



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:42 PM UTC

PDB ID : 4KMU / pdb_00004kmu
Title : X-ray crystal structure of the Escherichia coli RNA polymerase in complex with Rifampin
Authors : Murakami, K.S.
Deposited on : 2013-05-08
Resolution : 3.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

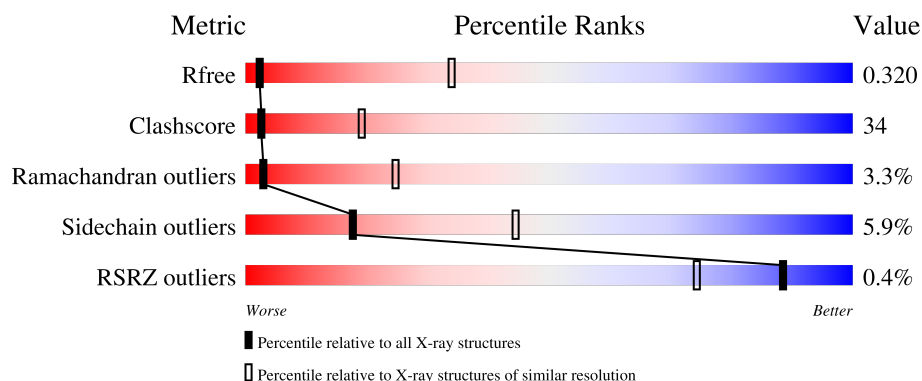
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)

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	329	
1	B	329	
1	F	329	
1	G	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	H	1342	48% 45% 6% ..
3	D	1407	31% 45% 5% 18%
3	I	1407	34% 43% 5% 18%
4	E	91	51% 43% . ..
4	J	91	% 44% 35% . . 16%
5	X	613	43% 39% . 16%
5	Y	613	36% 36% . 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56315 atoms, of which 116 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2514	1571	443	492	8			
1	B	221	Total	C	N	O	S	0	0	0
			1706	1065	300	335	6			
1	F	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			
1	G	217	Total	C	N	O	S	0	0	0
			1671	1045	293	327	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			
2	H	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			
3	I	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			

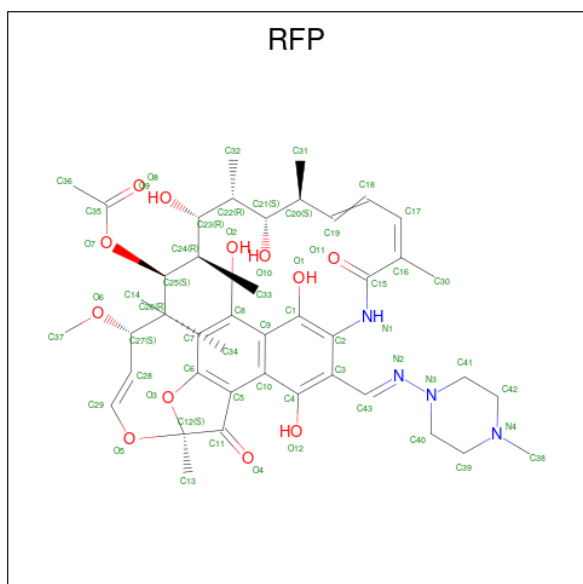
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	517	Total	C	N	O	S	0	0	0
			4198	2621	745	806	26			
5	Y	458	Total	C	N	O	S	0	0	0
			3732	2335	671	703	23			

- Molecule 6 is RIFAMPICIN (CCD ID: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			117	43	58	4	12		
6	H	1	Total	C	H	N	O	0	0
			117	43	58	4	12		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	I	2	Total	Zn	0	0
			2	2		

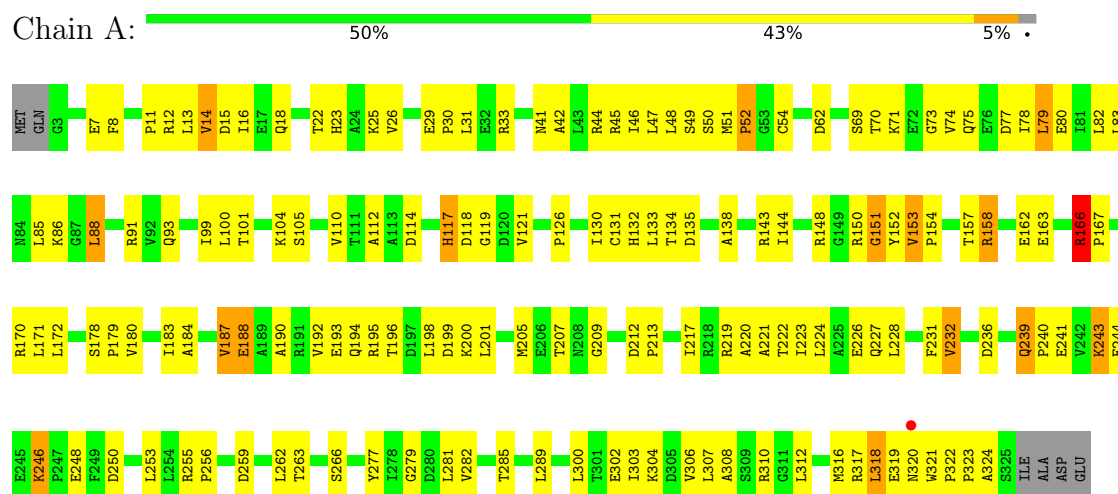
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total 1	Mg 1	0	0
8	I	1	Total 1	Mg 1	0	0

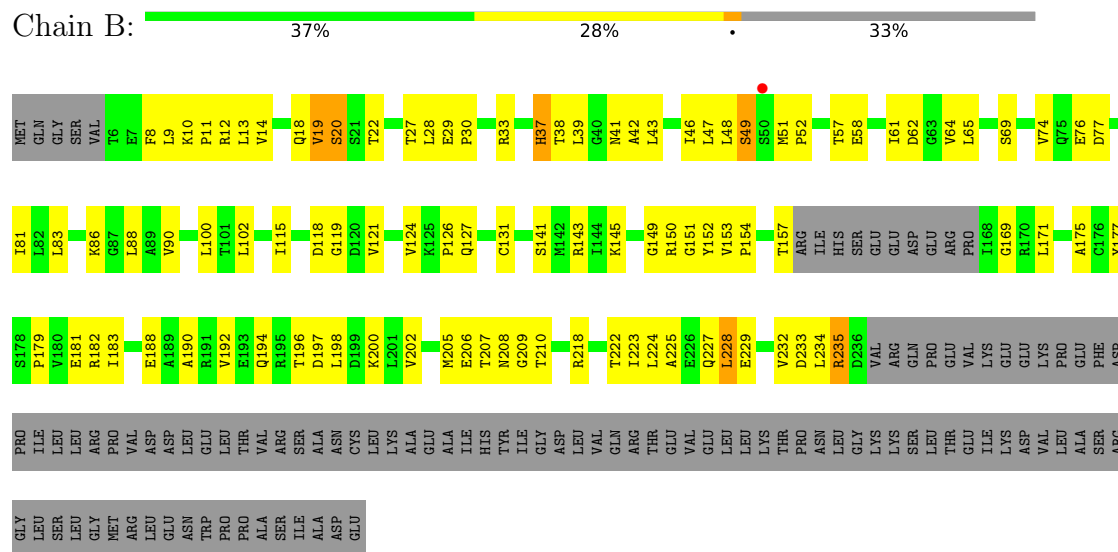
3 Residue-property plots

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.

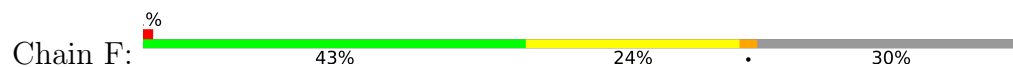
• Molecule 1: DNA-directed RNA polymerase subunit alpha

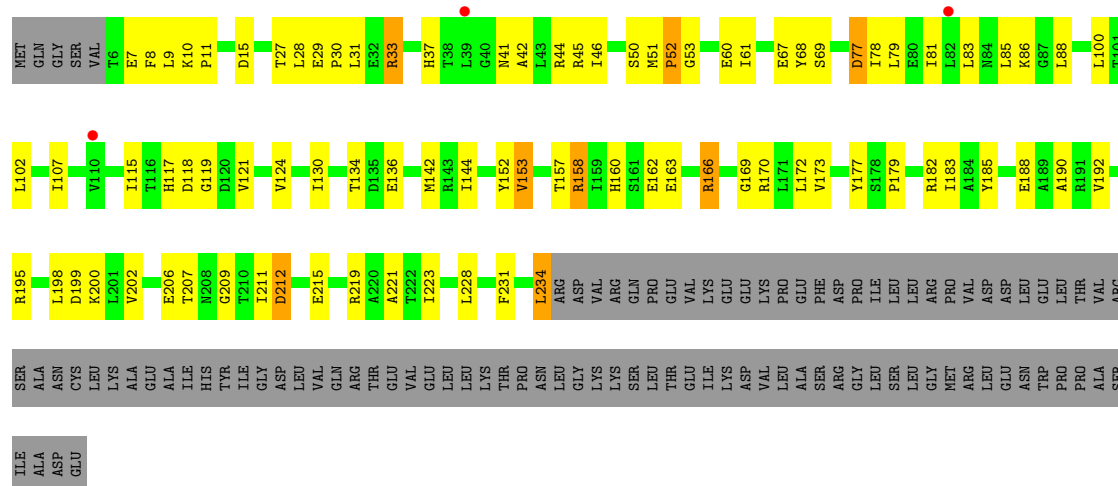


• Molecule 1: DNA-directed RNA polymerase subunit alpha

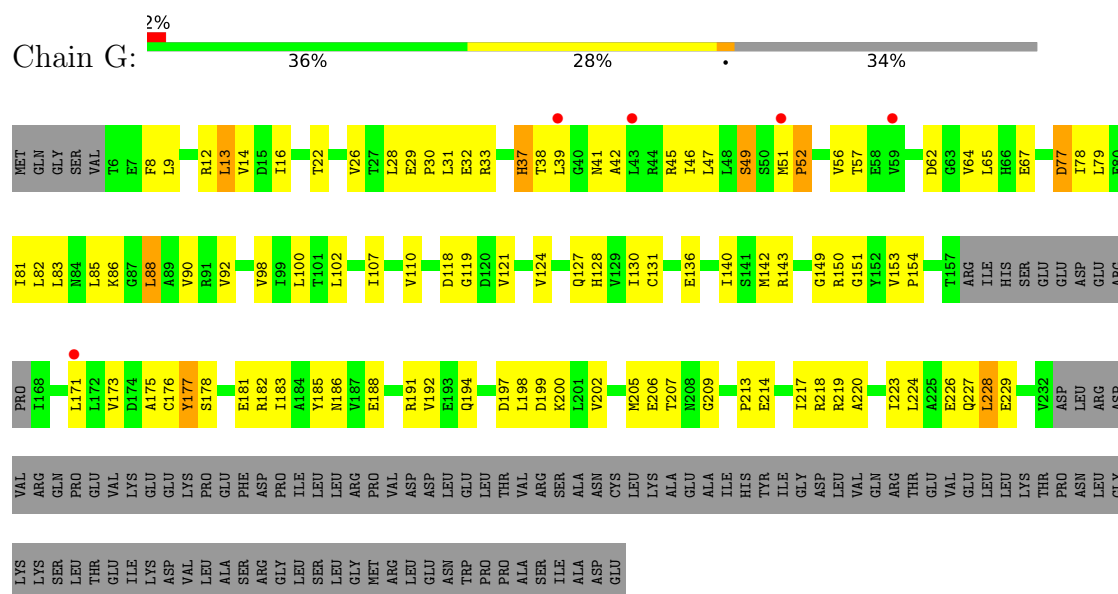


• Molecule 1: DNA-directed RNA polymerase subunit alpha

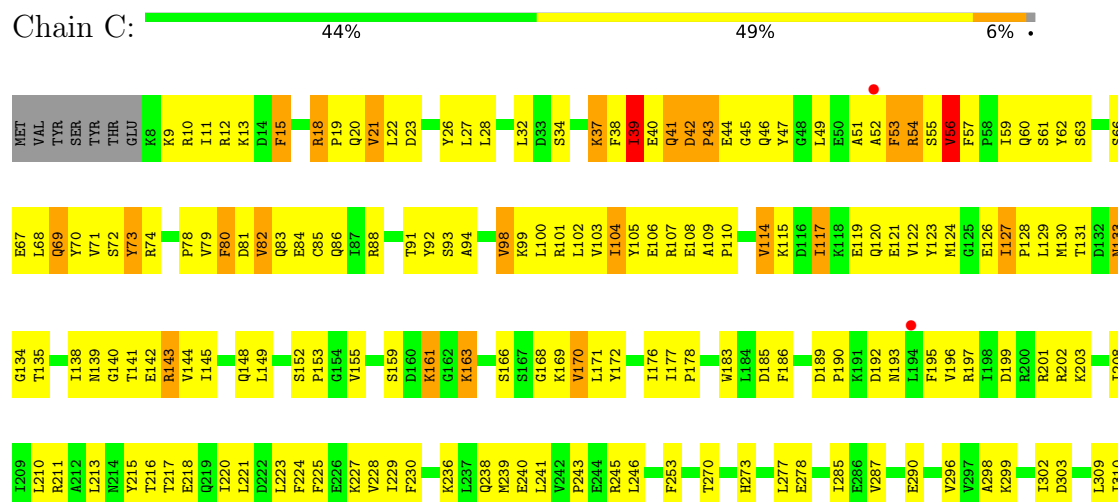


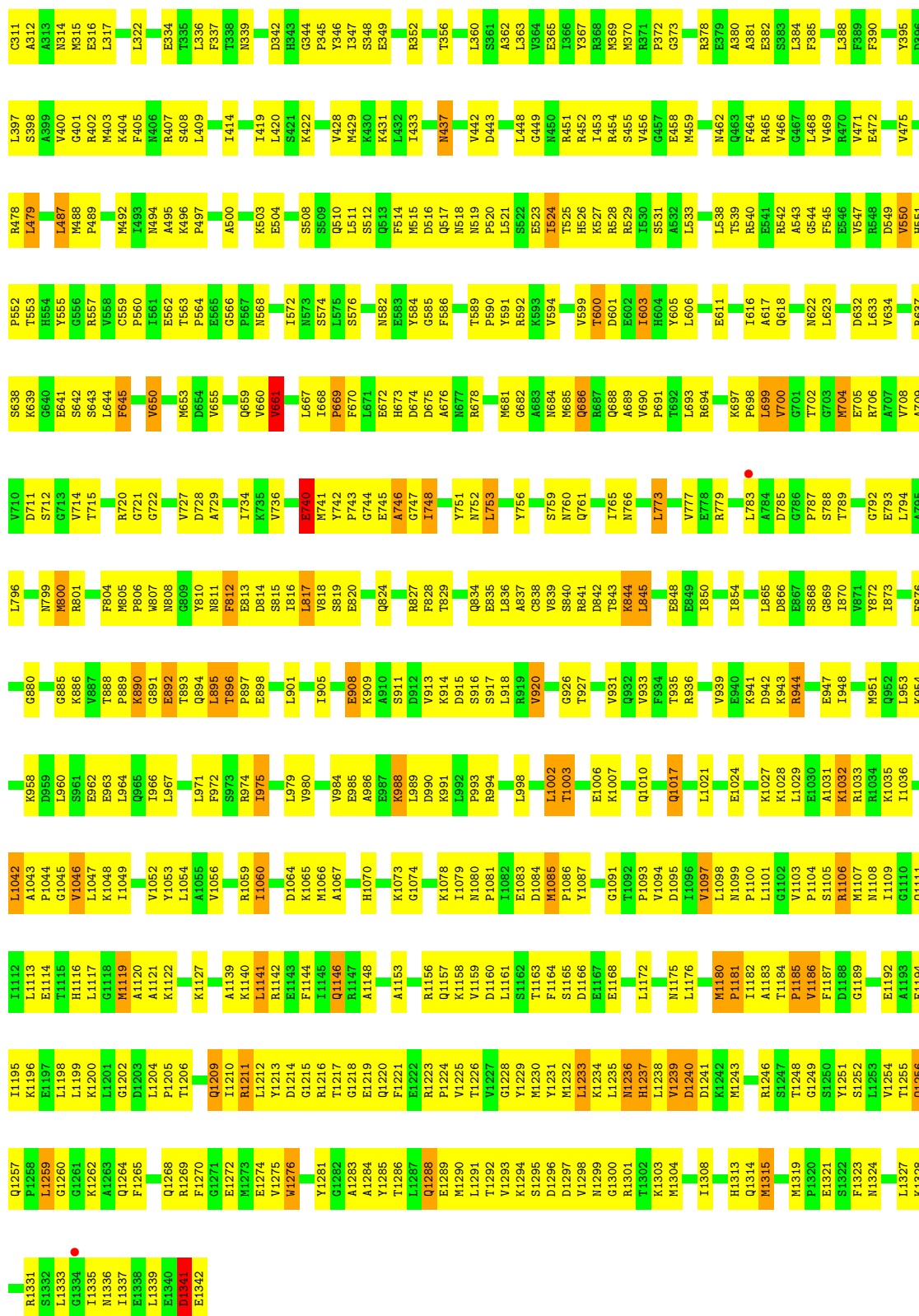


• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta

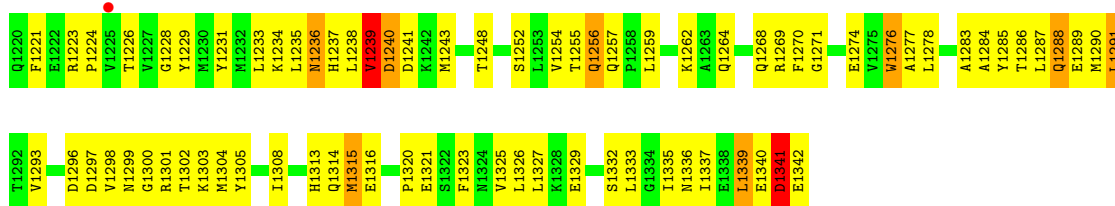




• Molecule 2: DNA-directed RNA polymerase subunit beta

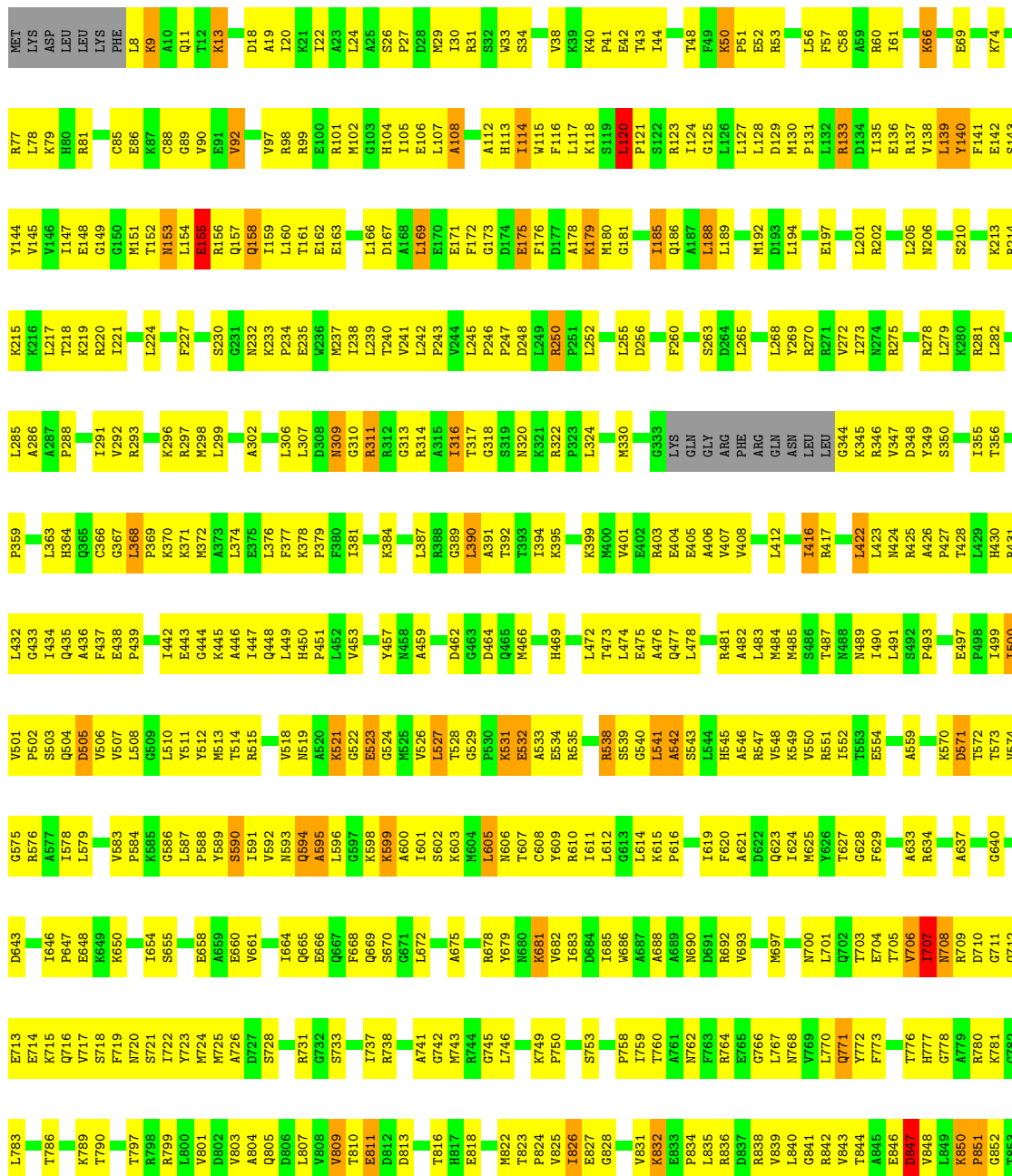
Chain H: 48% 45% 6% ..

F1144	K1073	V980	L902	T816	Y742	S666	N582	G507	I435	Y346	F136	L68	MET
I1145	G1074	V981	L905	L817	P743	L667	G585	S508	R436	I347	Y137	Q69	VAL
R1146	V1075	V984	V905	S818	A746	T668	G586	L511	R437	L351	I138	V70	TYR
R1147	I1076	S819	E908	P669	A747	P669	F586	L512	G438	L356	N139	V71	SER
A1148	S1077	E920	K909	F670	G747	E670	E588	Q513	R439	T356	G140	S72	THR
R1156	K1078	E987	K909	L671	I748	L671	E589	F514	Y442	L360	T141	Y73	
Q1157	I1079	K988	A910	E672	D749	E672	T593	F515	D443	L361	E142	R74	GLU
Q1158	M1080	L989	S911	H673		H673	P590	H615			R143		K8
P1159	P1081	D990	D912	F678	N752	A679	Y591	D516	D446	Y144	P78		K9
D1160	I1082	V913	V913	L753	L753	L753	R592	Q517	H447	I145	V79		R10
T1163	D1084	P993	S916	T830	Y756	L680	V599	N519	L448	E365	D81		R12
F1164	M1085	R994	S917	T831	Y757	H681	T600	P520		T366	V82		K13
S1165	P1086	D995	L918	L831	S759		D601	L521	R452	Y367	Q148		D14
E1166	Y1087	R996	R919	C839	N760	N684	E602	S522	R453	R151		Q86	F15
E1167	Y1087	R997	V920	S840	T763	Q686	T603	E523	R454	S152		R88	
E1168	T1092	L998	P921	S940	T764	R687	Q687	L524		P153			R18
R1171	P1093	G923	N922	D842	T765	Q688	S607	H526	F458	L241		T91	P19
L1172	V1094	G924	G924	T843	T766	A689	E610	K527	M459	V242		Y92	Q20
A1173	V1097	S925	S925	T844	T767	V690	E611	R528	M462	F156		S93	V21
E1174	N1098	G926	G926	L845	Q767	M768	P691	R529	Q463	D158		D23	L22
N1175	N1099	T927	T927	L846	P769	P691	L616		F464	S159		P95	V24
L1176	P1100	V933	V933	E848	C770	K697	A617	P535	R465	K161		L96	P25
R1177	G1102	Q1010	Q1010	E849	T771	P698	Q618	L538	V466	G162		R97	Y26
A1178	V1103	Q1013	Q1013	T850	S772	L699	A619	L539	C467	K163		V98	L27
G1179	P1104	A1014	A1014	L854	L773	V700	L623	T539	L468			K99	L28
M1180	S1105	A1015	K941	T854	G774	T702	A543		R470	S166		R101	S29
P1181	R1106	E1016	D942	V857	E775	T702	H628		V471	S167		L102	I30
N1182	M1107	Q1017	K943	V857	L783	G703	F629	V547	E472	R173		Q31	Q31
A1183	N1108	R944	R944	D866	A784	E705		R546		V287		I104	Q36
T1184	I1109	L946	A945	E967	T785	R706	D632	R549	V475	D393		Y105	K37
V1185	G1110	L947	E947	S868	Q786	A707	L633	V550	R476	L171		Y106	K38
F1186	P1111	E948	E948	G669	P787		H511	H551	E477	Y172		E107	F38
F1187	L1112	L870	S788	S788	S788		P552	T553	R478	N173		R107	I39
D1188	E1114	V871	L791	V872	L791	D711	R637	H554	L479	A174		E108	
G1189	T1115	E950	G792		G792	S712	S638	R554	S480	R175		A109	
L1199	H1116	R951	E793	E876	E793	S713	K639	R555	L481	I177		P110	
K1200	A1043	L953	L794	V877	L794	T715	S643	R557	L484	P178		V114	
L1201	P1044	L953	A795		A795	A716	L644	V568	D485			I117	
G1202	V1045	K958	L796	L883	L796	V717	S646	C559	T486			K118	
D1203	L1046	V884		G885		A718	R647	E562	L487			E119	
L1204	L1047	G886	N799	G886	N799	Q725		T563	M488			Q120	
P1205	L1054	K886	R801	R886	R801	V726	V650	P564	P489			E121	
T1206	A1055	V887	V802	T888	V802	D727	M653		D491			Y122	
S1207	V1056	P889	V802	P889	V802	D728	V654		M492			M124	
G1208	K1057	Q865	N805	K890	N805	A729	R661	N568	L493			G125	
Q1209	R1058	I966	P806	G891	P806		V655	I572	L494			E126	
I1210	R1059	I967	N807	E892	N807	T732		R573	M494			I127	
R1211	I1060	L971	N808	T893	N808	V733	Q658	S574	D427			P58	
Y1213	Q1134	L971	Q809	Q894	G809	L734	Q659	L576	V428			I59	
D1214	K1065	L975	N811	L895	Y810	K735	V660	S576	M429			M130	
G1215	A1139	T896	N811	T896	N811	V736	S662	V577	K430			T131	
R1216	K1140	P897	R812	P897	R812		S663	V578	K431			D132	
T1217	L1141	A977	E813	E899	E813	D739	V664	A579	L432			N133	
G1218	R1142	V978	D814	E999	D814	E740	G664	F505	G344			G134	
E1219	E1143	L979	S815	L901	S815	M741	A665	T581	F506			T135	



• Molecule 3: DNA-directed RNA polymerase subunit beta'

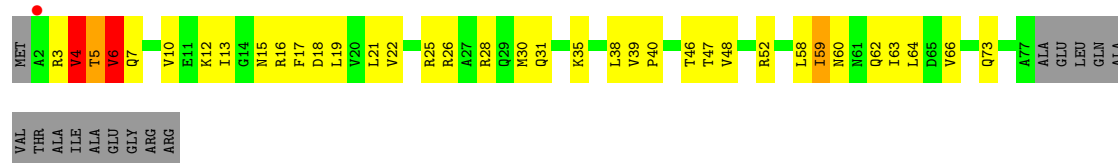
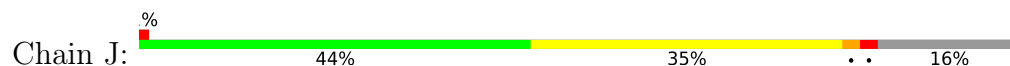
Chain D: 31% 45% 5% 18%



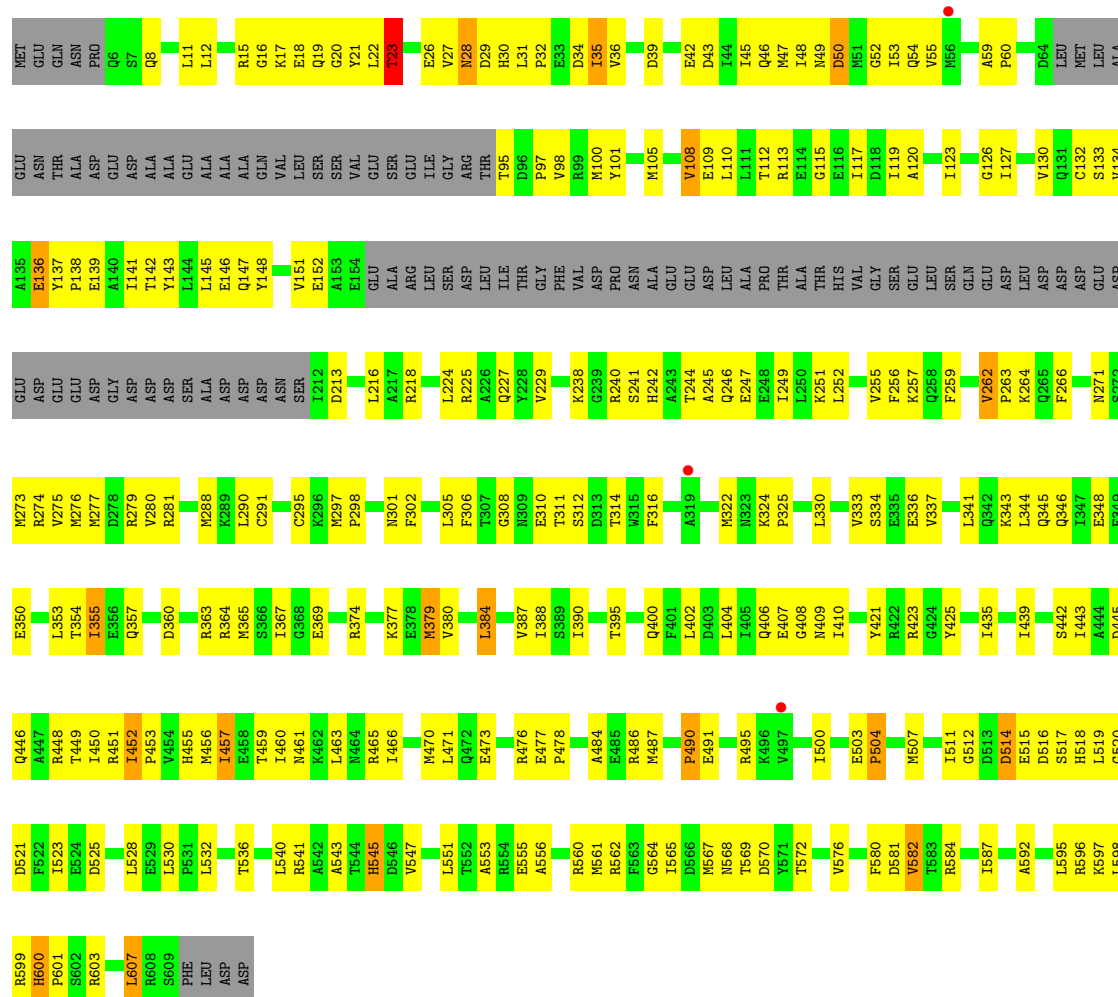




- Molecule 4: DNA-directed RNA polymerase subunit omega

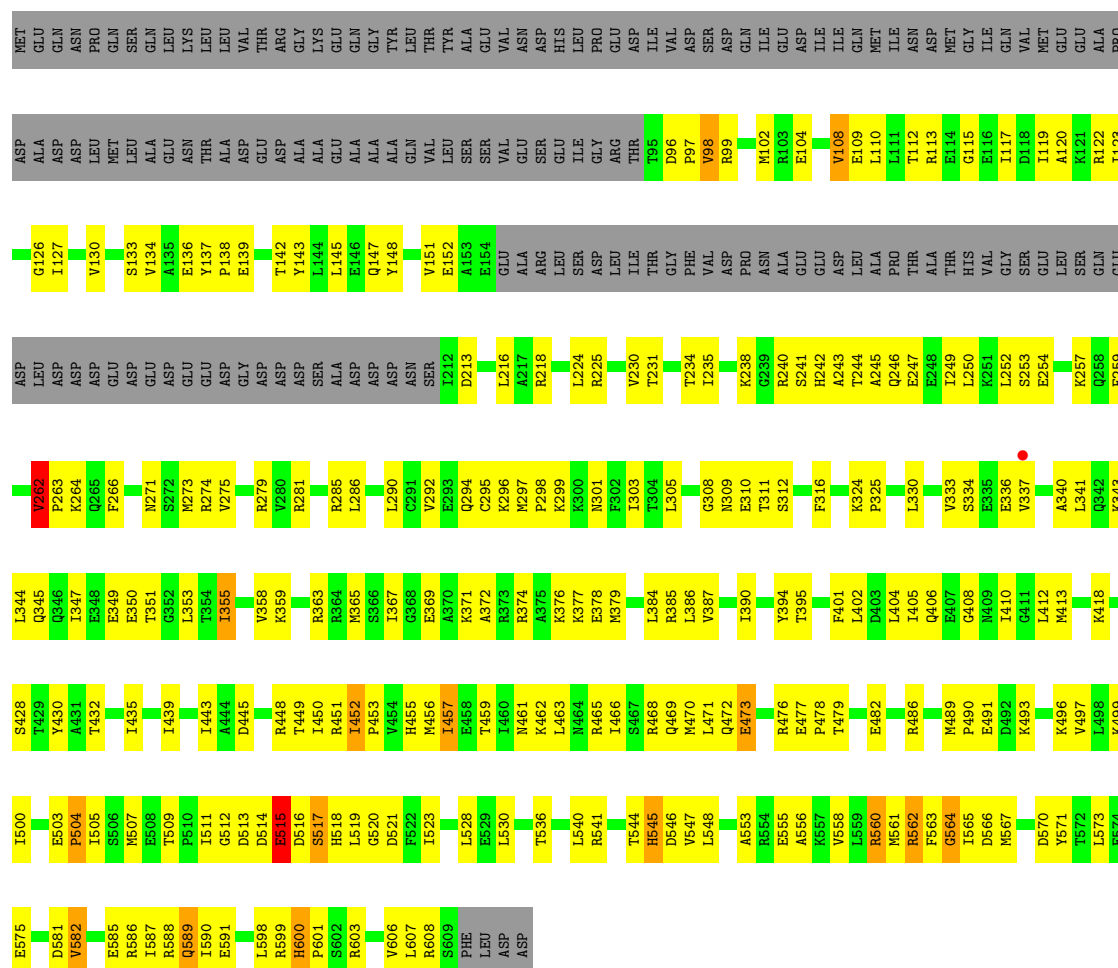


- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 5: RNA polymerase sigma factor RpoD

Chain Y:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.52Å 203.87Å 307.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 3.85 29.97 – 3.85	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.97-3.85) 87.2 (29.97-3.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.54 (at 3.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.264 , 0.321 0.265 , 0.320	Depositor DCC
R_{free} test set	5158 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	117.3	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	56315	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: MG, RFP, ZN

