



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:22 PM BST

PDB ID : 4V8L
EMDB ID: : EMD-2238
Title : Cryo-EM Structure of the Mycobacterial Fatty Acid Synthase
Authors : Boehringer, D.; Ban, N.; Leibundgut, M.
Deposited on : 2012-12-06
Resolution : 7.50 Å(reported)
Based on PDB ID : 2UV8

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

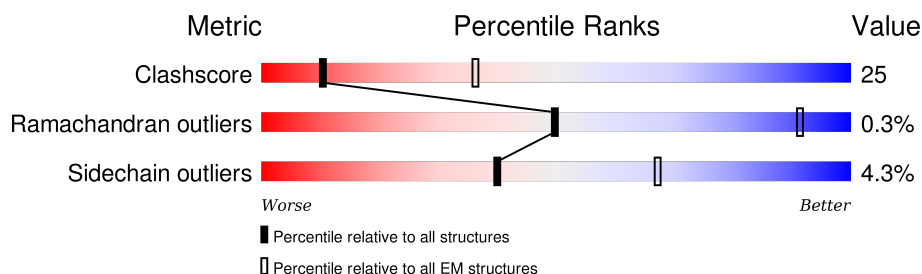
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	3089	56% 33% • 9%
1	B	3089	56% 33% • 9%
1	C	3089	56% 33% • 9%
1	D	3089	88% • 9%
1	E	3089	88% • 9%
1	F	3089	88% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 126306 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 FATTY ACID SYNTHASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	2822	Total 21020	C 13294	N 3662	O 3998	S 66	0	0
1	E	2822	Total 21020	C 13294	N 3662	O 3998	S 66	0	0
1	F	2822	Total 21020	C 13294	N 3662	O 3998	S 66	0	0
1	A	2822	Total 21020	C 13294	N 3662	O 3998	S 66	0	0
1	B	2822	Total 21020	C 13294	N 3662	O 3998	S 66	0	0
1	C	2822	Total 21020	C 13294	N 3662	O 3998	S 66	0	0

There are 1086 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	929	UNK	GLU	CONFLICT	UNP A0R1H7
D	930	UNK	PRO	CONFLICT	UNP A0R1H7
D	931	UNK	VAL	CONFLICT	UNP A0R1H7
D	932	UNK	GLU	CONFLICT	UNP A0R1H7
D	933	UNK	VAL	CONFLICT	UNP A0R1H7
D	934	UNK	LEU	CONFLICT	UNP A0R1H7
D	935	UNK	SER	CONFLICT	UNP A0R1H7
D	936	UNK	ARG	CONFLICT	UNP A0R1H7
D	937	UNK	ARG	CONFLICT	UNP A0R1H7
D	938	UNK	GLN	CONFLICT	UNP A0R1H7
D	939	UNK	ALA	CONFLICT	UNP A0R1H7
D	940	UNK	ARG	CONFLICT	UNP A0R1H7
D	941	UNK	ARG	CONFLICT	UNP A0R1H7
D	942	UNK	ASP	CONFLICT	UNP A0R1H7
D	943	UNK	ALA	CONFLICT	UNP A0R1H7
D	944	UNK	SER	CONFLICT	UNP A0R1H7
D	974	UNK	THR	CONFLICT	UNP A0R1H7
D	975	UNK	GLU	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	976	UNK	TRP	CONFLICT	UNP A0R1H7
D	977	UNK	GLN	CONFLICT	UNP A0R1H7
D	978	UNK	VAL	CONFLICT	UNP A0R1H7
D	979	UNK	ARG	CONFLICT	UNP A0R1H7
D	980	UNK	GLU	CONFLICT	UNP A0R1H7
D	981	UNK	GLY	CONFLICT	UNP A0R1H7
D	982	UNK	SER	CONFLICT	UNP A0R1H7
D	983	UNK	ASP	CONFLICT	UNP A0R1H7
D	984	UNK	ASN	CONFLICT	UNP A0R1H7
D	985	UNK	ARG	CONFLICT	UNP A0R1H7
D	986	UNK	SER	CONFLICT	UNP A0R1H7
D	987	UNK	ALA	CONFLICT	UNP A0R1H7
D	988	UNK	SER	CONFLICT	UNP A0R1H7
D	989	UNK	HIS	CONFLICT	UNP A0R1H7
D	990	UNK	PRO	CONFLICT	UNP A0R1H7
D	991	UNK	SER	CONFLICT	UNP A0R1H7
D	992	UNK	THR	CONFLICT	UNP A0R1H7
D	993	UNK	GLY	CONFLICT	UNP A0R1H7
D	994	UNK	ALA	CONFLICT	UNP A0R1H7
D	995	UNK	ARG	CONFLICT	UNP A0R1H7
D	996	UNK	LEU	CONFLICT	UNP A0R1H7
D	997	UNK	GLU	CONFLICT	UNP A0R1H7
D	998	UNK	VAL	CONFLICT	UNP A0R1H7
D	999	UNK	ALA	CONFLICT	UNP A0R1H7
D	1000	UNK	ASP	CONFLICT	UNP A0R1H7
D	1001	UNK	ASP	CONFLICT	UNP A0R1H7
D	1002	UNK	GLN	CONFLICT	UNP A0R1H7
D	1003	UNK	HIS	CONFLICT	UNP A0R1H7
