



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:53 AM UTC

PDB ID : 1N6E / pdb_00001n6e
Title : tricorn protease in complex with a tridecapeptide chloromethyl ketone derivative
Authors : Kim, J.-S.; Groll, M.; Huber, R.; Brandstetter, H.
Deposited on : 2002-11-10
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

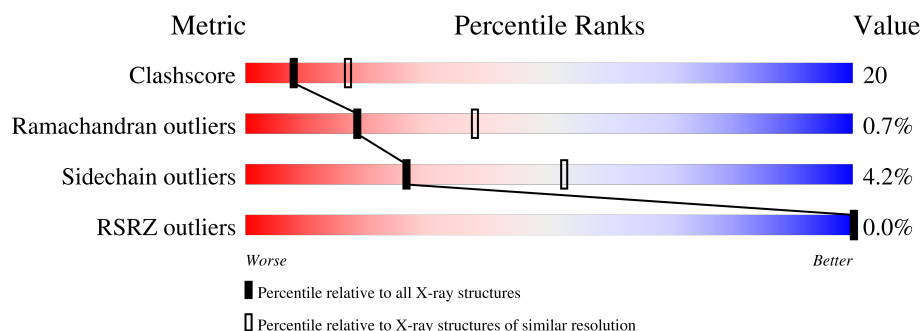
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	1071	
1	C	1071	
1	E	1071	
1	G	1071	
1	I	1071	
1	K	1071	

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Mol	Chain	Length	Quality of chain
2	B	14	50% 29% 7% 14%
2	D	14	50% 29% 7% 14%
2	F	14	36% 36% 14% 14%
2	H	14	50% 29% 7% 14%
2	J	14	50% 29% 7% 14%
2	L	14	7% 43% 29% 14% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 50544 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tricorn protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	C	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	E	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	G	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	I	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	K	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			

- Molecule 2 is a protein called DQTQKAAAELTFF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	0	0	1
			87	58	13	16			
2	D	12	Total	C	N	O	0	0	1
			87	58	13	16			
2	F	12	Total	C	N	O	0	0	1
			87	58	13	16			
2	H	12	Total	C	N	O	0	0	1
			87	58	13	16			
2	J	12	Total	C	N	O	0	0	1
			87	58	13	16			
2	L	12	Total	C	N	O	0	0	1
			87	58	13	16			

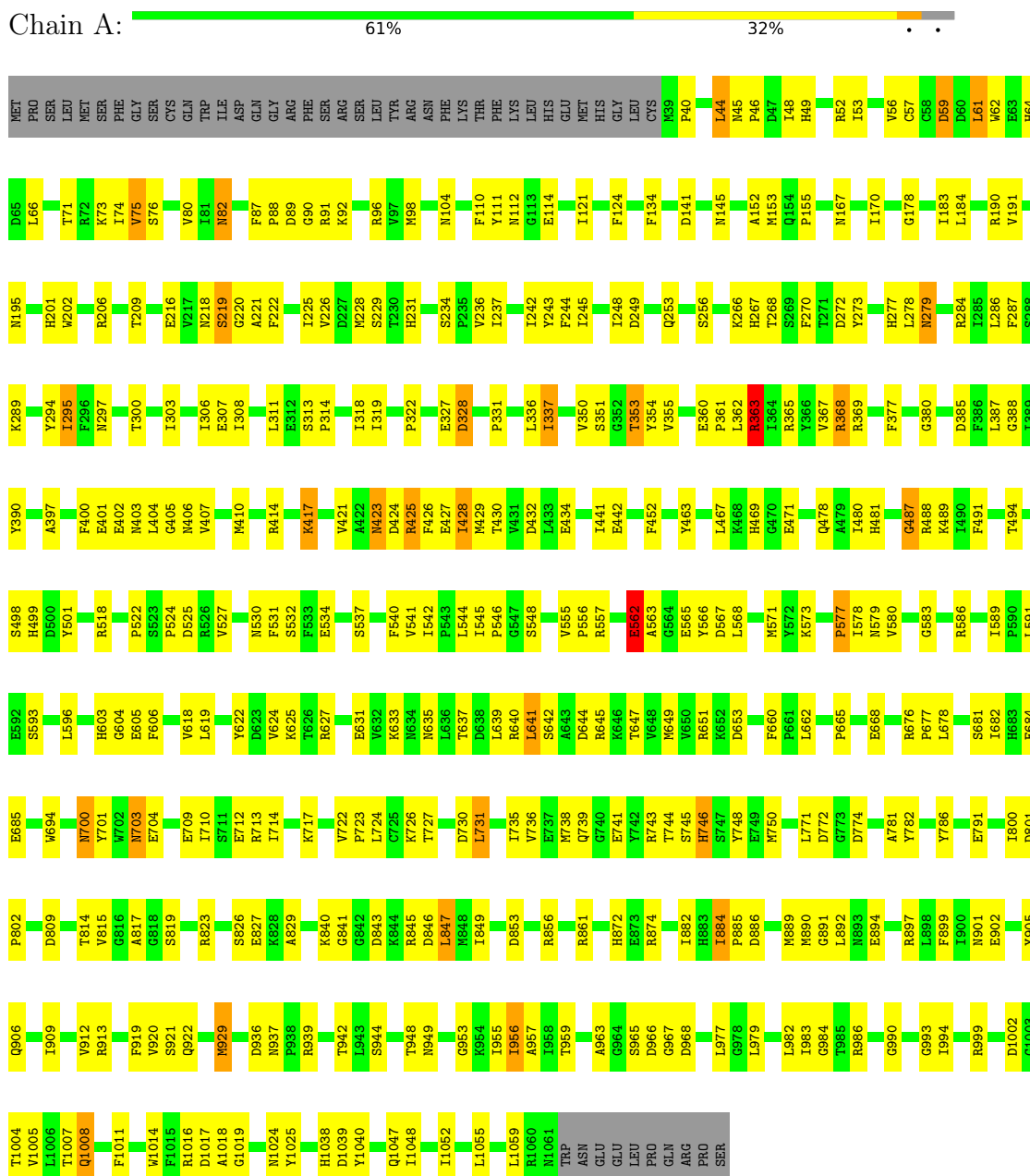
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total 178	O 178	0	0
3	B	2	Total 2	O 2	0	0
3	C	172	Total 172	O 172	0	0
3	D	2	Total 2	O 2	0	0
3	E	138	Total 138	O 138	0	0
3	F	5	Total 5	O 5	0	0
3	G	154	Total 154	O 154	0	0
3	H	2	Total 2	O 2	0	0
3	I	157	Total 157	O 157	0	0
3	J	2	Total 2	O 2	0	0
3	K	146	Total 146	O 146	0	0
3	L	2	Total 2	O 2	0	0

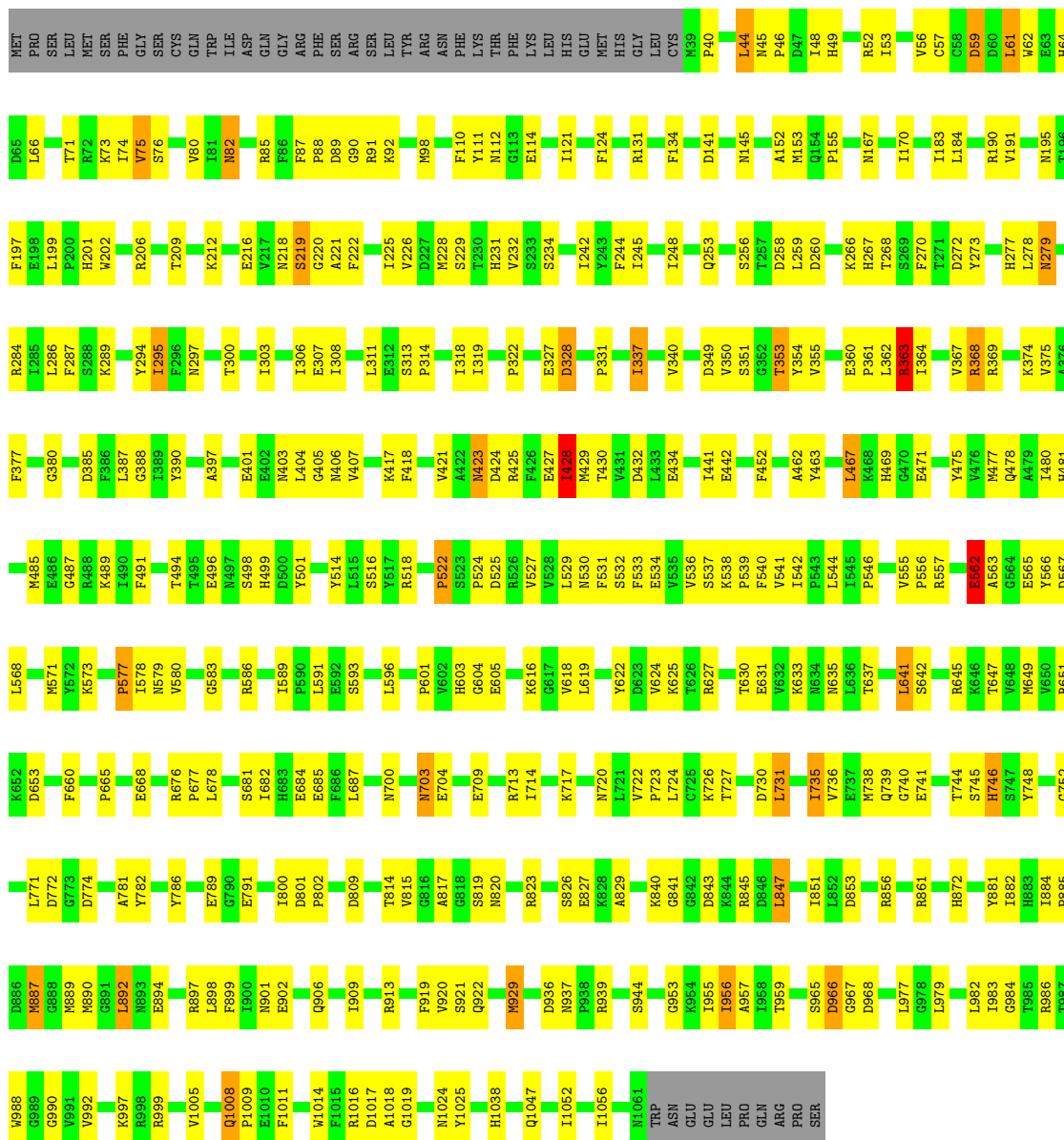
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

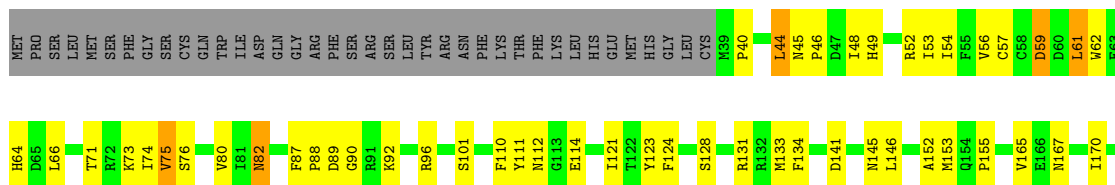
- Molecule 1: Tricorn protease



Chain C: 61% 32% . .



Chain E: 56% 36% . .

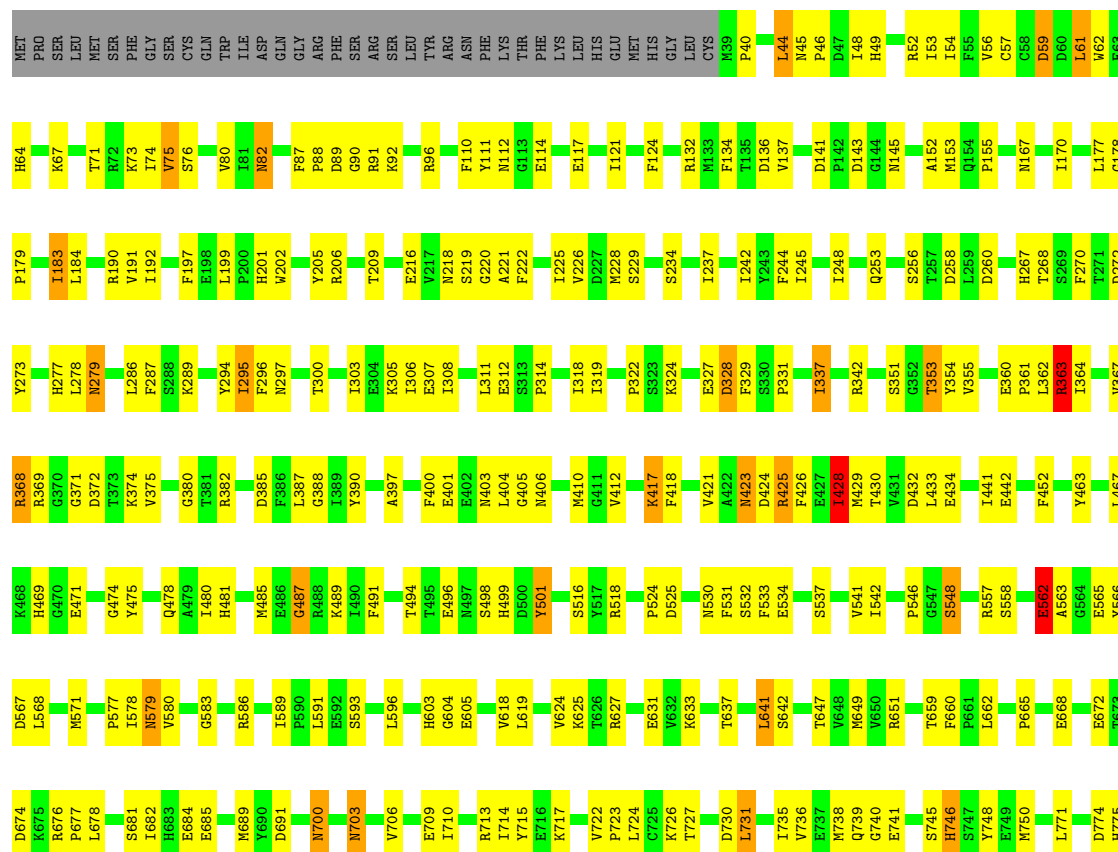


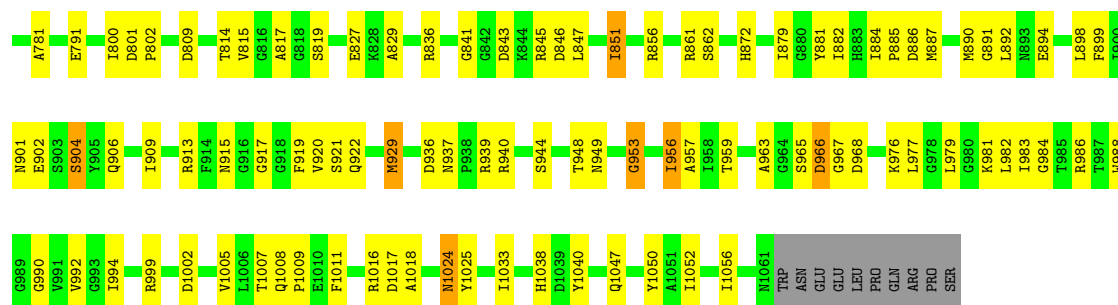
Q1008	P1009	E1010	F1011	W1014	F1015	A1016	D1017	C1018	G1019	N1024	Y1025	P1029	I1033	A1036	P1037	H1038	D1039	Y1040	D1045	P1046	Q1047	H1048	Y1049	Y1050	A1051	I1052	L1055	I1056	L1059	R1060	I1061	TRP	ASN	GLU	GLU	LEU	PRO	GLN	ARG	PRO	SER											
E926	N929	D936	N937	P938	S944	Y946	P947	T948	N949	G953	I956	A957	T958	T959	Y962	S965	D966	G967	D968	I969	F970	L977	G978	L979	G980	X981	L982	L983	G984	T985	R986	T987	W988	G989	G990	V991	G992	G993	I994	K997	R998	R999	D1002	G1003	T1004	V1005	T1006	T1007				
K844	R845	D846	L847	I851	L852	D853	R856	R859	E860	S861	S862	W863	H872	Y881	I882	H883	L884	P885	D886	K887	G888	M889	A781	Y782	C891	L892	H893	E894	F895	G896	R897	L898	F899	I900	N901	E902	Y905	Q906	T909	V912	R913	F914	N915	G916	G917	G918	F919	G1003	T1004	S921	Q922	T923
E737	M738	Q739	G740	E741	Y742	R743	T744	S745	H746	S747	Y748	E749	M750	S762	C767	L771	D772	G773	D774	H775	Y776	K780	A781	Y782	E791	I800	D801	P802	D809	G812	E813	T814	V815	G816	A817	G818	S819	N820	I821	Y822	R823	S826	E827	K828	A829	K840	G841	G842	D843			
P539	F540	V541	I542	P546	L554	R557	E562	A563	G564	E565	Y566	D567	L568	M571	E672	T673	D674	P677	L678	S681	I682	H683	E684	E685	A697	N700	Y701	Y702	W703	V706	E709	R713	I714	Y715	E716	K717	V722	P723	L724	C725	K726	L731	I735	V736	S737	K538						
I441	E442	D451	F452	A462	Y463	L467	K468	H469	D473	G474	Y475	Q478	A479	I480	H481	M485	E486	G487	R488	K489	F491	T494	T495	E496	N497	S498	H499	E500	Y501	D506	L515	S516	Y517	R518	P524	D525	V528	L529	N530	F531	S532	F533	E534	V535	V536	S537	K538					
E360	P361	L362	R363	I364	V367	R368	D372	V375	A376	F377	I378	H379	G380	D385	F386	L387	G388	I389	Y390	R393	A397	F400	E401	E402	M403	L404	G405	N406	V407	M410	G411	V412	K417	F418	V421	A422	M423	D424	R425	F426	E427	M429	F432	T430	F431	D432	L433	E434				
D258	L259	D260	H267	T268	S269	F270	I271	Y272	H277	L278	N279	L280	D281	L286	F287	K289	Y294	I295	F296	I303	I306	E307	G220	E401	I308	L311	P314	I318	I319	P322	E327	D328	F329	P331	I337	D349	V350	S351	G352	T353	Y354	V355	V358	P359								
G178	P179	A180	I183	I184	R190	V191	I192	N195	T196	F197	E198	P200	H201	W202	K203	G204	R206	T209	E216	V217	N218	S219	E220	A221	F222	K223	K224	I225	V226	D227	M228	S229	T230	H231	V232	S233	P234	P235	V236	I237	I242	Y243	F244	I245	I248	Q253	S256	T257				

● Molecule 1: Tricorn protease

Chain G:  60% 32%

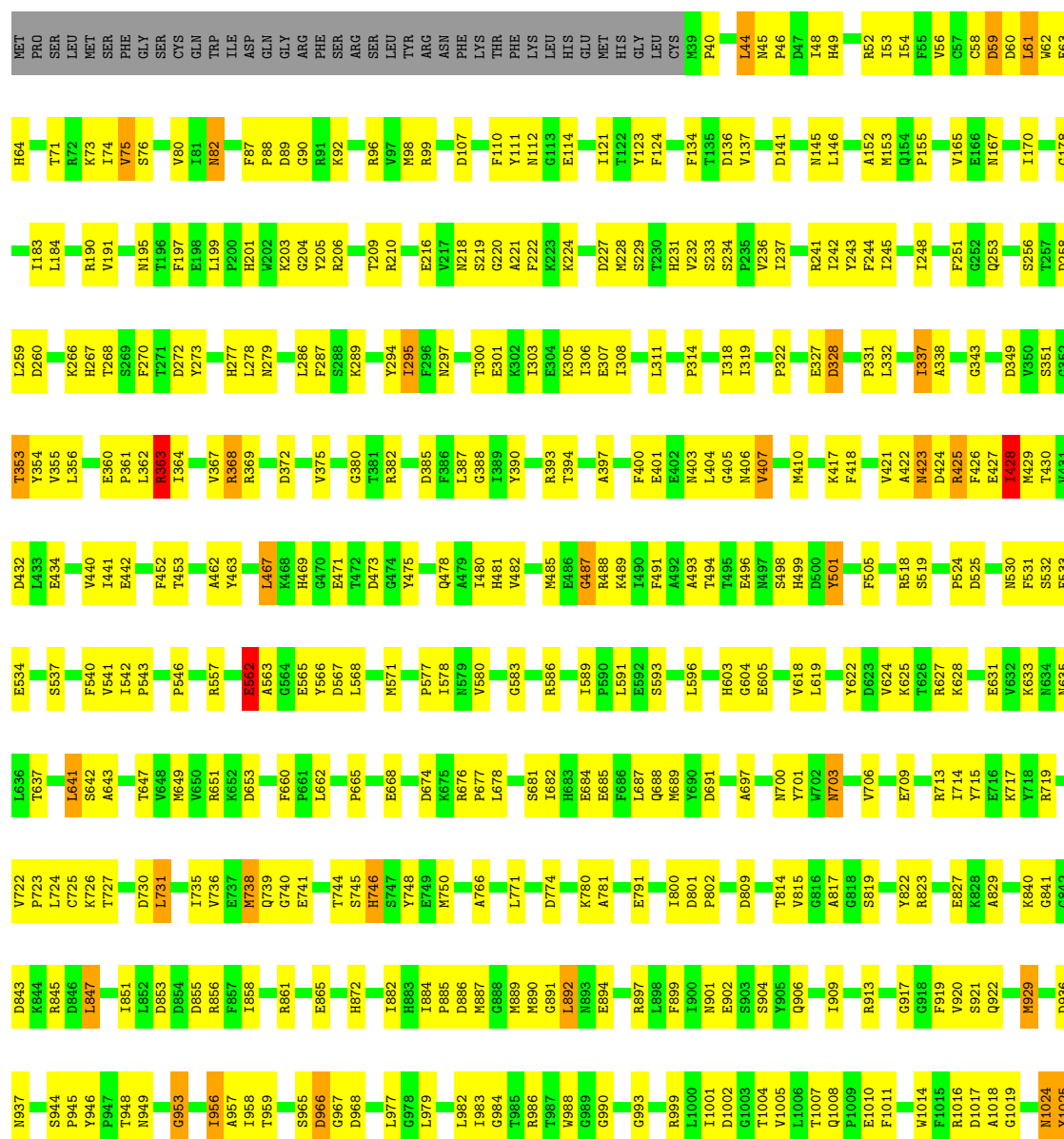
MET	PRO	SER	LEU	MET	SER	PHE	GLY	SER	CYS	GLN	TRP	ILE	ASP	GLN	GLY	ARG	PHE	SER	ARG	SER	LEU	TYR	ASN	ARG	PHE	LYS	THR	PHE	LYS	LEU	HIS	GLU	MET	HIS	GLY	LEU	CYS	M59	M39	P40	L44	M45	P46	D47	M48	H49	R52	I53	I54	F55	V56	C57	G58	D59	D60	L61	W62	E63
	H64	D65	L66	T71	R72	K73	I74	V75	S76	V80	I81	N82	F87	P88	D89	G90	R96	N104	F110	Y111	N112	G113	E114	E117	I121	F124	R131	F134	T135	D141	P142	D143	G144	N145	S149	T150	A151	M153	Q154	P155	N167	I170	L177															
	G178	T181	H182	I183	L184	R190	V191	F197	E198	L199	P200	H201	W202	Y205	R206	T209	E216	V217	N218	S219	A221	K223	K224	D227	M228	S229	S234	P235	V236	I237	I242	Y243	F244	I245	I248	Q253	S256	L259	L265	H267	T268	S269	F270	T271	D272													
Y273	R276	H277	L278	M279	R284	L285	L286	F287	S288	K289	Y294	I295	F296	N297	T300	I303	I306	E307	I308	L311	F312	S313	P314	I318	I319	P322	E327	D328	F329	S330	P331	I337	Q344	V350	S351	G352	T353	Y354	V355	L356	K357	E360	P361	L362	R363													





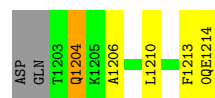
• Molecule 1: Tricorn protease

Chain K: 57% 35%

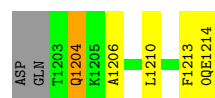




• Molecule 2: DQTQKAAAELTFF



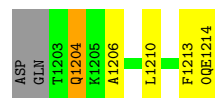
• Molecule 2: DQTQKAAAELTFF



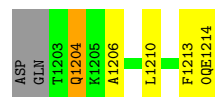
• Molecule 2: DQTQKAAAELTFF



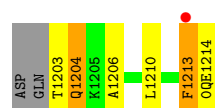
• Molecule 2: DQTQKAAAELTFF



• Molecule 2: DQTQKAAAELTFF



• Molecule 2: DQTQKAAAELTFF



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.47Å 245.10Å 157.89Å 90.00° 105.19° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60 6.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.6 (6.00-2.60) 85.4 (6.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.288 0.264 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50544	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0QE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	1/8367 (0.0%)	1.04	23/11311 (0.2%)
1	C	0.85	1/8367 (0.0%)	1.04	24/11311 (0.2%)
1	E	0.79	2/8367 (0.0%)	1.04	24/11311 (0.2%)
1	G	0.80	0/8367	1.04	20/11311 (0.2%)
1	I	0.81	1/8367 (0.0%)	1.04	22/11311 (0.2%)
1	K	0.79	0/8367	1.03	21/11311 (0.2%)
2	B	1.21	1/87 (1.1%)	0.87	0/116
2	D	1.24	1/87 (1.1%)	0.84	0/116
2	F	1.13	1/87 (1.1%)	0.84	0/116
2	H	1.25	1/87 (1.1%)	0.85	0/116
2	J	1.16	1/87 (1.1%)	0.83	0/116
2	L	1.02	1/87 (1.1%)	0.86	0/116
All	All	0.82	11/50724 (0.0%)	1.04	134/68562 (0.2%)

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	E	0	2
1	K	0	2
All	All	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1213	PHE	C-O	10.58	1.44	1.23
2	D	1213	PHE	C-O	10.34	1.44	1.23
2	B	1213	PHE	C-O	9.81	1.43	1.23
2	J	1213	PHE	C-O	9.73	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1213	PHE	C-O	9.05	1.41	1.23
2	L	1213	PHE	C-O	7.72	1.39	1.23
1	E	946	TYR	CA-CB	5.25	1.59	1.53
1	C	887	MET	SD-CE	5.19	1.92	1.79
1	A	694	TRP	NE1-CE2	-5.14	1.31	1.37
1	E	234	SER	C-O	-5.10	1.21	1.23
1	I	689	MET	SD-CE	5.01	1.92	1.79

