45
1:C:918:U:H2'	1:C:918:U:O2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:905:G:H5'	1:D:905:G:H8	1.82	0.45
2:A:17:TRP:CZ2	2:A:803:GLU:HG3	2.52	0.45
2:B:266:SER:O	2:B:269:ALA:HB3	2.16	0.45
2:B:306:ILE:HG12	2:B:307:ILE:N	2.31	0.45
2:B:411:LYS:HA	2:B:416:GLU:CD	2.37	0.45
2:B:676:TYR:HA	2:B:697:LEU:CD2	2.46	0.45
2:B:729:MET:CE	2:B:729:MET:HA	2.47	0.45
2:B:953:LYS:HB3	2:B:953:LYS:NZ	2.30	0.45
2:A:294:LYS:N	2:A:294:LYS:HD2	2.32	0.45
2:A:377:GLU:C	2:A:377:GLU:CD	2.75	0.45
2:A:544:HIS:CD2	2:A:544:HIS:N	2.85	0.45
2:A:582:LYS:H	2:A:582:LYS:HD2	1.81	0.45
2:A:713:GLU:O	2:A:714:TYR:C	2.53	0.45
2:A:838:PHE:HE2	2:A:922:ASN:HD21	1.63	0.45
2:B:142:PHE:O	2:B:144:VAL:N	2.49	0.45
2:B:231:ARG:HB3	2:B:233:GLU:CD	2.37	0.45
2:B:342:GLU:OE2	2:B:342:GLU:N	2.50	0.45
2:B:393:LEU:C	2:B:395:GLN:N	2.70	0.45
2:B:393:LEU:CD1	2:B:396:ALA:HB3	2.46	0.45
2:B:713:GLU:CA	2:B:713:GLU:OE2	2.65	0.45
2:B:711:PHE:HE1	2:B:783:LEU:HD23	1.82	0.45
1:D:944:C:H2'	1:D:945:C:H6	1.81	0.45
2:A:80:TRP:CD1	2:A:130:MET:HG3	2.51	0.45
2:A:557:GLU:O	2:A:559:LEU:N	2.49	0.45
2:B:123:ILE:HD11	2:B:155:LEU:CD1	2.47	0.45
2:B:252:ALA:HB2	2:B:282:VAL:HA	1.99	0.45
2:B:232:PRO:HG2	2:B:428:ALA:HB2	1.99	0.45
2:B:55:ARG:HD2	2:B:687:PHE:CD1	2.51	0.45
2:B:730:LEU:HA	2:B:730:LEU:HD23	1.84	0.45
2:B:742:ASN:O	2:B:745:GLU:N	2.50	0.45
2:B:83:THR:HG22	2:B:153:THR:HG22	1.97	0.45
2:B:921:ILE:HB	2:B:928:ARG:HH22	1.77	0.45
1:C:960:C:H4'	1:C:961:C:OP2	2.17	0.45
2:A:112:PRO:HB2	2:A:115:ILE:HG13	1.99	0.45
2:A:210:ILE:O	2:A:210:ILE:HG13	2.16	0.45
2:A:211:ILE:HG21	2:A:319:THR:HG21	1.99	0.45
2:A:218:GLU:OE2	2:A:294:LYS:HE2	2.16	0.45
2:A:211:ILE:HA	2:A:227:ALA:O	2.17	0.45
2:A:341:ARG:HG2	2:A:341:ARG:HH11	1.81	0.45
2:A:426:ALA:HA	2:A:429:LYS:CE	2.31	0.45
2:A:277:ASP:HB2	2:A:460:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:717:LYS:C	2:A:717:LYS:CD	2.83	0.45
2:A:93:ARG:HG3	2:A:93:ARG:NH1	2.32	0.45
2:B:51:VAL:O	2:B:54:ALA:CB	2.62	0.45
2:B:54:ALA:CB	2:B:661:PHE:CD1	3.00	0.45
2:A:266:SER:O	2:A:269:ALA:HB3	2.17	0.45
2:A:482:LEU:C	2:A:482:LEU:CD2	2.85	0.45
2:A:61:ASP:OD2	2:A:674:ARG:NH1	2.48	0.45
2:A:831:THR:O	2:A:835:GLU:CG	2.65	0.45
2:A:840:ARG:HE	2:A:840:ARG:HB3	1.60	0.45
2:B:227:ALA:HA	2:B:321:VAL:O	2.15	0.45
2:B:245:PRO:O	2:B:288:GLY:HA3	2.17	0.45
2:B:387:GLN:HE21	2:B:387:GLN:HA	1.82	0.45
2:B:387:GLN:HG3	2:B:388:LYS:N	2.32	0.45
2:B:766:TRP:HZ3	2:B:836:GLU:CG	2.30	0.45
2:B:7:LYS:HZ3	2:B:7:LYS:HB2	1.81	0.45
2:B:731:HIS:HE1	2:B:833:GLU:OE1	2.00	0.45
2:B:950:LYS:H	2:B:953:LYS:NZ	2.15	0.45
1:C:916:C:H5'	1:C:917:C:H5	1.66	0.45
1:C:939:A:H4'	1:C:939:A:OP1	2.16	0.45
1:D:921:U:OP2	1:D:922:C:H3'	2.17	0.45
2:A:250:VAL:HG12	2:A:285:GLU:HG3	1.99	0.45
2:A:463:ASP:O	2:A:464:GLN:C	2.55	0.45
2:A:568:PHE:CB	2:A:569:LEU:HD12	2.46	0.45
2:A:728:TRP:HE3	2:A:729:MET:CA	2.29	0.45
2:B:28:ARG:HG3	2:B:28:ARG:NH1	2.30	0.45
2:B:713:GLU:O	2:B:714:TYR:C	2.55	0.45
2:B:682:GLU:OE1	2:B:748:ARG:NH1	2.49	0.45
2:B:890:LEU:O	2:B:892:LYS:N	2.50	0.45
2:B:911:ILE:O	2:B:911:ILE:HG13	2.16	0.45
2:A:94:ILE:HD11	2:A:120:GLU:CA	2.46	0.44
2:A:518:LEU:HD12	2:A:524:TRP:HB3	1.98	0.44
2:A:553:LYS:NZ	2:A:553:LYS:HB3	2.32	0.44
2:A:800:HIS:C	2:A:802:CYS:N	2.70	0.44
2:A:800:HIS:C	2:A:802:CYS:H	2.21	0.44
2:A:902:GLU:C	2:A:904:ALA:H	2.21	0.44
2:A:916:PHE:HB3	2:A:917:ASP:H	1.67	0.44
2:B:373:PHE:N	2:B:374:PRO:CD	2.80	0.44
2:B:860:ARG:HB3	2:B:966:ILE:CG2	2.40	0.44
1:D:960:C:H4'	1:D:961:C:H5''	1.98	0.44
2:A:26:ASN:C	2:A:28:ARG:HH21	2.20	0.44
2:A:67:LYS:HE2	2:A:70:GLN:HE22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:GLU:O	2:B:296:VAL:HA	2.17	0.44
2:B:429:LYS:HZ2	2:B:429:LYS:HB3	1.82	0.44
2:B:42:PHE:N	2:B:42:PHE:CD1	2.85	0.44
2:B:511:LYS:HE3	2:B:524:TRP:CE2	2.51	0.44
2:B:714:TYR:CD2	2:B:714:TYR:N	2.73	0.44
2:A:119:PHE:C	2:A:121:ASP:N	2.69	0.44
2:A:31:PRO:HD2	2:A:34:LYS:HG3	1.98	0.44
2:A:482:LEU:O	2:A:493:ARG:NH1	2.50	0.44
2:A:69:MET:HB3	2:A:818:ALA:O	2.17	0.44
2:A:768:LEU:O	2:A:770:ARG:N	2.49	0.44
2:A:85:SER:N	2:A:86:PRO:CD	2.77	0.44
2:B:170:LEU:CB	2:B:176:ILE:HD11	2.41	0.44
2:B:211:ILE:O	2:B:211:ILE:HG13	2.16	0.44
2:B:234:THR:HA	2:B:355:ILE:CD1	2.47	0.44
2:B:476:GLU:HA	2:B:479:ARG:NH1	2.32	0.44
2:B:57:TYR:O	2:B:60:PRO:CG	2.62	0.44
2:B:809:LEU:O	2:B:810:GLY:C	2.56	0.44
2:B:860:ARG:O	2:B:860:ARG:NH1	2.50	0.44
2:B:902:GLU:C	2:B:904:ALA:H	2.21	0.44
2:A:234:THR:HB	2:A:325:VAL:HG21	1.99	0.44
2:A:400:ILE:HD12	2:A:400:ILE:C	2.37	0.44
2:A:432:LEU:HD11	2:A:439:ILE:CG1	2.45	0.44
2:A:730:LEU:CA	2:A:827:TRP:HE1	2.30	0.44
2:A:766:TRP:O	2:A:770:ARG:N	2.47	0.44
2:B:150:PHE:C	2:B:150:PHE:CD1	2.90	0.44
2:B:186:ASP:OD2	2:B:188:VAL:HG13	2.18	0.44
2:B:518:LEU:HD22	2:B:520:TRP:CZ2	2.52	0.44
2:B:742:ASN:ND2	2:B:742:ASN:N	2.65	0.44
2:A:703:ARG:HG2	2:A:761:MET:CE	2.48	0.44
2:A:872:LYS:HA	2:A:872:LYS:HZ2	1.83	0.44
2:A:878:SER:HB2	2:A:914:ARG:HB2	1.99	0.44
2:A:933:PHE:CE1	2:A:937:GLU:HB2	2.51	0.44
2:B:340:LYS:HG2	2:B:341:ARG:NH1	2.32	0.44
2:B:490:GLU:C	2:B:492:ARG:H	2.21	0.44
2:B:718:GLY:O	2:B:720:VAL:HG13	2.18	0.44
2:B:750:ARG:HB3	2:B:750:ARG:HE	1.50	0.44
2:B:679:SER:HA	2:B:753:VAL:HG11	2.00	0.44
2:B:783:LEU:N	2:B:783:LEU:HD12	2.33	0.44
2:B:846:ILE:HG12	2:B:964:ILE:HD12	1.94	0.44
2:B:866:ALA:H	2:B:955:LYS:HZ1	1.57	0.44
2:A:518:LEU:HD22	2:A:520:TRP:CZ2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:789:VAL:O	2:A:791:VAL:N	2.50	0.44
2:B:216:LEU:O	2:B:216:LEU:HG	2.17	0.44
2:B:393:LEU:O	2:B:395:GLN:N	2.51	0.44
2:B:330:PRO:HD3	2:B:400:ILE:HG12	2.00	0.44
2:B:725:ILE:HG21	2:B:771:THR:HG21	1.99	0.44
2:B:768:LEU:O	2:B:769:ARG:C	2.55	0.44
1:D:902:C:H2'	1:D:903:G:C4'	2.47	0.44
1:D:972:U:H5''	1:D:973:C:OP2	2.18	0.44
2:A:244:ASN:HB2	2:A:313:VAL:HG23	1.99	0.44
2:A:50:HIS:CE1	2:A:53:HIS:CE1	3.06	0.44
2:A:862:TYR:HB2	2:A:964:ILE:HA	1.99	0.44
2:B:218:GLU:CD	2:B:219:ASN:ND2	2.70	0.44
2:B:261:GLU:HB2	2:B:263:TRP:HE1	1.81	0.44
2:B:339:LEU:HD13	2:B:339:LEU:N	2.33	0.44
2:B:449:ILE:HG23	2:B:454:ASN:O	2.18	0.44
2:B:908:GLN:HE22	2:B:958:MET:HG3	1.83	0.44
1:C:957:G:C2	1:C:958:U:C2	3.06	0.44
2:A:863:ILE:CG2	2:A:953:LYS:HD3	2.48	0.44
2:B:168:TRP:NE1	2:B:519:PRO:HB2	2.33	0.44
2:B:250:VAL:HG12	2:B:285:GLU:HG3	2.00	0.44
2:B:463:ASP:O	2:B:464:GLN:C	2.56	0.44
2:B:75:LEU:HD22	2:B:601:TRP:CD1	2.53	0.44
2:B:104:ILE:HG21	2:B:653:LYS:HD3	1.99	0.44