D	1004	UNK	VAL	CONFLICT	UNP A0R1H7
D	1005	UNK	VAL	CONFLICT	UNP A0R1H7
D	1006	UNK	LEU	CONFLICT	UNP A0R1H7
D	1007	UNK	SER	CONFLICT	UNP A0R1H7
D	1008	UNK	VAL	CONFLICT	UNP A0R1H7
D	1009	UNK	PRO	CONFLICT	UNP A0R1H7
D	1010	UNK	LEU	CONFLICT	UNP A0R1H7
D	1011	UNK	SER	CONFLICT	UNP A0R1H7
D	1012	UNK	GLY	CONFLICT	UNP A0R1H7
D	1013	UNK	THR	CONFLICT	UNP A0R1H7
D	1014	UNK	TRP	CONFLICT	UNP A0R1H7
D	1196	UNK	GLY	CONFLICT	UNP A0R1H7
D	1197	UNK	ARG	CONFLICT	UNP A0R1H7
D	1198	UNK	THR	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1199	UNK	GLY	CONFLICT	UNP A0R1H7
D	1200	UNK	ALA	CONFLICT	UNP A0R1H7
D	1201	UNK	ALA	CONFLICT	UNP A0R1H7
D	1202	UNK	GLU	CONFLICT	UNP A0R1H7
D	1203	UNK	LEU	CONFLICT	UNP A0R1H7
D	1204	UNK	THR	CONFLICT	UNP A0R1H7
D	1205	UNK	ASP	CONFLICT	UNP A0R1H7
D	1206	UNK	PRO	CONFLICT	UNP A0R1H7
D	1207	UNK	VAL	CONFLICT	UNP A0R1H7
D	1208	UNK	ARG	CONFLICT	UNP A0R1H7
D	1209	UNK	ALA	CONFLICT	UNP A0R1H7
D	1210	UNK	GLY	CONFLICT	UNP A0R1H7
D	1211	UNK	GLY	CONFLICT	UNP A0R1H7
D	1212	UNK	ALA	CONFLICT	UNP A0R1H7
D	1213	UNK	ILE	CONFLICT	UNP A0R1H7
D	1214	UNK	SER	CONFLICT	UNP A0R1H7
D	1215	UNK	ASP	CONFLICT	UNP A0R1H7
D	1216	UNK	ASN	CONFLICT	UNP A0R1H7
D	1217	UNK	ALA	CONFLICT	UNP A0R1H7
D	1218	UNK	THR	CONFLICT	UNP A0R1H7
D	1219	UNK	ASP	CONFLICT	UNP A0R1H7
D	1220	UNK	THR	CONFLICT	UNP A0R1H7
D	1221	UNK	PRO	CONFLICT	UNP A0R1H7
D	1222	UNK	ARG	CONFLICT	UNP A0R1H7
D	1223	UNK	ARG	CONFLICT	UNP A0R1H7
D	1224	UNK	ARG	CONFLICT	UNP A0R1H7
D	1225	UNK	ARG	CONFLICT	UNP A0R1H7
D	1226	UNK	ARG	CONFLICT	UNP A0R1H7
D	1227	UNK	ASP	CONFLICT	UNP A0R1H7
D	2076	UNK	GLY	CONFLICT	UNP A0R1H7
D	2077	UNK	ASP	CONFLICT	UNP A0R1H7
D	2078	UNK	ILE	CONFLICT	UNP A0R1H7
D	2079	UNK	ASP	CONFLICT	UNP A0R1H7
D	2080	UNK	ALA	CONFLICT	UNP A0R1H7
D	2081	UNK	GLN	CONFLICT	UNP A0R1H7
D	2082	UNK	TRP	CONFLICT	UNP A0R1H7
D	2083	UNK	GLU	CONFLICT	UNP A0R1H7
D	2084	UNK	GLN	CONFLICT	UNP A0R1H7
D	2085	UNK	LEU	CONFLICT	UNP A0R1H7
D	2086	UNK	SER	CONFLICT	UNP A0R1H7
D	2087	UNK	GLN	CONFLICT	UNP A0R1H7
D	2088	UNK	ARG	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2089	UNK	PHE	CONFLICT	UNP A0R1H7
D	2090	UNK	GLU	CONFLICT	UNP A0R1H7
D	2091	UNK	GLY	CONFLICT	UNP A0R1H7
D	2092	UNK	THR	CONFLICT	UNP A0R1H7
D	2093	UNK	GLY	CONFLICT	UNP A0R1H7
D	2094	UNK	HIS	CONFLICT	UNP A0R1H7
D	2095	UNK	VAL	CONFLICT	UNP A0R1H7
D	2096	UNK	VAL	CONFLICT	UNP A0R1H7
D	2097	UNK	ALA	CONFLICT	UNP A0R1H7
D	2098	UNK	THR	CONFLICT	UNP A0R1H7
D	2099	UNK	GLN	CONFLICT	UNP A0R1H7
D	2100	UNK	ALA	CONFLICT	UNP A0R1H7
D	2101	UNK	ASN	CONFLICT	UNP A0R1H7
D	2102	UNK	TRP	CONFLICT	UNP A0R1H7
D	2103	UNK	TRP	CONFLICT	UNP A0R1H7
D	2104	UNK	GLN	CONFLICT	UNP A0R1H7
D	2105	UNK	GLY	CONFLICT	UNP A0R1H7
D	2106	UNK	LYS	CONFLICT	UNP A0R1H7
D	2107	UNK	ALA	CONFLICT	UNP A0R1H7