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	0.26	0/2548	0.74	5/3454 (0.1%)
1	B	0.26	0/1725	0.75	0/2337
1	F	0.27	0/1797	0.77	4/2436 (0.2%)
1	G	0.25	0/1690	0.75	0/2290
2	C	0.27	0/10690	0.77	12/14423 (0.1%)
2	H	0.27	1/10690 (0.0%)	0.75	16/14423 (0.1%)
3	D	0.26	0/9198	0.77	13/12413 (0.1%)
3	I	0.26	0/9198	0.76	12/12413 (0.1%)
4	E	0.25	0/710	0.71	0/956
4	J	0.25	0/607	0.70	0/817
5	X	0.25	0/4253	0.72	2/5719 (0.0%)
5	Y	0.25	0/3783	0.72	2/5083 (0.0%)
All	All	0.26	1/56889 (0.0%)	0.75	66/76764 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	663	VAL	CA-C	5.63	1.60	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	120	LEU	CA-C-N	-8.62	110.39	120.13
3	D	120	LEU	C-N-CA	-8.62	110.39	120.13
2	C	42	ASP	CA-C-N	6.72	128.24	119.84
2	C	42	ASP	C-N-CA	6.72	128.24	119.84
3	I	120	LEU	CA-C-N	-6.65	112.62	120.13
3	I	120	LEU	C-N-CA	-6.65	112.62	120.13
3	I	529	GLY	CA-C-N	6.24	126.43	119.32
3	I	529	GLY	C-N-CA	6.24	126.43	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	368	LEU	CA-C-N	6.22	126.24	119.89
3	D	368	LEU	C-N-CA	6.22	126.24	119.89
3	D	904	ALA	N-CA-C	-6.11	105.32	112.89
2	C	1085	MET	CA-C-N	6.01	127.35	119.84
2	C	1085	MET	C-N-CA	6.01	127.35	119.84
2	H	1323	PHE	N-CA-C	-6.00	107.78	114.62
2	C	566	GLY	CA-C-N	5.95	125.65	119.64
2	C	566	GLY	C-N-CA	5.95	125.65	119.64
3	D	130	MET	CA-C-N	5.90	125.91	119.89
3	D	130	MET	C-N-CA	5.90	125.91	119.89
2	H	986	ALA	CB-CA-C	-5.89	109.77	116.54
3	I	854	ALA	CB-CA-C	-5.87	109.82	116.63
3	D	497	GLU	CA-C-N	5.87	125.82	119.78
3	D	497	GLU	C-N-CA	5.87	125.82	119.78
3	D	854	ALA	CB-CA-C	-5.85	109.84	116.63
2	H	45	GLY	N-CA-C	5.83	115.51	110.21
3	D	529	GLY	CA-C-N	5.72	125.85	119.32
3	D	529	GLY	C-N-CA	5.72	125.85	119.32
2	C	986	ALA	CB-CA-C	-5.57	110.14	116.54
2	H	1184	THR	CA-C-N	5.56	126.79	119.84
2	H	1184	THR	C-N-CA	5.56	126.79	119.84
3	D	599	LYS	N-CA-C	-5.53	107.19	114.04
1	A	241	GLU	CB-CA-C	-5.52	110.23	116.63
1	A	166	ARG	CA-C-N	5.46	126.66	119.84
1	A	166	ARG	C-N-CA	5.46	126.66	119.84
3	I	501	VAL	CA-C-N	5.45	125.46	119.90
3	I	501	VAL	C-N-CA	5.45	125.46	119.90
3	I	827	GLU	N-CA-C	-5.43	106.42	113.16
2	H	242	VAL	CA-C-N	5.41	125.49	119.32
2	H	242	VAL	C-N-CA	5.41	125.49	119.32
2	C	892	GLU	CB-CA-C	-5.40	109.88	117.23
2	H	127	ILE	CA-C-N	5.37	125.31	119.78
2	H	127	ILE	C-N-CA	5.37	125.31	119.78
5	Y	262	VAL	CA-C-N	5.34	126.52	119.84
5	Y	262	VAL	C-N-CA	5.34	126.52	119.84
1	A	212	ASP	CA-C-N	5.33	124.99	119.56
1	A	212	ASP	C-N-CA	5.33	124.99	119.56
2	H	1080	ASN	CA-C-N	5.32	125.26	119.78
2	H	1080	ASN	C-N-CA	5.32	125.26	119.78
5	X	262	VAL	CA-C-N	5.32	125.38	119.32
5	X	262	VAL	C-N-CA	5.32	125.38	119.32
2	C	54	ARG	N-CA-C	5.30	121.14	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	449	GLY	N-CA-C	-5.25	106.90	115.46
3	I	1184	ASP	CA-C-N	5.23	126.38	119.84
3	I	1184	ASP	C-N-CA	5.23	126.38	119.84
3	I	826	ILE	N-CA-C	5.21	114.24	106.85
1	F	212	ASP	CA-C-N	5.16	124.96	119.28
1	F	212	ASP	C-N-CA	5.16	124.96	119.28
2	C	896	THR	CA-C-N	5.14	126.26	119.84
2	C	896	THR	C-N-CA	5.14	126.26	119.84
2	H	1085	MET	CA-C-N	5.14	126.26	119.84
2	H	1085	MET	C-N-CA	5.14	126.26	119.84
2	H	664	GLY	N-CA-C	-5.08	106.63	112.83
3	I	904	ALA	N-CA-C	-5.05	106.62	112.89
2	H	896	THR	CA-C-N	5.02	126.11	119.84
2	H	896	THR	C-N-CA	5.02	126.11	119.84
1	F	166	ARG	CA-C-N	5.01	126.10	119.84
1	F	166	ARG	C-N-CA	5.01	126.10	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2514	0	2566	170	0
1	B	1706	0	1738	108	0
1	F	1775	0	1800	77	0
1	G	1671	0	1706	95	0
2	C	10523	0	10546	834	0
2	H	10523	0	10546	719	0
3	D	9060	0	9257	832	0
3	I	9060	0	9257	769	0
4	E	708	0	719	52	0
4	J	605	0	612	44	0
5	X	4198	0	4250	256	0
5	Y	3732	0	3809	218	0
6	C	59	58	56	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	59	58	56	14	0
7	D	2	0	0	0	0
7	I	2	0	0	0	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
All	All	56199	116	56918	3861	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (3861) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.20	1.17
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.26	1.14
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.29	1.14
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.30	1.12
3:I:1173:ARG:HA	3:I:1174:ARG:HB2	1.28	1.12
2:H:54:ARG:H	2:H:55:SER:HB2	1.16	1.10
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.34	1.09
3:D:610:ARG:HG3	3:D:864:LEU:HD13	1.34	1.09
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.27	1.08
2:C:42:ASP:HB3	2:C:43:PRO:HD2	1.34	1.08
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.36	1.07
2:H:488:MET:HB2	2:H:490:GLN:H	1.13	1.07
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.33	1.06
3:D:310:GLY:HA3	3:D:311:ARG:HB2	1.15	1.05
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.38	1.05
3:I:850:LYS:HD2	3:I:851:PRO:HD2	1.32	1.05
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.41	1.02
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.41	1.02
3:I:858:VAL:HB	3:I:859:PRO:HD3	1.40	1.02
1:B:83:LEU:HD11	3:D:527:LEU:HA	1.41	1.02
3:D:858:VAL:HB	3:D:859:PRO:HD3	1.42	1.02
2:H:876:GLU:HG3	2:H:927:THR:HG22	1.41	1.02
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.43	0.99
3:I:186:GLN:HB2	3:I:238:ILE:HD11	1.43	0.99
2:C:524:ILE:HD11	2:C:712:SER:HB2	1.41	0.99
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.45	0.98
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.45	0.98
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.45	0.97
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.44	0.97
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.43	0.96
3:D:142:GLU:HA	3:D:180:MET:HE2	1.47	0.96
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.47	0.96
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.44	0.96
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	1.46	0.96
3:I:842:ARG:HD2	3:I:882:VAL:HG21	1.45	0.96
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.27	0.96
2:C:54:ARG:H	2:C:55:SER:HB2	1.29	0.95
1:G:192:VAL:HG21	1:G:198:LEU:HD12	1.47	0.95
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.49	0.95
3:I:1173:ARG:HG2	3:I:1189:MET:HE1	1.44	0.94
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.50	0.94
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.49	0.94
2:H:255:ILE:HD12	2:H:263:VAL:HB	1.50	0.93
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.33	0.93
3:D:230:SER:HB2	3:D:1339:GLY:H	1.33	0.93
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.49	0.93
3:D:1301:THR:HG23	3:I:1301:THR:HG23	1.47	0.93
2:H:487:LEU:HB3	2:H:488:MET:HA	1.48	0.93
2:H:845:LEU:HD23	2:H:889:PRO:HG2	1.50	0.93
5:X:139:GLU:HA	5:X:142:THR:HG22	1.51	0.93
1:B:192:VAL:HG21	1:B:198:LEU:HD12	1.49	0.93
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.50	0.93
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.51	0.92
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.49	0.92
2:C:876:GLU:HG3	2:C:927:THR:HG22	1.51	0.92
3:D:803:VAL:HG13	3:D:1259:GLN:HE22	1.34	0.92
3:I:905:ARG:HH22	4:J:10:VAL:HG11	1.33	0.92
3:I:546:ALA:H	3:I:547:ARG:HA	1.34	0.92
2:H:800:MET:HA	2:H:800:MET:HE3	1.52	0.92
2:H:908:GLU:HG2	2:H:909:LYS:H	1.34	0.92
3:I:145:VAL:HG13	3:I:180:MET:HB3	1.52	0.91
2:H:27:LEU:HD13	2:H:528:ARG:HH21	1.35	0.91
2:H:55:SER:HB3	2:H:56:VAL:HG13	1.52	0.91
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.51	0.91
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.53	0.91
3:D:310:GLY:CA	3:D:311:ARG:HB2	2.01	0.90
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.52	0.90
2:H:131:THR:HG23	2:H:133:ASN:H	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:487:LEU:CB	2:H:488:MET:HA	2.00	0.90
4:E:10:VAL:HG21	4:E:16:ARG:HG2	1.54	0.90
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.53	0.90
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.51	0.90
2:H:488:MET:HB2	2:H:490:GLN:N	1.86	0.90
3:D:128:LEU:HA	3:D:192:MET:HE1	1.53	0.89
3:D:1247:LYS:HD3	3:D:1247:LYS:H	1.36	0.89
3:D:186:GLN:HB2	3:D:238:ILE:HD11	1.52	0.89
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.52	0.89
2:H:660:VAL:HG13	2:H:661:VAL:HG13	1.51	0.89
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.53	0.89
4:J:5:THR:HA	4:J:6:VAL:CB	2.03	0.89
4:E:5:THR:HA	4:E:6:VAL:CB	2.03	0.88
3:D:546:ALA:H	3:D:547:ARG:HA	1.37	0.88
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	1.52	0.88
3:I:1247:LYS:H	3:I:1247:LYS:HD3	1.38	0.88
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.56	0.88
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.56	0.88
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.56	0.88
3:I:697:MET:HE1	3:I:738:ARG:HA	1.56	0.87
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.01	0.87
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.55	0.87
1:B:12:ARG:H	1:B:30:PRO:HG2	1.37	0.87
2:C:133:ASN:O	2:C:527:LYS:NZ	2.08	0.87
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.57	0.87
5:X:466:ILE:HD12	5:X:487:MET:HE2	1.57	0.87
2:C:800:MET:HA	2:C:800:MET:HE3	1.53	0.87
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.39	0.87
3:D:697:MET:HE1	3:D:738:ARG:HA	1.56	0.87
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.57	0.86
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.57	0.86
2:C:55:SER:HB3	2:C:56:VAL:HG22	1.57	0.86
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.56	0.86
2:C:59:ILE:HD13	2:C:479:LEU:HD22	1.54	0.86
3:D:154:LEU:HD21	3:D:160:LEU:HD21	1.55	0.86
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.55	0.86
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.41	0.86
5:Y:546:ASP:HB3	5:Y:603:ARG:HH22	1.37	0.86
3:I:263:SER:HB2	5:Y:507:MET:HE2	1.58	0.86
2:C:933:VAL:HG12	2:C:948:ILE:HD11	1.56	0.86
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:864:LEU:HD11	3:I:901:ARG:HH12	1.41	0.86
2:C:524:ILE:HD11	2:C:712:SER:CB	2.05	0.85
3:I:259:ARG:HH21	5:Y:504:PRO:HB2	1.41	0.85
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.57	0.85
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.39	0.85
1:A:205:MET:HE1	1:A:217:ILE:HD11	1.57	0.85
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.55	0.85
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.40	0.85
2:H:898:GLU:HB2	5:Y:540:LEU:HD21	1.57	0.85
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.57	0.85
2:H:794:LEU:HD21	2:H:796:LEU:HG	1.57	0.85
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.57	0.85
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.58	0.85
2:C:520:PRO:HB3	2:C:714:VAL:HG11	1.59	0.85
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.58	0.85
5:X:240:ARG:HD3	5:X:244:THR:HB	1.57	0.85
2:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.58	0.85
5:Y:262:VAL:HG13	5:Y:263:PRO:HD2	1.58	0.85
5:X:471:LEU:HB3	5:X:478:PRO:HD3	1.58	0.85
2:H:808:ASN:H	3:I:633:ALA:HB2	1.42	0.84
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.59	0.84
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.42	0.84
2:H:131:THR:HG21	2:H:135:THR:HG22	1.59	0.84
4:J:38:LEU:HD13	4:J:58:LEU:HD23	1.59	0.84
2:H:828:PHE:HB2	2:H:1060:ILE:HD13	1.59	0.84
2:H:1073:LYS:HD3	3:I:462:ASP:HB3	1.60	0.84
3:D:145:VAL:HG13	3:D:180:MET:HB3	1.60	0.84
3:I:128:LEU:HD21	3:I:188:LEU:HD13	1.59	0.84
3:D:842:ARG:HD2	3:D:882:VAL:HG21	1.60	0.84
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.57	0.84
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.58	0.84
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.59	0.84
3:D:828:GLY:HA2	3:D:832:LYS:H	1.43	0.84
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.60	0.84
2:C:816:ILE:HD13	2:C:1074:GLY:HA3	1.59	0.83
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.59	0.83
2:H:488:MET:CB	2:H:490:GLN:H	1.91	0.83
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.04	0.83
4:J:10:VAL:HG21	4:J:16:ARG:HG2	1.61	0.83
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.59	0.83
5:Y:402:LEU:HD13	5:Y:405:ILE:HD11	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:VAL:HG23	2:C:171:LEU:H	1.42	0.83
2:C:400:VAL:HG12	2:C:404:LYS:HE2	1.61	0.83
6:C:1401:RFP:H311	6:C:1401:RFP:H323	1.61	0.83
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.61	0.82
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.60	0.82
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.61	0.82
2:H:564:PRO:HA	2:H:684:ASN:HD21	1.44	0.82
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.61	0.82
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.60	0.82
2:H:54:ARG:N	2:H:55:SER:HB2	1.93	0.82
2:H:1105:SER:HB2	3:I:731:ARG:HB2	1.61	0.82
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	1.60	0.82
2:H:194:LEU:HD23	2:H:429:MET:HE3	1.60	0.82
2:C:55:SER:HB3	2:C:56:VAL:HG13	1.60	0.82
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.60	0.82
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.59	0.82
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.45	0.82
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.61	0.82
2:H:131:THR:CG2	2:H:135:THR:HG22	2.10	0.81
2:C:403:MET:HG3	2:C:414:ILE:HB	1.62	0.81
2:H:1101:LEU:HD13	3:I:504:GLN:HB2	1.62	0.81
1:B:11:PRO:HA	1:B:30:PRO:HB2	1.62	0.81
2:C:131:THR:CG2	2:C:135:THR:HG22	2.11	0.81
3:D:107:LEU:HD23	3:D:299:LEU:HD21	1.62	0.81
5:Y:469:GLN:HE21	5:Y:473:GLU:HG3	1.46	0.81
1:B:49:SER:HA	1:B:151:GLY:HA2	1.62	0.81
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.42	0.81
3:I:803:VAL:HG13	3:I:1259:GLN:HE22	1.45	0.81
2:C:131:THR:HG21	2:C:135:THR:HG22	1.61	0.81
4:J:5:THR:HA	4:J:6:VAL:HB	1.62	0.81
2:C:131:THR:HG23	2:C:133:ASN:H	1.45	0.81
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.62	0.81
4:E:5:THR:HA	4:E:6:VAL:CG1	2.11	0.80
2:H:28:LEU:HD22	2:H:527:LYS:HD2	1.62	0.80
2:H:55:SER:HB3	2:H:56:VAL:HG22	1.63	0.80
1:F:163:GLU:HG3	1:F:170:ARG:HH12	1.44	0.80
3:I:145:VAL:HG22	3:I:180:MET:SD	2.21	0.80
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.64	0.80
2:C:487:LEU:HB2	2:C:489:PRO:HD3	1.63	0.80
3:D:518:VAL:HG12	3:D:519:ASN:HD22	1.47	0.80
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:128:LEU:HD11	3:D:188:LEU:HD22	1.63	0.80
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.47	0.80
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.63	0.80
4:J:5:THR:HA	4:J:6:VAL:CG1	2.11	0.80
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.63	0.79
3:D:512:TYR:HD2	3:D:724:MET:HE1	1.47	0.79
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.17	0.79
3:D:112:ALA:HA	3:D:238:ILE:HG22	1.62	0.79
2:H:1042:LEU:HD13	2:H:1042:LEU:H	1.46	0.79
2:C:1243:MET:HE3	3:D:372:MET:HB2	1.64	0.79
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.63	0.79
5:X:59:ALA:HB3	5:X:60:PRO:HD3	1.65	0.79
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.17	0.79
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.62	0.79
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	1.63	0.79
4:E:5:THR:HA	4:E:6:VAL:HB	1.62	0.79
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.64	0.79
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.65	0.79
2:H:700:VAL:HG11	2:H:1114:GLU:CG	2.13	0.79
3:I:298:MET:HE3	5:Y:402:LEU:HB3	1.64	0.79
2:C:309:LEU:HD23	2:C:309:LEU:H	1.48	0.78
2:C:13:LYS:CD	2:C:1181:PRO:HG2	2.13	0.78
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.65	0.78
1:G:192:VAL:HG12	1:G:194:GLN:HG2	1.64	0.78
4:J:5:THR:HA	4:J:6:VAL:HG12	1.64	0.78
2:C:564:PRO:HA	2:C:684:ASN:HD21	1.49	0.78
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.63	0.78
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.65	0.78
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.66	0.78
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.64	0.78
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.64	0.78
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.63	0.78
5:X:35:ILE:HG13	5:X:36:VAL:H	1.46	0.78
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.66	0.78
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	1.65	0.78
2:C:54:ARG:HG2	2:C:55:SER:HB2	1.64	0.78
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.66	0.78
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.65	0.78
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.64	0.78
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.65	0.78
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.07	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:487:LEU:HB3	2:H:488:MET:CA	2.14	0.78
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.64	0.77
2:C:617:ALA:HB2	2:C:650:VAL:HG21	1.64	0.77
2:H:1223:ARG:HD2	3:I:637:ALA:HA	1.66	0.77
2:C:189:ASP:OD1	2:C:193:ASN:N	2.16	0.77
3:D:1254:GLU:O	3:D:1257:VAL:HG12	1.84	0.77
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.65	0.77
2:C:736:VAL:HG11	2:C:740:GLU:HA	1.65	0.77
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.67	0.77
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.66	0.77
3:D:545:HIS:HB2	3:D:546:ALA:HB2	1.67	0.77
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.66	0.77
3:D:275:ARG:HD2	3:D:302:ALA:HB2	1.65	0.77
2:C:27:LEU:O	2:C:528:ARG:NH1	2.18	0.77
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.67	0.77
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.65	0.77
2:C:562:GLU:HG2	2:C:574:SER:CB	2.15	0.77
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.66	0.77
4:E:5:THR:HA	4:E:6:VAL:HG12	1.64	0.77
3:I:828:GLY:HA2	3:I:832:LYS:H	1.48	0.77
2:C:39:ILE:HG22	2:C:40:GLU:HG2	1.67	0.76
1:G:45:ARG:O	3:I:538:ARG:NH2	2.18	0.76
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.65	0.76
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.20	0.76
3:D:1149:ARG:HD3	3:D:1149:ARG:H	1.49	0.76
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.65	0.76
3:D:151:MET:SD	3:D:151:MET:N	2.59	0.76
3:I:1343:GLU:HA	3:I:1344:LEU:HB2	1.68	0.76
3:D:1155:ILE:HG12	3:D:1211:SER:HB2	1.66	0.76
3:I:518:VAL:HG12	3:I:519:ASN:HD22	1.51	0.76
3:I:1155:ILE:HG12	3:I:1211:SER:HB2	1.68	0.76
2:C:526:HIS:HA	2:C:529:ARG:NH1	2.00	0.76
2:H:309:LEU:HD23	2:H:309:LEU:H	1.50	0.76
2:H:562:GLU:HG2	2:H:574:SER:CB	2.15	0.76
3:I:546:ALA:N	3:I:547:ARG:HA	2.00	0.76
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.21	0.76
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.67	0.76
2:H:13:LYS:CD	2:H:1181:PRO:HG2	2.16	0.76
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.67	0.76
3:D:822:MET:SD	3:D:838:ARG:NH1	2.58	0.76
2:H:1288:GLN:HA	2:H:1288:GLN:HE21	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:905:ARG:HH22	4:E:10:VAL:HG11	1.50	0.76
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.67	0.75
1:B:29:GLU:HA	1:B:200:LYS:CB	2.16	0.75
2:H:146:VAL:HG13	2:H:513:GLN:HG3	1.67	0.75
2:C:660:VAL:HG22	2:C:661:VAL:H	1.52	0.75
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.67	0.75
3:D:30:ILE:HG23	3:D:243:PRO:HB3	1.66	0.75
3:D:405:GLU:O	3:D:407:VAL:N	2.19	0.75
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.68	0.75
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.68	0.75
3:D:140:TYR:HA	3:D:181:GLY:HA2	1.68	0.75
3:D:664:ILE:HG21	3:D:681:LYS:HD2	1.66	0.75
2:C:143:ARG:NH1	2:C:512:SER:O	2.20	0.75
2:H:142:GLU:HG2	2:H:515:MET:SD	2.27	0.75
3:I:1155:ILE:HG13	3:I:1210:ILE:HG23	1.69	0.75
5:Y:145:LEU:HD21	5:Y:225:ARG:HH21	1.51	0.75
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.69	0.75
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.49	0.75
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.22	0.75
2:H:1284:ALA:HA	3:I:1357:ILE:HD13	1.69	0.75
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.67	0.75
2:H:1256:GLN:HB3	2:H:1301:ARG:HH22	1.51	0.75
2:C:829:THR:HG22	2:C:1059:ARG:HG2	1.67	0.75
3:I:761:ALA:HB3	3:I:767:LEU:HD13	1.68	0.75
3:I:850:LYS:O	3:I:852:GLY:N	2.18	0.75
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.69	0.74
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.17	0.74
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.00	0.74
2:C:645:PHE:HE1	2:C:650:VAL:HB	1.52	0.74
3:D:291:ILE:HD11	5:X:384:LEU:HD21	1.70	0.74
2:H:21:VAL:HG13	2:H:22:LEU:H	1.51	0.74
2:C:197:ARG:NH1	5:X:29:ASP:OD1	2.21	0.74
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.70	0.74
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.69	0.74
3:D:546:ALA:H	3:D:547:ARG:CA	2.01	0.74
3:D:932:MET:SD	3:D:932:MET:N	2.59	0.74
5:Y:453:PRO:HD2	5:Y:456:MET:HB2	1.68	0.74
2:C:134:GLY:O	2:C:527:LYS:NZ	2.18	0.74
1:G:65:LEU:HD23	1:G:65:LEU:H	1.53	0.74
1:G:227:GLN:C	1:G:228:LEU:HD23	2.12	0.74
4:J:10:VAL:CG2	4:J:16:ARG:HG2	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:515:MET:HE3	2:C:527:LYS:HE2	1.68	0.74
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.23	0.74
5:Y:264:LYS:HD2	5:Y:264:LYS:H	1.53	0.74
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.69	0.73
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.22	0.73
2:C:538:LEU:HD21	2:C:547:VAL:HG11	1.70	0.73
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.69	0.73
2:C:1042:LEU:HD13	2:C:1042:LEU:H	1.53	0.73
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.69	0.73
3:I:1173:ARG:HB3	3:I:1174:ARG:O	1.88	0.73
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.70	0.73
3:D:505:ASP:HB3	3:D:629:PHE:HE2	1.54	0.73
3:D:1297:LYS:HE3	3:I:1267:VAL:HB	1.69	0.73
3:I:828:GLY:HA2	3:I:832:LYS:N	2.03	0.73
5:X:511:ILE:HG23	5:X:512:GLY:H	1.52	0.73
3:I:20:ILE:CD1	3:I:1320:ILE:HD11	2.17	0.73
2:C:700:VAL:CG1	2:C:1114:GLU:HG3	2.13	0.73
1:F:234:LEU:HD22	1:G:214:GLU:OE2	1.88	0.73
3:I:186:GLN:CB	3:I:238:ILE:HD11	2.18	0.73
2:H:664:GLY:O	2:H:686:GLN:NE2	2.21	0.73
3:I:770:LEU:HD13	3:I:774:ILE:HD13	1.70	0.73
2:C:104:ILE:HD11	2:C:115:LYS:HB2	1.69	0.73
1:F:102:LEU:HG	1:F:115:ILE:HG12	1.70	0.73
2:C:765:ILE:HG13	2:C:787:PRO:HG2	1.70	0.73
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.69	0.73
1:F:158:ARG:HH11	1:F:172:LEU:HD11	1.52	0.73
2:H:59:ILE:HD13	2:H:479:LEU:HD12	1.70	0.73
1:B:33:ARG:NH1	2:C:820:GLU:OE2	2.22	0.73
2:C:1140:LYS:CE	2:C:1166:ASP:HB3	2.19	0.73
3:D:1260:MET:HE2	3:D:1306:LEU:HD11	1.69	0.73
5:X:264:LYS:H	5:X:264:LYS:HD2	1.54	0.73
3:D:33:TRP:HB3	3:D:102:MET:HG3	1.68	0.72
3:D:828:GLY:HA2	3:D:832:LYS:N	2.04	0.72
2:H:1252:SER:OG	2:H:1255:THR:O	2.07	0.72
5:Y:108:VAL:HG23	5:Y:109:GLU:H	1.54	0.72
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.72	0.72
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.18	0.72
2:H:347:ILE:HD11	2:H:433:ILE:HD11	1.70	0.72
2:H:971:LEU:HD21	2:H:1017:GLN:HE21	1.54	0.72
3:I:546:ALA:H	3:I:547:ARG:CA	2.02	0.72
3:I:610:ARG:CG	3:I:864:LEU:HD13	2.16	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.18	0.72
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.24	0.72
3:I:385:LEU:HD21	3:I:411:ILE:HG13	1.71	0.72
3:D:56:LEU:O	3:D:250:ARG:NH2	2.21	0.72
2:H:163:LYS:H	2:H:163:LYS:HD3	1.54	0.72
3:I:367:GLY:HA3	3:I:448:GLN:HB2	1.70	0.72
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.19	0.72
3:I:230:SER:HB2	3:I:1339:GLY:H	1.52	0.72
2:C:521:LEU:O	2:C:525:THR:HG22	1.88	0.72
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.17	0.72
5:X:108:VAL:HG23	5:X:109:GLU:H	1.53	0.72
2:H:59:ILE:HG21	2:H:479:LEU:HB3	1.69	0.72
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.20	0.72
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.23	0.72
2:C:55:SER:CB	2:C:56:VAL:HG22	2.20	0.72
2:C:1211:ARG:O	2:C:1211:ARG:NE	2.22	0.72
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.71	0.72
2:H:143:ARG:NH1	2:H:512:SER:O	2.23	0.72
3:I:222:LYS:NZ	3:I:1276:GLU:HB2	2.04	0.72
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.72	0.72
3:D:546:ALA:N	3:D:547:ARG:HA	2.03	0.72
5:Y:585:GLU:HB3	5:Y:589:GLN:HE22	1.53	0.72
2:C:302:ILE:HA	2:C:309:LEU:HA	1.71	0.71
2:C:54:ARG:N	2:C:55:SER:HB2	2.04	0.71
2:C:514:PHE:HB2	6:C:1401:RFP:O8	1.89	0.71
3:D:720:ASN:O	3:D:722:ILE:N	2.23	0.71
3:D:746:LEU:CD1	3:D:758:PRO:HG3	2.20	0.71
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	1.89	0.71
1:F:44:ARG:HG3	1:F:183:ILE:HG22	1.72	0.71
2:H:94:ALA:HB2	2:H:129:LEU:HD11	1.70	0.71
3:I:903:LEU:HD11	3:I:909:ILE:HG22	1.70	0.71
2:C:842:ASP:HB2	2:C:1046:VAL:HG21	1.73	0.71
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.72	0.71
3:I:588:PRO:CG	3:I:591:ILE:HD11	2.20	0.71
3:I:647:PRO:HG3	3:I:697:MET:HA	1.71	0.71
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.24	0.71
2:C:402:ARG:NH2	2:C:419:ILE:O	2.24	0.71
1:G:14:VAL:HG22	1:G:28:LEU:HD22	1.71	0.71
2:H:590:PRO:O	2:H:659:GLN:NE2	2.23	0.71
3:I:1344:LEU:H	3:I:1345:ARG:HG3	1.56	0.71
2:C:28:LEU:HD21	2:C:524:ILE:HG23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:838:CYS:HB2	2:C:918:LEU:HB2	1.71	0.71
2:C:1153:ALA:HB2	2:C:1194:GLU:HG2	1.73	0.71
5:X:457:ILE:O	5:X:461:ASN:ND2	2.23	0.71
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.72	0.71
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.21	0.71
3:D:614:LEU:HG	4:E:7:GLN:HG3	1.71	0.71
2:H:592:ARG:HB2	2:H:653:MET:HB3	1.73	0.71
2:C:1304:MET:HE1	2:C:1308:ILE:HD11	1.72	0.71
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.26	0.71
5:X:448:ARG:HD2	5:X:452:ILE:HD12	1.72	0.71
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.72	0.71
2:H:170:VAL:HG23	2:H:171:LEU:H	1.56	0.71
3:I:160:LEU:HA	3:I:164:GLN:NE2	2.05	0.71
2:H:1239:VAL:HG12	2:H:1240:ASP:H	1.55	0.71
3:D:128:LEU:HD21	3:D:188:LEU:HD22	1.73	0.70
2:C:524:ILE:CD1	2:C:712:SER:HB2	2.18	0.70
2:H:54:ARG:H	2:H:55:SER:CB	2.00	0.70
3:I:514:THR:HG23	3:I:576:ARG:HE	1.56	0.70
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.72	0.70
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.20	0.70
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.21	0.70
1:F:231:PHE:CZ	1:G:39:LEU:HD13	2.26	0.70
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.72	0.70
2:H:488:MET:HE3	2:H:489:PRO:HA	1.72	0.70
2:H:1085:MET:HE2	2:H:1094:VAL:HG23	1.72	0.70
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.21	0.70
5:Y:573:LEU:HD21	5:Y:588:ARG:HD3	1.73	0.70
1:A:45:ARG:HH12	2:C:1084:ASP:HB3	1.57	0.70
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.06	0.70
2:H:817:LEU:HB3	2:H:1097:VAL:HG13	1.72	0.70
1:B:47:LEU:HD13	1:B:205:MET:HE2	1.72	0.70
3:D:850:LYS:O	3:D:852:GLY:N	2.23	0.70
5:X:12:LEU:HD23	5:X:27:VAL:HG21	1.74	0.70
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.73	0.70
5:Y:511:ILE:CG2	5:Y:517:SER:HB2	2.22	0.70
3:D:316:ILE:HG23	3:D:317:THR:H	1.56	0.70
2:C:130:MET:CG	2:C:134:GLY:HA2	2.21	0.69
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.74	0.69
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.74	0.69
3:I:436:ALA:HB3	3:I:485:MET:HA	1.72	0.69
1:A:42:ALA:O	1:A:46:ILE:HG12	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1401:RFP:O9	6:C:1401:RFP:O10	2.02	0.69
3:D:145:VAL:HG22	3:D:180:MET:SD	2.32	0.69
3:D:1362:GLY:O	3:D:1364:ALA:N	2.25	0.69
2:H:127:ILE:H	2:H:127:ILE:HD13	1.58	0.69
3:I:298:MET:CE	5:Y:402:LEU:HB3	2.22	0.69
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.23	0.69
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.27	0.69
3:I:473:THR:HB	3:I:476:ALA:CB	2.22	0.69
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.25	0.69
3:D:389:GLY:O	3:D:391:ALA:N	2.26	0.69
5:Y:119:ILE:HD12	5:Y:122:ARG:HH21	1.56	0.69
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.72	0.69
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.74	0.69
2:H:28:LEU:HD22	2:H:527:LYS:CD	2.22	0.69
1:A:263:THR:HG23	1:A:266:SER:H	1.58	0.69
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.22	0.69
2:C:221:LEU:HD21	2:C:314:ASN:HD22	1.57	0.69
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.74	0.69
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.74	0.69
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.22	0.69
5:X:298:PRO:HB2	5:X:301:ASN:HD22	1.56	0.69
2:H:660:VAL:HG22	2:H:661:VAL:H	1.57	0.69
3:I:886:VAL:HG11	3:I:1230:THR:HG21	1.74	0.69
5:Y:120:ALA:HA	5:Y:123:ILE:HD12	1.74	0.69
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.23	0.69
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.28	0.69
2:H:62:TYR:HD2	2:H:480:SER:HB3	1.58	0.69
2:H:600:THR:HG22	2:H:601:ASP:H	1.57	0.69
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.73	0.69
1:F:45:ARG:HH12	2:H:1216:ARG:HA	1.58	0.69
2:H:152:SER:HG	2:H:404:LYS:HZ2	1.41	0.69
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.75	0.69
5:Y:561:MET:HA	5:Y:567:MET:SD	2.33	0.69
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.28	0.68
2:H:736:VAL:HG11	2:H:740:GLU:HB3	1.75	0.68
3:I:142:GLU:HA	3:I:180:MET:HE2	1.75	0.68
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.22	0.68
2:C:11:ILE:HD13	2:C:697:LYS:NZ	2.08	0.68
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.57	0.68
3:D:864:LEU:HD11	3:D:901:ARG:HH12	1.57	0.68
3:D:1225:GLY:CA	3:I:1294:ALA:HA	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:27:VAL:HA	5:X:30:HIS:HD2	1.57	0.68
2:C:1335:ILE:HD11	3:D:22:ILE:CD1	2.24	0.68
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.75	0.68
2:H:1283:ALA:HB1	2:H:1286:THR:HB	1.74	0.68
5:Y:556:ALA:O	5:Y:560:ARG:HB2	1.93	0.68
1:B:42:ALA:O	1:B:46:ILE:HG12	1.93	0.68
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.29	0.68
1:G:49:SER:OG	3:I:538:ARG:NH2	2.26	0.68
2:H:1046:VAL:HG22	2:H:1047:LEU:HD13	1.75	0.68
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.22	0.68
1:B:27:THR:HG22	1:B:202:VAL:HG22	1.76	0.68
3:D:473:THR:HB	3:D:476:ALA:CB	2.24	0.68
2:H:727:VAL:HG22	2:H:773:LEU:HB3	1.73	0.68
3:D:131:PRO:HG2	3:D:135:ILE:HD13	1.75	0.68
3:D:1261:LEU:HD21	3:D:1306:LEU:HD22	1.75	0.68
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.75	0.68
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.28	0.68
5:Y:448:ARG:HD3	5:Y:450:ILE:HG13	1.76	0.68
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.57	0.68
2:C:400:VAL:HG12	2:C:404:LYS:CE	2.23	0.68
2:C:1212:LEU:HD12	2:C:1225:VAL:HG21	1.76	0.68
3:D:230:SER:HB2	3:D:1339:GLY:N	2.07	0.68
5:Y:108:VAL:HB	5:Y:110:LEU:HG	1.75	0.68
3:D:213:LYS:O	3:D:217:LEU:HG	1.93	0.68
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.76	0.68
3:D:822:MET:HG2	3:D:839:VAL:HG23	1.76	0.68
3:D:1171:GLY:HA3	3:D:1172:LYS:HB2	1.76	0.68
3:I:185:ILE:HG22	3:I:238:ILE:HD13	1.75	0.68
3:D:20:ILE:CD1	3:D:1320:ILE:HD11	2.24	0.68
3:D:932:MET:O	3:D:933:ARG:HG3	1.93	0.68
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.74	0.68
3:I:1287:ILE:HG22	3:I:1290:ARG:HE	1.59	0.68
1:A:110:VAL:HB	1:A:131:CYS:HB2	1.77	0.67
2:C:1119:MET:HG2	2:C:1228:GLY:CA	2.19	0.67
3:D:510:LEU:HD12	3:D:601:ILE:HD11	1.75	0.67
3:D:711:GLY:O	3:D:712:GLN:HG2	1.92	0.67
2:H:735:LYS:HA	2:H:748:ILE:HA	1.76	0.67
3:I:288:PRO:HB2	3:I:291:ILE:HG12	1.76	0.67
3:I:473:THR:HB	3:I:476:ALA:HB2	1.75	0.67
3:I:800:LEU:HB3	3:I:920:ALA:HB1	1.74	0.67
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:473:THR:HB	3:D:476:ALA:HB2	1.76	0.67
3:D:647:PRO:HG3	3:D:697:MET:HA	1.74	0.67
3:I:827:GLU:O	3:I:831:VAL:HG12	1.93	0.67
5:Y:138:PRO:HG3	5:Y:353:LEU:HD21	1.77	0.67
1:A:80:GLU:HB2	2:C:694:ARG:HH22	1.60	0.67
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.30	0.67
2:C:20:GLN:O	2:C:22:LEU:N	2.28	0.67
2:C:42:ASP:CB	2:C:43:PRO:HD2	2.13	0.67
3:D:573:THR:HG22	3:D:576:ARG:CG	2.24	0.67
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.27	0.67
3:I:621:ALA:HA	3:I:624:ILE:HG12	1.75	0.67
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.29	0.67
1:B:181:GLU:HG2	3:D:531:LYS:HD3	1.77	0.67
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.24	0.67
2:C:487:LEU:CD1	2:C:488:MET:H	2.07	0.67
2:H:699:LEU:HB2	2:H:799:ASN:ND2	2.10	0.67
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.76	0.67
3:I:824:PRO:CB	3:I:836:ARG:HD3	2.25	0.67
3:D:156:ARG:NH1	3:D:157:GLN:OE1	2.28	0.67
3:D:572:THR:HG22	3:D:594:GLN:NE2	2.09	0.67
1:F:10:LYS:HE3	1:G:226:GLU:HB3	1.75	0.67
1:F:29:GLU:HB3	1:F:30:PRO:HD3	1.77	0.67
1:F:52:PRO:HG2	1:F:219:ARG:HH21	1.59	0.67
2:H:816:ILE:HD13	2:H:1074:GLY:HA3	1.76	0.67
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.10	0.67
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.58	0.67
5:Y:546:ASP:HB3	5:Y:603:ARG:NH2	2.07	0.67
2:C:488:MET:N	2:C:489:PRO:HD3	2.10	0.67
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.18	0.67
3:I:579:LEU:HD23	3:I:627:THR:HG21	1.75	0.67
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	1.77	0.67
2:C:600:THR:HG22	2:C:601:ASP:H	1.59	0.67
2:C:1319:MET:HE3	2:C:1324:ASN:HB2	1.76	0.67
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.77	0.67
3:I:590:SER:HB3	3:I:594:GLN:HE22	1.60	0.67
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.76	0.67
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.77	0.67
2:C:808:ASN:H	3:D:633:ALA:HB2	1.59	0.67
2:C:841:ARG:NH1	3:D:256:ASP:HB3	2.09	0.67
3:D:124:ILE:HD11	3:D:189:LEU:HD11	1.76	0.67
3:D:147:ILE:HA	3:D:178:ALA:HB1	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:442:SER:OG	5:X:446:GLN:NE2	2.28	0.67
3:D:528:THR:HG22	3:D:551:ARG:HB2	1.76	0.67
3:D:643:ASP:O	3:D:720:ASN:ND2	2.15	0.67
2:H:817:LEU:HB3	2:H:1097:VAL:CG1	2.24	0.67
2:C:1237:HIS:O	2:C:1238:LEU:HG	1.95	0.67
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.76	0.67
3:D:147:ILE:HA	3:D:178:ALA:CB	2.25	0.67
3:D:478:LEU:CD1	4:E:47:THR:HG23	2.25	0.67
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.27	0.67
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.77	0.67
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.28	0.67
2:H:1210:ILE:HG23	2:H:1211:ARG:NH1	2.10	0.67
3:I:541:LEU:HD23	3:I:541:LEU:H	1.60	0.67
3:I:720:ASN:O	3:I:722:ILE:N	2.28	0.67
1:A:158:ARG:HH11	1:A:172:LEU:HD11	1.60	0.66
1:B:179:PRO:HB3	1:B:210:THR:HB	1.76	0.66
2:C:448:LEU:HB2	2:C:553:THR:CG2	2.24	0.66
2:H:230:PHE:HB2	2:H:333:ILE:HB	1.77	0.66
2:H:484:LEU:H	2:H:484:LEU:HD22	1.60	0.66
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.60	0.66
3:I:545:HIS:HB2	3:I:546:ALA:HB2	1.76	0.66
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.77	0.66
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.76	0.66
1:F:11:PRO:HB3	1:F:31:LEU:HD21	1.77	0.66
4:J:5:THR:CA	4:J:6:VAL:HB	2.25	0.66
5:Y:496:LYS:HE3	5:Y:499:LYS:HD3	1.76	0.66
2:C:845:LEU:HD13	2:C:845:LEU:H	1.59	0.66
3:D:147:ILE:HD12	3:D:178:ALA:HB2	1.77	0.66
3:D:524:GLY:HA2	3:D:548:VAL:HG23	1.78	0.66
3:D:848:VAL:HG11	3:D:880:VAL:HA	1.77	0.66
5:X:476:ARG:H	5:X:476:ARG:HD2	1.59	0.66
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.77	0.66
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.78	0.66
2:H:628:HIS:HB3	2:H:647:ARG:NH2	2.09	0.66
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.77	0.66
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.25	0.66
2:H:360:LEU:HD13	2:H:378:ARG:HH11	1.60	0.66
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.78	0.66
5:Y:511:ILE:HG23	5:Y:512:GLY:H	1.60	0.66
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.29	0.66
3:D:124:ILE:CD1	3:D:189:LEU:HD11	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:TYR:CD1	1:F:79:LEU:HD11	2.31	0.66
2:H:505:PHE:O	2:H:512:SER:OG	2.12	0.66
2:H:576:SER:HB3	2:H:579:ALA:HB2	1.78	0.66
2:H:843:THR:HB	2:H:845:LEU:CD2	2.26	0.66
2:H:1335:ILE:HD11	3:I:22:ILE:CD1	2.24	0.66
3:I:711:GLY:O	3:I:712:GLN:HG2	1.95	0.66
3:I:1266:ILE:HG13	3:I:1274:PHE:O	1.96	0.66
3:D:77:ARG:HG3	3:D:78:LEU:H	1.58	0.66
3:D:270:ARG:HE	5:X:449:THR:HG22	1.61	0.66
3:D:423:LEU:HB3	3:D:466:MET:CE	2.26	0.66
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.26	0.66
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.78	0.66
1:A:45:ARG:NE	1:B:38:THR:OG1	2.25	0.66
2:H:55:SER:CB	2:H:56:VAL:HG22	2.25	0.66
3:I:491:LEU:HB2	3:I:904:ALA:HA	1.77	0.66
2:C:94:ALA:N	2:C:126:GLU:OE2	2.21	0.66
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.77	0.66
2:H:208:ILE:HD11	2:H:365:GLU:HB3	1.77	0.66
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.25	0.66
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.78	0.66
5:X:407:GLU:HA	5:X:410:ILE:HG22	1.77	0.66
2:H:645:PHE:HE1	2:H:650:VAL:HB	1.59	0.66
3:I:305:ALA:O	3:I:309:ASN:ND2	2.29	0.66
2:C:1002:LEU:HD13	2:C:1003:THR:H	1.60	0.66
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.78	0.66
3:D:610:ARG:CG	3:D:864:LEU:HD13	2.19	0.66
3:D:697:MET:SD	3:D:741:ALA:HB3	2.36	0.66
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.26	0.66
2:H:524:ILE:HA	2:H:527:LYS:HD2	1.76	0.66
2:C:1270:PHE:CZ	2:C:1290:MET:HG2	2.32	0.65
3:D:759:ILE:CG2	3:D:771:GLN:HG3	2.26	0.65
3:D:1173:ARG:HG2	3:D:1189:MET:HE1	1.77	0.65
5:X:139:GLU:HA	5:X:142:THR:CG2	2.26	0.65
2:H:766:ASN:H	2:H:787:PRO:HG3	1.61	0.65
2:H:908:GLU:HG2	2:H:909:LYS:N	2.11	0.65
3:I:382:TYR:HE1	3:I:401:VAL:HG21	1.62	0.65
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.26	0.65
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.79	0.65
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.26	0.65
3:D:1287:ILE:HG22	3:D:1290:ARG:HE	1.61	0.65
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:877:VAL:HG11	2:H:883:LEU:HD21	1.78	0.65
2:H:989:LEU:HD11	2:H:992:LEU:HD22	1.79	0.65
2:H:1148:ALA:HA	2:H:1201:LEU:HD21	1.79	0.65
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.11	0.65
1:B:192:VAL:CG2	1:B:198:LEU:HD12	2.24	0.65
3:D:478:LEU:HD12	4:E:47:THR:HG23	1.77	0.65
2:H:732:ILE:HD11	2:H:769:PRO:CB	2.25	0.65
3:I:512:TYR:HD2	3:I:724:MET:HE1	1.60	0.65
2:C:812:PHE:H	2:C:815:SER:HB2	1.58	0.65
3:D:1162:ILE:HG12	3:D:1203:ARG:HG2	1.79	0.65
2:H:1180:MET:HB3	2:H:1181:PRO:CA	2.25	0.65
3:I:108:ALA:CB	3:I:279:LEU:HD12	2.26	0.65
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	1.77	0.65
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.77	0.65
3:D:1180:VAL:HG22	3:D:1185:PRO:HA	1.77	0.65
1:F:11:PRO:HG2	1:G:228:LEU:H	1.61	0.65
3:I:288:PRO:HG2	5:Y:413:MET:HE2	1.77	0.65
3:I:1297:LYS:HA	3:I:1297:LYS:NZ	2.11	0.65
5:Y:449:THR:OG1	5:Y:503:GLU:O	2.15	0.65
5:X:448:ARG:HD3	5:X:450:ILE:HG13	1.78	0.65
2:H:13:LYS:HE3	2:H:1183:ALA:HB2	1.77	0.65
3:I:152:THR:O	3:I:154:LEU:N	2.29	0.65
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.79	0.65
2:C:704:MET:HE3	2:C:704:MET:HA	1.78	0.65
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.78	0.65
5:X:213:ASP:HB2	5:X:216:LEU:CB	2.27	0.65
1:F:11:PRO:CG	1:G:228:LEU:H	2.10	0.65
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.12	0.65
2:C:11:ILE:HG21	2:C:697:LYS:HZ2	1.61	0.65
2:C:102:LEU:HB3	2:C:117:ILE:HD11	1.78	0.65
2:H:18:ARG:HG3	2:H:19:PRO:HD2	1.78	0.65
2:C:845:LEU:HD23	2:C:889:PRO:HG2	1.77	0.65
2:C:1200:LYS:O	2:C:1202:GLY:N	2.29	0.65
5:X:28:ASN:HD22	5:X:29:ASP:N	1.95	0.65
2:H:1269:ARG:HG3	3:I:346:ARG:CG	2.22	0.65
2:C:854:ILE:HD11	2:C:885:GLY:HA2	1.79	0.65
2:H:1122:LYS:HG2	2:H:1229:TYR:CE2	2.32	0.65
3:I:1145:PHE:HB3	3:I:1309:ILE:CD1	2.27	0.65
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.62	0.64
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.27	0.64
2:H:496:LYS:HE2	5:Y:471:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:894:GLN:HE21	3:I:77:ARG:HH11	1.45	0.64
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.32	0.64
2:C:816:ILE:HG13	2:C:1098:LEU:CD2	2.24	0.64
3:D:589:TYR:O	3:D:591:ILE:N	2.28	0.64
2:H:459:MET:SD	2:H:511:LEU:HD22	2.37	0.64
3:D:425:ARG:NH2	3:D:464:ASP:OD2	2.29	0.64
3:D:1237:VAL:O	3:D:1240:VAL:HG22	1.97	0.64
3:I:1297:LYS:HA	3:I:1297:LYS:HZ3	1.61	0.64
1:A:253:LEU:HB3	1:A:321:TRP:CH2	2.33	0.64
2:C:660:VAL:O	2:C:661:VAL:HG22	1.98	0.64
2:C:842:ASP:CB	2:C:1046:VAL:HG21	2.27	0.64
3:D:930:LEU:CD2	3:D:1244:GLN:HG3	2.28	0.64
2:H:843:THR:HB	2:H:845:LEU:HD22	1.78	0.64
5:Y:279:ARG:NH2	5:Y:350:GLU:OE1	2.29	0.64
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.32	0.64
1:B:61:ILE:HB	1:B:64:VAL:HB	1.80	0.64
2:C:59:ILE:HG21	2:C:479:LEU:HD22	1.79	0.64
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.79	0.64
3:I:381:ILE:HD11	3:I:412:LEU:HD13	1.80	0.64
3:I:554:GLU:HA	3:I:589:TYR:HD2	1.63	0.64
3:I:704:GLU:HB2	3:I:718:SER:OG	1.97	0.64
5:Y:139:GLU:HG3	5:Y:351:THR:HA	1.78	0.64
2:C:1087:TYR:HE2	2:C:1215:GLY:HA2	1.62	0.64
3:D:114:ILE:HD12	3:D:311:ARG:HD3	1.78	0.64
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.77	0.64
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.33	0.64
3:I:1268:ASN:HB3	3:I:1300:ALA:HB1	1.79	0.64
2:C:843:THR:HB	2:C:845:LEU:CD2	2.28	0.64
2:C:1141:LEU:HD13	2:C:1141:LEU:H	1.63	0.64
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.80	0.64
1:A:100:LEU:HD11	1:A:121:VAL:HG11	1.80	0.64
2:C:130:MET:HG3	2:C:134:GLY:HA2	1.80	0.64
2:C:1239:VAL:O	2:C:1241:ASP:N	2.30	0.64
5:X:240:ARG:HD3	5:X:244:THR:CB	2.28	0.64
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.63	0.64
3:I:19:ALA:HA	3:I:1344:LEU:HD12	1.79	0.64
2:C:746:ALA:HB2	2:C:971:LEU:HD23	1.80	0.64
2:C:1108:ASN:ND2	2:C:1111:GLN:OE1	2.30	0.64
2:C:1219:GLU:OE2	3:D:634:ARG:NH1	2.29	0.64
3:D:143:SER:HB2	5:X:100:MET:HE2	1.80	0.64
3:D:1173:ARG:HB3	3:D:1174:ARG:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:10:VAL:CG2	4:E:16:ARG:HG2	2.27	0.64
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.31	0.64
2:H:1066:MET:HG3	2:H:1234:LYS:HA	1.80	0.64
3:I:832:LYS:HA	3:I:832:LYS:HZ1	1.61	0.64
5:Y:511:ILE:HG23	5:Y:517:SER:HB2	1.79	0.64
5:Y:573:LEU:HD22	5:Y:588:ARG:HB2	1.79	0.64
1:A:48:LEU:HG	1:A:183:ILE:HB	1.79	0.63
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.33	0.63
3:D:767:LEU:HB3	3:D:771:GLN:HE22	1.63	0.63
5:X:584:ARG:O	5:X:587:ILE:HG22	1.98	0.63
3:I:253:VAL:HG11	5:Y:523:ILE:HG21	1.80	0.63
3:I:1173:ARG:CZ	3:I:1176:VAL:HG21	2.28	0.63
3:I:1362:GLY:O	3:I:1364:ALA:N	2.30	0.63
2:C:1251:TYR:O	5:X:525:ASP:N	2.30	0.63
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.28	0.63
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.33	0.63
2:H:36:GLN:O	2:H:39:ILE:HG22	1.98	0.63
2:H:356:THR:HG21	2:H:362:ALA:HA	1.81	0.63
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.26	0.63
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.28	0.63
3:I:589:TYR:O	3:I:591:ILE:N	2.27	0.63
5:Y:571:TYR:HB3	5:Y:575:GLU:HB2	1.79	0.63
2:C:145:ILE:CG2	2:C:456:VAL:HG22	2.28	0.63
3:D:363:LEU:HA	3:D:450:HIS:ND1	2.13	0.63
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.29	0.63
3:I:850:LYS:HD2	3:I:851:PRO:CD	2.21	0.63
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.32	0.63
3:D:13:LYS:HA	3:D:13:LYS:NZ	2.13	0.63
2:H:55:SER:CB	2:H:56:VAL:HG13	2.26	0.63
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.62	0.63
3:I:524:GLY:HA2	3:I:548:VAL:HG23	1.80	0.63
5:Y:243:ALA:O	5:Y:247:GLU:HG3	1.99	0.63
1:A:45:ARG:NH1	2:C:1084:ASP:HB3	2.12	0.63
2:C:517:GLN:HE21	2:C:760:ASN:H	1.45	0.63
2:C:1085:MET:HE2	2:C:1094:VAL:HG23	1.79	0.63
3:D:1341:ARG:NH2	3:D:1343:GLU:OE1	2.32	0.63
5:X:240:ARG:O	5:X:242:HIS:N	2.31	0.63
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.31	0.63
3:I:151:MET:SD	3:I:151:MET:N	2.72	0.63
3:I:242:LEU:HD12	3:I:243:PRO:HD2	1.79	0.63
3:I:508:LEU:CD1	3:I:725:MET:HG2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:640:GLY:N	3:I:643:ASP:OD2	2.30	0.63
2:C:21:VAL:HG21	2:C:592:ARG:HD3	1.81	0.63
3:D:608:CYS:O	3:D:612:LEU:HB2	1.98	0.63
1:F:60:GLU:HG3	1:F:169:GLY:O	1.98	0.63
3:I:510:LEU:HD12	3:I:601:ILE:HD11	1.80	0.63
2:C:92:TYR:HD1	2:C:129:LEU:HB2	1.62	0.63
2:C:213:LEU:HD13	2:C:422:LYS:CB	2.29	0.63
2:C:897:PRO:HB3	5:X:564:GLY:O	1.97	0.63
3:D:591:ILE:HD12	3:D:592:VAL:N	2.14	0.63
5:X:379:MET:HE2	5:X:379:MET:HA	1.81	0.63
2:H:519:ASN:ND2	2:H:689:ALA:O	2.31	0.63
2:H:520:PRO:HB3	2:H:714:VAL:HG11	1.80	0.63
2:H:1141:LEU:HD13	2:H:1141:LEU:H	1.62	0.63
2:C:202:ARG:NE	2:C:369:MET:HG2	2.13	0.63
2:C:448:LEU:HB2	2:C:553:THR:HG21	1.80	0.63
2:C:842:ASP:N	2:C:1046:VAL:HG11	2.14	0.63
3:D:349:TYR:CD2	3:D:472:LEU:HD21	2.33	0.63
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.24	0.63
3:I:77:ARG:HG3	3:I:78:LEU:H	1.63	0.63
3:I:733:SER:O	3:I:737:ILE:HG12	1.99	0.63
1:B:65:LEU:HD23	1:B:65:LEU:H	1.64	0.63
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.79	0.63
2:C:1161:LEU:HD23	2:C:1164:PHE:HD1	1.63	0.63
3:D:205:LEU:HD22	3:D:217:LEU:CD2	2.28	0.63
3:D:298:MET:HE3	5:X:402:LEU:HB3	1.79	0.63
2:H:699:LEU:HD23	2:H:799:ASN:CG	2.22	0.63
2:H:1078:LYS:HG2	2:H:1079:ILE:H	1.64	0.63
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.64	0.63
2:C:843:THR:HB	2:C:845:LEU:HD22	1.80	0.62
2:C:1223:ARG:HD2	3:D:637:ALA:HA	1.80	0.62
3:D:137:ARG:NH1	5:X:95:THR:HG23	2.13	0.62
3:D:646:ILE:HG22	3:D:741:ALA:O	1.99	0.62
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.34	0.62
2:H:68:LEU:HG	2:H:100:LEU:HD23	1.80	0.62
3:I:213:LYS:O	3:I:217:LEU:HG	1.99	0.62
3:I:264:ASP:HB3	3:I:324:LEU:HB3	1.80	0.62
3:I:392:THR:CG2	5:Y:606:VAL:HG11	2.29	0.62
3:I:767:LEU:HB3	3:I:771:GLN:NE2	2.14	0.62
5:Y:457:ILE:O	5:Y:461:ASN:ND2	2.32	0.62
3:D:588:PRO:CG	3:D:591:ILE:HD11	2.29	0.62
5:X:101:TYR:OH	5:X:384:LEU:HD11	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:517:SER:O	5:X:518:HIS:ND1	2.32	0.62
3:I:107:LEU:H	3:I:107:LEU:HD12	1.63	0.62
1:A:282:VAL:CG2	1:A:316:MET:HE2	2.28	0.62
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.29	0.62
3:D:512:TYR:CD2	3:D:724:MET:HE1	2.31	0.62
2:H:1239:VAL:O	2:H:1241:ASP:N	2.32	0.62
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.28	0.62
3:I:128:LEU:HD12	3:I:192:MET:CE	2.29	0.62
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.82	0.62
4:J:15:ASN:HD22	4:J:18:ASP:H	1.47	0.62
1:B:27:THR:HG22	1:B:202:VAL:HG13	1.79	0.62
2:C:54:ARG:HG2	2:C:55:SER:CB	2.28	0.62
3:D:107:LEU:H	3:D:107:LEU:HD12	1.64	0.62
3:D:514:THR:HG23	3:D:576:ARG:HE	1.64	0.62
3:D:664:ILE:HG21	3:D:681:LYS:CD	2.29	0.62
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.30	0.62
2:H:38:PHE:HE2	2:H:49:LEU:HD12	1.65	0.62
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.34	0.62
2:C:756:TYR:H	2:C:766:ASN:CB	2.12	0.62
2:C:1268:GLN:HB2	3:D:350:SER:HB3	1.81	0.62
3:D:116:PHE:HB3	3:D:237:MET:HE1	1.82	0.62
4:E:45:LYS:O	4:E:49:ILE:HG12	1.99	0.62
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.28	0.62
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.81	0.62
2:H:26:TYR:CE2	2:H:28:LEU:HB2	2.35	0.62
3:D:709:ARG:HD2	3:D:714:GLU:HB2	1.82	0.62
3:D:827:GLU:O	3:D:831:VAL:HG12	1.99	0.62
2:H:55:SER:HB3	2:H:56:VAL:CB	2.30	0.62
2:H:91:THR:HB	2:H:138:ILE:HD13	1.80	0.62
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.33	0.62