2:B:729:MET:HE2	2:B:729:MET:HB2	1.78	0.44
1:D:937:C:H2'	1:D:937:C:O2	2.18	0.44
2:A:243:VAL:HG23	2:A:244:ASN:N	2.33	0.44
2:A:803:GLU:HA	2:A:815:VAL:HG21	1.98	0.44
2:B:331:PHE:O	2:B:334:VAL:HG23	2.17	0.44
2:B:58:THR:HA	2:B:142:PHE:HE1	1.83	0.44
2:B:739:GLU:HB3	2:B:755:TRP:CD1	2.53	0.44
2:B:79:ALA:HB2	2:B:539:TYR:CE2	2.51	0.44
1:D:953:A:H1'	2:B:849:ILE:CG2	2.48	0.44
2:A:49:LEU:HD22	2:A:137:PHE:HE1	1.83	0.43
2:A:238:VAL:HG13	2:A:238:VAL:O	2.16	0.43
2:A:245:PRO:O	2:A:288:GLY:HA3	2.18	0.43
2:A:636:LYS:HB3	2:A:636:LYS:NZ	2.32	0.43
2:A:703:ARG:HG3	2:A:707:LEU:CD1	2.47	0.43
2:A:767:TYR:CE2	2:A:783:LEU:HD11	2.52	0.43
2:A:824:VAL:CG1	2:A:827:TRP:CE3	3.00	0.43
2:A:966:ILE:HG13	2:A:966:ILE:O	2.17	0.43
2:B:267:LYS:O	2:B:270:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:459:LYS:HZ2	2:B:461:ILE:HD13	1.82	0.43
2:B:57:TYR:O	2:B:60:PRO:HD2	2.17	0.43
2:B:724:ASP:OD2	2:B:928:ARG:HD3	2.18	0.43
2:B:738:LYS:HB3	2:B:738:LYS:NZ	2.33	0.43
2:B:711:PHE:CE1	2:B:783:LEU:HD23	2.53	0.43
1:C:937:C:H2'	1:C:938:A:O4'	2.18	0.43
1:C:941:A:H4'	2:A:699:LYS:HZ1	1.82	0.43
1:C:958:U:C3'	1:C:958:U:C6	3.01	0.43
1:C:972:U:H5'	1:C:973:C:OP2	2.18	0.43
1:D:923:A:HO2'	1:D:924:A:P	2.40	0.43
2:A:381:LYS:HZ2	2:A:381:LYS:HB3	1.83	0.43
2:A:420:VAL:HG12	2:A:424:LYS:HZ1	1.82	0.43
2:A:83:THR:O	2:A:528:SER:HB3	2.17	0.43
2:A:677:ILE:HD11	2:A:689:TRP:HZ3	1.83	0.43
2:A:675:LEU:CD1	2:A:697:LEU:HD21	2.48	0.43
2:A:701:ILE:O	2:A:704:PHE:HB3	2.16	0.43
2:A:81:HIS:HD2	2:A:152:THR:HG21	1.83	0.43
2:A:890:LEU:O	2:A:892:LYS:N	2.51	0.43
2:A:921:ILE:O	2:A:924:GLU:HB3	2.17	0.43
2:B:331:PHE:HD1	2:B:334:VAL:HG21	1.83	0.43
2:B:355:ILE:HG23	2:B:412:VAL:CG1	2.49	0.43
2:B:742:ASN:O	2:B:744:LEU:N	2.51	0.43
2:A:244:ASN:HD22	2:A:313:VAL:HG23	1.82	0.43
2:A:490:GLU:C	2:A:492:ARG:H	2.22	0.43
2:A:166:GLN:NE2	2:A:534:ILE:HG12	2.33	0.43
2:A:58:THR:HG22	2:A:62:VAL:CG2	2.49	0.43
2:A:75:LEU:CD1	2:A:75:LEU:C	2.84	0.43
2:A:824:VAL:HB	2:A:827:TRP:CE3	2.53	0.43
2:B:188:VAL:HG23	2:B:190:GLY:H	1.84	0.43
2:B:339:LEU:HD22	2:B:340:LYS:HG3	2.00	0.43
2:B:449:ILE:HG22	2:B:450:SER:N	2.33	0.43
2:B:618:LEU:HA	2:B:618:LEU:HD23	1.88	0.43
2:B:911:ILE:O	2:B:912:LYS:HG3	2.18	0.43
2:A:919:LYS:H	2:A:919:LYS:HE2	1.82	0.43
2:B:163:ILE:HA	2:B:163:ILE:HD13	1.92	0.43
2:B:210:ILE:HG22	2:B:439:ILE:HG12	1.99	0.43
2:B:373:PHE:N	2:B:373:PHE:CD1	2.86	0.43
2:B:412:VAL:HG23	2:B:414:PRO:HD2	2.00	0.43
2:B:577:GLU:OE1	2:B:592:HIS:HB2	2.18	0.43
2:B:644:GLY:HA2	2:B:687:PHE:O	2.18	0.43
2:B:860:ARG:HH12	2:B:861:ALA:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:877:VAL:HG22	2:B:906:ILE:HG23	2.01	0.43
1:C:985:A:H61	2:A:504:ASP:CB	2.24	0.43
1:D:917:C:C2	1:D:918:U:C5	3.06	0.43
2:A:446:LYS:HD2	2:A:446:LYS:H	1.84	0.43
2:A:460:ILE:HD12	2:A:460:ILE:N	2.33	0.43
1:C:988:A:N7	2:A:529:LEU:HD21	2.33	0.43
2:A:623:PHE:O	2:A:624:ASN:C	2.56	0.43
2:A:884:LYS:C	2:A:886:SER:N	2.72	0.43
2:B:119:PHE:C	2:B:121:ASP:N	2.70	0.43
2:B:310:ALA:HB1	2:B:312:PHE:CE1	2.53	0.43
2:A:183:VAL:CG1	2:A:183:VAL:O	2.65	0.43
2:A:27:ILE:HG12	2:A:28:ARG:CZ	2.49	0.43
2:A:330:PRO:CD	2:A:400:ILE:HG12	2.48	0.43
2:A:508:CYS:O	2:A:508:CYS:SG	2.77	0.43
2:A:45:LEU:CD1	2:A:80:TRP:HB3	2.47	0.43
2:B:114:GLU:OE1	2:B:114:GLU:HA	2.18	0.43
2:B:198:LEU:H	2:B:198:LEU:CD1	2.29	0.43
2:B:340:LYS:CE	2:B:341:ARG:HH12	2.32	0.43
2:B:401:TYR:OH	2:B:424:LYS:HE3	2.19	0.43
2:B:171:LYS:HD2	2:B:520:TRP:CE3	2.54	0.43
2:B:62:VAL:HG21	2:B:678:MET:HE2	1.98	0.43
1:C:964:G:O2'	1:C:965:G:H5'	2.18	0.43
2:A:138:ILE:HD12	2:A:138:ILE:HA	1.87	0.43
2:A:273:LEU:HD21	2:A:440:MET:HG3	2.00	0.43
2:A:703:ARG:O	2:A:707:LEU:HD12	2.18	0.43
2:A:728:TRP:O	2:A:730:LEU:N	2.51	0.43
2:A:960:LEU:CD2	2:A:960:LEU:N	2.81	0.43
1:C:955:G:P	2:A:961:LYS:HZ3	2.40	0.43
2:B:45:LEU:HD11	2:B:130:MET:HG3	2.00	0.43
2:B:183:VAL:O	2:B:184:ARG:C	2.57	0.43
2:B:211:ILE:HA	2:B:227:ALA:O	2.19	0.43
2:B:546:ASN:HA	2:B:546:ASN:HD22	1.59	0.43
2:B:573:SER:HB2	2:B:576:LYS:HG2	2.00	0.43
2:B:922:ASN:ND2	2:B:923:GLU:N	2.63	0.43
2:B:923:GLU:HB2	2:B:945:ASN:HD21	1.84	0.43
2:A:128:TYR:O	2:A:128:TYR:CD1	2.71	0.43
2:A:198:LEU:HD22	2:A:202:GLU:CB	2.49	0.43
2:A:36:PHE:O	2:A:38:ILE:HG22	2.18	0.43
2:A:742:ASN:O	2:A:745:GLU:N	2.52	0.43
2:A:94:ILE:HD12	2:A:94:ILE:C	2.39	0.43
2:B:173:LYS:HD2	2:B:175:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:GLU:O	2:B:219:ASN:C	2.56	0.43
2:B:337:GLU:HG2	2:B:337:GLU:O	2.18	0.43
2:B:379:VAL:O	2:B:383:GLY:HA3	2.19	0.43
2:B:481:ALA:O	2:B:484:ARG:N	2.34	0.43
1:C:986:C:O3'	2:A:510:ARG:HD2	2.19	0.43
1:D:976:C:O2'	1:D:977:G:H5'	2.18	0.43
2:A:182:ARG:O	2:A:183:VAL:CB	2.66	0.43
2:A:246:ASN:OD1	2:A:247:ALA:N	2.52	0.43
2:A:380:ASN:O	2:A:384:ILE:HG13	2.19	0.43
2:A:37:TYR:CE2	2:A:39:THR:CG2	3.01	0.43
2:A:566:TYR:OH	2:A:572:PHE:HD1	2.01	0.43
2:B:25:PRO:HD2	2:B:145:ASP:OD2	2.19	0.43
2:B:273:LEU:CB	2:B:280:ILE:HD11	2.49	0.43
2:B:33:GLU:N	2:B:33:GLU:OE2	2.39	0.43
2:B:343:THR:HG23	2:B:344:GLU:HG2	2.00	0.43
2:B:539:TYR:HA	2:B:542:SER:HB2	2.01	0.43
2:B:646:LEU:O	2:B:647:GLU:HB2	2.19	0.43
2:B:728:TRP:HZ3	2:B:729:MET:CE	2.32	0.43
2:B:803:GLU:CG	2:B:815:VAL:HG12	2.49	0.43
2:B:864:TYR:OH	2:B:871:TRP:HZ2	2.02	0.43
2:B:953:LYS:O	2:B:954:LYS:C	2.57	0.43
1:D:969:G:O2'	1:D:970:A:H5'	2.18	0.43
2:A:231:ARG:O	2:A:234:THR:OG1	2.36	0.43
2:A:214:PHE:HA	2:A:299:PRO:CG	2.49	0.43
2:A:511:LYS:HE2	2:A:524:TRP:CE2	2.53	0.43
2:A:544:HIS:HE1	2:A:593:GLU:OE2	2.01	0.43
2:B:231:ARG:O	2:B:234:THR:OG1	2.37	0.43
2:B:471:ASN:OD1	2:B:473:GLU:HG2	2.18	0.43
2:B:560:THR:O	2:B:563:PHE:HB3	2.19	0.43
2:B:98:ASP:OD2	2:B:99:PRO:HD2	2.19	0.43
2:A:184:ARG:HD3	2:A:198:LEU:HD21	2.01	0.42
2:A:232:PRO:O	2:A:427:ILE:HG21	2.19	0.42
2:A:311:GLU:OE2	2:A:335:ALA:HB2	2.19	0.42
2:A:384:ILE:CG2	2:A:385:LYS:H	2.19	0.42
2:A:198:LEU:HD23	2:A:448:VAL:HG13	2.01	0.42
2:A:470:GLY:O	2:A:471:ASN:C	2.57	0.42
2:A:475:LYS:HE3	2:A:500:ILE:O	2.19	0.42
2:A:521:ASP:N	2:A:522:PRO:HD3	2.34	0.42
2:A:884:LYS:HZ3	2:A:884:LYS:HB2	1.82	0.42
2:B:223:ILE:HG23	2:B:223:ILE:O	2.19	0.42
2:B:22:ILE:HA	2:B:22:ILE:HD12	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:PHE:HB2	2:B:374:PRO:HD3	2.02	0.42
2:B:374:PRO:HG3	2:B:379:VAL:CG2	2.49	0.42
2:B:614:ILE:HA	2:B:618:LEU:HB2	2.01	0.42
2:B:698:ARG:O	2:B:701:ILE:HB	2.18	0.42
2:B:680:LEU:C	2:B:750:ARG:HG3	2.39	0.42
2:B:737:ILE:HG22	2:B:823:PRO:HD3	2.00	0.42