D	2108	UNK	LEU	CONFLICT	UNP A0R1H7
D	2109	UNK	ALA	CONFLICT	UNP A0R1H7
D	2110	UNK	ALA	CONFLICT	UNP A0R1H7
D	2111	UNK	GLY	CONFLICT	UNP A0R1H7
D	2112	UNK	ARG	CONFLICT	UNP A0R1H7
D	2113	UNK	ASN	CONFLICT	UNP A0R1H7
D	2114	UNK	VAL	CONFLICT	UNP A0R1H7
D	2115	UNK	HIS	CONFLICT	UNP A0R1H7
D	2116	UNK	ALA	CONFLICT	UNP A0R1H7
D	2117	UNK	SER	CONFLICT	UNP A0R1H7
D	2118	UNK	LEU	CONFLICT	UNP A0R1H7
D	2119	UNK	PHE	CONFLICT	UNP A0R1H7
D	2120	UNK	GLY	CONFLICT	UNP A0R1H7
D	2121	UNK	ARG	CONFLICT	UNP A0R1H7
D	2122	UNK	ILE	CONFLICT	UNP A0R1H7
D	2123	UNK	ALA	CONFLICT	UNP A0R1H7
D	2124	UNK	ALA	CONFLICT	UNP A0R1H7
D	2125	UNK	GLY	CONFLICT	UNP A0R1H7
D	2126	UNK	ALA	CONFLICT	UNP A0R1H7
D	2127	UNK	GLU	CONFLICT	UNP A0R1H7
D	2128	UNK	ASN	CONFLICT	UNP A0R1H7
D	2129	UNK	PRO	CONFLICT	UNP A0R1H7
D	2130	UNK	GLY	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2131	UNK	LYS	CONFLICT	UNP A0R1H7
D	2132	UNK	GLY	CONFLICT	UNP A0R1H7
D	2133	UNK	ARG	CONFLICT	UNP A0R1H7
D	2134	UNK	TYR	CONFLICT	UNP A0R1H7
D	2135	UNK	SER	CONFLICT	UNP A0R1H7
D	2422	UNK	GLU	CONFLICT	UNP A0R1H7
D	2423	UNK	SER	CONFLICT	UNP A0R1H7
D	2424	UNK	ASP	CONFLICT	UNP A0R1H7
D	2425	UNK	ASP	CONFLICT	UNP A0R1H7
D	2426	UNK	GLU	CONFLICT	UNP A0R1H7
D	2427	UNK	ALA	CONFLICT	UNP A0R1H7
D	2428	UNK	PRO	CONFLICT	UNP A0R1H7
D	2429	UNK	ALA	CONFLICT	UNP A0R1H7
D	2430	UNK	GLY	CONFLICT	UNP A0R1H7
D	2431	UNK	THR	CONFLICT	UNP A0R1H7
D	2432	UNK	ILE	CONFLICT	UNP A0R1H7
D	2433	UNK	ARG	CONFLICT	UNP A0R1H7
D	2434	UNK	ALA	CONFLICT	UNP A0R1H7
D	2435	UNK	LEU	CONFLICT	UNP A0R1H7
D	2436	UNK	PRO	CONFLICT	UNP A0R1H7
D	2437	UNK	SER	CONFLICT	UNP A0R1H7
D	2438	UNK	PRO	CONFLICT	UNP A0R1H7
D	2439	UNK	PRO	CONFLICT	UNP A0R1H7
D	2440	UNK	ARG	CONFLICT	UNP A0R1H7
D	2441	UNK	GLY	CONFLICT	UNP A0R1H7
D	2442	UNK	TYR	CONFLICT	UNP A0R1H7
D	2443	UNK	ASN	CONFLICT	UNP A0R1H7
D	2444	UNK	PRO	CONFLICT	UNP A0R1H7
D	2445	UNK	ALA	CONFLICT	UNP A0R1H7
D	2446	UNK	PRO	CONFLICT	UNP A0R1H7
D	2447	UNK	ALA	CONFLICT	UNP A0R1H7
D	2448	UNK	PRO	CONFLICT	UNP A0R1H7
D	2449	UNK	GLU	CONFLICT	UNP A0R1H7
D	2450	UNK	TRP	CONFLICT	UNP A0R1H7
D	2451	UNK	ASP	CONFLICT	UNP A0R1H7
D	2452	UNK	ASP	CONFLICT	UNP A0R1H7
D	2453	UNK	LEU	CONFLICT	UNP A0R1H7
E	929	UNK	GLU	CONFLICT	UNP A0R1H7
E	930	UNK	PRO	CONFLICT	UNP A0R1H7
E	931	UNK	VAL	CONFLICT	UNP A0R1H7
E	932	UNK	GLU	CONFLICT	UNP A0R1H7
E	933	UNK	VAL	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	934	UNK	LEU	CONFLICT	UNP A0R1H7
E	935	UNK	SER	CONFLICT	UNP A0R1H7
E	936	UNK	ARG	CONFLICT	UNP A0R1H7
E	937	UNK	ARG	CONFLICT	UNP A0R1H7
E	938	UNK	GLN	CONFLICT	UNP A0R1H7
E	939	UNK	ALA	CONFLICT	UNP A0R1H7
E	940	UNK	ARG	CONFLICT	UNP A0R1H7
E	941	UNK	ARG	CONFLICT	UNP A0R1H7
E	942	UNK	ASP	CONFLICT	UNP A0R1H7
E	943	UNK	ALA	CONFLICT	UNP A0R1H7
E	944	UNK	SER	CONFLICT	UNP A0R1H7