3:I:128:LEU:HD12	3:I:192:MET:HE3	1.82	0.62
3:I:147:ILE:HD12	3:I:178:ALA:CB	2.30	0.62
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.00	0.62
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.80	0.62
2:C:740:GLU:HB2	2:C:741:MET:SD	2.40	0.62
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.34	0.62
3:D:824:PRO:CB	3:D:836:ARG:HD3	2.30	0.62
4:E:6:VAL:HG23	4:E:51:LEU:HD13	1.81	0.62
2:H:91:THR:HG22	2:H:139:ASN:N	2.14	0.62
1:A:13:LEU:HD11	1:A:16:ILE:HG12	1.82	0.62
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:MET:HE1	1:G:219:ARG:HG2	1.82	0.62
3:I:128:LEU:HD13	3:I:189:LEU:HD23	1.81	0.62
3:I:591:ILE:HD12	3:I:592:VAL:N	2.14	0.62
3:I:646:ILE:HG22	3:I:741:ALA:O	2.00	0.62
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.28	0.62
3:D:767:LEU:HB3	3:D:771:GLN:NE2	2.14	0.62
3:D:822:MET:HG2	3:D:839:VAL:CG2	2.28	0.62
5:X:213:ASP:HB2	5:X:216:LEU:HB3	1.82	0.62
2:H:73:TYR:HD2	2:H:74:ARG:H	1.48	0.62
2:H:448:LEU:HB2	2:H:553:THR:HG21	1.80	0.62
2:H:618:GLN:OE1	3:I:770:LEU:HB2	2.00	0.62
2:H:660:VAL:O	2:H:661:VAL:HG22	2.00	0.62
2:H:892:GLU:O	2:H:893:THR:OG1	2.17	0.62
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.33	0.62
2:C:18:ARG:HG3	2:C:19:PRO:HD2	1.82	0.62
2:C:55:SER:HB3	2:C:56:VAL:CB	2.30	0.62
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.35	0.62
2:H:516:ASP:HB2	6:H:1401:RFP:H323	1.80	0.62
3:I:389:GLY:O	3:I:391:ALA:N	2.33	0.62
2:C:41:GLN:CD	2:C:42:ASP:H	2.08	0.61
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.30	0.61
3:D:1191:PRO:O	3:D:1193:TRP:N	2.31	0.61
2:H:1176:LEU:HD22	2:H:1180:MET:O	2.00	0.61
3:I:513:MET:O	3:I:575:GLY:HA3	2.00	0.61
2:C:218:GLU:HG2	2:C:299:LYS:HA	1.81	0.61
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.82	0.61
3:D:527:LEU:H	3:D:550:VAL:HG12	1.65	0.61
2:H:521:LEU:O	2:H:525:THR:HG22	1.99	0.61
3:I:88:CYS:O	3:I:90:VAL:N	2.34	0.61
3:I:316:ILE:HD13	3:I:316:ILE:H	1.64	0.61
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.30	0.61
2:C:678:ARG:HD3	2:C:681:MET:HG3	1.81	0.61
2:C:868:SER:OG	2:C:942:ASP:OD1	2.15	0.61
1:F:234:LEU:HD12	1:F:234:LEU:N	2.15	0.61
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.64	0.61
2:H:1336:ASN:HB2	3:I:33:TRP:HH2	1.65	0.61
3:I:527:LEU:HD13	3:I:531:LYS:CB	2.30	0.61
2:C:21:VAL:HG13	2:C:22:LEU:H	1.65	0.61
3:D:316:ILE:HG23	3:D:317:THR:N	2.15	0.61
3:D:1177:ILE:HD11	3:D:1196:LEU:HD11	1.80	0.61
4:E:5:THR:CA	4:E:6:VAL:HB	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:448:LEU:HB2	2:H:553:THR:CG2	2.30	0.61
3:I:1191:PRO:O	3:I:1193:TRP:N	2.33	0.61
2:C:1252:SER:OG	2:C:1255:THR:O	2.19	0.61
3:D:450:HIS:HD2	3:D:451:PRO:HD2	1.64	0.61
2:H:106:GLU:N	2:H:107:ARG:HA	2.15	0.61
2:H:1200:LYS:O	2:H:1202:GLY:N	2.32	0.61
3:I:31:ARG:NH2	3:I:106:GLU:OE2	2.29	0.61
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.82	0.61
5:Y:108:VAL:HA	5:Y:385:ARG:HH12	1.66	0.61
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.35	0.61
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.29	0.61
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.30	0.61
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.35	0.61
2:H:1156:ARG:HH11	2:H:1157:GLN:H	1.48	0.61
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.00	0.61
5:Y:264:LYS:HD2	5:Y:264:LYS:N	2.14	0.61
2:C:816:ILE:HD13	2:C:1074:GLY:CA	2.30	0.61
3:D:841:GLY:CA	3:D:901:ARG:HD3	2.30	0.61
2:H:926:GLY:CA	2:H:1056:VAL:HG12	2.26	0.61
2:H:1211:ARG:NE	2:H:1211:ARG:O	2.33	0.61
1:A:221:ALA:HB1	1:B:228:LEU:HD13	1.82	0.61
3:D:451:PRO:HG2	3:D:625:MET:SD	2.40	0.61
2:H:1336:ASN:HB2	3:I:33:TRP:CH2	2.35	0.61
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.36	0.61
1:A:45:ARG:HH22	2:C:1216:ARG:CA	2.12	0.61
2:C:127:ILE:H	2:C:127:ILE:HD13	1.65	0.61
2:C:229:ILE:HB	2:C:240:GLU:CD	2.26	0.61
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.82	0.61
5:X:48:ILE:HG13	5:X:49:ASN:H	1.65	0.61
2:H:400:VAL:HG12	2:H:404:LYS:HE2	1.81	0.61
3:I:186:GLN:HB2	3:I:238:ILE:CD1	2.24	0.61
3:I:349:TYR:CE2	3:I:379:PRO:HG2	2.31	0.61
3:I:534:GLU:O	3:I:538:ARG:HB2	2.01	0.61
3:I:824:PRO:O	3:I:826:ILE:HG13	2.01	0.61
1:A:163:GLU:CB	1:A:166:ARG:HB3	2.30	0.61
2:C:800:MET:HA	2:C:800:MET:CE	2.28	0.61
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.15	0.61
2:C:1078:LYS:HG2	2:C:1079:ILE:H	1.66	0.61
2:C:1105:SER:HB2	3:D:731:ARG:HB2	1.82	0.61
2:H:26:TYR:HE2	2:H:28:LEU:HB2	1.65	0.61
2:H:1304:MET:HE1	2:H:1308:ILE:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:56:LEU:HB3	3:I:250:ARG:NH2	2.16	0.61
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.00	0.61
5:Y:412:LEU:HB2	5:Y:435:ILE:HD11	1.83	0.61
2:C:514:PHE:HE2	2:C:760:ASN:HB3	1.66	0.60
2:C:898:GLU:HG3	5:X:565:ILE:CD1	2.31	0.60
3:D:230:SER:CB	3:D:1339:GLY:H	2.13	0.60
2:H:845:LEU:HD13	2:H:845:LEU:H	1.65	0.60
3:I:1140:ARG:HH21	3:I:1236:GLU:CG	2.13	0.60
3:D:500:ILE:H	3:D:500:ILE:HD13	1.66	0.60
3:D:515:ARG:HH22	3:D:717:VAL:C	2.09	0.60
3:D:1343:GLU:HA	3:D:1344:LEU:HB2	1.82	0.60
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.83	0.60
3:I:138:VAL:O	3:I:143:SER:HB3	2.00	0.60
2:C:59:ILE:CG2	2:C:479:LEU:HD13	2.32	0.60
2:C:72:SER:O	2:C:98:VAL:HG23	2.02	0.60
2:C:752:ASN:O	2:C:753:LEU:HG	2.01	0.60
2:C:1204:LEU:CD2	2:C:1205:PRO:HD2	2.32	0.60
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.19	0.60
3:D:147:ILE:HG13	3:D:148:GLU:N	2.17	0.60
5:X:145:LEU:HD21	5:X:225:ARG:HE	1.65	0.60
5:X:264:LYS:HD2	5:X:264:LYS:N	2.16	0.60
2:H:131:THR:HG23	2:H:133:ASN:N	2.11	0.60
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.83	0.60
1:A:23:HIS:HE1	1:A:25:LYS:HE3	1.66	0.60
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.34	0.60
2:H:504:GLU:O	2:H:508:SER:HB3	2.01	0.60
2:H:800:MET:HA	2:H:800:MET:CE	2.30	0.60
3:I:355:ILE:HG12	3:I:464:ASP:O	2.00	0.60
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.13	0.60
3:D:13:LYS:HA	3:D:13:LYS:HZ3	1.66	0.60
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.67	0.60
4:E:5:THR:HB	4:E:7:GLN:HB2	1.83	0.60
2:H:28:LEU:CD2	2:H:524:ILE:HG23	2.32	0.60
2:H:1286:THR:N	3:I:479:GLU:OE2	2.33	0.60
3:I:858:VAL:CB	3:I:859:PRO:HD3	2.24	0.60
5:Y:213:ASP:HB2	5:Y:216:LEU:HB3	1.81	0.60
2:C:37:LYS:HA	2:C:37:LYS:HE3	1.84	0.60
2:C:517:GLN:HG3	2:C:759:SER:OG	2.01	0.60
3:D:137:ARG:CZ	5:X:95:THR:HG23	2.30	0.60
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.16	0.60
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.37	0.60
2:H:303:ASP:HB2	2:H:310:ILE:CD1	2.28	0.60
2:H:813:GLU:HG2	3:I:504:GLN:NE2	2.16	0.60
5:Y:238:LYS:HE2	5:Y:242:HIS:HE1	1.65	0.60
1:B:64:VAL:HG13	1:B:69:SER:OG	2.02	0.60
1:B:179:PRO:O	1:B:207:THR:OG1	2.15	0.60
2:C:740:GLU:OE2	2:C:974:ARG:NH2	2.34	0.60
3:I:1140:ARG:HG2	3:I:1240:VAL:HG11	1.83	0.60
1:A:42:ALA:HA	1:B:38:THR:HG23	1.83	0.60
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.01	0.60
5:X:390:ILE:HD11	5:X:435:ILE:CG2	2.31	0.60
2:H:218:GLU:HG2	2:H:299:LYS:HA	1.83	0.60
2:C:13:LYS:NZ	2:C:793:GLU:OE1	2.31	0.60
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.17	0.60
3:D:128:LEU:HD12	3:D:192:MET:CE	2.29	0.60
3:D:139:LEU:HD11	3:D:185:ILE:HD13	1.83	0.60
2:H:59:ILE:HD11	2:H:63:SER:HB3	1.83	0.60
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.01	0.60
1:A:80:GLU:HG3	2:C:694:ARG:HH12	1.67	0.60
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.32	0.60
1:G:56:VAL:HG12	1:G:173:VAL:HG11	1.84	0.60
2:H:91:THR:HG22	2:H:139:ASN:H	1.65	0.60
6:H:1401:RFP:O1	6:H:1401:RFP:O11	2.19	0.60
3:I:140:TYR:HA	3:I:181:GLY:HA2	1.84	0.60
3:I:222:LYS:HZ3	3:I:1276:GLU:HB2	1.67	0.60
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.36	0.60
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.84	0.59
2:C:93:SER:HB2	2:C:126:GLU:CD	2.26	0.59
2:C:691:PRO:HA	2:C:788:SER:OG	2.02	0.59
3:D:1292:LEU:HD21	3:I:1284:ARG:HH22	1.67	0.59
3:I:30:ILE:HG23	3:I:243:PRO:HB3	1.84	0.59
3:D:27:PRO:O	3:D:31:ARG:HD3	2.01	0.59
3:D:789:LYS:HB3	3:D:932:MET:SD	2.42	0.59
5:X:16:GLY:HA2	5:X:19:GLN:HG3	1.83	0.59
5:X:363:ARG:O	5:X:367:ILE:HG12	2.02	0.59
2:H:514:PHE:N	6:H:1401:RFP:O8	2.35	0.59
2:H:663:VAL:HA	2:H:666:SER:HB3	1.84	0.59
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.67	0.59
3:I:701:LEU:HD21	3:I:723:TYR:HB2	1.83	0.59
3:I:1329:THR:O	3:I:1333:THR:OG1	2.19	0.59
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:LYS:HD2	2:C:1181:PRO:HG2	1.84	0.59
2:C:744:GLY:HA2	2:C:974:ARG:HH11	1.68	0.59
2:C:1285:TYR:HA	2:C:1288:GLN:HB3	1.83	0.59
3:D:173:GLY:O	3:D:175:GLU:HG3	2.03	0.59
4:E:30:MET:HE1	4:E:49:ILE:HG22	1.83	0.59
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.31	0.59
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.83	0.59
1:B:190:ALA:HB2	1:B:200:LYS:HB3	1.84	0.59
2:C:11:ILE:HG21	2:C:697:LYS:NZ	2.17	0.59
2:C:59:ILE:CG2	2:C:479:LEU:HB3	2.32	0.59
2:C:105:TYR:CD1	2:C:106:GLU:HB2	2.38	0.59
3:D:139:LEU:HD13	3:D:140:TYR:N	2.17	0.59
5:X:119:ILE:O	5:X:123:ILE:HG13	2.02	0.59
5:X:600:HIS:H	5:X:601:PRO:HD2	1.67	0.59
2:H:766:ASN:N	2:H:787:PRO:HG3	2.18	0.59
3:I:147:ILE:HG13	3:I:148:GLU:N	2.17	0.59
3:I:205:LEU:HD22	3:I:217:LEU:CD2	2.33	0.59
5:Y:512:GLY:H	5:Y:517:SER:CB	2.15	0.59
1:A:22:THR:O	1:A:207:THR:HG22	2.03	0.59
1:A:158:ARG:HE	1:A:172:LEU:HD13	1.67	0.59
1:B:83:LEU:HD11	3:D:527:LEU:CA	2.26	0.59
2:C:216:THR:O	2:C:220:ILE:HG13	2.03	0.59
2:C:634:VAL:H	2:C:645:PHE:HE2	1.50	0.59
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.83	0.59
3:D:202:ARG:O	3:D:206:ASN:ND2	2.33	0.59
3:D:899:TYR:CE1	3:D:915:ILE:HD12	2.38	0.59
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.17	0.59
3:I:50:LYS:HB3	3:I:50:LYS:NZ	2.18	0.59
2:C:302:ILE:HG22	2:C:309:LEU:HB3	1.84	0.59
2:C:837:ALA:C	2:C:918:LEU:HD22	2.27	0.59
3:D:50:LYS:HB3	3:D:50:LYS:NZ	2.16	0.59
3:D:116:PHE:HB3	3:D:237:MET:CE	2.33	0.59
5:X:112:THR:HG22	5:X:113:ARG:H	1.66	0.59
2:H:1296:ASP:OD2	2:H:1320:PRO:HB2	2.01	0.59
3:I:262:THR:OG1	3:I:266:ASN:ND2	2.30	0.59
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.17	0.59
1:A:195:ARG:HH21	1:A:198:LEU:HD21	1.67	0.59
1:A:320:ASN:O	1:A:323:PRO:HD3	2.02	0.59
2:C:51:ALA:HB3	2:C:465:ARG:HH11	1.67	0.59
2:C:452:ARG:HH22	2:C:458:GLU:CD	2.10	0.59
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:459:MET:HE1	2:C:511:LEU:HD22	1.84	0.59
2:C:1002:LEU:HG	2:C:1007:LYS:HG2	1.83	0.59
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.83	0.59
3:D:614:LEU:CG	4:E:7:GLN:HG3	2.31	0.59
2:H:11:ILE:HD13	2:H:697:LYS:NZ	2.18	0.59
2:H:747:GLY:O	2:H:748:ILE:HG13	2.02	0.59
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.84	0.59
3:I:1173:ARG:NH1	3:I:1176:VAL:HG21	2.17	0.59
2:C:131:THR:HG22	2:C:135:THR:N	2.17	0.59
2:C:403:MET:HG2	2:C:407:ARG:NH1	2.17	0.59
2:C:510:GLN:O	2:C:511:LEU:HB2	2.03	0.59
2:C:839:VAL:HG13	2:C:1049:ILE:HG22	1.84	0.59
2:C:841:ARG:HA	2:C:1046:VAL:CG1	2.33	0.59
3:D:546:ALA:HB3	3:D:547:ARG:O	2.03	0.59
3:D:1347:LEU:CD2	3:D:1358:PRO:HG2	2.32	0.59
5:X:448:ARG:CD	5:X:452:ILE:HD12	2.32	0.59
2:H:1335:ILE:HD11	3:I:22:ILE:CG1	2.32	0.59
3:I:394:ILE:HG23	5:Y:536:THR:HG22	1.85	0.59
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.84	0.59
1:B:14:VAL:HG22	1:B:28:LEU:HD22	1.85	0.59
2:C:452:ARG:HH11	2:C:585:GLY:HA3	1.67	0.59
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.35	0.59
5:X:23:THR:HB	5:X:26:GLU:HG3	1.85	0.59
5:X:507:MET:HB3	5:X:520:GLY:HA3	1.85	0.59
2:H:607:SER:H	2:H:610:GLU:HB2	1.68	0.59
3:I:708:ASN:OD1	3:I:712:GLN:HB2	2.03	0.59
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.67	0.59
2:C:841:ARG:HA	2:C:1046:VAL:HG13	1.83	0.58
3:D:124:ILE:CG1	3:D:189:LEU:HD11	2.33	0.58
3:D:169:LEU:HD13	3:D:173:GLY:HA3	1.84	0.58
3:D:598:LYS:NZ	3:D:726:ALA:O	2.36	0.58
3:D:858:VAL:CB	3:D:859:PRO:HD3	2.26	0.58
3:D:901:ARG:HA	3:D:908:ILE:HA	1.85	0.58
4:E:60:ASN:HB2	4:E:63:ILE:HG12	1.83	0.58
5:X:561:MET:SD	5:X:576:VAL:HG22	2.43	0.58
1:G:64:VAL:HG12	1:G:171:LEU:HD11	1.84	0.58
2:H:28:LEU:HD21	2:H:524:ILE:HG23	1.84	0.58
3:I:490:ILE:HG23	3:I:500:ILE:HD11	1.85	0.58
3:I:512:TYR:CD2	3:I:724:MET:HE1	2.38	0.58
3:I:527:LEU:HB2	3:I:535:ARG:NH1	2.18	0.58
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ILE:HD13	1:B:205:MET:HA	1.85	0.58
2:C:39:ILE:CG2	2:C:40:GLU:HG2	2.32	0.58
2:C:106:GLU:HG2	2:C:109:ALA:H	1.68	0.58
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.38	0.58
2:C:316:GLU:HG3	2:C:352:ARG:HH12	1.68	0.58
2:C:562:GLU:HG2	2:C:574:SER:HB3	1.84	0.58
2:C:617:ALA:HB2	2:C:650:VAL:CG2	2.33	0.58
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.31	0.58
3:D:9:LYS:HE3	3:D:11:GLN:HG2	1.83	0.58
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.84	0.58
5:X:242:HIS:O	5:X:246:GLN:HB2	2.03	0.58
1:F:182:ARG:NH2	1:F:206:GLU:OE1	2.35	0.58
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.38	0.58
2:H:406:ASN:HB3	2:H:411:ARG:HB2	1.84	0.58
2:H:516:ASP:HB2	6:H:1401:RFP:H20C	1.83	0.58
2:H:901:LEU:O	2:H:905:ILE:HG13	2.02	0.58
3:I:508:LEU:HD11	3:I:725:MET:HG2	1.84	0.58
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.84	0.58
3:D:127:LEU:HD11	3:D:194:LEU:HD11	1.84	0.58
3:D:139:LEU:O	3:D:139:LEU:HD22	2.03	0.58
3:D:545:HIS:HB2	3:D:546:ALA:CB	2.33	0.58
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.32	0.58
3:D:1158:GLU:HA	3:D:1223:LEU:CD2	2.32	0.58
1:F:68:TYR:HD1	1:F:79:LEU:HD11	1.68	0.58
1:F:118:ASP:OD1	1:F:119:GLY:N	2.36	0.58
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.37	0.58
3:I:40:LYS:HB3	3:I:42:GLU:HG2	1.85	0.58
3:I:144:TYR:HE1	3:I:161:THR:HG23	1.68	0.58
3:I:270:ARG:HE	5:Y:449:THR:HG22	1.67	0.58
3:I:886:VAL:HG13	3:I:1230:THR:HG21	1.85	0.58
3:I:1180:VAL:HG22	3:I:1185:PRO:HA	1.85	0.58
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.86	0.58
2:C:1142:ARG:O	2:C:1146:GLN:HB2	2.04	0.58
3:D:85:CYS:HB3	3:D:88:CYS:O	2.04	0.58
3:D:149:GLY:HA2	3:D:156:ARG:HG2	1.84	0.58
3:D:825:VAL:CG2	3:D:835:LEU:HB2	2.33	0.58
3:D:864:LEU:CD1	3:D:901:ARG:HH12	2.16	0.58
2:H:523:GLU:C	2:H:527:LYS:HE2	2.28	0.58
2:H:1214:ASP:HB3	2:H:1218:GLY:H	1.68	0.58
2:H:1237:HIS:O	2:H:1238:LEU:HG	2.02	0.58
3:I:583:VAL:HG13	3:I:587:LEU:HD22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:611:ILE:HG22	3:I:865:HIS:CE1	2.39	0.58
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	1.86	0.58
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.03	0.58
2:C:363:LEU:HD13	2:C:382:GLU:HG2	1.85	0.58
2:C:838:CYS:HB2	2:C:918:LEU:CB	2.33	0.58
3:D:552:ILE:HD13	3:D:570:LYS:HB2	1.85	0.58
2:H:237:LEU:HD13	2:H:292:ILE:HD12	1.84	0.58
2:H:753:LEU:HD12	2:H:753:LEU:O	2.03	0.58
2:H:963:GLU:O	2:H:967:LEU:HD13	2.02	0.58
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.17	0.58
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.39	0.58
2:C:345:PRO:O	2:C:349:GLU:HG2	2.03	0.58
2:C:520:PRO:O	2:C:524:ILE:HG12	2.04	0.58
2:C:854:ILE:HD11	2:C:885:GLY:CA	2.33	0.58
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.39	0.58
3:D:141:PHE:O	3:D:297:ARG:HD3	2.03	0.58
3:D:655:SER:HA	3:D:658:GLU:HG2	1.84	0.58
2:H:516:ASP:OD2	2:H:518:ASN:ND2	2.37	0.58
2:H:716:ALA:HB3	2:H:784:ALA:HB3	1.85	0.58
3:I:139:LEU:HD13	3:I:140:TYR:N	2.18	0.58
3:I:394:ILE:CG2	5:Y:536:THR:HG22	2.33	0.58
3:D:50:LYS:HG2	3:D:51:PRO:CD	2.34	0.58
5:X:126:GLY:O	5:X:130:VAL:HG23	2.03	0.58
5:X:503:GLU:N	5:X:504:PRO:HA	2.19	0.58
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.39	0.58
2:H:53:PHE:HA	2:H:56:VAL:HG23	1.85	0.58
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.34	0.58
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.36	0.58
3:I:527:LEU:HD13	3:I:531:LYS:HB3	1.85	0.58
3:I:543:SER:O	3:I:574:VAL:HB	2.04	0.58
3:I:1148:ARG:NH2	3:I:1149:ARG:O	2.36	0.58
4:J:39:VAL:CG1	4:J:40:PRO:HD2	2.33	0.58
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.69	0.58
1:B:86:LYS:NZ	3:D:526:VAL:O	2.35	0.58
1:B:192:VAL:HG21	1:B:198:LEU:CD1	2.27	0.58
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.03	0.58
2:C:1073:LYS:HD3	3:D:462:ASP:HB3	1.86	0.58
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.84	0.58
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.34	0.58
3:D:832:LYS:HA	3:D:832:LYS:HZ2	1.69	0.58
5:X:466:ILE:CD1	5:X:487:MET:HE2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:768:MET:O	2:H:785:ASP:N	2.35	0.58
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.34	0.58
5:Y:471:LEU:HB3	5:Y:478:PRO:HD3	1.86	0.58
2:C:515:MET:CE	2:C:527:LYS:HE2	2.34	0.58
3:D:133:ARG:HB2	3:D:133:ARG:NH2	2.19	0.58
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.86	0.58
1:A:13:LEU:CD2	1:A:16:ILE:HD11	2.19	0.58
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.04	0.58
3:D:1174:ARG:HA	3:D:1192:LYS:HG3	1.85	0.58
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.85	0.58
3:I:709:ARG:O	3:I:711:GLY:N	2.37	0.58
2:C:524:ILE:HD13	2:C:524:ILE:N	2.19	0.57
3:D:120:LEU:CB	3:D:121:PRO:CD	2.82	0.57
5:X:301:ASN:O	5:X:305:LEU:HD13	2.03	0.57
2:H:1274:GLU:OE1	2:H:1274:GLU:N	2.37	0.57
3:I:245:LEU:O	3:I:250:ARG:NH1	2.35	0.57
3:I:544:LEU:HD13	3:I:719:PHE:HE1	1.68	0.57
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.37	0.57
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.36	0.57
3:D:58:CYS:SG	3:D:61:ILE:N	2.69	0.57
3:D:298:MET:CE	5:X:402:LEU:HB3	2.34	0.57
3:D:858:VAL:HB	3:D:859:PRO:CD	2.26	0.57
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.86	0.57
2:H:96:LEU:HD22	2:H:127:ILE:HD12	1.86	0.57
2:H:500:ALA:O	2:H:504:GLU:HB2	2.04	0.57
3:I:139:LEU:HD21	3:I:185:ILE:HD13	1.86	0.57
2:C:142:GLU:HG2	2:C:515:MET:SD	2.44	0.57
3:D:543:SER:O	3:D:574:VAL:HB	2.03	0.57
3:D:733:SER:O	3:D:737:ILE:HG12	2.04	0.57
5:X:224:LEU:HB2	5:X:259:PHE:CE1	2.38	0.57
2:H:629:PHE:HB2	2:H:647:ARG:HH12	1.69	0.57
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.30	0.57
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.38	0.57
1:A:134:THR:HG21	2:C:727:VAL:O	2.03	0.57
2:C:1029:LEU:O	2:C:1032:LYS:HG3	2.03	0.57
2:H:740:GLU:HB2	2:H:741:MET:SD	2.44	0.57
3:I:40:LYS:HE3	3:I:42:GLU:HG3	1.86	0.57
2:C:400:VAL:O	2:C:404:LYS:HE2	2.04	0.57
2:C:568:ASN:HB3	2:C:572:ILE:CD1	2.35	0.57
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.04	0.57
2:C:698:PRO:HB3	2:C:1231:TYR:CZ	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:355:ILE:O	5:X:355:ILE:HD13	2.05	0.57
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.39	0.57
2:H:384:LEU:O	2:H:388:LEU:HG	2.05	0.57
2:H:807:TRP:HH2	2:H:1216:ARG:HE	1.51	0.57
2:H:817:LEU:CB	2:H:1097:VAL:HG13	2.35	0.57
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	1.86	0.57
3:I:230:SER:CB	3:I:1339:GLY:H	2.17	0.57
3:I:515:ARG:HH22	3:I:717:VAL:C	2.12	0.57
3:I:614:LEU:HD23	4:J:7:GLN:HG3	1.86	0.57
3:I:1290:ARG:NH1	3:I:1296:GLY:O	2.37	0.57
1:A:300:LEU:CD1	1:A:304:LYS:HE2	2.34	0.57
2:C:953:LEU:HD21	2:C:1033:ARG:HG3	1.85	0.57
3:D:66:LYS:HG3	3:D:69:GLU:OE2	2.04	0.57
3:D:1145:PHE:CD2	3:D:1256:ILE:HD11	2.40	0.57
3:D:1197:ASN:HD22	3:D:1212:ASP:HB3	1.69	0.57
4:E:44:ASP:HB2	4:E:49:ILE:HD11	1.87	0.57
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.85	0.57
3:I:648:GLU:OE2	3:I:648:GLU:N	2.37	0.57
3:I:1270:GLY:HA3	3:I:1299:GLY:HA2	1.87	0.57
2:C:829:THR:CG2	2:C:1059:ARG:HG2	2.35	0.57
3:D:227:PHE:HE1	3:D:234:PRO:HD3	1.70	0.57
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.85	0.57
2:H:1204:LEU:CD2	2:H:1205:PRO:HD2	2.35	0.57
3:I:1287:ILE:HA	3:I:1290:ARG:HG2	1.85	0.57
1:A:219:ARG:O	1:A:223:ILE:HG13	2.03	0.57
2:C:59:ILE:HD11	2:C:63:SER:OG	2.04	0.57
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.85	0.57
2:C:514:PHE:CE2	2:C:760:ASN:HB3	2.39	0.57
2:C:670:PHE:HZ	2:C:1117:LEU:HD22	1.70	0.57
3:D:660:GLU:HG2	3:D:685:ILE:HD13	1.85	0.57
3:D:809:VAL:HG13	3:D:912:GLY:H	1.69	0.57
5:X:27:VAL:HA	5:X:30:HIS:CD2	2.37	0.57
1:F:44:ARG:HA	1:F:183:ILE:HG21	1.85	0.57
1:F:158:ARG:NH2	1:F:162:GLU:HB3	2.20	0.57
2:H:94:ALA:N	2:H:126:GLU:OE2	2.24	0.57
2:H:555:TYR:HE2	2:H:616:ILE:HD13	1.68	0.57
2:H:658:GLN:HB3	2:H:1186:VAL:HG11	1.86	0.57
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.30	0.57
3:I:1345:ARG:HH21	3:I:1373:ARG:HH21	1.52	0.57
5:Y:98:VAL:O	5:Y:102:MET:HG2	2.04	0.57
2:C:526:HIS:HA	2:C:529:ARG:HH12	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:549:ASP:OD1	3:D:750:PRO:HB3	2.04	0.57
3:D:554:GLU:HA	3:D:589:TYR:HD2	1.70	0.57
3:D:1369:ARG:HB3	3:D:1369:ARG:NH1	2.19	0.57
5:X:525:ASP:OD1	5:X:528:LEU:HG	2.05	0.57
2:H:159:SER:OG	2:H:442:VAL:HG11	2.04	0.57
2:H:645:PHE:CD1	2:H:650:VAL:HB	2.40	0.57
3:I:412:LEU:O	3:I:416:ILE:HG23	2.04	0.57
3:I:678:ARG:HA	3:I:681:LYS:HG3	1.87	0.57
1:A:310:ARG:NE	1:A:310:ARG:HA	2.20	0.57
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.05	0.57
3:D:120:LEU:CG	5:X:46:GLN:HB2	2.35	0.57
3:D:514:THR:HG21	3:D:595:ALA:O	2.04	0.57
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	1.86	0.57
1:F:134:THR:HG21	2:H:727:VAL:O	2.05	0.57
2:H:1304:MET:O	2:H:1308:ILE:HG13	2.05	0.57
3:I:513:MET:CE	3:I:579:LEU:HB2	2.34	0.57
3:I:583:VAL:CG1	3:I:587:LEU:HD22	2.34	0.57
5:Y:453:PRO:HD2	5:Y:456:MET:CB	2.35	0.57
1:A:231:PHE:CD2	1:B:43:LEU:HD11	2.39	0.56
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.39	0.56
1:B:118:ASP:OD1	1:B:119:GLY:N	2.38	0.56
3:D:609:TYR:HD1	3:D:610:ARG:HD2	1.70	0.56
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.05	0.56
2:H:27:LEU:HD13	2:H:528:ARG:NH2	2.14	0.56
2:H:616:ILE:HB	2:H:637:ARG:HB2	1.86	0.56
3:I:601:ILE:HD12	3:I:604:MET:CE	2.35	0.56
3:I:608:CYS:O	3:I:612:LEU:HB2	2.05	0.56
3:I:620:PHE:O	3:I:624:ILE:HG23	2.05	0.56
1:A:300:LEU:HD13	1:A:304:LYS:HE2	1.87	0.56
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.71	0.56
2:C:177:ILE:HG13	2:C:183:TRP:CZ3	2.40	0.56
2:C:753:LEU:O	2:C:753:LEU:HD12	2.05	0.56
3:D:661:VAL:HG23	3:D:682:VAL:HB	1.85	0.56
1:G:42:ALA:O	1:G:46:ILE:HG12	2.06	0.56
1:G:110:VAL:HB	1:G:131:CYS:HB2	1.86	0.56
2:H:568:ASN:HB3	2:H:572:ILE:HD12	1.87	0.56
3:I:230:SER:HB2	3:I:1339:GLY:N	2.18	0.56
1:A:78:ILE:O	1:A:82:LEU:HG	2.04	0.56
2:C:1304:MET:O	2:C:1308:ILE:HG13	2.05	0.56
3:D:144:TYR:HB3	3:D:159:ILE:CG2	2.34	0.56
3:D:252:LEU:HD23	3:D:252:LEU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:505:ASP:HB3	3:D:629:PHE:CE2	2.37	0.56
3:D:1284:ARG:NH2	3:I:1292:LEU:HD11	2.20	0.56
2:H:521:LEU:CD2	2:H:686:GLN:HB3	2.35	0.56
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.86	0.56
2:H:989:LEU:CD1	2:H:992:LEU:HD22	2.34	0.56
2:H:1141:LEU:H	2:H:1141:LEU:CD1	2.18	0.56
3:I:141:PHE:O	3:I:297:ARG:HD3	2.05	0.56
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.32	0.56
3:I:619:ILE:O	3:I:623:GLN:HG2	2.05	0.56
2:C:1029:LEU:HD12	2:C:1032:LYS:HE3	1.88	0.56
2:C:1141:LEU:H	2:C:1141:LEU:CD1	2.18	0.56
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.87	0.56
2:H:661:VAL:HG23	2:H:662:SER:O	2.06	0.56
2:H:808:ASN:N	3:I:633:ALA:HB2	2.19	0.56
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.30	0.56
3:I:382:TYR:CE1	3:I:401:VAL:HG21	2.41	0.56
3:I:1268:ASN:HB3	3:I:1300:ALA:CB	2.35	0.56
2:C:42:ASP:HB3	2:C:43:PRO:CD	2.23	0.56
2:C:131:THR:HG22	2:C:135:THR:H	1.69	0.56
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.86	0.56
3:D:919:ALA:O	3:D:923:ILE:HG12	2.05	0.56
2:H:484:LEU:HB3	2:H:486:THR:HG22	1.88	0.56
2:H:521:LEU:HD23	2:H:686:GLN:HB3	1.86	0.56
2:H:734:ILE:O	2:H:749:ASP:N	2.38	0.56
2:H:810:TYR:CD2	3:I:359:PRO:HG2	2.40	0.56
2:H:936:ARG:HD2	2:H:1047:LEU:H	1.70	0.56
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.35	0.56
2:C:616:ILE:HB	2:C:637:ARG:HB2	1.88	0.56
3:D:263:SER:HB2	5:X:507:MET:HE2	1.88	0.56
3:D:589:TYR:O	3:D:591:ILE:HG13	2.05	0.56
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.88	0.56
3:D:1229:VAL:O	3:D:1233:ILE:HG13	2.06	0.56
1:F:11:PRO:HD3	1:G:227:GLN:HG3	1.87	0.56
1:G:29:GLU:HA	1:G:200:LYS:CB	2.36	0.56
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.39	0.56
3:I:363:LEU:HA	3:I:450:HIS:ND1	2.20	0.56
1:A:131:CYS:O	1:A:132:HIS:ND1	2.39	0.56
1:A:152:TYR:CE2	2:C:824:GLN:HG2	2.41	0.56
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.20	0.56
2:C:51:ALA:HA	2:C:54:ARG:HB3	1.88	0.56
2:C:80:PHE:HB3	2:C:85:CYS:SG	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1142:ARG:HH22	2:C:1165:SER:N	2.04	0.56
5:X:461:ASN:HB3	5:X:465:ARG:CZ	2.35	0.56
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.41	0.56
3:I:573:THR:HG22	3:I:576:ARG:HG3	1.88	0.56
3:I:1195:GLN:OE1	3:I:1195:GLN:N	2.38	0.56
1:A:11:PRO:HG3	1:B:228:LEU:H	1.71	0.56
2:C:618:GLN:HG2	2:C:637:ARG:HH22	1.70	0.56
2:C:634:VAL:HG22	2:C:645:PHE:HE2	1.70	0.56
3:D:205:LEU:CD2	3:D:217:LEU:HD22	2.34	0.56
3:D:437:PHE:HZ	3:D:453:VAL:HG21	1.69	0.56
3:D:841:GLY:HA3	3:D:901:ARG:HD3	1.88	0.56
3:D:1290:ARG:NH1	3:D:1296:GLY:O	2.39	0.56
2:H:105:TYR:CD1	2:H:114:VAL:HG13	2.41	0.56
2:H:794:LEU:HD21	2:H:796:LEU:CG	2.33	0.56
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.20	0.56
2:C:106:GLU:N	2:C:107:ARG:HA	2.19	0.56
2:C:163:LYS:H	2:C:163:LYS:HD3	1.69	0.56
2:C:1084:ASP:HB2	2:C:1216:ARG:HG2	1.88	0.56
2:C:1341:ASP:HB2	2:C:1342:GLU:OE1	2.06	0.56
3:D:648:GLU:N	3:D:648:GLU:OE2	2.38	0.56
1:G:52:PRO:HG3	1:G:150:ARG:HH12	1.71	0.56
3:I:85:CYS:HB3	3:I:88:CYS:O	2.06	0.56
3:I:147:ILE:HG23	3:I:156:ARG:C	2.30	0.56
3:I:449:LEU:HD12	3:I:450:HIS:H	1.70	0.56
3:I:767:LEU:HB3	3:I:771:GLN:HE22	1.69	0.56
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.06	0.56
3:I:1366:HIS:O	3:I:1370:MET:HB2	2.06	0.56
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.87	0.56
1:B:18:GLN:C	1:B:20:SER:H	2.14	0.56
2:C:563:THR:HG21	3:D:780:ARG:CZ	2.35	0.56
2:C:894:GLN:O	2:C:895:LEU:HB2	2.06	0.56
3:D:1264:ALA:HB1	3:D:1303:SER:O	2.06	0.56
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.87	0.56
2:H:467:GLY:HA2	2:H:470:ARG:HG3	1.88	0.56
2:H:568:ASN:HB3	2:H:572:ILE:CD1	2.36	0.56
3:I:1154:ALA:HB1	3:I:1211:SER:HB3	1.86	0.56
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.06	0.56
3:D:703:THR:HA	3:D:717:VAL:HA	1.86	0.55
5:X:452:ILE:HD11	5:X:500:ILE:HG22	1.88	0.55
1:F:45:ARG:NH1	2:H:1216:ARG:HA	2.21	0.55
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:92:TYR:CD1	2:H:129:LEU:HB2	2.41	0.55
2:H:367:TYR:CD1	2:H:384:LEU:HD13	2.41	0.55
2:H:898:GLU:CB	5:Y:540:LEU:HD21	2.34	0.55
3:I:288:PRO:HB2	3:I:291:ILE:CG1	2.36	0.55
5:Y:439:ILE:O	5:Y:443:ILE:HG13	2.06	0.55
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.21	0.55
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	1.88	0.55
1:A:184:ALA:HB2	2:C:1091:GLY:N	2.22	0.55
2:C:202:ARG:HA	5:X:29:ASP:OD1	2.06	0.55
2:C:936:ARG:HB3	2:C:939:VAL:HG21	1.88	0.55
3:D:824:PRO:HD3	3:D:836:ARG:HE	1.71	0.55
3:D:1372:ARG:NH2	3:I:853:THR:HG21	2.21	0.55
5:X:130:VAL:O	5:X:134:VAL:HG23	2.06	0.55
5:X:139:GLU:CA	5:X:142:THR:HG22	2.32	0.55
1:G:192:VAL:HG21	1:G:198:LEU:CD1	2.29	0.55
2:H:18:ARG:N	2:H:1188:ASP:OD2	2.26	0.55
2:H:742:TYR:CB	2:H:743:PRO:HD3	2.35	0.55
2:H:933:VAL:CG1	2:H:948:ILE:HD11	2.34	0.55
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.21	0.55
3:I:382:TYR:HE1	3:I:401:VAL:CG2	2.19	0.55
3:I:405:GLU:O	3:I:407:VAL:N	2.39	0.55
5:Y:428:SER:O	5:Y:432:THR:OG1	2.25	0.55
2:C:59:ILE:HG21	2:C:479:LEU:HB3	1.88	0.55
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.34	0.55
2:C:1046:VAL:HG22	2:C:1047:LEU:HD13	1.89	0.55
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.35	0.55
3:D:29:MET:HA	3:D:29:MET:HE3	1.87	0.55
3:D:40:LYS:HB3	3:D:42:GLU:HG2	1.87	0.55
3:D:930:LEU:HD22	3:D:1244:GLN:HG3	1.88	0.55
3:D:1270:GLY:HA3	3:D:1299:GLY:HA2	1.88	0.55
3:I:131:PRO:HG2	3:I:135:ILE:HD13	1.89	0.55
3:I:474:LEU:HD22	3:I:477:GLN:NE2	2.22	0.55
3:I:490:ILE:HA	3:I:500:ILE:HD12	1.88	0.55
1:A:317:ARG:C	1:A:318:LEU:HD13	2.31	0.55
2:C:55:SER:CB	2:C:56:VAL:HG13	2.34	0.55
2:C:643:SER:C	2:C:644:LEU:HD12	2.31	0.55
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.06	0.55
5:X:595:LEU:O	5:X:599:ARG:NH1	2.38	0.55
2:H:1087:TYR:O	2:H:1213:TYR:N	2.27	0.55
2:H:1291:LEU:HD13	3:I:345:LYS:NZ	2.21	0.55
3:I:120:LEU:CB	3:I:121:PRO:CD	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:370:LYS:HG3	3:I:371:LYS:H	1.72	0.55
3:I:768:ASN:O	3:I:771:GLN:NE2	2.39	0.55
5:Y:126:GLY:O	5:Y:130:VAL:HG23	2.07	0.55
5:Y:511:ILE:HG22	5:Y:517:SER:HB2	1.88	0.55
1:A:91:ARG:NH2	1:A:209:GLY:O	2.40	0.55
2:C:518:ASN:HD21	2:C:761:GLN:HG2	1.72	0.55
2:C:582:ASN:N	2:C:586:PHE:O	2.38	0.55
3:D:156:ARG:HD3	3:D:157:GLN:HG3	1.89	0.55
3:D:316:ILE:HG13	3:D:317:THR:N	2.21	0.55
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.39	0.55
1:G:186:ASN:HB2	1:G:202:VAL:HB	1.87	0.55
2:H:1252:SER:HB3	2:H:1259:LEU:CD2	2.36	0.55
3:I:857:LEU:HB2	3:I:860:ARG:HB2	1.88	0.55
5:Y:558:VAL:HG22	5:Y:587:ILE:HD11	1.88	0.55
1:A:243:LYS:HB2	1:A:243:LYS:HZ3	1.72	0.55
2:C:144:VAL:HB	2:C:526:HIS:CE1	2.42	0.55
2:C:1087:TYR:CE2	2:C:1215:GLY:HA2	2.42	0.55
3:D:349:TYR:CE2	3:D:379:PRO:HG2	2.42	0.55
3:D:664:ILE:CD1	3:D:681:LYS:HE3	2.33	0.55
4:E:39:VAL:CG1	4:E:40:PRO:HD2	2.37	0.55
2:H:263:VAL:HG22	2:H:273:HIS:CD2	2.41	0.55
2:H:634:VAL:H	2:H:645:PHE:HE2	1.55	0.55
3:I:863:LEU:HB2	3:I:866:GLU:HB2	1.89	0.55
5:Y:562:ARG:HG3	5:Y:591:GLU:OE1	2.06	0.55
2:C:10:ARG:HD3	2:C:1175:ASN:HD21	1.72	0.55
2:C:163:LYS:H	2:C:163:LYS:CD	2.19	0.55
2:C:980:VAL:O	2:C:984:VAL:HG22	2.06	0.55
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.06	0.55
5:X:143:TYR:O	5:X:147:GLN:HG2	2.06	0.55
5:X:439:ILE:O	5:X:443:ILE:HG13	2.07	0.55
5:X:518:HIS:HB2	5:X:521:ASP:OD2	2.06	0.55
1:G:90:VAL:HG13	1:G:121:VAL:HG13	1.87	0.55
3:I:27:PRO:O	3:I:31:ARG:NH1	2.40	0.55
3:I:144:TYR:CE1	3:I:161:THR:HG23	2.42	0.55
3:I:197:GLU:O	3:I:201:LEU:HD23	2.06	0.55
3:I:546:ALA:HB3	3:I:547:ARG:O	2.07	0.55
5:Y:445:ASP:OD1	5:Y:445:ASP:N	2.39	0.55
5:Y:547:VAL:CG2	5:Y:603:ARG:HD2	2.37	0.55
5:Y:562:ARG:NH1	5:Y:591:GLU:OE2	2.39	0.55
2:C:82:VAL:HB	2:C:92:TYR:CE2	2.41	0.55
2:C:1314:GLN:HG3	4:E:28:ARG:NH1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1314:GLN:HG3	4:E:28:ARG:HH12	1.72	0.55
3:D:120:LEU:HG	5:X:46:GLN:CB	2.35	0.55
3:D:154:LEU:CD2	3:D:160:LEU:HD21	2.32	0.55
3:D:1284:ARG:HH22	3:I:1292:LEU:HD21	1.71	0.55
5:X:133:SER:OG	5:X:365:MET:HB2	2.07	0.55
1:G:118:ASP:OD1	1:G:119:GLY:N	2.38	0.55
2:H:442:VAL:HG12	2:H:443:ASP:H	1.71	0.55
2:H:1313:HIS:HD2	3:I:474:LEU:HD23	1.72	0.55
3:I:154:LEU:HD21	3:I:160:LEU:HD21	1.89	0.55
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.07	0.55
2:C:54:ARG:H	2:C:55:SER:CB	2.10	0.55
2:C:685:MET:CE	2:C:1235:LEU:HD11	2.36	0.55
2:C:942:ASP:HB2	2:C:1048:LYS:NZ	2.22	0.55
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.22	0.55
2:H:590:PRO:HB2	2:H:655:VAL:HG21	1.88	0.55
2:H:821:ARG:NE	2:H:1082:ILE:HD13	2.22	0.55
2:H:951:MET:HA	2:H:951:MET:HE3	1.89	0.55
2:H:1268:GLN:O	3:I:346:ARG:HA	2.06	0.55
3:I:24:LEU:HD11	3:I:116:PHE:CZ	2.41	0.55
1:A:13:LEU:HD21	1:A:16:ILE:CD1	2.19	0.55
2:C:557:ARG:NH2	2:C:606:LEU:O	2.40	0.55
2:C:901:LEU:O	2:C:905:ILE:HG13	2.07	0.55
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.36	0.55
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.37	0.55
4:E:59:ILE:HG23	4:E:64:LEU:HD21	1.89	0.55
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.38	0.55
2:H:177:ILE:HG13	2:H:183:TRP:CZ3	2.42	0.55
2:H:840:SER:HB3	2:H:850:ILE:HD11	1.89	0.55
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.07	0.55
5:Y:138:PRO:CG	5:Y:353:LEU:HD21	2.37	0.55
5:Y:469:GLN:HG2	5:Y:473:GLU:HB2	1.89	0.55
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.06	0.54
2:C:812:PHE:N	2:C:815:SER:HB2	2.22	0.54
3:D:395:LYS:HG3	5:X:536:THR:HG21	1.88	0.54
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.07	0.54
5:X:503:GLU:HB3	5:X:504:PRO:O	2.07	0.54
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.42	0.54
2:H:403:MET:HG2	2:H:407:ARG:HH12	1.72	0.54
2:H:866:ASP:HA	2:H:872:TYR:CZ	2.42	0.54
5:Y:148:TYR:OH	5:Y:218:ARG:HG2	2.07	0.54
5:Y:253:SER:O	5:Y:257:LYS:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:747:GLY:O	2:C:748:ILE:HG13	2.06	0.54
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.07	0.54
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.72	0.54
3:D:88:CYS:O	3:D:90:VAL:N	2.40	0.54
1:F:45:ARG:NE	1:G:38:THR:OG1	2.38	0.54
1:F:158:ARG:NH2	1:F:158:ARG:HB2	2.22	0.54
2:H:28:LEU:CD2	2:H:527:LYS:HD2	2.33	0.54
2:H:725:GLN:HE22	2:H:966:ILE:HD11	1.73	0.54
3:I:363:LEU:O	3:I:486:SER:OG	2.21	0.54
3:I:697:MET:SD	3:I:741:ALA:HB3	2.46	0.54
3:I:807:LEU:HD23	3:I:1259:GLN:HG2	1.89	0.54
1:A:192:VAL:O	1:A:194:GLN:N	2.40	0.54
2:C:59:ILE:CD1	2:C:479:LEU:HD22	2.34	0.54
2:C:224:PHE:CD2	2:C:347:ILE:HG21	2.43	0.54
2:C:533:LEU:HD23	2:C:533:LEU:H	1.71	0.54
1:G:49:SER:HA	1:G:151:GLY:HA2	1.90	0.54
2:H:12:ARG:O	2:H:13:LYS:HG2	2.07	0.54
2:H:86:GLN:HA	2:H:140:GLY:HA2	1.89	0.54
2:H:752:ASN:O	2:H:753:LEU:HG	2.07	0.54
2:H:1298:VAL:HG13	2:H:1321:GLU:HG3	1.88	0.54
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.88	0.54
2:C:73:TYR:HA	2:C:98:VAL:HA	1.89	0.54
2:C:539:THR:O	2:C:540:ARG:HG3	2.06	0.54
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.22	0.54
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.43	0.54
1:G:67:GLU:O	1:G:78:ILE:HB	2.07	0.54
2:H:59:ILE:HB	2:H:480:SER:OG	2.06	0.54
3:I:347:VAL:HG23	3:I:350:SER:OG	2.07	0.54
3:I:508:LEU:O	3:I:508:LEU:HD23	2.08	0.54
3:I:601:ILE:HD12	3:I:604:MET:HE2	1.88	0.54
3:I:1145:PHE:CD2	3:I:1256:ILE:HD11	2.41	0.54
3:I:1270:GLY:HA2	3:I:1298:VAL:C	2.32	0.54
2:C:9:LYS:N	2:C:9:LYS:HD3	2.22	0.54
3:D:169:LEU:HD22	3:D:176:PHE:CE2	2.43	0.54
3:D:355:ILE:HG12	3:D:464:ASP:O	2.08	0.54
5:X:354:THR:HG23	5:X:357:GLN:HB3	1.89	0.54
1:F:44:ARG:HG3	1:F:183:ILE:CG2	2.37	0.54
2:H:759:SER:HB3	2:H:763:THR:H	1.73	0.54
2:H:866:ASP:HA	2:H:872:TYR:OH	2.08	0.54
3:I:140:TYR:OH	3:I:312:ARG:NH1	2.39	0.54
2:C:898:GLU:HG3	5:X:565:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.08	0.54
3:D:152:THR:O	3:D:154:LEU:N	2.40	0.54
3:D:513:MET:O	3:D:575:GLY:HA3	2.08	0.54
3:D:621:ALA:HA	3:D:624:ILE:HG12	1.89	0.54
2:H:207:THR:HG21	2:H:351:LEU:HG	1.90	0.54
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.89	0.54
3:I:155:GLU:CD	3:I:158:GLN:HB2	2.31	0.54
3:I:278:ARG:O	3:I:282:LEU:HG	2.08	0.54
3:I:369:PRO:HB2	3:I:372:MET:HB2	1.89	0.54
1:A:100:LEU:HD21	1:A:121:VAL:CG2	2.30	0.54
2:C:1342:GLU:HG3	3:D:18:ASP:OD2	2.08	0.54
3:D:422:LEU:HA	3:D:436:ALA:HA	1.90	0.54
3:D:501:VAL:CG2	3:D:602:SER:HB2	2.34	0.54
4:E:15:ASN:OD1	4:E:17:PHE:HB2	2.08	0.54
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.39	0.54
2:H:1142:ARG:O	2:H:1146:GLN:HB2	2.08	0.54
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.90	0.54
3:D:864:LEU:CG	3:D:901:ARG:HH12	2.21	0.54
3:D:1141:VAL:HG22	3:D:1240:VAL:HG21	1.88	0.54
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.90	0.54
5:X:592:ALA:O	5:X:596:ARG:HG2	2.07	0.54
1:F:79:LEU:O	1:F:83:LEU:HD13	2.08	0.54
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.89	0.54
2:H:839:VAL:O	2:H:886:LYS:NZ	2.39	0.54
2:H:943:LYS:O	2:H:947:GLU:HG2	2.07	0.54
2:H:1277:ALA:HB3	3:I:434:ILE:HD13	1.90	0.54
2:H:1313:HIS:CD2	3:I:474:LEU:HD23	2.43	0.54
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.43	0.54
2:C:873:ILE:HD11	2:C:931:VAL:HG22	1.89	0.54
3:D:125:GLY:O	3:D:129:ASP:N	2.41	0.54
5:X:357:GLN:NE2	5:X:360:ASP:OD2	2.40	0.54
2:H:101:ARG:HG3	2:H:118:LYS:H	1.73	0.54
2:H:468:LEU:O	2:H:471:VAL:HG22	2.08	0.54
2:H:819:SER:HB2	2:H:1085:MET:SD	2.48	0.54
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.38	0.54
3:I:535:ARG:HB3	3:I:541:LEU:CD1	2.34	0.54
3:I:824:PRO:HD3	3:I:836:ARG:HE	1.73	0.54
5:Y:147:GLN:O	5:Y:151:VAL:HG23	2.08	0.54
2:C:888:THR:HG23	2:C:916:SER:HB3	1.90	0.54
2:C:1212:LEU:CD1	2:C:1225:VAL:HG21	2.38	0.54
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:579:LEU:HD23	3:D:627:THR:HG21	1.89	0.54
3:D:797:THR:O	3:D:801:VAL:HG23	2.08	0.54
3:D:864:LEU:HD21	3:D:901:ARG:HH22	1.71	0.54
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.90	0.54
3:D:1215:GLU:HB3	3:D:1220:ILE:HD11	1.89	0.54
5:X:117:ILE:HG13	5:X:421:TYR:HB2	1.90	0.54
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.89	0.54
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	1.90	0.54
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.89	0.54
3:I:546:ALA:N	3:I:547:ARG:CA	2.67	0.54
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.41	0.54
3:I:1194:ARG:N	3:I:1194:ARG:HD2	2.23	0.54
1:B:14:VAL:HG13	1:B:28:LEU:CD2	2.37	0.53
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.88	0.53
3:D:474:LEU:HA	3:D:477:GLN:HE21	1.72	0.53
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.08	0.53
3:D:709:ARG:O	3:D:711:GLY:N	2.41	0.53
3:D:1301:THR:CG2	3:I:1301:THR:HG23	2.31	0.53
5:X:17:LYS:N	5:X:18:GLU:HA	2.23	0.53
2:H:549:ASP:OD1	2:H:550:VAL:N	2.40	0.53
3:I:115:TRP:CE2	3:I:1329:THR:HG23	2.43	0.53
3:I:128:LEU:HA	3:I:192:MET:HE1	1.89	0.53
3:I:222:LYS:HZ2	3:I:1276:GLU:HB2	1.71	0.53
3:I:252:LEU:H	3:I:252:LEU:HD23	1.72	0.53
3:I:264:ASP:OD2	3:I:324:LEU:HA	2.09	0.53
3:I:502:PRO:HB3	3:I:506:VAL:HG11	1.90	0.53
4:J:4:VAL:O	4:J:5:THR:OG1	2.24	0.53
1:A:18:GLN:HE22	1:A:213:PRO:CG	2.11	0.53
1:A:134:THR:HG21	2:C:727:VAL:HG23	1.90	0.53
1:A:318:LEU:O	1:A:320:ASN:N	2.37	0.53
1:B:83:LEU:HD12	1:B:86:LYS:HD2	1.89	0.53
2:C:681:MET:O	2:C:685:MET:HG2	2.08	0.53
3:D:260:PHE:O	5:X:504:PRO:HG2	2.08	0.53
5:X:333:VAL:HG22	5:X:336:GLU:HB2	1.89	0.53
1:F:31:LEU:HB2	1:F:199:ASP:O	2.08	0.53
2:H:54:ARG:HG2	2:H:55:SER:CB	2.38	0.53
2:H:639:LYS:HA	2:H:639:LYS:HE2	1.89	0.53
3:I:1234:VAL:HA	3:I:1253:ILE:HG21	1.88	0.53
3:I:1241:TYR:HB3	3:I:1246:VAL:HG23	1.90	0.53
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.08	0.53
2:C:347:ILE:HD11	2:C:433:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:367:TYR:CD1	2:C:381:ALA:HA	2.43	0.53
2:C:594:VAL:CG2	2:C:599:VAL:HG22	2.37	0.53
2:C:840:SER:CB	2:C:850:ILE:HD11	2.29	0.53
5:X:290:LEU:HD13	5:X:336:GLU:HB3	1.89	0.53
5:X:365:MET:O	5:X:369:GLU:HG3	2.07	0.53
5:X:374:ARG:HH21	5:X:377:LYS:HD2	1.72	0.53
2:H:496:LYS:N	2:H:497:PRO:HD2	2.24	0.53
2:H:812:PHE:H	2:H:815:SER:HB2	1.74	0.53
3:I:29:MET:HA	3:I:29:MET:HE3	1.90	0.53
3:I:57:PHE:CE1	3:I:252:LEU:HD22	2.44	0.53
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.89	0.53
4:J:3:ARG:O	4:J:4:VAL:HG13	2.08	0.53
1:A:79:LEU:O	1:A:83:LEU:HD13	2.08	0.53
2:C:12:ARG:O	2:C:13:LYS:HG2	2.09	0.53
2:C:975:ILE:O	2:C:975:ILE:HD13	2.08	0.53
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.08	0.53
3:D:33:TRP:O	3:D:102:MET:HB2	2.08	0.53
3:D:810:THR:OG1	3:D:811:GLU:N	2.39	0.53
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.08	0.53
3:D:1322:ALA:HB3	3:D:1331:VAL:HG21	1.90	0.53
5:X:271:ASN:O	5:X:275:VAL:HG23	2.07	0.53
2:H:818:VAL:HG22	2:H:819:SER:H	1.73	0.53
2:H:1287:LEU:HD23	3:I:1357:ILE:HG12	1.91	0.53
3:I:544:LEU:HD13	3:I:719:PHE:CE1	2.43	0.53
4:J:48:VAL:O	4:J:52:ARG:HG3	2.07	0.53
2:C:806:PRO:HD3	2:C:1100:PRO:HG3	1.90	0.53
2:C:960:LEU:HD12	2:C:1032:LYS:HD3	1.89	0.53
3:D:546:ALA:N	3:D:547:ARG:CA	2.68	0.53
3:D:1346:GLY:HA3	3:D:1349:GLU:OE2	2.09	0.53
1:F:9:LEU:O	1:G:227:GLN:NE2	2.42	0.53
1:F:190:ALA:HB2	1:F:200:LYS:CB	2.38	0.53
2:H:994:ARG:HD3	2:H:994:ARG:N	2.24	0.53
3:I:930:LEU:HD11	3:I:1241:TYR:HE2	1.72	0.53
3:I:1247:LYS:H	3:I:1247:LYS:CD	2.14	0.53
2:C:312:ALA:HB3	2:C:315:MET:HE3	1.90	0.53
2:C:681:MET:HE3	2:C:1073:LYS:HE3	1.90	0.53
2:C:699:LEU:HB2	2:C:799:ASN:ND2	2.24	0.53
2:C:892:GLU:O	2:C:893:THR:OG1	2.21	0.53
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.08	0.53
3:D:40:LYS:HE3	3:D:42:GLU:HG3	1.90	0.53
3:D:501:VAL:HG23	3:D:502:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:573:THR:HG23	3:D:576:ARG:H	1.73	0.53
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.91	0.53
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.91	0.53
2:H:896:THR:CG2	2:H:897:PRO:HD2	2.39	0.53
2:H:1335:ILE:CD1	3:I:22:ILE:HD11	2.36	0.53
3:I:918:ILE:HD13	3:I:919:ALA:N	2.23	0.53
3:I:1287:ILE:O	3:I:1291:GLU:HG2	2.07	0.53
5:Y:476:ARG:H	5:Y:476:ARG:HD2	1.72	0.53
1:A:183:ILE:CD1	1:A:205:MET:HG3	2.39	0.53
2:C:590:PRO:HD3	2:C:605:TYR:HE1	1.72	0.53
2:C:618:GLN:HG2	2:C:637:ARG:NH2	2.23	0.53
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.91	0.53
2:H:122:VAL:HG23	2:H:490:GLN:HG3	1.91	0.53
2:H:828:PHE:CB	2:H:1060:ILE:HD13	2.35	0.53
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.40	0.53
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.08	0.53
2:C:810:TYR:CD2	3:D:359:PRO:HG2	2.44	0.53
2:C:1293:VAL:HG23	2:C:1301:ARG:HA	1.91	0.53
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.38	0.53
3:D:749:LYS:NZ	3:D:753:SER:HB2	2.23	0.53
3:D:905:ARG:NH2	4:E:10:VAL:HG11	2.20	0.53
3:D:1252:HIS:O	3:D:1256:ILE:HG23	2.09	0.53
5:X:540:LEU:HD13	5:X:607:LEU:HG	1.91	0.53
2:H:522:SER:HA	2:H:525:THR:CG2	2.39	0.53
2:H:582:ASN:HD22	2:H:588:GLU:CD	2.17	0.53
2:H:632:ASP:O	2:H:633:LEU:HD23	2.09	0.53
2:C:67:GLU:HG2	2:C:103:VAL:CG1	2.38	0.53
2:C:149:LEU:HD12	2:C:452:ARG:O	2.09	0.53
3:D:584:PRO:O	3:D:589:TYR:OH	2.23	0.53
3:D:619:ILE:O	3:D:623:GLN:HG2	2.09	0.53
3:D:654:ILE:HD13	3:D:760:THR:HB	1.90	0.53
5:X:11:LEU:HD22	5:X:15:ARG:NH2	2.24	0.53
5:X:123:ILE:O	5:X:127:ILE:HG12	2.09	0.53
1:G:88:LEU:HG	1:G:128:HIS:HD2	1.74	0.53
2:H:528:ARG:HH22	2:H:663:VAL:CG2	2.22	0.53
2:H:1291:LEU:HD13	3:I:345:LYS:HZ1	1.74	0.53
5:Y:585:GLU:HB3	5:Y:589:GLN:NE2	2.21	0.53
1:B:48:LEU:HD22	3:D:534:GLU:HG3	1.90	0.53
2:C:828:PHE:HB2	2:C:1060:ILE:HD13	1.91	0.53
3:D:58:CYS:SG	3:D:61:ILE:HG13	2.49	0.53
3:D:227:PHE:O	3:D:230:SER:OG	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:620:PHE:O	3:D:624:ILE:HG23	2.09	0.53
3:D:1266:ILE:HG13	3:D:1274:PHE:O	2.09	0.53
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.24	0.53
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.08	0.53
5:X:453:PRO:HD2	5:X:456:MET:HB2	1.90	0.53
5:X:600:HIS:H	5:X:601:PRO:CD	2.21	0.53
1:F:50:SER:HB3	1:G:8:PHE:CZ	2.44	0.53
2:H:57:PHE:CE2	2:H:472:GLU:HG3	2.44	0.53
2:H:88:ARG:NH2	2:H:1040:ASP:OD1	2.42	0.53
2:H:514:PHE:HB2	6:H:1401:RFP:O8	2.09	0.53
2:H:516:ASP:HB2	6:H:1401:RFP:C32	2.39	0.53
2:H:522:SER:HA	2:H:525:THR:HG22	1.89	0.53
3:I:423:LEU:HB3	3:I:466:MET:CE	2.38	0.53
3:I:451:PRO:HG2	3:I:625:MET:SD	2.49	0.53
3:I:858:VAL:HB	3:I:859:PRO:CD	2.25	0.53
3:I:1176:VAL:HG22	3:I:1189:MET:SD	2.49	0.53
5:Y:130:VAL:O	5:Y:134:VAL:HG23	2.09	0.53
5:Y:355:ILE:HD13	5:Y:355:ILE:O	2.09	0.53
2:C:92:TYR:HE1	2:C:129:LEU:HD12	1.73	0.52
2:C:384:LEU:O	2:C:388:LEU:HG	2.09	0.52
2:C:943:LYS:O	2:C:947:GLU:HG2	2.09	0.52
1:G:33:ARG:NH1	2:H:820:GLU:OE2	2.43	0.52
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.90	0.52
2:H:21:VAL:HG13	2:H:22:LEU:N	2.22	0.52
2:H:27:LEU:HD22	2:H:528:ARG:NH2	2.23	0.52
2:H:582:ASN:HB3	2:H:586:PHE:C	2.34	0.52
2:H:1339:LEU:H	2:H:1339:LEU:HD12	1.73	0.52
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.91	0.52
3:I:169:LEU:HD13	3:I:173:GLY:HA2	1.90	0.52
3:I:1347:LEU:CD2	3:I:1358:PRO:HG2	2.38	0.52
1:A:11:PRO:HB3	1:A:31:LEU:HD21	1.91	0.52
2:C:538:LEU:CD2	2:C:547:VAL:HG11	2.39	0.52
2:C:706:ARG:HA	2:C:792:GLY:O	2.09	0.52
2:C:804:PHE:HZ	2:C:1230:MET:HE1	1.75	0.52
2:H:494:ASN:OD1	2:H:495:ALA:N	2.42	0.52
3:I:316:ILE:HD13	3:I:316:ILE:N	2.25	0.52
3:I:797:THR:O	3:I:801:VAL:HG23	2.08	0.52
2:C:68:LEU:HD22	2:C:475:VAL:HG21	1.90	0.52
2:C:1066:MET:HG3	2:C:1234:LYS:HA	1.89	0.52
2:C:1081:PRO:CB	2:C:1083:GLU:HG2	2.39	0.52
2:C:1335:ILE:CD1	3:D:22:ILE:HD11	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:279:LEU:HD21	3:D:296:LYS:HG2	1.91	0.52
3:D:436:ALA:HB3	3:D:485:MET:HA	1.91	0.52
4:E:31:GLN:HB2	4:E:46:THR:HG21	1.91	0.52
1:G:98:VAL:HG11	1:G:121:VAL:HG22	1.91	0.52
2:H:1252:SER:HB3	2:H:1259:LEU:HD21	1.92	0.52
3:I:681:LYS:HB2	3:I:681:LYS:NZ	2.25	0.52
3:I:1290:ARG:HD2	3:I:1299:GLY:HA3	1.90	0.52
2:C:510:GLN:C	2:C:512:SER:H	2.17	0.52
2:C:747:GLY:C	2:C:748:ILE:HG13	2.33	0.52
2:C:988:LYS:O	2:C:991:LYS:HE3	2.09	0.52
2:C:1146:GLN:CD	2:C:1160:ASP:HB2	2.35	0.52
2:C:1153:ALA:CB	2:C:1194:GLU:HG2	2.39	0.52
2:C:1223:ARG:HG3	2:C:1224:PRO:HD2	1.91	0.52
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.10	0.52
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.91	0.52
5:X:141:ILE:HG13	5:X:256:PHE:CD1	2.45	0.52
1:F:67:GLU:O	1:F:78:ILE:HB	2.10	0.52
2:H:684:ASN:HB3	2:H:687:ARG:HH12	1.75	0.52
2:H:691:PRO:HA	2:H:788:SER:OG	2.09	0.52
2:H:1124:ILE:HG21	2:H:1180:MET:HE2	1.90	0.52
3:I:545:HIS:CE1	3:I:574:VAL:HG21	2.45	0.52
3:I:1256:ILE:O	3:I:1260:MET:HB2	2.09	0.52
5:Y:493:LYS:O	5:Y:497:VAL:HG23	2.10	0.52
1:B:74:VAL:HG12	1:B:76:GLU:H	1.75	0.52
1:B:83:LEU:CD1	3:D:527:LEU:HA	2.27	0.52
2:C:699:LEU:H	2:C:799:ASN:HD21	1.56	0.52
3:D:185:ILE:HG22	3:D:238:ILE:HD13	1.91	0.52
3:I:1264:ALA:HB1	3:I:1303:SER:O	2.09	0.52
4:J:60:ASN:H	4:J:63:ILE:CG1	2.23	0.52
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.22	0.52
1:A:22:THR:HB	1:A:207:THR:O	2.09	0.52
1:A:236:ASP:HA	1:B:14:VAL:HB	1.90	0.52
1:A:285:THR:O	1:A:289:LEU:HG	2.09	0.52
2:C:299:LYS:HE3	2:C:334:GLU:OE1	2.10	0.52
2:C:840:SER:HB3	2:C:850:ILE:CD1	2.29	0.52
2:C:1120:ALA:HB1	2:C:1198:LEU:HB3	1.92	0.52
2:C:1313:HIS:CD2	3:D:474:LEU:HD23	2.45	0.52
3:D:20:ILE:HD13	3:D:1320:ILE:HD11	1.92	0.52
3:D:423:LEU:O	3:D:434:ILE:HA	2.09	0.52
3:D:701:LEU:HD21	3:D:723:TYR:HB2	1.90	0.52
5:X:132:CYS:SG	5:X:257:LYS:HD2	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:VAL:CG1	1:G:171:LEU:HD11	2.40	0.52
2:H:131:THR:HG22	2:H:135:THR:N	2.25	0.52
5:Y:600:HIS:HB2	5:Y:601:PRO:HD3	1.91	0.52
1:B:19:VAL:O	1:B:20:SER:HB3	2.09	0.52
2:C:989:LEU:HG	2:C:990:ASP:H	1.75	0.52
6:C:1401:RFP:H332	6:C:1401:RFP:C35	2.39	0.52
3:D:292:VAL:HG22	3:D:296:LYS:HE3	1.92	0.52
2:H:337:PHE:O	2:H:338:THR:OG1	2.27	0.52
2:H:1210:ILE:HG23	2:H:1211:ARG:HH11	1.73	0.52
3:I:425:ARG:NH2	3:I:464:ASP:OD2	2.42	0.52
3:I:807:LEU:HD12	3:I:807:LEU:O	2.10	0.52
3:I:846:GLU:HA	3:I:858:VAL:HA	1.92	0.52
3:I:856:ILE:HG13	3:I:857:LEU:O	2.09	0.52
5:Y:240:ARG:HD3	5:Y:244:THR:CB	2.39	0.52
2:C:1304:MET:CE	2:C:1308:ILE:HD11	2.40	0.52
3:D:573:THR:CG2	3:D:576:ARG:HG3	2.36	0.52
2:H:106:GLU:HG2	2:H:109:ALA:H	1.75	0.52
2:H:194:LEU:CD2	2:H:429:MET:HE3	2.38	0.52
2:H:395:TYR:CE2	2:H:420:LEU:HG	2.45	0.52
2:H:902:LEU:HD21	5:Y:608:ARG:HG3	1.91	0.52
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.25	0.52
2:H:1223:ARG:HG3	2:H:1224:PRO:HD2	1.90	0.52
2:H:1234:LYS:HE2	2:H:1238:LEU:HD22	1.91	0.52
3:I:161:THR:H	3:I:164:GLN:CD	2.18	0.52
3:I:864:LEU:HD11	3:I:901:ARG:NH1	2.18	0.52
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.92	0.52
2:C:1204:LEU:HD22	2:C:1205:PRO:HD2	1.92	0.52