2:B:840:ARG:O	2:B:844:GLU:HG3	2.18	0.42
1:C:941:A:H2'	1:C:942:U:H6	1.84	0.42
1:C:964:G:N2	1:C:975:C:C2	2.86	0.42
1:D:920:G:H5''	1:D:921:U:C5	2.48	0.42
2:A:314:ASP:HA	2:A:315:PRO:HD3	1.89	0.42
2:A:675:LEU:CD1	2:A:697:LEU:HD11	2.48	0.42
2:A:714:TYR:N	2:A:714:TYR:CD2	2.88	0.42
2:A:786:LEU:C	2:A:786:LEU:HD23	2.40	0.42
2:A:854:LYS:HG3	2:A:855:ILE:H	1.83	0.42
2:A:890:LEU:C	2:A:892:LYS:N	2.72	0.42
2:A:959:PRO:C	2:A:960:LEU:CD2	2.87	0.42
2:B:355:ILE:CG2	2:B:410:PHE:CE1	3.02	0.42
2:B:54:ALA:HB2	2:B:661:PHE:CD1	2.54	0.42
2:B:706:GLU:O	2:B:709:SER:HB2	2.19	0.42
2:B:872:LYS:HA	2:B:872:LYS:HD3	1.88	0.42
1:C:958:U:H2'	1:C:959:U:O5'	2.19	0.42
1:D:958:U:H2'	1:D:959:U:O5'	2.19	0.42
1:D:916:C:O2'	1:D:972:U:O3'	2.36	0.42
2:A:244:ASN:ND2	2:A:313:VAL:HG23	2.34	0.42
2:A:469:TYR:CE2	2:A:620:PHE:CD1	3.07	0.42
2:A:774:ARG:HG2	2:A:775:ASP:N	2.34	0.42
2:B:159:PHE:O	2:B:162:PHE:HB3	2.19	0.42
2:B:165:TRP:HZ2	2:B:565:ASP:OD2	2.02	0.42
2:B:827:TRP:HD1	2:B:827:TRP:O	2.02	0.42
2:B:884:LYS:O	2:B:885:SER:C	2.57	0.42
1:C:960:C:C2	1:C:971:A:H1'	2.54	0.42
2:A:218:GLU:O	2:A:219:ASN:C	2.57	0.42
2:A:373:PHE:N	2:A:374:PRO:CD	2.83	0.42
2:A:572:PHE:HE1	2:A:595:LYS:HB3	1.85	0.42
2:A:614:ILE:HA	2:A:618:LEU:HB2	2.02	0.42
2:A:691:ARG:CG	2:A:691:ARG:NH1	2.80	0.42
2:A:860:ARG:NH2	2:A:862:TYR:CB	2.77	0.42
2:B:388:LYS:H	2:B:390:LYS:HE2	1.84	0.42
2:B:720:VAL:CG1	2:B:777:GLU:HG2	2.48	0.42
1:D:953:A:HO2'	1:D:954:G:H8	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:191:THR:HA	2:A:192:PRO:HD3	1.88	0.42
2:A:195:ASP:C	2:A:202:GLU:OE1	2.57	0.42
2:A:160:SER:HB3	2:A:516:THR:HG23	2.01	0.42
2:A:724:ASP:C	2:A:726:ASP:N	2.73	0.42
2:A:733:LEU:HD11	2:A:789:VAL:CG2	2.48	0.42
2:B:225:LEU:HD12	2:B:264:ILE:O	2.20	0.42
2:B:800:HIS:O	2:B:802:CYS:N	2.53	0.42
2:B:819:LYS:HD2	2:B:819:LYS:N	2.34	0.42
1:C:985:A:O3'	1:C:986:C:C6	2.72	0.42
2:A:211:ILE:HG12	2:A:438:GLU:O	2.20	0.42
2:A:256:ARG:NH1	2:A:278:ARG:NH1	2.68	0.42
2:A:37:TYR:OH	2:A:536:MET:O	2.30	0.42
2:A:911:ILE:HG13	2:A:912:LYS:HG3	2.02	0.42
2:B:581:GLU:HG3	2:B:586:ILE:O	2.20	0.42
2:B:616:ASN:O	2:B:619:THR:N	2.52	0.42
1:C:982:C:O5'	1:C:982:C:H6	2.02	0.42
1:D:922:C:H4'	1:D:923:A:C5'	2.46	0.42
2:A:145:ASP:OD1	2:A:147:SER:N	2.52	0.42
2:A:83:THR:HA	2:A:153:THR:HG22	2.02	0.42
2:A:276:GLN:HE21	2:A:276:GLN:HB3	1.62	0.42
2:A:379:VAL:O	2:A:383:GLY:HA3	2.19	0.42
2:A:730:LEU:HD23	2:A:730:LEU:HA	1.90	0.42
2:A:767:TYR:OH	2:A:782:VAL:HG21	2.19	0.42
2:A:947:THR:CG2	2:A:948:GLU:H	2.33	0.42
2:B:176:ILE:HD13	2:B:520:TRP:CH2	2.55	0.42
2:B:470:GLY:O	2:B:471:ASN:C	2.58	0.42
2:B:469:TYR:HB2	2:B:504:ASP:O	2.20	0.42
2:B:645:THR:OG1	2:B:688:ASP:OD1	2.28	0.42
2:B:721:GLU:HA	2:B:721:GLU:OE2	2.19	0.42
2:B:728:TRP:O	2:B:730:LEU:N	2.53	0.42
2:B:764:LEU:HD13	2:B:786:LEU:CD1	2.48	0.42
2:B:766:TRP:O	2:B:770:ARG:N	2.45	0.42
2:B:890:LEU:C	2:B:892:LYS:N	2.71	0.42
1:D:922:C:H5''	1:D:923:A:OP1	2.20	0.42
2:A:560:THR:O	2:A:563:PHE:N	2.52	0.42
2:A:544:HIS:HE1	2:A:593:GLU:CD	2.23	0.42
2:A:711:PHE:CD1	2:A:711:PHE:N	2.88	0.42
2:A:931:LYS:NZ	2:A:935:GLU:OE2	2.42	0.42
2:B:129:PHE:HA	2:B:132:ALA:HB3	2.01	0.42
2:B:478:ALA:HB2	2:B:623:PHE:CD1	2.55	0.42
2:B:661:PHE:O	2:B:665:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:775:ASP:O	2:B:775:ASP:OD1	2.38	0.42
2:B:921:ILE:HD12	2:B:928:ARG:HH12	1.85	0.42
2:A:12:LYS:HZ1	2:A:16:ARG:HH22	1.67	0.42
2:A:181:HIS:ND1	2:A:182:ARG:O	2.52	0.42
2:A:519:PRO:HG2	2:A:520:TRP:CE3	2.55	0.42
2:A:67:LYS:HA	2:A:70:GLN:HB2	2.01	0.42
2:B:152:THR:HG22	2:B:159:PHE:CE1	2.55	0.42
2:B:277:ASP:OD2	2:B:462:HIS:CE1	2.73	0.42
2:B:317:ASN:O	2:B:318:ALA:HB3	2.20	0.42
2:B:147:SER:OG	2:B:543:ARG:HG3	2.20	0.42
2:B:576:LYS:O	2:B:580:LEU:HD13	2.20	0.42
2:B:725:ILE:CD1	2:B:770:ARG:NE	2.82	0.42
2:B:714:TYR:CD1	2:B:780:ARG:HD3	2.55	0.42
2:B:871:TRP:CD2	2:B:920:ARG:NH2	2.80	0.42
1:C:927:G:C6	1:C:928:C:C4	3.08	0.42
1:C:953:A:C5'	1:C:954:G:OP1	2.68	0.42
2:A:290:LYS:HE3	2:A:290:LYS:HB3	1.95	0.42
2:A:347:GLU:C	2:A:347:GLU:CD	2.78	0.42
2:A:402:LYS:O	2:A:403:ALA:C	2.58	0.42
2:A:418:LYS:HB3	2:A:422:GLU:OE2	2.20	0.42
2:A:434:LYS:HB3	2:A:436:ILE:CG1	2.46	0.42
2:A:708:ILE:HD12	2:A:791:VAL:CG2	2.49	0.42
2:A:887:MET:CE	2:A:891:MET:HG2	2.49	0.42
2:A:924:GLU:HA	2:A:927:LEU:HB3	2.02	0.42
2:B:567:ILE:HG21	2:B:594:MET:HE3	2.01	0.42
2:B:32:LYS:HA	2:B:600:TYR:CE1	2.55	0.42
2:B:734:ASN:HA	2:B:734:ASN:HD22	1.51	0.42
2:B:800:HIS:C	2:B:802:CYS:N	2.72	0.42
1:D:923:A:O2'	1:D:924:A:OP2	2.30	0.42
2:A:123:ILE:HD11	2:A:155:LEU:HD11	2.02	0.41
2:A:235:VAL:HG11	2:A:431:MET:HE3	2.02	0.41
2:A:87:ILE:O	2:A:90:ILE:HB	2.20	0.41
2:B:325:VAL:N	2:B:332:ASP:OD2	2.51	0.41
2:B:553:LYS:HE3	2:B:553:LYS:HB3	1.80	0.41
2:B:671:ASP:HB3	2:B:798:THR:HG22	2.02	0.41
1:D:953:A:N1	2:B:966:ILE:HG12	2.35	0.41
1:C:923:A:O2'	1:C:924:A:OP2	2.34	0.41
1:C:926:G:O2'	1:C:927:G:H5'	2.20	0.41
1:D:903:G:H2'	1:D:904:G:O4'	2.20	0.41
2:A:711:PHE:O	2:A:784:ARG:HG2	2.20	0.41
2:A:824:VAL:O	2:A:825:GLU:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:VAL:O	2:B:416:GLU:OE1	2.37	0.41
2:B:677:ILE:HD13	2:B:677:ILE:HA	1.85	0.41
2:B:728:TRP:HE3	2:B:729:MET:N	2.18	0.41
2:B:768:LEU:O	2:B:770:ARG:N	2.52	0.41
2:B:803:GLU:CD	2:B:815:VAL:HG12	2.41	0.41
2:B:824:VAL:HG12	2:B:825:GLU:N	2.35	0.41
2:B:825:GLU:O	2:B:825:GLU:CG	2.68	0.41
1:C:976:C:C2'	1:C:977:G:H5'	2.50	0.41
2:A:236:TYR:CE2	2:A:414:PRO:HG2	2.55	0.41
2:A:250:VAL:CG1	2:A:285:GLU:HG3	2.50	0.41
2:A:264:ILE:O	2:A:264:ILE:HG22	2.18	0.41
2:A:341:ARG:N	2:A:341:ARG:HD3	2.36	0.41
2:A:691:ARG:O	2:A:694:VAL:CG1	2.64	0.41
2:A:9:ILE:HD13	2:A:804:GLU:HG2	2.02	0.41
2:A:871:TRP:CE3	2:A:920:ARG:NH2	2.88	0.41
2:B:263:TRP:CD1	2:B:263:TRP:N	2.88	0.41
2:B:264:ILE:HG23	2:B:286:PHE:CE2	2.55	0.41
2:B:289:GLU:N	2:B:289:GLU:OE2	2.53	0.41
1:D:988:A:N7	2:B:529:LEU:HD21	2.36	0.41
2:B:934:MET:O	2:B:938:LEU:HD13	2.21	0.41
1:C:970:A:O2'	1:C:971:A:O5'	2.38	0.41
2:A:12:LYS:NZ	2:A:16:ARG:HH22	2.18	0.41
2:A:459:LYS:CG	2:A:460:ILE:N	2.83	0.41
2:A:499:ILE:HG12	2:A:615:PRO:HA	2.02	0.41
2:A:148:ARG:HB3	2:A:542:SER:HB3	2.02	0.41
2:A:710:GLN:O	2:A:711:PHE:C	2.57	0.41
2:A:909:LYS:NZ	2:A:913:GLU:O	2.52	0.41
2:B:173:LYS:HD2	2:B:175:TYR:HE2	1.85	0.41
2:B:212:ILE:CD1	2:B:235:VAL:HG12	2.47	0.41
2:B:510:ARG:HA	2:B:510:ARG:HE	1.84	0.41
2:B:730:LEU:O	2:B:827:TRP:NE1	2.53	0.41
2:B:847:LYS:HE3	2:B:847:LYS:HB2	1.89	0.41