E	974	UNK	THR	CONFLICT	UNP A0R1H7
E	975	UNK	GLU	CONFLICT	UNP A0R1H7
E	976	UNK	TRP	CONFLICT	UNP A0R1H7
E	977	UNK	GLN	CONFLICT	UNP A0R1H7
E	978	UNK	VAL	CONFLICT	UNP A0R1H7
E	979	UNK	ARG	CONFLICT	UNP A0R1H7
E	980	UNK	GLU	CONFLICT	UNP A0R1H7
E	981	UNK	GLY	CONFLICT	UNP A0R1H7
E	982	UNK	SER	CONFLICT	UNP A0R1H7
E	983	UNK	ASP	CONFLICT	UNP A0R1H7
E	984	UNK	ASN	CONFLICT	UNP A0R1H7
E	985	UNK	ARG	CONFLICT	UNP A0R1H7
E	986	UNK	SER	CONFLICT	UNP A0R1H7
E	987	UNK	ALA	CONFLICT	UNP A0R1H7
E	988	UNK	SER	CONFLICT	UNP A0R1H7
E	989	UNK	HIS	CONFLICT	UNP A0R1H7
E	990	UNK	PRO	CONFLICT	UNP A0R1H7
E	991	UNK	SER	CONFLICT	UNP A0R1H7
E	992	UNK	THR	CONFLICT	UNP A0R1H7
E	993	UNK	GLY	CONFLICT	UNP A0R1H7
E	994	UNK	ALA	CONFLICT	UNP A0R1H7
E	995	UNK	ARG	CONFLICT	UNP A0R1H7
E	996	UNK	LEU	CONFLICT	UNP A0R1H7
E	997	UNK	GLU	CONFLICT	UNP A0R1H7
E	998	UNK	VAL	CONFLICT	UNP A0R1H7
E	999	UNK	ALA	CONFLICT	UNP A0R1H7
E	1000	UNK	ASP	CONFLICT	UNP A0R1H7
E	1001	UNK	ASP	CONFLICT	UNP A0R1H7
E	1002	UNK	GLN	CONFLICT	UNP A0R1H7
E	1003	UNK	HIS	CONFLICT	UNP A0R1H7
E	1004	UNK	VAL	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1005	UNK	VAL	CONFLICT	UNP A0R1H7
E	1006	UNK	LEU	CONFLICT	UNP A0R1H7
E	1007	UNK	SER	CONFLICT	UNP A0R1H7
E	1008	UNK	VAL	CONFLICT	UNP A0R1H7
E	1009	UNK	PRO	CONFLICT	UNP A0R1H7
E	1010	UNK	LEU	CONFLICT	UNP A0R1H7
E	1011	UNK	SER	CONFLICT	UNP A0R1H7
E	1012	UNK	GLY	CONFLICT	UNP A0R1H7
E	1013	UNK	THR	CONFLICT	UNP A0R1H7
E	1014	UNK	TRP	CONFLICT	UNP A0R1H7
E	1196	UNK	GLY	CONFLICT	UNP A0R1H7
E	1197	UNK	ARG	CONFLICT	UNP A0R1H7
E	1198	UNK	THR	CONFLICT	UNP A0R1H7
E	1199	UNK	GLY	CONFLICT	UNP A0R1H7
E	1200	UNK	ALA	CONFLICT	UNP A0R1H7
E	1201	UNK	ALA	CONFLICT	UNP A0R1H7
E	1202	UNK	GLU	CONFLICT	UNP A0R1H7
E	1203	UNK	LEU	CONFLICT	UNP A0R1H7
E	1204	UNK	THR	CONFLICT	UNP A0R1H7
E	1205	UNK	ASP	CONFLICT	UNP A0R1H7
E	1206	UNK	PRO	CONFLICT	UNP A0R1H7
E	1207	UNK	VAL	CONFLICT	UNP A0R1H7
E	1208	UNK	ARG	CONFLICT	UNP A0R1H7
E	1209	UNK	ALA	CONFLICT	UNP A0R1H7
E	1210	UNK	GLY	CONFLICT	UNP A0R1H7
E	1211	UNK	GLY	CONFLICT	UNP A0R1H7
E	1212	UNK	ALA	CONFLICT	UNP A0R1H7
E	1213	UNK	ILE	CONFLICT	UNP A0R1H7
E	1214	UNK	SER	CONFLICT	UNP A0R1H7
E	1215	UNK	ASP	CONFLICT	UNP A0R1H7
E	1216	UNK	ASN	CONFLICT	UNP A0R1H7
E	1217	UNK	ALA	CONFLICT	UNP A0R1H7
E	1218	UNK	THR	CONFLICT	UNP A0R1H7
E	1219	UNK	ASP	CONFLICT	UNP A0R1H7
E	1220	UNK	THR	CONFLICT	UNP A0R1H7
E	1221	UNK	PRO	CONFLICT	UNP A0R1H7
E	1222	UNK	ARG	CONFLICT	UNP A0R1H7
E	1223	UNK	ARG	CONFLICT	UNP A0R1H7
E	1224	UNK	ARG	CONFLICT	UNP A0R1H7
E	1225	UNK	ARG	CONFLICT	UNP A0R1H7
E	1226	UNK	ARG	CONFLICT	UNP A0R1H7
E	1227	UNK	ASP	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2076	UNK	GLY	CONFLICT	UNP A0R1H7
E	2077	UNK	ASP	CONFLICT	UNP A0R1H7
E	2078	UNK	ILE	CONFLICT	UNP A0R1H7