3:D:24:LEU:H	3:D:232:ASN:ND2	2.07	0.52
3:D:58:CYS:SG	3:D:60:ARG:N	2.83	0.52
3:D:143:SER:HB2	5:X:100:MET:CE	2.39	0.52
3:D:807:LEU:HD12	3:D:807:LEU:O	2.10	0.52
5:X:459:THR:O	5:X:463:LEU:HD13	2.09	0.52
1:G:31:LEU:HB2	1:G:199:ASP:O	2.10	0.52
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.44	0.52
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.10	0.52
3:I:355:ILE:HA	3:I:447:ILE:HG23	1.92	0.52
3:I:474:LEU:HB3	4:J:28:ARG:HH21	1.74	0.52
3:I:492:SER:HB2	3:I:499:ILE:HB	1.91	0.52
3:I:643:ASP:O	3:I:720:ASN:ND2	2.19	0.52
5:Y:401:PHE:O	5:Y:405:ILE:HG23	2.09	0.52
2:C:130:MET:SD	2:C:134:GLY:HA2	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:311:CYS:SG	2:C:315:MET:HB2	2.50	0.52
3:D:428:THR:HG23	3:D:433:GLY:HA3	1.91	0.52
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.09	0.52
5:X:551:LEU:HD22	5:X:597:LYS:HD2	1.90	0.52
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.09	0.52
3:I:50:LYS:HG2	3:I:51:PRO:CD	2.40	0.52
3:I:227:PHE:HE1	3:I:234:PRO:HD3	1.75	0.52
3:I:526:VAL:HG12	3:I:549:LYS:HB2	1.92	0.52
5:Y:298:PRO:HB2	5:Y:301:ASN:HD22	1.75	0.52
1:A:130:ILE:HG22	1:A:131:CYS:SG	2.50	0.51
3:D:370:LYS:HG3	3:D:371:LYS:H	1.74	0.51
3:D:449:LEU:HD12	3:D:450:HIS:H	1.75	0.51
3:D:697:MET:CE	3:D:738:ARG:HA	2.36	0.51
3:D:789:LYS:HD2	3:D:932:MET:SD	2.49	0.51
3:D:1171:GLY:N	3:D:1172:LYS:O	2.41	0.51
5:X:224:LEU:HB2	5:X:259:PHE:CZ	2.45	0.51
2:H:1200:LYS:HE2	2:H:1206:THR:HB	1.92	0.51
3:I:428:THR:HG23	3:I:433:GLY:HA3	1.91	0.51
5:Y:213:ASP:HB2	5:Y:216:LEU:CB	2.39	0.51
1:A:13:LEU:HD11	1:A:16:ILE:CG1	2.40	0.51
1:B:77:ASP:O	1:B:81:ILE:HG13	2.09	0.51
1:B:153:VAL:O	1:B:175:ALA:N	2.42	0.51
2:C:685:MET:HE3	2:C:1235:LEU:HD11	1.92	0.51
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.25	0.51
3:D:66:LYS:HB2	3:D:69:GLU:HG2	1.91	0.51
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.91	0.51
3:D:1269:ALA:N	3:D:1300:ALA:HB2	2.20	0.51
5:X:35:ILE:HG23	5:X:36:VAL:HG13	1.92	0.51
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.91	0.51
2:H:886:LYS:HD3	2:H:916:SER:O	2.09	0.51
3:I:42:GLU:HG3	5:Y:451:ARG:HH21	1.74	0.51
3:I:161:THR:HG22	3:I:162:GLU:H	1.75	0.51
3:I:263:SER:HB2	5:Y:507:MET:CE	2.34	0.51
3:I:450:HIS:NE2	3:I:625:MET:SD	2.84	0.51
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.10	0.51
5:Y:585:GLU:O	5:Y:589:GLN:N	2.40	0.51
1:A:180:VAL:CG1	1:A:183:ILE:HG12	2.40	0.51
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.24	0.51
2:C:560:PRO:HB2	3:D:776:THR:OG1	2.10	0.51
2:C:926:GLY:CA	2:C:1056:VAL:HG12	2.38	0.51
2:C:1161:LEU:HD23	2:C:1164:PHE:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:369:PRO:HG3	3:D:446:ALA:O	2.10	0.51
3:D:918:ILE:HD13	3:D:919:ALA:N	2.26	0.51
3:D:930:LEU:HD11	3:D:1241:TYR:HE2	1.74	0.51
2:H:11:ILE:HD13	2:H:697:LYS:HZ3	1.75	0.51
2:H:53:PHE:HA	2:H:56:VAL:CG2	2.40	0.51
2:H:992:LEU:HD23	2:H:996:ARG:HG3	1.93	0.51
3:I:524:GLY:C	3:I:548:VAL:HG23	2.36	0.51
3:I:1346:GLY:HA3	3:I:1349:GLU:CD	2.35	0.51
5:Y:119:ILE:O	5:Y:123:ILE:HG13	2.09	0.51
1:A:190:ALA:HB2	1:A:200:LYS:HB3	1.92	0.51
2:C:67:GLU:HG2	2:C:103:VAL:HG12	1.91	0.51
2:C:905:ILE:HG12	5:X:595:LEU:HD22	1.90	0.51
3:D:139:LEU:HD13	3:D:140:TYR:HB3	1.91	0.51
2:H:818:VAL:HG22	2:H:819:SER:N	2.26	0.51
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.92	0.51
2:H:1293:VAL:HG21	2:H:1304:MET:CB	2.40	0.51
3:I:413:ASP:HA	3:I:416:ILE:HD12	1.91	0.51
3:I:664:ILE:HD12	3:I:681:LYS:HE3	1.91	0.51
3:I:700:ASN:O	3:I:704:GLU:HG2	2.10	0.51
3:I:778:GLY:HA2	3:I:781:LYS:HE3	1.92	0.51
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	1.92	0.51
1:A:118:ASP:OD1	1:A:119:GLY:N	2.44	0.51
2:C:42:ASP:O	2:C:44:GLU:HG2	2.10	0.51
2:C:51:ALA:C	2:C:53:PHE:H	2.18	0.51
2:C:149:LEU:HD23	2:C:451:ARG:HE	1.75	0.51
2:C:496:LYS:N	2:C:497:PRO:HD2	2.24	0.51
3:D:412:LEU:O	3:D:416:ILE:HD12	2.10	0.51
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.40	0.51
1:G:124:VAL:HG11	1:G:209:GLY:CA	2.34	0.51
2:H:119:GLU:HG2	2:H:120:GLN:N	2.25	0.51
3:I:1156:LEU:HA	3:I:1208:ASP:O	2.10	0.51
2:C:518:ASN:OD1	2:C:1236:ASN:ND2	2.43	0.51
2:C:667:LEU:HD11	2:C:708:VAL:HG21	1.92	0.51
2:C:720:ARG:HE	2:C:736:VAL:CG2	2.23	0.51
2:C:848:GLU:HG2	2:C:888:THR:HA	1.92	0.51
3:D:48:THR:OG1	3:D:50:LYS:NZ	2.44	0.51
3:D:363:LEU:HA	3:D:450:HIS:CE1	2.46	0.51
3:D:886:VAL:HG13	3:D:1230:THR:HG21	1.92	0.51
5:X:35:ILE:HG23	5:X:36:VAL:N	2.25	0.51
5:X:213:ASP:HB2	5:X:216:LEU:HB2	1.92	0.51
1:G:22:THR:HB	1:G:207:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:157:PHE:CZ	2:H:431:LYS:HD3	2.46	0.51
2:H:829:THR:HG22	2:H:1059:ARG:HG2	1.92	0.51
2:H:1314:GLN:HG3	4:J:28:ARG:HH12	1.73	0.51
3:I:919:ALA:O	3:I:923:ILE:HG12	2.11	0.51
2:C:92:TYR:CE1	2:C:129:LEU:HB2	2.46	0.51
2:C:660:VAL:HG22	2:C:661:VAL:N	2.22	0.51
2:C:866:ASP:HA	2:C:872:TYR:OH	2.11	0.51
2:C:1290:MET:SD	2:C:1294:LYS:HD3	2.51	0.51
3:D:422:LEU:HD12	3:D:469:HIS:HB2	1.92	0.51
3:D:482:ALA:C	3:D:483:LEU:HD12	2.35	0.51
3:D:611:ILE:HG13	3:D:612:LEU:CD2	2.40	0.51
3:D:813:ASP:HA	3:D:895:CYS:SG	2.51	0.51
3:D:1247:LYS:H	3:D:1247:LYS:CD	2.15	0.51
2:H:747:GLY:C	2:H:748:ILE:HG13	2.36	0.51
2:H:1187:PHE:HZ	3:I:772:TYR:HD2	1.57	0.51
3:I:762:ASN:OD1	3:I:764:ARG:HB3	2.10	0.51
1:A:14:VAL:HG21	1:A:29:GLU:HB2	1.92	0.51
1:A:41:ASN:HD21	2:C:1218:GLY:CA	2.24	0.51
2:C:639:LYS:HE2	2:C:639:LYS:HA	1.93	0.51
3:D:545:HIS:CE1	3:D:574:VAL:HG21	2.46	0.51
3:D:678:ARG:HD2	3:D:678:ARG:C	2.35	0.51
2:H:9:LYS:HD3	2:H:9:LYS:N	2.25	0.51
3:I:217:LEU:O	3:I:221:ILE:HG12	2.10	0.51
3:I:678:ARG:HA	3:I:681:LYS:CG	2.41	0.51
3:I:856:ILE:HA	3:I:860:ARG:HH21	1.75	0.51
5:Y:231:THR:HB	5:Y:252:LEU:HD22	1.92	0.51
5:Y:240:ARG:HH11	5:Y:244:THR:HG21	1.76	0.51
5:Y:598:LEU:O	5:Y:599:ARG:HD2	2.11	0.51
2:C:49:LEU:HD11	2:C:464:PHE:CG	2.46	0.51
2:C:221:LEU:HD13	2:C:298:ALA:HA	1.92	0.51
2:C:542:ARG:O	2:C:544:GLY:N	2.39	0.51
2:C:785:ASP:CG	2:C:789:THR:HG23	2.35	0.51
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.93	0.51
3:D:930:LEU:HA	3:D:1244:GLN:OE1	2.10	0.51
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.26	0.51
5:X:240:ARG:HD3	5:X:244:THR:CG2	2.41	0.51
5:X:442:SER:HG	5:X:446:GLN:HE21	1.58	0.51
2:H:99:LYS:HD3	2:H:99:LYS:N	2.26	0.51
2:H:453:ILE:O	2:H:453:ILE:HG23	2.11	0.51
3:I:147:ILE:HD12	3:I:178:ALA:HB2	1.93	0.51
3:I:390:LEU:N	3:I:390:LEU:HD12	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:38:LEU:HD13	4:J:58:LEU:CD2	2.38	0.51
5:Y:271:ASN:O	5:Y:275:VAL:HG23	2.11	0.51
1:A:180:VAL:HG11	1:A:183:ILE:HG12	1.92	0.51
2:C:227:LYS:NZ	2:C:334:GLU:OE2	2.36	0.51
2:C:590:PRO:O	2:C:659:GLN:NE2	2.44	0.51
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.26	0.51
3:D:588:PRO:HG2	3:D:591:ILE:HD11	1.92	0.51
3:D:640:GLY:N	3:D:643:ASP:OD2	2.43	0.51
2:H:82:VAL:HB	2:H:92:TYR:CE2	2.45	0.51
2:H:741:MET:SD	2:H:741:MET:N	2.83	0.51
2:H:1314:GLN:O	3:I:473:THR:HG23	2.11	0.51
3:I:33:TRP:O	3:I:102:MET:HB2	2.11	0.51
3:I:800:LEU:O	3:I:803:VAL:HG12	2.11	0.51
3:I:932:MET:O	3:I:933:ARG:HG3	2.10	0.51
1:A:71:LYS:HB3	1:A:74:VAL:HG21	1.92	0.50
1:B:227:GLN:O	1:B:228:LEU:HG	2.10	0.50
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.92	0.50
2:C:166:SER:O	2:C:168:GLY:N	2.36	0.50
2:C:1105:SER:HB2	3:D:731:ARG:HD3	1.93	0.50
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.25	0.50
3:D:136:GLU:HA	3:D:139:LEU:HD12	1.94	0.50
3:D:179:LYS:H	3:D:179:LYS:HD3	1.76	0.50
3:D:835:LEU:HD22	3:D:1242:ARG:NH1	2.25	0.50
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.93	0.50
2:H:607:SER:N	2:H:610:GLU:HB2	2.26	0.50
2:H:998:LEU:O	2:H:998:LEU:HD13	2.11	0.50
3:I:205:LEU:CD2	3:I:217:LEU:HD22	2.36	0.50
5:Y:513:ASP:N	5:Y:517:SER:OG	2.45	0.50
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.77	0.50
2:C:138:ILE:O	2:C:141:THR:OG1	2.30	0.50
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.94	0.50
2:C:478:ARG:HD3	2:C:492:MET:HG3	1.92	0.50
2:C:550:VAL:HG11	3:D:776:THR:HG23	1.93	0.50
2:C:564:PRO:HA	2:C:684:ASN:ND2	2.23	0.50
2:C:689:ALA:HB2	2:C:1233:LEU:HD22	1.94	0.50
2:C:880:GLY:H	2:C:920:VAL:HG13	1.77	0.50
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.92	0.50
3:D:697:MET:HE1	3:D:738:ARG:CA	2.37	0.50
3:D:803:VAL:HG13	3:D:1259:GLN:NE2	2.14	0.50
4:E:5:THR:HB	4:E:7:GLN:N	2.27	0.50
2:H:166:SER:O	2:H:168:GLY:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:518:ASN:OD1	2:H:1236:ASN:ND2	2.44	0.50
2:H:1204:LEU:HD22	2:H:1205:PRO:HD2	1.94	0.50
3:I:27:PRO:HD3	3:I:236:TRP:CE3	2.46	0.50
3:I:1159:ILE:HD12	3:I:1186:TYR:CE2	2.42	0.50
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.11	0.50
5:Y:262:VAL:HG13	5:Y:263:PRO:CD	2.35	0.50
5:Y:515:GLU:HA	5:Y:516:ASP:CB	2.40	0.50
1:A:82:LEU:HD11	1:A:171:LEU:HD13	1.93	0.50
1:A:151:GLY:O	1:A:153:VAL:HG23	2.11	0.50
1:A:158:ARG:HE	1:A:172:LEU:CD1	2.24	0.50
1:A:248:GLU:N	1:A:248:GLU:OE1	2.43	0.50
2:C:21:VAL:HG13	2:C:22:LEU:N	2.26	0.50
2:C:676:ALA:HB2	3:D:772:TYR:CE1	2.46	0.50
2:C:800:MET:HE1	2:C:827:ARG:HD3	1.94	0.50
2:C:1116:HIS:HE1	2:C:1226:THR:HG23	1.74	0.50
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.93	0.50
3:D:161:THR:HG22	3:D:162:GLU:H	1.75	0.50
3:D:412:LEU:O	3:D:416:ILE:HG23	2.11	0.50
3:D:778:GLY:HA2	3:D:781:LYS:HE3	1.92	0.50
3:D:1320:ILE:HG22	3:D:1352:ILE:CD1	2.38	0.50
5:X:384:LEU:O	5:X:384:LEU:HD13	2.11	0.50
2:H:151:ARG:HH22	2:H:175:ARG:HH11	1.60	0.50
3:I:473:THR:HG22	3:I:475:GLU:HG2	1.91	0.50
3:I:1148:ARG:NH2	3:I:1148:ARG:HB2	2.27	0.50
4:J:15:ASN:HD21	4:J:17:PHE:HB2	1.76	0.50
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.94	0.50
1:A:54:CYS:SG	1:A:148:ARG:HD3	2.51	0.50
2:C:839:VAL:HG22	2:C:1049:ILE:CG2	2.41	0.50
3:D:583:VAL:HG13	3:D:584:PRO:HD2	1.94	0.50
3:D:610:ARG:HG2	3:D:864:LEU:HD22	1.91	0.50
1:F:195:ARG:HH21	1:F:198:LEU:HD21	1.76	0.50
2:H:517:GLN:HE21	2:H:760:ASN:H	1.60	0.50
3:I:58:CYS:SG	3:I:61:ILE:N	2.71	0.50
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.47	0.50
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.40	0.50
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.41	0.50
3:D:197:GLU:O	3:D:201:LEU:HD23	2.12	0.50
3:D:1226:VAL:HG11	3:I:1292:LEU:HA	1.92	0.50
2:H:13:LYS:NZ	2:H:793:GLU:OE1	2.41	0.50
2:H:513:GLN:HA	6:H:1401:RFP:C37	2.42	0.50
3:I:116:PHE:HB3	3:I:237:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:590:SER:O	3:I:594:GLN:N	2.44	0.50
1:A:183:ILE:HD11	1:A:205:MET:HG3	1.92	0.50
2:C:356:THR:HG21	2:C:362:ALA:HA	1.94	0.50
3:D:52:GLU:OE1	5:X:451:ARG:HD2	2.11	0.50
3:D:356:THR:O	3:D:448:GLN:HA	2.11	0.50
3:D:534:GLU:O	3:D:538:ARG:HB2	2.11	0.50
3:D:813:ASP:OD1	3:D:896:ALA:HB3	2.12	0.50
3:D:932:MET:HB3	3:D:1139:PRO:HG2	1.93	0.50
5:X:17:LYS:NZ	5:X:17:LYS:HB3	2.25	0.50
5:X:244:THR:HA	5:X:247:GLU:HG3	1.94	0.50
1:G:41:ASN:OD1	2:H:1217:THR:HA	2.12	0.50
1:G:41:ASN:CG	2:H:1217:THR:HA	2.36	0.50
1:G:191:ARG:NH2	3:I:441:LEU:O	2.44	0.50
2:H:944:ARG:O	2:H:944:ARG:HD3	2.11	0.50
6:H:1401:RFP:H341	6:H:1401:RFP:H29C	1.93	0.50
3:I:265:LEU:HD11	3:I:330:MET:SD	2.51	0.50
3:I:482:ALA:C	3:I:483:LEU:HD12	2.37	0.50
4:J:16:ARG:O	4:J:19:LEU:HB3	2.11	0.50
5:Y:402:LEU:O	5:Y:406:GLN:HB2	2.11	0.50
1:A:104:LYS:HD3	1:A:105:SER:N	2.26	0.50
1:B:218:ARG:NH1	1:B:222:THR:OG1	2.44	0.50
2:C:611:GLU:HG3	2:C:616:ILE:HD11	1.93	0.50
2:C:954:LYS:HE3	2:C:958:LYS:HE2	1.94	0.50
3:D:30:ILE:HD12	3:D:243:PRO:HG3	1.94	0.50
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.12	0.50
5:X:8:GLN:HE21	5:X:32:PRO:CD	2.25	0.50
2:H:487:LEU:HB3	2:H:488:MET:HG3	1.94	0.50
2:H:524:ILE:HA	2:H:527:LYS:CD	2.41	0.50
3:I:474:LEU:HA	3:I:477:GLN:NE2	2.21	0.50
1:A:104:LYS:HD2	1:A:110:VAL:HG22	1.93	0.50
2:C:841:ARG:HH12	3:D:256:ASP:HB3	1.74	0.50
3:D:374:LEU:HD22	3:D:381:ILE:CD1	2.42	0.50
3:D:401:VAL:HG12	3:D:408:VAL:HG21	1.92	0.50
3:D:824:PRO:O	3:D:826:ILE:HG13	2.12	0.50
2:H:629:PHE:H	2:H:647:ARG:HH22	1.59	0.50
3:I:260:PHE:O	5:Y:504:PRO:HG2	2.12	0.50
3:I:810:THR:OG1	3:I:811:GLU:N	2.41	0.50
3:I:1157:ALA:O	3:I:1207:GLY:N	2.45	0.50
5:Y:99:ARG:O	5:Y:99:ARG:HD3	2.12	0.50
3:D:533:ALA:HB2	3:D:578:ILE:HD13	1.93	0.50
3:D:552:ILE:HG12	3:D:590:SER:OG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:LEU:HB3	2:H:655:VAL:CG1	2.42	0.50
2:H:1045:GLY:O	2:H:1046:VAL:HB	2.12	0.50
3:I:720:ASN:O	3:I:720:ASN:ND2	2.45	0.50
3:D:128:LEU:HD11	3:D:188:LEU:CD2	2.37	0.49
3:D:217:LEU:O	3:D:221:ILE:HG12	2.12	0.49
3:D:279:LEU:HD21	3:D:296:LYS:CG	2.42	0.49
3:D:513:MET:HE2	3:D:579:LEU:HB2	1.94	0.49
3:D:841:GLY:HA2	3:D:901:ARG:HD3	1.93	0.49
3:D:899:TYR:O	3:D:1251:LYS:HD3	2.11	0.49
3:D:1177:ILE:HG13	3:D:1190:ILE:HD13	1.94	0.49
5:X:115:GLY:O	5:X:119:ILE:HG12	2.11	0.49
5:X:541:ARG:O	5:X:545:HIS:HB2	2.12	0.49
5:X:598:LEU:O	5:X:599:ARG:HD2	2.11	0.49
2:H:47:TYR:CD1	2:H:70:TYR:HE2	2.30	0.49
2:H:671:LEU:HD23	2:H:1186:VAL:CG2	2.42	0.49
2:H:1028:LYS:O	2:H:1032:LYS:HG2	2.12	0.49
3:I:116:PHE:HB3	3:I:237:MET:CE	2.42	0.49
3:I:514:THR:HG21	3:I:595:ALA:O	2.12	0.49
3:I:600:ALA:CA	3:I:603:LYS:HB3	2.38	0.49
3:I:899:TYR:CE2	3:I:1251:LYS:HD2	2.47	0.49
4:J:60:ASN:H	4:J:63:ILE:HB	1.77	0.49
1:A:244:GLU:HB2	1:A:246:LYS:CE	2.41	0.49
2:C:487:LEU:HD13	2:C:488:MET:H	1.75	0.49
2:C:891:GLY:O	2:C:893:THR:HG23	2.12	0.49
3:D:435:GLN:HB2	3:D:457:TYR:OH	2.12	0.49
3:D:539:SER:OG	3:D:540:GLY:N	2.45	0.49
2:H:10:ARG:HE	2:H:1171:ARG:HE	1.61	0.49
2:H:1006:GLU:H	2:H:1006:GLU:CD	2.20	0.49
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.27	0.49
2:H:1255:THR:O	2:H:1257:GLN:N	2.42	0.49
2:H:1301:ARG:HG3	2:H:1302:THR:N	2.26	0.49
3:I:58:CYS:SG	3:I:60:ARG:N	2.85	0.49
3:I:293:ARG:NH1	5:Y:104:GLU:HB2	2.27	0.49
3:I:545:HIS:HB2	3:I:546:ALA:CB	2.41	0.49
3:I:1348:LYS:O	3:I:1352:ILE:HG12	2.12	0.49
5:Y:402:LEU:HA	5:Y:405:ILE:HG12	1.94	0.49
1:A:18:GLN:NE2	1:A:213:PRO:HG2	2.11	0.49
2:C:559:CYS:SG	2:C:661:VAL:HA	2.52	0.49
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.41	0.49
3:D:128:LEU:HD21	3:D:188:LEU:HD13	1.93	0.49
3:D:1155:ILE:O	3:D:1156:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1087:TYR:CE2	2:H:1215:GLY:HA2	2.43	0.49
3:I:589:TYR:O	3:I:591:ILE:HG13	2.12	0.49
1:B:29:GLU:HA	1:B:200:LYS:HB3	1.93	0.49
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.48	0.49
3:D:138:VAL:O	3:D:143:SER:HB3	2.13	0.49
3:D:425:ARG:CD	3:D:459:ALA:HB2	2.42	0.49
3:D:527:LEU:HD12	3:D:535:ARG:CZ	2.43	0.49
3:D:541:LEU:HD23	3:D:541:LEU:H	1.78	0.49
3:D:1195:GLN:OE1	3:D:1195:GLN:N	2.45	0.49
3:D:1270:GLY:CA	3:D:1299:GLY:HA2	2.43	0.49
3:I:29:MET:HE2	3:I:33:TRP:NE1	2.28	0.49
2:C:59:ILE:HG12	2:C:66:SER:HB3	1.93	0.49
3:D:583:VAL:CG1	3:D:587:LEU:HD22	2.43	0.49
3:D:824:PRO:HD3	3:D:836:ARG:NE	2.27	0.49
3:D:1329:THR:O	3:D:1333:THR:OG1	2.28	0.49
5:X:453:PRO:O	5:X:456:MET:HB2	2.12	0.49
3:I:126:LEU:HD21	3:I:223:LEU:CD1	2.42	0.49
3:I:490:ILE:O	3:I:499:ILE:HG22	2.12	0.49
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.13	0.49
5:Y:299:LYS:O	5:Y:303:ILE:HG12	2.12	0.49
1:A:163:GLU:HG3	1:A:170:ARG:NH1	2.26	0.49
1:B:227:GLN:C	1:B:229:GLU:H	2.20	0.49
2:C:339:ASN:O	2:C:345:PRO:HD3	2.12	0.49
2:C:816:ILE:CD1	2:C:1074:GLY:HA3	2.36	0.49
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.95	0.49
2:C:1313:HIS:HD2	3:D:474:LEU:HD23	1.78	0.49
3:D:31:ARG:NE	3:D:241:VAL:HG21	2.28	0.49
3:D:848:VAL:HG11	3:D:880:VAL:HG12	1.93	0.49
2:H:176:ILE:HD11	2:H:428:VAL:HG21	1.94	0.49
2:H:805:MET:HE1	2:H:1221:PHE:CE1	2.47	0.49
2:H:985:GLU:HG2	2:H:989:LEU:HD13	1.95	0.49
2:H:1133:LYS:HG3	2:H:1134:GLN:HG3	1.95	0.49
2:H:1276:TRP:HA	2:H:1276:TRP:CE3	2.47	0.49
3:I:325:LYS:HZ3	3:I:330:MET:HG2	1.78	0.49
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.12	0.49
5:Y:145:LEU:CD2	5:Y:225:ARG:HH21	2.24	0.49
5:Y:295:CYS:SG	5:Y:330:LEU:HD23	2.52	0.49
2:C:805:MET:HE1	2:C:1221:PHE:CE1	2.48	0.49
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.93	0.49
5:X:560:ARG:HG2	5:X:565:ILE:HG23	1.93	0.49
2:H:741:MET:HG2	2:H:743:PRO:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:765:ILE:HG13	2:H:787:PRO:HG2	1.95	0.49
3:I:31:ARG:HA	3:I:34:SER:OG	2.12	0.49
3:I:126:LEU:HD21	3:I:223:LEU:HD13	1.95	0.49
3:I:155:GLU:HG3	3:I:158:GLN:HB2	1.94	0.49
3:I:259:ARG:HH21	5:Y:504:PRO:CB	2.17	0.49
3:I:500:ILE:HD13	3:I:500:ILE:H	1.77	0.49
3:I:515:ARG:NH2	3:I:718:SER:O	2.44	0.49
3:I:707:ILE:HG22	3:I:708:ASN:H	1.76	0.49
3:I:888:CYS:HB2	3:I:898:CYS:SG	2.52	0.49
5:Y:469:GLN:O	5:Y:473:GLU:N	2.40	0.49
1:A:44:ARG:HG3	1:A:183:ILE:CG2	2.38	0.49
2:C:12:ARG:NH1	2:C:1159:VAL:HG21	2.28	0.49
2:C:487:LEU:HD12	2:C:488:MET:H	1.78	0.49
2:C:545:PHE:HZ	3:D:781:LYS:HA	1.76	0.49
3:D:1346:GLY:HA3	3:D:1349:GLU:CD	2.37	0.49
3:D:1368:ASP:O	3:D:1372:ARG:HB2	2.12	0.49
5:X:346:GLN:O	5:X:350:GLU:HG3	2.11	0.49
2:H:11:ILE:HG21	2:H:697:LYS:HZ2	1.77	0.49
2:H:51:ALA:C	2:H:53:PHE:H	2.21	0.49
2:H:96:LEU:HB2	2:H:127:ILE:CD1	2.43	0.49
2:H:145:ILE:HD11	2:H:506:PHE:CD2	2.48	0.49
2:H:989:LEU:HG	2:H:990:ASP:H	1.78	0.49
2:H:1297:ASP:OD1	2:H:1300:GLY:HA3	2.12	0.49
3:I:614:LEU:CD2	4:J:7:GLN:HG3	2.42	0.49
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.12	0.49
2:C:590:PRO:CB	2:C:655:VAL:HG21	2.39	0.49
2:C:748:ILE:HD12	2:C:748:ILE:O	2.12	0.49
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.47	0.49
2:C:1121:ALA:O	2:C:1180:MET:N	2.45	0.49
2:C:1243:MET:SD	3:D:445:LYS:HB3	2.53	0.49
2:C:1314:GLN:HA	4:E:28:ARG:NH2	2.28	0.49
3:D:1157:ALA:O	3:D:1207:GLY:N	2.46	0.49
3:D:1197:ASN:ND2	3:D:1212:ASP:HB3	2.28	0.49
1:F:42:ALA:O	1:F:46:ILE:HG12	2.13	0.49
1:F:200:LYS:HG3	1:F:200:LYS:O	2.13	0.49
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.94	0.49
2:H:20:GLN:O	2:H:22:LEU:N	2.45	0.49
2:H:479:LEU:CD2	2:H:492:MET:HE1	2.42	0.49
2:H:896:THR:HG22	2:H:898:GLU:OE1	2.13	0.49
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.13	0.49
3:I:56:LEU:HB3	3:I:250:ARG:HH21	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:127:LEU:HD21	3:I:234:PRO:HB3	1.94	0.49
3:I:242:LEU:HD12	3:I:243:PRO:CD	2.43	0.49
3:I:393:THR:HG23	3:I:396:ALA:H	1.78	0.49
3:I:1165:PHE:CD2	3:I:1168:GLU:HG3	2.47	0.49
3:I:1361:THR:O	4:J:21:LEU:HD21	2.13	0.49
5:Y:333:VAL:HG22	5:Y:336:GLU:HB2	1.93	0.49
5:Y:528:LEU:HD12	5:Y:528:LEU:O	2.12	0.49
2:C:9:LYS:HE3	2:C:12:ARG:HH21	1.77	0.49
2:C:123:TYR:OH	2:C:126:GLU:HB2	2.13	0.49
2:C:1108:ASN:ND2	2:C:1108:ASN:O	2.45	0.49
3:D:369:PRO:HB3	3:D:444:GLY:O	2.13	0.49
3:D:844:THR:HB	3:D:858:VAL:O	2.13	0.49
5:X:245:ALA:O	5:X:249:ILE:HG13	2.13	0.49
2:H:94:ALA:HB2	2:H:129:LEU:CD1	2.42	0.49
3:I:210:SER:O	3:I:214:ARG:HG3	2.12	0.49
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.94	0.49
3:I:1205:GLU:HB2	3:I:1208:ASP:OD1	2.12	0.49
4:J:26:ARG:HE	4:J:30:MET:HE3	1.78	0.49
1:A:253:LEU:HB3	1:A:321:TRP:HH2	1.74	0.48
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.48	0.48
2:C:801:ARG:HD2	2:C:1229:TYR:OH	2.14	0.48
1:G:191:ARG:HH22	3:I:442:ILE:HA	1.78	0.48
2:H:923:GLY:HA2	3:I:371:LYS:HE3	1.95	0.48
3:I:154:LEU:CD2	3:I:160:LEU:HD21	2.43	0.48
3:I:329:ASP:OD1	3:I:332:LYS:HE3	2.12	0.48
3:I:436:ALA:N	3:I:484:MET:O	2.33	0.48
3:I:524:GLY:CA	3:I:548:VAL:HG23	2.43	0.48
3:I:583:VAL:HG13	3:I:584:PRO:HD2	1.95	0.48
3:I:746:LEU:H	3:I:746:LEU:HD22	1.78	0.48
5:Y:240:ARG:O	5:Y:242:HIS:N	2.46	0.48
5:Y:477:GLU:OE1	5:Y:477:GLU:N	2.45	0.48
1:A:282:VAL:HG22	1:A:316:MET:HE2	1.94	0.48
2:C:94:ALA:O	2:C:126:GLU:HG2	2.12	0.48
2:C:494:ASN:OD1	2:C:495:ALA:N	2.45	0.48
2:C:611:GLU:CD	2:C:616:ILE:HD11	2.38	0.48
2:C:634:VAL:HG22	2:C:645:PHE:CZ	2.47	0.48
3:D:147:ILE:HD12	3:D:178:ALA:CB	2.42	0.48
3:D:316:ILE:HG13	3:D:317:THR:H	1.78	0.48
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.94	0.48
3:D:678:ARG:O	3:D:681:LYS:HG3	2.13	0.48
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:379:MET:HA	5:X:379:MET:CE	2.43	0.48
2:H:488:MET:HB2	2:H:489:PRO:CA	2.43	0.48
2:H:643:SER:C	2:H:644:LEU:HD12	2.39	0.48
2:H:1065:LYS:HG2	2:H:1235:LEU:HD12	1.95	0.48
1:B:49:SER:CA	1:B:151:GLY:HA2	2.39	0.48
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.28	0.48
2:C:1276:TRP:HA	2:C:1276:TRP:CE3	2.49	0.48
2:C:1297:ASP:OD1	2:C:1300:GLY:HA3	2.13	0.48
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	1.94	0.48
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.96	0.48
3:D:120:LEU:CD2	3:D:1330:ARG:HD2	2.43	0.48
3:D:706:VAL:C	3:D:707:ILE:HG13	2.38	0.48
2:H:516:ASP:OD1	2:H:522:SER:OG	2.30	0.48
3:I:362:ARG:HD2	3:I:364:HIS:HE1	1.78	0.48
3:I:661:VAL:O	3:I:665:GLN:HG3	2.13	0.48
3:I:766:GLY:C	3:I:767:LEU:HD22	2.39	0.48
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.29	0.48
5:Y:310:GLU:O	5:Y:344:LEU:HD23	2.13	0.48
2:C:453:ILE:HG23	2:C:453:ILE:O	2.13	0.48
2:C:1006:GLU:H	2:C:1006:GLU:CD	2.21	0.48
2:C:1276:TRP:HA	2:C:1276:TRP:HE3	1.79	0.48
3:D:20:ILE:HD11	3:D:1320:ILE:HD11	1.94	0.48
3:D:118:LYS:NZ	5:X:43:ASP:OD2	2.45	0.48
3:D:286:ALA:C	3:D:288:PRO:HD3	2.38	0.48
3:D:366:CYS:SG	3:D:437:PHE:HB2	2.54	0.48
3:D:481:ARG:HA	3:D:485:MET:HE2	1.94	0.48
3:D:860:ARG:NH1	3:D:866:GLU:HG2	2.29	0.48
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.94	0.48
5:X:45:ILE:C	5:X:45:ILE:HD12	2.38	0.48
5:X:145:LEU:HD21	5:X:225:ARG:NE	2.29	0.48
5:X:316:PHE:CZ	5:X:334:SER:HA	2.48	0.48
5:X:580:PHE:O	5:X:582:VAL:N	2.46	0.48
1:G:185:TYR:HA	1:G:202:VAL:O	2.13	0.48
2:H:157:PHE:CE1	2:H:431:LYS:HD3	2.48	0.48
3:I:306:LEU:C	3:I:306:LEU:HD23	2.39	0.48
3:I:596:LEU:N	3:I:596:LEU:HD23	2.28	0.48
2:C:185:ASP:O	2:C:196:VAL:HG23	2.13	0.48
2:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.94	0.48
2:C:951:MET:HA	2:C:951:MET:HE3	1.95	0.48
2:C:963:GLU:O	2:C:967:LEU:HD13	2.12	0.48
3:D:490:ILE:HG23	3:D:500:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:ILE:HG22	2:H:476:LYS:HA	1.95	0.48
2:H:106:GLU:CB	2:H:107:ARG:HA	2.43	0.48
2:H:975:ILE:HD13	2:H:975:ILE:O	2.12	0.48
2:H:1058:ARG:HD3	2:H:1240:ASP:OD1	2.12	0.48
3:I:12:THR:O	3:I:13:LYS:HD2	2.13	0.48
3:I:145:VAL:HG21	3:I:165:TYR:CD2	2.48	0.48
3:I:773:PHE:O	3:I:776:THR:HG22	2.14	0.48
5:Y:450:ILE:HD11	5:Y:500:ILE:O	2.13	0.48
1:B:232:VAL:O	1:B:233:ASP:HB2	2.13	0.48
2:C:442:VAL:HG12	2:C:443:ASP:H	1.78	0.48
2:C:686:GLN:C	2:C:688:GLN:H	2.19	0.48
2:C:893:THR:O	2:C:895:LEU:N	2.41	0.48
3:D:588:PRO:HG2	3:D:592:VAL:HG13	1.95	0.48
3:D:799:ARG:NH1	3:D:1146:GLU:OE1	2.46	0.48
2:H:487:LEU:HB3	2:H:488:MET:CG	2.44	0.48
2:H:697:LYS:HG3	2:H:698:PRO:HD2	1.95	0.48
2:H:748:ILE:C	2:H:748:ILE:HD12	2.38	0.48
3:I:824:PRO:HD3	3:I:836:ARG:NE	2.28	0.48
5:Y:123:ILE:O	5:Y:127:ILE:HG12	2.13	0.48
2:C:9:LYS:CE	2:C:12:ARG:HH21	2.27	0.48
2:C:1105:SER:HB3	2:C:1106:ARG:HD2	1.95	0.48
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.96	0.48
3:D:355:ILE:HA	3:D:447:ILE:HG23	1.96	0.48
3:D:766:GLY:C	3:D:767:LEU:HD22	2.39	0.48
5:X:113:ARG:O	5:X:117:ILE:HD13	2.13	0.48
5:X:477:GLU:CD	5:X:477:GLU:H	2.22	0.48
5:X:519:LEU:O	5:X:519:LEU:HD13	2.14	0.48
2:H:1108:ASN:ND2	2:H:1108:ASN:O	2.46	0.48
3:I:306:LEU:O	3:I:326:SER:HB2	2.13	0.48
1:A:99:ILE:HA	1:A:144:ILE:O	2.14	0.48
2:C:591:TYR:O	2:C:603:ILE:HA	2.14	0.48
2:C:709:ALA:O	2:C:715:THR:HG22	2.14	0.48
2:C:720:ARG:HE	2:C:736:VAL:HG22	1.78	0.48
3:D:278:ARG:O	3:D:282:LEU:HG	2.13	0.48
3:D:313:GLY:O	3:D:314:ARG:HB2	2.14	0.48
1:F:45:ARG:HG2	2:H:1083:GLU:HB2	1.95	0.48
2:H:127:ILE:HD13	2:H:127:ILE:N	2.26	0.48
2:H:158:ASP:N	2:H:173:ASN:O	2.46	0.48
3:I:194:LEU:O	3:I:198:CYS:HB2	2.13	0.48
3:I:316:ILE:HA	3:I:323:PRO:HA	1.95	0.48
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:513:MET:HE1	3:I:579:LEU:HB2	1.96	0.48
3:I:1169:THR:HA	3:I:1173:ARG:HB3	1.96	0.48
3:I:1282:TYR:HA	3:I:1285:VAL:HG22	1.96	0.48
5:Y:250:LEU:O	5:Y:254:GLU:HG2	2.13	0.48
1:B:9:LEU:H	1:B:9:LEU:HD23	1.79	0.48
2:C:524:ILE:HD11	2:C:712:SER:OG	2.14	0.48
3:D:531:LYS:NZ	3:D:531:LYS:HB3	2.29	0.48
3:D:1284:ARG:HA	3:D:1287:ILE:CG1	2.44	0.48
4:E:4:VAL:O	4:E:5:THR:OG1	2.23	0.48
5:X:470:MET:HG2	5:X:486:ARG:HH11	1.79	0.48
5:X:560:ARG:CG	5:X:565:ILE:HG23	2.43	0.48
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.95	0.48
2:H:660:VAL:HG22	2:H:661:VAL:N	2.25	0.48
2:H:669:PRO:HG2	2:H:1070:HIS:HE1	1.79	0.48
2:H:699:LEU:HB2	2:H:799:ASN:HD21	1.77	0.48
3:I:132:LEU:O	3:I:136:GLU:HB2	2.14	0.48
3:I:361:LEU:HD23	3:I:366:CYS:HA	1.96	0.48
3:I:403:ARG:O	3:I:405:GLU:N	2.47	0.48
5:Y:316:PHE:HZ	5:Y:334:SER:HA	1.78	0.48
5:Y:489:MET:SD	5:Y:493:LYS:HB3	2.54	0.48
1:A:7:GLU:H	1:B:150:ARG:HH22	1.62	0.48
1:A:83:LEU:O	1:A:86:LYS:HB2	2.14	0.48
1:B:57:THR:HG21	1:B:177:TYR:OH	2.14	0.48
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.95	0.48
2:C:122:VAL:HG22	2:C:123:TYR:N	2.29	0.48
2:C:678:ARG:HE	2:C:1106:ARG:HG2	1.78	0.48
3:D:144:TYR:HB3	3:D:159:ILE:HG22	1.95	0.48
3:D:205:LEU:HB3	3:D:217:LEU:HD22	1.96	0.48
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.44	0.48
3:D:1148:ARG:HH21	3:D:1148:ARG:HB2	1.79	0.48
2:H:946:LEU:HD12	2:H:949:GLU:HG2	1.96	0.48
2:H:977:ALA:O	2:H:980:VAL:HG12	2.14	0.48
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.49	0.48
3:I:169:LEU:HD13	3:I:173:GLY:CA	2.44	0.48
3:I:413:ASP:HA	3:I:416:ILE:CD1	2.43	0.48
3:I:1346:GLY:O	3:I:1350:ASN:HB2	2.14	0.48
1:A:104:LYS:HD3	1:A:104:LYS:C	2.39	0.47
2:C:500:ALA:O	2:C:504:GLU:HB2	2.13	0.47
2:C:736:VAL:HG11	2:C:740:GLU:CA	2.41	0.47
3:D:1170:LYS:C	3:D:1173:ARG:HD2	2.39	0.47
5:X:48:ILE:HG13	5:X:49:ASN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:122:VAL:HG22	2:H:123:TYR:N	2.28	0.47
2:H:442:VAL:HG12	2:H:443:ASP:N	2.29	0.47
2:H:478:ARG:HD3	2:H:492:MET:HG3	1.96	0.47
2:H:1101:LEU:HD11	3:I:505:ASP:HA	1.95	0.47
2:H:1276:TRP:HA	2:H:1276:TRP:HE3	1.79	0.47
3:I:62:PHE:O	3:I:101:ARG:HG3	2.13	0.47
3:I:923:ILE:HD11	3:I:1252:HIS:HB2	1.95	0.47
5:Y:311:THR:HG23	5:Y:355:ILE:HG21	1.96	0.47
1:A:11:PRO:O	1:A:12:ARG:HG3	2.14	0.47
1:A:243:LYS:HD3	1:A:243:LYS:N	2.29	0.47
2:C:127:ILE:HD13	2:C:127:ILE:N	2.28	0.47
2:C:170:VAL:HG23	2:C:171:LEU:N	2.21	0.47
3:D:646:ILE:HD12	3:D:646:ILE:O	2.13	0.47
3:D:1262:ARG:O	3:D:1280:VAL:HG22	2.14	0.47
3:D:1287:ILE:HA	3:D:1290:ARG:HG2	1.95	0.47
2:H:94:ALA:O	2:H:126:GLU:HG2	2.15	0.47
2:H:1269:ARG:HD2	3:I:346:ARG:NE	2.30	0.47
4:J:25:ARG:HD3	4:J:64:LEU:HD12	1.96	0.47
2:C:210:LEU:O	2:C:215:TYR:HB2	2.14	0.47
2:C:533:LEU:HD23	2:C:533:LEU:N	2.28	0.47
2:C:542:ARG:HG2	2:C:543:ALA:N	2.29	0.47
2:C:697:LYS:HD2	2:C:793:GLU:CD	2.39	0.47
2:C:1065:LYS:O	2:C:1235:LEU:HB2	2.14	0.47
3:D:19:ALA:HB2	3:D:1343:GLU:CB	2.43	0.47
3:D:30:ILE:HD13	3:D:33:TRP:CZ3	2.49	0.47
3:D:30:ILE:CG2	3:D:243:PRO:HB3	2.39	0.47
3:D:690:ASN:ND2	3:D:745:GLY:HA3	2.30	0.47
2:H:169:LYS:HD3	2:H:169:LYS:HA	1.67	0.47
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.47	0.47
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.96	0.47
3:I:1262:ARG:HD3	3:I:1279:GLN:OE1	2.15	0.47
5:Y:281:ARG:O	5:Y:285:ARG:HB2	2.14	0.47
5:Y:452:ILE:HG21	5:Y:457:ILE:HG12	1.94	0.47
1:A:246:LYS:HD3	1:A:246:LYS:N	2.29	0.47
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.48	0.47
2:C:745:GLU:HA	2:C:1017:GLN:OE1	2.14	0.47
2:C:954:LYS:HE3	2:C:958:LYS:CE	2.44	0.47
2:C:1121:ALA:HA	2:C:1180:MET:HB2	1.96	0.47
2:C:1156:ARG:HH11	2:C:1157:GLN:H	1.62	0.47
2:C:1272:GLU:HA	2:C:1275:VAL:HG22	1.96	0.47
3:D:186:GLN:CB	3:D:238:ILE:HD11	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:542:ALA:HB3	3:D:545:HIS:ND1	2.29	0.47
3:D:1328:THR:HA	3:D:1331:VAL:CG1	2.44	0.47
1:G:192:VAL:CG1	1:G:194:GLN:HG2	2.37	0.47
2:H:71:VAL:O	2:H:72:SER:OG	2.24	0.47
2:H:106:GLU:H	2:H:107:ARG:HA	1.80	0.47
2:H:253:PHE:CZ	2:H:287:VAL:HG12	2.50	0.47
2:H:487:LEU:CG	2:H:488:MET:HA	2.44	0.47
2:H:660:VAL:C	2:H:661:VAL:HG13	2.40	0.47
2:H:1209:GLN:O	2:H:1210:ILE:HG13	2.14	0.47
3:I:147:ILE:HG13	3:I:149:GLY:H	1.79	0.47
1:A:178:SER:HA	1:A:179:PRO:HD3	1.73	0.47
2:C:372:PRO:HG3	5:X:36:VAL:HG22	1.97	0.47
2:C:741:MET:SD	2:C:741:MET:N	2.87	0.47
2:C:1172:LEU:O	2:C:1176:LEU:HG	2.14	0.47
3:D:213:LYS:C	3:D:217:LEU:HG	2.40	0.47
3:D:803:VAL:HB	3:D:1313:SER:HB3	1.97	0.47
1:F:41:ASN:CG	2:H:1218:GLY:HA3	2.39	0.47
2:H:725:GLN:NE2	2:H:966:ILE:HD11	2.30	0.47
2:H:802:VAL:HG23	2:H:1098:LEU:HG	1.97	0.47
2:H:842:ASP:N	2:H:1046:VAL:HG11	2.30	0.47
2:H:941:LYS:HD2	2:H:941:LYS:O	2.14	0.47
2:H:1219:GLU:OE2	3:I:634:ARG:NH1	2.48	0.47
3:I:120:LEU:HD22	3:I:1330:ARG:HD3	1.97	0.47
3:I:813:ASP:OD1	3:I:896:ALA:HB3	2.13	0.47
3:I:1140:ARG:HH21	3:I:1236:GLU:HG2	1.77	0.47
3:I:1290:ARG:CD	3:I:1299:GLY:HA3	2.44	0.47
1:A:47:LEU:HD21	1:A:220:ALA:HB2	1.96	0.47
2:C:728:ASP:OD2	2:C:729:ALA:N	2.47	0.47
2:C:1024:GLU:O	2:C:1028:LYS:HG3	2.15	0.47
2:C:1284:ALA:CB	3:D:1361:THR:HB	2.40	0.47
3:D:269:TYR:HA	3:D:272:VAL:HG12	1.95	0.47
3:D:535:ARG:HB3	3:D:541:LEU:CD2	2.38	0.47
3:D:773:PHE:O	3:D:776:THR:HG22	2.14	0.47
2:H:157:PHE:HA	2:H:174:ALA:HA	1.96	0.47
2:H:773:LEU:HD13	2:H:773:LEU:H	1.79	0.47
3:I:368:LEU:HD12	3:I:369:PRO:HD2	1.96	0.47
3:I:490:ILE:HG23	3:I:500:ILE:CD1	2.44	0.47
3:I:592:VAL:HG23	3:I:593:ASN:OD1	2.15	0.47
3:I:1207:GLY:HA2	3:I:1223:LEU:CD2	2.43	0.47
3:I:1280:VAL:HG11	3:I:1304:ARG:NE	2.23	0.47
1:A:47:LEU:CD2	1:A:220:ALA:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:THR:HG23	1:A:209:GLY:H	1.79	0.47
1:B:22:THR:HG22	1:B:208:ASN:O	2.14	0.47
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.49	0.47
2:C:429:MET:O	2:C:433:ILE:HG13	2.15	0.47
2:C:514:PHE:HB3	6:C:1401:RFP:H322	1.96	0.47
2:C:756:TYR:H	2:C:766:ASN:HB2	1.80	0.47
2:C:818:VAL:HG22	2:C:819:SER:N	2.30	0.47
2:C:845:LEU:CD2	2:C:889:PRO:HG2	2.43	0.47
2:C:936:ARG:HH11	5:X:495:ARG:HD3	1.80	0.47
2:C:998:LEU:HD13	2:C:998:LEU:O	2.14	0.47
2:C:1106:ARG:HD2	2:C:1106:ARG:N	2.30	0.47
2:C:1286:THR:O	2:C:1290:MET:HB2	2.15	0.47
2:C:1303:LYS:HE2	2:C:1303:LYS:HA	1.96	0.47
3:D:306:LEU:C	3:D:306:LEU:HD23	2.40	0.47
3:D:474:LEU:HD11	4:E:27:ALA:HB3	1.96	0.47
3:D:834:PRO:C	3:D:835:LEU:HD12	2.40	0.47
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.79	0.47
5:X:28:ASN:HD22	5:X:29:ASP:H	1.61	0.47
1:G:14:VAL:HG22	1:G:28:LEU:CD2	2.43	0.47
1:G:191:ARG:NH2	3:I:442:ILE:HA	2.30	0.47
2:H:106:GLU:HG3	2:H:108:GLU:N	2.30	0.47
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.50	0.47
2:H:559:CYS:SG	2:H:661:VAL:HA	2.54	0.47
2:H:633:LEU:HD22	2:H:645:PHE:O	2.15	0.47
2:H:673:HIS:O	2:H:1109:ILE:HG22	2.14	0.47
2:H:681:MET:HE3	2:H:1073:LYS:HE3	1.97	0.47
2:H:773:LEU:H	2:H:773:LEU:CD1	2.28	0.47
2:H:1252:SER:O	2:H:1256:GLN:NE2	2.48	0.47
2:H:1305:TYR:HE1	3:I:379:PRO:HG3	1.80	0.47
3:I:392:THR:HG22	5:Y:606:VAL:HG11	1.96	0.47
3:I:579:LEU:O	3:I:579:LEU:HD13	2.14	0.47
3:I:660:GLU:O	3:I:664:ILE:HG12	2.13	0.47
3:I:800:LEU:HB3	3:I:920:ALA:CB	2.41	0.47
3:I:1171:GLY:N	3:I:1172:LYS:O	2.47	0.47
4:J:62:GLN:O	4:J:66:VAL:HG23	2.15	0.47
5:Y:120:ALA:HA	5:Y:123:ILE:CD1	2.42	0.47
5:Y:544:THR:O	5:Y:548:LEU:HG	2.14	0.47
1:A:85:LEU:HD22	1:A:88:LEU:HD12	1.96	0.47
1:A:226:GLU:HB3	1:B:10:LYS:NZ	2.29	0.47
1:B:181:GLU:HB2	1:B:206:GLU:O	2.14	0.47
2:C:515:MET:HE2	2:C:523:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:557:ARG:O	2:C:576:SER:HB3	2.14	0.47
2:C:818:VAL:HG22	2:C:819:SER:H	1.79	0.47
2:C:1239:VAL:HG12	2:C:1240:ASP:N	2.27	0.47
2:C:1255:THR:O	2:C:1257:GLN:N	2.41	0.47
3:D:179:LYS:HD3	3:D:179:LYS:N	2.29	0.47
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.97	0.47
5:X:277:MET:HE3	5:X:281:ARG:HG3	1.95	0.47
5:X:453:PRO:HD2	5:X:456:MET:HG3	1.96	0.47
5:X:528:LEU:O	5:X:528:LEU:HD12	2.14	0.47
1:F:15:ASP:HB3	1:F:27:THR:OG1	2.15	0.47
1:G:56:VAL:HG12	1:G:173:VAL:CG1	2.44	0.47
2:H:131:THR:HG22	2:H:135:THR:H	1.80	0.47
2:H:135:THR:OG1	2:H:143:ARG:O	2.23	0.47
3:I:155:GLU:CD	3:I:155:GLU:H	2.22	0.47
3:I:325:LYS:NZ	3:I:325:LYS:HB3	2.28	0.47
4:J:59:ILE:HG23	4:J:64:LEU:HD21	1.96	0.47
5:Y:224:LEU:HB2	5:Y:259:PHE:CE1	2.50	0.47
1:A:223:ILE:HD13	1:B:8:PHE:CE1	2.49	0.47
2:C:13:LYS:HE3	2:C:1183:ALA:HB2	1.97	0.47
2:C:15:PHE:CD2	2:C:1182:ILE:HD11	2.50	0.47
2:C:170:VAL:O	2:C:171:LEU:HB2	2.14	0.47
2:C:241:LEU:HD22	2:C:285:ILE:HG21	1.97	0.47
2:C:342:ASP:OD1	2:C:342:ASP:N	2.45	0.47
2:C:660:VAL:C	2:C:661:VAL:HG13	2.39	0.47
2:C:766:ASN:N	2:C:787:PRO:HG3	2.30	0.47
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.79	0.47
3:D:24:LEU:HD23	3:D:232:ASN:ND2	2.30	0.47
3:D:85:CYS:SG	3:D:86:GLU:N	2.88	0.47
3:D:139:LEU:HD13	3:D:139:LEU:C	2.40	0.47
4:E:5:THR:HB	4:E:7:GLN:H	1.78	0.47
5:X:310:GLU:O	5:X:344:LEU:HD23	2.15	0.47
5:X:470:MET:HG2	5:X:486:ARG:NH1	2.30	0.47
5:X:511:ILE:HG23	5:X:512:GLY:N	2.26	0.47
5:X:511:ILE:HG22	5:X:517:SER:HB3	1.96	0.47
5:X:525:ASP:HB3	5:X:528:LEU:HD21	1.97	0.47
1:F:68:TYR:HB3	2:H:756:TYR:CD1	2.50	0.47
1:G:154:PRO:HB3	3:I:525:MET:HE1	1.97	0.47
2:H:157:PHE:HD2	2:H:174:ALA:HB2	1.79	0.47
2:H:868:SER:OG	2:H:942:ASP:OD1	2.32	0.47
2:H:869:GLY:C	2:H:870:ILE:HD12	2.40	0.47
3:I:621:ALA:HA	3:I:624:ILE:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:744:ARG:HD2	3:I:763:PHE:CE1	2.50	0.47
3:I:822:MET:HG2	3:I:839:VAL:HG23	1.96	0.47
3:I:844:THR:HB	3:I:858:VAL:O	2.14	0.47
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.15	0.47
5:Y:545:HIS:NE2	5:Y:566:ASP:OD2	2.27	0.47
1:A:42:ALA:HA	1:B:38:THR:CG2	2.44	0.47
1:A:143:ARG:H	1:A:143:ARG:HD2	1.80	0.47
1:A:232:VAL:O	1:B:218:ARG:HG3	2.15	0.47
1:A:302:GLU:O	1:A:306:VAL:HG22	2.15	0.47
2:C:766:ASN:H	2:C:787:PRO:HG3	1.80	0.47
2:C:842:ASP:H	2:C:1046:VAL:HG11	1.77	0.47
3:D:50:LYS:HB3	3:D:50:LYS:HZ2	1.80	0.47
3:D:118:LYS:HE3	5:X:39:ASP:OD2	2.15	0.47
3:D:155:GLU:H	3:D:155:GLU:CD	2.22	0.47
3:D:901:ARG:HB3	3:D:908:ILE:HA	1.96	0.47
3:D:1157:ALA:O	3:D:1223:LEU:HD21	2.15	0.47
3:D:1359:ALA:HA	3:D:1363:TYR:HB2	1.96	0.47
5:X:484:ALA:HB1	5:X:490:PRO:O	2.14	0.47
2:H:37:LYS:HA	2:H:37:LYS:HE3	1.96	0.47
2:H:170:VAL:CG2	2:H:171:LEU:H	2.21	0.47
2:H:908:GLU:H	2:H:908:GLU:CD	2.23	0.47
2:H:975:ILE:O	2:H:979:LEU:HB2	2.15	0.47
3:I:120:LEU:HD22	3:I:1330:ARG:CD	2.45	0.47
5:Y:230:VAL:O	5:Y:234:THR:HG23	2.14	0.47
5:Y:573:LEU:CD2	5:Y:588:ARG:HB2	2.43	0.47
5:Y:582:VAL:CB	5:Y:586:ARG:HG2	2.45	0.47
2:C:26:TYR:HE2	2:C:28:LEU:HB2	1.80	0.46
2:C:348:SER:O	2:C:352:ARG:HG3	2.14	0.46
2:C:845:LEU:HD13	2:C:845:LEU:N	2.27	0.46
2:C:1122:LYS:HG2	2:C:1229:TYR:CE2	2.49	0.46
5:X:52:GLY:O	5:X:53:ILE:HB	2.14	0.46
1:F:142:MET:SD	1:F:144:ILE:HD11	2.56	0.46
2:H:157:PHE:CD2	2:H:174:ALA:HB2	2.50	0.46
2:H:1163:THR:HG22	2:H:1164:PHE:H	1.80	0.46
3:I:856:ILE:HD12	3:I:857:LEU:N	2.30	0.46
3:I:1247:LYS:HD3	3:I:1247:LYS:N	2.19	0.46
4:J:25:ARG:HD3	4:J:64:LEU:CD1	2.45	0.46
5:Y:138:PRO:CD	5:Y:353:LEU:HD21	2.45	0.46
2:C:103:VAL:HG22	2:C:104:ILE:N	2.29	0.46
2:C:756:TYR:H	2:C:766:ASN:HB3	1.78	0.46
2:C:1199:LEU:HD13	2:C:1206:THR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1252:SER:HA	5:X:523:ILE:O	2.14	0.46
3:D:34:SER:HB3	3:D:104:HIS:ND1	2.30	0.46
3:D:42:GLU:HG3	5:X:451:ARG:HH21	1.79	0.46
3:D:311:ARG:HG3	5:X:42:GLU:OE1	2.15	0.46
3:D:573:THR:HG22	3:D:576:ARG:CD	2.44	0.46
3:D:824:PRO:CD	3:D:836:ARG:HD3	2.46	0.46
5:X:377:LYS:HA	5:X:380:VAL:HG12	1.97	0.46
1:G:92:VAL:HG22	1:G:121:VAL:HG22	1.98	0.46
1:G:98:VAL:HG11	1:G:121:VAL:CG2	2.45	0.46
2:H:103:VAL:HG22	2:H:104:ILE:N	2.30	0.46
2:H:572:ILE:HD13	6:H:1401:RFP:C1	2.45	0.46
2:H:634:VAL:HG22	2:H:645:PHE:CZ	2.49	0.46
3:I:186:GLN:CA	3:I:238:ILE:HD11	2.45	0.46
3:I:503:SER:O	3:I:507:VAL:HG23	2.16	0.46
3:I:508:LEU:HD12	3:I:725:MET:HG2	1.97	0.46
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.98	0.46
3:I:841:GLY:HA3	3:I:901:ARG:HG2	1.98	0.46
5:Y:316:PHE:CD1	5:Y:337:VAL:HG11	2.50	0.46
1:A:29:GLU:O	1:A:31:LEU:N	2.47	0.46
1:A:85:LEU:HD21	1:A:130:ILE:HD13	1.96	0.46
1:A:184:ALA:HB2	2:C:1091:GLY:CA	2.46	0.46
2:C:201:ARG:HH12	5:X:36:VAL:HG11	1.79	0.46
2:C:1290:MET:HB2	2:C:1290:MET:HE2	1.81	0.46
3:D:252:LEU:HG	3:D:252:LEU:O	2.16	0.46
3:D:1158:GLU:HA	3:D:1223:LEU:HD21	1.95	0.46
5:X:456:MET:O	5:X:460:ILE:HG13	2.15	0.46
1:F:51:MET:HB2	1:F:179:PRO:HD2	1.97	0.46
1:G:33:ARG:HE	1:G:197:ASP:HB2	1.80	0.46
2:H:170:VAL:HG23	2:H:171:LEU:N	2.28	0.46
2:H:170:VAL:O	2:H:171:LEU:HB2	2.16	0.46
2:H:1087:TYR:HE2	2:H:1215:GLY:CA	2.28	0.46
3:I:107:LEU:HD11	3:I:242:LEU:HB3	1.96	0.46
3:I:279:LEU:HD23	3:I:295:GLU:HG3	1.98	0.46
3:I:421:VAL:HB	3:I:439:PRO:HG3	1.96	0.46
3:I:513:MET:HE2	3:I:579:LEU:HB2	1.97	0.46
5:Y:281:ARG:HD3	5:Y:359:LYS:NZ	2.30	0.46
1:A:232:VAL:HG13	1:B:218:ARG:CZ	2.45	0.46
1:B:154:PRO:O	1:B:157:THR:HG22	2.15	0.46
1:B:192:VAL:CG1	1:B:194:GLN:HG2	2.43	0.46
2:C:462:ASN:O	2:C:466:VAL:HG23	2.15	0.46
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:377:PHE:O	3:D:381:ILE:HG13	2.16	0.46
3:D:532:GLU:HG3	3:D:533:ALA:N	2.30	0.46
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.97	0.46
3:D:720:ASN:O	3:D:720:ASN:ND2	2.49	0.46
3:D:1159:ILE:HD12	3:D:1186:TYR:HE2	1.80	0.46
5:X:242:HIS:HA	5:X:245:ALA:HB3	1.96	0.46
1:G:12:ARG:H	1:G:30:PRO:HG2	1.80	0.46
2:H:403:MET:HG2	2:H:407:ARG:NH1	2.29	0.46
2:H:511:LEU:HA	2:H:513:GLN:HE21	1.80	0.46
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.44	0.46
3:I:263:SER:CB	5:Y:507:MET:HE2	2.38	0.46
3:I:286:ALA:O	3:I:288:PRO:HD3	2.15	0.46
3:I:847:ASP:H	3:I:858:VAL:HA	1.80	0.46
3:I:1174:ARG:HA	3:I:1192:LYS:HG3	1.96	0.46
3:I:1297:LYS:HA	3:I:1297:LYS:CE	2.45	0.46
2:C:92:TYR:CE1	2:C:129:LEU:HD12	2.49	0.46
2:C:568:ASN:HB3	2:C:572:ILE:HD12	1.98	0.46
2:C:799:ASN:O	2:C:800:MET:HE3	2.16	0.46
2:C:1161:LEU:HD21	2:C:1172:LEU:HD11	1.97	0.46
2:C:1246:ARG:NH2	2:C:1249:GLY:H	2.12	0.46
2:C:1335:ILE:HD11	3:D:22:ILE:CG1	2.45	0.46
3:D:392:THR:HG22	5:X:603:ARG:HG2	1.97	0.46
3:D:478:LEU:HB3	4:E:20:VAL:HG13	1.97	0.46
5:X:311:THR:HG23	5:X:355:ILE:HG21	1.98	0.46
5:X:322:MET:HG2	5:X:324:LYS:HG2	1.98	0.46
2:H:18:ARG:HD3	2:H:619:ALA:O	2.15	0.46
2:H:92:TYR:CE1	2:H:129:LEU:HB2	2.51	0.46
2:H:216:THR:OG1	2:H:219:GLN:HG3	2.16	0.46
2:H:538:LEU:HD11	2:H:547:VAL:HG11	1.98	0.46
2:H:557:ARG:NH2	2:H:607:SER:O	2.48	0.46
2:H:773:LEU:O	2:H:773:LEU:HD22	2.15	0.46
2:H:807:TRP:HE1	2:H:1086:PRO:HD3	1.80	0.46
2:H:848:GLU:HG2	2:H:888:THR:HA	1.98	0.46
2:H:1335:ILE:HD11	3:I:22:ILE:HG13	1.98	0.46
3:I:310:GLY:HA2	3:I:314:ARG:HE	1.81	0.46
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.15	0.46
5:Y:309:ASN:ND2	5:Y:312:SER:HB3	2.31	0.46
1:A:16:ILE:HG23	1:A:26:VAL:HG22	1.98	0.46
2:C:777:VAL:HG21	2:C:783:LEU:HD21	1.97	0.46
2:C:886:LYS:HD3	2:C:916:SER:O	2.14	0.46
2:C:896:THR:HG22	2:C:898:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:26:SER:O	3:D:29:MET:HB3	2.16	0.46
3:D:44:ILE:HG22	5:X:450:ILE:HG22	1.97	0.46
3:D:147:ILE:HG23	3:D:156:ARG:C	2.41	0.46
3:D:205:LEU:HD13	3:D:217:LEU:HA	1.97	0.46
3:D:899:TYR:CZ	3:D:915:ILE:HD12	2.51	0.46
5:X:387:VAL:HG13	5:X:408:GLY:HA3	1.97	0.46
5:X:451:ARG:O	5:X:452:ILE:HG13	2.16	0.46
1:G:227:GLN:C	1:G:229:GLU:H	2.23	0.46
2:H:130:MET:HE3	2:H:136:PHE:CZ	2.51	0.46
2:H:1277:ALA:CB	3:I:434:ILE:HD13	2.46	0.46
3:I:12:THR:C	3:I:13:LYS:HD2	2.40	0.46
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.98	0.46
3:I:679:TYR:O	3:I:683:ILE:HG13	2.16	0.46
3:I:1357:ILE:H	3:I:1357:ILE:HD12	1.80	0.46
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.16	0.46
5:Y:511:ILE:HG23	5:Y:517:SER:CB	2.45	0.46
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.16	0.46
1:B:19:VAL:O	1:B:20:SER:CB	2.64	0.46
2:C:11:ILE:HD13	2:C:697:LYS:CE	2.45	0.46
2:C:245:ARG:HB3	2:C:337:PHE:CE2	2.50	0.46
2:C:442:VAL:HG12	2:C:443:ASP:N	2.30	0.46
2:C:589:THR:OG1	2:C:590:PRO:HD2	2.16	0.46
2:C:1101:LEU:HD11	3:D:505:ASP:HA	1.96	0.46
3:D:298:MET:SD	5:X:402:LEU:HB3	2.56	0.46
3:D:390:LEU:N	3:D:390:LEU:HD12	2.30	0.46
3:D:546:ALA:H	3:D:547:ARG:C	2.23	0.46
3:D:824:PRO:HD3	3:D:836:ARG:HD3	1.97	0.46
5:X:251:LYS:O	5:X:255:VAL:HG23	2.16	0.46
5:X:453:PRO:HB2	5:X:455:HIS:CE1	2.51	0.46
2:H:446:ASP:HB2	2:H:551:HIS:CD2	2.51	0.46
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.51	0.46
2:H:1060:ILE:HA	2:H:1064:ASP:OD2	2.16	0.46
2:H:1199:LEU:HD13	2:H:1206:THR:HA	1.97	0.46
2:H:1339:LEU:HD12	2:H:1339:LEU:N	2.31	0.46
3:I:145:VAL:HA	3:I:180:MET:HB3	1.96	0.46
3:I:834:PRO:C	3:I:835:LEU:HD12	2.41	0.46
3:I:1230:THR:O	3:I:1234:VAL:HG12	2.16	0.46
2:C:843:THR:HG22	2:C:844:LYS:H	1.80	0.46
3:D:614:LEU:CD2	4:E:7:GLN:HG3	2.45	0.46
3:D:818:GLU:HA	3:D:881:LYS:HE2	1.97	0.46
5:X:515:GLU:N	5:X:516:ASP:HA	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:ILE:HG23	1:G:131:CYS:SG	2.56	0.46
2:H:807:TRP:HE1	2:H:1086:PRO:CD	2.28	0.46
2:H:848:GLU:CD	2:H:888:THR:HG22	2.41	0.46
3:I:801:VAL:HG13	3:I:917:VAL:HG12	1.98	0.46
3:I:886:VAL:HG22	3:I:1257:VAL:CG1	2.46	0.46
5:Y:238:LYS:HE2	5:Y:242:HIS:CE1	2.49	0.46
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.81	0.46
2:C:43:PRO:HD3	2:C:47:TYR:CD2	2.51	0.46
2:C:360:LEU:HD13	2:C:378:ARG:HH11	1.79	0.46
2:C:1148:ALA:HB1	2:C:1180:MET:CE	2.46	0.46
2:C:1319:MET:HE3	2:C:1324:ASN:CB	2.43	0.46
3:D:97:VAL:HG13	3:D:101:ARG:NH2	2.30	0.46
3:D:161:THR:HG22	3:D:162:GLU:N	2.31	0.46
3:D:1165:PHE:CD2	3:D:1168:GLU:HG3	2.51	0.46
3:D:1346:GLY:O	3:D:1350:ASN:HB2	2.15	0.46
5:X:11:LEU:HB3	5:X:15:ARG:NH1	2.30	0.46
2:H:513:GLN:HA	6:H:1401:RFP:H371	1.98	0.46
2:H:678:ARG:HE	2:H:1106:ARG:HG2	1.81	0.46
2:H:690:VAL:HG11	2:H:830:THR:HG21	1.97	0.46
3:I:160:LEU:HA	3:I:164:GLN:HE22	1.79	0.46
3:I:161:THR:HG22	3:I:162:GLU:CD	2.41	0.46
3:I:621:ALA:O	3:I:624:ILE:HG12	2.16	0.46
3:I:1292:LEU:HD12	3:I:1292:LEU:N	2.31	0.46
1:B:126:PRO:HG2	1:B:127:GLN:OE1	2.15	0.46
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.51	0.46
2:C:678:ARG:NH1	2:C:681:MET:HE2	2.30	0.46
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.46	0.46
3:D:886:VAL:CG1	3:D:1230:THR:HG21	2.46	0.46
3:D:1205:GLU:HB2	3:D:1208:ASP:OD1	2.15	0.46
3:D:1361:THR:O	4:E:21:LEU:HD21	2.15	0.46
4:E:16:ARG:O	4:E:20:VAL:HG23	2.16	0.46
5:X:22:LEU:HD13	5:X:48:ILE:HD12	1.97	0.46
5:X:514:ASP:C	5:X:516:ASP:HA	2.41	0.46
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.97	0.46
2:H:342:ASP:OD1	2:H:342:ASP:N	2.43	0.46
2:H:429:MET:O	2:H:433:ILE:HG13	2.16	0.46
3:I:161:THR:HG22	3:I:162:GLU:N	2.31	0.46
3:I:349:TYR:CD1	3:I:472:LEU:HD11	2.51	0.46
3:I:747:MET:O	3:I:755:ILE:HG22	2.16	0.46
3:I:1320:ILE:HG22	3:I:1352:ILE:CD1	2.45	0.46
3:I:1338:ALA:O	3:I:1340:LYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:448:ARG:HD3	5:Y:450:ILE:CG1	2.44	0.46
5:Y:449:THR:HG23	5:Y:503:GLU:OE1	2.16	0.46
5:Y:586:ARG:HH22	5:Y:590:ILE:HD11	1.81	0.46
1:B:33:ARG:HE	1:B:197:ASP:HB2	1.81	0.45
2:C:705:GLU:H	2:C:705:GLU:CD	2.25	0.45
2:C:1064:ASP:OD1	2:C:1238:LEU:HB2	2.15	0.45
3:D:489:ASN:HA	3:D:904:ALA:CB	2.46	0.45
3:D:521:LYS:HB2	3:D:542:ALA:HB2	1.98	0.45
3:D:749:LYS:HZ2	3:D:753:SER:HB2	1.80	0.45
3:D:786:THR:O	3:D:790:THR:HG23	2.16	0.45
4:E:3:ARG:O	4:E:4:VAL:HG13	2.16	0.45
2:H:127:ILE:O	2:H:127:ILE:HG12	2.16	0.45
2:H:1166:ASP:C	2:H:1168:GLU:H	2.23	0.45
2:H:1298:VAL:HG23	2:H:1299:ASN:N	2.29	0.45
3:I:179:LYS:HE3	3:I:179:LYS:H	1.81	0.45
3:I:262:THR:O	5:Y:507:MET:N	2.37	0.45
3:I:313:GLY:O	3:I:314:ARG:HB2	2.16	0.45
3:I:527:LEU:HB2	3:I:535:ARG:CZ	2.46	0.45
5:Y:479:THR:OG1	5:Y:482:GLU:HB2	2.16	0.45
5:Y:608:ARG:HB3	5:Y:608:ARG:NH1	2.31	0.45
2:C:71:VAL:O	2:C:72:SER:OG	2.27	0.45
2:C:73:TYR:O	2:C:74:ARG:HB2	2.15	0.45
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.51	0.45
2:C:869:GLY:C	2:C:870:ILE:HD12	2.41	0.45
3:D:600:ALA:CA	3:D:603:LYS:HB3	2.37	0.45
3:D:700:ASN:O	3:D:704:GLU:HG2	2.15	0.45
3:D:804:ALA:HB2	3:D:1259:GLN:NE2	2.31	0.45
3:D:1148:ARG:HB2	3:D:1148:ARG:NH2	2.31	0.45
3:D:1290:ARG:HD2	3:D:1299:GLY:HA3	1.97	0.45
1:G:51:MET:HE1	1:G:219:ARG:CG	2.46	0.45
2:H:216:THR:O	2:H:220:ILE:HG13	2.16	0.45
2:H:528:ARG:NH2	2:H:663:VAL:HB	2.31	0.45
2:H:838:CYS:HB2	2:H:918:LEU:HB2	1.98	0.45
2:H:884:VAL:HB	2:H:918:LEU:HB3	1.97	0.45
2:H:993:PRO:HB2	2:H:994:ARG:H	1.57	0.45
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.17	0.45
3:I:591:ILE:HD12	3:I:592:VAL:HG13	1.97	0.45
5:Y:292:VAL:HG13	5:Y:297:MET:O	2.16	0.45
2:C:56:VAL:HB	2:C:57:PHE:H	1.46	0.45
2:C:106:GLU:H	2:C:107:ARG:HA	1.81	0.45
2:C:230:PHE:CE1	2:C:239:MET:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:591:TYR:CE1	2:C:616:ILE:HG23	2.51	0.45
2:C:603:ILE:HD12	2:C:603:ILE:O	2.16	0.45
3:D:79:LYS:HE3	5:X:569:THR:N	2.32	0.45
3:D:81:ARG:HA	3:D:92:VAL:O	2.16	0.45
3:D:344:GLY:O	3:D:345:LYS:HB2	2.17	0.45
3:D:424:ASN:HB2	3:D:434:ILE:HG13	1.98	0.45
3:D:704:GLU:O	3:D:705:THR:OG1	2.29	0.45
3:D:1221:LEU:HD23	3:D:1226:VAL:HA	1.98	0.45
3:D:1234:VAL:HG13	3:D:1235:ASN:N	2.31	0.45
5:X:445:ASP:OD1	5:X:445:ASP:N	2.34	0.45
2:H:10:ARG:HD3	2:H:1175:ASN:HD21	1.82	0.45
2:H:572:ILE:HD13	6:H:1401:RFP:O1	2.16	0.45
2:H:810:TYR:CE1	2:H:1078:LYS:HD2	2.50	0.45
3:I:149:GLY:HA2	3:I:156:ARG:HG2	1.97	0.45
3:I:746:LEU:HD22	3:I:746:LEU:N	2.31	0.45
1:A:80:GLU:HG3	2:C:694:ARG:NH1	2.31	0.45
2:C:403:MET:HG2	2:C:407:ARG:HH12	1.82	0.45
2:C:555:TYR:OH	2:C:637:ARG:NH2	2.50	0.45
2:C:686:GLN:O	2:C:688:GLN:N	2.41	0.45
2:C:702:THR:HA	2:C:1184:THR:O	2.15	0.45
3:D:309:ASN:HD22	3:D:314:ARG:HA	1.82	0.45
5:X:276:MET:O	5:X:280:VAL:HG23	2.17	0.45
5:X:572:THR:O	5:X:576:VAL:HG23	2.16	0.45
1:G:57:THR:HG22	1:G:175:ALA:HB2	1.98	0.45
2:H:812:PHE:N	2:H:815:SER:HB2	2.31	0.45
2:H:993:PRO:HD2	2:H:996:ARG:HB3	1.99	0.45
3:I:279:LEU:HD23	3:I:295:GLU:CG	2.46	0.45
3:I:378:LYS:HG3	3:I:382:TYR:CZ	2.51	0.45
3:I:646:ILE:HD12	3:I:646:ILE:O	2.15	0.45
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.16	0.45
2:C:408:SER:O	2:C:431:LYS:NZ	2.47	0.45
2:C:475:VAL:HG23	2:C:492:MET:SD	2.57	0.45
2:C:641:GLU:HG3	2:C:642:SER:H	1.80	0.45
2:C:1024:GLU:HG3	2:C:1028:LYS:HD2	1.99	0.45
3:D:510:LEU:HD12	3:D:601:ILE:CD1	2.43	0.45
3:D:607:THR:O	3:D:611:ILE:HG12	2.17	0.45
1:F:52:PRO:HG2	1:F:219:ARG:NH2	2.27	0.45
2:H:31:GLN:O	2:H:130:MET:HE1	2.17	0.45
2:H:705:GLU:H	2:H:705:GLU:CD	2.25	0.45
2:H:944:ARG:HD3	2:H:944:ARG:C	2.42	0.45
3:I:252:LEU:HG	3:I:252:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:385:LEU:HD23	3:I:411:ILE:HG13	1.98	0.45
3:I:504:GLN:HG3	3:I:505:ASP:H	1.82	0.45
3:I:590:SER:HB3	3:I:594:GLN:NE2	2.29	0.45
3:I:860:ARG:NH1	3:I:866:GLU:HG2	2.32	0.45
5:Y:286:LEU:HD23	5:Y:340:ALA:HB2	1.99	0.45
5:Y:386:LEU:O	5:Y:390:ILE:HG23	2.15	0.45
1:B:81:ILE:HG12	1:B:131:CYS:SG	2.57	0.45
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.99	0.45
2:C:515:MET:CE	2:C:527:LYS:CE	2.94	0.45
3:D:318:GLY:C	3:D:320:ASN:H	2.25	0.45
3:D:364:HIS:HB3	3:D:487:THR:HG21	1.99	0.45
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.98	0.45
3:D:587:LEU:HD12	3:D:611:ILE:HD11	1.98	0.45
4:E:12:LYS:HA	4:E:12:LYS:HD3	1.80	0.45
5:X:148:TYR:OH	5:X:218:ARG:HA	2.16	0.45
1:G:227:GLN:O	1:G:229:GLU:N	2.50	0.45
2:H:106:GLU:HB3	2:H:107:ARG:CA	2.47	0.45
3:I:97:VAL:HG13	3:I:101:ARG:NH2	2.31	0.45
3:I:522:GLY:O	3:I:523:GLU:HG2	2.17	0.45
3:I:611:ILE:HG13	3:I:612:LEU:CD2	2.47	0.45