2:A:45:LEU:HD13	2:A:130:MET:CB	2.51	0.41
2:A:16:ARG:NH1	2:A:16:ARG:HG3	2.36	0.41
2:A:317:ASN:O	2:A:318:ALA:HB3	2.21	0.41
2:A:395:GLN:HG3	2:A:396:ALA:N	2.34	0.41
2:A:410:PHE:CZ	2:A:412:VAL:HG21	2.54	0.41
2:A:574:GLU:HA	2:A:577:GLU:OE1	2.20	0.41
2:A:61:ASP:O	2:A:64:ALA:N	2.53	0.41
2:A:767:TYR:OH	2:A:782:VAL:HG11	2.21	0.41
2:B:182:ARG:O	2:B:183:VAL:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:506:LYS:HE3	2:B:527:GLU:OE1	2.21	0.41
2:B:570:GLU:OE1	2:B:576:LYS:HG3	2.20	0.41
2:B:774:ARG:CG	2:B:775:ASP:N	2.84	0.41
1:C:987:C:H5	2:A:506:LYS:NZ	2.18	0.41
2:A:544:HIS:CE1	2:A:593:GLU:OE2	2.73	0.41
2:A:540:THR:HG21	2:A:598:PHE:CD1	2.55	0.41
2:A:711:PHE:HA	2:A:714:TYR:CE2	2.56	0.41
2:B:196:HIS:CD2	2:B:197:ASP:N	2.89	0.41
2:B:241:MET:HG3	2:B:296:VAL:CG2	2.51	0.41
2:B:725:ILE:HD13	2:B:770:ARG:NE	2.36	0.41
2:B:884:LYS:C	2:B:886:SER:N	2.73	0.41
1:C:960:C:H2'	1:C:971:A:H1'	2.03	0.41
1:D:902:C:H2'	1:D:903:G:C5'	2.51	0.41
2:A:412:VAL:H	2:A:416:GLU:HG2	1.86	0.41
2:A:612:ASP:OD1	2:A:613:LEU:HD23	2.21	0.41
2:A:614:ILE:N	2:A:615:PRO:CD	2.83	0.41
2:A:7:LYS:HZ3	2:A:7:LYS:HB2	1.85	0.41
2:A:950:LYS:H	2:A:953:LYS:HZ3	1.68	0.41
2:B:136:THR:HG23	2:B:662:ILE:HB	2.02	0.41
2:B:856:GLU:O	2:B:857:ASN:O	2.38	0.41
2:B:880:LYS:O	2:B:881:ARG:C	2.59	0.41
2:B:863:ILE:HG13	2:B:945:ASN:HA	2.03	0.41
1:C:920:G:C4'	1:C:920:G:OP1	2.68	0.41
2:A:116:LEU:C	2:A:116:LEU:HD23	2.41	0.41
2:A:382:LEU:C	2:A:384:ILE:N	2.74	0.41
2:A:405:TYR:HE2	2:A:424:LYS:HZ3	1.68	0.41
2:A:181:HIS:HD2	2:A:466:PHE:CE1	2.38	0.41
2:A:626:VAL:HG12	2:A:634:TRP:CD2	2.56	0.41
2:A:676:TYR:O	2:A:679:SER:HB3	2.21	0.41
2:A:793:LEU:HD23	2:A:821:PRO:HG3	2.03	0.41
2:A:884:LYS:O	2:A:885:SER:C	2.58	0.41
2:B:276:GLN:HE21	2:B:460:ILE:HD11	1.86	0.41
2:B:471:ASN:C	2:B:471:ASN:HD22	2.23	0.41
2:B:623:PHE:O	2:B:626:VAL:HG22	2.21	0.41
2:B:65:ARG:HA	2:B:68:ARG:HH11	1.81	0.41
1:D:944:C:OP1	2:B:765:ARG:HD3	2.20	0.41
2:B:860:ARG:HH21	2:B:860:ARG:HB2	1.86	0.41
2:A:112:PRO:HD2	2:A:115:ILE:HD12	2.02	0.41
2:A:293:GLY:O	2:A:295:TYR:CD1	2.74	0.41
2:A:406:HIS:ND1	2:A:421:GLN:OE1	2.54	0.41
2:A:467:ILE:CG1	2:A:508:CYS:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:644:GLY:HA2	2:A:687:PHE:O	2.20	0.41
2:A:872:LYS:O	2:A:876:VAL:CG2	2.65	0.41
2:B:749:THR:O	2:B:750:ARG:C	2.57	0.41
2:B:849:ILE:HD12	2:B:964:ILE:CD1	2.51	0.41
2:A:175:TYR:CE1	2:A:474:TRP:HB2	2.56	0.41
2:A:714:TYR:CE1	2:A:780:ARG:HG2	2.56	0.41
2:A:831:THR:O	2:A:834:ALA:HB3	2.21	0.41
2:A:872:LYS:HA	2:A:875:GLU:CD	2.41	0.41
2:A:882:ASP:C	2:A:883:PHE:HD1	2.24	0.41
2:B:560:THR:HB	2:B:561:PRO:CD	2.51	0.41
2:B:652:SER:HG	2:B:655:LYS:HB2	1.85	0.41
2:B:725:ILE:HB	2:B:929:GLU:OE1	2.20	0.41
2:B:846:ILE:HD12	2:B:938:LEU:CD2	2.51	0.41
2:B:944:ILE:HG22	2:B:945:ASN:N	2.36	0.41
2:B:964:ILE:HG13	2:B:965:PHE:N	2.34	0.41
1:C:914:A:H1'	1:C:925:A:N1	2.36	0.41
1:C:958:U:C2'	1:C:959:U:O5'	2.68	0.41
1:D:925:A:H2'	1:D:926:G:O4'	2.21	0.41
2:A:135:GLU:O	2:A:139:ARG:HB2	2.21	0.41
2:A:173:LYS:CB	2:A:175:TYR:CE2	3.04	0.41
2:A:232:PRO:O	2:A:235:VAL:HG22	2.21	0.41
2:A:252:ALA:HB1	2:A:281:GLU:O	2.21	0.41
2:A:168:TRP:CZ3	2:A:520:TRP:CE3	3.09	0.41
2:B:412:VAL:O	2:B:413:PRO:C	2.60	0.41
2:B:488:LEU:HA	2:B:488:LEU:HD23	1.81	0.41
2:B:771:THR:HB	2:B:774:ARG:HD3	2.03	0.41
2:B:786:LEU:HD23	2:B:786:LEU:C	2.41	0.41
2:B:846:ILE:HA	2:B:849:ILE:HD12	2.03	0.41
2:B:870:LYS:HE3	2:B:905:LYS:CE	2.40	0.41
2:A:9:ILE:O	2:A:12:LYS:HB3	2.22	0.40
2:A:345:ILE:O	2:A:346:LEU:HB2	2.20	0.40
1:C:986:C:C2	2:A:507:ALA:N	2.89	0.40
2:A:581:GLU:HG3	2:A:586:ILE:O	2.21	0.40
2:B:152:THR:HG22	2:B:159:PHE:CZ	2.56	0.40
2:B:155:LEU:C	2:B:157:PRO:HD3	2.42	0.40
2:B:240:ASN:O	2:B:324:SER:HB3	2.21	0.40
2:B:334:VAL:HG13	2:B:388:LYS:O	2.20	0.40
2:B:381:LYS:C	2:B:381:LYS:HD2	2.40	0.40
2:B:482:LEU:C	2:B:482:LEU:HD23	2.41	0.40
2:B:704:PHE:HD1	2:B:790:TRP:CH2	2.39	0.40
2:B:914:ARG:CZ	2:B:915:THR:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:914:ARG:HH21	2:B:915:THR:CG2	2.27	0.40
2:B:914:ARG:NH2	2:B:915:THR:HG23	2.29	0.40
2:B:949:ASP:HB2	2:B:954:LYS:CE	2.45	0.40
1:C:980:C:H2'	1:C:981:C:H6	1.86	0.40
2:A:339:LEU:N	2:A:339:LEU:HD13	2.36	0.40
2:A:232:PRO:CG	2:A:428:ALA:HB2	2.51	0.40
2:A:646:LEU:O	2:A:647:GLU:CB	2.69	0.40
2:A:713:GLU:O	2:A:714:TYR:O	2.40	0.40
2:A:733:LEU:HD11	2:A:789:VAL:HB	2.02	0.40
2:A:803:GLU:HA	2:A:803:GLU:OE1	2.20	0.40
2:A:824:VAL:CG1	2:A:825:GLU:N	2.84	0.40
2:A:914:ARG:HH21	2:A:915:THR:C	2.25	0.40
2:A:9:ILE:O	2:A:10:GLU:C	2.60	0.40
2:B:497:GLU:O	2:B:500:ILE:N	2.54	0.40
2:A:173:LYS:HD3	2:A:175:TYR:HE2	1.86	0.40
2:A:441:TYR:O	2:A:442:GLU:OE2	2.40	0.40
2:A:50:HIS:H	2:A:53:HIS:HD2	1.68	0.40
2:A:959:PRO:O	2:A:960:LEU:HB2	2.20	0.40
2:B:186:ASP:CB	2:B:193:LEU:HD11	2.42	0.40
2:B:216:LEU:HB2	2:B:296:VAL:HG12	2.04	0.40
2:B:337:GLU:O	2:B:339:LEU:HD12	2.21	0.40
2:B:461:ILE:HB	2:B:464:GLN:HB2	2.03	0.40
2:B:597:GLU:O	2:B:600:TYR:N	2.53	0.40
2:B:783:LEU:N	2:B:783:LEU:CD1	2.84	0.40
2:B:13:TRP:CZ2	2:B:803:GLU:HB3	2.53	0.40
2:B:871:TRP:HZ3	2:B:918:VAL:HA	1.87	0.40
2:B:915:THR:O	2:B:916:PHE:CD2	2.74	0.40
2:A:14:GLN:H	2:A:14:GLN:HG3	1.61	0.40
2:A:217:ARG:HE	2:A:217:ARG:HB3	1.62	0.40
2:A:497:GLU:O	2:A:500:ILE:N	2.54	0.40
2:A:518:LEU:C	2:A:520:TRP:H	2.24	0.40
2:A:77:PRO:HG3	2:A:539:TYR:CD1	2.56	0.40
2:A:918:VAL:HG11	2:A:920:ARG:NH1	2.37	0.40
2:A:953:LYS:O	2:A:954:LYS:C	2.59	0.40
2:B:48:HIS:NE2	2:B:132:ALA:HB1	2.36	0.40
2:B:349:TYR:O	2:B:349:TYR:CG	2.74	0.40
2:B:555:ASP:OD2	2:B:557:GLU:HB2	2.22	0.40
2:B:718:GLY:O	2:B:719:ASN:C	2.60	0.40
2:B:70:GLN:HB3	2:B:72:TYR:CE1	2.56	0.40
2:B:849:ILE:HD12	2:B:964:ILE:HD11	2.04	0.40
2:A:330:PRO:HD3	2:A:400:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:559:LEU:HA	2:A:563:PHE:CD2	2.57	0.40
2:A:867:GLU:N	2:A:867:GLU:OE1	2.38	0.40
2:A:96:ASN:ND2	2:A:96:ASN:N	2.70	0.40
2:B:44:TYR:O	2:B:46:SER:N	2.54	0.40
2:B:525:VAL:HG13	2:B:525:VAL:O	2.22	0.40
2:B:646:LEU:O	2:B:647:GLU:CB	2.69	0.40
2:B:724:ASP:C	2:B:726:ASP:N	2.75	0.40
2:B:780:ARG:O	2:B:781:TYR:C	2.59	0.40
2:B:919:LYS:NZ	2:B:960:LEU:HD11	2.36	0.40
2:B:921:ILE:O	2:B:924:GLU:CB	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	944/967 (98%)	630 (67%)	211 (22%)	103 (11%)	0	3
2	B	944/967 (98%)	632 (67%)	208 (22%)	104 (11%)	0	2
All	All	1888/1934 (98%)	1262 (67%)	419 (22%)	207 (11%)	0	2