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	487	GLY	N-CA-C	-7.57	106.08	115.08
1	G	362	LEU	N-CA-C	7.53	120.03	110.24
1	I	425	ARG	N-CA-C	-7.33	104.07	113.16
1	K	425	ARG	N-CA-C	-7.32	104.09	113.16
1	A	746	HIS	N-CA-C	7.31	121.48	111.54
1	E	487	GLY	N-CA-C	-7.29	106.41	115.08
1	A	355	VAL	N-CA-C	7.27	118.29	108.11
1	E	884	ILE	CA-C-N	7.18	126.68	118.85
1	E	884	ILE	C-N-CA	7.18	126.68	118.85
1	I	362	LEU	N-CA-C	7.14	119.52	110.24
1	G	487	GLY	N-CA-C	-7.09	106.25	114.69
1	A	487	GLY	N-CA-C	-7.00	106.75	115.08
1	A	884	ILE	CA-C-N	6.96	126.78	119.05
1	A	884	ILE	C-N-CA	6.96	126.78	119.05
1	E	362	LEU	N-CA-C	6.90	119.22	110.24
1	I	487	GLY	N-CA-C	-6.77	106.64	114.69
1	K	884	ILE	CA-C-N	6.76	126.36	119.19
1	K	884	ILE	C-N-CA	6.76	126.36	119.19
1	C	884	ILE	CA-C-N	6.73	126.19	118.85
1	C	884	ILE	C-N-CA	6.73	126.19	118.85
1	K	362	LEU	N-CA-C	6.71	118.97	110.24
1	A	362	LEU	N-CA-C	6.71	118.96	110.24
1	C	425	ARG	N-CA-C	-6.64	104.92	113.16
1	E	428	ILE	N-CA-C	-6.61	98.96	108.48
1	C	746	HIS	N-CA-C	6.59	120.51	111.54
1	K	428	ILE	N-CA-C	-6.56	99.03	108.48
1	G	425	ARG	N-CA-C	-6.55	105.03	113.16
1	A	425	ARG	N-CA-C	-6.53	105.07	113.16
1	E	355	VAL	N-CA-C	6.47	117.17	108.11
1	G	355	VAL	N-CA-C	6.44	117.12	108.11
1	I	746	HIS	N-CA-C	6.41	120.25	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	355	VAL	N-CA-C	6.39	117.06	108.11
1	C	801	ASP	CA-C-N	6.39	126.08	119.82
1	C	801	ASP	C-N-CA	6.39	126.08	119.82
1	E	364	ILE	N-CA-C	-6.34	98.73	107.99
1	K	355	VAL	N-CA-C	6.34	117.61	108.48
1	I	904	SER	N-CA-C	6.31	119.70	112.57
1	A	801	ASP	CA-C-N	6.30	126.00	119.82
1	A	801	ASP	C-N-CA	6.30	126.00	119.82
1	K	746	HIS	N-CA-C	6.27	120.07	111.54
1	C	362	LEU	N-CA-C	6.24	118.35	110.24
1	I	884	ILE	CA-C-N	6.24	125.65	118.85
1	I	884	ILE	C-N-CA	6.24	125.65	118.85
1	K	966	ASP	N-CA-C	-6.21	104.80	112.38
1	A	527	VAL	N-CA-C	6.19	116.51	111.62
1	I	966	ASP	N-CA-C	-6.19	104.83	112.38
1	K	134	PHE	N-CA-C	6.18	118.02	110.41
1	E	746	HIS	N-CA-C	6.18	119.94	111.54
1	C	735	ILE	N-CA-C	6.17	116.35	110.42
1	I	364	ILE	N-CA-C	-6.15	99.01	107.99
1	C	487	GLY	N-CA-C	-6.13	107.39	114.69
1	E	425	ARG	N-CA-C	-6.11	105.69	113.02
1	C	134	PHE	N-CA-C	6.10	117.91	110.41
1	G	884	ILE	CA-C-N	6.10	125.50	118.85
1	G	884	ILE	C-N-CA	6.10	125.50	118.85
1	E	134	PHE	N-CA-C	6.08	117.89	110.41
1	C	428	ILE	N-CA-C	-6.00	99.83	108.48
1	G	801	ASP	CA-C-N	5.99	125.67	119.56
1	G	801	ASP	C-N-CA	5.99	125.67	119.56
1	G	134	PHE	N-CA-C	5.96	117.75	110.41
1	I	134	PHE	N-CA-C	5.93	117.70	110.41
1	A	134	PHE	N-CA-C	5.90	117.66	110.41
1	E	965	SER	CB-CA-C	-5.89	109.22	117.23
1	G	904	SER	N-CA-C	5.88	119.22	112.57
1	I	953	GLY	N-CA-C	5.88	120.13	110.77
1	C	355	VAL	N-CA-C	5.83	116.88	108.48
1	G	364	ILE	N-CA-C	-5.80	99.52	107.99
1	C	577	PRO	CA-C-N	-5.77	115.66	123.10
1	C	577	PRO	C-N-CA	-5.77	115.66	123.10
1	A	577	PRO	CA-C-N	-5.75	115.69	123.10
1	A	577	PRO	C-N-CA	-5.75	115.69	123.10
1	K	801	ASP	CA-C-N	5.74	125.44	119.82
1	K	801	ASP	C-N-CA	5.74	125.44	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	ASP	N-CA-C	-5.73	106.13	113.23
1	G	746	HIS	N-CA-C	5.72	119.33	111.54
1	A	782	TYR	N-CA-C	5.71	118.52	110.23
1	A	700	ASN	N-CA-C	5.67	120.36	113.38
1	E	501	TYR	N-CA-C	5.65	115.69	108.24
1	K	364	ILE	N-CA-C	-5.64	99.76	107.99
1	G	966	ASP	N-CA-C	-5.63	105.50	112.38
1	K	407	VAL	N-CA-C	5.63	116.32	108.89
1	E	801	ASP	CA-C-N	5.56	125.23	119.56
1	E	801	ASP	C-N-CA	5.56	125.23	119.56
1	C	853	ASP	N-CA-C	-5.55	106.34	113.23
1	A	428	ILE	N-CA-C	-5.55	100.49	108.48
1	C	349	ASP	N-CA-C	-5.54	102.32	110.52
1	I	801	ASP	CA-C-N	5.52	125.23	119.82
1	I	801	ASP	C-N-CA	5.52	125.23	119.82
1	I	862	SER	N-CA-C	-5.47	105.22	111.07
1	C	527	VAL	N-CA-C	5.39	115.88	111.62
1	C	752	GLY	N-CA-C	-5.37	105.83	112.33
1	E	853	ASP	N-CA-C	-5.37	106.57	113.23
1	E	358	VAL	N-CA-C	-5.35	104.03	108.63
1	C	966	ASP	N-CA-C	-5.33	105.88	112.38
1	A	849	ILE	N-CA-C	5.32	115.96	108.36
1	K	993	GLY	N-CA-C	5.30	120.63	112.51
1	E	506	ASP	N-CA-C	-5.29	103.40	110.55
1	E	988	TRP	N-CA-C	5.29	120.10	111.37
1	E	993	GLY	N-CA-C	5.29	120.60	112.51
1	A	606	PHE	N-CA-C	5.28	116.72	111.07
1	E	782	TYR	N-CA-C	5.28	118.09	110.28
1	I	428	ILE	N-CA-C	-5.27	100.89	108.48
1	G	606	PHE	N-CA-C	5.26	116.70	111.07
1	E	606	PHE	N-CA-C	5.25	116.68	111.07
1	G	963	ALA	N-CA-C	-5.24	100.69	109.24
1	G	700	ASN	N-CA-C	5.23	119.81	113.38
1	K	349	ASP	N-CA-C	-5.23	103.01	110.59
1	C	968	ASP	N-CA-C	-5.22	105.50	111.14
1	E	847	LEU	N-CA-C	5.21	118.06	109.72
1	I	501	TYR	N-CA-C	5.21	115.42	108.38
1	K	853	ASP	N-CA-C	-5.21	106.77	113.23
1	G	501	TYR	N-CA-C	5.20	115.40	108.38
1	K	904	SER	N-CA-C	5.18	119.10	112.26
1	A	963	ALA	N-CA-C	-5.17	100.81	109.24
1	A	1039	ASP	N-CA-C	-5.17	105.72	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	364	ILE	N-CA-C	-5.17	100.45	107.99
1	C	847	LEU	N-CA-C	5.15	117.96	109.72
1	A	993	GLY	N-CA-C	5.15	120.39	112.51
1	I	879	ILE	N-CA-C	5.13	115.50	108.12
1	E	966	ASP	N-CA-C	-5.13	106.12	112.38
1	G	517	TYR	N-CA-C	-5.11	103.94	111.81
1	I	577	PRO	CA-C-N	-5.10	116.52	123.10
1	I	577	PRO	C-N-CA	-5.10	116.52	123.10
1	I	700	ASN	N-CA-C	5.10	119.65	113.38
1	K	847	LEU	N-CA-C	5.09	117.86	109.72
1	C	782	TYR	N-CA-C	5.08	117.81	110.28
1	G	853	ASP	N-CA-C	-5.08	106.93	113.23
1	I	963	ALA	N-CA-C	-5.07	100.98	109.24
1	K	501	TYR	N-CA-C	5.06	114.92	108.24
1	K	953	GLY	N-CA-C	5.05	118.80	110.77
1	A	847	LEU	N-CA-C	5.03	117.77	109.72
1	G	993	GLY	N-CA-C	5.03	120.20	112.51
1	C	522	PRO	N-CA-C	5.02	120.06	111.68
1	E	349	ASP	N-CA-C	-5.02	103.09	110.52

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	776	TYR	Sidechain
1	E	822	TYR	Sidechain
1	K	1025	TYR	Sidechain
1	K	822	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8177	0	8002	319	1
1	C	8177	0	8002	307	1
1	E	8177	0	8002	367	0
1	G	8177	0	8002	324	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	8177	0	8002	320	1
1	K	8177	0	8002	349	0
2	B	87	0	84	5	0
2	D	87	0	84	5	0
2	F	87	0	84	9	0
2	H	87	0	84	4	0
2	J	87	0	84	5	0
2	L	87	0	84	8	0
3	A	178	0	0	29	0
3	B	2	0	0	0	0
3	C	172	0	0	25	0
3	D	2	0	0	0	0
3	E	138	0	0	55	0
3	F	5	0	0	2	0
3	G	154	0	0	32	0
3	H	2	0	0	1	0
3	I	157	0	0	19	0
3	J	2	0	0	0	0
3	K	146	0	0	56	0
3	L	2	0	0	1	0
All	All	50544	0	48516	1902	2

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 20.