5:Y:343:LYS:O	5:Y:347:ILE:HG13	2.16	0.45
1:A:49:SER:OG	1:A:50:SER:N	2.50	0.45
1:A:303:ILE:O	1:A:307:LEU:HD13	2.17	0.45
2:C:192:ASP:HB3	2:C:346:TYR:CD1	2.52	0.45
2:C:518:ASN:ND2	2:C:761:GLN:HG2	2.31	0.45
2:C:697:LYS:HD2	2:C:793:GLU:OE2	2.16	0.45
2:C:975:ILE:O	2:C:979:LEU:HB2	2.17	0.45
2:C:1284:ALA:HA	3:D:1357:ILE:HD13	1.99	0.45
3:D:372:MET:O	3:D:376:LEU:HG	2.16	0.45
3:D:478:LEU:HD11	4:E:47:THR:HG23	1.99	0.45
3:D:665:GLN:HG2	3:D:678:ARG:NH1	2.32	0.45
3:D:746:LEU:H	3:D:746:LEU:HD22	1.82	0.45
3:D:768:ASN:O	3:D:771:GLN:NE2	2.50	0.45
3:D:840:LEU:HD12	3:D:840:LEU:O	2.17	0.45
3:D:1154:ALA:HB1	3:D:1211:SER:HB3	1.99	0.45
2:H:54:ARG:N	2:H:55:SER:C	2.74	0.45
2:H:99:LYS:C	2:H:100:LEU:HD12	2.42	0.45
2:H:142:GLU:O	2:H:143:ARG:HB2	2.16	0.45
2:H:562:GLU:HG2	2:H:574:SER:HB3	1.95	0.45
2:H:1043:ALA:C	2:H:1045:GLY:H	2.25	0.45
2:H:1293:VAL:HG21	2:H:1304:MET:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:8:LEU:HD23	3:I:8:LEU:N	2.32	0.45
3:I:703:THR:O	3:I:718:SER:N	2.50	0.45
3:I:801:VAL:HG12	3:I:805:GLN:HB3	1.99	0.45
2:C:44:GLU:HG3	2:C:45:GLY:N	2.32	0.45
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.52	0.45
2:C:911:SER:C	2:C:913:VAL:H	2.25	0.45
2:C:1045:GLY:O	2:C:1046:VAL:HB	2.16	0.45
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.78	0.45
3:D:167:ASP:O	3:D:171:GLU:HG2	2.16	0.45
3:D:169:LEU:HD22	3:D:176:PHE:HE2	1.82	0.45
3:D:215:LYS:O	3:D:219:LYS:HG3	2.17	0.45
3:D:270:ARG:NE	5:X:449:THR:HG22	2.29	0.45
3:D:474:LEU:HD11	4:E:27:ALA:CB	2.46	0.45
3:D:768:ASN:OD1	3:D:771:GLN:N	2.33	0.45
3:D:842:ARG:HD2	3:D:882:VAL:CG2	2.38	0.45
3:D:1140:ARG:NH2	3:D:1144:LEU:HD21	2.31	0.45
3:D:1178:THR:HG22	3:D:1187:GLU:HA	1.97	0.45
1:F:61:ILE:HG12	1:F:142:MET:HB3	1.99	0.45
1:G:176:CYS:O	1:G:178:SER:N	2.43	0.45
2:H:120:GLN:HG3	2:H:121:GLU:N	2.32	0.45
2:H:177:ILE:N	2:H:177:ILE:HD12	2.31	0.45
2:H:207:THR:O	2:H:211:ARG:HG3	2.17	0.45
2:H:628:HIS:HB3	2:H:647:ARG:HH21	1.78	0.45
2:H:1066:MET:HE2	2:H:1076:ILE:HD11	1.98	0.45
2:H:1285:TYR:HD2	3:I:1361:THR:HG21	1.81	0.45
3:I:664:ILE:HG21	3:I:681:LYS:HD2	1.98	0.45
3:I:1161:GLY:HA2	3:I:1181:ASP:HB2	1.99	0.45
3:D:316:ILE:O	3:D:317:THR:OG1	2.25	0.45
3:D:704:GLU:HB2	3:D:718:SER:OG	2.17	0.45
3:D:841:GLY:HA3	3:D:901:ARG:CD	2.47	0.45
3:D:1241:TYR:CD1	3:D:1248:ILE:HG21	2.52	0.45
3:D:1307:LEU:N	3:D:1307:LEU:HD23	2.31	0.45
5:X:225:ARG:O	5:X:229:VAL:HG13	2.16	0.45
1:F:152:TYR:CD2	2:H:824:GLN:HG2	2.52	0.45
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.84	0.45
2:H:771:VAL:HG23	2:H:775:GLU:CD	2.41	0.45
2:H:802:VAL:CG2	2:H:1098:LEU:HG	2.47	0.45
3:I:516:ASP:OD1	3:I:516:ASP:N	2.46	0.45
3:I:526:VAL:HG12	3:I:549:LYS:O	2.17	0.45
3:I:572:THR:HB	3:I:576:ARG:HD2	1.98	0.45
3:I:707:ILE:HD11	3:I:716:GLN:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:15:ASN:ND2	4:J:17:PHE:HB2	2.32	0.45
1:A:281:LEU:HG	1:A:307:LEU:HD21	1.98	0.45
2:C:53:PHE:HD1	2:C:57:PHE:CD2	2.34	0.45
2:C:54:ARG:N	2:C:55:SER:C	2.75	0.45
2:C:106:GLU:HG3	2:C:108:GLU:N	2.32	0.45
2:C:153:PRO:O	2:C:404:LYS:HE3	2.17	0.45
2:C:397:LEU:O	2:C:398:SER:OG	2.24	0.45
2:C:515:MET:HE2	2:C:523:GLU:CG	2.47	0.45
2:C:966:ILE:HG23	2:C:967:LEU:HD12	1.99	0.45
2:C:1210:ILE:HG23	2:C:1211:ARG:NH1	2.32	0.45
3:D:41:PRO:HG3	3:D:273:ILE:HG22	1.99	0.45
3:D:611:ILE:HG13	3:D:612:LEU:HD22	1.99	0.45
3:D:746:LEU:HD22	3:D:746:LEU:N	2.32	0.45
5:X:452:ILE:HD11	5:X:500:ILE:CG2	2.47	0.45
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	1.98	0.45
3:I:30:ILE:HD13	3:I:33:TRP:CZ3	2.52	0.45
3:I:239:LEU:HD12	3:I:239:LEU:O	2.17	0.45
3:I:372:MET:O	3:I:376:LEU:HG	2.16	0.45
3:I:527:LEU:HD13	3:I:531:LYS:HB2	1.97	0.45
3:I:848:VAL:HG11	3:I:880:VAL:HA	1.98	0.45
5:Y:134:VAL:HG22	5:Y:273:MET:HE1	1.99	0.45
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.99	0.44
2:C:178:PRO:HA	2:C:397:LEU:CD2	2.42	0.44
2:C:542:ARG:HG2	2:C:543:ALA:H	1.82	0.44
2:C:632:ASP:O	2:C:633:LEU:HD23	2.17	0.44
2:C:773:LEU:C	2:C:773:LEU:HD22	2.41	0.44
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.28	0.44
2:C:1342:GLU:HG3	3:D:18:ASP:CG	2.42	0.44
3:D:66:LYS:NZ	3:D:66:LYS:HB3	2.32	0.44
3:D:161:THR:HG22	3:D:162:GLU:CD	2.42	0.44
3:D:900:GLY:O	3:D:908:ILE:HG22	2.17	0.44
3:D:1184:ASP:HA	3:D:1185:PRO:HD3	1.75	0.44
5:X:47:MET:O	5:X:55:VAL:HG11	2.17	0.44
5:X:511:ILE:CG2	5:X:517:SER:HB3	2.48	0.44
1:F:85:LEU:CD2	1:F:130:ILE:HD13	2.47	0.44
2:H:18:ARG:HB2	2:H:1188:ASP:OD2	2.18	0.44
2:H:73:TYR:O	2:H:74:ARG:HB2	2.16	0.44
2:H:678:ARG:HD3	2:H:681:MET:HG3	1.98	0.44
2:H:1239:VAL:HG12	2:H:1240:ASP:N	2.28	0.44
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.79	0.44
3:I:159:ILE:N	3:I:159:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:325:LYS:HZ3	3:I:325:LYS:HB3	1.83	0.44
3:I:584:PRO:O	3:I:589:TYR:OH	2.22	0.44
3:I:610:ARG:HH21	3:I:901:ARG:NH2	2.14	0.44
4:J:10:VAL:HG11	4:J:16:ARG:CG	2.47	0.44
5:Y:586:ARG:O	5:Y:589:GLN:HB2	2.17	0.44
1:A:152:TYR:CE2	2:C:824:GLN:HA	2.51	0.44
2:C:80:PHE:O	2:C:84:GLU:HB3	2.16	0.44
2:C:296:VAL:O	2:C:336:LEU:N	2.50	0.44
2:C:988:LYS:NZ	2:C:988:LYS:HB3	2.31	0.44
2:C:1293:VAL:HG21	2:C:1304:MET:CB	2.48	0.44
3:D:159:ILE:N	3:D:159:ILE:HD12	2.32	0.44
3:D:572:THR:HB	3:D:576:ARG:HB2	2.00	0.44
5:X:311:THR:HB	5:X:345:GLN:HG2	1.99	0.44
5:X:556:ALA:O	5:X:560:ARG:HB2	2.17	0.44
2:H:582:ASN:HB2	2:H:588:GLU:HG3	1.99	0.44
2:H:877:VAL:HG11	2:H:883:LEU:CD2	2.45	0.44
3:I:73:GLY:O	3:I:76:LYS:HE3	2.17	0.44
3:I:1190:ILE:HD12	3:I:1190:ILE:N	2.32	0.44
5:Y:145:LEU:C	5:Y:145:LEU:HD13	2.42	0.44
5:Y:355:ILE:O	5:Y:358:VAL:HG22	2.17	0.44
2:C:94:ALA:C	2:C:126:GLU:HG2	2.42	0.44
2:C:177:ILE:N	2:C:177:ILE:HD12	2.33	0.44
2:C:1100:PRO:HB2	3:D:725:MET:HE1	2.00	0.44
3:D:545:HIS:HB2	3:D:546:ALA:CA	2.48	0.44
3:D:579:LEU:O	3:D:579:LEU:HD13	2.16	0.44
3:D:888:CYS:HB2	3:D:898:CYS:SG	2.58	0.44
5:X:101:TYR:HE2	5:X:388:ILE:HD11	1.82	0.44
1:G:9:LEU:HD23	1:G:9:LEU:H	1.83	0.44
2:H:1298:VAL:CG1	2:H:1321:GLU:HG3	2.47	0.44
3:I:145:VAL:CG1	3:I:180:MET:HB3	2.36	0.44
3:I:517:CYS:N	3:I:544:LEU:O	2.42	0.44
3:I:532:GLU:O	3:I:535:ARG:HB2	2.17	0.44
3:I:647:PRO:HG3	3:I:697:MET:CA	2.43	0.44
3:I:761:ALA:HB3	3:I:767:LEU:CD1	2.44	0.44
5:Y:471:LEU:HD12	5:Y:472:GLN:N	2.32	0.44
2:C:68:LEU:HD12	2:C:68:LEU:HA	1.83	0.44
2:C:98:VAL:HG11	2:C:124:MET:SD	2.57	0.44
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.98	0.44
2:C:712:SER:HB3	2:C:714:VAL:HG12	2.00	0.44
2:C:720:ARG:NH2	2:C:741:MET:HE1	2.33	0.44
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:387:LEU:HD23	3:D:387:LEU:C	2.43	0.44
3:D:473:THR:HB	3:D:476:ALA:HB3	1.98	0.44
3:D:535:ARG:HB3	3:D:541:LEU:HD11	2.00	0.44
3:D:588:PRO:HB2	3:D:591:ILE:HD11	2.00	0.44
3:D:822:MET:CG	3:D:838:ARG:HG3	2.47	0.44
3:D:844:THR:OG1	3:D:856:ILE:HD11	2.17	0.44
3:D:1180:VAL:HG22	3:D:1185:PRO:CA	2.46	0.44
5:X:134:VAL:HG22	5:X:273:MET:HE1	1.98	0.44
1:G:37:HIS:CE1	2:H:1216:ARG:HD3	2.53	0.44
3:I:16:GLU:HB3	3:I:1369:ARG:HH22	1.82	0.44
3:I:56:LEU:O	3:I:250:ARG:NH2	2.43	0.44
3:I:145:VAL:HA	3:I:180:MET:CB	2.48	0.44
3:I:614:LEU:CG	4:J:7:GLN:HG3	2.48	0.44
3:I:828:GLY:CA	3:I:832:LYS:HA	2.46	0.44
3:I:856:ILE:HD12	3:I:857:LEU:H	1.82	0.44
3:I:1148:ARG:HB2	3:I:1148:ARG:HH21	1.82	0.44
3:I:1307:LEU:N	3:I:1307:LEU:HD23	2.33	0.44
1:A:300:LEU:HD13	1:A:300:LEU:O	2.17	0.44
1:B:152:TYR:OH	3:D:535:ARG:NH1	2.43	0.44
2:C:270:THR:H	2:C:273:HIS:HD2	1.65	0.44
2:C:668:ILE:HG23	2:C:669:PRO:HD2	1.99	0.44
2:C:935:THR:HA	2:C:1048:LYS:HB3	1.99	0.44
2:C:1274:GLU:OE1	2:C:1274:GLU:N	2.50	0.44
3:D:384:LYS:HD2	3:D:384:LYS:HA	1.86	0.44
3:D:425:ARG:HH21	3:D:464:ASP:CG	2.26	0.44
3:D:1328:THR:HA	3:D:1331:VAL:HG12	1.99	0.44
5:X:35:ILE:HG13	5:X:36:VAL:N	2.25	0.44
5:X:316:PHE:CD1	5:X:337:VAL:HG11	2.52	0.44
2:H:736:VAL:HG11	2:H:740:GLU:CB	2.47	0.44
3:I:531:LYS:HB3	3:I:531:LYS:NZ	2.32	0.44
2:C:59:ILE:O	2:C:62:TYR:HB2	2.17	0.44
2:C:202:ARG:HH21	2:C:369:MET:HA	1.82	0.44
2:C:667:LEU:HD23	2:C:704:MET:HB3	1.98	0.44
2:C:682:GLY:HA2	2:C:685:MET:HG2	1.99	0.44
2:C:985:GLU:HG3	2:C:988:LYS:HB2	1.99	0.44
3:D:230:SER:CB	3:D:1338:ALA:HA	2.47	0.44
3:D:901:ARG:CA	3:D:908:ILE:HA	2.48	0.44
5:X:306:PHE:O	5:X:310:GLU:HG2	2.17	0.44
5:X:561:MET:HA	5:X:567:MET:SD	2.56	0.44
2:H:30:ILE:HD12	2:H:581:THR:HG22	2.00	0.44
2:H:127:ILE:HA	2:H:128:PRO:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:528:ARG:HH22	2:H:663:VAL:HG23	1.83	0.44
2:H:876:GLU:HG3	2:H:927:THR:CG2	2.30	0.44
2:H:924:VAL:HG12	2:H:1058:ARG:HH22	1.82	0.44
3:I:510:LEU:CD1	3:I:601:ILE:HD11	2.47	0.44
5:Y:470:MET:CB	5:Y:478:PRO:HB3	2.41	0.44
5:Y:519:LEU:HD13	5:Y:519:LEU:O	2.18	0.44
1:A:45:ARG:HG2	2:C:1083:GLU:OE1	2.18	0.44
1:A:180:VAL:HG11	1:A:183:ILE:CG1	2.48	0.44
2:C:57:PHE:CE1	2:C:475:VAL:HG11	2.53	0.44
2:C:117:ILE:HG21	2:C:487:LEU:HD23	2.00	0.44
2:C:127:ILE:O	2:C:127:ILE:HG12	2.18	0.44
3:D:112:ALA:HA	3:D:238:ILE:CG2	2.43	0.44
3:D:220:ARG:NE	3:D:224:LEU:HD11	2.33	0.44
3:D:268:LEU:HG	3:D:306:LEU:HA	2.00	0.44
5:X:343:LYS:O	5:X:346:GLN:HB3	2.18	0.44
2:H:475:VAL:O	2:H:479:LEU:HB2	2.18	0.44
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.33	0.44
3:I:214:ARG:O	3:I:218:THR:HG22	2.18	0.44
3:I:901:ARG:HA	3:I:908:ILE:HA	1.99	0.44
3:I:1278:GLU:HG3	3:I:1279:GLN:N	2.33	0.44
5:Y:108:VAL:HG23	5:Y:109:GLU:N	2.29	0.44
5:Y:455:HIS:O	5:Y:459:THR:HG23	2.18	0.44
1:A:256:PRO:HA	1:A:277:TYR:HA	2.00	0.44
2:C:103:VAL:HG22	2:C:104:ILE:H	1.82	0.44
2:C:1084:ASP:HB2	2:C:1216:ARG:CG	2.47	0.44
3:D:128:LEU:CD1	3:D:188:LEU:HD22	2.41	0.44
3:D:160:LEU:HD12	3:D:160:LEU:N	2.32	0.44
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.83	0.44
2:H:578:TYR:HB3	2:H:590:PRO:HG3	2.00	0.44
2:H:1214:ASP:OD1	2:H:1216:ARG:HB2	2.18	0.44
2:H:1254:VAL:HG23	2:H:1255:THR:N	2.33	0.44
3:I:149:GLY:CA	3:I:156:ARG:HG2	2.48	0.44
3:I:552:ILE:HG22	3:I:554:GLU:HG3	2.00	0.44
3:I:573:THR:HG22	3:I:576:ARG:CG	2.46	0.44
3:I:595:ALA:HB1	3:I:596:LEU:HD23	1.99	0.44
3:I:610:ARG:HH21	3:I:901:ARG:HH22	1.65	0.44
3:I:1234:VAL:HG13	3:I:1235:ASN:N	2.31	0.44
3:I:1258:ARG:HG3	3:I:1259:GLN:N	2.33	0.44
1:A:104:LYS:HG3	1:A:114:ASP:OD2	2.18	0.44
1:A:308:ALA:HA	1:A:312:LEU:O	2.17	0.44
1:B:102:LEU:O	1:B:141:SER:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:159:SER:HA	2:C:442:VAL:HG11	2.00	0.44
2:C:201:ARG:HD2	2:C:370:MET:SD	2.58	0.44
2:C:403:MET:HG2	2:C:407:ARG:CZ	2.47	0.44
2:C:465:ARG:O	2:C:469:VAL:HG23	2.18	0.44
2:C:516:ASP:OD1	2:C:518:ASN:ND2	2.51	0.44
2:C:1166:ASP:C	2:C:1168:GLU:H	2.26	0.44
6:C:1401:RFP:O1	6:C:1401:RFP:O11	2.35	0.44
3:D:490:ILE:HA	3:D:500:ILE:HD12	2.00	0.44
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.18	0.44
1:F:153:VAL:HG13	1:F:157:THR:OG1	2.17	0.44
2:H:153:PRO:HD2	2:H:452:ARG:HD3	2.00	0.44
2:H:670:PHE:CE2	2:H:1113:LEU:HB3	2.53	0.44
2:H:707:ALA:O	2:H:710:VAL:HG12	2.18	0.44
3:I:31:ARG:CZ	3:I:241:VAL:HG21	2.48	0.44
3:I:42:GLU:OE1	5:Y:451:ARG:HG2	2.17	0.44
3:I:202:ARG:O	3:I:206:ASN:ND2	2.45	0.44
3:I:494:ALA:HA	3:I:1252:HIS:HE1	1.83	0.44
3:I:686:TRP:HB3	3:I:758:PRO:HG2	1.99	0.44
1:A:23:HIS:CE1	1:A:25:LYS:HE3	2.50	0.43
1:A:222:THR:O	1:A:226:GLU:HG3	2.17	0.43
2:C:11:ILE:HD13	2:C:697:LYS:HE3	1.99	0.43
2:C:119:GLU:OE2	2:C:489:PRO:HB2	2.18	0.43
2:C:148:GLN:HA	2:C:531:SER:O	2.18	0.43
2:C:454:ARG:CD	2:C:459:MET:HG2	2.41	0.43
2:C:751:TYR:HE1	2:C:783:LEU:HD12	1.83	0.43
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.31	0.43
3:D:140:TYR:HA	3:D:181:GLY:CA	2.45	0.43
3:D:392:THR:CG2	5:X:603:ARG:HG2	2.48	0.43
3:D:610:ARG:HG3	3:D:864:LEU:CD1	2.25	0.43
5:X:406:GLN:HA	5:X:406:GLN:NE2	2.32	0.43
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.52	0.43
2:H:599:VAL:HG21	2:H:623:LEU:HD21	1.99	0.43
2:H:821:ARG:CZ	2:H:1082:ILE:HD13	2.48	0.43
6:H:1401:RFP:H341	6:H:1401:RFP:C29	2.47	0.43
3:I:416:ILE:HG13	3:I:441:LEU:CD2	2.48	0.43
3:I:598:LYS:HE3	3:I:599:LYS:HE3	1.99	0.43
3:I:901:ARG:CB	3:I:908:ILE:HA	2.47	0.43
3:I:1309:ILE:HG22	3:I:1310:THR:N	2.33	0.43
2:C:91:THR:HB	2:C:138:ILE:HD13	2.01	0.43
2:C:812:PHE:CE1	3:D:629:PHE:HZ	2.36	0.43
2:C:850:ILE:HD12	2:C:850:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:865:LEU:HG	2:C:869:GLY:C	2.42	0.43
2:C:1086:PRO:HA	2:C:1213:TYR:O	2.18	0.43
2:C:1140:LYS:C	2:C:1142:ARG:H	2.26	0.43
2:C:1209:GLN:O	2:C:1210:ILE:HG13	2.18	0.43
2:C:1214:ASP:HA	2:C:1221:PHE:CZ	2.52	0.43
3:D:43:THR:OG1	3:D:44:ILE:N	2.51	0.43
3:D:1158:GLU:HA	3:D:1223:LEU:HD22	1.99	0.43
4:E:60:ASN:H	4:E:63:ILE:HB	1.83	0.43
5:X:312:SER:OG	5:X:314:THR:HG23	2.18	0.43
1:G:183:ILE:HD11	1:G:205:MET:HE2	1.98	0.43
2:H:681:MET:O	2:H:685:MET:HG2	2.17	0.43
2:H:1293:VAL:HG21	2:H:1304:MET:HG3	2.00	0.43
2:H:1327:LEU:HD13	2:H:1339:LEU:HD11	1.99	0.43
3:I:801:VAL:CG1	3:I:805:GLN:HB3	2.48	0.43
3:I:1322:ALA:CB	3:I:1331:VAL:HG21	2.48	0.43
5:Y:133:SER:OG	5:Y:365:MET:HB2	2.18	0.43
5:Y:418:LYS:O	5:Y:430:TYR:OH	2.30	0.43
1:A:134:THR:CG2	2:C:727:VAL:HG23	2.47	0.43
1:B:19:VAL:O	1:B:19:VAL:HG12	2.18	0.43
1:B:227:GLN:O	1:B:229:GLU:N	2.44	0.43
2:C:46:GLN:O	2:C:49:LEU:HB3	2.19	0.43
2:C:119:GLU:HG2	2:C:120:GLN:N	2.33	0.43
2:C:309:LEU:H	2:C:309:LEU:CD2	2.24	0.43
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.53	0.43
2:C:1066:MET:HG2	2:C:1232:MET:HE2	2.00	0.43
3:D:478:LEU:HD22	4:E:24:ALA:HB2	2.00	0.43
3:D:1158:GLU:O	3:D:1223:LEU:HD11	2.19	0.43
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.18	0.43
3:D:1287:ILE:O	3:D:1291:GLU:HG2	2.18	0.43
3:D:1357:ILE:HD12	3:D:1357:ILE:N	2.33	0.43
4:E:38:LEU:HD13	4:E:58:LEU:CD2	2.37	0.43
5:X:142:THR:O	5:X:146:GLU:HG3	2.17	0.43
5:X:311:THR:HG21	5:X:348:GLU:CD	2.44	0.43
5:X:453:PRO:HD2	5:X:456:MET:CB	2.48	0.43
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.86	0.43
2:H:481:LEU:HD13	2:H:481:LEU:C	2.43	0.43
2:H:988:LYS:HB3	2:H:988:LYS:NZ	2.33	0.43
3:I:119:SER:HA	3:I:311:ARG:HH12	1.83	0.43
3:I:369:PRO:HG3	3:I:446:ALA:O	2.18	0.43
3:I:473:THR:HB	3:I:476:ALA:HB3	1.97	0.43
3:I:518:VAL:HG23	3:I:716:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:799:ARG:HD2	3:I:1310:THR:CG2	2.48	0.43
5:Y:365:MET:O	5:Y:369:GLU:HG3	2.18	0.43
1:A:318:LEU:HD13	1:A:318:LEU:N	2.33	0.43
1:B:47:LEU:HA	1:B:51:MET:HG2	1.99	0.43
2:C:57:PHE:O	2:C:67:GLU:HA	2.19	0.43
2:C:105:TYR:HA	2:C:106:GLU:HB2	2.00	0.43
2:C:149:LEU:CD2	2:C:451:ARG:HE	2.31	0.43
2:C:228:VAL:HG22	2:C:245:ARG:NH1	2.33	0.43
2:C:243:PRO:HB2	2:C:278:GLU:HG3	2.00	0.43
2:C:892:GLU:C	2:C:894:GLN:H	2.27	0.43
3:D:121:PRO:O	3:D:123:ARG:HD2	2.18	0.43
3:D:247:PRO:HA	3:D:250:ARG:NH1	2.33	0.43
3:D:515:ARG:HG3	3:D:719:PHE:CZ	2.52	0.43
3:D:681:LYS:O	3:D:685:ILE:HG13	2.19	0.43
3:D:823:THR:OG1	3:D:824:PRO:HD2	2.17	0.43
3:D:1332:LEU:HD12	3:D:1332:LEU:HA	1.87	0.43
1:F:11:PRO:HA	1:F:30:PRO:O	2.18	0.43
2:H:684:ASN:CB	2:H:687:ARG:HH12	2.31	0.43
3:I:120:LEU:N	3:I:120:LEU:HD12	2.33	0.43
1:B:118:ASP:HB3	1:B:121:VAL:HB	2.00	0.43
2:C:22:LEU:HB3	2:C:655:VAL:CG1	2.48	0.43
2:C:161:LYS:NZ	2:C:161:LYS:HB3	2.34	0.43
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.00	0.43
2:C:1043:ALA:C	2:C:1045:GLY:H	2.26	0.43
3:D:8:LEU:HD23	3:D:8:LEU:N	2.33	0.43
3:D:349:TYR:CE1	3:D:472:LEU:HD11	2.53	0.43
3:D:1180:VAL:HG21	3:D:1185:PRO:HB3	2.00	0.43
4:E:19:LEU:HD13	4:E:19:LEU:C	2.44	0.43
5:X:240:ARG:CD	5:X:244:THR:HB	2.38	0.43
1:F:207:THR:HG23	1:F:209:GLY:H	1.84	0.43
1:G:83:LEU:HD21	3:I:551:ARG:HB2	2.00	0.43
1:G:85:LEU:CD2	1:G:130:ILE:HD13	2.49	0.43
2:H:756:TYR:H	2:H:766:ASN:CB	2.32	0.43
2:H:773:LEU:HD22	2:H:773:LEU:C	2.43	0.43
2:H:894:GLN:HE21	3:I:77:ARG:NH1	2.14	0.43
2:H:924:VAL:CG1	2:H:1058:ARG:HH22	2.31	0.43
3:I:799:ARG:NH1	3:I:1146:GLU:OE1	2.52	0.43
1:A:73:GLY:O	1:A:133:LEU:HA	2.19	0.43
1:B:37:HIS:NE2	2:C:1216:ARG:HD3	2.34	0.43
2:C:342:ASP:O	2:C:437:ASN:ND2	2.52	0.43
2:C:637:ARG:O	2:C:638:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:785:ASP:OD1	2:C:789:THR:HG23	2.19	0.43
2:C:980:VAL:CG2	2:C:984:VAL:HG13	2.48	0.43
3:D:515:ARG:NH2	3:D:717:VAL:HG12	2.33	0.43
3:D:532:GLU:O	3:D:535:ARG:HB2	2.18	0.43
3:D:668:PHE:HD2	3:D:675:ALA:CB	2.32	0.43
4:E:73:GLN:O	4:E:77:ALA:HB3	2.18	0.43
1:F:9:LEU:HD11	1:F:195:ARG:CZ	2.48	0.43
2:H:105:TYR:HA	2:H:106:GLU:HA	1.87	0.43
2:H:667:LEU:HD23	2:H:704:MET:HB3	1.99	0.43
2:H:1064:ASP:OD1	2:H:1239:VAL:HG23	2.19	0.43
3:I:450:HIS:HD2	3:I:451:PRO:HD2	1.79	0.43
3:I:452:LEU:C	3:I:454:CYS:H	2.27	0.43
3:I:605:LEU:HD22	3:I:620:PHE:CD2	2.54	0.43
3:I:701:LEU:HD23	3:I:723:TYR:HB2	2.00	0.43
3:I:708:ASN:HA	3:I:712:GLN:HA	2.00	0.43
5:Y:108:VAL:HA	5:Y:385:ARG:NH1	2.31	0.43
5:Y:316:PHE:CZ	5:Y:334:SER:HA	2.54	0.43
5:Y:374:ARG:HH21	5:Y:377:LYS:HD2	1.83	0.43
1:B:100:LEU:HD21	1:B:121:VAL:HG21	2.01	0.43
2:C:676:ALA:HA	3:D:772:TYR:OH	2.19	0.43
3:D:286:ALA:O	3:D:288:PRO:HD3	2.18	0.43
3:D:591:ILE:HD12	3:D:591:ILE:C	2.43	0.43
3:D:592:VAL:HG23	3:D:593:ASN:OD1	2.19	0.43
3:D:799:ARG:HB3	3:D:1309:ILE:HG21	1.99	0.43
3:D:1274:PHE:HD2	3:D:1275:LEU:HG	1.83	0.43
5:X:395:THR:HA	5:X:404:LEU:CD2	2.48	0.43
1:F:7:GLU:O	1:F:8:PHE:HB2	2.18	0.43
1:G:29:GLU:HA	1:G:200:LYS:HB2	1.99	0.43
2:H:152:SER:OG	2:H:404:LYS:NZ	2.23	0.43
2:H:431:LYS:O	2:H:435:ILE:HG13	2.19	0.43
2:H:479:LEU:HD23	2:H:492:MET:HE1	2.00	0.43
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.52	0.43
2:H:843:THR:HB	2:H:845:LEU:HD21	2.00	0.43
2:H:893:THR:O	2:H:895:LEU:N	2.45	0.43
2:H:984:VAL:HG12	2:H:986:ALA:HB2	2.00	0.43
2:H:1108:ASN:ND2	2:H:1111:GLN:OE1	2.52	0.43
3:I:704:GLU:HB3	3:I:705:THR:H	1.70	0.43
1:A:166:ARG:HB2	1:A:166:ARG:CZ	2.48	0.43
2:C:169:LYS:HD3	2:C:169:LYS:HA	1.69	0.43
2:C:221:LEU:HD21	2:C:314:ASN:ND2	2.28	0.43
2:C:850:ILE:HG23	2:C:885:GLY:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:GLU:HG2	3:D:163:GLU:N	2.33	0.43
3:D:364:HIS:HB3	3:D:487:THR:HG23	2.00	0.43
3:D:596:LEU:N	3:D:596:LEU:HD23	2.34	0.43
3:D:686:TRP:O	3:D:690:ASN:N	2.49	0.43
3:D:714:GLU:HG2	3:D:715:LYS:H	1.83	0.43
3:D:899:TYR:HE1	3:D:915:ILE:HG23	1.82	0.43
3:D:1216:ALA:O	3:D:1220:ILE:HG13	2.19	0.43
3:D:1266:ILE:HA	3:D:1302:TYR:HA	2.00	0.43
3:D:1301:THR:HG22	3:I:1290:ARG:HH22	1.83	0.43
5:X:291:CYS:O	5:X:295:CYS:HB2	2.19	0.43
5:X:453:PRO:HD2	5:X:456:MET:CG	2.48	0.43
2:H:106:GLU:CB	2:H:107:ARG:CA	2.96	0.43
2:H:452:ARG:HH22	2:H:458:GLU:CD	2.25	0.43
2:H:564:PRO:HA	2:H:684:ASN:ND2	2.24	0.43
2:H:946:LEU:O	2:H:949:GLU:HG3	2.19	0.43
2:H:1116:HIS:CE1	2:H:1226:THR:HG23	2.49	0.43
2:H:1243:MET:SD	3:I:445:LYS:HE3	2.58	0.43
3:I:160:LEU:HD12	3:I:160:LEU:N	2.34	0.43
3:I:166:LEU:HD12	3:I:167:ASP:N	2.34	0.43
3:I:276:ASN:O	3:I:280:LYS:HG3	2.19	0.43
3:I:384:LYS:HD2	3:I:384:LYS:HA	1.83	0.43
3:I:387:LEU:HD23	3:I:387:LEU:C	2.43	0.43
3:I:621:ALA:CA	3:I:624:ILE:HG12	2.47	0.43
3:I:735:ALA:O	3:I:739:GLN:HG3	2.18	0.43
1:B:64:VAL:HG12	1:B:171:LEU:HD11	2.01	0.43
2:C:836:LEU:O	2:C:1052:VAL:N	2.38	0.43
2:C:866:ASP:CG	2:C:868:SER:H	2.26	0.43
2:C:944:ARG:HG3	2:C:944:ARG:HH11	1.84	0.43
2:C:1298:VAL:HG23	2:C:1299:ASN:N	2.34	0.43
2:C:1331:ARG:HG3	3:D:33:TRP:CZ3	2.54	0.43
3:D:27:PRO:HG3	3:D:240:THR:HG22	2.01	0.43
3:D:522:GLY:O	3:D:523:GLU:HG2	2.19	0.43
3:D:1343:GLU:HB2	3:D:1373:ARG:HH22	1.84	0.43
1:F:51:MET:HA	1:F:52:PRO:HD3	1.83	0.43
1:F:69:SER:O	1:F:78:ILE:HG12	2.19	0.43
1:F:212:ASP:OD2	1:F:215:GLU:HG2	2.19	0.43
1:G:79:LEU:HD23	1:G:82:LEU:HD12	2.00	0.43
2:H:103:VAL:HG22	2:H:104:ILE:H	1.84	0.43
2:H:462:ASN:O	2:H:466:VAL:HG23	2.19	0.43
2:H:603:ILE:HD12	2:H:603:ILE:O	2.19	0.43
3:I:96:LYS:O	3:I:99:ARG:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:140:TYR:OH	3:I:300:GLN:HG2	2.19	0.43
3:I:481:ARG:HA	3:I:485:MET:HE2	1.99	0.43
5:Y:511:ILE:HG23	5:Y:512:GLY:N	2.28	0.43
1:A:100:LEU:CD2	1:A:121:VAL:HG21	2.37	0.43
1:A:246:LYS:HG2	1:A:246:LYS:O	2.19	0.43
1:B:22:THR:HB	1:B:207:THR:O	2.18	0.43
2:C:92:TYR:O	2:C:128:PRO:HA	2.18	0.43
2:C:807:TRP:HH2	2:C:1216:ARG:HE	1.64	0.43
3:D:31:ARG:HD2	3:D:241:VAL:HG11	2.00	0.43
3:D:205:LEU:HD13	3:D:217:LEU:HD22	2.00	0.43
3:D:519:ASN:ND2	3:D:709:ARG:HA	2.34	0.43
3:D:545:HIS:HA	3:D:546:ALA:HA	1.81	0.43
3:D:864:LEU:HD21	3:D:901:ARG:NH2	2.34	0.43
3:D:1284:ARG:CA	3:D:1287:ILE:HG12	2.48	0.43
3:D:1307:LEU:HD23	3:D:1307:LEU:H	1.84	0.43
5:X:27:VAL:O	5:X:31:LEU:HG	2.19	0.43
5:X:407:GLU:HB2	5:X:439:ILE:HG22	2.01	0.43
1:G:82:LEU:O	1:G:86:LYS:HG3	2.18	0.43
2:H:13:LYS:HD2	2:H:1181:PRO:HG2	1.95	0.43
2:H:57:PHE:HA	2:H:476:LYS:HZ1	1.82	0.43
2:H:178:PRO:HG2	2:H:182:SER:O	2.19	0.43
2:H:702:THR:HA	2:H:1184:THR:O	2.19	0.43
2:H:896:THR:HG23	2:H:897:PRO:HD2	2.00	0.43
2:H:944:ARG:O	2:H:947:GLU:HB2	2.19	0.43
2:H:1290:MET:HE2	2:H:1290:MET:HB2	1.92	0.43
3:I:63:GLY:O	3:I:98:ARG:NH2	2.51	0.43
3:I:262:THR:O	5:Y:507:MET:HG3	2.18	0.43
3:I:286:ALA:C	3:I:288:PRO:HD3	2.44	0.43
3:I:425:ARG:CD	3:I:459:ALA:HB2	2.49	0.43
3:I:704:GLU:O	3:I:705:THR:OG1	2.31	0.43
3:I:770:LEU:HD13	3:I:770:LEU:C	2.44	0.43
3:I:1278:GLU:HG3	3:I:1279:GLN:H	1.84	0.43
3:I:1357:ILE:HD12	3:I:1357:ILE:N	2.34	0.43
5:Y:231:THR:O	5:Y:235:ILE:HG13	2.19	0.43
5:Y:372:ALA:O	5:Y:376:LYS:HG3	2.18	0.43
5:Y:394:TYR:CG	5:Y:439:ILE:HD11	2.54	0.43
1:A:310:ARG:HA	1:A:310:ARG:HE	1.80	0.42
2:C:192:ASP:HB3	2:C:346:TYR:HD1	1.84	0.42
2:C:211:ARG:NH2	2:C:217:THR:OG1	2.46	0.42
2:C:405:PHE:O	2:C:409:LEU:HD23	2.19	0.42
2:C:1086:PRO:O	2:C:1094:VAL:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.52	0.42
2:C:1214:ASP:OD1	2:C:1216:ARG:HB2	2.19	0.42
3:D:767:LEU:HD12	3:D:771:GLN:CD	2.45	0.42
3:D:901:ARG:CB	3:D:908:ILE:HA	2.49	0.42
3:D:918:ILE:HD11	3:D:1252:HIS:NE2	2.33	0.42
3:D:1149:ARG:HA	3:D:1150:PRO:HD3	1.89	0.42
5:X:120:ALA:HA	5:X:123:ILE:HD12	2.00	0.42
5:X:400:GLN:CD	5:X:400:GLN:H	2.27	0.42
5:X:530:LEU:HD12	5:X:530:LEU:H	1.84	0.42
1:F:192:VAL:HG21	1:F:198:LEU:HD12	2.01	0.42
1:F:221:ALA:HB1	1:G:228:LEU:HD12	2.01	0.42
2:H:453:ILE:HG22	2:H:585:GLY:O	2.19	0.42
2:H:714:VAL:HG23	2:H:787:PRO:HD2	2.00	0.42
2:H:1054:LEU:HD12	2:H:1054:LEU:O	2.18	0.42
3:I:124:ILE:HG13	3:I:189:LEU:HD11	2.01	0.42
3:I:482:ALA:O	3:I:488:ASN:ND2	2.52	0.42
3:I:535:ARG:CB	3:I:541:LEU:HD11	2.43	0.42
3:I:550:VAL:HG23	3:I:552:ILE:HD11	2.00	0.42
3:I:809:VAL:HG13	3:I:912:GLY:H	1.84	0.42
1:A:227:GLN:HE22	1:B:11:PRO:HD3	1.84	0.42
1:B:88:LEU:HD22	1:B:90:VAL:CG2	2.49	0.42
1:B:183:ILE:HD11	1:B:205:MET:HG3	2.01	0.42
2:C:91:THR:HG22	2:C:139:ASN:H	1.84	0.42
2:C:317:LEU:HD13	2:C:322:LEU:HD21	2.01	0.42
2:C:681:MET:CE	2:C:1073:LYS:HE3	2.48	0.42
2:C:840:SER:OG	2:C:1047:LEU:HB3	2.19	0.42
2:C:994:ARG:HD3	2:C:994:ARG:N	2.34	0.42
2:C:1327:LEU:HA	2:C:1337:ILE:HD11	2.01	0.42
3:D:214:ARG:O	3:D:218:THR:HG22	2.18	0.42
3:D:401:VAL:HG12	3:D:408:VAL:CG2	2.49	0.42
3:D:771:GLN:HE21	3:D:772:TYR:N	2.17	0.42
3:D:1167:LYS:HE3	3:D:1173:ARG:NH1	2.20	0.42
3:D:1221:LEU:HD13	3:D:1221:LEU:C	2.44	0.42
1:F:68:TYR:OH	2:H:1057:LYS:HD2	2.19	0.42
1:G:100:LEU:HD11	1:G:121:VAL:HG11	2.01	0.42
2:H:38:PHE:O	2:H:39:ILE:HB	2.19	0.42
2:H:161:LYS:NZ	2:H:161:LYS:HB3	2.34	0.42
2:H:391:SER:OG	2:H:393:ASP:OD1	2.29	0.42
2:H:400:VAL:HA	2:H:403:MET:HE2	2.01	0.42
3:I:25:ALA:HB3	3:I:30:ILE:HD11	2.01	0.42
3:I:50:LYS:HG2	3:I:51:PRO:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:119:SER:HA	3:I:311:ARG:NH1	2.34	0.42
3:I:205:LEU:HB3	3:I:217:LEU:HD22	2.01	0.42
3:I:268:LEU:HG	3:I:306:LEU:HA	2.00	0.42
3:I:650:LYS:HE2	3:I:765:GLU:OE1	2.18	0.42
3:I:703:THR:HA	3:I:717:VAL:HA	2.00	0.42
3:I:836:ARG:HD2	3:I:836:ARG:HA	1.77	0.42
5:Y:242:HIS:O	5:Y:246:GLN:HB2	2.19	0.42
2:C:155:VAL:HG12	2:C:405:PHE:HA	2.01	0.42
2:C:704:MET:HA	2:C:704:MET:CE	2.46	0.42
3:D:526:VAL:HG12	3:D:549:LYS:O	2.19	0.42
3:D:869:CYS:HA	3:D:872:LEU:HD13	2.02	0.42
4:E:72:GLN:O	4:E:76:GLU:HB2	2.19	0.42
2:H:718:ALA:HB2	2:H:783:LEU:HG	2.00	0.42
3:I:298:MET:SD	5:Y:402:LEU:HB3	2.58	0.42
3:I:1259:GLN:H	3:I:1259:GLN:HG3	1.68	0.42
5:Y:96:ASP:CG	5:Y:97:PRO:HD2	2.44	0.42
2:C:49:LEU:HD23	2:C:49:LEU:C	2.45	0.42
2:C:73:TYR:N	2:C:73:TYR:CD2	2.87	0.42
2:C:131:THR:HG23	2:C:133:ASN:N	2.22	0.42
2:C:170:VAL:HG11	2:C:172:TYR:OH	2.19	0.42
2:C:225:PHE:CB	2:C:336:LEU:HD22	2.49	0.42
2:C:310:ILE:O	2:C:311:CYS:HB3	2.20	0.42
2:C:1054:LEU:O	2:C:1054:LEU:HD12	2.20	0.42
3:D:511:TYR:CE2	3:D:596:LEU:HD12	2.54	0.42
3:D:586:GLY:O	3:D:587:LEU:HB2	2.19	0.42
3:D:650:LYS:NZ	3:D:760:THR:O	2.51	0.42
3:D:915:ILE:O	3:D:918:ILE:HG23	2.20	0.42
3:D:1171:GLY:CA	3:D:1172:LYS:C	2.92	0.42
3:D:1267:VAL:O	3:D:1268:ASN:HB2	2.19	0.42
5:X:288:MET:HA	5:X:302:PHE:CZ	2.54	0.42
5:X:423:ARG:HG3	5:X:425:TYR:H	1.84	0.42
2:H:68:LEU:HD12	2:H:68:LEU:HA	1.86	0.42
2:H:102:LEU:HB3	2:H:117:ILE:HD11	2.01	0.42
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.18	0.42
2:H:145:ILE:HD11	2:H:506:PHE:CE2	2.54	0.42
2:H:854:ILE:O	2:H:857:VAL:HG22	2.19	0.42
2:H:901:LEU:HD13	5:Y:563:PHE:CE2	2.54	0.42
3:I:105:ILE:HG13	3:I:244:VAL:CG2	2.49	0.42
3:I:909:ILE:HD12	3:I:909:ILE:O	2.20	0.42
5:Y:410:ILE:HD12	5:Y:413:MET:HB3	2.01	0.42
5:Y:462:LYS:O	5:Y:466:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:866:ASP:HA	2:C:872:TYR:CZ	2.54	0.42
2:C:971:LEU:C	2:C:971:LEU:HD13	2.44	0.42
2:C:1314:GLN:HG2	2:C:1315:MET:H	1.84	0.42
3:D:79:LYS:HE3	5:X:568:ASN:C	2.44	0.42
3:D:399:LYS:NZ	3:D:403:ARG:HH11	2.17	0.42
3:D:423:LEU:HB3	3:D:466:MET:HE1	2.00	0.42
3:D:647:PRO:HG3	3:D:697:MET:CA	2.45	0.42
3:D:709:ARG:O	3:D:709:ARG:NH1	2.35	0.42
1:G:77:ASP:O	1:G:81:ILE:HG13	2.18	0.42
2:H:333:ILE:N	2:H:333:ILE:HD12	2.34	0.42
2:H:403:MET:O	2:H:407:ARG:NH1	2.52	0.42
2:H:505:PHE:HD2	2:H:506:PHE:CD1	2.37	0.42
3:I:125:GLY:O	3:I:129:ASP:N	2.52	0.42
3:I:270:ARG:NE	5:Y:449:THR:HG22	2.34	0.42
1:A:47:LEU:HD23	1:A:51:MET:SD	2.59	0.42
1:A:75:GLN:HA	2:C:728:ASP:HA	2.01	0.42
1:A:282:VAL:O	1:A:316:MET:N	2.49	0.42
1:B:27:THR:CG2	1:B:202:VAL:HG22	2.47	0.42
1:B:200:LYS:HG3	1:B:200:LYS:O	2.19	0.42
2:C:52:ALA:O	2:C:53:PHE:HB2	2.20	0.42
2:C:225:PHE:HB2	2:C:336:LEU:HD22	2.02	0.42
3:D:20:ILE:HD11	3:D:1319:PHE:CZ	2.55	0.42
3:D:909:ILE:HD12	3:D:909:ILE:O	2.19	0.42
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.19	0.42
5:X:528:LEU:HD12	5:X:528:LEU:C	2.45	0.42
5:X:543:ALA:O	5:X:547:VAL:HG23	2.19	0.42
1:G:16:ILE:HG12	1:G:26:VAL:HG22	2.02	0.42
2:H:325:LEU:C	2:H:328:SER:HG	2.27	0.42
3:I:139:LEU:C	3:I:139:LEU:HD22	2.45	0.42
3:I:281:ARG:O	3:I:285:LEU:HG	2.20	0.42
3:I:591:ILE:HD12	3:I:591:ILE:C	2.44	0.42
3:I:721:SER:O	3:I:725:MET:HG3	2.20	0.42
3:I:1166:GLY:O	3:I:1176:VAL:HB	2.19	0.42
5:Y:143:TYR:O	5:Y:147:GLN:HG2	2.20	0.42
1:B:65:LEU:HA	1:B:169:GLY:HA2	2.00	0.42
2:C:69:GLN:HE22	2:C:101:ARG:NH2	2.18	0.42
2:C:186:PHE:HA	2:C:195:PHE:O	2.18	0.42
2:C:1042:LEU:HB2	2:C:1043:ALA:H	1.73	0.42
3:D:128:LEU:CD2	3:D:188:LEU:HD22	2.48	0.42
3:D:281:ARG:O	3:D:285:LEU:HG	2.20	0.42
3:D:355:ILE:HA	3:D:447:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:532:GLU:OE1	3:D:578:ILE:HB	2.20	0.42
5:X:132:CYS:SG	5:X:257:LYS:NZ	2.82	0.42
5:X:607:LEU:O	5:X:607:LEU:HD12	2.20	0.42
1:G:47:LEU:CD2	1:G:220:ALA:HB2	2.50	0.42
1:G:200:LYS:HG3	1:G:200:LYS:O	2.20	0.42
2:H:151:ARG:CZ	2:H:156:PHE:HZ	2.33	0.42
2:H:174:ALA:N	2:H:186:PHE:O	2.51	0.42
2:H:360:LEU:HD13	2:H:378:ARG:NH1	2.31	0.42
2:H:367:TYR:HD2	2:H:376:PRO:HG3	1.85	0.42
2:H:488:MET:HB2	2:H:489:PRO:HA	2.01	0.42
2:H:854:ILE:HB	2:H:857:VAL:HG11	2.01	0.42
4:J:5:THR:HB	4:J:7:GLN:HB2	2.02	0.42
1:A:184:ALA:HB2	2:C:1091:GLY:HA2	2.02	0.42
2:C:197:ARG:NH1	2:C:201:ARG:O	2.52	0.42
2:C:685:MET:HE2	2:C:1067:ALA:CB	2.49	0.42
2:C:876:GLU:N	2:C:876:GLU:OE2	2.53	0.42
2:C:890:LYS:HB3	2:C:890:LYS:NZ	2.35	0.42
2:C:1029:LEU:HD12	2:C:1032:LYS:CE	2.50	0.42
2:C:1142:ARG:HH22	2:C:1164:PHE:HB2	1.84	0.42
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.55	0.42
3:D:1190:ILE:HD12	3:D:1190:ILE:N	2.34	0.42
5:X:408:GLY:HA2	5:X:435:ILE:HG23	2.00	0.42
2:H:223:LEU:HD13	2:H:426:ILE:HD13	2.00	0.42
2:H:1278:LEU:HD21	2:H:1286:THR:HG22	2.01	0.42
2:H:1287:LEU:HD23	3:I:1357:ILE:CG1	2.49	0.42
2:H:1293:VAL:HG23	2:H:1301:ARG:HA	2.01	0.42
3:I:545:HIS:HA	3:I:546:ALA:HA	1.79	0.42
1:B:151:GLY:O	1:B:177:TYR:HB2	2.20	0.42
2:C:202:ARG:CZ	2:C:369:MET:HG2	2.50	0.42
2:C:454:ARG:NH1	2:C:462:ASN:OD1	2.53	0.42
2:C:563:THR:HG21	3:D:780:ARG:NE	2.35	0.42
3:D:513:MET:HE2	3:D:513:MET:HB3	1.95	0.42
3:D:708:ASN:HA	3:D:712:GLN:HA	2.01	0.42
3:D:901:ARG:HB2	3:D:907:HIS:O	2.20	0.42
3:D:1292:LEU:HD11	3:I:1284:ARG:NH2	2.34	0.42
5:X:130:VAL:HG13	5:X:365:MET:HG3	2.02	0.42
1:G:217:ILE:HG13	1:G:218:ARG:N	2.35	0.42
2:H:138:ILE:O	2:H:141:THR:OG1	2.35	0.42
2:H:465:ARG:O	2:H:469:VAL:HG23	2.20	0.42
2:H:517:GLN:NE2	2:H:760:ASN:OD1	2.53	0.42
2:H:526:HIS:ND1	2:H:526:HIS:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:557:ARG:HH12	2:H:611:GLU:CD	2.28	0.42
2:H:699:LEU:HD13	2:H:1181:PRO:HB3	2.00	0.42
3:I:40:LYS:HE3	3:I:42:GLU:CG	2.49	0.42
3:I:1149:ARG:HA	3:I:1150:PRO:HD3	1.93	0.42
4:J:12:LYS:HA	4:J:12:LYS:HD3	1.88	0.42
1:A:69:SER:OG	1:A:70:THR:N	2.53	0.42
2:C:367:TYR:CE1	2:C:380:ALA:HB1	2.54	0.42
2:C:678:ARG:O	2:C:681:MET:HB2	2.19	0.42
2:C:800:MET:HE2	2:C:1095:ASP:OD2	2.20	0.42
2:C:843:THR:HB	2:C:845:LEU:HD21	2.02	0.42
2:C:1319:MET:HG3	2:C:1323:PHE:HD2	1.85	0.42
3:D:155:GLU:CD	3:D:158:GLN:HB2	2.44	0.42
3:D:285:LEU:CD1	5:X:410:ILE:HD11	2.50	0.42
3:D:422:LEU:HD22	3:D:484:MET:CE	2.50	0.42
3:D:591:ILE:HD12	3:D:592:VAL:HG13	2.02	0.42
4:E:65:ASP:O	4:E:69:ARG:HG3	2.20	0.42
5:X:43:ASP:HA	5:X:46:GLN:CD	2.45	0.42
2:H:10:ARG:O	2:H:1172:LEU:HA	2.20	0.42
2:H:728:ASP:OD2	2:H:729:ALA:N	2.52	0.42
3:I:41:PRO:HB3	3:I:270:ARG:HG3	2.00	0.42
3:I:139:LEU:HD22	3:I:139:LEU:O	2.19	0.42
3:I:513:MET:HE2	3:I:513:MET:HB3	1.94	0.42
3:I:846:GLU:HA	3:I:858:VAL:HG13	2.02	0.42
5:Y:553:ALA:C	5:Y:555:GLU:H	2.27	0.42
1:A:158:ARG:NH2	1:A:158:ARG:HB2	2.35	0.41
2:C:34:SER:OG	2:C:455:SER:HB2	2.20	0.41
2:C:73:TYR:CG	2:C:74:ARG:N	2.87	0.41
2:C:106:GLU:CB	2:C:107:ARG:HA	2.48	0.41
2:C:106:GLU:CG	2:C:109:ALA:H	2.30	0.41
2:C:218:GLU:CG	2:C:299:LYS:HA	2.49	0.41
2:C:344:GLY:HA2	2:C:345:PRO:HD3	1.85	0.41
2:C:835:GLU:HG3	2:C:1053:TYR:HE1	1.85	0.41
2:C:844:LYS:HB2	2:C:844:LYS:NZ	2.34	0.41
3:D:101:ARG:O	3:D:246:PRO:HG3	2.21	0.41
3:D:145:VAL:CG1	3:D:180:MET:HB3	2.42	0.41
3:D:291:ILE:HD12	5:X:409:ASN:CG	2.45	0.41
3:D:588:PRO:CB	3:D:591:ILE:HD11	2.50	0.41
3:D:670:SER:O	3:D:672:LEU:HD13	2.20	0.41
3:D:905:ARG:HH12	4:E:10:VAL:HG12	1.85	0.41
5:X:291:CYS:O	5:X:297:MET:HB3	2.20	0.41
1:F:53:GLY:HA3	1:F:177:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:911:SER:OG	2:H:913:VAL:HG12	2.20	0.41
2:H:1270:PHE:HB3	2:H:1271:GLY:H	1.59	0.41
3:I:85:CYS:SG	3:I:86:GLU:N	2.93	0.41
3:I:545:HIS:HB2	3:I:546:ALA:CA	2.50	0.41
3:I:670:SER:O	3:I:672:LEU:HD13	2.20	0.41
3:I:1216:ALA:HB3	3:I:1219:ASP:OD1	2.20	0.41
4:J:19:LEU:HD13	4:J:19:LEU:C	2.45	0.41
5:Y:515:GLU:HA	5:Y:516:ASP:HB2	2.01	0.41
5:Y:564:GLY:HA3	5:Y:570:ASP:HB3	2.01	0.41
1:A:135:ASP:OD1	1:A:138:ALA:HB2	2.20	0.41
1:A:166:ARG:HG3	1:A:166:ARG:O	2.20	0.41
2:C:807:TRP:HE1	2:C:1086:PRO:HD3	1.85	0.41
2:C:980:VAL:HG23	2:C:984:VAL:HG13	2.02	0.41
2:C:1163:THR:HG22	2:C:1164:PHE:H	1.86	0.41
2:C:1180:MET:CB	2:C:1181:PRO:HA	2.49	0.41
2:C:1220:GLN:HG2	2:C:1221:PHE:O	2.20	0.41
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.55	0.41
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.55	0.41
3:D:1270:GLY:HA2	3:D:1298:VAL:C	2.45	0.41
3:D:1324:SER:CB	3:D:1348:LYS:HD3	2.50	0.41
5:X:112:THR:HG22	5:X:113:ARG:N	2.33	0.41
5:X:337:VAL:O	5:X:341:LEU:HG	2.21	0.41
2:H:27:LEU:CD1	2:H:528:ARG:HH21	2.19	0.41
2:H:97:ARG:HA	2:H:122:VAL:O	2.20	0.41
2:H:681:MET:CE	2:H:1073:LYS:HE3	2.50	0.41
2:H:843:THR:HG22	2:H:844:LYS:H	1.85	0.41
3:I:392:THR:HG21	5:Y:606:VAL:HG11	2.00	0.41
3:I:1166:GLY:O	3:I:1167:LYS:HB2	2.20	0.41
5:Y:240:ARG:NH1	5:Y:244:THR:HG21	2.35	0.41
5:Y:528:LEU:HD12	5:Y:528:LEU:C	2.46	0.41
1:B:153:VAL:HG21	1:B:177:TYR:CE2	2.55	0.41
2:C:721:GLY:HA3	2:C:779:ARG:N	2.35	0.41
2:C:886:LYS:HB3	2:C:917:SER:HA	2.02	0.41
2:C:898:GLU:OE1	2:C:898:GLU:N	2.43	0.41
2:C:1233:LEU:O	2:C:1233:LEU:HD12	2.20	0.41
3:D:24:LEU:HD23	3:D:232:ASN:HD22	1.86	0.41
3:D:843:VAL:HA	3:D:861:ASN:HA	2.03	0.41
3:D:1170:LYS:O	3:D:1173:ARG:HD2	2.20	0.41
5:X:145:LEU:HD13	5:X:145:LEU:C	2.45	0.41
1:G:98:VAL:HG21	1:G:121:VAL:HG23	2.01	0.41
2:H:396:ASP:CG	2:H:398:SER:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:600:THR:HG22	2:H:601:ASP:N	2.31	0.41
2:H:700:VAL:CG1	2:H:1114:GLU:HG3	2.29	0.41
2:H:764:CYS:HB2	2:H:831:ILE:HB	2.01	0.41
3:I:33:TRP:HB3	3:I:102:MET:HG3	2.01	0.41
3:I:133:ARG:O	3:I:133:ARG:NH2	2.43	0.41
3:I:162:GLU:HG2	3:I:163:GLU:N	2.36	0.41
3:I:1171:GLY:CA	3:I:1172:LYS:C	2.94	0.41
1:A:44:ARG:HA	1:A:183:ILE:HG21	2.02	0.41
1:A:190:ALA:HB2	1:A:200:LYS:CB	2.50	0.41
2:C:57:PHE:HE1	2:C:472:GLU:HA	1.83	0.41
2:C:1328:LYS:HD2	3:D:102:MET:SD	2.60	0.41
6:C:1401:RFP:C35	6:C:1401:RFP:C33	2.98	0.41
3:D:155:GLU:CG	3:D:158:GLN:HB2	2.50	0.41
3:D:707:ILE:HD11	3:D:716:GLN:CD	2.44	0.41
3:D:783:LEU:O	3:D:786:THR:HB	2.21	0.41
3:D:825:VAL:HG23	3:D:835:LEU:HB2	2.00	0.41
5:X:274:ARG:NH1	5:X:369:GLU:OE2	2.52	0.41
5:X:297:MET:HE3	5:X:330:LEU:HD21	2.02	0.41
2:H:56:VAL:HB	2:H:57:PHE:H	1.38	0.41
2:H:106:GLU:CG	2:H:109:ALA:H	2.33	0.41
2:H:408:SER:O	2:H:431:LYS:NZ	2.42	0.41
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.20	0.41
2:H:967:LEU:O	2:H:971:LEU:HB2	2.21	0.41
3:I:475:GLU:HG2	3:I:475:GLU:H	1.70	0.41
3:I:573:THR:HG22	3:I:576:ARG:CD	2.51	0.41
3:I:887:SER:O	3:I:888:CYS:HB3	2.21	0.41
3:I:1171:GLY:HA3	3:I:1172:LYS:C	2.45	0.41
5:Y:470:MET:HG2	5:Y:486:ARG:HH11	1.85	0.41
1:B:58:GLU:HB2	1:B:145:LYS:HB3	2.02	0.41
1:B:222:THR:O	1:B:225:ALA:HB3	2.20	0.41
2:C:22:LEU:HD13	2:C:23:ASP:O	2.21	0.41
2:C:215:TYR:CE1	2:C:223:LEU:HD11	2.55	0.41
2:C:504:GLU:O	2:C:508:SER:HB3	2.20	0.41
2:C:748:ILE:HD12	2:C:748:ILE:C	2.45	0.41
2:C:842:ASP:HB3	2:C:1046:VAL:HG21	2.01	0.41
2:C:1117:LEU:HD13	2:C:1195:ILE:HG12	2.02	0.41
2:C:1321:GLU:C	2:C:1323:PHE:H	2.29	0.41
3:D:147:ILE:CG1	3:D:148:GLU:N	2.83	0.41
3:D:153:ASN:HB2	3:D:172:PHE:CZ	2.56	0.41
3:D:614:LEU:HD23	4:E:7:GLN:HG3	2.02	0.41
3:D:873:GLU:OE2	3:D:877:VAL:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:899:TYR:CE1	3:D:915:ILE:HG23	2.55	0.41
3:D:1292:LEU:HD12	3:D:1292:LEU:N	2.35	0.41
5:X:240:ARG:HB3	5:X:244:THR:HB	2.01	0.41
2:H:10:ARG:CZ	2:H:1171:ARG:HH21	2.32	0.41
2:H:680:LEU:O	2:H:680:LEU:HD23	2.20	0.41
2:H:1313:HIS:CG	4:J:31:GLN:HE22	2.38	0.41
3:I:130:MET:HA	3:I:131:PRO:HD3	1.93	0.41
3:I:473:THR:O	3:I:477:GLN:HG3	2.20	0.41
3:I:504:GLN:HA	3:I:730:ALA:HA	2.01	0.41
3:I:1140:ARG:O	3:I:1144:LEU:HG	2.20	0.41
1:A:200:LYS:HG3	1:A:200:LYS:O	2.20	0.41
1:B:232:VAL:HG12	1:B:233:ASP:O	2.20	0.41
2:C:152:SER:HA	2:C:153:PRO:HD3	1.88	0.41
2:C:384:LEU:HD23	2:C:385:PHE:N	2.35	0.41
2:C:468:LEU:O	2:C:471:VAL:HG22	2.20	0.41
2:C:1087:TYR:HE2	2:C:1215:GLY:CA	2.33	0.41
2:C:1211:ARG:HB2	2:C:1220:GLN:HE21	1.84	0.41
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.90	0.41
3:D:513:MET:CE	3:D:579:LEU:HB2	2.50	0.41
3:D:526:VAL:HG12	3:D:549:LYS:HB2	2.02	0.41
3:D:846:GLU:O	3:D:847:ASP:C	2.63	0.41
5:X:238:LYS:HD3	5:X:242:HIS:HE1	1.86	0.41
5:X:324:LYS:HB3	5:X:325:PRO:HD2	2.01	0.41
2:H:338:THR:OG1	2:H:345:PRO:HG3	2.21	0.41
2:H:514:PHE:HB2	6:H:1401:RFP:C35	2.50	0.41
2:H:958:LYS:HE2	2:H:958:LYS:HB2	1.90	0.41
3:I:19:ALA:HB2	3:I:1343:GLU:CB	2.50	0.41
3:I:644:MET:O	3:I:764:ARG:NH1	2.54	0.41
3:I:681:LYS:O	3:I:685:ILE:HG13	2.21	0.41
3:I:1262:ARG:O	3:I:1280:VAL:HG22	2.21	0.41
1:A:143:ARG:HD2	1:A:143:ARG:N	2.36	0.41
1:A:150:ARG:HB3	1:A:150:ARG:NH1	2.35	0.41
1:A:154:PRO:HD2	1:A:157:THR:OG1	2.21	0.41
1:A:231:PHE:CE2	1:B:43:LEU:HD11	2.55	0.41
1:B:41:ASN:CG	2:C:1217:THR:HA	2.45	0.41
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.60	0.41
3:D:238:ILE:O	3:D:238:ILE:HG13	2.20	0.41
3:D:888:CYS:C	3:D:890:THR:H	2.29	0.41
3:D:921:GLN:O	3:D:925:GLU:HB2	2.21	0.41
5:X:553:ALA:C	5:X:555:GLU:H	2.29	0.41
1:G:67:GLU:HA	1:G:78:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:VAL:HG11	1:G:140:ILE:HD11	2.02	0.41
1:G:181:GLU:HG2	3:I:531:LYS:HD3	2.03	0.41
2:H:894:GLN:O	2:H:895:LEU:HB2	2.20	0.41
3:I:122:SER:HB2	3:I:132:LEU:HD22	2.02	0.41
3:I:260:PHE:O	5:Y:505:ILE:HG22	2.21	0.41
3:I:271:ARG:HH12	3:I:317:THR:HG21	1.86	0.41
3:I:478:LEU:HD12	4:J:47:THR:HG23	2.02	0.41
3:I:759:ILE:CG2	3:I:771:GLN:HG3	2.38	0.41
3:I:873:GLU:H	3:I:873:GLU:HG3	1.65	0.41
5:Y:408:GLY:HA2	5:Y:435:ILE:HG23	2.02	0.41
5:Y:587:ILE:HD12	5:Y:587:ILE:HA	1.93	0.41
1:A:62:ASP:OD1	1:A:143:ARG:NH1	2.42	0.41
1:A:232:VAL:HG13	1:B:218:ARG:NE	2.36	0.41
2:C:145:ILE:HA	2:C:511:LEU:O	2.21	0.41
2:C:290:GLU:OE1	2:C:290:GLU:N	2.52	0.41
2:C:811:ASN:O	2:C:1099:ASN:HB2	2.20	0.41
2:C:914:LYS:HG2	2:C:915:ASP:H	1.85	0.41
2:C:1106:ARG:O	2:C:1108:ASN:N	2.48	0.41
3:D:291:ILE:HD11	5:X:384:LEU:CD2	2.45	0.41
3:D:1171:GLY:HA3	3:D:1172:LYS:C	2.45	0.41
4:E:48:VAL:O	4:E:52:ARG:HG3	2.21	0.41
1:F:219:ARG:O	1:F:223:ILE:HG13	2.20	0.41
2:H:712:SER:HB3	2:H:714:VAL:HG12	2.02	0.41
2:H:1092:THR:HA	2:H:1093:PRO:HD3	1.90	0.41
2:H:1333:LEU:HB2	2:H:1335:ILE:HG22	2.01	0.41
3:I:524:GLY:HA2	3:I:548:VAL:HA	2.01	0.41
3:I:609:TYR:HD1	3:I:610:ARG:HD2	1.85	0.41
3:I:613:GLY:O	3:I:617:THR:OG1	2.29	0.41
3:I:1170:LYS:C	3:I:1173:ARG:HD2	2.45	0.41
3:I:1284:ARG:HA	3:I:1287:ILE:CG1	2.47	0.41
1:A:228:LEU:HD21	1:B:224:LEU:HD23	2.02	0.41
1:A:250:ASP:HB3	1:A:253:LEU:HD13	2.03	0.41
1:B:149:GLY:HA3	1:B:177:TYR:CG	2.55	0.41
2:C:57:PHE:CE1	2:C:472:GLU:HA	2.56	0.41
2:C:60:GLN:O	2:C:61:SER:OG	2.33	0.41
2:C:202:ARG:HD3	5:X:35:ILE:HB	2.03	0.41
2:C:562:GLU:O	2:C:562:GLU:HG3	2.19	0.41
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.56	0.41
2:C:834:GLN:O	2:C:1053:TYR:HA	2.21	0.41
2:C:972:PHE:CA	2:C:975:ILE:HG22	2.49	0.41
2:C:1212:LEU:HG	2:C:1225:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1232:MET:HE2	2:C:1232:MET:HB3	1.95	0.41
2:C:1314:GLN:O	3:D:473:THR:HG23	2.21	0.41
2:C:1315:MET:HE2	3:D:473:THR:OG1	2.21	0.41
2:C:1331:ARG:HG3	3:D:33:TRP:CH2	2.55	0.41
3:D:97:VAL:HG13	3:D:101:ARG:CZ	2.50	0.41
3:D:185:ILE:O	3:D:189:LEU:HG	2.20	0.41
3:D:297:ARG:NH1	5:X:97:PRO:HA	2.35	0.41
3:D:688:ALA:O	3:D:692:ARG:HG2	2.21	0.41
3:D:846:GLU:HA	3:D:858:VAL:HA	2.03	0.41
3:D:1145:PHE:HB3	3:D:1309:ILE:CD1	2.48	0.41
3:D:1171:GLY:HA3	3:D:1172:LYS:CB	2.45	0.41
3:D:1256:ILE:O	3:D:1260:MET:HB2	2.21	0.41
5:X:12:LEU:CD2	5:X:27:VAL:HG11	2.51	0.41
5:X:47:MET:HA	5:X:55:VAL:HG21	2.02	0.41
5:X:290:LEU:CD1	5:X:336:GLU:HB3	2.49	0.41
5:X:532:LEU:C	5:X:532:LEU:HD13	2.45	0.41
1:F:117:HIS:O	1:F:117:HIS:ND1	2.49	0.41
2:H:53:PHE:HZ	2:H:68:LEU:HB3	1.85	0.41
2:H:73:TYR:CD2	2:H:73:TYR:N	2.89	0.41
2:H:163:LYS:H	2:H:163:LYS:CD	2.27	0.41
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.56	0.41
2:H:811:ASN:HA	2:H:815:SER:HB2	2.03	0.41
2:H:870:ILE:HG22	2:H:944:ARG:NH1	2.35	0.41
2:H:933:VAL:HG12	2:H:948:ILE:CD1	2.41	0.41
2:H:1308:ILE:HG21	3:I:379:PRO:HB2	2.03	0.41
2:H:1314:GLN:HA	4:J:28:ARG:NH2	2.35	0.41
3:I:31:ARG:HD2	3:I:104:HIS:CD2	2.56	0.41
3:I:42:GLU:HB3	5:Y:451:ARG:NE	2.36	0.41
3:I:66:LYS:NZ	3:I:66:LYS:HB3	2.35	0.41
3:I:147:ILE:CG1	3:I:148:GLU:N	2.83	0.41
3:I:841:GLY:CA	3:I:901:ARG:HG2	2.50	0.41
3:I:846:GLU:O	3:I:847:ASP:C	2.63	0.41
3:I:888:CYS:C	3:I:890:THR:H	2.29	0.41
3:I:895:CYS:HB3	3:I:898:CYS:SG	2.60	0.41
5:Y:122:ARG:HH22	5:Y:378:GLU:CD	2.29	0.41
5:Y:345:GLN:O	5:Y:349:GLU:HG3	2.21	0.41
5:Y:387:VAL:HG22	5:Y:435:ILE:HD13	2.01	0.41
1:A:14:VAL:HG12	1:A:15:ASP:N	2.36	0.41
1:A:187:VAL:O	1:A:188:GLU:HB2	2.21	0.41
2:C:99:LYS:C	2:C:100:LEU:HD12	2.46	0.41
2:C:213:LEU:HD13	2:C:422:LYS:HB3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:243:PRO:HB3	2:C:277:LEU:HB2	2.03	0.41
2:C:302:ILE:HG22	2:C:309:LEU:CB	2.50	0.41
2:C:1103:VAL:N	2:C:1104:PRO:CD	2.83	0.41
3:D:220:ARG:HG2	3:D:224:LEU:HG	2.02	0.41
3:D:431:ARG:NH2	3:D:493:PRO:HG3	2.35	0.41
3:D:503:SER:O	3:D:507:VAL:HG23	2.21	0.41
3:D:605:LEU:HD22	3:D:620:PHE:CD2	2.56	0.41
3:D:666:GLU:O	3:D:669:GLN:HB3	2.21	0.41
3:D:841:GLY:HA3	3:D:901:ARG:CG	2.51	0.41
3:D:856:ILE:HD12	3:D:857:LEU:H	1.86	0.41
3:D:856:ILE:HD12	3:D:857:LEU:N	2.36	0.41
3:D:1167:LYS:HB3	3:D:1170:LYS:HB2	2.02	0.41
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	2.03	0.41
5:X:108:VAL:HB	5:X:110:LEU:HG	2.02	0.41
1:G:219:ARG:O	1:G:223:ILE:HG13	2.21	0.41
2:H:297:VAL:HB	2:H:317:LEU:HD21	2.04	0.41
2:H:493:ILE:HG13	2:H:493:ILE:O	2.20	0.41
2:H:714:VAL:CG2	2:H:787:PRO:HD2	2.50	0.41
2:H:1205:PRO:O	2:H:1207:SER:N	2.48	0.41
2:H:1329:GLU:O	2:H:1332:SER:HB3	2.21	0.41
3:I:169:LEU:HD22	3:I:176:PHE:CZ	2.56	0.41
3:I:539:SER:O	3:I:541:LEU:N	2.53	0.41
3:I:680:ASN:O	3:I:683:ILE:HB	2.20	0.41
3:I:884:SER:OG	3:I:1254:GLU:OE1	2.37	0.41
5:Y:608:ARG:HB3	5:Y:608:ARG:HH11	1.86	0.41
1:A:227:GLN:NE2	1:B:11:PRO:HD3	2.37	0.40
2:C:49:LEU:HD21	2:C:464:PHE:CD2	2.55	0.40
2:C:81:ASP:OD1	2:C:83:GLN:HG2	2.21	0.40
2:C:153:PRO:HD2	2:C:404:LYS:NZ	2.36	0.40
2:C:876:GLU:HG3	2:C:927:THR:CG2	2.37	0.40
3:D:265:LEU:HD11	3:D:330:MET:SD	2.61	0.40
3:D:500:ILE:H	3:D:500:ILE:CD1	2.31	0.40
5:X:30:HIS:O	5:X:31:LEU:HD23	2.22	0.40
1:F:27:THR:HG22	1:F:202:VAL:HG22	2.03	0.40
1:F:41:ASN:OD1	1:F:185:TYR:OH	2.39	0.40
1:G:32:GLU:HA	1:G:198:LEU:HD22	2.03	0.40
2:H:765:ILE:HA	2:H:787:PRO:CG	2.50	0.40
2:H:805:MET:HE3	3:I:636:GLY:HA2	2.04	0.40
2:H:842:ASP:HB2	2:H:1046:VAL:HG11	2.02	0.40
2:H:845:LEU:HD13	2:H:845:LEU:N	2.33	0.40
2:H:898:GLU:OE1	2:H:898:GLU:N	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1180:MET:CB	2:H:1181:PRO:HA	2.50	0.40
2:H:1241:ASP:N	2:H:1241:ASP:OD2	2.54	0.40
2:H:1305:TYR:HD1	3:I:349:TYR:OH	2.05	0.40
2:H:1332:SER:O	3:I:243:PRO:HG2	2.22	0.40
2:H:1337:ILE:HG22	3:I:22:ILE:HB	2.03	0.40
3:I:697:MET:SD	3:I:742:GLY:N	2.94	0.40
5:Y:311:THR:O	5:Y:341:LEU:HB3	2.21	0.40
5:Y:530:LEU:HD12	5:Y:530:LEU:H	1.85	0.40
1:B:234:LEU:O	1:B:235:ARG:HB2	2.21	0.40
2:C:82:VAL:HG13	2:C:83:GLN:H	1.87	0.40
2:C:106:GLU:HB3	2:C:107:ARG:CA	2.50	0.40
2:C:896:THR:CG2	2:C:897:PRO:HD2	2.51	0.40
2:C:958:LYS:O	2:C:962:GLU:HG2	2.21	0.40
2:C:1204:LEU:HD23	2:C:1205:PRO:HD2	2.01	0.40
3:D:166:LEU:HD12	3:D:167:ASP:N	2.36	0.40
3:D:605:LEU:HD23	3:D:624:ILE:HD13	2.03	0.40
3:D:809:VAL:HG23	3:D:894:VAL:O	2.20	0.40
3:D:873:GLU:H	3:D:873:GLU:HG3	1.67	0.40
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.56	0.40
5:X:49:ASN:CG	5:X:50:ASP:H	2.26	0.40
5:X:147:GLN:O	5:X:151:VAL:HG23	2.20	0.40
5:X:551:LEU:CD2	5:X:597:LYS:HD2	2.51	0.40
1:G:13:LEU:O	1:G:28:LEU:HA	2.21	0.40
1:G:41:ASN:OD1	2:H:1217:THR:HG22	2.22	0.40
1:G:213:PRO:O	1:G:217:ILE:HG12	2.21	0.40
2:H:18:ARG:HE	2:H:18:ARG:HA	1.85	0.40
2:H:148:GLN:HB2	2:H:511:LEU:HD21	2.03	0.40
2:H:205:PRO:O	2:H:208:ILE:HG22	2.21	0.40
2:H:564:PRO:HG3	6:H:1401:RFP:H302	2.02	0.40
2:H:618:GLN:OE1	3:I:769:VAL:HG13	2.21	0.40
2:H:1054:LEU:HD12	2:H:1054:LEU:C	2.46	0.40
3:I:526:VAL:CG1	3:I:549:LYS:HB2	2.52	0.40
3:I:532:GLU:HG2	3:I:577:ALA:HB3	2.02	0.40
3:I:805:GLN:HE21	3:I:805:GLN:HB2	1.67	0.40
5:Y:108:VAL:HG12	5:Y:385:ARG:CZ	2.51	0.40
2:C:213:LEU:HD13	2:C:422:LYS:HB2	2.01	0.40
2:C:395:TYR:CE2	2:C:420:LEU:HG	2.56	0.40
2:C:515:MET:HE3	2:C:527:LYS:CE	2.44	0.40
2:C:622:ASN:OD1	2:C:623:LEU:N	2.54	0.40
2:C:645:PHE:CD2	2:C:645:PHE:C	2.98	0.40
2:C:699:LEU:HB2	2:C:799:ASN:HD21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:722:GLY:N	2:C:734:ILE:HD11	2.35	0.40
2:C:1101:LEU:O	2:C:1104:PRO:HD2	2.22	0.40
3:D:58:CYS:HB3	3:D:61:ILE:HB	2.03	0.40
3:D:293:ARG:NH2	3:D:297:ARG:HE	2.19	0.40
1:F:86:LYS:CE	1:F:173:VAL:HG23	2.51	0.40
1:F:124:VAL:HG11	1:F:209:GLY:HA3	2.03	0.40
2:H:122:VAL:HG13	2:H:124:MET:HG3	2.03	0.40
2:H:578:TYR:CD2	2:H:659:GLN:HA	2.56	0.40
2:H:921:PRO:HG2	2:H:924:VAL:HG21	2.03	0.40
2:H:1013:GLN:HA	2:H:1016:GLU:HB2	2.02	0.40
2:H:1187:PHE:CZ	3:I:772:TYR:HD2	2.35	0.40
2:H:1315:MET:O	2:H:1316:GLU:HB2	2.22	0.40
3:I:83:VAL:HG12	3:I:84:ILE:O	2.22	0.40
3:I:591:ILE:CD1	3:I:592:VAL:HG13	2.51	0.40
3:I:888:CYS:SG	3:I:890:THR:HB	2.61	0.40
3:I:1344:LEU:O	3:I:1350:ASN:ND2	2.55	0.40
2:C:572:ILE:HD13	6:C:1401:RFP:O1	2.21	0.40
2:C:697:LYS:HG3	2:C:698:PRO:HD2	2.04	0.40
2:C:1246:ARG:NE	3:D:348:ASP:OD2	2.40	0.40
2:C:1256:GLN:HG3	2:C:1298:VAL:CG1	2.52	0.40
3:D:230:SER:HB3	3:D:1338:ALA:HA	2.03	0.40
3:D:394:ILE:HG21	5:X:536:THR:HA	2.03	0.40
3:D:432:LEU:HD12	3:D:499:ILE:HG12	2.03	0.40
3:D:483:LEU:HD12	3:D:483:LEU:N	2.36	0.40
3:D:549:LYS:HG2	3:D:571:ASP:OD1	2.21	0.40
3:D:609:TYR:CD1	3:D:610:ARG:HD2	2.53	0.40
1:F:28:LEU:O	1:F:200:LYS:HA	2.21	0.40
1:F:33:ARG:HA	1:F:33:ARG:HD3	1.82	0.40
1:F:77:ASP:O	1:F:81:ILE:HG13	2.21	0.40
2:H:59:ILE:HG12	2:H:65:ASN:O	2.22	0.40
2:H:387:ASN:HB3	2:H:394:ARG:HG3	2.04	0.40
2:H:734:ILE:HG23	2:H:749:ASP:HB2	2.04	0.40
3:I:114:ILE:HG13	3:I:304:ASP:HB3	2.02	0.40
3:I:131:PRO:O	3:I:136:GLU:HG2	2.21	0.40
3:I:262:THR:C	5:Y:507:MET:HG3	2.47	0.40
3:I:412:LEU:O	3:I:416:ILE:HD12	2.22	0.40
3:I:1167:LYS:NZ	3:I:1173:ARG:HH12	2.19	0.40
3:I:1269:ALA:H	3:I:1300:ALA:HB2	1.86	0.40
3:I:1280:VAL:HG21	3:I:1304:ARG:NH2	2.37	0.40
5:Y:250:LEU:O	5:Y:253:SER:HB2	2.21	0.40
1:A:33:ARG:NH1	1:A:199:ASP:OD2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:MET:HA	1:A:52:PRO:HD3	1.81	0.40
1:A:195:ARG:NH2	1:A:198:LEU:HD21	2.35	0.40
2:C:134:GLY:C	2:C:527:LYS:HZ3	2.16	0.40
2:C:590:PRO:CD	2:C:605:TYR:HE1	2.35	0.40
2:C:848:GLU:CD	2:C:888:THR:HG22	2.47	0.40
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.21	0.40
2:C:1054:LEU:HD12	2:C:1054:LEU:C	2.47	0.40
2:C:1335:ILE:HD11	3:D:22:ILE:HG13	2.04	0.40
3:D:316:ILE:HD11	3:D:320:ASN:O	2.21	0.40
5:X:227:GLN:HG3	5:X:252:LEU:HB2	2.02	0.40
5:X:279:ARG:NH2	5:X:350:GLU:OE1	2.54	0.40
2:H:958:LYS:O	2:H:962:GLU:HG2	2.22	0.40
2:H:966:ILE:HG23	2:H:967:LEU:HD12	2.04	0.40
2:H:1132:LEU:HD13	2:H:1174:GLU:OE2	2.21	0.40
3:I:172:PHE:HB3	3:I:175:GLU:OE1	2.22	0.40
3:I:905:ARG:NH2	4:J:16:ARG:HG3	2.36	0.40
4:J:18:ASP:O	4:J:22:VAL:HG12	2.22	0.40
5:Y:296:LYS:HA	5:Y:296:LYS:HD3	1.85	0.40
5:Y:395:THR:HA	5:Y:404:LEU:CD2	2.52	0.40
5:Y:507:MET:C	5:Y:509:THR:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/329 (98%)	254 (79%)	52 (16%)	15 (5%)	2	19
1	B	217/329 (66%)	188 (87%)	23 (11%)	6 (3%)	4	27
1	F	227/329 (69%)	194 (86%)	28 (12%)	5 (2%)	5	31
1	G	213/329 (65%)	188 (88%)	20 (9%)	5 (2%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1333/1342 (99%)	1066 (80%)	225 (17%)	42 (3%)	3	25
2	H	1333/1342 (99%)	1065 (80%)	222 (17%)	46 (4%)	3	23
3	D	1154/1407 (82%)	919 (80%)	193 (17%)	42 (4%)	2	23
3	I	1154/1407 (82%)	925 (80%)	192 (17%)	37 (3%)	3	25
4	E	88/91 (97%)	76 (86%)	7 (8%)	5 (6%)	1	16
4	J	74/91 (81%)	64 (86%)	5 (7%)	5 (7%)	1	14
5	X	511/613 (83%)	444 (87%)	54 (11%)	13 (2%)	4	29
5	Y	454/613 (74%)	410 (90%)	33 (7%)	11 (2%)	4	30
All	All	7079/8222 (86%)	5793 (82%)	1054 (15%)	232 (3%)	3	25