All (207) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	74	VAL
2	A	110	LYS
2	A	143	SER
2	A	183	VAL
2	A	188	VAL
2	A	276	GLN
2	A	333	HIS
2	A	347	GLU

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Mol	Chain	Res	Type
2	A	377	GLU
2	A	378	GLU
2	A	552	GLY
2	A	630	ARG
2	A	714	TYR
2	A	854	LYS
2	A	867	GLU
2	A	871	TRP
2	A	883	PHE
2	A	913	GLU
2	A	914	ARG
2	A	929	GLU
2	A	953	LYS
2	B	45	LEU
2	B	74	VAL
2	B	110	LYS
2	B	183	VAL
2	B	188	VAL
2	B	276	GLN
2	B	333	HIS
2	B	347	GLU
2	B	377	GLU
2	B	378	GLU
2	B	552	GLY
2	B	630	ARG
2	B	714	TYR
2	B	854	LYS
2	B	867	GLU
2	B	871	TRP
2	B	883	PHE
2	B	913	GLU
2	B	914	ARG
2	B	929	GLU
2	B	953	LYS
2	A	45	LEU
2	A	113	GLU
2	A	181	HIS
2	A	201	GLY
2	A	219	ASN
2	A	301	SER
2	A	343	THR
2	A	374	PRO