All (1902) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:351:SER:OG	1:I:353:THR:HG22	1.41	1.17
1:C:351:SER:OG	1:C:353:THR:HG22	1.46	1.16
1:G:351:SER:OG	1:G:353:THR:HG22	1.47	1.15
1:A:351:SER:OG	1:A:353:THR:HG22	1.45	1.14
1:E:351:SER:OG	1:E:353:THR:HG22	1.46	1.13
1:K:351:SER:OG	1:K:353:THR:HG22	1.52	1.10
3:E:1083:HOH:O	2:F:1213:PHE:HA	1.49	1.09
1:I:342:ARG:HG3	3:I:1095:HOH:O	1.54	1.08
1:K:241:ARG:HB3	3:K:1099:HOH:O	1.54	1.06
2:F:1213:PHE:O	3:F:239:HOH:O	1.73	1.04
1:E:702:TRP:HB3	3:E:1189:HOH:O	1.57	1.03
1:E:889:MET:HE3	3:E:1133:HOH:O	1.58	1.02
1:E:128:SER:HB2	3:E:1077:HOH:O	1.63	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:557:ARG:HH22	1:G:562:GLU:HB2	1.25	0.98
1:A:206:ARG:H	1:A:1024:ASN:HD21	1.11	0.98
1:K:557:ARG:HH22	1:K:562:GLU:HB2	1.28	0.97
1:G:276:ARG:HD3	3:G:1079:HOH:O	1.65	0.96
1:A:557:ARG:HH22	1:A:562:GLU:HB2	1.32	0.95
1:E:982:LEU:HG	3:E:1113:HOH:O	1.67	0.95
1:K:689:MET:HE3	3:K:1180:HOH:O	1.66	0.95
1:C:557:ARG:HH22	1:C:562:GLU:HB2	1.32	0.94
1:I:557:ARG:HH22	1:I:562:GLU:HB2	1.29	0.94
1:E:762:SER:HA	3:E:1135:HOH:O	1.66	0.94
1:E:557:ARG:HH22	1:E:562:GLU:HB2	1.30	0.93
1:K:858:ILE:HG13	3:K:1126:HOH:O	1.68	0.93
1:C:471:GLU:HA	3:C:1159:HOH:O	1.70	0.92
1:E:480:ILE:H	1:E:494:THR:CG2	1.83	0.92
1:K:351:SER:HG	1:K:353:THR:HG22	1.33	0.92
1:A:206:ARG:H	1:A:1024:ASN:ND2	1.68	0.91
1:A:480:ILE:H	1:A:494:THR:CG2	1.84	0.90
1:I:351:SER:HG	1:I:353:THR:HG22	1.34	0.90
1:I:206:ARG:H	1:I:1024:ASN:HD21	1.17	0.90
1:C:206:ARG:H	1:C:1024:ASN:HD21	1.16	0.90
1:G:480:ILE:H	1:G:494:THR:CG2	1.83	0.89
1:K:256:SER:HB2	3:K:1099:HOH:O	1.72	0.89
1:G:913:ARG:HH21	1:G:1047:GLN:HE21	1.20	0.89
1:E:74:ILE:HG13	1:E:75:VAL:HG12	1.54	0.88
1:E:351:SER:HG	1:E:353:THR:HG22	1.31	0.88
1:K:480:ILE:H	1:K:494:THR:CG2	1.85	0.88
1:C:351:SER:HG	1:C:353:THR:HG22	1.33	0.88
1:K:206:ARG:H	1:K:1024:ASN:HD21	1.17	0.88
1:K:251:PHE:HB3	3:K:1174:HOH:O	1.73	0.88
1:I:480:ILE:H	1:I:494:THR:CG2	1.87	0.87
1:I:525:ASP:HA	3:K:1090:HOH:O	1.72	0.87
1:I:913:ARG:HH21	1:I:1047:GLN:HE21	1.22	0.87
1:C:480:ILE:H	1:C:494:THR:CG2	1.86	0.87
1:G:736:VAL:HA	1:G:739:GLN:HE21	1.39	0.87
1:G:74:ILE:HG13	1:G:75:VAL:HG12	1.58	0.86
1:K:206:ARG:H	1:K:1024:ASN:ND2	1.72	0.86
1:E:206:ARG:H	1:E:1024:ASN:HD21	1.16	0.86
1:E:206:ARG:H	1:E:1024:ASN:ND2	1.73	0.85
1:I:206:ARG:H	1:I:1024:ASN:ND2	1.73	0.85
1:C:206:ARG:H	1:C:1024:ASN:ND2	1.74	0.85
1:K:736:VAL:HA	1:K:739:GLN:HE21	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:351:SER:HG	1:G:353:THR:HG22	1.39	0.84
1:E:736:VAL:HA	1:E:739:GLN:HE21	1.40	0.84
1:A:736:VAL:HA	1:A:739:GLN:HE21	1.41	0.84
1:G:40:PRO:HG2	1:G:724:LEU:HD22	1.59	0.84
1:K:73:LYS:HD3	1:K:76:SER:HB3	1.58	0.84
1:C:736:VAL:HA	1:C:739:GLN:HE21	1.40	0.84
1:A:351:SER:HG	1:A:353:THR:HG22	1.38	0.84
1:E:889:MET:HG2	3:E:1133:HOH:O	1.78	0.83
1:G:167:ASN:HB2	1:G:170:ILE:HB	1.61	0.83
1:I:736:VAL:HA	1:I:739:GLN:HE21	1.42	0.83
1:K:1001:ILE:HG23	3:K:1086:HOH:O	1.76	0.83
1:A:40:PRO:HG2	1:A:724:LEU:HD22	1.61	0.83
1:E:167:ASN:HB2	1:E:170:ILE:HB	1.58	0.83
1:C:40:PRO:HG2	1:C:724:LEU:HD22	1.59	0.83
1:K:167:ASN:HB2	1:K:170:ILE:HB	1.61	0.83
1:E:533:PHE:N	3:E:1181:HOH:O	2.11	0.83
1:G:206:ARG:H	1:G:1024:ASN:HD21	1.26	0.83
1:A:480:ILE:H	1:A:494:THR:HG22	1.43	0.82
1:K:337:ILE:HG13	1:K:649:MET:HE1	1.59	0.82
1:C:74:ILE:HG13	1:C:75:VAL:HG12	1.62	0.82
3:E:1181:HOH:O	1:G:525:ASP:HA	1.79	0.82
1:G:206:ARG:H	1:G:1024:ASN:ND2	1.78	0.82
1:I:167:ASN:HB2	1:I:170:ILE:HB	1.60	0.82
1:K:74:ILE:HG13	1:K:75:VAL:HG12	1.62	0.82
1:E:40:PRO:HG2	1:E:724:LEU:HD22	1.62	0.82
1:K:913:ARG:HH21	1:K:1047:GLN:HE21	1.27	0.81
1:K:643:ALA:HA	3:K:1107:HOH:O	1.79	0.81
1:I:40:PRO:HG2	1:I:724:LEU:HD22	1.61	0.81
1:A:703:ASN:C	1:A:703:ASN:HD22	1.89	0.81
1:E:337:ILE:HG13	1:E:649:MET:HE1	1.64	0.80
1:G:681:SER:HB3	1:G:684:GLU:HG2	1.61	0.80
1:K:394:THR:HB	3:K:1150:HOH:O	1.81	0.80
1:G:221:ALA:HB1	3:G:1113:HOH:O	1.80	0.80
1:E:913:ARG:HH21	1:E:1047:GLN:HE21	1.27	0.80
1:E:586:ARG:CZ	2:F:1206:ALA:HB3	2.10	0.80
1:E:703:ASN:HD22	1:E:703:ASN:C	1.89	0.80
1:E:1011:PHE:HB3	1:G:936:ASP:OD2	1.82	0.80
1:C:167:ASN:HB2	1:C:170:ILE:HB	1.62	0.80
1:K:709:GLU:OE2	1:K:713:ARG:HD3	1.82	0.80
1:I:74:ILE:HG13	1:I:75:VAL:HG12	1.62	0.79
1:I:337:ILE:HG13	1:I:649:MET:HE1	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:480:ILE:H	1:E:494:THR:HG22	1.46	0.79
1:G:480:ILE:H	1:G:494:THR:HG22	1.48	0.79
1:A:206:ARG:N	1:A:1024:ASN:HD21	1.81	0.78
1:A:74:ILE:HG13	1:A:75:VAL:HG12	1.64	0.78
1:E:73:LYS:HD3	1:E:76:SER:HB3	1.64	0.78
1:G:557:ARG:NH2	1:G:562:GLU:HB2	1.97	0.78
1:I:480:ILE:H	1:I:494:THR:HG22	1.48	0.78
1:G:625:LYS:HG3	3:G:1200:HOH:O	1.83	0.78
1:C:703:ASN:HD22	1:C:703:ASN:C	1.91	0.78
1:C:635:ASN:HA	3:C:1079:HOH:O	1.83	0.78
1:A:167:ASN:HB2	1:A:170:ILE:HB	1.66	0.77
1:K:40:PRO:HG2	1:K:724:LEU:HD22	1.64	0.77
1:K:440:VAL:HG12	3:K:1100:HOH:O	1.82	0.77
1:K:557:ARG:NH2	1:K:562:GLU:HB2	1.99	0.77
1:G:46:PRO:HB2	1:G:286:LEU:HD23	1.65	0.77
1:E:1033:ILE:HB	3:E:1123:HOH:O	1.82	0.77
1:I:709:GLU:OE2	1:I:713:ARG:HD3	1.84	0.77
1:G:337:ILE:HG13	1:G:649:MET:HE1	1.65	0.77
1:I:46:PRO:HB2	1:I:286:LEU:HD23	1.66	0.77
1:C:337:ILE:HG13	1:C:649:MET:HE1	1.67	0.77
1:E:46:PRO:HB2	1:E:286:LEU:HD23	1.66	0.77
1:K:203:LYS:HG2	3:K:1166:HOH:O	1.83	0.77
1:C:480:ILE:H	1:C:494:THR:HG22	1.48	0.76
1:E:709:GLU:OE2	1:E:713:ARG:HD3	1.85	0.76
1:G:709:GLU:OE2	1:G:713:ARG:HD3	1.84	0.76
1:I:53:ILE:HG23	1:I:286:LEU:HD21	1.66	0.76
1:I:73:LYS:HD3	1:I:76:SER:HB3	1.66	0.76
1:A:87:PHE:HB3	1:A:88:PRO:HD2	1.67	0.76
1:K:46:PRO:HB2	1:K:286:LEU:HD23	1.67	0.76
1:K:586:ARG:CZ	2:L:1206:ALA:HB3	2.15	0.76
1:K:999:ARG:HG2	1:K:1005:VAL:HG22	1.67	0.76
1:C:586:ARG:CZ	2:D:1206:ALA:HB3	2.16	0.76
1:E:992:VAL:CG1	3:E:1189:HOH:O	2.33	0.75
1:I:703:ASN:C	1:I:703:ASN:HD22	1.94	0.75
1:I:681:SER:HB3	1:I:684:GLU:HG2	1.67	0.75
1:C:279:ASN:ND2	3:C:1184:HOH:O	2.18	0.75
1:A:586:ARG:CZ	2:B:1206:ALA:HB3	2.17	0.75
1:C:284:ARG:HD3	3:C:1092:HOH:O	1.85	0.75
1:K:533:PHE:N	3:K:1090:HOH:O	2.19	0.75
1:K:233:SER:N	3:K:1097:HOH:O	2.20	0.75
1:K:681:SER:HB3	1:K:684:GLU:HG2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:LYS:HD3	1:C:76:SER:HB3	1.67	0.75
1:C:913:ARG:HH21	1:C:1047:GLN:HE21	1.33	0.74
1:E:557:ARG:NH2	1:E:562:GLU:HB2	2.02	0.74
1:K:505:PHE:HD1	3:K:1176:HOH:O	1.68	0.74
1:K:703:ASN:HD22	1:K:703:ASN:C	1.96	0.74
1:A:73:LYS:HD3	1:A:76:SER:HB3	1.69	0.74
1:G:53:ILE:HG23	1:G:286:LEU:HD21	1.70	0.74
1:K:480:ILE:H	1:K:494:THR:HG22	1.49	0.74
1:E:999:ARG:HG2	1:E:1005:VAL:HG22	1.68	0.74
1:E:331:PRO:HB3	1:E:649:MET:HE3	1.69	0.74
1:C:936:ASP:HB3	1:C:944:SER:HB2	1.70	0.74
1:I:557:ARG:NH2	1:I:562:GLU:HB2	2.03	0.74
1:C:789:GLU:OE1	3:C:1119:HOH:O	2.06	0.74
1:E:681:SER:HB3	1:E:684:GLU:HG2	1.70	0.74
1:K:1010:GLU:OE1	3:K:1079:HOH:O	2.06	0.73
1:A:61:LEU:HB3	1:A:75:VAL:HG13	1.68	0.73
1:A:557:ARG:NH2	1:A:562:GLU:HB2	2.01	0.73
1:E:498:SER:HB2	3:E:1107:HOH:O	1.86	0.73
1:I:586:ARG:CZ	2:J:1206:ALA:HB3	2.17	0.73
1:A:681:SER:HB3	1:A:684:GLU:HG2	1.71	0.73
1:A:936:ASP:HB3	1:A:944:SER:HB2	1.70	0.73
1:G:586:ARG:CZ	2:H:1206:ALA:HB3	2.19	0.73
1:I:190:ARG:CZ	3:I:1087:HOH:O	2.36	0.73
1:I:936:ASP:OD2	1:K:1011:PHE:HB3	1.88	0.73
1:K:936:ASP:HB3	1:K:944:SER:HB2	1.71	0.73
1:E:46:PRO:HB2	1:E:286:LEU:CD2	2.18	0.72
1:G:73:LYS:HD3	1:G:76:SER:HB3	1.70	0.72
3:K:1104:HOH:O	2:L:1213:PHE:HA	1.89	0.72
1:C:87:PHE:HB3	1:C:88:PRO:HD2	1.71	0.72
1:G:703:ASN:C	1:G:703:ASN:HD22	1.97	0.72
1:A:913:ARG:HH21	1:A:1047:GLN:HE21	1.33	0.72
1:C:557:ARG:NH2	1:C:562:GLU:HB2	2.04	0.72
1:A:365:ARG:HA	3:A:1133:HOH:O	1.90	0.72
1:C:228:MET:HE1	1:C:244:PHE:CE1	2.25	0.72
1:C:709:GLU:OE2	1:C:713:ARG:HD3	1.88	0.72
1:K:1008:GLN:NE2	3:K:1182:HOH:O	2.22	0.72
1:C:351:SER:OG	1:C:353:THR:CG2	2.33	0.72
1:I:403:ASN:HD22	1:I:404:LEU:N	1.87	0.72
1:A:253:GLN:HE22	1:A:270:PHE:H	1.38	0.72
1:A:337:ILE:HG13	1:A:649:MET:HE1	1.72	0.72
1:G:936:ASP:HB3	1:G:944:SER:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:403:ASN:ND2	1:I:405:GLY:H	1.87	0.72
1:I:1011:PHE:HB3	1:K:936:ASP:OD2	1.90	0.71
1:C:593:SER:O	1:C:624:VAL:HG22	1.90	0.71
1:I:351:SER:OG	1:I:353:THR:CG2	2.30	0.71
1:I:791:GLU:CD	1:I:861:ARG:HE	1.97	0.71
1:K:61:LEU:HB3	1:K:75:VAL:HG13	1.70	0.71
1:K:331:PRO:HB3	1:K:649:MET:HE3	1.71	0.71
1:A:228:MET:HE1	1:A:244:PHE:CE1	2.26	0.71
1:C:720:ASN:ND2	3:C:1186:HOH:O	2.12	0.71
1:E:206:ARG:N	1:E:1024:ASN:HD21	1.87	0.71
1:G:403:ASN:HD22	1:G:404:LEU:N	1.88	0.71
1:A:709:GLU:OE2	1:A:713:ARG:HD3	1.90	0.71
1:E:133:MET:HA	3:E:1077:HOH:O	1.91	0.71
1:E:948:THR:H	1:G:922:GLN:HE22	1.37	0.71
1:C:46:PRO:HB2	1:C:286:LEU:HD23	1.71	0.71
1:E:936:ASP:OD2	1:G:1011:PHE:HB3	1.90	0.71
1:I:913:ARG:HH21	1:I:1047:GLN:NE2	1.88	0.70
1:E:984:GLY:HA2	3:E:1123:HOH:O	1.90	0.70
1:K:87:PHE:HB3	1:K:88:PRO:HD2	1.73	0.70
1:G:351:SER:OG	1:G:353:THR:CG2	2.35	0.70
1:C:53:ILE:HG23	1:C:286:LEU:HD21	1.74	0.70
1:E:936:ASP:HB3	1:E:944:SER:HB2	1.71	0.70
1:I:206:ARG:N	1:I:1024:ASN:HD21	1.90	0.70
1:K:53:ILE:HG23	1:K:286:LEU:HD21	1.72	0.70
1:C:403:ASN:HD22	1:C:404:LEU:N	1.89	0.70
1:A:593:SER:O	1:A:624:VAL:HG22	1.92	0.70
1:G:1016:ARG:HG3	3:G:1099:HOH:O	1.90	0.70
1:I:929:MET:HE2	3:I:1166:HOH:O	1.92	0.70
1:E:557:ARG:NH1	3:E:1152:HOH:O	2.23	0.69
1:I:87:PHE:HB3	1:I:88:PRO:HD2	1.72	0.69
1:I:936:ASP:HB3	1:I:944:SER:HB2	1.72	0.69
1:E:403:ASN:HD22	1:E:404:LEU:N	1.90	0.69
1:G:530:ASN:ND2	1:G:531:PHE:H	1.90	0.69
1:E:372:ASP:HB2	3:E:1112:HOH:O	1.91	0.69
1:E:812:GLY:HA3	3:E:1150:HOH:O	1.91	0.69
1:G:999:ARG:HG2	1:G:1005:VAL:HG22	1.75	0.69
1:A:403:ASN:HD22	1:A:404:LEU:N	1.90	0.69
1:G:61:LEU:HD13	1:G:74:ILE:HD11	1.75	0.69
1:K:519:SER:OG	3:K:1125:HOH:O	2.10	0.69
1:G:253:GLN:HE22	1:G:270:PHE:H	1.39	0.69
1:C:681:SER:HB3	1:C:684:GLU:HG2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:HB3	1:C:75:VAL:HG13	1.75	0.68
1:E:351:SER:OG	1:E:353:THR:CG2	2.35	0.68
1:G:46:PRO:HB2	1:G:286:LEU:CD2	2.23	0.68
1:E:87:PHE:HB3	1:E:88:PRO:HD2	1.76	0.68
1:K:82:ASN:H	1:K:82:ASN:HD22	1.40	0.68
1:A:530:ASN:ND2	1:A:531:PHE:H	1.91	0.68
1:E:228:MET:HE1	1:E:244:PHE:CE1	2.28	0.68
1:E:61:LEU:HD13	1:E:74:ILE:HD11	1.76	0.68
1:I:228:MET:HE1	1:I:244:PHE:CE1	2.28	0.68
1:K:46:PRO:HB2	1:K:286:LEU:CD2	2.23	0.68
1:K:206:ARG:N	1:K:1024:ASN:HD21	1.90	0.68
1:G:87:PHE:HB3	1:G:88:PRO:HD2	1.75	0.68
1:K:403:ASN:ND2	1:K:405:GLY:H	1.91	0.68
1:G:403:ASN:ND2	1:G:405:GLY:H	1.92	0.68
1:G:557:ARG:HH22	1:G:562:GLU:CB	2.05	0.68
1:E:61:LEU:HB3	1:E:75:VAL:HG13	1.75	0.67
1:G:331:PRO:HB3	1:G:649:MET:HE3	1.74	0.67
1:G:913:ARG:HH21	1:G:1047:GLN:NE2	1.91	0.67
1:E:403:ASN:ND2	1:E:405:GLY:H	1.93	0.67
1:A:403:ASN:ND2	1:A:405:GLY:H	1.92	0.67
1:K:403:ASN:HD22	1:K:404:LEU:N	1.91	0.67
1:K:498:SER:HB2	3:K:1073:HOH:O	1.93	0.67
1:A:46:PRO:HB2	1:A:286:LEU:HD23	1.76	0.67
1:E:253:GLN:HE22	1:E:270:PHE:H	1.42	0.67
1:I:253:GLN:HE22	1:I:270:PHE:H	1.40	0.67
1:I:331:PRO:HB3	1:I:649:MET:HE3	1.76	0.67
1:K:228:MET:HE1	1:K:244:PHE:CE1	2.29	0.67
1:E:949:ASN:ND2	1:G:475:TYR:OH	2.25	0.67
1:I:530:ASN:ND2	1:I:531:PHE:H	1.94	0.67
1:I:999:ARG:HG2	1:I:1005:VAL:HG22	1.75	0.67
1:A:53:ILE:HG23	1:A:286:LEU:HD21	1.77	0.66
1:C:206:ARG:N	1:C:1024:ASN:HD21	1.89	0.66
1:E:82:ASN:H	1:E:82:ASN:HD22	1.44	0.66
1:G:218:ASN:HB3	1:G:221:ALA:HB3	1.77	0.66
1:C:999:ARG:HG2	1:C:1005:VAL:HG22	1.78	0.66
1:G:61:LEU:HB3	1:G:75:VAL:HG13	1.76	0.66
1:G:82:ASN:HD22	1:G:82:ASN:H	1.43	0.66
1:K:543:PRO:HB3	3:K:1202:HOH:O	1.95	0.66
1:C:253:GLN:HE22	1:C:270:PHE:H	1.44	0.66
1:A:471:GLU:HA	3:A:1170:HOH:O	1.95	0.66
1:A:591:LEU:HD12	1:A:596:LEU:HD23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1148:HOH:O	1:C:477:MET:HG2	1.95	0.66
2:F:1209:GLU:O	3:F:525:HOH:O	2.14	0.66
1:A:351:SER:OG	1:A:353:THR:CG2	2.34	0.66
1:A:999:ARG:HG2	1:A:1005:VAL:HG22	1.77	0.66
1:C:403:ASN:ND2	1:C:405:GLY:H	1.93	0.66
1:C:591:LEU:HD12	1:C:596:LEU:HD23	1.78	0.66
1:E:53:ILE:HG23	1:E:286:LEU:HD21	1.77	0.66
1:E:218:ASN:HB3	1:E:221:ALA:HB3	1.78	0.66
3:K:1170:HOH:O	2:L:1203:THR:HG23	1.95	0.65
1:A:82:ASN:HD22	1:A:82:ASN:H	1.44	0.65
1:A:284:ARG:HD3	3:A:1095:HOH:O	1.96	0.65
1:C:791:GLU:CD	1:C:861:ARG:HE	2.03	0.65
1:C:892:LEU:HD13	1:C:920:VAL:HG21	1.79	0.65
1:E:913:ARG:HH21	1:E:1047:GLN:NE2	1.95	0.65
1:K:746:HIS:CE1	3:K:1104:HOH:O	2.49	0.65
1:A:61:LEU:HD13	1:A:74:ILE:HD11	1.78	0.65
1:I:1002:ASP:HA	3:I:1095:HOH:O	1.96	0.65
1:C:331:PRO:HB3	1:C:649:MET:HE3	1.79	0.65
1:G:228:MET:HE1	1:G:244:PHE:CE1	2.31	0.65
1:K:322:PRO:HA	1:K:678:LEU:HD22	1.79	0.65
1:G:909:ILE:HG12	1:G:956:ILE:CG2	2.27	0.65
1:K:256:SER:OG	1:K:267:HIS:HE1	1.79	0.65
1:K:301:GLU:HB3	3:K:1195:HOH:O	1.96	0.65
1:E:815:VAL:HA	1:E:819:SER:HB3	1.79	0.65
1:C:82:ASN:H	1:C:82:ASN:HD22	1.43	0.65
1:I:46:PRO:HB2	1:I:286:LEU:CD2	2.26	0.65
1:K:557:ARG:HH22	1:K:562:GLU:CB	2.08	0.65
1:K:591:LEU:HD12	1:K:596:LEU:HD23	1.78	0.65
1:G:322:PRO:HA	1:G:678:LEU:HD22	1.78	0.64
1:K:319:ILE:HG23	1:K:677:PRO:HB3	1.79	0.64
1:A:279:ASN:ND2	3:A:1111:HOH:O	2.30	0.64
1:G:791:GLU:CD	1:G:861:ARG:HE	2.05	0.64
1:K:253:GLN:HE22	1:K:270:PHE:H	1.46	0.64
1:K:351:SER:OG	1:K:353:THR:CG2	2.39	0.64
1:A:331:PRO:HB3	1:A:649:MET:HE3	1.79	0.64
1:G:558:SER:HA	1:K:393:ARG:HE	1.60	0.64
1:K:52:ARG:NH1	1:K:90:GLY:O	2.29	0.64
1:A:815:VAL:HA	1:A:819:SER:HB3	1.80	0.64
1:C:46:PRO:HB2	1:C:286:LEU:CD2	2.27	0.64
1:C:52:ARG:NH1	1:C:90:GLY:O	2.30	0.64
1:G:589:ILE:HD13	1:G:641:LEU:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:61:LEU:HB3	1:I:75:VAL:HG13	1.80	0.64
1:A:791:GLU:CD	1:A:861:ARG:HE	2.05	0.64
1:K:791:GLU:CD	1:K:861:ARG:HE	2.06	0.64
1:C:530:ASN:ND2	1:C:531:PHE:H	1.95	0.64
1:E:948:THR:HA	3:E:1102:HOH:O	1.97	0.64
1:G:591:LEU:HD12	1:G:596:LEU:HD23	1.78	0.64
1:I:132:ARG:HA	3:I:1207:HOH:O	1.98	0.64
1:C:700:ASN:HD22	1:C:1008:GLN:NE2	1.96	0.64
1:I:67:LYS:HD2	3:I:1203:HOH:O	1.98	0.64
1:I:913:ARG:NH2	1:I:1047:GLN:HE21	1.94	0.64
1:A:46:PRO:HB2	1:A:286:LEU:CD2	2.28	0.63
1:I:909:ILE:HG12	1:I:956:ILE:CG2	2.28	0.63
1:G:593:SER:O	1:G:624:VAL:HG22	1.98	0.63
1:I:322:PRO:HA	1:I:678:LEU:HD22	1.80	0.63
1:A:228:MET:HE1	1:A:244:PHE:CZ	2.34	0.63
1:C:677:PRO:HD2	1:I:827:GLU:O	1.97	0.63
1:G:660:PHE:HB3	1:G:668:GLU:HB3	1.80	0.63
1:C:322:PRO:HA	1:C:678:LEU:HD22	1.79	0.63
1:G:206:ARG:N	1:G:1024:ASN:HD21	1.95	0.63
1:A:676:ARG:CD	3:A:1073:HOH:O	2.47	0.63
1:I:403:ASN:HD22	1:I:403:ASN:C	2.07	0.63
1:I:548:SER:O	3:I:1178:HOH:O	2.15	0.63
1:E:393:ARG:HE	1:I:558:SER:HA	1.63	0.63
1:I:61:LEU:HD13	1:I:74:ILE:HD11	1.79	0.63
1:I:949:ASN:ND2	1:K:475:TYR:OH	2.24	0.63
1:K:537:SER:HB3	1:K:583:GLY:O	1.99	0.62
1:A:322:PRO:HA	1:A:678:LEU:HD22	1.80	0.62
1:G:596:LEU:HD12	1:G:619:LEU:HD11	1.81	0.62
1:K:406:ASN:HB2	1:K:424:ASP:CG	2.24	0.62
1:K:660:PHE:HB3	1:K:668:GLU:HB3	1.82	0.62
1:E:52:ARG:NH1	1:E:90:GLY:O	2.33	0.62
1:I:82:ASN:HD22	1:I:82:ASN:H	1.45	0.62
1:K:356:LEU:HD23	3:K:1137:HOH:O	1.98	0.62
1:E:983:ILE:HG23	3:E:1123:HOH:O	1.99	0.62
1:K:815:VAL:HA	1:K:819:SER:HB3	1.81	0.62
1:K:892:LEU:HD13	1:K:920:VAL:HG21	1.81	0.62
1:A:596:LEU:HD12	1:A:619:LEU:HD11	1.82	0.62
1:I:700:ASN:HD22	1:I:1008:GLN:NE2	1.97	0.62
1:I:922:GLN:HE22	1:K:948:THR:H	1.48	0.62
1:K:593:SER:O	1:K:624:VAL:HG22	1.99	0.62
1:K:913:ARG:HH21	1:K:1047:GLN:NE2	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:530:ASN:ND2	1:K:531:PHE:H	1.98	0.61
1:A:534:GLU:HG3	1:C:534:GLU:OE2	2.00	0.61
1:C:61:LEU:HD13	1:C:74:ILE:HD11	1.82	0.61
1:E:596:LEU:HD12	1:E:619:LEU:HD11	1.83	0.61
1:K:61:LEU:CB	1:K:75:VAL:HG13	2.30	0.61
1:A:676:ARG:HD2	3:A:1073:HOH:O	2.01	0.61
1:E:319:ILE:HG23	1:E:677:PRO:HB3	1.82	0.61
1:K:800:ILE:HG21	1:K:845:ARG:NH2	2.15	0.61
1:A:319:ILE:HG23	1:A:677:PRO:HB3	1.82	0.61
1:A:414:ARG:HD3	3:A:1162:HOH:O	1.99	0.61
1:C:295:ILE:HG13	1:C:306:ILE:HD11	1.82	0.61
1:E:791:GLU:CD	1:E:861:ARG:HE	2.09	0.61
1:G:319:ILE:HG23	1:G:677:PRO:HB3	1.82	0.61
1:I:660:PHE:HB3	1:I:668:GLU:HB3	1.83	0.61
1:A:556:PRO:HD3	1:I:354:TYR:CD1	2.36	0.61
1:E:541:VAL:HG22	1:E:542:ILE:N	2.16	0.61
1:E:591:LEU:HD12	1:E:596:LEU:HD23	1.81	0.61
1:E:922:GLN:HE22	1:G:948:THR:H	1.48	0.61
1:A:892:LEU:HD13	1:A:920:VAL:HG21	1.82	0.61
1:G:815:VAL:HA	1:G:819:SER:HB3	1.81	0.61
1:K:61:LEU:HD13	1:K:74:ILE:HD11	1.82	0.61
1:A:218:ASN:HB3	1:A:221:ALA:HB3	1.82	0.61
1:A:478:GLN:HB3	1:A:499:HIS:HD2	1.66	0.61
1:C:40:PRO:HG2	1:C:724:LEU:CD2	2.30	0.61
1:I:218:ASN:HB3	1:I:221:ALA:HB3	1.82	0.61
1:E:401:GLU:H	1:E:401:GLU:CD	2.08	0.61
1:K:700:ASN:HD22	1:K:1008:GLN:NE2	1.99	0.61
1:G:52:ARG:NH1	1:G:90:GLY:O	2.33	0.61
1:E:256:SER:OG	1:E:267:HIS:HE1	1.83	0.60
1:A:534:GLU:OE2	1:C:534:GLU:HG3	2.01	0.60
1:C:228:MET:HE1	1:C:244:PHE:CZ	2.37	0.60
1:A:52:ARG:NH1	1:A:90:GLY:O	2.34	0.60
1:C:401:GLU:CD	1:C:401:GLU:H	2.08	0.60
1:C:556:PRO:HD3	1:G:354:TYR:CD1	2.35	0.60
1:A:401:GLU:CD	1:A:401:GLU:H	2.08	0.60
1:G:401:GLU:H	1:G:401:GLU:CD	2.09	0.60
1:G:403:ASN:HD22	1:G:403:ASN:C	2.10	0.60
1:I:53:ILE:CG2	1:I:286:LEU:HD21	2.31	0.60
1:A:537:SER:HB3	1:A:583:GLY:O	2.02	0.60
1:C:660:PHE:HB3	1:C:668:GLU:HB3	1.84	0.60
1:G:390:TYR:HD1	1:G:397:ALA:HB2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:986:ARG:HD2	1:K:1025:TYR:O	2.02	0.60
1:A:929:MET:HE3	1:A:979:LEU:HD11	1.84	0.60
1:C:603:HIS:HD2	1:C:604:GLY:O	1.85	0.60
1:E:478:GLN:HB3	1:E:499:HIS:HD2	1.66	0.60
1:E:530:ASN:ND2	1:E:531:PHE:H	2.00	0.60
1:K:432:ASP:OD1	1:K:434:GLU:HB3	2.01	0.60
1:K:774:ASP:HA	1:K:817:ALA:HB2	1.84	0.60
1:K:977:LEU:HB2	1:K:979:LEU:HD13	1.82	0.60
1:A:300:THR:HG21	3:A:1178:HOH:O	2.00	0.59
1:G:537:SER:HB3	1:G:583:GLY:O	2.01	0.59
1:G:977:LEU:HB2	1:G:979:LEU:HD13	1.83	0.59
1:K:909:ILE:HG12	1:K:956:ILE:CG2	2.31	0.59
1:A:480:ILE:N	1:A:494:THR:HG22	2.16	0.59
1:C:815:VAL:HA	1:C:819:SER:HB3	1.84	0.59
1:A:677:PRO:HD2	1:G:827:GLU:O	2.01	0.59
1:C:319:ILE:HG23	1:C:677:PRO:HB3	1.83	0.59
1:E:101:SER:N	3:E:1094:HOH:O	2.34	0.59
1:E:781:ALA:HB2	1:E:802:PRO:HG2	1.83	0.59
1:K:107:ASP:OD2	3:K:1131:HOH:O	2.16	0.59
1:K:218:ASN:HB3	1:K:221:ALA:HB3	1.84	0.59
1:K:390:TYR:HD1	1:K:397:ALA:HB2	1.67	0.59
1:G:753:THR:HB	3:G:1163:HOH:O	2.02	0.59
1:G:882:ILE:HD11	1:G:899:PHE:HA	1.84	0.59
1:A:557:ARG:HH22	1:A:562:GLU:CB	2.10	0.59
1:A:774:ASP:HA	1:A:817:ALA:HB2	1.85	0.59
1:C:218:ASN:HB3	1:C:221:ALA:HB3	1.84	0.59
1:E:229:SER:HB3	1:E:248:ILE:HD11	1.84	0.59
1:E:322:PRO:HA	1:E:678:LEU:HD22	1.84	0.59
1:E:774:ASP:HA	1:E:817:ALA:HB2	1.84	0.59
1:I:537:SER:HB3	1:I:583:GLY:O	2.02	0.59
1:I:557:ARG:HH22	1:I:562:GLU:CB	2.10	0.59
1:A:700:ASN:HD22	1:A:1008:GLN:NE2	2.00	0.59
1:E:61:LEU:CB	1:E:75:VAL:HG13	2.33	0.59
1:E:295:ILE:HG13	1:E:306:ILE:HD11	1.85	0.59
1:K:800:ILE:HG21	1:K:845:ARG:HH22	1.68	0.59
1:G:141:ASP:OD1	1:G:145:ASN:HB2	2.03	0.59
1:G:800:ILE:HG21	1:G:845:ARG:NH2	2.17	0.59
1:A:660:PHE:HB3	1:A:668:GLU:HB3	1.84	0.59
1:E:660:PHE:HB3	1:E:668:GLU:HB3	1.85	0.59
1:A:256:SER:OG	1:A:267:HIS:HE1	1.86	0.59
1:I:319:ILE:HG23	1:I:677:PRO:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:541:VAL:HG22	1:K:542:ILE:N	2.17	0.59
1:C:809:ASP:HB3	1:C:814:THR:HA	1.85	0.59
1:E:557:ARG:HH22	1:E:562:GLU:CB	2.11	0.59
1:I:229:SER:HB3	1:I:248:ILE:HD11	1.83	0.59
1:K:229:SER:HB3	1:K:248:ILE:HD11	1.85	0.59
1:C:746:HIS:NE2	2:D:1214:OQE:C1	2.66	0.58
1:I:342:ARG:NH2	3:I:1095:HOH:O	2.34	0.58
1:I:480:ILE:N	1:I:494:THR:HG22	2.18	0.58
1:I:800:ILE:HG21	1:I:845:ARG:NH2	2.18	0.58
1:K:440:VAL:CG1	3:K:1100:HOH:O	2.45	0.58
1:A:603:HIS:HD2	1:A:604:GLY:O	1.86	0.58
1:A:800:ILE:HG21	1:A:845:ARG:HH22	1.67	0.58
1:E:929:MET:HE3	1:E:979:LEU:HD11	1.85	0.58
1:G:131:ARG:HB2	3:G:1131:HOH:O	2.02	0.58
1:I:478:GLN:HB3	1:I:499:HIS:HD2	1.67	0.58
1:I:589:ILE:HD13	1:I:641:LEU:HD12	1.85	0.58
1:C:557:ARG:HH22	1:C:562:GLU:CB	2.11	0.58
1:E:430:THR:HG23	1:E:441:ILE:HD11	1.84	0.58
1:E:593:SER:O	1:E:624:VAL:HG22	2.04	0.58
1:E:800:ILE:HG21	1:E:845:ARG:NH2	2.18	0.58
1:E:909:ILE:HG12	1:E:956:ILE:CG2	2.33	0.58
1:G:800:ILE:HG21	1:G:845:ARG:HH22	1.67	0.58
1:G:913:ARG:NH2	1:G:1047:GLN:HE21	1.96	0.58
1:I:286:LEU:HD12	1:I:295:ILE:HG12	1.86	0.58
1:C:307:GLU:C	1:C:308:ILE:HD12	2.29	0.58
1:G:681:SER:CB	1:G:684:GLU:HG2	2.33	0.58
1:A:909:ILE:HG12	1:A:956:ILE:CG2	2.33	0.58
1:E:863:TRP:CD1	3:E:1114:HOH:O	2.55	0.58
1:G:478:GLN:HB3	1:G:499:HIS:HD2	1.69	0.58
1:I:591:LEU:HD12	1:I:596:LEU:HD23	1.84	0.58
1:I:815:VAL:HA	1:I:819:SER:HB3	1.85	0.58
1:K:307:GLU:HG2	3:K:1177:HOH:O	2.04	0.58
1:E:222:PHE:HB2	1:E:1038:HIS:HD2	1.69	0.58
1:A:40:PRO:HG2	1:A:724:LEU:CD2	2.31	0.58
1:A:61:LEU:CB	1:A:75:VAL:HG13	2.34	0.58
1:I:593:SER:O	1:I:624:VAL:HG22	2.02	0.58
1:K:286:LEU:HD12	1:K:295:ILE:HG12	1.84	0.58
1:C:977:LEU:HB2	1:C:979:LEU:HD13	1.84	0.58
1:E:314:PRO:HD2	1:E:726:LYS:HG2	1.86	0.58
1:G:700:ASN:HD22	1:G:1008:GLN:NE2	2.01	0.58
1:K:73:LYS:HD3	1:K:76:SER:CB	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:480:ILE:N	1:K:494:THR:HG22	2.17	0.58
1:G:40:PRO:HG2	1:G:724:LEU:CD2	2.32	0.58
1:I:190:ARG:NH1	3:I:1087:HOH:O	2.34	0.58
1:I:885:PRO:O	1:I:915:ASN:HA	2.04	0.58
1:A:744:THR:HA	3:A:1151:HOH:O	2.02	0.58
1:A:800:ILE:HG21	1:A:845:ARG:NH2	2.17	0.58
1:C:124:PHE:CE2	1:C:153:MET:HE1	2.39	0.58
1:C:403:ASN:HD22	1:C:403:ASN:C	2.12	0.58
1:E:889:MET:CE	3:E:1133:HOH:O	2.28	0.58
1:I:141:ASP:OD1	1:I:145:ASN:HB2	2.04	0.58
1:I:781:ALA:HB2	1:I:802:PRO:HG2	1.85	0.58