All (232) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	B	20	SER
1	B	52	PRO
2	C	21	VAL
2	C	39	ILE
2	C	43	PRO
2	C	53	PHE
2	C	110	PRO
2	C	114	VAL
2	C	170	VAL
2	C	661	VAL
2	C	669	PRO
2	C	699	LEU
2	C	748	ILE
2	C	993	PRO
2	C	1185	PRO
2	C	1341	ASP
3	D	120	LEU
3	D	155	GLU
3	D	311	ARG
3	D	390	LEU
3	D	404	GLU
3	D	406	ALA
3	D	708	ASN
3	D	721	SER
3	D	901	ARG

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Mol	Chain	Res	Type
3	D	913	GLU
3	D	914	ALA
3	D	1268	ASN
4	E	6	VAL
4	E	35	LYS
5	X	241	SER
5	X	490	PRO
1	F	52	PRO
1	G	52	PRO
1	G	228	LEU
2	H	21	VAL
2	H	39	ILE
2	H	53	PHE
2	H	79	VAL
2	H	110	PRO
2	H	114	VAL
2	H	661	VAL
2	H	748	ILE
2	H	993	PRO
2	H	1185	PRO
2	H	1341	ASP
3	I	108	ALA
3	I	120	LEU
3	I	390	LEU
3	I	404	GLU
3	I	406	ALA
3	I	595	ALA
3	I	710	ASP
3	I	851	PRO
3	I	914	ALA
3	I	1268	ASN
4	J	4	VAL
4	J	6	VAL
4	J	35	LYS
5	Y	241	SER
1	A	93	GLN
1	A	193	GLU
1	A	319	GLU
1	B	19	VAL
2	C	56	VAL
2	C	79	VAL
2	C	437	ASN