E	2079	UNK	ASP	CONFLICT	UNP A0R1H7
E	2080	UNK	ALA	CONFLICT	UNP A0R1H7
E	2081	UNK	GLN	CONFLICT	UNP A0R1H7
E	2082	UNK	TRP	CONFLICT	UNP A0R1H7
E	2083	UNK	GLU	CONFLICT	UNP A0R1H7
E	2084	UNK	GLN	CONFLICT	UNP A0R1H7
E	2085	UNK	LEU	CONFLICT	UNP A0R1H7
E	2086	UNK	SER	CONFLICT	UNP A0R1H7
E	2087	UNK	GLN	CONFLICT	UNP A0R1H7
E	2088	UNK	ARG	CONFLICT	UNP A0R1H7
E	2089	UNK	PHE	CONFLICT	UNP A0R1H7
E	2090	UNK	GLU	CONFLICT	UNP A0R1H7
E	2091	UNK	GLY	CONFLICT	UNP A0R1H7
E	2092	UNK	THR	CONFLICT	UNP A0R1H7
E	2093	UNK	GLY	CONFLICT	UNP A0R1H7
E	2094	UNK	HIS	CONFLICT	UNP A0R1H7
E	2095	UNK	VAL	CONFLICT	UNP A0R1H7
E	2096	UNK	VAL	CONFLICT	UNP A0R1H7
E	2097	UNK	ALA	CONFLICT	UNP A0R1H7
E	2098	UNK	THR	CONFLICT	UNP A0R1H7
E	2099	UNK	GLN	CONFLICT	UNP A0R1H7
E	2100	UNK	ALA	CONFLICT	UNP A0R1H7
E	2101	UNK	ASN	CONFLICT	UNP A0R1H7
E	2102	UNK	TRP	CONFLICT	UNP A0R1H7
E	2103	UNK	TRP	CONFLICT	UNP A0R1H7
E	2104	UNK	GLN	CONFLICT	UNP A0R1H7
E	2105	UNK	GLY	CONFLICT	UNP A0R1H7
E	2106	UNK	LYS	CONFLICT	UNP A0R1H7
E	2107	UNK	ALA	CONFLICT	UNP A0R1H7
E	2108	UNK	LEU	CONFLICT	UNP A0R1H7
E	2109	UNK	ALA	CONFLICT	UNP A0R1H7
E	2110	UNK	ALA	CONFLICT	UNP A0R1H7
E	2111	UNK	GLY	CONFLICT	UNP A0R1H7
E	2112	UNK	ARG	CONFLICT	UNP A0R1H7
E	2113	UNK	ASN	CONFLICT	UNP A0R1H7
E	2114	UNK	VAL	CONFLICT	UNP A0R1H7
E	2115	UNK	HIS	CONFLICT	UNP A0R1H7
E	2116	UNK	ALA	CONFLICT	UNP A0R1H7
E	2117	UNK	SER	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2118	UNK	LEU	CONFLICT	UNP A0R1H7
E	2119	UNK	PHE	CONFLICT	UNP A0R1H7
E	2120	UNK	GLY	CONFLICT	UNP A0R1H7
E	2121	UNK	ARG	CONFLICT	UNP A0R1H7
E	2122	UNK	ILE	CONFLICT	UNP A0R1H7
E	2123	UNK	ALA	CONFLICT	UNP A0R1H7
E	2124	UNK	ALA	CONFLICT	UNP A0R1H7
E	2125	UNK	GLY	CONFLICT	UNP A0R1H7
E	2126	UNK	ALA	CONFLICT	UNP A0R1H7
E	2127	UNK	GLU	CONFLICT	UNP A0R1H7
E	2128	UNK	ASN	CONFLICT	UNP A0R1H7
E	2129	UNK	PRO	CONFLICT	UNP A0R1H7
E	2130	UNK	GLY	CONFLICT	UNP A0R1H7
E	2131	UNK	LYS	CONFLICT	UNP A0R1H7
E	2132	UNK	GLY	CONFLICT	UNP A0R1H7
E	2133	UNK	ARG	CONFLICT	UNP A0R1H7
E	2134	UNK	TYR	CONFLICT	UNP A0R1H7
E	2135	UNK	SER	CONFLICT	UNP A0R1H7
E	2422	UNK	GLU	CONFLICT	UNP A0R1H7
E	2423	UNK	SER	CONFLICT	UNP A0R1H7
E	2424	UNK	ASP	CONFLICT	UNP A0R1H7
E	2425	UNK	ASP	CONFLICT	UNP A0R1H7
E	2426	UNK	GLU	CONFLICT	UNP A0R1H7
E	2427	UNK	ALA	CONFLICT	UNP A0R1H7
E	2428	UNK	PRO	CONFLICT	UNP A0R1H7
E	2429	UNK	ALA	CONFLICT	UNP A0R1H7
E	2430	UNK	GLY	CONFLICT	UNP A0R1H7
E	2431	UNK	THR	CONFLICT	UNP A0R1H7
E	2432	UNK	ILE	CONFLICT	UNP A0R1H7
E	2433	UNK	ARG	CONFLICT	UNP A0R1H7
E	2434	UNK	ALA	CONFLICT	UNP A0R1H7
E	2435	UNK	LEU	CONFLICT	UNP A0R1H7
E	2436	UNK	PRO	CONFLICT	UNP A0R1H7
E	2437	UNK	SER	CONFLICT	UNP A0R1H7
E	2438	UNK	PRO	CONFLICT	UNP A0R1H7
E	2439	UNK	PRO	CONFLICT	UNP A0R1H7
E	2440	UNK	ARG	CONFLICT	UNP A0R1H7
E	2441	UNK	GLY	CONFLICT	UNP A0R1H7