1:A:618:VAL:CG2	1:A:631:GLU:HG3	2.34	0.57
1:K:781:ALA:HB2	1:K:802:PRO:HG2	1.86	0.57
1:C:390:TYR:HD1	1:C:397:ALA:HB2	1.69	0.57
1:E:480:ILE:N	1:E:494:THR:HG22	2.18	0.57
1:G:307:GLU:C	1:G:308:ILE:HD12	2.29	0.57
1:I:307:GLU:C	1:I:308:ILE:HD12	2.29	0.57
1:I:475:TYR:OH	1:K:949:ASN:ND2	2.36	0.57
1:A:155:PRO:O	1:A:856:ARG:HD2	2.05	0.57
1:A:403:ASN:HD22	1:A:403:ASN:C	2.13	0.57
1:A:913:ARG:HH21	1:A:1047:GLN:NE2	2.01	0.57
1:K:363:ARG:HB3	1:K:380:GLY:O	2.04	0.57
1:K:403:ASN:HD22	1:K:403:ASN:C	2.11	0.57
1:C:88:PRO:HG2	1:C:89:ASP:H	1.68	0.57
1:C:220:GLY:O	1:C:1038:HIS:HB3	2.04	0.57
1:C:596:LEU:HD12	1:C:619:LEU:HD11	1.86	0.57
1:E:286:LEU:HD12	1:E:295:ILE:HG12	1.86	0.57
1:A:229:SER:HB3	1:A:248:ILE:HD11	1.87	0.57
1:C:286:LEU:HD12	1:C:295:ILE:HG12	1.86	0.57
1:A:286:LEU:HD12	1:A:295:ILE:HG12	1.87	0.57
1:C:774:ASP:HA	1:C:817:ALA:HB2	1.86	0.57
1:E:423:ASN:HD22	1:E:423:ASN:C	2.12	0.57
1:A:406:ASN:HB2	1:A:424:ASP:CG	2.30	0.57
1:C:800:ILE:HG21	1:C:845:ARG:NH2	2.19	0.57
1:E:363:ARG:HB3	1:E:380:GLY:O	2.03	0.57
1:I:746:HIS:NE2	2:J:1214:OQE:C1	2.67	0.57
1:K:63:GLU:C	3:K:1152:HOH:O	2.47	0.57
1:K:746:HIS:NE2	2:L:1214:OQE:C1	2.67	0.57
1:C:489:LYS:HG3	1:C:491:PHE:CE1	2.40	0.57
1:E:948:THR:H	1:G:922:GLN:NE2	2.02	0.57
1:K:278:LEU:HD23	1:K:287:PHE:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:929:MET:HE3	1:C:979:LEU:HD11	1.87	0.57
1:E:475:TYR:OH	1:G:949:ASN:ND2	2.34	0.57
1:G:61:LEU:CB	1:G:75:VAL:HG13	2.35	0.57
1:G:568:LEU:HB3	1:G:571:MET:HE2	1.85	0.57
1:I:401:GLU:CD	1:I:401:GLU:H	2.13	0.57
1:I:774:ASP:HA	1:I:817:ALA:HB2	1.86	0.57
1:A:124:PHE:CE2	1:A:153:MET:HE1	2.39	0.57
1:A:568:LEU:HB3	1:A:571:MET:HE2	1.86	0.57
1:C:229:SER:HB3	1:C:248:ILE:HD11	1.85	0.57
1:A:727:THR:O	1:A:730:ASP:HB2	2.05	0.56
1:A:874:ARG:NE	3:A:1176:HOH:O	2.38	0.56
1:C:478:GLN:HB3	1:C:499:HIS:HD2	1.70	0.56
1:G:286:LEU:HD12	1:G:295:ILE:HG12	1.87	0.56
1:I:390:TYR:HD1	1:I:397:ALA:HB2	1.68	0.56
1:K:809:ASP:HB3	1:K:814:THR:HA	1.87	0.56
1:K:929:MET:HE3	1:K:979:LEU:HD11	1.87	0.56
1:A:218:ASN:O	1:A:220:GLY:N	2.37	0.56
1:A:589:ILE:HD13	1:A:641:LEU:HD12	1.85	0.56
1:C:586:ARG:HG3	2:D:1204:GLN:HG3	1.87	0.56
1:E:1047:GLN:HG2	3:E:1123:HOH:O	2.05	0.56
1:G:88:PRO:HG2	1:G:89:ASP:H	1.70	0.56
1:K:53:ILE:CG2	1:K:286:LEU:HD21	2.35	0.56
1:K:735:ILE:O	1:K:739:GLN:HG3	2.05	0.56
1:A:88:PRO:HG2	1:A:89:ASP:H	1.69	0.56
1:A:498:SER:OG	1:A:518:ARG:HG2	2.05	0.56
1:C:314:PRO:HD2	1:C:726:LYS:HG2	1.86	0.56
1:C:676:ARG:HD2	3:C:1072:HOH:O	2.04	0.56
1:E:228:MET:HE1	1:E:244:PHE:CZ	2.40	0.56
1:E:537:SER:HB3	1:E:583:GLY:O	2.04	0.56
1:E:737:GLU:HG2	3:E:1197:HOH:O	2.05	0.56
1:E:913:ARG:NH2	1:E:1047:GLN:HE21	2.01	0.56
1:I:546:PRO:HG2	1:I:567:ASP:HB3	1.87	0.56
1:I:977:LEU:HB2	1:I:979:LEU:HD13	1.88	0.56
1:K:220:GLY:O	1:K:1038:HIS:HB3	2.05	0.56
1:C:124:PHE:CD2	1:C:153:MET:HE1	2.39	0.56
1:I:909:ILE:HA	1:I:956:ILE:HG22	1.87	0.56
1:K:478:GLN:HB3	1:K:499:HIS:HD2	1.70	0.56
1:E:882:ILE:HD11	1:E:899:PHE:HA	1.88	0.56
1:G:314:PRO:HD2	1:G:726:LYS:HG2	1.87	0.56
1:I:228:MET:HE1	1:I:244:PHE:CZ	2.41	0.56
1:K:44:LEU:HD12	1:K:56:VAL:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:ASN:C	1:C:423:ASN:HD22	2.14	0.56
1:C:913:ARG:HH21	1:C:1047:GLN:NE2	1.99	0.56
1:E:390:TYR:HD1	1:E:397:ALA:HB2	1.71	0.56
1:G:674:ASP:HB2	3:G:1150:HOH:O	2.06	0.56
1:A:743:ARG:O	3:A:1151:HOH:O	2.18	0.56
1:A:977:LEU:HB2	1:A:979:LEU:HD13	1.88	0.56
1:E:800:ILE:HG21	1:E:845:ARG:HH22	1.70	0.56
1:K:603:HIS:HD2	1:K:604:GLY:O	1.88	0.56
1:K:882:ILE:HD11	1:K:899:PHE:HA	1.87	0.56
1:E:406:ASN:HB2	1:E:424:ASP:CG	2.30	0.56
1:E:977:LEU:HB2	1:E:979:LEU:HD13	1.87	0.56
1:G:278:LEU:HD23	1:G:287:PHE:HB3	1.88	0.56
1:I:318:ILE:HG21	1:I:682:ILE:HD11	1.87	0.56
1:I:295:ILE:HG13	1:I:306:ILE:HD11	1.88	0.56
1:K:546:PRO:HG2	1:K:567:ASP:HB3	1.88	0.56
1:K:746:HIS:HA	1:K:748:TYR:CZ	2.41	0.56
1:C:589:ILE:HD13	1:C:641:LEU:HD12	1.88	0.55
1:E:722:VAL:N	1:E:723:PRO:HD2	2.22	0.55
1:I:53:ILE:HG23	1:I:286:LEU:CD2	2.36	0.55
1:I:88:PRO:HG2	1:I:89:ASP:H	1.71	0.55
1:K:228:MET:HE1	1:K:244:PHE:CZ	2.40	0.55
1:A:278:LEU:HD23	1:A:287:PHE:HB3	1.88	0.55
1:A:314:PRO:HD2	1:A:726:LYS:HG2	1.86	0.55
1:C:253:GLN:NE2	1:C:268:THR:OG1	2.39	0.55
1:C:909:ILE:HG12	1:C:956:ILE:CG2	2.36	0.55
1:C:929:MET:HE3	1:C:979:LEU:CD1	2.37	0.55
1:E:809:ASP:HB3	1:E:814:THR:HA	1.88	0.55
1:G:728:ARG:HD3	3:G:1073:HOH:O	2.04	0.55
1:G:781:ALA:HB2	1:G:802:PRO:HG2	1.88	0.55
1:G:909:ILE:HA	1:G:956:ILE:HG22	1.88	0.55
1:K:596:LEU:HD12	1:K:619:LEU:HD11	1.88	0.55
1:A:363:ARG:HB3	1:A:380:GLY:O	2.07	0.55
1:A:390:TYR:HD1	1:A:397:ALA:HB2	1.71	0.55
1:A:417:LYS:NZ	3:A:1164:HOH:O	2.37	0.55
1:C:155:PRO:O	1:C:856:ARG:HD2	2.06	0.55
1:C:190:ARG:HG3	1:C:216:GLU:OE2	2.05	0.55
1:E:929:MET:HE3	1:E:979:LEU:CD1	2.36	0.55
1:I:52:ARG:NH1	1:I:90:GLY:O	2.38	0.55
1:K:887:MET:HB2	1:K:917:GLY:C	2.30	0.55
1:G:124:PHE:CE2	1:G:153:MET:HE1	2.41	0.55
1:G:432:ASP:OD1	1:G:434:GLU:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:809:ASP:HB3	1:G:814:THR:HA	1.89	0.55
1:G:892:LEU:HD13	1:G:920:VAL:HG21	1.88	0.55
1:I:278:LEU:HD23	1:I:287:PHE:HB3	1.88	0.55
1:G:703:ASN:ND2	1:G:706:VAL:H	2.04	0.55
1:I:800:ILE:HG21	1:I:845:ARG:HH22	1.70	0.55
1:K:401:GLU:H	1:K:401:GLU:CD	2.14	0.55
1:K:714:ILE:HG21	1:K:741:GLU:HG3	1.89	0.55
1:C:256:SER:OG	1:C:267:HIS:HE1	1.89	0.55
1:E:268:THR:HG22	1:E:303:ILE:HD11	1.89	0.55
1:K:62:TRP:HB3	3:K:1152:HOH:O	2.07	0.55
1:A:220:GLY:O	1:A:1038:HIS:HB3	2.06	0.55
1:A:253:GLN:NE2	1:A:268:THR:OG1	2.40	0.55
1:C:781:ALA:HB2	1:C:802:PRO:HG2	1.88	0.55
1:G:184:LEU:HB2	1:G:191:VAL:HB	1.89	0.55
1:G:746:HIS:HA	1:G:748:TYR:CZ	2.42	0.55
1:G:774:ASP:HA	1:G:817:ALA:HB2	1.88	0.55
1:I:872:HIS:HE1	1:I:902:GLU:OE1	1.89	0.55
1:K:295:ILE:HG13	1:K:306:ILE:HD11	1.88	0.55
1:G:363:ARG:HB3	1:G:380:GLY:O	2.06	0.55
1:I:44:LEU:HD12	1:I:56:VAL:HB	1.88	0.55
1:K:681:SER:CB	1:K:684:GLU:HG2	2.35	0.55
1:G:295:ILE:HG13	1:G:306:ILE:HD11	1.89	0.55
1:A:882:ILE:HD11	1:A:899:PHE:HA	1.89	0.55
1:C:387:LEU:HD13	1:C:388:GLY:N	2.22	0.55
1:E:546:PRO:HG2	1:E:567:ASP:HB3	1.89	0.55
1:E:736:VAL:HB	3:E:1197:HOH:O	2.06	0.55
1:E:532:SER:HB2	1:G:525:ASP:OD1	2.06	0.54
1:E:568:LEU:HB3	1:E:571:MET:HE2	1.90	0.54
1:E:746:HIS:HA	1:E:748:TYR:CZ	2.42	0.54
1:E:993:GLY:HA2	3:E:1083:HOH:O	2.04	0.54
1:E:703:ASN:C	1:E:703:ASN:ND2	2.59	0.54
1:G:53:ILE:CG2	1:G:286:LEU:HD21	2.36	0.54
1:I:882:ILE:HD11	1:I:899:PHE:HA	1.89	0.54
1:K:190:ARG:HG3	1:K:216:GLU:OE2	2.07	0.54
1:K:498:SER:CB	3:K:1073:HOH:O	2.48	0.54
1:K:565:GLU:HG2	1:K:566:TYR:N	2.22	0.54
1:E:1016:ARG:O	1:E:1017:ASP:HB2	2.07	0.54
1:G:489:LYS:HG3	1:G:491:PHE:CE1	2.43	0.54
1:I:568:LEU:HB3	1:I:571:MET:HE2	1.89	0.54
1:I:703:ASN:C	1:I:703:ASN:ND2	2.64	0.54
1:K:1002:ASP:N	3:K:1180:HOH:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:ASP:HB3	1:A:814:THR:HA	1.88	0.54
1:C:245:ILE:HD11	1:C:278:LEU:HG	1.90	0.54
1:E:681:SER:CB	1:E:684:GLU:HG2	2.36	0.54
1:E:746:HIS:NE2	2:F:1214:OQE:C1	2.71	0.54
1:K:533:PHE:C	3:K:1090:HOH:O	2.50	0.54
1:A:87:PHE:CB	1:A:88:PRO:HD2	2.35	0.54
1:A:874:ARG:CZ	3:A:1176:HOH:O	2.55	0.54
1:C:541:VAL:HG22	1:C:542:ILE:N	2.23	0.54
1:E:403:ASN:HD22	1:E:403:ASN:C	2.12	0.54
1:E:700:ASN:HD22	1:E:1008:GLN:NE2	2.05	0.54
1:E:887:MET:HB2	1:E:917:GLY:C	2.32	0.54
1:I:324:LYS:HD2	3:I:1117:HOH:O	2.05	0.54
1:I:892:LEU:HD13	1:I:920:VAL:HG21	1.89	0.54
1:A:112:ASN:OD1	1:A:114:GLU:HB3	2.08	0.54
1:A:781:ALA:HB2	1:A:802:PRO:HG2	1.89	0.54
1:C:1052:ILE:O	1:C:1056:ILE:HG13	2.07	0.54
1:E:256:SER:OG	1:E:267:HIS:CE1	2.60	0.54
1:G:190:ARG:HG3	1:G:216:GLU:OE2	2.08	0.54
1:I:124:PHE:CE2	1:I:153:MET:HE1	2.43	0.54
1:K:703:ASN:C	1:K:703:ASN:ND2	2.65	0.54
1:C:278:LEU:HD23	1:C:287:PHE:HB3	1.90	0.54
1:C:363:ARG:HB3	1:C:380:GLY:O	2.07	0.54
1:C:800:ILE:HG21	1:C:845:ARG:HH22	1.71	0.54
1:E:44:LEU:HD12	1:E:56:VAL:HB	1.90	0.54
1:E:956:ILE:HD13	1:E:957:ALA:N	2.21	0.54
1:G:541:VAL:HG22	1:G:542:ILE:N	2.22	0.54
1:G:681:SER:HB3	1:G:684:GLU:CG	2.35	0.54
1:G:929:MET:HE3	1:G:979:LEU:HD11	1.89	0.54
1:K:423:ASN:C	1:K:423:ASN:HD22	2.16	0.54
1:K:565:GLU:HG2	3:K:1178:HOH:O	2.07	0.54
1:A:124:PHE:CD2	1:A:153:MET:HE1	2.43	0.54
1:A:746:HIS:NE2	2:B:1214:OQE:C1	2.71	0.54
1:C:746:HIS:HA	1:C:748:TYR:CZ	2.43	0.54
1:E:220:GLY:O	1:E:1038:HIS:HB3	2.08	0.54
1:G:406:ASN:HB2	1:G:424:ASP:CG	2.32	0.54
1:G:480:ILE:N	1:G:494:THR:HG22	2.19	0.54
1:G:956:ILE:HD13	1:G:957:ALA:N	2.22	0.54
1:I:681:SER:CB	1:I:684:GLU:HG2	2.34	0.54
1:K:184:LEU:HB2	1:K:191:VAL:HB	1.89	0.54
1:K:684:GLU:HG3	1:K:685:GLU:N	2.23	0.54
1:C:268:THR:HG22	1:C:303:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:HIS:HE1	3:E:1155:HOH:O	1.90	0.54
1:I:525:ASP:OD1	1:K:532:SER:HB2	2.07	0.54
1:I:901:ASN:HB3	1:K:469:HIS:ND1	2.22	0.54
1:K:337:ILE:HG13	1:K:649:MET:CE	2.35	0.54
1:K:1016:ARG:O	1:K:1017:ASP:HB2	2.08	0.54
1:A:430:THR:HG23	1:A:441:ILE:HD11	1.90	0.54
1:E:278:LEU:HD23	1:E:287:PHE:HB3	1.89	0.54
1:E:565:GLU:HG2	1:E:566:TYR:H	1.73	0.54
1:G:744:THR:HA	3:G:1174:HOH:O	2.08	0.54
1:A:295:ILE:HG13	1:A:306:ILE:HD11	1.90	0.53
1:A:522:PRO:HG2	1:C:889:MET:SD	2.48	0.53
1:C:882:ILE:HD11	1:C:899:PHE:HA	1.90	0.53
1:E:201:HIS:HB3	1:E:736:VAL:HG13	1.91	0.53
1:E:603:HIS:HD2	1:E:604:GLY:O	1.90	0.53
1:E:986:ARG:HD2	1:E:1025:TYR:O	2.06	0.53
1:G:110:PHE:CD2	1:G:121:ILE:HG13	2.43	0.53
1:K:253:GLN:HA	1:K:253:GLN:NE2	2.22	0.53
1:K:591:LEU:HD13	1:K:662:LEU:HD21	1.90	0.53
1:A:633:LYS:NZ	1:A:665:PRO:O	2.40	0.53
1:A:889:MET:SD	1:C:522:PRO:HG2	2.49	0.53
1:C:714:ILE:HG21	1:C:741:GLU:HG3	1.91	0.53
1:E:701:TYR:O	1:G:939:ARG:HD3	2.08	0.53
1:G:268:THR:HG22	1:G:303:ILE:HD11	1.91	0.53
1:G:731:LEU:HD22	1:G:735:ILE:CD1	2.38	0.53
1:I:314:PRO:HD2	1:I:726:LYS:HG2	1.89	0.53
1:I:618:VAL:CG2	1:I:631:GLU:HG3	2.38	0.53
1:K:343:GLY:HA2	3:K:1095:HOH:O	2.07	0.53
1:A:268:THR:HG22	1:A:303:ILE:HD11	1.91	0.53
1:A:402:GLU:HB2	3:A:1195:HOH:O	2.08	0.53
1:E:565:GLU:HG2	1:E:566:TYR:N	2.23	0.53
1:K:112:ASN:OD1	1:K:114:GLU:HB3	2.08	0.53
1:A:541:VAL:HG22	1:A:542:ILE:N	2.22	0.53
1:C:909:ILE:HA	1:C:956:ILE:HG22	1.90	0.53
1:E:432:ASP:OD1	1:E:434:GLU:HB3	2.08	0.53
1:G:124:PHE:HB3	1:G:152:ALA:CB	2.39	0.53
1:I:222:PHE:HB2	1:I:1038:HIS:HD2	1.74	0.53
1:C:300:THR:HG21	3:C:1154:HOH:O	2.08	0.53
1:E:909:ILE:HA	1:E:956:ILE:HG22	1.90	0.53
1:E:1029:PRO:HB3	3:E:1113:HOH:O	2.09	0.53
1:G:229:SER:HB3	1:G:248:ILE:HD11	1.90	0.53
1:G:387:LEU:HD13	1:G:388:GLY:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:681:SER:O	1:G:684:GLU:HG2	2.08	0.53
1:A:909:ILE:HA	1:A:956:ILE:HG22	1.90	0.53
1:C:568:LEU:HB3	1:C:571:MET:HE2	1.90	0.53
1:C:840:LYS:HE2	3:C:1213:HOH:O	2.08	0.53
1:E:525:ASP:OD1	1:G:532:SER:HB2	2.07	0.53
1:G:618:VAL:CG2	1:G:631:GLU:HG3	2.38	0.53
1:I:124:PHE:HB3	1:I:152:ALA:CB	2.39	0.53
1:K:909:ILE:HA	1:K:956:ILE:HG22	1.91	0.53
1:A:423:ASN:C	1:A:423:ASN:HD22	2.15	0.53
1:A:524:PRO:HD3	1:C:605:GLU:CG	2.39	0.53
1:A:555:VAL:HG22	1:I:354:TYR:OH	2.08	0.53
1:A:714:ILE:HG21	1:A:741:GLU:HG3	1.91	0.53
1:C:44:LEU:HD12	1:C:56:VAL:HB	1.90	0.53
1:C:727:THR:O	1:C:730:ASP:HB2	2.08	0.53
1:G:746:HIS:NE2	2:H:1214:OQE:C1	2.72	0.53
1:I:532:SER:HB2	1:K:525:ASP:OD1	2.08	0.53
1:A:681:SER:CB	1:A:684:GLU:HG2	2.38	0.53
1:A:1016:ARG:O	1:A:1017:ASP:HB2	2.08	0.53
1:E:73:LYS:HD3	1:E:76:SER:CB	2.38	0.53
1:E:184:LEU:HB2	1:E:191:VAL:HB	1.91	0.53
1:G:220:GLY:O	1:G:1038:HIS:HB3	2.08	0.53
1:I:432:ASP:OD1	1:I:434:GLU:HB3	2.08	0.53
1:K:124:PHE:CD2	1:K:153:MET:HE1	2.44	0.53
1:C:406:ASN:HB2	1:C:424:ASP:CG	2.32	0.53
1:I:596:LEU:HD12	1:I:619:LEU:HD11	1.90	0.53
1:K:480:ILE:H	1:K:494:THR:HG21	1.73	0.53
1:G:546:PRO:HG2	1:G:567:ASP:HB3	1.90	0.53
1:I:809:ASP:HB3	1:I:814:THR:HA	1.91	0.53
1:K:929:MET:HE3	1:K:979:LEU:CD1	2.38	0.53
1:E:218:ASN:O	1:E:220:GLY:N	2.42	0.52
1:G:222:PHE:HB2	1:G:1038:HIS:HD2	1.74	0.52
1:G:322:PRO:HB3	1:G:678:LEU:HD13	1.91	0.52
1:G:926:GLU:CD	3:G:1160:HOH:O	2.52	0.52
1:G:1016:ARG:O	1:G:1017:ASP:HB2	2.09	0.52
1:I:179:PRO:HG2	3:I:1162:HOH:O	2.09	0.52
1:K:197:PHE:HE1	1:K:199:LEU:HD21	1.74	0.52
1:C:184:LEU:HB2	1:C:191:VAL:HB	1.90	0.52
1:E:146:LEU:HD23	1:E:165:VAL:HG21	1.91	0.52
1:G:87:PHE:CB	1:G:88:PRO:HD2	2.40	0.52
1:I:155:PRO:O	1:I:856:ARG:HD2	2.09	0.52
1:I:220:GLY:O	1:I:1038:HIS:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:256:SER:OG	1:I:267:HIS:HE1	1.91	0.52
1:I:1016:ARG:O	1:I:1017:ASP:HB2	2.08	0.52
1:K:222:PHE:HB2	1:K:1038:HIS:HD2	1.73	0.52
1:K:453:THR:HG23	3:K:1176:HOH:O	2.09	0.52
1:C:61:LEU:CB	1:C:75:VAL:HG13	2.38	0.52
1:C:498:SER:OG	1:C:518:ARG:HG2	2.09	0.52
1:C:618:VAL:CG2	1:C:631:GLU:HG3	2.40	0.52
1:E:892:LEU:HD13	1:E:920:VAL:HG21	1.90	0.52
1:I:229:SER:HB3	1:I:248:ILE:CD1	2.39	0.52
1:I:363:ARG:HB3	1:I:380:GLY:O	2.09	0.52
1:I:423:ASN:C	1:I:423:ASN:HD22	2.15	0.52
1:C:110:PHE:CD2	1:C:121:ILE:HG13	2.44	0.52
1:C:1016:ARG:O	1:C:1017:ASP:HB2	2.10	0.52
1:E:82:ASN:HD21	1:E:96:ARG:HG2	1.73	0.52
1:E:242:ILE:O	1:E:256:SER:HA	2.09	0.52
1:I:61:LEU:CB	1:I:75:VAL:HG13	2.39	0.52
1:K:363:ARG:NH2	3:K:1095:HOH:O	2.42	0.52
1:C:273:TYR:O	1:C:289:LYS:HD2	2.10	0.52
1:G:53:ILE:HG23	1:G:286:LEU:CD2	2.39	0.52
1:K:124:PHE:CE2	1:K:153:MET:HE1	2.44	0.52
1:K:242:ILE:O	1:K:256:SER:HA	2.09	0.52
1:K:256:SER:OG	1:K:267:HIS:CE1	2.60	0.52
1:K:681:SER:O	1:K:684:GLU:HG2	2.10	0.52
1:C:218:ASN:O	1:C:220:GLY:N	2.43	0.52
1:C:601:PRO:O	3:C:1096:HOH:O	2.19	0.52
1:G:684:GLU:HG3	1:G:685:GLU:N	2.23	0.52
1:I:110:PHE:CD2	1:I:121:ILE:HG13	2.44	0.52
1:I:353:THR:HG23	1:I:354:TYR:CD1	2.45	0.52
1:K:82:ASN:HD21	1:K:96:ARG:HG2	1.74	0.52
1:K:913:ARG:NH2	1:K:1047:GLN:HE21	2.03	0.52
1:A:184:LEU:HB2	1:A:191:VAL:HB	1.92	0.52
1:A:489:LYS:HG3	1:A:491:PHE:CE1	2.44	0.52
1:C:64:HIS:HD2	1:C:71:THR:OG1	1.92	0.52
1:C:430:THR:HG23	1:C:441:ILE:HD11	1.91	0.52
1:K:82:ASN:HD22	1:K:82:ASN:N	2.08	0.52
1:A:432:ASP:OD1	1:A:434:GLU:HB3	2.09	0.52
1:A:684:GLU:HG3	1:A:685:GLU:N	2.25	0.52
1:E:714:ILE:HG21	1:E:741:GLU:HG3	1.91	0.52
1:E:281:ASP:HA	3:E:1162:HOH:O	2.09	0.52
1:E:337:ILE:HG13	1:E:649:MET:CE	2.37	0.52
1:E:735:ILE:O	1:E:739:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:TYR:HA	1:G:1024:ASN:HD21	1.74	0.52
1:I:387:LEU:HD13	1:I:388:GLY:N	2.24	0.52
1:K:201:HIS:HB3	1:K:736:VAL:HG13	1.91	0.52
1:K:234:SER:HB3	1:K:278:LEU:H	1.75	0.52
1:K:633:LYS:NZ	1:K:665:PRO:O	2.42	0.52
1:E:273:TYR:O	1:E:289:LYS:HD2	2.10	0.52
1:E:591:LEU:HD13	1:E:662:LEU:HD21	1.92	0.52
1:I:124:PHE:CD2	1:I:153:MET:HE1	2.45	0.52
1:I:184:LEU:HB2	1:I:191:VAL:HB	1.92	0.52
1:K:565:GLU:HG2	1:K:566:TYR:H	1.72	0.52
1:K:890:MET:O	1:K:894:GLU:HG2	2.10	0.52
1:A:605:GLU:CG	1:C:524:PRO:HD3	2.39	0.51
1:A:704:GLU:HG3	1:C:939:ARG:HH11	1.73	0.51
1:C:565:GLU:HG2	1:C:566:TYR:N	2.25	0.51
1:I:956:ILE:HD13	1:I:957:ALA:N	2.25	0.51
1:K:591:LEU:CD1	1:K:662:LEU:HD21	2.40	0.51
1:A:273:TYR:O	1:A:289:LYS:HD2	2.09	0.51
1:A:307:GLU:C	1:A:308:ILE:HD12	2.34	0.51
1:A:327:GLU:O	1:A:328:ASP:O	2.28	0.51
1:A:586:ARG:HG3	2:B:1204:GLN:HG3	1.92	0.51
1:A:949:ASN:ND2	1:C:475:TYR:OH	2.39	0.51
1:C:112:ASN:OD1	1:C:114:GLU:HB3	2.10	0.51
1:C:616:LYS:HD3	3:C:1079:HOH:O	2.11	0.51
1:I:64:HIS:HD2	1:I:71:THR:OG1	1.93	0.51
1:K:110:PHE:CD2	1:K:121:ILE:HG13	2.45	0.51
1:A:318:ILE:HG21	1:A:682:ILE:HD11	1.92	0.51
1:E:609:TYR:CE1	3:E:1133:HOH:O	2.54	0.51
1:G:965:SER:HA	1:G:990:GLY:O	2.11	0.51
1:I:367:VAL:HG12	1:I:375:VAL:HG21	1.92	0.51
1:I:887:MET:HB2	1:I:917:GLY:C	2.35	0.51
1:I:1052:ILE:O	1:I:1056:ILE:HG13	2.10	0.51
1:K:124:PHE:HB3	1:K:152:ALA:CB	2.40	0.51
1:K:218:ASN:O	1:K:220:GLY:N	2.43	0.51
1:A:64:HIS:HD2	1:A:71:THR:OG1	1.93	0.51
1:A:245:ILE:HD11	1:A:278:LEU:HG	1.92	0.51
1:A:929:MET:HE3	1:A:979:LEU:CD1	2.40	0.51
1:A:948:THR:H	1:C:922:GLN:HE22	1.57	0.51
1:G:423:ASN:C	1:G:423:ASN:HD22	2.17	0.51
1:G:642:SER:HB2	1:G:647:THR:HB	1.92	0.51
1:I:87:PHE:CB	1:I:88:PRO:HD2	2.38	0.51
1:I:197:PHE:HE1	1:I:199:LEU:HD21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:746:HIS:HA	1:I:748:TYR:CZ	2.45	0.51
1:I:890:MET:O	1:I:894:GLU:HG2	2.10	0.51
1:K:253:GLN:NE2	1:K:268:THR:OG1	2.43	0.51
1:A:202:TRP:CH2	1:A:745:SER:HB3	2.46	0.51
1:A:256:SER:OG	1:A:267:HIS:CE1	2.63	0.51
1:C:322:PRO:HB3	1:C:678:LEU:HD13	1.91	0.51
1:C:480:ILE:N	1:C:494:THR:HG22	2.20	0.51
1:E:533:PHE:C	3:E:1181:HOH:O	2.53	0.51
1:G:228:MET:HE1	1:G:244:PHE:CZ	2.45	0.51
1:I:591:LEU:CD1	1:I:662:LEU:HD21	2.41	0.51
1:K:307:GLU:C	1:K:308:ILE:HD12	2.36	0.51
1:K:586:ARG:HG3	2:L:1204:GLN:HG3	1.93	0.51
1:K:681:SER:HB3	1:K:684:GLU:CG	2.40	0.51
1:A:841:GLY:C	1:A:843:ASP:H	2.19	0.51
1:C:681:SER:CB	1:C:684:GLU:HG2	2.39	0.51
1:E:53:ILE:HD12	1:E:66:LEU:HD21	1.93	0.51
1:I:546:PRO:CG	1:I:567:ASP:HB3	2.41	0.51
1:I:633:LYS:NZ	1:I:665:PRO:O	2.42	0.51
1:A:743:ARG:HB3	3:A:1090:HOH:O	2.10	0.51
1:G:44:LEU:HD12	1:G:56:VAL:HB	1.92	0.51
1:G:284:ARG:HD3	3:G:1179:HOH:O	2.09	0.51
1:G:591:LEU:HD13	1:G:662:LEU:HD21	1.92	0.51
1:I:190:ARG:HG3	1:I:216:GLU:OE2	2.10	0.51
1:I:429:MET:HA	1:I:441:ILE:HD13	1.93	0.51
1:I:565:GLU:HG2	1:I:566:TYR:N	2.25	0.51
1:A:110:PHE:CD2	1:A:121:ILE:HG13	2.46	0.51
1:G:112:ASN:OD1	1:G:114:GLU:HB3	2.11	0.51
1:G:890:MET:O	1:G:894:GLU:HG2	2.10	0.51
1:I:218:ASN:O	1:I:220:GLY:N	2.44	0.51
1:I:940:ARG:HD2	3:K:1098:HOH:O	2.10	0.51
1:K:385:ASP:HB2	1:K:405:GLY:O	2.11	0.51
1:K:1052:ILE:O	1:K:1056:ILE:HG13	2.11	0.51
1:A:640:ARG:HD2	3:A:1184:HOH:O	2.10	0.51
1:E:633:LYS:NZ	1:E:665:PRO:O	2.44	0.51
1:I:731:LEU:HD22	1:I:735:ILE:CD1	2.41	0.51
1:C:429:MET:HA	1:C:441:ILE:HD13	1.93	0.51
1:E:591:LEU:CD1	1:E:662:LEU:HD21	2.41	0.51
1:E:905:TYR:HB2	3:E:1086:HOH:O	2.11	0.51
1:G:82:ASN:HD22	1:G:82:ASN:N	2.09	0.51
1:C:432:ASP:OD1	1:C:434:GLU:HB3	2.11	0.50
1:C:703:ASN:C	1:C:703:ASN:ND2	2.62	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:925:ILE:HG22	3:E:1134:HOH:O	2.11	0.50
1:G:909:ILE:HG12	1:G:956:ILE:HG21	1.92	0.50
1:I:948:THR:H	1:K:922:GLN:HE22	1.57	0.50
1:K:87:PHE:CB	1:K:88:PRO:HD2	2.39	0.50
1:A:387:LEU:HD13	1:A:388:GLY:N	2.27	0.50
1:A:986:ARG:HD2	1:A:1025:TYR:O	2.11	0.50
1:C:222:PHE:HB2	1:C:1038:HIS:HD2	1.76	0.50
1:G:218:ASN:O	1:G:220:GLY:N	2.44	0.50
1:I:541:VAL:HG22	1:I:542:ILE:N	2.26	0.50
1:K:245:ILE:HD11	1:K:278:LEU:HG	1.92	0.50
1:A:722:VAL:N	1:A:723:PRO:HD2	2.27	0.50
1:A:965:SER:HA	1:A:990:GLY:O	2.11	0.50
1:G:124:PHE:CD2	1:G:153:MET:HE1	2.46	0.50
1:G:714:ILE:HG21	1:G:741:GLU:HG3	1.93	0.50
1:I:480:ILE:H	1:I:494:THR:HG21	1.75	0.50
1:I:618:VAL:HG21	1:I:631:GLU:HG3	1.93	0.50
1:E:110:PHE:CD2	1:E:121:ILE:HG13	2.45	0.50
1:G:591:LEU:CD1	1:G:662:LEU:HD21	2.42	0.50
1:I:82:ASN:HD22	1:I:82:ASN:N	2.09	0.50
1:I:112:ASN:OD1	1:I:114:GLU:HB3	2.11	0.50
1:I:684:GLU:HG3	1:I:685:GLU:N	2.26	0.50
1:K:273:TYR:O	1:K:289:LYS:HD2	2.10	0.50
1:K:872:HIS:HE1	1:K:902:GLU:OE1	1.94	0.50
1:K:956:ILE:HD13	1:K:957:ALA:N	2.27	0.50
1:G:986:ARG:HD2	1:G:1025:TYR:O	2.12	0.50
1:I:603:HIS:HD2	1:I:604:GLY:O	1.93	0.50
1:I:901:ASN:HB3	1:K:469:HIS:CE1	2.45	0.50
1:K:422:ALA:HB1	3:K:1091:HOH:O	2.12	0.50
1:A:637:THR:OG1	1:A:651:ARG:HG2	2.12	0.50
1:A:939:ARG:HH11	1:C:704:GLU:HG3	1.76	0.50
1:C:87:PHE:CB	1:C:88:PRO:HD2	2.37	0.50
1:G:367:VAL:O	1:G:368:ARG:HD3	2.12	0.50
1:G:546:PRO:CG	1:G:567:ASP:HB3	2.42	0.50
1:K:53:ILE:HG23	1:K:286:LEU:CD2	2.39	0.50
1:K:201:HIS:O	1:K:740:GLY:HA2	2.11	0.50
1:K:372:ASP:HB3	3:K:1197:HOH:O	2.12	0.50
1:A:44:LEU:HD12	1:A:56:VAL:HB	1.94	0.50
1:A:61:LEU:HB3	1:A:75:VAL:CG1	2.39	0.50
1:A:546:PRO:HG2	1:A:567:ASP:HB3	1.93	0.50
1:E:201:HIS:O	1:E:740:GLY:HA2	2.12	0.50
1:I:91:ARG:NH2	3:I:1202:HOH:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:565:GLU:HG2	1:I:566:TYR:H	1.76	0.50
1:K:64:HIS:HD2	1:K:71:THR:OG1	1.95	0.50
1:A:565:GLU:HG2	1:A:566:TYR:N	2.26	0.50
1:A:618:VAL:HG21	1:A:631:GLU:HG3	1.93	0.50
1:G:586:ARG:HG3	2:H:1204:GLN:HG3	1.92	0.50
1:I:681:SER:O	1:I:684:GLU:HG2	2.11	0.50
1:K:236:VAL:HG23	1:K:243:TYR:HB2	1.94	0.50
1:K:722:VAL:N	1:K:723:PRO:HD2	2.26	0.50
1:I:367:VAL:O	1:I:368:ARG:HD3	2.12	0.50
1:I:714:ILE:HG21	1:I:741:GLU:HG3	1.92	0.50
1:K:314:PRO:HD2	1:K:726:LYS:HG2	1.94	0.50
1:C:141:ASP:OD1	1:C:145:ASN:HB2	2.12	0.49
1:C:319:ILE:HD11	3:I:1179:HOH:O	2.12	0.49
1:C:544:LEU:N	3:C:1113:HOH:O	2.45	0.49
1:E:133:MET:HE1	3:E:1180:HOH:O	2.11	0.49
1:E:684:GLU:HG3	1:E:685:GLU:N	2.26	0.49
1:E:1052:ILE:O	1:E:1056:ILE:HG13	2.12	0.49
1:G:565:GLU:HG2	1:G:566:TYR:N	2.26	0.49
1:I:489:LYS:HG3	1:I:491:PHE:CE1	2.47	0.49
1:I:642:SER:HB2	1:I:647:THR:HB	1.92	0.49
1:E:905:TYR:N	3:E:1086:HOH:O	2.29	0.49
1:G:480:ILE:H	1:G:494:THR:HG21	1.72	0.49
1:G:633:LYS:NZ	1:G:665:PRO:O	2.46	0.49
1:G:929:MET:HE3	1:G:979:LEU:CD1	2.41	0.49
1:K:124:PHE:HB3	1:K:152:ALA:HB1	1.92	0.49
1:K:887:MET:HG3	1:K:966:ASP:OD2	2.13	0.49
1:A:141:ASP:OD1	1:A:145:ASN:HB2	2.11	0.49
1:E:64:HIS:HD2	1:E:71:THR:OG1	1.96	0.49
1:G:367:VAL:HG12	1:G:375:VAL:HG21	1.93	0.49
1:G:703:ASN:HA	3:G:1097:HOH:O	2.11	0.49
1:G:715:TYR:HB3	3:G:1186:HOH:O	2.11	0.49
1:I:234:SER:HB3	1:I:278:LEU:H	1.76	0.49
1:I:430:THR:HG23	1:I:441:ILE:HD11	1.94	0.49
1:I:929:MET:HE3	1:I:979:LEU:HD11	1.94	0.49
1:K:568:LEU:N	1:K:568:LEU:HD23	2.27	0.49
1:C:57:CYS:HB3	1:C:62:TRP:CD1	2.48	0.49
1:C:242:ILE:O	1:C:256:SER:HA	2.13	0.49
1:C:327:GLU:O	1:C:328:ASP:O	2.30	0.49
1:E:88:PRO:HG2	1:E:89:ASP:H	1.77	0.49
1:E:407:VAL:HG13	1:E:421:VAL:HG13	1.95	0.49