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Mol	Chain	Res	Type
2	C	686	GLN
2	C	753	LEU
2	C	1186	VAL
2	C	1236	ASN
2	C	1239	VAL
2	C	1256	GLN
3	D	89	GLY
3	D	255	LEU
3	D	316	ILE
3	D	542	ALA
3	D	590	SER
3	D	595	ALA
3	D	710	ASP
3	D	847	ASP
3	D	851	PRO
3	D	1363	TYR
4	E	4	VAL
5	X	581	ASP
2	H	56	VAL
2	H	78	PRO
2	H	170	VAL
2	H	437	ASN
2	H	535	PRO
2	H	669	PRO
2	H	753	LEU
2	H	1046	VAL
2	H	1186	VAL
2	H	1236	ASN
2	H	1239	VAL
3	I	89	GLY
3	I	153	ASN
3	I	155	GLU
3	I	417	ARG
3	I	542	ALA
3	I	590	SER
3	I	707	ILE
3	I	708	ASN
3	I	721	SER
3	I	847	ASP
3	I	901	ARG
3	I	913	GLU
3	I	1195	GLN

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Mol	Chain	Res	Type
5	Y	491	GLU
1	A	14	VAL
1	A	201	LEU
2	C	78	PRO
2	C	1003	THR
2	C	1046	VAL
2	C	1240	ASP
3	D	53	ARG
3	D	108	ALA
3	D	210	SER
3	D	417	ARG
3	D	559	ALA
3	D	1195	GLN
5	X	50	ASP
5	X	108	VAL
5	X	308	GLY
5	X	514	ASP
5	X	600	HIS
1	F	33	ARG
1	G	188	GLU
3	I	53	ARG
3	I	210	SER
3	I	559	ALA
3	I	1344	LEU
3	I	1363	TYR
5	Y	308	GLY
5	Y	490	PRO
5	Y	504	PRO
5	Y	515	GLU
1	A	166	ARG
1	A	188	GLU
1	B	188	GLU
1	B	235	ARG
2	C	908	GLU
2	C	1080	ASN
2	C	1093	PRO
2	C	1139	ALA
2	C	1315	MET
3	D	707	ILE
3	D	855	ASP
3	D	1344	LEU
4	E	5	THR