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Mol	Chain	Res	Type
2	A	376	VAL
2	A	415	TYR
2	A	464	GLN
2	A	494	ALA
2	A	502	TRP
2	A	528	SER
2	A	529	LEU
2	A	568	PHE
2	A	616	ASN
2	A	711	PHE
2	A	782	VAL
2	A	857	ASN
2	A	868	ASP
2	A	869	TRP
2	A	885	SER
2	A	900	GLY
2	A	921	ILE
2	A	922	ASN
2	A	950	LYS
2	A	954	LYS
2	A	955	LYS
2	B	113	GLU
2	B	143	SER
2	B	181	HIS
2	B	201	GLY
2	B	219	ASN
2	B	301	SER
2	B	343	THR
2	B	374	PRO
2	B	376	VAL
2	B	415	TYR
2	B	464	GLN
2	B	502	TRP
2	B	528	SER
2	B	529	LEU
2	B	568	PHE
2	B	616	ASN
2	B	782	VAL
2	B	857	ASN
2	B	868	ASP
2	B	869	TRP
2	B	885	SER

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Mol	Chain	Res	Type
2	B	900	GLY
2	B	921	ILE
2	B	922	ASN
2	B	950	LYS
2	B	954	LYS
2	B	955	LYS
2	A	73	ASN
2	A	223	ILE
2	A	240	ASN
2	A	453	GLY
2	A	482	LEU
2	A	558	LYS
2	A	631	GLU
2	A	775	ASP
2	A	825	GLU
2	A	895	GLU
2	A	911	ILE
2	B	73	ASN
2	B	96	ASN
2	B	220	GLY
2	B	223	ILE
2	B	240	ASN
2	B	453	GLY
2	B	494	ALA
2	B	558	LYS
2	B	631	GLU
2	B	711	PHE
2	B	775	ASP
2	B	825	GLU
2	B	891	MET
2	B	895	GLU
2	B	911	ILE
2	A	85	SER
2	A	96	ASN
2	A	117	TRP
2	A	220	GLY
2	A	283	ILE
2	A	421	GLN
2	A	542	SER
2	A	623	PHE
2	A	670	ALA
2	A	719	ASN