1:E:568:LEU:N	1:E:568:LEU:HD23	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:SER:OG	1:G:267:HIS:HE1	1.95	0.49
1:G:885:PRO:O	1:G:915:ASN:HA	2.12	0.49
1:I:202:TRP:CH2	1:I:745:SER:HB3	2.47	0.49
1:K:589:ILE:HD13	1:K:641:LEU:HD12	1.93	0.49
1:K:703:ASN:ND2	1:K:706:VAL:H	2.10	0.49
1:C:124:PHE:HB3	1:C:152:ALA:CB	2.42	0.49
1:C:337:ILE:HG13	1:C:649:MET:CE	2.39	0.49
1:C:374:LYS:HG3	3:C:1144:HOH:O	2.11	0.49
1:C:684:GLU:HG3	1:C:685:GLU:N	2.27	0.49
1:E:190:ARG:HG3	1:E:216:GLU:OE2	2.12	0.49
1:E:618:VAL:CG2	1:E:631:GLU:HG3	2.42	0.49
1:G:965:SER:O	1:G:968:ASP:N	2.44	0.49
1:K:546:PRO:CG	1:K:567:ASP:HB3	2.41	0.49
1:A:87:PHE:HB3	1:A:88:PRO:CD	2.41	0.49
1:A:242:ILE:O	1:A:256:SER:HA	2.12	0.49
1:E:48:ILE:HG12	1:E:49:HIS:N	2.27	0.49
1:E:124:PHE:HB3	1:E:152:ALA:CB	2.43	0.49
1:E:307:GLU:C	1:E:308:ILE:HD12	2.37	0.49
1:E:781:ALA:CB	1:E:802:PRO:HG2	2.43	0.49
1:K:353:THR:HG23	1:K:354:TYR:CD1	2.47	0.49
1:C:637:THR:OG1	1:C:651:ARG:HG2	2.13	0.49
1:C:722:VAL:N	1:C:723:PRO:HD2	2.27	0.49
1:E:589:ILE:HD13	1:E:641:LEU:HD12	1.93	0.49
1:E:681:SER:O	1:E:684:GLU:HG2	2.12	0.49
1:G:565:GLU:HG2	1:G:566:TYR:H	1.77	0.49
1:I:222:PHE:H	1:I:1038:HIS:CD2	2.29	0.49
1:C:45:ASN:HA	1:C:277:HIS:CD2	2.48	0.49
1:E:418:PHE:CE1	1:E:485:MET:HE2	2.48	0.49
1:E:532:SER:HB2	3:E:1181:HOH:O	2.11	0.49
1:E:642:SER:HB2	1:E:647:THR:HB	1.94	0.49
1:E:965:SER:C	1:E:967:GLY:N	2.70	0.49
1:G:124:PHE:HB3	1:G:152:ALA:HB1	1.94	0.49
1:I:268:THR:HG22	1:I:303:ILE:HD11	1.95	0.49
1:K:40:PRO:HG2	1:K:724:LEU:CD2	2.41	0.49
1:A:746:HIS:HA	1:A:748:TYR:CZ	2.48	0.49
1:A:939:ARG:NH1	1:C:704:GLU:HG3	2.28	0.49
1:E:245:ILE:HD11	1:E:278:LEU:HG	1.94	0.49
1:G:353:THR:HG23	1:G:354:TYR:CD1	2.48	0.49
1:G:872:HIS:HE1	1:G:902:GLU:OE1	1.95	0.49
1:I:959:THR:O	1:I:984:GLY:HA3	2.13	0.49
1:K:63:GLU:N	3:K:1152:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:840:LYS:CE	3:C:1213:HOH:O	2.59	0.49
1:E:353:THR:HG23	1:E:354:TYR:CD1	2.48	0.49
1:G:222:PHE:H	1:G:1038:HIS:CD2	2.31	0.49
1:G:430:THR:HG23	1:G:441:ILE:HD11	1.95	0.49
1:I:322:PRO:HB3	1:I:678:LEU:HD13	1.94	0.49
1:A:124:PHE:HB3	1:A:152:ALA:CB	2.42	0.48
1:A:190:ARG:HG3	1:A:216:GLU:OE2	2.13	0.48
1:A:959:THR:O	1:A:984:GLY:HA3	2.13	0.48
1:C:229:SER:HB3	1:C:248:ILE:CD1	2.42	0.48
1:C:633:LYS:NZ	1:C:665:PRO:O	2.45	0.48
1:I:965:SER:HA	1:I:990:GLY:O	2.12	0.48
1:A:641:LEU:HD23	1:A:647:THR:O	2.13	0.48
1:C:442:GLU:OE2	1:C:481:HIS:HD2	1.96	0.48
1:C:546:PRO:HG2	1:C:567:ASP:HB3	1.95	0.48
1:C:586:ARG:NE	2:D:1206:ALA:HB3	2.28	0.48
1:E:197:PHE:HE1	1:E:199:LEU:HD21	1.77	0.48
1:E:859:ARG:NH1	3:E:1122:HOH:O	2.46	0.48
1:G:641:LEU:HD23	1:G:647:THR:O	2.13	0.48
1:I:273:TYR:O	1:I:289:LYS:HD2	2.12	0.48
1:I:591:LEU:HD13	1:I:662:LEU:HD21	1.95	0.48
1:K:452:PHE:HB3	1:K:463:TYR:HB3	1.96	0.48
1:A:429:MET:HA	1:A:441:ILE:HD13	1.95	0.48
1:A:704:GLU:HG3	1:C:939:ARG:NH1	2.28	0.48
1:E:429:MET:HA	1:E:441:ILE:HD13	1.95	0.48
1:E:641:LEU:HD23	1:E:647:THR:O	2.14	0.48
1:E:827:GLU:O	1:K:677:PRO:HD2	2.13	0.48
1:E:885:PRO:HG2	1:E:890:MET:HG2	1.95	0.48
1:E:959:THR:HG22	3:E:1113:HOH:O	2.12	0.48
1:E:992:VAL:HG13	3:E:1189:HOH:O	2.06	0.48
1:I:403:ASN:HD22	1:I:405:GLY:H	1.60	0.48
1:K:210:ARG:N	3:K:1083:HOH:O	2.45	0.48
1:E:605:GLU:CG	1:G:524:PRO:HD3	2.42	0.48
1:I:775:HIS:HA	3:I:1188:HOH:O	2.13	0.48
1:K:268:THR:HG22	1:K:303:ILE:HD11	1.95	0.48
1:K:410:MET:HG2	1:K:421:VAL:HG22	1.96	0.48
1:A:201:HIS:HB3	1:A:736:VAL:HG13	1.94	0.48
1:A:530:ASN:ND2	1:A:531:PHE:N	2.61	0.48
1:C:921:SER:HB3	1:C:966:ASP:OD2	2.13	0.48
1:E:40:PRO:HG2	1:E:724:LEU:CD2	2.37	0.48
1:G:337:ILE:HG13	1:G:649:MET:CE	2.39	0.48
1:G:735:ILE:O	1:G:739:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:124:PHE:HB3	1:I:152:ALA:HB1	1.93	0.48
1:I:242:ILE:O	1:I:256:SER:HA	2.13	0.48
1:I:516:SER:HB3	1:I:518:ARG:HG3	1.96	0.48
1:K:430:THR:HG23	1:K:441:ILE:HD11	1.95	0.48
1:A:300:THR:O	1:A:300:THR:HG22	2.13	0.48
1:A:540:PHE:HA	1:A:577:PRO:HA	1.96	0.48
1:C:641:LEU:HD23	1:C:647:THR:O	2.14	0.48
1:C:676:ARG:CD	3:C:1072:HOH:O	2.59	0.48
1:E:410:MET:HG2	1:E:421:VAL:HG22	1.96	0.48
1:E:425:ARG:O	1:E:426:PHE:HB2	2.14	0.48
3:E:1181:HOH:O	1:G:525:ASP:CG	2.57	0.48
1:A:469:HIS:ND1	1:C:901:ASN:HB3	2.27	0.48
1:C:124:PHE:HB3	1:C:152:ALA:HB1	1.94	0.48
1:E:546:PRO:CG	1:E:567:ASP:HB3	2.44	0.48
1:G:429:MET:HA	1:G:441:ILE:HD13	1.95	0.48
1:I:201:HIS:O	1:I:740:GLY:HA2	2.14	0.48
1:I:406:ASN:HB2	1:I:424:ASP:CG	2.39	0.48
1:I:727:THR:O	1:I:730:ASP:HB2	2.14	0.48
1:K:61:LEU:HB3	1:K:75:VAL:CG1	2.39	0.48
1:K:731:LEU:HD22	1:K:735:ILE:CD1	2.43	0.48
1:E:124:PHE:HB3	1:E:152:ALA:HB1	1.95	0.48
1:E:131:ARG:HH21	1:E:131:ARG:HG2	1.79	0.48
1:E:637:THR:OG1	1:E:651:ARG:HG2	2.13	0.48
1:I:190:ARG:NH2	1:I:222:PHE:HZ	2.12	0.48
1:I:586:ARG:HG3	2:J:1204:GLN:HG3	1.95	0.48
1:I:710:ILE:O	1:I:714:ILE:HG12	2.13	0.48
1:K:141:ASP:OD1	1:K:145:ASN:HB2	2.14	0.48
1:K:387:LEU:HD13	1:K:388:GLY:N	2.28	0.48
1:E:124:PHE:CE2	1:E:153:MET:HE1	2.49	0.48
1:E:586:ARG:NE	2:F:1206:ALA:HB3	2.28	0.48
1:G:273:TYR:O	1:G:289:LYS:HD2	2.14	0.48
1:G:766:ALA:HA	1:G:855:ASP:OD1	2.13	0.48
1:I:988:TRP:CZ3	1:I:990:GLY:HA3	2.49	0.48
1:K:184:LEU:HD13	1:K:237:ILE:HG13	1.96	0.48
1:K:253:GLN:HA	1:K:253:GLN:HE21	1.78	0.48
1:K:557:ARG:NE	3:K:1164:HOH:O	2.46	0.48
1:K:676:ARG:HD2	3:K:1169:HOH:O	2.14	0.48
1:A:712:GLU:HG3	3:A:1190:HOH:O	2.13	0.47
1:A:1011:PHE:HB3	1:C:936:ASP:OD2	2.14	0.47
1:E:498:SER:OG	1:E:518:ARG:HG2	2.14	0.47
1:E:965:SER:HA	1:E:990:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:318:ILE:HG21	1:G:682:ILE:HD11	1.96	0.47
1:I:367:VAL:CG1	1:I:375:VAL:HG21	2.43	0.47
1:A:82:ASN:HD22	1:A:82:ASN:N	2.10	0.47
1:A:739:GLN:NE2	3:A:1104:HOH:O	2.45	0.47
1:C:202:TRP:CH2	1:C:745:SER:HB3	2.49	0.47
1:E:452:PHE:HB3	1:E:463:TYR:HB3	1.96	0.47
1:E:554:LEU:N	3:E:1174:HOH:O	2.47	0.47
1:E:703:ASN:ND2	1:E:706:VAL:H	2.11	0.47
1:G:82:ASN:HD21	1:G:96:ARG:HG2	1.78	0.47
1:I:59:ASP:HB3	1:I:80:VAL:HA	1.97	0.47
1:I:681:SER:HB3	1:I:684:GLU:CG	2.40	0.47
1:I:703:ASN:ND2	1:I:706:VAL:H	2.12	0.47
1:K:841:GLY:C	1:K:843:ASP:H	2.22	0.47
1:K:921:SER:HB3	1:K:966:ASP:OD2	2.14	0.47
1:C:353:THR:HG23	1:C:354:TYR:CD1	2.49	0.47
1:C:735:ILE:O	1:C:739:GLN:HG3	2.14	0.47
1:C:841:GLY:C	1:C:843:ASP:H	2.21	0.47
1:E:894:GLU:OE1	1:E:897:ARG:NH2	2.47	0.47
1:G:425:ARG:O	1:G:426:PHE:HB2	2.15	0.47
1:K:88:PRO:HG2	1:K:89:ASP:H	1.79	0.47
1:K:959:THR:O	1:K:984:GLY:HA3	2.14	0.47
1:A:906:GLN:O	1:A:953:GLY:HA3	2.14	0.47
1:C:272:ASP:O	1:C:717:LYS:HE2	2.15	0.47
1:C:385:ASP:HB2	1:C:405:GLY:O	2.15	0.47
1:C:516:SER:HB3	1:C:518:ARG:HG3	1.96	0.47
1:E:225:ILE:HG13	1:E:226:VAL:HG23	1.97	0.47
1:E:322:PRO:HB3	1:E:678:LEU:HD13	1.96	0.47
1:E:385:ASP:HB2	1:E:405:GLY:O	2.14	0.47
1:E:922:GLN:NE2	1:G:948:THR:H	2.11	0.47
1:G:64:HIS:HD2	1:G:71:THR:OG1	1.98	0.47
1:G:710:ILE:O	1:G:714:ILE:HG12	2.13	0.47
1:I:363:ARG:HD3	1:I:363:ARG:HA	1.52	0.47
1:I:637:THR:OG1	1:I:651:ARG:HG2	2.13	0.47
1:E:586:ARG:HG3	2:F:1204:GLN:HG3	1.96	0.47
1:E:737:GLU:N	3:E:1197:HOH:O	2.46	0.47
1:G:61:LEU:HB3	1:G:75:VAL:CG1	2.43	0.47
1:K:568:LEU:HB3	1:K:571:MET:HE2	1.96	0.47
1:E:872:HIS:HE1	1:E:902:GLU:OE1	1.98	0.47
1:A:57:CYS:HB3	1:A:62:TRP:CD1	2.50	0.47
1:A:82:ASN:HD21	1:A:96:ARG:HG2	1.79	0.47
1:A:546:PRO:CG	1:A:567:ASP:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:LYS:HD3	1:C:76:SER:CB	2.40	0.47
1:C:367:VAL:O	1:C:368:ARG:HD3	2.14	0.47
1:E:57:CYS:HB3	1:E:62:TRP:CD1	2.50	0.47
1:E:234:SER:HB3	1:E:278:LEU:H	1.79	0.47
1:E:387:LEU:HD13	1:E:388:GLY:N	2.30	0.47
1:G:151:ASP:OD1	3:G:1094:HOH:O	2.20	0.47
1:G:297:ASN:HD22	1:G:297:ASN:C	2.21	0.47
1:I:40:PRO:HG2	1:I:724:LEU:CD2	2.37	0.47
1:I:586:ARG:NE	2:J:1206:ALA:HB3	2.30	0.47
1:K:637:THR:OG1	1:K:651:ARG:HG2	2.15	0.47
1:K:982:LEU:C	1:K:983:ILE:HD12	2.40	0.47
2:L:1206:ALA:HA	3:L:921:HOH:O	2.13	0.47
1:A:360:GLU:HG3	1:A:377:PHE:CZ	2.50	0.47
1:A:642:SER:HB2	1:A:647:THR:HB	1.97	0.47
1:C:890:MET:O	1:C:894:GLU:HG2	2.15	0.47
1:E:61:LEU:HB3	1:E:75:VAL:CG1	2.45	0.47
1:E:681:SER:HB3	1:E:684:GLU:CG	2.43	0.47
1:E:841:GLY:C	1:E:843:ASP:H	2.23	0.47
1:E:887:MET:HG3	1:E:966:ASP:OD2	2.15	0.47
1:G:637:THR:OG1	1:G:651:ARG:HG2	2.15	0.47
1:A:942:THR:HG21	3:C:1159:HOH:O	2.14	0.47
1:I:178:GLY:HA3	1:I:1040:TYR:CD1	2.50	0.47
1:I:722:VAL:N	1:I:723:PRO:HD2	2.30	0.47
1:K:322:PRO:HB3	1:K:678:LEU:HD13	1.95	0.47
1:C:85:ARG:HD3	3:C:1228:HOH:O	2.15	0.47
1:C:642:SER:HB2	1:C:647:THR:HB	1.96	0.47
1:C:885:PRO:HG2	1:C:890:MET:HG2	1.96	0.47
1:C:956:ILE:HD13	1:C:957:ALA:N	2.30	0.47
1:E:921:SER:HB3	1:E:966:ASP:OD2	2.15	0.47
1:E:926:GLU:N	3:E:1134:HOH:O	2.47	0.47
1:E:1002:ASP:OD1	1:E:1004:THR:OG1	2.32	0.47
1:G:224:LYS:NZ	1:G:227:ASP:OD2	2.38	0.47
1:G:229:SER:HB3	1:G:248:ILE:CD1	2.45	0.47
1:G:704:GLU:CD	3:G:1110:HOH:O	2.58	0.47
1:I:534:GLU:N	3:I:1082:HOH:O	2.40	0.47
1:A:872:HIS:HE1	1:A:902:GLU:OE1	1.97	0.46
1:C:555:VAL:HG22	1:G:354:TYR:OH	2.15	0.46
1:C:992:VAL:HG11	1:C:1009:PRO:HB2	1.96	0.46
1:E:229:SER:HB3	1:E:248:ILE:CD1	2.45	0.46
1:G:367:VAL:CG1	1:G:375:VAL:HG21	2.45	0.46
1:G:887:MET:HB2	1:G:917:GLY:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:618:VAL:CG2	1:K:631:GLU:HG3	2.44	0.46
1:K:642:SER:HB2	1:K:647:THR:HB	1.97	0.46
1:A:367:VAL:O	1:A:368:ARG:HD3	2.15	0.46
1:C:256:SER:OG	1:C:267:HIS:CE1	2.68	0.46
1:C:565:GLU:HG2	1:C:566:TYR:H	1.79	0.46
1:E:253:GLN:NE2	1:E:253:GLN:HA	2.30	0.46
1:E:524:PRO:HD3	1:G:605:GLU:CG	2.44	0.46
1:E:605:GLU:HG2	1:G:524:PRO:HD3	1.98	0.46
1:E:829:ALA:HA	1:E:851:ILE:HG22	1.97	0.46
1:I:452:PHE:HB3	1:I:463:TYR:HB3	1.98	0.46
1:K:501:TYR:CD2	1:K:501:TYR:N	2.83	0.46
1:A:322:PRO:HB3	1:A:678:LEU:HD13	1.97	0.46
1:A:913:ARG:NH2	1:A:1047:GLN:HE21	2.08	0.46
1:C:48:ILE:HG12	1:C:49:HIS:N	2.30	0.46
1:G:57:CYS:HB3	1:G:62:TRP:CD1	2.50	0.46
1:G:155:PRO:O	1:G:856:ARG:HD2	2.14	0.46
1:G:329:PHE:HD1	1:G:649:MET:SD	2.38	0.46
1:G:471:GLU:O	1:G:471:GLU:HG3	2.15	0.46
1:I:836:ARG:N	3:I:1191:HOH:O	2.48	0.46
1:I:887:MET:HG3	1:I:966:ASP:OD2	2.15	0.46
1:A:956:ILE:HD13	1:A:957:ALA:N	2.31	0.46
1:C:540:PHE:HA	1:C:577:PRO:HA	1.97	0.46
1:C:622:TYR:OH	1:C:627:ARG:HG2	2.15	0.46
1:E:367:VAL:HG12	1:E:375:VAL:HG21	1.97	0.46
1:E:387:LEU:HD12	1:E:400:PHE:CE1	2.50	0.46
1:K:429:MET:HA	1:K:441:ILE:HD13	1.97	0.46
1:A:994:ILE:HG22	1:A:1008:GLN:O	2.15	0.46
1:E:363:ARG:HD3	1:E:363:ARG:HA	1.50	0.46
1:E:401:GLU:CD	1:E:401:GLU:N	2.73	0.46
1:E:946:TYR:CE1	1:G:922:GLN:HB3	2.51	0.46
1:G:184:LEU:HD13	1:G:237:ILE:HG13	1.98	0.46
1:G:906:GLN:O	1:G:953:GLY:HA3	2.14	0.46
1:I:533:PHE:N	1:K:525:ASP:OD1	2.39	0.46
1:I:906:GLN:O	1:I:953:GLY:HA3	2.15	0.46
1:K:319:ILE:CG2	1:K:677:PRO:HB3	2.46	0.46
1:K:1001:ILE:CG1	3:K:1180:HOH:O	2.64	0.46
1:E:1014:TRP:CD1	1:E:1019:GLY:HA2	2.51	0.46
1:I:57:CYS:HB3	1:I:62:TRP:CD1	2.50	0.46
1:I:471:GLU:O	1:I:471:GLU:HG3	2.15	0.46
1:K:425:ARG:O	1:K:426:PHE:HB2	2.14	0.46
1:A:524:PRO:HD3	1:C:605:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:GLU:HG2	1:C:524:PRO:HD3	1.97	0.46
1:C:253:GLN:NE2	1:C:253:GLN:HA	2.30	0.46
1:E:112:ASN:OD1	1:E:114:GLU:HB3	2.16	0.46
1:E:540:PHE:HA	1:E:577:PRO:HA	1.97	0.46
1:K:59:ASP:HB3	1:K:80:VAL:HA	1.97	0.46
1:K:318:ILE:HG21	1:K:682:ILE:HD11	1.98	0.46
1:K:322:PRO:HG2	1:K:674:ASP:OD1	2.16	0.46
1:K:367:VAL:O	1:K:368:ARG:HD3	2.16	0.46
1:K:965:SER:C	1:K:967:GLY:N	2.72	0.46
1:A:562:GLU:O	1:A:563:ALA:HB3	2.15	0.46
1:G:442:GLU:OE2	1:G:481:HIS:HD2	1.98	0.46
1:I:872:HIS:CE1	1:I:902:GLU:OE1	2.67	0.46
1:K:462:ALA:HA	1:K:481:HIS:O	2.16	0.46
1:C:533:PHE:HB3	1:C:536:VAL:HG11	1.97	0.46
1:E:258:ASP:OD1	1:E:260:ASP:HB2	2.16	0.46
1:E:697:ALA:CB	1:E:738:MET:HE1	2.46	0.46
1:G:234:SER:HB3	1:G:278:LEU:H	1.81	0.46
1:G:965:SER:C	1:G:967:GLY:N	2.70	0.46
1:G:1002:ASP:OD1	1:G:1004:THR:OG1	2.31	0.46
1:I:534:GLU:HG3	1:K:534:GLU:OE2	2.15	0.46
1:A:827:GLU:O	1:G:677:PRO:HD2	2.16	0.46
1:C:401:GLU:CD	1:C:401:GLU:N	2.74	0.46
1:I:45:ASN:HA	1:I:277:HIS:CD2	2.51	0.46
1:I:256:SER:OG	1:I:267:HIS:CE1	2.69	0.46
1:I:524:PRO:HD3	1:K:605:GLU:CG	2.46	0.46
1:K:146:LEU:HD23	1:K:165:VAL:HG21	1.97	0.46
1:A:48:ILE:HG12	1:A:49:HIS:N	2.30	0.45
1:C:360:GLU:HG3	1:C:377:PHE:CZ	2.51	0.45
1:E:180:ALA:HA	3:E:1072:HOH:O	2.16	0.45
1:E:541:VAL:CG2	1:E:542:ILE:N	2.78	0.45
1:E:562:GLU:O	1:E:563:ALA:HB3	2.16	0.45
1:G:197:PHE:HE1	1:G:199:LEU:HD21	1.81	0.45
1:G:295:ILE:O	1:G:303:ILE:HA	2.16	0.45
1:I:641:LEU:HD23	1:I:647:THR:O	2.17	0.45
1:K:228:MET:HE3	1:K:232:VAL:HG21	1.97	0.45
1:A:45:ASN:HA	1:A:277:HIS:CD2	2.51	0.45
1:C:988:TRP:CZ3	1:C:990:GLY:HA3	2.50	0.45
1:E:190:ARG:NH2	1:E:222:PHE:HZ	2.14	0.45
1:G:59:ASP:HB3	1:G:80:VAL:HA	1.98	0.45
1:G:190:ARG:NH2	1:G:222:PHE:HZ	2.14	0.45
1:G:885:PRO:HG2	1:G:890:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:921:SER:HB3	1:G:966:ASP:OD2	2.16	0.45
1:G:959:THR:O	1:G:984:GLY:HA3	2.15	0.45
1:I:184:LEU:HD13	1:I:237:ILE:HG13	1.97	0.45
1:I:387:LEU:HD12	1:I:400:PHE:CE1	2.51	0.45
1:I:841:GLY:C	1:I:843:ASP:H	2.25	0.45
1:I:886:ASP:O	1:I:891:GLY:HA3	2.17	0.45
1:K:865:GLU:HB3	3:K:1144:HOH:O	2.16	0.45
1:K:885:PRO:HG2	1:K:890:MET:HG2	1.98	0.45
1:A:218:ASN:O	1:A:219:SER:C	2.59	0.45
1:A:249:ASP:HB2	3:A:1208:HOH:O	2.17	0.45
1:A:731:LEU:HD22	1:A:735:ILE:CD1	2.47	0.45
1:A:894:GLU:OE1	1:A:897:ARG:NH2	2.49	0.45
1:E:639:LEU:HD23	1:E:639:LEU:C	2.41	0.45
1:G:530:ASN:ND2	1:G:531:PHE:N	2.62	0.45
1:G:894:GLU:OE1	1:G:897:ARG:NH2	2.49	0.45
1:G:1016:ARG:NH1	3:G:1216:HOH:O	2.39	0.45
1:I:329:PHE:HD1	1:I:649:MET:SD	2.39	0.45
1:I:562:GLU:HB3	1:I:563:ALA:H	1.58	0.45
1:I:965:SER:O	1:I:968:ASP:HB2	2.16	0.45
1:K:387:LEU:HD12	1:K:400:PHE:CE1	2.51	0.45
1:K:909:ILE:HG12	1:K:956:ILE:HG21	1.97	0.45
1:A:337:ILE:HG13	1:A:649:MET:CE	2.44	0.45
1:A:360:GLU:OE2	1:A:361:PRO:HD2	2.16	0.45
1:A:703:ASN:C	1:A:703:ASN:ND2	2.61	0.45
1:A:840:LYS:O	1:A:843:ASP:HB2	2.17	0.45
1:C:141:ASP:C	1:C:141:ASP:OD2	2.60	0.45
1:C:462:ALA:HA	1:C:481:HIS:O	2.17	0.45
1:C:562:GLU:O	1:C:563:ALA:HB3	2.17	0.45
1:E:124:PHE:CD2	1:E:153:MET:HE1	2.50	0.45
1:E:731:LEU:HD22	1:E:735:ILE:CD1	2.47	0.45
1:G:515:LEU:HD23	1:G:539:PRO:HA	1.99	0.45
1:I:226:VAL:HG13	1:I:228:MET:HE2	1.97	0.45
1:I:929:MET:HE3	1:I:979:LEU:CD1	2.46	0.45
1:K:586:ARG:NE	2:L:1206:ALA:HB3	2.31	0.45
1:A:222:PHE:H	1:A:1038:HIS:CD2	2.33	0.45
1:A:401:GLU:CD	1:A:401:GLU:N	2.75	0.45
1:A:676:ARG:HD3	3:A:1073:HOH:O	2.15	0.45
1:C:226:VAL:HG13	1:C:228:MET:HE2	1.98	0.45
1:C:300:THR:HG22	1:C:300:THR:O	2.15	0.45
1:C:681:SER:O	1:C:684:GLU:HG2	2.16	0.45
1:C:827:GLU:O	1:I:677:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:894:GLU:OE1	1:C:897:ARG:NH2	2.50	0.45
1:E:92:LYS:HA	1:E:111:TYR:O	2.17	0.45
1:E:141:ASP:OD1	1:E:145:ASN:HB2	2.17	0.45
1:E:195:ASN:O	1:E:231:HIS:HE1	1.99	0.45
1:E:318:ILE:HG21	1:E:682:ILE:HD11	1.98	0.45
1:E:997:LYS:NZ	3:E:1136:HOH:O	2.41	0.45
1:I:385:ASP:HB2	1:I:405:GLY:O	2.17	0.45
1:K:872:HIS:CE1	1:K:902:GLU:OE1	2.69	0.45
1:A:353:THR:HG23	1:A:354:TYR:CD1	2.52	0.45
1:A:452:PHE:HB3	1:A:463:TYR:HB3	1.99	0.45
1:A:936:ASP:OD2	1:C:1011:PHE:HB3	2.16	0.45
1:E:59:ASP:HB3	1:E:80:VAL:HA	1.98	0.45
1:E:155:PRO:O	1:E:856:ARG:HD2	2.17	0.45
1:I:562:GLU:O	1:I:563:ALA:HB3	2.16	0.45
1:I:605:GLU:CG	1:K:524:PRO:HD3	2.47	0.45
1:I:885:PRO:HG2	1:I:890:MET:HG2	1.99	0.45
1:A:363:ARG:HD3	1:A:363:ARG:HA	1.55	0.45
1:E:959:THR:O	1:E:984:GLY:HA3	2.17	0.45
1:G:540:PHE:HA	1:G:577:PRO:HA	1.99	0.45
1:I:300:THR:O	1:I:300:THR:HG22	2.17	0.45
1:I:360:GLU:OE2	1:I:361:PRO:HD2	2.17	0.45
1:I:418:PHE:CE1	1:I:485:MET:HE2	2.52	0.45
1:K:894:GLU:OE1	1:K:897:ARG:NH2	2.50	0.45
1:A:253:GLN:HG3	1:A:266:LYS:HE2	1.98	0.45
1:A:573:LYS:HE2	1:C:786:TYR:CZ	2.52	0.45
1:C:212:LYS:HE3	3:C:1126:HOH:O	2.17	0.45
1:C:630:THR:HG23	3:C:1225:HOH:O	2.17	0.45
1:C:922:GLN:NE2	3:C:1132:HOH:O	2.31	0.45
1:E:982:LEU:C	1:E:983:ILE:HD12	2.42	0.45
1:E:984:GLY:CA	3:E:1123:HOH:O	2.58	0.45
1:G:177:LEU:O	3:G:1089:HOH:O	2.21	0.45
1:G:243:TYR:CD2	1:G:256:SER:HB3	2.52	0.45
1:K:48:ILE:HG12	1:K:49:HIS:N	2.31	0.45
1:A:385:ASP:HB2	1:A:405:GLY:O	2.16	0.45
1:A:425:ARG:O	1:A:426:PHE:HB2	2.17	0.45
1:A:480:ILE:H	1:A:494:THR:HG21	1.76	0.45
1:C:913:ARG:NH2	1:C:1047:GLN:HE21	2.07	0.45
1:E:87:PHE:CB	1:E:88:PRO:HD2	2.41	0.45
1:E:635:ASN:HB3	1:E:653:ASP:OD1	2.17	0.45
1:E:826:SER:CB	3:E:1135:HOH:O	2.64	0.45
1:G:245:ILE:HD11	1:G:278:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:445:ARG:NH1	3:G:1167:HOH:O	2.49	0.45
1:G:562:GLU:O	1:G:563:ALA:HB3	2.17	0.45
1:G:841:GLY:C	1:G:843:ASP:H	2.25	0.45
1:I:57:CYS:HB3	1:I:62:TRP:NE1	2.32	0.45
1:I:425:ARG:O	1:I:426:PHE:HB2	2.17	0.45
1:I:442:GLU:OE2	1:I:481:HIS:HD2	2.00	0.45
1:K:906:GLN:O	1:K:953:GLY:HA3	2.17	0.45
1:A:717:LYS:N	3:A:1229:HOH:O	2.31	0.45
1:E:442:GLU:OE2	1:E:481:HIS:HD2	2.00	0.45
1:G:722:VAL:N	1:G:723:PRO:HD2	2.31	0.45
1:G:727:THR:O	1:G:730:ASP:HB2	2.16	0.45
1:I:82:ASN:HD21	1:I:96:ARG:HG2	1.80	0.45
1:I:136:ASP:OD2	1:I:137:VAL:N	2.44	0.45
1:I:735:ILE:O	1:I:739:GLN:HG3	2.16	0.45
1:K:360:GLU:OE2	1:K:361:PRO:HD2	2.17	0.45
1:E:272:ASP:O	1:E:717:LYS:HE2	2.17	0.44
1:E:840:LYS:O	1:E:843:ASP:HB2	2.17	0.44
1:E:901:ASN:HB3	1:G:469:HIS:CE1	2.53	0.44
1:G:360:GLU:OE2	1:G:361:PRO:HD2	2.16	0.44
1:G:618:VAL:HG21	1:G:631:GLU:HG3	1.98	0.44
1:I:337:ILE:HG13	1:I:649:MET:CE	2.40	0.44
1:I:390:TYR:CD1	1:I:397:ALA:HB2	2.50	0.44
1:K:295:ILE:O	1:K:303:ILE:HA	2.17	0.44
1:K:591:LEU:HD12	1:K:596:LEU:CD2	2.47	0.44
1:C:53:ILE:CG2	1:C:286:LEU:HD21	2.46	0.44
1:C:965:SER:HA	1:C:990:GLY:O	2.17	0.44
1:E:57:CYS:HB3	1:E:62:TRP:NE1	2.31	0.44
1:G:382:ARG:HD2	1:G:691:ASP:CG	2.42	0.44
1:K:541:VAL:CG2	1:K:542:ILE:N	2.80	0.44
1:C:57:CYS:HB3	1:C:62:TRP:NE1	2.31	0.44
1:C:87:PHE:HB3	1:C:88:PRO:CD	2.45	0.44
1:C:418:PHE:CE1	1:C:485:MET:HE2	2.53	0.44
1:C:772:ASP:OD1	1:C:772:ASP:C	2.60	0.44
1:C:982:LEU:C	1:C:983:ILE:HD12	2.42	0.44
1:C:1014:TRP:CD1	1:C:1019:GLY:HA2	2.52	0.44
1:E:123:TYR:OH	1:E:823:ARG:HD3	2.16	0.44
1:E:473:ASP:HA	1:G:904:SER:OG	2.17	0.44
1:E:890:MET:O	1:E:894:GLU:HG2	2.16	0.44
1:G:45:ASN:HA	1:G:277:HIS:CD2	2.52	0.44
1:G:287:PHE:CE1	1:G:294:TYR:HB2	2.52	0.44
1:I:295:ILE:O	1:I:303:ILE:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:568:LEU:HD23	1:I:568:LEU:N	2.31	0.44
1:I:829:ALA:HA	1:I:851:ILE:HG22	1.98	0.44
1:I:909:ILE:HG12	1:I:956:ILE:HG21	1.96	0.44
1:K:178:GLY:HA3	1:K:1040:TYR:CD1	2.53	0.44
1:A:243:TYR:CD2	1:A:256:SER:HB3	2.52	0.44
1:A:736:VAL:HG22	3:A:1104:HOH:O	2.16	0.44
1:C:586:ARG:HH21	2:D:1204:GLN:HB3	1.81	0.44
1:E:367:VAL:O	1:E:368:ARG:HD3	2.17	0.44
1:E:534:GLU:OE2	1:G:534:GLU:HG3	2.17	0.44
1:E:677:PRO:HD3	3:K:1136:HOH:O	2.18	0.44
1:E:800:ILE:CG2	1:E:845:ARG:HH22	2.31	0.44
1:G:141:ASP:OD2	1:G:141:ASP:C	2.61	0.44
1:G:1017:ASP:N	3:G:1099:HOH:O	2.49	0.44
1:I:177:LEU:HD21	3:I:1087:HOH:O	2.17	0.44
1:C:201:HIS:O	1:C:740:GLY:HA2	2.17	0.44
1:C:872:HIS:HE1	1:C:902:GLU:OE1	2.00	0.44
1:E:489:LYS:HG3	1:E:491:PHE:CE1	2.52	0.44
1:E:965:SER:O	1:E:968:ASP:N	2.50	0.44
1:G:568:LEU:N	1:G:568:LEU:HD23	2.32	0.44
1:I:54:ILE:HA	1:I:62:TRP:O	2.18	0.44
1:I:605:GLU:HG2	1:K:524:PRO:HD3	1.98	0.44
1:I:986:ARG:HD2	1:I:1025:TYR:O	2.17	0.44
1:K:155:PRO:O	1:K:856:ARG:HD2	2.17	0.44
1:A:253:GLN:NE2	1:A:253:GLN:HA	2.33	0.44
1:A:565:GLU:HG2	1:A:566:TYR:H	1.81	0.44
1:C:618:VAL:HG21	1:C:631:GLU:HG3	1.98	0.44
1:E:45:ASN:HA	1:E:277:HIS:CD2	2.53	0.44
1:E:501:TYR:CD2	1:E:501:TYR:N	2.86	0.44
1:K:390:TYR:CD1	1:K:397:ALA:HB2	2.49	0.44
1:A:272:ASP:O	1:A:717:LYS:HE2	2.17	0.44
1:C:98:MET:HE3	1:C:98:MET:HB2	1.84	0.44
1:C:1008:GLN:NE2	3:C:1190:HOH:O	2.50	0.44
1:E:222:PHE:H	1:E:1038:HIS:CD2	2.36	0.44
1:E:258:ASP:C	1:E:260:ASP:H	2.26	0.44
1:G:57:CYS:HB3	1:G:62:TRP:NE1	2.33	0.44
1:G:586:ARG:NE	2:H:1206:ALA:HB3	2.32	0.44
1:G:703:ASN:C	1:G:703:ASN:ND2	2.67	0.44
1:G:1016:ARG:HA	3:G:1099:HOH:O	2.17	0.44
1:I:73:LYS:HD3	1:I:76:SER:CB	2.42	0.44
1:I:253:GLN:NE2	1:I:268:THR:OG1	2.49	0.44
1:I:800:ILE:CG2	1:I:845:ARG:HH22	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:337:ILE:HD11	3:K:1165:HOH:O	2.17	0.44
1:K:407:VAL:HG13	1:K:421:VAL:HG13	2.00	0.44
1:K:418:PHE:CE1	1:K:485:MET:HE2	2.52	0.44
1:K:800:ILE:CG2	1:K:845:ARG:HH22	2.30	0.44
1:A:525:ASP:OD1	1:C:532:SER:HB2	2.18	0.44
1:I:992:VAL:HG11	1:I:1009:PRO:HB2	2.00	0.44
1:A:53:ILE:HD12	1:A:66:LEU:HD21	1.99	0.44
1:C:687:LEU:HD23	1:C:687:LEU:HA	1.86	0.44
1:E:268:THR:HG22	1:E:303:ILE:CD1	2.47	0.44
1:E:295:ILE:O	1:E:303:ILE:HA	2.18	0.44
1:E:633:LYS:HE2	1:E:633:LYS:HB2	1.84	0.44
1:E:909:ILE:HG12	1:E:956:ILE:HG21	1.99	0.44
1:G:202:TRP:CH2	1:G:745:SER:HB3	2.53	0.44
1:G:418:PHE:CE1	1:G:485:MET:HE2	2.53	0.44
1:I:205:TYR:HA	1:I:1024:ASN:HD21	1.83	0.44
1:I:225:ILE:HG13	1:I:226:VAL:HG23	1.99	0.44
1:I:272:ASP:O	1:I:717:LYS:HE2	2.18	0.44
1:A:407:VAL:HG13	1:A:421:VAL:HG13	1.98	0.43
1:A:897:ARG:NH1	3:A:1146:HOH:O	2.43	0.43
1:A:965:SER:O	1:A:968:ASP:N	2.50	0.43
1:C:59:ASP:HB3	1:C:80:VAL:HA	2.00	0.43
1:C:363:ARG:HD3	1:C:363:ARG:HA	1.55	0.43
1:C:546:PRO:CG	1:C:567:ASP:HB3	2.48	0.43
1:E:469:HIS:ND1	1:G:901:ASN:HB3	2.32	0.43
1:E:516:SER:HB3	1:E:518:ARG:HG3	1.99	0.43
1:E:528:VAL:HG21	1:E:896:TYR:CD2	2.53	0.43
1:E:591:LEU:HD12	1:E:596:LEU:CD2	2.48	0.43
1:G:134:PHE:HB2	3:G:1094:HOH:O	2.18	0.43
1:G:272:ASP:O	1:G:717:LYS:HE2	2.18	0.43
1:I:524:PRO:HD3	1:K:605:GLU:HG2	1.99	0.43
1:I:534:GLU:OE2	1:K:534:GLU:HG3	2.17	0.43
1:I:781:ALA:CB	1:I:802:PRO:HG2	2.48	0.43