E	2442	UNK	TYR	CONFLICT	UNP A0R1H7
E	2443	UNK	ASN	CONFLICT	UNP A0R1H7
E	2444	UNK	PRO	CONFLICT	UNP A0R1H7
E	2445	UNK	ALA	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2446	UNK	PRO	CONFLICT	UNP A0R1H7
E	2447	UNK	ALA	CONFLICT	UNP A0R1H7
E	2448	UNK	PRO	CONFLICT	UNP A0R1H7
E	2449	UNK	GLU	CONFLICT	UNP A0R1H7
E	2450	UNK	TRP	CONFLICT	UNP A0R1H7
E	2451	UNK	ASP	CONFLICT	UNP A0R1H7
E	2452	UNK	ASP	CONFLICT	UNP A0R1H7
E	2453	UNK	LEU	CONFLICT	UNP A0R1H7
F	929	UNK	GLU	CONFLICT	UNP A0R1H7
F	930	UNK	PRO	CONFLICT	UNP A0R1H7
F	931	UNK	VAL	CONFLICT	UNP A0R1H7
F	932	UNK	GLU	CONFLICT	UNP A0R1H7
F	933	UNK	VAL	CONFLICT	UNP A0R1H7
F	934	UNK	LEU	CONFLICT	UNP A0R1H7
F	935	UNK	SER	CONFLICT	UNP A0R1H7
F	936	UNK	ARG	CONFLICT	UNP A0R1H7
F	937	UNK	ARG	CONFLICT	UNP A0R1H7
F	938	UNK	GLN	CONFLICT	UNP A0R1H7
F	939	UNK	ALA	CONFLICT	UNP A0R1H7
F	940	UNK	ARG	CONFLICT	UNP A0R1H7
F	941	UNK	ARG	CONFLICT	UNP A0R1H7
F	942	UNK	ASP	CONFLICT	UNP A0R1H7
F	943	UNK	ALA	CONFLICT	UNP A0R1H7
F	944	UNK	SER	CONFLICT	UNP A0R1H7
F	974	UNK	THR	CONFLICT	UNP A0R1H7
F	975	UNK	GLU	CONFLICT	UNP A0R1H7
F	976	UNK	TRP	CONFLICT	UNP A0R1H7
F	977	UNK	GLN	CONFLICT	UNP A0R1H7
F	978	UNK	VAL	CONFLICT	UNP A0R1H7
F	979	UNK	ARG	CONFLICT	UNP A0R1H7
F	980	UNK	GLU	CONFLICT	UNP A0R1H7
F	981	UNK	GLY	CONFLICT	UNP A0R1H7
F	982	UNK	SER	CONFLICT	UNP A0R1H7
F	983	UNK	ASP	CONFLICT	UNP A0R1H7
F	984	UNK	ASN	CONFLICT	UNP A0R1H7
F	985	UNK	ARG	CONFLICT	UNP A0R1H7
F	986	UNK	SER	CONFLICT	UNP A0R1H7
F	987	UNK	ALA	CONFLICT	UNP A0R1H7
F	988	UNK	SER	CONFLICT	UNP A0R1H7
F	989	UNK	HIS	CONFLICT	UNP A0R1H7
F	990	UNK	PRO	CONFLICT	UNP A0R1H7
F	991	UNK	SER	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	992	UNK	THR	CONFLICT	UNP A0R1H7
F	993	UNK	GLY	CONFLICT	UNP A0R1H7
F	994	UNK	ALA	CONFLICT	UNP A0R1H7
F	995	UNK	ARG	CONFLICT	UNP A0R1H7
F	996	UNK	LEU	CONFLICT	UNP A0R1H7
F	997	UNK	GLU	CONFLICT	UNP A0R1H7
F	998	UNK	VAL	CONFLICT	UNP A0R1H7
F	999	UNK	ALA	CONFLICT	UNP A0R1H7
F	1000	UNK	ASP	CONFLICT	UNP A0R1H7
F	1001	UNK	ASP	CONFLICT	UNP A0R1H7
F	1002	UNK	GLN	CONFLICT	UNP A0R1H7
F	1003	UNK	HIS	CONFLICT	UNP A0R1H7
F	1004	UNK	VAL	CONFLICT	UNP A0R1H7
F	1005	UNK	VAL	CONFLICT	UNP A0R1H7
F	1006	UNK	LEU	CONFLICT	UNP A0R1H7
F	1007	UNK	SER	CONFLICT	UNP A0R1H7
F	1008	UNK	VAL	CONFLICT	UNP A0R1H7
F	1009	UNK	PRO	CONFLICT	UNP A0R1H7
F	1010	UNK	LEU	CONFLICT	UNP A0R1H7
F	1011	UNK	SER	CONFLICT	UNP A0R1H7
F	1012	UNK	GLY	CONFLICT	UNP A0R1H7
F	1013	UNK	THR	CONFLICT	UNP A0R1H7
F	1014	UNK	TRP	CONFLICT	UNP A0R1H7
F	1196	UNK	GLY	CONFLICT	UNP A0R1H7
F	1197	UNK	ARG	CONFLICT	UNP A0R1H7
F	1198	UNK	THR	CONFLICT	UNP A0R1H7
F	1199	UNK	GLY	CONFLICT	UNP A0R1H7
F	1200	UNK	ALA	CONFLICT	UNP A0R1H7
F	1201	UNK	ALA	CONFLICT	UNP A0R1H7
F	1202	UNK	GLU	CONFLICT	UNP A0R1H7