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Mol	Chain	Res	Type
2	A	856	GLU
2	A	881	ARG
2	A	891	MET
2	A	903	VAL
2	A	907	VAL
2	B	85	SER
2	B	117	TRP
2	B	421	GLN
2	B	482	LEU
2	B	623	PHE
2	B	670	ALA
2	B	719	ASN
2	B	790	TRP
2	B	856	GLU
2	B	881	ARG
2	B	903	VAL
2	B	907	VAL
2	A	157	PRO
2	A	337	GLU
2	A	339	LEU
2	A	394	GLU
2	A	452	PHE
2	A	519	PRO
2	A	790	TRP
2	A	878	SER
2	A	898	LYS
2	B	157	PRO
2	B	283	ILE
2	B	339	LEU
2	B	403	ALA
2	B	452	PHE
2	B	519	PRO
2	B	540	THR
2	B	542	SER
2	B	743	ALA
2	B	878	SER
2	A	303	ASP
2	A	403	ALA
2	A	743	ALA
2	A	813	GLY
2	B	337	GLU
2	B	394	GLU

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Mol	Chain	Res	Type
2	B	495	GLN
2	A	945	ASN
2	A	946	PRO
2	B	945	ASN
2	B	946	PRO
2	A	88	VAL
2	A	471	ASN
2	A	522	PRO
2	A	823	PRO
2	B	471	ASN
2	B	522	PRO
2	B	789	VAL
2	A	302	GLY
2	A	353	PRO
2	A	355	ILE
2	A	384	ILE
2	B	222	VAL
2	B	302	GLY
2	B	353	PRO
2	B	355	ILE
2	B	384	ILE
2	A	115	ILE
2	A	222	VAL
2	A	329	ALA
2	A	330	PRO
2	B	88	VAL
2	B	115	ILE
2	B	329	ALA
2	B	330	PRO
2	B	813	GLY
2	B	823	PRO

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	841/857 (98%)	731 (87%)	110 (13%)	4 20
2	B	841/857 (98%)	752 (89%)	89 (11%)	7 30
All	All	1682/1714 (98%)	1483 (88%)	199 (12%)	6 25

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	16	ARG
2	A	28	ARG
2	A	29	ASP
2	A	35	LYS
2	A	37	TYR
2	A	38	ILE
2	A	42	PHE
2	A	70	GLN
2	A	75	LEU
2	A	77	PRO
2	A	107	ASP
2	A	124	ASN
2	A	135	GLU
2	A	138	ILE
2	A	139	ARG
2	A	157	PRO
2	A	172	GLU
2	A	173	LYS
2	A	183	VAL
2	A	196	HIS
2	A	203	ASP
2	A	213	LYS
2	A	217	ARG
2	A	230	LEU
2	A	233	GLU
2	A	234	THR
2	A	239	THR
2	A	246	ASN
2	A	276	GLN
2	A	278	ARG
2	A	289	GLU
2	A	294	LYS

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Mol	Chain	Res	Type
2	A	317	ASN
2	A	331	PHE
2	A	339	LEU
2	A	341	ARG
2	A	347	GLU
2	A	349	TYR
2	A	373	PHE
2	A	381	LYS
2	A	433	GLU
2	A	446	LYS
2	A	455	ARG
2	A	463	ASP
2	A	492	ARG
2	A	527	GLU
2	A	529	LEU
2	A	531	ASP
2	A	536	MET
2	A	540	THR
2	A	551	GLU
2	A	562	GLU
2	A	569	LEU
2	A	590	ILE
2	A	602	TYR
2	A	616	ASN
2	A	624	ASN
2	A	625	HIS
2	A	636	LYS
2	A	640	VAL
2	A	645	THR
2	A	649	GLN
2	A	658	VAL
2	A	678	MET
2	A	679	SER
2	A	685	SER
2	A	691	ARG
2	A	700	GLN
2	A	703	ARG
2	A	707	LEU
2	A	720	VAL
2	A	722	LEU
2	A	727	ARG
2	A	732	ARG

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Mol	Chain	Res	Type
2	A	733	LEU
2	A	744	LEU
2	A	747	PHE
2	A	771	THR
2	A	776	ASP
2	A	784	ARG
2	A	792	ARG
2	A	809	LEU
2	A	815	VAL
2	A	817	LEU
2	A	819	LYS
2	A	820	TRP
2	A	823	PRO
2	A	825	GLU
2	A	826	GLU
2	A	828	TRP
2	A	829	ASN
2	A	852	VAL
2	A	860	ARG
2	A	862	TYR
2	A	869	TRP
2	A	872	LYS
2	A	879	GLU
2	A	881	ARG
2	A	884	LYS
2	A	910	LEU
2	A	916	PHE
2	A	917	ASP
2	A	919	LYS
2	A	922	ASN
2	A	923	GLU
2	A	932	GLU
2	A	933	PHE
2	A	942	ILE
2	A	953	LYS
2	A	964	ILE
2	B	7	LYS
2	B	18	LEU
2	B	42	PHE
2	B	44	TYR
2	B	70	GLN
2	B	97	ARG