1:K:297:ASN:O	1:K:301:GLU:N	2.49	0.43
1:K:440:VAL:CB	3:K:1100:HOH:O	2.66	0.43
1:K:829:ALA:HA	1:K:851:ILE:HG22	2.00	0.43
1:A:487:GLY:HA3	1:A:489:LYS:NZ	2.33	0.43
1:A:557:ARG:HH22	1:A:562:GLU:H	1.66	0.43
1:A:701:TYR:O	1:C:939:ARG:HD3	2.18	0.43
1:A:921:SER:HB3	1:A:966:ASP:OD2	2.18	0.43
1:C:201:HIS:HB3	1:C:736:VAL:HG13	2.00	0.43
1:C:313:SER:O	1:I:117:GLU:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:VAL:HG13	1:C:421:VAL:HG13	1.99	0.43
1:C:428:ILE:HD13	1:C:429:MET:N	2.33	0.43
1:E:183:ILE:HD12	1:E:192:ILE:HD13	1.99	0.43
1:E:487:GLY:O	1:E:488:ARG:C	2.61	0.43
1:E:823:ARG:O	1:E:826:SER:HB3	2.17	0.43
1:E:881:TYR:O	1:E:898:LEU:HD23	2.18	0.43
1:E:906:GLN:O	1:E:953:GLY:HA3	2.18	0.43
1:G:1053:ASP:OD2	3:G:1223:HOH:O	2.21	0.43
1:K:195:ASN:O	1:K:231:HIS:HE1	2.02	0.43
1:K:622:TYR:OH	1:K:627:ARG:HG2	2.18	0.43
1:K:1001:ILE:HG12	3:K:1180:HOH:O	2.18	0.43
1:A:190:ARG:NH2	1:A:222:PHE:HZ	2.16	0.43
1:A:222:PHE:HB2	1:A:1038:HIS:HD2	1.82	0.43
1:A:532:SER:HB2	1:C:525:ASP:OD1	2.17	0.43
1:A:744:THR:HG22	1:A:745:SER:N	2.33	0.43
1:E:184:LEU:HD13	1:E:237:ILE:HG13	2.00	0.43
1:E:921:SER:HB2	1:E:970:PHE:HB2	2.00	0.43
1:E:922:GLN:HB3	1:G:946:TYR:CE1	2.53	0.43
1:E:992:VAL:HG11	1:E:1009:PRO:HB2	2.00	0.43
1:I:474:GLY:HA2	1:K:945:PRO:HD2	2.01	0.43
1:I:579:ASN:HD22	1:I:627:ARG:HH22	1.66	0.43
1:I:659:THR:O	1:I:668:GLU:HA	2.18	0.43
1:A:501:TYR:CD2	1:A:501:TYR:N	2.86	0.43
1:E:322:PRO:HG2	1:E:674:ASP:OD1	2.18	0.43
1:E:423:ASN:ND2	1:E:427:GLU:H	2.16	0.43
1:E:462:ALA:HA	1:E:481:HIS:O	2.17	0.43
1:E:962:TYR:HA	3:E:1167:HOH:O	2.17	0.43
1:G:253:GLN:NE2	1:G:268:THR:OG1	2.50	0.43
1:G:558:SER:O	1:K:393:ARG:HG3	2.18	0.43
1:I:922:GLN:NE2	1:K:948:THR:H	2.15	0.43
1:K:45:ASN:HA	1:K:277:HIS:CD2	2.53	0.43
1:A:562:GLU:HB3	1:A:563:ALA:H	1.59	0.43
1:A:982:LEU:C	1:A:983:ILE:HD12	2.44	0.43
1:C:563:ALA:N	3:C:1164:HOH:O	2.50	0.43
1:E:451:ASP:OD1	2:F:1205:LYS:HD2	2.18	0.43
1:E:524:PRO:HD3	1:G:605:GLU:HG2	1.99	0.43
1:E:981:LYS:HE2	3:E:1168:HOH:O	2.19	0.43
1:G:581:ASP:HB2	3:G:1149:HOH:O	2.18	0.43
1:I:245:ILE:HD11	1:I:278:LEU:HG	2.00	0.43
1:K:307:GLU:N	3:K:1177:HOH:O	2.50	0.43
1:K:688:GLN:HA	3:K:1161:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:965:SER:HA	1:K:990:GLY:O	2.19	0.43
1:A:229:SER:HB3	1:A:248:ILE:CD1	2.48	0.43
1:A:234:SER:HB3	1:A:278:LEU:H	1.83	0.43
1:C:452:PHE:HB3	1:C:463:TYR:HB3	1.99	0.43
1:E:236:VAL:HG23	1:E:243:TYR:HB2	2.00	0.43
1:G:633:LYS:HB2	1:G:633:LYS:HE2	1.82	0.43
1:G:927:LYS:HD3	3:G:1128:HOH:O	2.18	0.43
1:I:279:ASN:HD22	1:I:279:ASN:HA	1.72	0.43
1:K:840:LYS:O	1:K:843:ASP:HB2	2.19	0.43
1:A:92:LYS:HA	1:A:111:TYR:O	2.19	0.43
1:A:313:SER:O	1:G:117:GLU:HA	2.19	0.43
1:C:82:ASN:HD22	1:C:82:ASN:N	2.12	0.43
1:E:53:ILE:CG2	1:E:286:LEU:HD21	2.46	0.43
1:E:82:ASN:HD22	1:E:82:ASN:N	2.13	0.43
1:E:360:GLU:HG3	1:E:377:PHE:CZ	2.53	0.43
1:E:586:ARG:HH21	2:F:1204:GLN:HB3	1.84	0.43
1:E:886:ASP:O	1:E:891:GLY:HA3	2.19	0.43
1:G:363:ARG:HD3	1:G:363:ARG:HA	1.50	0.43
1:I:297:ASN:C	1:I:297:ASN:HD22	2.25	0.43
1:K:222:PHE:H	1:K:1038:HIS:CD2	2.37	0.43
1:K:628:LYS:HA	3:K:1181:HOH:O	2.19	0.43
1:K:635:ASN:HB3	1:K:653:ASP:OD1	2.19	0.43
1:K:727:THR:O	1:K:730:ASP:HB2	2.18	0.43
1:C:501:TYR:CD2	1:C:501:TYR:N	2.86	0.43
1:E:467:LEU:HD11	1:E:496:GLU:HB2	2.00	0.43
1:G:800:ILE:CG2	1:G:845:ARG:HH22	2.30	0.43
1:K:327:GLU:O	1:K:328:ASP:O	2.37	0.43
1:K:428:ILE:HG22	1:K:442:GLU:O	2.18	0.43
1:K:467:LEU:HD11	1:K:496:GLU:HB2	2.01	0.43
1:A:568:LEU:HD23	1:A:568:LEU:N	2.33	0.43
1:A:681:SER:O	1:A:684:GLU:HG2	2.18	0.43
1:A:727:THR:HG22	3:A:1092:HOH:O	2.19	0.43
1:A:735:ILE:O	1:A:739:GLN:HG3	2.18	0.43
1:E:390:TYR:CD1	1:E:397:ALA:HB2	2.52	0.43
1:E:1033:ILE:HD11	1:E:1050:TYR:CD2	2.54	0.43
1:G:467:LEU:HD11	1:G:496:GLU:HB2	2.01	0.43
1:G:884:ILE:HB	1:G:912:VAL:HG12	2.01	0.43
1:I:498:SER:OG	1:I:518:ARG:HG2	2.18	0.43
1:K:988:TRP:CZ3	1:K:990:GLY:HA3	2.54	0.43
1:A:829:ALA:HB3	3:A:1132:HOH:O	2.18	0.43
1:C:731:LEU:HD22	1:C:735:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:780:LYS:HD3	1:E:782:TYR:CZ	2.54	0.43
1:E:1055:LEU:O	1:E:1059:LEU:HD13	2.19	0.43
1:G:781:ALA:CB	1:G:802:PRO:HG2	2.49	0.43
1:K:92:LYS:HA	1:K:111:TYR:O	2.19	0.43
1:K:725:CYS:SG	1:K:730:ASP:HB3	2.59	0.43
1:A:1002:ASP:OD1	1:A:1004:THR:OG1	2.35	0.42
1:C:234:SER:HB3	1:C:278:LEU:H	1.84	0.42
1:C:423:ASN:ND2	1:C:427:GLU:H	2.17	0.42
1:C:514:TYR:HE1	3:C:1106:HOH:O	2.02	0.42
1:C:562:GLU:HB3	1:C:563:ALA:H	1.59	0.42
1:C:616:LYS:HE2	1:C:653:ASP:CB	2.49	0.42
1:C:906:GLN:O	1:C:953:GLY:HA3	2.18	0.42
1:E:131:ARG:HG2	1:E:131:ARG:NH2	2.34	0.42
1:G:390:TYR:CD1	1:G:397:ALA:HB2	2.50	0.42
1:I:183:ILE:HD12	1:I:192:ILE:HD13	2.00	0.42
1:K:1045:ASP:HB3	1:K:1048:ILE:HG22	2.01	0.42
1:A:471:GLU:O	1:A:471:GLU:HG3	2.19	0.42
1:A:786:TYR:CZ	1:C:573:LYS:HE2	2.53	0.42
1:C:228:MET:HE3	1:C:232:VAL:HG21	2.00	0.42
1:C:253:GLN:HG3	1:C:266:LYS:HE2	2.00	0.42
1:E:123:TYR:HB3	3:E:1135:HOH:O	2.18	0.42
1:E:912:VAL:HG11	1:E:970:PHE:CE2	2.54	0.42
1:G:502:ALA:HB1	3:G:1078:HOH:O	2.19	0.42
1:G:533:PHE:HB3	1:G:536:VAL:HG11	2.01	0.42
1:G:591:LEU:HD12	1:G:596:LEU:CD2	2.46	0.42
1:G:886:ASP:O	1:G:891:GLY:HA3	2.18	0.42
1:I:403:ASN:ND2	1:I:403:ASN:C	2.75	0.42
1:K:471:GLU:O	1:K:471:GLU:HG3	2.18	0.42
1:K:498:SER:OG	1:K:518:ARG:HG2	2.19	0.42
1:K:540:PHE:HA	1:K:577:PRO:HA	2.01	0.42
1:A:544:LEU:N	3:A:1144:HOH:O	2.52	0.42
1:A:586:ARG:NE	2:B:1206:ALA:HB3	2.32	0.42
1:A:710:ILE:O	1:A:714:ILE:HG12	2.19	0.42
1:A:800:ILE:CG2	1:A:845:ARG:HH22	2.31	0.42
1:A:884:ILE:HB	1:A:912:VAL:HG12	2.01	0.42
1:C:195:ASN:O	1:C:231:HIS:HE1	2.03	0.42
1:C:318:ILE:HG21	1:C:682:ILE:HD11	1.99	0.42
1:E:287:PHE:CZ	1:E:294:TYR:HB2	2.54	0.42
1:E:308:ILE:CG2	1:E:311:LEU:HD13	2.49	0.42
1:E:378:ILE:HD11	1:E:410:MET:HG3	2.01	0.42
1:G:53:ILE:HD12	1:G:66:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:ILE:O	1:G:256:SER:HA	2.19	0.42
1:I:312:GLU:HG2	1:I:314:PRO:HD3	2.01	0.42
1:I:586:ARG:HH21	2:J:1204:GLN:HB3	1.85	0.42
1:I:1033:ILE:HD11	1:I:1050:TYR:CD2	2.54	0.42
1:K:956:ILE:CG2	1:K:956:ILE:O	2.68	0.42
1:A:922:GLN:NE2	1:C:529:LEU:HD23	2.33	0.42
1:A:965:SER:C	1:A:967:GLY:N	2.77	0.42
1:C:167:ASN:HB2	1:C:170:ILE:CB	2.42	0.42
1:C:360:GLU:OE2	1:C:361:PRO:HD2	2.19	0.42
1:C:959:THR:O	1:C:984:GLY:HA3	2.18	0.42
1:E:87:PHE:HB3	1:E:88:PRO:CD	2.48	0.42
1:E:412:VAL:HG13	1:E:433:LEU:HD11	2.01	0.42
1:G:988:TRP:CZ3	1:G:990:GLY:HA3	2.54	0.42
1:I:87:PHE:HB3	1:I:88:PRO:CD	2.46	0.42
1:I:201:HIS:HB3	1:I:736:VAL:HG13	2.01	0.42
1:I:412:VAL:HG13	1:I:433:LEU:HD11	2.02	0.42
1:K:123:TYR:OH	1:K:823:ARG:HD3	2.19	0.42
1:K:190:ARG:NH2	1:K:222:PHE:HZ	2.18	0.42
1:K:229:SER:HB3	1:K:248:ILE:CD1	2.48	0.42
1:K:442:GLU:OE2	1:K:481:HIS:HD2	2.02	0.42
1:K:562:GLU:O	1:K:563:ALA:HB3	2.18	0.42
1:A:545:ILE:O	1:A:548:SER:HB2	2.19	0.42
1:A:885:PRO:HG2	1:A:890:MET:HG2	2.00	0.42
1:A:886:ASP:O	1:A:891:GLY:HA3	2.20	0.42
1:A:955:ILE:HG22	1:A:956:ILE:N	2.33	0.42
1:C:53:ILE:HD12	1:C:66:LEU:HD21	2.01	0.42
1:C:222:PHE:H	1:C:1038:HIS:CD2	2.37	0.42
1:C:537:SER:HB3	1:C:583:GLY:O	2.19	0.42
1:E:228:MET:HE3	1:E:232:VAL:HG21	2.01	0.42
1:E:744:THR:HG22	1:E:745:SER:N	2.34	0.42
1:E:767:CYS:C	3:E:1122:HOH:O	2.61	0.42
1:G:82:ASN:HD21	1:G:96:ARG:HH21	1.66	0.42
1:G:131:ARG:H	1:G:131:ARG:HG2	1.61	0.42
1:I:141:ASP:C	1:I:141:ASP:OD2	2.62	0.42
1:I:904:SER:OG	1:K:473:ASP:HA	2.19	0.42
1:K:300:THR:O	1:K:300:THR:HG22	2.19	0.42
1:K:482:VAL:HG23	1:K:493:ALA:HB2	2.02	0.42
1:K:750:MET:HE2	1:K:1007:THR:CG2	2.50	0.42
1:K:886:ASP:O	1:K:891:GLY:HA3	2.18	0.42
1:A:287:PHE:CZ	1:A:294:TYR:HB2	2.55	0.42
1:A:295:ILE:O	1:A:303:ILE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:ARG:O	1:A:826:SER:HB3	2.19	0.42
1:C:909:ILE:HG12	1:C:956:ILE:HG21	2.01	0.42
1:C:986:ARG:HD2	1:C:1025:TYR:O	2.19	0.42
1:E:422:ALA:HB1	3:E:1087:HOH:O	2.19	0.42
1:I:327:GLU:O	1:I:328:ASP:O	2.36	0.42
1:C:297:ASN:C	1:C:297:ASN:HD22	2.27	0.42
1:C:471:GLU:HG3	1:C:471:GLU:O	2.19	0.42
1:C:541:VAL:CG2	1:C:542:ILE:N	2.83	0.42
1:C:955:ILE:HG22	1:C:956:ILE:N	2.33	0.42
1:E:203:LYS:O	1:E:743:ARG:HG2	2.18	0.42
1:E:393:ARG:HG3	1:I:558:SER:O	2.19	0.42
1:E:984:GLY:N	3:E:1123:HOH:O	2.53	0.42
1:E:1036:ALA:O	1:E:1039:ASP:HB2	2.19	0.42
1:G:141:ASP:CG	1:G:145:ASN:HB2	2.44	0.42
1:G:423:ASN:ND2	1:G:427:GLU:H	2.17	0.42
1:G:499:HIS:CE1	3:H:885:HOH:O	2.73	0.42
1:G:535:VAL:HG23	1:G:535:VAL:O	2.19	0.42
1:I:982:LEU:C	1:I:983:ILE:HD12	2.44	0.42
1:K:1002:ASP:OD1	1:K:1004:THR:OG1	2.37	0.42
1:A:641:LEU:HD22	1:A:645:ARG:HA	2.00	0.42
1:A:772:ASP:C	1:A:772:ASP:OD1	2.62	0.42
1:A:901:ASN:HB3	1:C:469:HIS:ND1	2.34	0.42
1:C:61:LEU:HB3	1:C:75:VAL:CG1	2.46	0.42
1:E:319:ILE:CG2	1:E:677:PRO:HB3	2.49	0.42
1:E:428:ILE:HG22	1:E:442:GLU:O	2.20	0.42
1:E:772:ASP:OD1	1:E:772:ASP:C	2.63	0.42
1:G:54:ILE:HA	1:G:62:TRP:O	2.20	0.42
1:G:181:THR:HG22	1:G:182:HIS:CE1	2.55	0.42
1:G:236:VAL:HG23	1:G:243:TYR:HB2	2.02	0.42
1:G:487:GLY:HA3	1:G:489:LYS:NZ	2.34	0.42
1:G:809:ASP:HA	1:G:815:VAL:HG22	2.02	0.42
1:I:190:ARG:NH2	1:I:222:PHE:CZ	2.88	0.42
1:K:641:LEU:HD23	1:K:647:THR:O	2.19	0.42
1:K:965:SER:O	1:K:968:ASP:N	2.52	0.42
1:A:124:PHE:HB3	1:A:152:ALA:HB1	2.01	0.42
1:A:406:ASN:O	1:A:423:ASN:HA	2.19	0.42
1:C:287:PHE:CZ	1:C:294:TYR:HB2	2.54	0.42
1:C:308:ILE:HD12	1:C:308:ILE:N	2.35	0.42
1:E:901:ASN:HB3	1:G:469:HIS:ND1	2.35	0.42
1:G:104:ASN:H	1:G:104:ASN:ND2	2.18	0.42
1:G:287:PHE:CZ	1:G:294:TYR:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:327:GLU:O	1:G:328:ASP:O	2.38	0.42
1:G:867:ASN:HD22	1:G:867:ASN:HA	1.64	0.42
1:I:322:PRO:HG2	1:I:674:ASP:OD1	2.20	0.42
1:I:649:MET:HE3	1:I:649:MET:HB2	1.88	0.42
1:I:750:MET:HE2	1:I:1007:THR:CG2	2.50	0.42
1:K:676:ARG:CD	3:K:1169:HOH:O	2.68	0.42
1:K:746:HIS:HE1	1:K:990:GLY:O	2.03	0.42
1:C:197:PHE:HE1	1:C:199:LEU:HD21	1.85	0.42
1:E:178:GLY:HA3	1:E:1040:TYR:CD1	2.54	0.42
1:E:329:PHE:HD1	1:E:649:MET:SD	2.43	0.42
1:E:533:PHE:HB3	1:E:536:VAL:HG11	2.00	0.42
1:G:716:GLU:HB3	3:G:1142:HOH:O	2.19	0.42
1:I:579:ASN:HD22	1:I:627:ARG:NH2	2.16	0.42
1:I:881:TYR:O	1:I:898:LEU:HD23	2.20	0.42
1:I:921:SER:HB3	1:I:966:ASP:OD2	2.19	0.42
1:I:939:ARG:HD3	1:K:701:TYR:O	2.19	0.42
1:K:489:LYS:HG3	1:K:491:PHE:CE1	2.55	0.42
1:A:98:MET:HE3	1:A:98:MET:HB2	1.89	0.41
1:A:1014:TRP:CD1	1:A:1019:GLY:HA2	2.55	0.41
1:C:591:LEU:HD12	1:C:596:LEU:CD2	2.48	0.41
1:C:744:THR:HG22	1:C:745:SER:N	2.35	0.41
1:C:887:MET:HG3	1:C:966:ASP:OD2	2.20	0.41
1:E:110:PHE:CE2	1:E:121:ILE:HG13	2.55	0.41
1:I:141:ASP:CG	1:I:145:ASN:HB2	2.45	0.41
1:K:382:ARG:HD2	1:K:691:ASP:CG	2.45	0.41
1:K:687:LEU:HD22	1:K:719:ARG:NH2	2.35	0.41
1:K:780:LYS:CE	3:K:1214:HOH:O	2.67	0.41
1:A:91:ARG:HG3	1:A:91:ARG:HH21	1.84	0.41
1:A:410:MET:HG2	1:A:421:VAL:HG22	2.01	0.41
1:A:591:LEU:HD12	1:A:596:LEU:CD2	2.48	0.41
1:C:965:SER:C	1:C:967:GLY:N	2.76	0.41
1:E:287:PHE:CE1	1:E:294:TYR:HB2	2.55	0.41
1:E:367:VAL:CG1	1:E:375:VAL:HG21	2.50	0.41
1:E:677:PRO:HD2	1:K:827:GLU:O	2.21	0.41
1:I:530:ASN:ND2	1:I:531:PHE:N	2.64	0.41
1:I:846:ASP:C	1:I:846:ASP:OD2	2.63	0.41
1:K:258:ASP:C	1:K:260:ASP:H	2.28	0.41
1:K:297:ASN:C	1:K:297:ASN:HD22	2.26	0.41
1:K:403:ASN:HD22	1:K:405:GLY:H	1.67	0.41
1:K:480:ILE:N	1:K:494:THR:CG2	2.67	0.41
1:K:586:ARG:HH21	2:L:1204:GLN:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:CYS:HB3	1:A:62:TRP:NE1	2.35	0.41
1:A:195:ASN:O	1:A:231:HIS:HE1	2.03	0.41
1:A:225:ILE:HG13	1:A:226:VAL:HG23	2.02	0.41
1:A:297:ASN:HD22	1:A:297:ASN:C	2.27	0.41
1:A:703:ASN:HD22	1:A:704:GLU:N	2.18	0.41
1:C:225:ILE:HG13	1:C:226:VAL:HG23	2.02	0.41
1:E:406:ASN:O	1:E:423:ASN:HA	2.20	0.41
1:E:618:VAL:HG21	1:E:631:GLU:HG3	2.02	0.41
1:E:872:HIS:CE1	1:E:902:GLU:OE1	2.72	0.41
1:E:988:TRP:CZ3	1:E:990:GLY:HA3	2.55	0.41
1:G:300:THR:O	1:G:300:THR:HG22	2.19	0.41
1:G:387:LEU:HD12	1:G:400:PHE:CE1	2.55	0.41
1:G:929:MET:CE	3:G:1084:HOH:O	2.67	0.41
1:I:61:LEU:HB3	1:I:75:VAL:CG1	2.49	0.41
1:I:92:LYS:HA	1:I:111:TYR:O	2.21	0.41
1:I:401:GLU:CD	1:I:401:GLU:N	2.78	0.41
1:I:965:SER:C	1:I:967:GLY:N	2.74	0.41
1:A:586:ARG:HH21	2:B:1204:GLN:HB3	1.85	0.41
1:C:226:VAL:CG1	1:C:228:MET:HE2	2.50	0.41
1:C:579:ASN:HA	3:C:1171:HOH:O	2.20	0.41
1:E:53:ILE:HG23	1:E:286:LEU:CD2	2.45	0.41
1:G:178:GLY:HA3	1:G:1040:TYR:CD1	2.56	0.41
1:G:360:GLU:HG3	1:G:377:PHE:CZ	2.56	0.41
1:G:498:SER:OG	1:G:518:ARG:HG2	2.21	0.41
1:I:382:ARG:HD2	1:I:691:ASP:CG	2.46	0.41
1:I:469:HIS:CE1	1:K:901:ASN:HB3	2.55	0.41
1:I:981:LYS:HA	1:I:981:LYS:HD3	1.87	0.41
1:K:234:SER:CB	1:K:278:LEU:H	2.33	0.41
1:K:272:ASP:O	1:K:717:LYS:HE2	2.21	0.41
1:K:781:ALA:CB	1:K:802:PRO:HG2	2.50	0.41
1:A:591:LEU:CD1	1:A:662:LEU:HD21	2.50	0.41
1:A:846:ASP:C	1:A:846:ASP:OD2	2.62	0.41
1:A:909:ILE:HG12	1:A:956:ILE:HG21	1.99	0.41
1:A:948:THR:H	1:C:922:GLN:NE2	2.17	0.41
1:C:367:VAL:CG1	1:C:375:VAL:HG21	2.50	0.41
1:C:467:LEU:HD11	1:C:496:GLU:HB2	2.03	0.41
1:C:568:LEU:N	1:C:568:LEU:HD23	2.35	0.41
1:C:829:ALA:HA	1:C:851:ILE:HG22	2.02	0.41
1:E:253:GLN:HA	1:E:253:GLN:HE21	1.85	0.41
1:E:327:GLU:O	1:E:328:ASP:O	2.38	0.41
1:E:994:ILE:HG22	1:E:1008:GLN:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1045:ASP:HB3	1:E:1048:ILE:HG22	2.03	0.41
1:G:73:LYS:HD3	1:G:76:SER:CB	2.45	0.41
1:G:887:MET:HG3	1:G:966:ASP:OD2	2.21	0.41
1:K:224:LYS:HD2	1:K:227:ASP:HB2	2.02	0.41
1:K:363:ARG:HD3	1:K:363:ARG:HA	1.51	0.41
1:K:369:ARG:NH2	3:K:1160:HOH:O	2.53	0.41
1:A:809:ASP:HA	1:A:815:VAL:HG22	2.03	0.41
1:A:965:SER:O	1:A:968:ASP:HB2	2.21	0.41
1:C:327:GLU:HG3	1:C:340:VAL:HG12	2.02	0.41
1:C:579:ASN:HD22	1:C:627:ARG:NH2	2.17	0.41
1:C:840:LYS:O	1:C:843:ASP:HB2	2.21	0.41
1:E:360:GLU:OE2	1:E:361:PRO:HD2	2.20	0.41
1:E:469:HIS:CE1	1:G:901:ASN:HB3	2.56	0.41
1:G:639:LEU:HD23	1:G:639:LEU:C	2.45	0.41
1:G:977:LEU:HB3	3:G:1084:HOH:O	2.21	0.41
1:I:48:ILE:HG12	1:I:49:HIS:N	2.36	0.41
1:I:167:ASN:HB2	1:I:170:ILE:CB	2.43	0.41
1:I:633:LYS:HE2	1:I:633:LYS:HB2	1.82	0.41
1:I:809:ASP:HA	1:I:815:VAL:HG22	2.02	0.41
1:K:403:ASN:ND2	1:K:403:ASN:C	2.78	0.41
1:A:541:VAL:CG2	1:A:542:ILE:N	2.84	0.41
1:A:622:TYR:OH	1:A:627:ARG:HG2	2.21	0.41
1:C:53:ILE:HG23	1:C:286:LEU:CD2	2.47	0.41
1:C:268:THR:HG22	1:C:303:ILE:CD1	2.51	0.41
1:C:997:LYS:NZ	3:C:1236:HOH:O	2.49	0.41
1:E:54:ILE:HA	1:E:62:TRP:O	2.21	0.41
1:E:515:LEU:HD23	1:E:539:PRO:HA	2.02	0.41
1:E:534:GLU:HG3	1:G:534:GLU:OE2	2.21	0.41
1:E:885:PRO:CG	1:E:890:MET:HG2	2.51	0.41
1:G:344:GLN:OE1	1:G:357:LYS:HE3	2.21	0.41
1:G:501:TYR:N	1:G:501:TYR:CD2	2.88	0.41
1:G:569:ASN:HA	3:G:1137:HOH:O	2.20	0.41
1:I:501:TYR:CD2	1:I:501:TYR:N	2.88	0.41
1:I:676:ARG:HA	1:I:677:PRO:HD3	1.90	0.41
1:K:99:ARG:NH1	3:K:1135:HOH:O	2.51	0.41
1:K:401:GLU:CD	1:K:401:GLU:N	2.79	0.41
1:K:744:THR:HG22	1:K:745:SER:N	2.36	0.41
1:A:53:ILE:CG2	1:A:286:LEU:HD21	2.49	0.41
1:A:236:VAL:HG23	1:A:243:TYR:HB2	2.02	0.41
1:A:555:VAL:HG13	1:I:354:TYR:CE2	2.56	0.41
1:A:635:ASN:HB3	1:A:653:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:MET:HA	1:A:889:MET:HE2	2.02	0.41
1:C:641:LEU:HD22	1:C:645:ARG:HA	2.01	0.41
1:G:823:ARG:O	1:G:826:SER:HB3	2.20	0.41
1:I:190:ARG:HH21	1:I:222:PHE:HZ	1.68	0.41
1:I:234:SER:CB	1:I:278:LEU:H	2.34	0.41
1:I:296:PHE:HD1	1:I:303:ILE:HG12	1.85	0.41
1:A:178:GLY:HA3	1:A:1040:TYR:CD1	2.55	0.41
1:A:387:LEU:HD12	1:A:400:PHE:CE1	2.56	0.41
1:A:423:ASN:ND2	1:A:427:GLU:H	2.19	0.41
1:A:1048:ILE:O	1:A:1052:ILE:HG13	2.21	0.41
1:C:92:LYS:HA	1:C:111:TYR:O	2.21	0.41
1:C:295:ILE:O	1:C:303:ILE:HA	2.20	0.41
1:C:809:ASP:HA	1:C:815:VAL:HG22	2.03	0.41
1:E:224:LYS:NZ	1:E:227:ASP:OD2	2.48	0.41
1:E:253:GLN:NE2	1:E:268:THR:OG1	2.51	0.41
1:E:351:SER:O	1:E:672:GLU:HB2	2.21	0.41
1:E:746:HIS:CE1	3:E:1083:HOH:O	2.73	0.41
1:E:885:PRO:O	1:E:915:ASN:HA	2.21	0.41
1:G:48:ILE:HG12	1:G:49:HIS:N	2.34	0.41
1:G:135:THR:HA	1:G:149:SER:O	2.21	0.41
1:G:312:GLU:HG2	1:G:314:PRO:HD3	2.02	0.41
1:G:337:ILE:HD13	1:G:350:VAL:HG12	2.03	0.41
1:G:452:PHE:HB3	1:G:463:TYR:HB3	2.02	0.41
1:I:319:ILE:CG2	1:I:677:PRO:HB3	2.51	0.41
1:I:469:HIS:ND1	1:K:901:ASN:HB3	2.36	0.41
1:K:136:ASP:CG	1:K:137:VAL:H	2.28	0.41
1:K:487:GLY:O	1:K:488:ARG:C	2.63	0.41
1:K:958:ILE:HD11	1:K:1051:ALA:CB	2.50	0.41
1:A:141:ASP:OD2	1:A:141:ASP:C	2.64	0.41
1:C:131:ARG:HH21	1:C:131:ARG:HG2	1.86	0.41
1:C:218:ASN:O	1:C:219:SER:C	2.63	0.41
1:C:649:MET:HE3	1:C:649:MET:HB2	1.85	0.41
1:C:676:ARG:HA	1:C:677:PRO:HD3	1.94	0.41
1:C:781:ALA:CB	1:C:802:PRO:HG2	2.50	0.41
1:E:204:GLY:O	1:E:206:ARG:HG3	2.21	0.41
1:E:649:MET:HE3	1:E:649:MET:HB2	1.94	0.41
1:G:307:GLU:HA	1:G:307:GLU:OE2	2.21	0.41
1:I:294:TYR:CE2	1:I:305:LYS:HB2	2.55	0.41
1:I:367:VAL:HG12	1:I:375:VAL:CG2	2.51	0.41
1:I:374:LYS:HG3	3:I:1210:HOH:O	2.20	0.41
1:I:410:MET:HG2	1:I:421:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:98:MET:HE3	1:K:98:MET:HB2	1.85	0.41
1:K:205:TYR:HA	1:K:1024:ASN:HD21	1.85	0.41
1:K:332:LEU:HD11	1:K:338:ALA:HB2	2.03	0.41
1:K:367:VAL:CG1	1:K:375:VAL:HG21	2.51	0.41
1:K:618:VAL:HG21	1:K:631:GLU:HG3	2.02	0.41
1:K:889:MET:HE2	1:K:889:MET:HA	2.02	0.41
1:A:59:ASP:HB3	1:A:80:VAL:HA	2.03	0.40
1:A:73:LYS:HD3	1:A:76:SER:CB	2.43	0.40
1:A:184:LEU:HD13	1:A:237:ILE:HG13	2.02	0.40
1:A:403:ASN:ND2	1:A:403:ASN:C	2.79	0.40
1:A:957:ALA:HB3	1:A:982:LEU:HD12	2.03	0.40
1:E:141:ASP:OD2	1:E:141:ASP:C	2.63	0.40
1:E:296:PHE:HD1	1:E:303:ILE:HG12	1.86	0.40
1:E:780:LYS:CE	3:E:1130:HOH:O	2.69	0.40
1:G:190:ARG:HH21	1:G:222:PHE:HZ	1.70	0.40
1:I:258:ASP:C	1:I:260:ASP:H	2.30	0.40
1:I:994:ILE:HG22	1:I:1008:GLN:O	2.21	0.40
1:K:87:PHE:HB3	1:K:88:PRO:CD	2.45	0.40
1:K:423:ASN:ND2	1:K:427:GLU:H	2.19	0.40
1:K:956:ILE:O	1:K:956:ILE:HG23	2.21	0.40
1:A:390:TYR:CD1	1:A:397:ALA:HB2	2.53	0.40
1:A:442:GLU:OE2	1:A:481:HIS:HD2	2.03	0.40
1:A:905:TYR:HB2	3:A:1180:HOH:O	2.21	0.40
1:A:1055:LEU:O	1:A:1059:LEU:HD13	2.20	0.40
1:C:480:ILE:H	1:C:494:THR:HG21	1.81	0.40
1:C:538:LYS:HG2	1:C:539:PRO:HD2	2.03	0.40
1:C:823:ARG:O	1:C:826:SER:HB3	2.21	0.40
1:E:742:TYR:O	1:E:743:ARG:C	2.63	0.40
1:E:750:MET:HE2	1:E:1007:THR:CG2	2.51	0.40
1:G:525:ASP:HB3	1:G:528:VAL:O	2.21	0.40
1:G:635:ASN:HB3	1:G:653:ASP:OD1	2.22	0.40
1:I:387:LEU:HB2	1:I:404:LEU:HD11	2.03	0.40
1:I:417:LYS:HE3	1:I:417:LYS:HB2	1.99	0.40
1:I:428:ILE:HG22	1:I:442:GLU:O	2.21	0.40
1:I:487:GLY:HA3	1:I:489:LYS:NZ	2.36	0.40
1:K:204:GLY:O	1:K:206:ARG:HG3	2.21	0.40
1:K:367:VAL:HG12	1:K:375:VAL:HG21	2.03	0.40
1:K:1014:TRP:CD1	1:K:1019:GLY:HA2	2.56	0.40
1:A:487:GLY:O	1:A:488:ARG:C	2.64	0.40
1:A:750:MET:HE2	1:A:1007:THR:HG23	2.03	0.40
1:C:530:ASN:ND2	1:C:531:PHE:N	2.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:633:LYS:HB2	1:C:633:LYS:HE2	1.81	0.40
1:E:202:TRP:CH2	1:E:745:SER:HB3	2.56	0.40
1:G:201:HIS:HB3	1:G:736:VAL:HG13	2.02	0.40
1:G:482:VAL:HG23	1:G:493:ALA:HB2	2.02	0.40
1:G:1052:ILE:O	1:G:1056:ILE:HG13	2.21	0.40
1:I:371:GLY:O	1:I:372:ASP:C	2.65	0.40
1:K:58:CYS:C	1:K:60:ASP:H	2.29	0.40
1:A:141:ASP:CG	1:A:145:ASN:HB2	2.47	0.40
1:A:190:ARG:HH21	1:A:222:PHE:HZ	1.69	0.40
1:A:279:ASN:HD22	1:A:279:ASN:HA	1.79	0.40
1:A:336:LEU:C	1:A:337:ILE:HD12	2.46	0.40
1:A:579:ASN:HD22	1:A:627:ARG:NH2	2.20	0.40
1:A:633:LYS:HE2	1:A:633:LYS:HB2	1.87	0.40
1:A:639:LEU:C	1:A:639:LEU:HD23	2.46	0.40
1:A:642:SER:OG	1:A:644:ASP:OD2	2.37	0.40
1:C:258:ASP:C	1:C:260:ASP:H	2.29	0.40
1:C:881:TYR:O	1:C:898:LEU:HD23	2.20	0.40
1:G:319:ILE:CG2	1:G:677:PRO:HB3	2.48	0.40
1:G:378:ILE:HD13	1:G:378:ILE:HA	1.91	0.40
1:G:424:ASP:OD2	3:G:1076:HOH:O	2.22	0.40
1:G:566:TYR:O	3:G:1157:HOH:O	2.22	0.40
1:G:579:ASN:HD22	1:G:627:ARG:NH2	2.20	0.40
1:K:294:TYR:CE2	1:K:305:LYS:HB2	2.57	0.40
1:K:766:ALA:HA	1:K:855:ASP:OD1	2.20	0.40
1:K:1036:ALA:O	1:K:1039:ASP:HB2	2.20	0.40
1:A:153:MET:O	3:A:1130:HOH:O	2.21	0.40
1:A:417:LYS:HE3	1:A:417:LYS:HB2	1.99	0.40
1:A:645:ARG:HH21	1:A:645:ARG:HG3	1.86	0.40
1:C:91:ARG:HG3	1:C:91:ARG:HH21	1.86	0.40
1:C:319:ILE:CG2	1:C:677:PRO:HB3	2.51	0.40
1:E:776:TYR:CZ	1:E:821:ILE:HG22	2.57	0.40
1:G:131:ARG:HG2	1:G:131:ARG:NH2	2.37	0.40
1:G:374:LYS:HG3	3:G:1165:HOH:O	2.21	0.40
1:G:462:ALA:HA	1:G:481:HIS:O	2.22	0.40
1:G:913:ARG:HD3	1:G:958:ILE:HG22	2.03	0.40
1:G:1055:LEU:O	1:G:1059:LEU:HD13	2.22	0.40
1:I:177:LEU:HD13	1:I:192:ILE:HD11	2.03	0.40
1:I:351:SER:O	1:I:672:GLU:HB2	2.22	0.40
1:I:922:GLN:HB3	1:K:946:TYR:CE1	2.56	0.40
1:I:976:LYS:NZ	3:I:1134:HOH:O	2.38	0.40
1:K:54:ILE:HA	1:K:62:TRP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:253:GLN:HG3	1:K:266:LYS:HE2	2.04	0.40
1:K:697:ALA:CB	1:K:738:MET:HE1	2.52	0.40
1:K:1024:ASN:HD22	1:K:1024:ASN:HA	1.68	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASN:N	1:I:143:ASP:OD2[2_545]	2.06	0.14
1:C:167:ASN:N	1:G:143:ASP:OD2[2_455]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1021/1071 (95%)	948 (93%)	67 (7%)	6 (1%)	21	42
1	C	1021/1071 (95%)	947 (93%)	66 (6%)	8 (1%)	16	34
1	E	1021/1071 (95%)	950 (93%)	63 (6%)	8 (1%)	16	34
1	G	1021/1071 (95%)	950 (93%)	63 (6%)	8 (1%)	16	34
1	I	1021/1071 (95%)	949 (93%)	64 (6%)	8 (1%)	16	34
1	K	1021/1071 (95%)	947 (93%)	66 (6%)	8 (1%)	16	34
2	B	9/14 (64%)	4 (44%)	5 (56%)	0	100	100
2	D	9/14 (64%)	4 (44%)	5 (56%)	0	100	100
2	F	9/14 (64%)	6 (67%)	3 (33%)	0	100	100
2	H	9/14 (64%)	5 (56%)	4 (44%)	0	100	100
2	J	9/14 (64%)	6 (67%)	3 (33%)	0	100	100
2	L	9/14 (64%)	5 (56%)	4 (44%)	0	100	100
All	All	6180/6510 (95%)	5721 (93%)	413 (7%)	46 (1%)	18	38