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Mol	Chain	Res	Type
5	X	23	THR
5	X	491	GLU
5	X	504	PRO
1	F	153	VAL
1	F	166	ARG
1	G	177	TYR
2	H	43	PRO
2	H	487	LEU
2	H	699	LEU
2	H	895	LEU
2	H	908	GLU
2	H	1003	THR
2	H	1080	ASN
2	H	1093	PRO
2	H	1139	ALA
2	H	1240	ASP
2	H	1256	GLN
2	H	1315	MET
3	I	255	LEU
3	I	855	ASP
4	J	5	THR
5	Y	108	VAL
5	Y	514	ASP
5	Y	581	ASP
1	A	117	HIS
1	A	196	THR
1	A	232	VAL
1	A	322	PRO
2	C	740	GLU
3	D	811	GLU
3	D	902	ASP
3	D	1174	ARG
1	F	188	GLU
2	H	488	MET
2	H	543	ALA
2	H	740	GLU
2	H	746	ALA
2	H	812	PHE
5	Y	600	HIS
1	B	49	SER
2	C	69	GLN
2	C	143	ARG

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Mol	Chain	Res	Type
2	C	746	ALA
2	C	812	PHE
2	C	895	LEU
2	C	1237	HIS
3	D	153	ASN
3	D	728	SER
3	D	850	LYS
3	D	888	CYS
3	D	1173	ARG
4	E	59	ILE
1	G	49	SER
2	H	13	LYS
2	H	104	ILE
2	H	739	ASP
3	I	850	LYS
3	I	1174	ARG
3	I	1194	ARG
4	J	59	ILE
1	A	153	VAL
2	C	104	ILE
5	X	20	GLY
2	C	373	GLY
5	X	35	ILE
2	H	373	GLY
2	H	736	VAL
3	I	706	VAL
3	I	1339	GLY
1	A	187	VAL
3	D	742	GLY
3	D	1339	GLY
3	I	540	GLY
1	A	151	GLY
3	D	706	VAL
3	I	471	PRO
5	Y	564	GLY
2	H	489	PRO
2	H	1181	PRO
2	C	1181	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/286 (98%)	270 (96%)	11 (4%)	28	52
1	B	189/286 (66%)	185 (98%)	4 (2%)	47	65
1	F	197/286 (69%)	191 (97%)	6 (3%)	36	57
1	G	185/286 (65%)	180 (97%)	5 (3%)	39	60
2	C	1150/1157 (99%)	1073 (93%)	77 (7%)	15	41
2	H	1150/1157 (99%)	1075 (94%)	75 (6%)	15	42
3	D	971/1168 (83%)	902 (93%)	69 (7%)	13	40
3	I	971/1168 (83%)	904 (93%)	67 (7%)	14	41
4	E	74/75 (99%)	70 (95%)	4 (5%)	20	46
4	J	65/75 (87%)	61 (94%)	4 (6%)	16	43
5	X	460/540 (85%)	443 (96%)	17 (4%)	30	54
5	Y	407/540 (75%)	387 (95%)	20 (5%)	22	48
All	All	6100/7024 (87%)	5741 (94%)	359 (6%)	18	44

All (359) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	79	LEU
1	A	88	LEU
1	A	101	THR
1	A	117	HIS
1	A	158	ARG
1	A	239	GLN
1	A	243	LYS
1	A	246	LYS
1	A	262	LEU
1	A	318	LEU
1	B	13	LEU
1	B	37	HIS
1	B	182	ARG

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Mol	Chain	Res	Type
1	B	228	LEU
2	C	15	PHE
2	C	18	ARG
2	C	32	LEU
2	C	37	LYS
2	C	39	ILE
2	C	41	GLN
2	C	56	VAL
2	C	70	TYR
2	C	73	TYR
2	C	80	PHE
2	C	82	VAL
2	C	88	ARG
2	C	98	VAL
2	C	117	ILE
2	C	121	GLU
2	C	127	ILE
2	C	133	ASN
2	C	161	LYS
2	C	163	LYS
2	C	203	LYS
2	C	479	LEU
2	C	487	LEU
2	C	524	ILE
2	C	550	VAL
2	C	600	THR
2	C	603	ILE
2	C	645	PHE
2	C	650	VAL
2	C	661	VAL
2	C	690	VAL
2	C	693	LEU
2	C	700	VAL
2	C	704	MET
2	C	711	ASP
2	C	740	GLU
2	C	773	LEU
2	C	800	MET
2	C	817	LEU
2	C	844	LYS
2	C	845	LEU
2	C	890	LYS

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Mol	Chain	Res	Type
2	C	908	GLU
2	C	909	LYS
2	C	920	VAL
2	C	941	LYS
2	C	944	ARG
2	C	964	LEU
2	C	975	ILE
2	C	988	LYS
2	C	1002	LEU
2	C	1010	GLN
2	C	1017	GLN
2	C	1027	LYS
2	C	1032	LYS
2	C	1042	LEU
2	C	1060	ILE
2	C	1097	VAL
2	C	1106	ARG
2	C	1119	MET
2	C	1141	LEU
2	C	1146	GLN
2	C	1158	LYS
2	C	1180	MET
2	C	1209	GLN
2	C	1211	ARG
2	C	1233	LEU
2	C	1248	THR
2	C	1259	LEU
2	C	1262	LYS
2	C	1264	GLN
2	C	1265	PHE
2	C	1276	TRP
2	C	1288	GLN
2	C	1291	LEU
2	C	1336	ASN
2	C	1339	LEU
2	C	1341	ASP
3	D	9	LYS
3	D	13	LYS
3	D	50	LYS
3	D	66	LYS
3	D	74	LYS
3	D	92	VAL

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Mol	Chain	Res	Type
3	D	114	ILE
3	D	117	LEU
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	155	GLU
3	D	158	GLN
3	D	169	LEU
3	D	175	GLU
3	D	179	LYS
3	D	185	ILE
3	D	188	LEU
3	D	235	GLU
3	D	239	LEU
3	D	250	ARG
3	D	309	ASN
3	D	324	LEU
3	D	416	ILE
3	D	422	LEU
3	D	442	ILE
3	D	475	GLU
3	D	500	ILE
3	D	505	ASP
3	D	508	LEU
3	D	521	LYS
3	D	523	GLU
3	D	527	LEU
3	D	531	LYS
3	D	532	GLU
3	D	538	ARG
3	D	541	LEU
3	D	571	ASP
3	D	594	GLN
3	D	605	LEU
3	D	681	LYS
3	D	707	ILE
3	D	713	GLU
3	D	771	GLN
3	D	805	GLN
3	D	809	VAL
3	D	816	THR
3	D	826	ILE

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Mol	Chain	Res	Type
3	D	832	LYS
3	D	847	ASP
3	D	864	LEU
3	D	867	GLN
3	D	873	GLU
3	D	882	VAL
3	D	909	ILE
3	D	911	LYS
3	D	918	ILE
3	D	932	MET
3	D	933	ARG
3	D	1134	ILE
3	D	1148	ARG
3	D	1155	ILE
3	D	1188	GLU
3	D	1226	VAL
3	D	1247	LYS
3	D	1256	ILE
3	D	1257	VAL
3	D	1297	LYS
3	D	1306	LEU
4	E	4	VAL
4	E	6	VAL
4	E	13	ILE
4	E	73	GLN
5	X	21	TYR
5	X	23	THR
5	X	28	ASN
5	X	54	GLN
5	X	98	VAL
5	X	136	GLU
5	X	266	PHE
5	X	355	ILE
5	X	379	MET
5	X	384	LEU
5	X	452	ILE
5	X	457	ILE
5	X	473	GLU
5	X	545	HIS
5	X	562	ARG
5	X	582	VAL
5	X	607	LEU

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Mol	Chain	Res	Type
1	F	37	HIS
1	F	77	ASP
1	F	88	LEU
1	F	158	ARG
1	F	160	HIS
1	F	234	LEU
1	G	13	LEU
1	G	37	HIS
1	G	77	ASP
1	G	88	LEU
1	G	127	GLN
2	H	9	LYS
2	H	15	PHE
2	H	18	ARG
2	H	37	LYS
2	H	42	ASP
2	H	46	GLN
2	H	56	VAL
2	H	73	TYR
2	H	80	PHE
2	H	82	VAL
2	H	88	ARG
2	H	98	VAL
2	H	99	LYS
2	H	117	ILE
2	H	127	ILE
2	H	161	LYS
2	H	203	LYS
2	H	311	CYS
2	H	379	GLU
2	H	479	LEU
2	H	529	ARG
2	H	539	THR
2	H	550	VAL
2	H	600	THR
2	H	603	ILE
2	H	645	PHE
2	H	661	VAL
2	H	663	VAL
2	H	690	VAL
2	H	700	VAL
2	H	704	MET

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Mol	Chain	Res	Type
2	H	711	ASP
2	H	740	GLU
2	H	765	ILE
2	H	773	LEU
2	H	791	LEU
2	H	800	MET
2	H	817	LEU
2	H	844	LYS
2	H	845	LEU
2	H	890	LYS
2	H	909	LYS
2	H	920	VAL
2	H	953	LEU
2	H	964	LEU
2	H	971	LEU
2	H	975	ILE
2	H	988	LYS
2	H	1002	LEU
2	H	1005	GLU
2	H	1010	GLN
2	H	1017	GLN
2	H	1027	LYS
2	H	1032	LYS
2	H	1042	LEU
2	H	1060	ILE
2	H	1097	VAL
2	H	1119	MET
2	H	1141	LEU
2	H	1158	LYS
2	H	1180	MET
2	H	1209	GLN
2	H	1210	ILE
2	H	1211	ARG
2	H	1233	LEU
2	H	1239	VAL
2	H	1248	THR
2	H	1262	LYS
2	H	1264	GLN
2	H	1276	TRP
2	H	1288	GLN
2	H	1291	LEU
2	H	1326	LEU

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Mol	Chain	Res	Type
2	H	1339	LEU
2	H	1341	ASP
3	I	9	LYS
3	I	31	ARG
3	I	50	LYS
3	I	66	LYS
3	I	74	LYS
3	I	92	VAL
3	I	114	ILE
3	I	117	LEU
3	I	133	ARG
3	I	139	LEU
3	I	140	TYR
3	I	141	PHE
3	I	151	MET
3	I	155	GLU
3	I	158	GLN
3	I	169	LEU
3	I	179	LYS
3	I	185	ILE
3	I	188	LEU
3	I	235	GLU
3	I	250	ARG
3	I	301	GLU
3	I	316	ILE
3	I	325	LYS
3	I	416	ILE
3	I	442	ILE
3	I	475	GLU
3	I	500	ILE
3	I	516	ASP
3	I	521	LYS
3	I	523	GLU
3	I	527	LEU
3	I	531	LYS
3	I	532	GLU
3	I	538	ARG
3	I	541	LEU
3	I	571	ASP
3	I	594	GLN
3	I	605	LEU
3	I	681	LYS

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Mol	Chain	Res	Type
3	I	707	ILE
3	I	771	GLN
3	I	805	GLN
3	I	809	VAL
3	I	816	THR
3	I	826	ILE
3	I	832	LYS
3	I	847	ASP
3	I	856	ILE
3	I	864	LEU
3	I	867	GLN
3	I	873	GLU
3	I	882	VAL
3	I	909	ILE
3	I	911	LYS
3	I	918	ILE
3	I	932	MET
3	I	933	ARG
3	I	1134	ILE
3	I	1148	ARG
3	I	1155	ILE
3	I	1226	VAL
3	I	1247	LYS
3	I	1256	ILE
3	I	1297	LYS
3	I	1306	LEU
3	I	1366	HIS
4	J	4	VAL
4	J	6	VAL
4	J	13	ILE
4	J	73	GLN
5	Y	98	VAL
5	Y	136	GLU
5	Y	262	VAL
5	Y	266	PHE
5	Y	355	ILE
5	Y	371	LYS
5	Y	379	MET
5	Y	384	LEU
5	Y	452	ILE
5	Y	457	ILE
5	Y	473	GLU

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Mol	Chain	Res	Type
5	Y	515	GLU
5	Y	517	SER
5	Y	545	HIS
5	Y	560	ARG
5	Y	562	ARG
5	Y	565	ILE
5	Y	582	VAL
5	Y	589	GLN
5	Y	607	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	23	HIS
1	A	75	GLN
1	A	84	ASN
1	A	227	GLN
1	A	239	GLN
1	B	66	HIS
1	B	84	ASN
1	B	147	GLN
2	C	69	GLN
2	C	133	ASN
2	C	139	ASN
2	C	238	GLN
2	C	273	HIS
2	C	314	ASN
2	C	437	ASN
2	C	450	ASN
2	C	517	GLN
2	C	518	ASN
2	C	573	ASN
2	C	582	ASN
2	C	673	HIS
2	C	684	ASN
2	C	725	GLN
2	C	760	ASN
2	C	799	ASN
2	C	808	ASN
2	C	922	ASN
2	C	952	GLN

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Mol	Chain	Res	Type
2	C	955	GLN
2	C	1010	GLN
2	C	1017	GLN
2	C	1072	ASN
2	C	1134	GLN
2	C	1146	GLN
2	C	1175	ASN
2	C	1220	GLN
2	C	1236	ASN
2	C	1264	GLN
3	D	164	GLN
3	D	209	ASN
3	D	294	ASN
3	D	309	ASN
3	D	419	HIS
3	D	477	GLN
3	D	519	ASN
3	D	545	HIS
3	D	680	ASN
3	D	690	ASN
3	D	739	GLN
3	D	792	ASN
3	D	875	ASN
3	D	910	ASN
3	D	1197	ASN
3	D	1268	ASN
3	D	1350	ASN
3	D	1366	HIS
4	E	31	GLN
5	X	8	GLN
5	X	28	ASN
5	X	30	HIS
5	X	46	GLN
5	X	54	GLN
5	X	242	HIS
5	X	283	GLN
5	X	301	ASN
5	X	317	ASN
5	X	342	GLN
5	X	345	GLN
5	X	406	GLN
5	X	437	GLN

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Mol	Chain	Res	Type
5	X	446	GLN
5	X	455	HIS
1	F	23	HIS
1	F	66	HIS
1	F	84	ASN
1	G	66	HIS
2	H	46	GLN
2	H	69	GLN
2	H	133	ASN
2	H	238	GLN
2	H	510	GLN
2	H	513	GLN
2	H	517	GLN
2	H	573	ASN
2	H	582	ASN
2	H	628	HIS
2	H	684	ASN
2	H	686	GLN
2	H	725	GLN
2	H	761	GLN
2	H	799	ASN
2	H	834	GLN
2	H	894	GLN
2	H	965	GLN
2	H	1072	ASN
2	H	1116	HIS
2	H	1134	GLN
2	H	1175	ASN
2	H	1236	ASN
2	H	1264	GLN
2	H	1288	GLN
2	H	1313	HIS
3	I	153	ASN
3	I	164	GLN
3	I	209	ASN
3	I	300	GLN
3	I	477	GLN
3	I	488	ASN
3	I	489	ASN
3	I	504	GLN
3	I	519	ASN
3	I	623	GLN

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Mol	Chain	Res	Type
3	I	680	ASN
3	I	1268	ASN
3	I	1350	ASN
4	J	15	ASN
4	J	31	GLN
5	Y	128	ASN
5	Y	242	HIS
5	Y	301	ASN
5	Y	331	HIS
5	Y	342	GLN
5	Y	400	GLN
5	Y	437	GLN
5	Y	455	HIS
5	Y	469	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](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	RFP	H	1401	-	63,63,63	2.20	10 (15%)	94,94,94	1.92	26 (27%)
6	RFP	C	1401	-	63,63,63	2.15	11 (17%)	94,94,94	2.28	28 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	RFP	H	1401	-	-	18/60/85/85	0/5/5/5
6	RFP	C	1401	-	-	39/60/85/85	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	RFP	O3-C6	10.86	1.57	1.37
6	H	1401	RFP	O3-C6	10.74	1.57	1.37
6	H	1401	RFP	C15-N1	6.97	1.50	1.35
6	C	1401	RFP	C15-N1	6.31	1.48	1.35
6	C	1401	RFP	C12-C11	-4.58	1.36	1.54
6	H	1401	RFP	C12-C11	-4.53	1.36	1.54
6	C	1401	RFP	C18-C17	4.06	1.55	1.43
6	H	1401	RFP	C3-C43	3.98	1.55	1.46
6	H	1401	RFP	O7-C25	-3.71	1.39	1.44
6	H	1401	RFP	C18-C17	3.52	1.54	1.43
6	C	1401	RFP	C3-C43	3.28	1.53	1.46
6	C	1401	RFP	O7-C35	3.26	1.42	1.35
6	C	1401	RFP	O7-C25	-3.02	1.40	1.44
6	H	1401	RFP	C2-N1	2.69	1.48	1.43
6	H	1401	RFP	O7-C35	2.56	1.40	1.35
6	H	1401	RFP	C43-N2	2.55	1.34	1.27
6	C	1401	RFP	C17-C16	2.46	1.41	1.34
6	C	1401	RFP	C18-C19	2.34	1.42	1.33
6	C	1401	RFP	C43-N2	2.25	1.33	1.27
6	H	1401	RFP	O6-C27	-2.24	1.38	1.43
6	C	1401	RFP	C2-N1	2.14	1.47	1.43

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	RFP	C2-C3-C43	-8.46	115.01	123.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	RFP	O7-C35-C36	5.63	121.14	111.09
6	C	1401	RFP	O4-C11-C5	-5.21	122.02	131.63
6	H	1401	RFP	C17-C18-C19	-5.10	112.60	124.43
6	C	1401	RFP	C37-O6-C27	5.01	124.47	112.99
6	H	1401	RFP	O4-C11-C5	-5.01	122.40	131.63
6	C	1401	RFP	C12-C11-C5	4.83	116.64	107.30
6	H	1401	RFP	O7-C35-C36	4.72	119.51	111.09
6	H	1401	RFP	C41-N3-N2	4.67	138.52	113.99
6	C	1401	RFP	C38-N4-C42	4.46	119.14	110.63
6	C	1401	RFP	C41-N3-N2	4.42	137.21	113.99
6	C	1401	RFP	C3-C2-N1	-4.28	112.00	119.33
6	C	1401	RFP	C38-N4-C39	4.26	118.76	110.63
6	H	1401	RFP	C41-C42-N4	4.08	117.42	110.86
6	H	1401	RFP	C38-N4-C39	4.07	118.39	110.63
6	C	1401	RFP	C40-N3-N2	-3.83	93.88	113.99
6	C	1401	RFP	C3-C2-C1	3.81	123.39	120.68
6	H	1401	RFP	C12-C11-C5	3.81	114.67	107.30
6	H	1401	RFP	C38-N4-C42	3.49	117.28	110.63
6	H	1401	RFP	C25-O7-C35	3.48	123.13	117.72
6	C	1401	RFP	C17-C16-C15	-3.48	110.58	120.83
6	C	1401	RFP	O7-C25-C26	3.45	115.47	107.52
6	C	1401	RFP	C3-C43-N2	-3.43	115.97	121.58
6	H	1401	RFP	C30-C16-C17	-3.43	115.33	123.67
6	H	1401	RFP	C2-C3-C43	-3.40	120.38	123.99
6	C	1401	RFP	C5-C10-C9	-3.27	114.30	119.77
6	H	1401	RFP	C12-O3-C6	-3.19	102.36	107.69
6	C	1401	RFP	C13-C12-C11	-3.17	106.10	113.90
6	C	1401	RFP	C25-O7-C35	3.04	122.45	117.72
6	H	1401	RFP	C5-C10-C9	-3.03	114.69	119.77
6	H	1401	RFP	C12-O5-C29	2.80	124.72	117.84
6	C	1401	RFP	C23-C22-C21	-2.80	106.95	112.55
6	H	1401	RFP	C37-O6-C27	2.72	119.21	112.99
6	H	1401	RFP	C32-C22-C23	-2.71	106.11	111.43
6	C	1401	RFP	O8-C35-C36	-2.68	115.28	124.77
6	H	1401	RFP	C3-C2-N1	-2.66	114.78	119.33
6	C	1401	RFP	C18-C17-C16	-2.62	119.23	126.64
6	H	1401	RFP	C31-C20-C19	-2.56	104.11	109.91
6	H	1401	RFP	O3-C6-C7	2.55	125.48	121.16
6	C	1401	RFP	O3-C6-C5	-2.55	106.59	113.56
6	C	1401	RFP	O3-C6-C7	2.53	125.45	121.16
6	C	1401	RFP	O5-C12-C13	2.46	113.34	106.98
6	H	1401	RFP	C40-N3-N2	-2.44	101.14	113.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	RFP	C17-C18-C19	-2.40	118.86	124.43
6	H	1401	RFP	C26-C27-C28	2.35	117.19	112.11
6	H	1401	RFP	O3-C6-C5	-2.31	107.25	113.56
6	H	1401	RFP	C41-N3-C40	2.27	120.07	113.44
6	C	1401	RFP	C31-C20-C19	-2.21	104.91	109.91
6	H	1401	RFP	C42-N4-C39	2.19	113.03	109.54
6	C	1401	RFP	C30-C16-C17	-2.14	118.46	123.67
6	H	1401	RFP	C4-C3-C43	2.09	119.31	116.63
6	C	1401	RFP	C8-C9-C10	2.06	123.58	119.41
6	H	1401	RFP	C17-C16-C15	-2.06	114.76	120.83
6	C	1401	RFP	O6-C27-C26	2.02	112.13	107.97

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1401	RFP	C4-C3-C43-N2
6	C	1401	RFP	C17-C18-C19-C20
6	C	1401	RFP	C23-C24-C25-C26
6	C	1401	RFP	C23-C24-C25-O7
6	C	1401	RFP	C33-C24-C25-C26
6	C	1401	RFP	C33-C24-C25-O7
6	C	1401	RFP	O7-C25-C26-C27
6	C	1401	RFP	O7-C25-C26-C34
6	C	1401	RFP	C26-C27-C28-C29
6	C	1401	RFP	C26-C27-O6-C37
6	C	1401	RFP	C28-C27-O6-C37
6	C	1401	RFP	C43-N2-N3-C40
6	C	1401	RFP	C43-N2-N3-C41
6	H	1401	RFP	C4-C3-C43-N2
6	H	1401	RFP	C13-C12-O5-C29
6	H	1401	RFP	C15-C16-C17-C18
6	C	1401	RFP	C36-C35-O7-C25
6	H	1401	RFP	C3-C2-N1-C15
6	H	1401	RFP	C3-C43-N2-N3
6	C	1401	RFP	C3-C2-N1-C15
6	C	1401	RFP	C3-C43-N2-N3
6	H	1401	RFP	C18-C19-C20-C31
6	C	1401	RFP	C21-C22-C23-O9
6	C	1401	RFP	C32-C22-C23-O9
6	C	1401	RFP	C32-C22-C23-C24
6	C	1401	RFP	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
6	H	1401	RFP	C1-C2-N1-C15
6	C	1401	RFP	C24-C25-C26-C34
6	C	1401	RFP	C24-C25-C26-C27
6	H	1401	RFP	C26-C27-C28-C29
6	C	1401	RFP	C2-C3-C43-N2
6	C	1401	RFP	O10-C21-C22-C23
6	C	1401	RFP	C15-C16-C17-C18
6	C	1401	RFP	O10-C21-C22-C32
6	C	1401	RFP	O11-C15-C16-C30
6	C	1401	RFP	C24-C25-O7-C35
6	H	1401	RFP	C33-C24-C25-C26
6	C	1401	RFP	C27-C28-C29-O5
6	H	1401	RFP	C27-C28-C29-O5
6	C	1401	RFP	O6-C27-C28-C29
6	H	1401	RFP	C11-C12-O5-C29
6	H	1401	RFP	O3-C12-O5-C29
6	C	1401	RFP	C1-C2-N1-C15
6	C	1401	RFP	N1-C15-C16-C30
6	C	1401	RFP	C26-C25-O7-C35
6	C	1401	RFP	C20-C21-C22-C32
6	C	1401	RFP	C22-C23-C24-C33
6	H	1401	RFP	C23-C24-C25-C26
6	C	1401	RFP	O9-C23-C24-C33
6	H	1401	RFP	C33-C24-C25-O7
6	H	1401	RFP	C21-C22-C23-C24
6	C	1401	RFP	C28-C29-O5-C12
6	H	1401	RFP	C28-C29-O5-C12
6	C	1401	RFP	C20-C21-C22-C23
6	C	1401	RFP	N1-C15-C16-C17
6	H	1401	RFP	C17-C18-C19-C20
6	H	1401	RFP	C23-C24-C25-O7

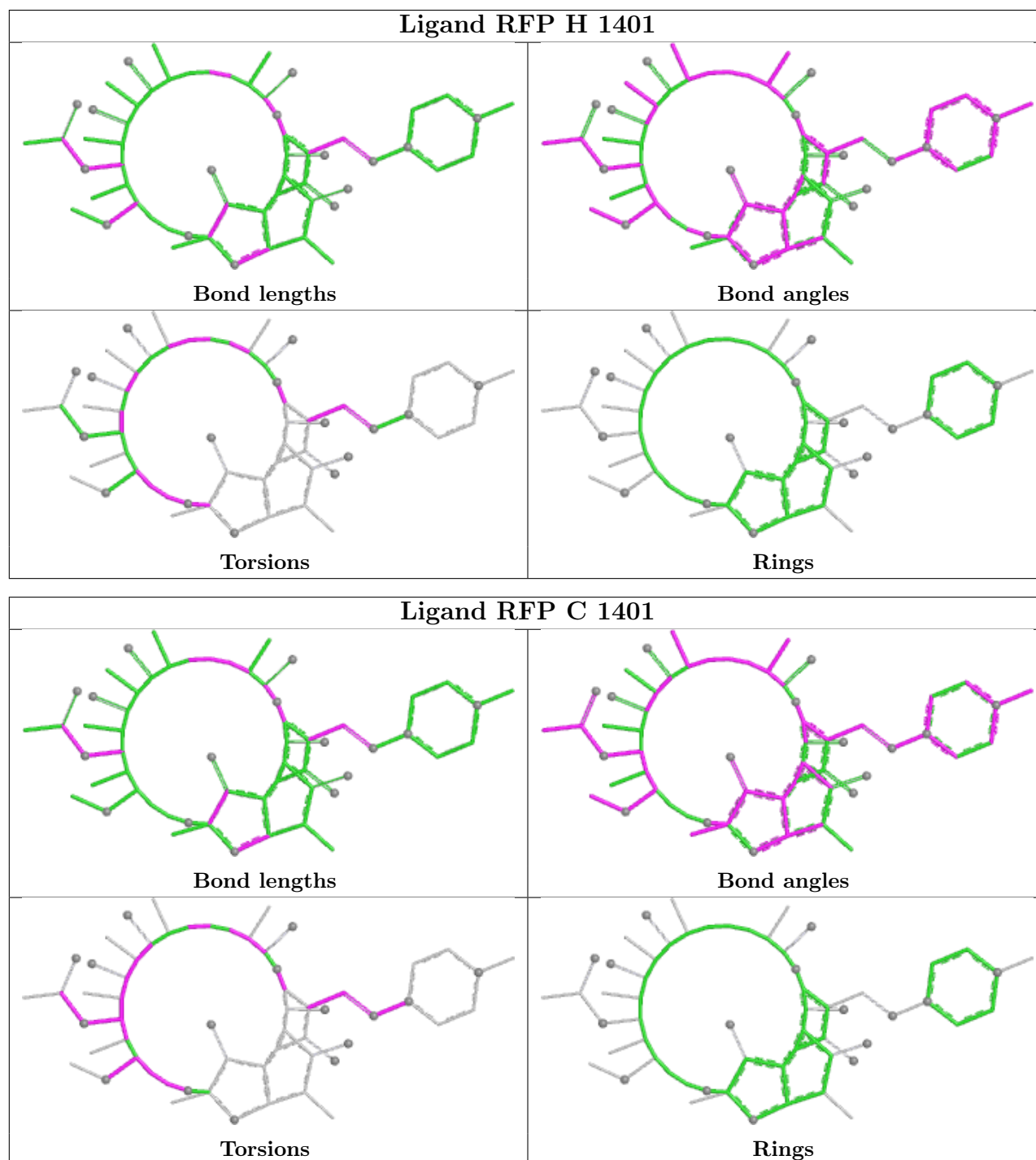
There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1401	RFP	14	0
6	C	1401	RFP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/329 (98%)	-0.56	1 (0%) 90 77	0, 73, 165, 263	0
1	B	221/329 (67%)	-0.32	1 (0%) 87 71	3, 97, 189, 266	0
1	F	229/329 (69%)	-0.33	3 (1%) 75 53	16, 121, 201, 266	0
1	G	217/329 (65%)	-0.37	5 (2%) 61 43	39, 111, 186, 215	0
2	C	1335/1342 (99%)	-0.49	4 (0%) 90 77	0, 48, 166, 284	0
2	H	1335/1342 (99%)	-0.51	2 (0%) 92 87	1, 86, 201, 341	0
3	D	1160/1407 (82%)	-0.50	1 (0%) 92 87	0, 40, 157, 284	0
3	I	1160/1407 (82%)	-0.47	4 (0%) 90 77	1, 52, 180, 322	0
4	E	90/91 (98%)	-0.62	0 100 100	0, 40, 109, 159	0
4	J	76/91 (83%)	-0.54	1 (1%) 75 53	5, 76, 155, 167	0
5	X	517/613 (84%)	-0.51	3 (0%) 85 68	3, 99, 228, 365	0
5	Y	458/613 (74%)	-0.50	1 (0%) 91 81	2, 102, 219, 328	0
All	All	7121/8222 (86%)	-0.49	26 (0%) 88 74	0, 70, 190, 365	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	59	VAL	4.5
5	Y	337	VAL	4.0
3	I	637	ALA	3.5
1	G	39	LEU	3.4
5	X	56	MET	3.2
2	C	194	LEU	3.1
1	B	50	SER	3.1
3	I	1215	GLU	3.0
1	F	110	VAL	2.9
2	H	1225	VAL	2.9
1	F	82	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
5	X	319	ALA	2.6
2	C	783	LEU	2.5
3	I	453	VAL	2.4
1	G	171	LEU	2.3
2	H	52	ALA	2.2
3	D	1273	ASP	2.1
3	I	333	GLY	2.1
2	C	52	ALA	2.1
5	X	497	VAL	2.1
1	G	51	MET	2.1
1	G	43	LEU	2.1
2	C	1334	GLY	2.0
1	F	39	LEU	2.0
1	A	320	ASN	2.0
4	J	2	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

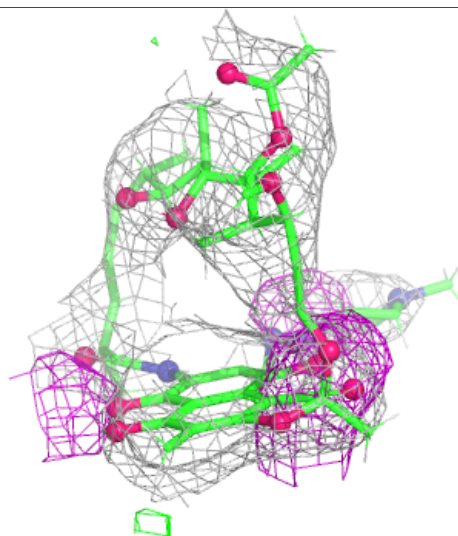
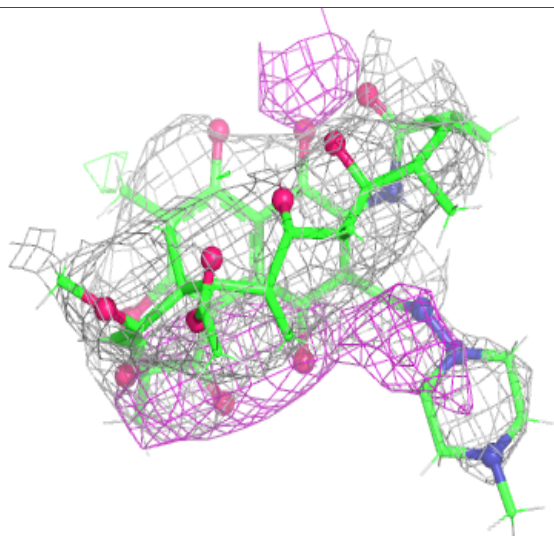
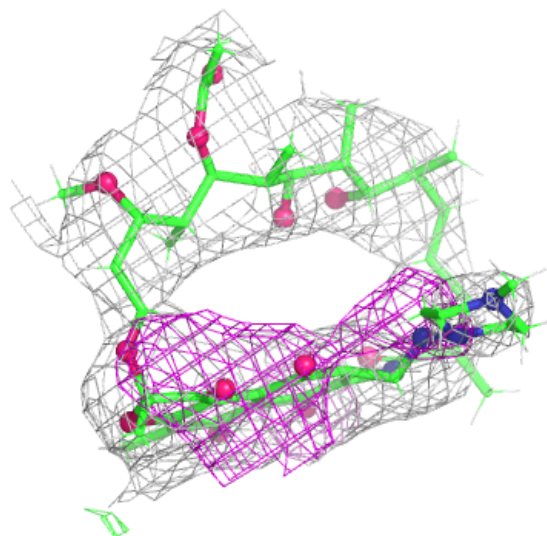
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	RFP	C	1401	59/59	0.82	0.09	20,20,20,20	0
6	RFP	H	1401	59/59	0.84	0.09	20,20,20,20	0
8	MG	I	1503	1/1	0.92	0.18	20,20,20,20	0
8	MG	D	1503	1/1	0.97	0.05	24,24,24,24	0
7	ZN	I	1502	1/1	0.98	0.08	49,49,49,49	0
7	ZN	I	1501	1/1	0.99	0.02	60,60,60,60	0
7	ZN	D	1501	1/1	1.00	0.02	54,54,54,54	0
7	ZN	D	1502	1/1	1.00	0.04	8,8,8,8	0

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

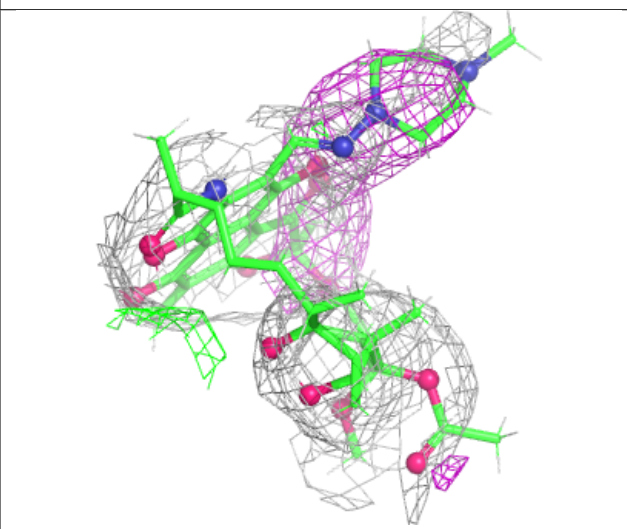
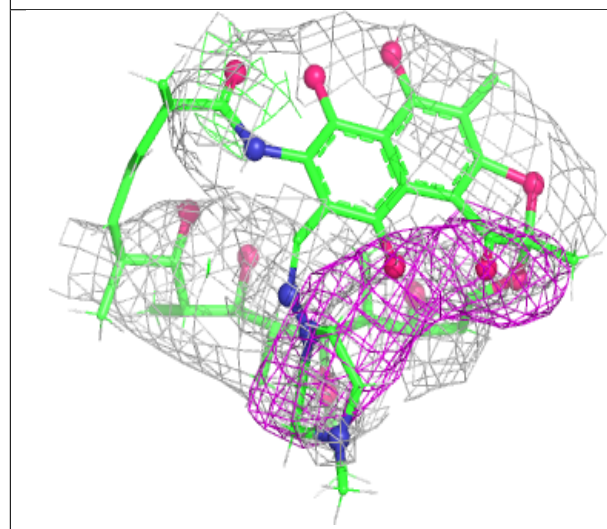
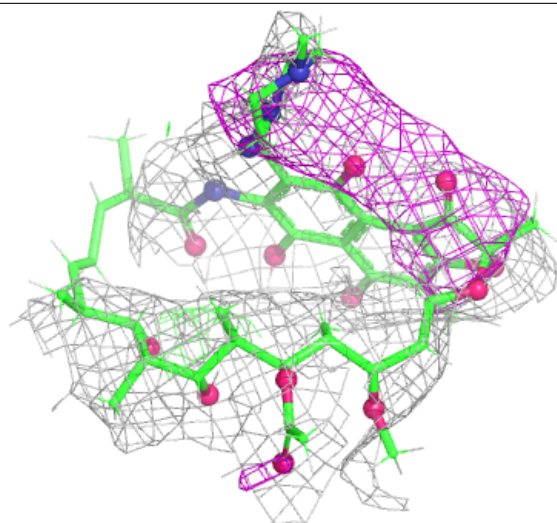
Electron density around RFP C 1401:

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



Electron density around RFP H 1401:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.