F	1203	UNK	LEU	CONFLICT	UNP A0R1H7
F	1204	UNK	THR	CONFLICT	UNP A0R1H7
F	1205	UNK	ASP	CONFLICT	UNP A0R1H7
F	1206	UNK	PRO	CONFLICT	UNP A0R1H7
F	1207	UNK	VAL	CONFLICT	UNP A0R1H7
F	1208	UNK	ARG	CONFLICT	UNP A0R1H7
F	1209	UNK	ALA	CONFLICT	UNP A0R1H7
F	1210	UNK	GLY	CONFLICT	UNP A0R1H7
F	1211	UNK	GLY	CONFLICT	UNP A0R1H7
F	1212	UNK	ALA	CONFLICT	UNP A0R1H7
F	1213	UNK	ILE	CONFLICT	UNP A0R1H7
F	1214	UNK	SER	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1215	UNK	ASP	CONFLICT	UNP A0R1H7
F	1216	UNK	ASN	CONFLICT	UNP A0R1H7
F	1217	UNK	ALA	CONFLICT	UNP A0R1H7
F	1218	UNK	THR	CONFLICT	UNP A0R1H7
F	1219	UNK	ASP	CONFLICT	UNP A0R1H7
F	1220	UNK	THR	CONFLICT	UNP A0R1H7
F	1221	UNK	PRO	CONFLICT	UNP A0R1H7
F	1222	UNK	ARG	CONFLICT	UNP A0R1H7
F	1223	UNK	ARG	CONFLICT	UNP A0R1H7
F	1224	UNK	ARG	CONFLICT	UNP A0R1H7
F	1225	UNK	ARG	CONFLICT	UNP A0R1H7
F	1226	UNK	ARG	CONFLICT	UNP A0R1H7
F	1227	UNK	ASP	CONFLICT	UNP A0R1H7
F	2076	UNK	GLY	CONFLICT	UNP A0R1H7
F	2077	UNK	ASP	CONFLICT	UNP A0R1H7
F	2078	UNK	ILE	CONFLICT	UNP A0R1H7
F	2079	UNK	ASP	CONFLICT	UNP A0R1H7
F	2080	UNK	ALA	CONFLICT	UNP A0R1H7
F	2081	UNK	GLN	CONFLICT	UNP A0R1H7
F	2082	UNK	TRP	CONFLICT	UNP A0R1H7
F	2083	UNK	GLU	CONFLICT	UNP A0R1H7
F	2084	UNK	GLN	CONFLICT	UNP A0R1H7
F	2085	UNK	LEU	CONFLICT	UNP A0R1H7
F	2086	UNK	SER	CONFLICT	UNP A0R1H7
F	2087	UNK	GLN	CONFLICT	UNP A0R1H7
F	2088	UNK	ARG	CONFLICT	UNP A0R1H7
F	2089	UNK	PHE	CONFLICT	UNP A0R1H7
F	2090	UNK	GLU	CONFLICT	UNP A0R1H7
F	2091	UNK	GLY	CONFLICT	UNP A0R1H7
F	2092	UNK	THR	CONFLICT	UNP A0R1H7
F	2093	UNK	GLY	CONFLICT	UNP A0R1H7
F	2094	UNK	HIS	CONFLICT	UNP A0R1H7
F	2095	UNK	VAL	CONFLICT	UNP A0R1H7
F	2096	UNK	VAL	CONFLICT	UNP A0R1H7
F	2097	UNK	ALA	CONFLICT	UNP A0R1H7
F	2098	UNK	THR	CONFLICT	UNP A0R1H7
F	2099	UNK	GLN	CONFLICT	UNP A0R1H7
F	2100	UNK	ALA	CONFLICT	UNP A0R1H7
F	2101	UNK	ASN	CONFLICT	UNP A0R1H7
F	2102	UNK	TRP	CONFLICT	UNP A0R1H7
F	2103	UNK	TRP	CONFLICT	UNP A0R1H7
F	2104	UNK	GLN	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	2105	UNK	GLY	CONFLICT	UNP A0R1H7
F	2106	UNK	LYS	CONFLICT	UNP A0R1H7
F	2107	UNK	ALA	CONFLICT	UNP A0R1H7
F	2108	UNK	LEU	CONFLICT	UNP A0R1H7
F	2109	UNK	ALA	CONFLICT	UNP A0R1H7
F	2110	UNK	ALA	CONFLICT	UNP A0R1H7
F	2111	UNK	GLY	CONFLICT	UNP A0R1H7
F	2112	UNK	ARG	CONFLICT	UNP A0R1H7
F	2113	UNK	ASN	CONFLICT	UNP A0R1H7
F	2114	UNK	VAL	CONFLICT	UNP A0R1H7
F	2115	UNK	HIS	CONFLICT	UNP A0R1H7
F	2116	UNK	ALA	CONFLICT	UNP A0R1H7
F	2117	UNK	SER	CONFLICT	UNP A0R1H7
F	2118	UNK	LEU	CONFLICT	UNP A0R1H7
F	2119	UNK	PHE	CONFLICT	UNP A0R1H7
F	2120	UNK	GLY	CONFLICT	UNP A0R1H7
F	2121	UNK	ARG	CONFLICT	UNP A0R1H7
F	2122	UNK	ILE	CONFLICT	UNP A0R1H7
F	2123	UNK	ALA	CONFLICT	UNP A0R1H7
F	2124	UNK	ALA	CONFLICT	UNP A0R1H7
F	2125	UNK	GLY	CONFLICT	UNP A0R1H7
F	2126	UNK	ALA	CONFLICT	UNP A0R1H7