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	SER
1	C	219	SER
1	E	219	SER
1	E	1018	ALA
1	G	219	SER
1	G	1018	ALA
1	I	219	SER
1	K	219	SER
1	A	328	ASP
1	A	1018	ALA
1	C	328	ASP
1	C	1018	ALA
1	I	1018	ALA
1	K	1018	ALA
1	E	328	ASP
1	E	562	GLU
1	G	328	ASP
1	G	363	ARG
1	I	328	ASP
1	I	363	ARG
1	I	562	GLU
1	I	579	ASN
1	K	328	ASP
1	K	562	GLU
1	A	363	ARG
1	A	562	GLU
1	C	259	LEU
1	C	363	ARG
1	C	562	GLU
1	E	259	LEU
1	E	363	ARG
1	G	562	GLU
1	G	579	ASN
1	G	919	PHE
1	K	259	LEU
1	A	919	PHE
1	C	919	PHE
1	E	715	TYR
1	E	919	PHE
1	G	259	LEU
1	I	715	TYR
1	K	363	ARG

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Mol	Chain	Res	Type
1	K	919	PHE
1	C	820	ASN
1	I	919	PHE
1	K	715	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	883/928 (95%)	848 (96%)	35 (4%)	28	55
1	C	883/928 (95%)	848 (96%)	35 (4%)	28	55
1	E	883/928 (95%)	848 (96%)	35 (4%)	28	55
1	G	883/928 (95%)	846 (96%)	37 (4%)	26	52
1	I	883/928 (95%)	847 (96%)	36 (4%)	27	54
1	K	883/928 (95%)	850 (96%)	33 (4%)	30	57
2	B	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	D	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	F	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	H	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	J	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	L	8/10 (80%)	6 (75%)	2 (25%)	0	1
All	All	5346/5628 (95%)	5123 (96%)	223 (4%)	26	52