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Mol	Chain	Res	Type
2	B	139	ARG
2	B	151	TYR
2	B	172	GLU
2	B	196	HIS
2	B	197	ASP
2	B	203	ASP
2	B	213	LYS
2	B	218	GLU
2	B	230	LEU
2	B	233	GLU
2	B	234	THR
2	B	271	TYR
2	B	276	GLN
2	B	285	GLU
2	B	298	ASN
2	B	303	ASP
2	B	331	PHE
2	B	332	ASP
2	B	338	ASP
2	B	339	LEU
2	B	341	ARG
2	B	347	GLU
2	B	381	LYS
2	B	405	TYR
2	B	415	TYR
2	B	429	LYS
2	B	451	ARG
2	B	471	ASN
2	B	479	ARG
2	B	504	ASP
2	B	505	LYS
2	B	510	ARG
2	B	511	LYS
2	B	528	SER
2	B	533	THR
2	B	536	MET
2	B	540	THR
2	B	546	ASN
2	B	547	LYS
2	B	551	GLU
2	B	557	GLU
2	B	565	ASP

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Mol	Chain	Res	Type
2	B	599	GLU
2	B	602	TYR
2	B	607	ARG
2	B	624	ASN
2	B	625	HIS
2	B	630	ARG
2	B	641	ASN
2	B	649	GLN
2	B	650	LYS
2	B	658	VAL
2	B	674	ARG
2	B	675	LEU
2	B	690	ARG
2	B	703	ARG
2	B	714	TYR
2	B	722	LEU
2	B	726	ASP
2	B	729	MET
2	B	734	ASN
2	B	744	LEU
2	B	748	ARG
2	B	750	ARG
2	B	812	GLU
2	B	819	LYS
2	B	820	TRP
2	B	825	GLU
2	B	826	GLU
2	B	828	TRP
2	B	829	ASN
2	B	855	ILE
2	B	860	ARG
2	B	869	TRP
2	B	885	SER
2	B	886	SER
2	B	889	GLU
2	B	917	ASP
2	B	919	LYS
2	B	920	ARG
2	B	940	ILE
2	B	953	LYS
2	B	964	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such

sidechains are listed below:

Mol	Chain	Res	Type
2	A	5	ASN
2	A	53	HIS
2	A	70	GLN
2	A	73	ASN
2	A	81	HIS
2	A	96	ASN
2	A	124	ASN
2	A	166	GLN
2	A	196	HIS
2	A	219	ASN
2	A	276	GLN
2	A	317	ASN
2	A	421	GLN
2	A	447	ASN
2	A	464	GLN
2	A	544	HIS
2	A	546	ASN
2	A	616	ASN
2	A	624	ASN
2	A	625	HIS
2	A	683	HIS
2	A	731	HIS
2	A	742	ASN
2	A	800	HIS
2	A	922	ASN
2	B	53	HIS
2	B	70	GLN
2	B	73	ASN
2	B	124	ASN
2	B	166	GLN
2	B	196	HIS
2	B	276	GLN
2	B	298	ASN
2	B	317	ASN
2	B	387	GLN
2	B	421	GLN
2	B	447	ASN
2	B	471	ASN
2	B	495	GLN
2	B	546	ASN
2	B	616	ASN
2	B	731	HIS

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Mol	Chain	Res	Type
2	B	734	ASN
2	B	742	ASN
2	B	908	GLN
2	B	922	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	87/88 (98%)	24 (27%)	7 (8%)
1	D	87/88 (98%)	22 (25%)	8 (9%)
All	All	174/176 (98%)	46 (26%)	15 (8%)

All (46) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	907	G
1	C	908	U
1	C	910	G
1	C	916	C
1	C	917	C
1	C	918	U
1	C	919	G
1	C	920	G
1	C	921	U
1	C	922	C
1	C	923	A
1	C	924	A
1	C	936	U
1	C	937	C
1	C	952	U
1	C	953	A
1	C	954	G
1	C	961	C
1	C	968	C
1	C	971	A
1	C	972	U
1	C	983	G
1	C	987	C
1	C	988	A
1	D	903	G
1	D	905	G

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Mol	Chain	Res	Type
1	D	908	U
1	D	909	U
1	D	910	G
1	D	917	C
1	D	918	U
1	D	919	G
1	D	920	G
1	D	921	U
1	D	923	A
1	D	924	A
1	D	936	U
1	D	952	U
1	D	961	C
1	D	971	A
1	D	972	U
1	D	973	C
1	D	984	C
1	D	985	A
1	D	987	C
1	D	988	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	907	G
1	C	922	C
1	C	923	A
1	C	953	A
1	C	960	C
1	C	970	A
1	C	972	U
1	D	907	G
1	D	920	G
1	D	922	C
1	D	923	A
1	D	953	A
1	D	960	C
1	D	970	A
1	D	972	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	88/88 (100%)	0.20	4 (4%) 33 22	53, 78, 126, 149	0
1	D	88/88 (100%)	0.41	7 (7%) 12 7	53, 91, 146, 150	0
2	A	948/967 (98%)	-0.09	26 (2%) 54 41	8, 59, 131, 150	0
2	B	948/967 (98%)	0.26	53 (5%) 24 14	48, 102, 149, 150	0
All	All	2072/2110 (98%)	0.10	90 (4%) 35 23	8, 82, 143, 150	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	407	LYS	5.3
1	D	936	U	5.3
2	B	524	TRP	5.1
1	D	939	A	4.9
2	B	236	TYR	4.9
2	B	386	SER	4.7
2	B	862	TYR	4.6
2	A	456	ALA	4.1
2	B	403	ALA	3.9
2	B	920	ARG	3.8
2	A	457	VAL	3.8
2	B	895	GLU	3.7
2	A	406	HIS	3.6
2	B	891	MET	3.6
2	B	869	TRP	3.6
2	B	265	VAL	3.6
2	A	869	TRP	3.5
2	A	455	ARG	3.5
2	B	583	LYS	3.4
1	D	909	U	3.4
2	B	457	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	291	LEU	3.2
2	B	167	PHE	3.2
1	D	988	A	3.2
2	B	310	ALA	3.2
2	B	405	TYR	3.2
2	A	915	THR	3.1
2	B	887	MET	3.1
2	A	586	ILE	3.1
1	D	986	C	3.0
2	B	280	ILE	3.0
2	B	255	ARG	2.9
2	B	784	ARG	2.9
2	A	291	LEU	2.9
2	A	404	GLU	2.9
2	A	450	SER	2.8
2	B	300	VAL	2.8
2	B	387	GLN	2.8
2	B	929	GLU	2.8
2	B	938	LEU	2.7
2	B	966	ILE	2.7
2	B	263	TRP	2.7
1	D	907	G	2.6
2	B	264	ILE	2.6
2	B	399	THR	2.6
2	B	883	PHE	2.6
2	B	238	VAL	2.6
2	A	447	ASN	2.6
2	A	191	THR	2.5
2	B	865	THR	2.5
2	A	448	VAL	2.5
2	A	917	ASP	2.5
2	B	455	ARG	2.5
2	B	381	LYS	2.5
1	C	987	C	2.4
2	B	355	ILE	2.4
2	A	862	TYR	2.4
2	B	242	TRP	2.4
1	C	986	C	2.3
2	B	870	LYS	2.3
2	A	868	ASP	2.3
2	A	449	ILE	2.3
2	A	502	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	453	GLY	2.3
2	B	919	LYS	2.3
2	B	353	PRO	2.3
2	B	400	ILE	2.3
2	B	964	ILE	2.2
2	B	279	GLU	2.2
2	A	584	THR	2.2
2	B	286	PHE	2.2
2	B	323	MET	2.2
1	D	940	G	2.2
2	B	404	GLU	2.2
2	B	352	ASP	2.1
2	B	251	LYS	2.1
2	B	409	ILE	2.1
2	B	458	ILE	2.1
2	B	354	ARG	2.1
2	B	967	GLU	2.1
1	C	939	A	2.1
2	B	319	THR	2.1
2	A	190	GLY	2.1
2	A	195	ASP	2.1
2	A	452	PHE	2.0
1	C	988	A	2.0
2	A	206	ILE	2.0
2	A	194	GLY	2.0
2	B	464	GLN	2.0
2	A	890	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.