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	59	ASP
1	A	61	LEU
1	A	75	VAL
1	A	82	ASN
1	A	104	ASN

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Mol	Chain	Res	Type
1	A	183	ILE
1	A	209	THR
1	A	279	ASN
1	A	295	ILE
1	A	311	LEU
1	A	337	ILE
1	A	350	VAL
1	A	353	THR
1	A	363	ARG
1	A	368	ARG
1	A	369	ARG
1	A	417	LYS
1	A	423	ASN
1	A	428	ILE
1	A	467	LEU
1	A	562	GLU
1	A	578	ILE
1	A	580	VAL
1	A	625	LYS
1	A	641	LEU
1	A	703	ASN
1	A	731	LEU
1	A	738	MET
1	A	771	LEU
1	A	847	LEU
1	A	929	MET
1	A	937	ASN
1	A	956	ILE
1	A	1008	GLN
2	B	1204	GLN
2	B	1210	LEU
1	C	44	LEU
1	C	59	ASP
1	C	61	LEU
1	C	75	VAL
1	C	82	ASN
1	C	183	ILE
1	C	209	THR
1	C	279	ASN
1	C	295	ILE
1	C	311	LEU
1	C	337	ILE

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Mol	Chain	Res	Type
1	C	350	VAL
1	C	353	THR
1	C	363	ARG
1	C	368	ARG
1	C	369	ARG
1	C	417	LYS
1	C	423	ASN
1	C	428	ILE
1	C	467	LEU
1	C	562	GLU
1	C	578	ILE
1	C	580	VAL
1	C	625	LYS
1	C	641	LEU
1	C	703	ASN
1	C	731	LEU
1	C	738	MET
1	C	771	LEU
1	C	847	LEU
1	C	892	LEU
1	C	929	MET
1	C	937	ASN
1	C	956	ILE
1	C	1008	GLN
2	D	1204	GLN
2	D	1210	LEU
1	E	44	LEU
1	E	59	ASP
1	E	61	LEU
1	E	75	VAL
1	E	82	ASN
1	E	183	ILE
1	E	209	THR
1	E	279	ASN
1	E	295	ILE
1	E	311	LEU
1	E	337	ILE
1	E	350	VAL
1	E	353	THR
1	E	363	ARG
1	E	368	ARG
1	E	417	LYS

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Mol	Chain	Res	Type
1	E	423	ASN
1	E	428	ILE
1	E	467	LEU
1	E	562	GLU
1	E	578	ILE
1	E	580	VAL
1	E	625	LYS
1	E	641	LEU
1	E	703	ASN
1	E	731	LEU
1	E	738	MET
1	E	771	LEU
1	E	847	LEU
1	E	892	LEU
1	E	929	MET
1	E	937	ASN
1	E	938	PRO
1	E	956	ILE
1	E	1024	ASN
2	F	1204	GLN
2	F	1210	LEU
1	G	44	LEU
1	G	59	ASP
1	G	61	LEU
1	G	75	VAL
1	G	82	ASN
1	G	104	ASN
1	G	183	ILE
1	G	209	THR
1	G	279	ASN
1	G	295	ILE
1	G	311	LEU
1	G	337	ILE
1	G	350	VAL
1	G	353	THR
1	G	363	ARG
1	G	368	ARG
1	G	417	LYS
1	G	423	ASN
1	G	428	ILE
1	G	467	LEU
1	G	496	GLU

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Mol	Chain	Res	Type
1	G	562	GLU
1	G	578	ILE
1	G	580	VAL
1	G	625	LYS
1	G	641	LEU
1	G	703	ASN
1	G	731	LEU
1	G	738	MET
1	G	771	LEU
1	G	847	LEU
1	G	929	MET
1	G	937	ASN
1	G	938	PRO
1	G	956	ILE
1	G	1008	GLN
1	G	1024	ASN
2	H	1204	GLN
2	H	1210	LEU
1	I	44	LEU
1	I	59	ASP
1	I	61	LEU
1	I	75	VAL
1	I	82	ASN
1	I	183	ILE
1	I	209	THR
1	I	279	ASN
1	I	295	ILE
1	I	311	LEU
1	I	337	ILE
1	I	353	THR
1	I	363	ARG
1	I	368	ARG
1	I	369	ARG
1	I	417	LYS
1	I	423	ASN
1	I	428	ILE
1	I	467	LEU
1	I	496	GLU
1	I	548	SER
1	I	562	GLU
1	I	578	ILE
1	I	580	VAL

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Mol	Chain	Res	Type
1	I	625	LYS
1	I	641	LEU
1	I	703	ASN
1	I	731	LEU
1	I	738	MET
1	I	771	LEU
1	I	847	LEU
1	I	851	ILE
1	I	929	MET
1	I	937	ASN
1	I	956	ILE
1	I	1024	ASN
2	J	1204	GLN
2	J	1210	LEU
1	K	44	LEU
1	K	59	ASP
1	K	61	LEU
1	K	75	VAL
1	K	82	ASN
1	K	183	ILE
1	K	209	THR
1	K	279	ASN
1	K	295	ILE
1	K	311	LEU
1	K	337	ILE
1	K	353	THR
1	K	363	ARG
1	K	368	ARG
1	K	417	LYS
1	K	423	ASN
1	K	428	ILE
1	K	467	LEU
1	K	562	GLU
1	K	578	ILE
1	K	580	VAL
1	K	625	LYS
1	K	641	LEU
1	K	703	ASN
1	K	731	LEU
1	K	738	MET
1	K	771	LEU
1	K	847	LEU

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Mol	Chain	Res	Type
1	K	892	LEU
1	K	929	MET
1	K	937	ASN
1	K	956	ILE
1	K	1024	ASN
2	L	1204	GLN
2	L	1210	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	82	ASN
1	A	145	ASN
1	A	167	ASN
1	A	176	ASN
1	A	195	ASN
1	A	253	GLN
1	A	267	HIS
1	A	277	HIS
1	A	279	ASN
1	A	297	ASN
1	A	403	ASN
1	A	423	ASN
1	A	481	HIS
1	A	511	ASN
1	A	530	ASN
1	A	579	ASN
1	A	603	HIS
1	A	611	GLN
1	A	683	HIS
1	A	688	GLN
1	A	703	ASN
1	A	733	ASN
1	A	739	GLN
1	A	867	ASN
1	A	872	HIS
1	A	922	GLN
1	A	930	ASN
1	A	937	ASN
1	A	949	ASN
1	A	1008	GLN

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Mol	Chain	Res	Type
1	A	1024	ASN
1	A	1038	HIS
1	A	1047	GLN
1	C	64	HIS
1	C	82	ASN
1	C	145	ASN
1	C	167	ASN
1	C	176	ASN
1	C	195	ASN
1	C	253	GLN
1	C	267	HIS
1	C	297	ASN
1	C	403	ASN
1	C	423	ASN
1	C	481	HIS
1	C	511	ASN
1	C	530	ASN
1	C	579	ASN
1	C	603	HIS
1	C	611	GLN
1	C	683	HIS
1	C	688	GLN
1	C	703	ASN
1	C	733	ASN
1	C	739	GLN
1	C	867	ASN
1	C	872	HIS
1	C	922	GLN
1	C	930	ASN
1	C	937	ASN
1	C	949	ASN
1	C	1008	GLN
1	C	1024	ASN
1	C	1038	HIS
1	C	1047	GLN
1	E	64	HIS
1	E	77	ASN
1	E	82	ASN
1	E	145	ASN
1	E	253	GLN
1	E	267	HIS
1	E	277	HIS

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Mol	Chain	Res	Type
1	E	279	ASN
1	E	297	ASN
1	E	403	ASN
1	E	415	ASN
1	E	423	ASN
1	E	481	HIS
1	E	499	HIS
1	E	511	ASN
1	E	530	ASN
1	E	579	ASN
1	E	603	HIS
1	E	611	GLN
1	E	688	GLN
1	E	703	ASN
1	E	733	ASN
1	E	739	GLN
1	E	775	HIS
1	E	867	ASN
1	E	872	HIS
1	E	922	GLN
1	E	930	ASN
1	E	937	ASN
1	E	949	ASN
1	E	1008	GLN
1	E	1024	ASN
1	E	1038	HIS
1	E	1047	GLN
1	G	64	HIS
1	G	82	ASN
1	G	145	ASN
1	G	176	ASN
1	G	253	GLN
1	G	267	HIS
1	G	277	HIS
1	G	279	ASN
1	G	297	ASN
1	G	403	ASN
1	G	423	ASN
1	G	481	HIS
1	G	499	HIS
1	G	511	ASN
1	G	530	ASN

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Mol	Chain	Res	Type
1	G	579	ASN
1	G	603	HIS
1	G	611	GLN
1	G	688	GLN
1	G	703	ASN
1	G	733	ASN
1	G	739	GLN
1	G	867	ASN
1	G	872	HIS
1	G	922	GLN
1	G	930	ASN
1	G	937	ASN
1	G	949	ASN
1	G	1008	GLN
1	G	1024	ASN
1	G	1038	HIS
1	G	1047	GLN
1	I	64	HIS
1	I	82	ASN
1	I	176	ASN
1	I	195	ASN
1	I	253	GLN
1	I	267	HIS
1	I	279	ASN
1	I	297	ASN
1	I	403	ASN
1	I	423	ASN
1	I	481	HIS
1	I	499	HIS
1	I	511	ASN
1	I	530	ASN
1	I	579	ASN
1	I	603	HIS
1	I	611	GLN
1	I	688	GLN
1	I	703	ASN
1	I	733	ASN
1	I	739	GLN
1	I	775	HIS
1	I	867	ASN
1	I	872	HIS
1	I	922	GLN

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Mol	Chain	Res	Type
1	I	930	ASN
1	I	937	ASN
1	I	949	ASN
1	I	1008	GLN
1	I	1024	ASN
1	I	1038	HIS
1	I	1047	GLN
1	K	64	HIS
1	K	82	ASN
1	K	145	ASN
1	K	167	ASN
1	K	176	ASN
1	K	253	GLN
1	K	267	HIS
1	K	277	HIS
1	K	279	ASN
1	K	297	ASN
1	K	403	ASN
1	K	423	ASN
1	K	481	HIS
1	K	511	ASN
1	K	530	ASN
1	K	579	ASN
1	K	603	HIS
1	K	611	GLN
1	K	683	HIS
1	K	688	GLN
1	K	703	ASN
1	K	733	ASN
1	K	739	GLN
1	K	775	HIS
1	K	867	ASN
1	K	872	HIS
1	K	922	GLN
1	K	930	ASN
1	K	937	ASN
1	K	949	ASN
1	K	1008	GLN
1	K	1024	ASN
1	K	1038	HIS
1	K	1047	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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(Å²)	Q<0.9
1	A	1023/1071 (95%)	-1.35	0	100	100	8, 35, 56, 78	20 (1%)
1	C	1023/1071 (95%)	-1.33	0	100	100	8, 36, 56, 78	20 (1%)
1	E	1023/1071 (95%)	-1.21	0	100	100	8, 39, 58, 80	20 (1%)
1	G	1023/1071 (95%)	-1.31	0	100	100	8, 36, 57, 78	20 (1%)
1	I	1023/1071 (95%)	-1.30	0	100	100	8, 37, 56, 78	20 (1%)
1	K	1023/1071 (95%)	-1.23	0	100	100	8, 39, 58, 79	20 (1%)
2	B	11/14 (78%)	-0.72	0	100	100	52, 84, 96, 99	0
2	D	11/14 (78%)	-0.74	0	100	100	52, 84, 96, 99	0
2	F	11/14 (78%)	-0.52	0	100	100	53, 85, 97, 98	0
2	H	11/14 (78%)	-0.78	0	100	100	52, 84, 96, 99	0
2	J	11/14 (78%)	-0.74	0	100	100	52, 84, 96, 99	0
2	L	11/14 (78%)	-0.26	1 (9%)	15	11	54, 84, 96, 99	0
All	All	6204/6510 (95%)	-1.28	1 (0%)	100	100	8, 37, 59, 99	120 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	1213	PHE	2.2

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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.