F	2127	UNK	GLU	CONFLICT	UNP A0R1H7
F	2128	UNK	ASN	CONFLICT	UNP A0R1H7
F	2129	UNK	PRO	CONFLICT	UNP A0R1H7
F	2130	UNK	GLY	CONFLICT	UNP A0R1H7
F	2131	UNK	LYS	CONFLICT	UNP A0R1H7
F	2132	UNK	GLY	CONFLICT	UNP A0R1H7
F	2133	UNK	ARG	CONFLICT	UNP A0R1H7
F	2134	UNK	TYR	CONFLICT	UNP A0R1H7
F	2135	UNK	SER	CONFLICT	UNP A0R1H7
F	2422	UNK	GLU	CONFLICT	UNP A0R1H7
F	2423	UNK	SER	CONFLICT	UNP A0R1H7
F	2424	UNK	ASP	CONFLICT	UNP A0R1H7
F	2425	UNK	ASP	CONFLICT	UNP A0R1H7
F	2426	UNK	GLU	CONFLICT	UNP A0R1H7
F	2427	UNK	ALA	CONFLICT	UNP A0R1H7
F	2428	UNK	PRO	CONFLICT	UNP A0R1H7
F	2429	UNK	ALA	CONFLICT	UNP A0R1H7
F	2430	UNK	GLY	CONFLICT	UNP A0R1H7
F	2431	UNK	THR	CONFLICT	UNP A0R1H7
F	2432	UNK	ILE	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	2433	UNK	ARG	CONFLICT	UNP A0R1H7
F	2434	UNK	ALA	CONFLICT	UNP A0R1H7
F	2435	UNK	LEU	CONFLICT	UNP A0R1H7
F	2436	UNK	PRO	CONFLICT	UNP A0R1H7
F	2437	UNK	SER	CONFLICT	UNP A0R1H7
F	2438	UNK	PRO	CONFLICT	UNP A0R1H7
F	2439	UNK	PRO	CONFLICT	UNP A0R1H7
F	2440	UNK	ARG	CONFLICT	UNP A0R1H7
F	2441	UNK	GLY	CONFLICT	UNP A0R1H7
F	2442	UNK	TYR	CONFLICT	UNP A0R1H7
F	2443	UNK	ASN	CONFLICT	UNP A0R1H7
F	2444	UNK	PRO	CONFLICT	UNP A0R1H7
F	2445	UNK	ALA	CONFLICT	UNP A0R1H7
F	2446	UNK	PRO	CONFLICT	UNP A0R1H7
F	2447	UNK	ALA	CONFLICT	UNP A0R1H7
F	2448	UNK	PRO	CONFLICT	UNP A0R1H7
F	2449	UNK	GLU	CONFLICT	UNP A0R1H7
F	2450	UNK	TRP	CONFLICT	UNP A0R1H7
F	2451	UNK	ASP	CONFLICT	UNP A0R1H7
F	2452	UNK	ASP	CONFLICT	UNP A0R1H7
F	2453	UNK	LEU	CONFLICT	UNP A0R1H7
A	929	UNK	GLU	CONFLICT	UNP A0R1H7
A	930	UNK	PRO	CONFLICT	UNP A0R1H7
A	931	UNK	VAL	CONFLICT	UNP A0R1H7
A	932	UNK	GLU	CONFLICT	UNP A0R1H7
A	933	UNK	VAL	CONFLICT	UNP A0R1H7
A	934	UNK	LEU	CONFLICT	UNP A0R1H7
A	935	UNK	SER	CONFLICT	UNP A0R1H7
A	936	UNK	ARG	CONFLICT	UNP A0R1H7
A	937	UNK	ARG	CONFLICT	UNP A0R1H7
A	938	UNK	GLN	CONFLICT	UNP A0R1H7
A	939	UNK	ALA	CONFLICT	UNP A0R1H7
A	940	UNK	ARG	CONFLICT	UNP A0R1H7
A	941	UNK	ARG	CONFLICT	UNP A0R1H7
A	942	UNK	ASP	CONFLICT	UNP A0R1H7
A	943	UNK	ALA	CONFLICT	UNP A0R1H7
A	944	UNK	SER	CONFLICT	UNP A0R1H7
A	974	UNK	THR	CONFLICT	UNP A0R1H7
A	975	UNK	GLU	CONFLICT	UNP A0R1H7
A	976	UNK	TRP	CONFLICT	UNP A0R1H7
A	977	UNK	GLN	CONFLICT	UNP A0R1H7
A	978	UNK	VAL	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	979	UNK	ARG	CONFLICT	UNP A0R1H7
A	980	UNK	GLU	CONFLICT	UNP A0R1H7
A	981	UNK	GLY	CONFLICT	UNP A0R1H7
A	982	UNK	SER	CONFLICT	UNP A0R1H7
A	983	UNK	ASP	CONFLICT	UNP A0R1H7
A	984	UNK	ASN	CONFLICT	UNP A0R1H7
A	985	UNK	ARG	CONFLICT	UNP A0R1H7
A	986	UNK	SER	CONFLICT	UNP A0R1H7
A	987	UNK	ALA	CONFLICT	UNP A0R1H7
A	988	UNK	SER	CONFLICT	UNP A0R1H7
A	989	UNK	HIS	CONFLICT	UNP A0R1H7
A	990	UNK	PRO	CONFLICT	UNP A0R1H7
A	991	UNK	SER	CONFLICT	UNP A0R1H7
A	992	UNK	THR	CONFLICT	UNP A0R1H7
A	993	UNK	GLY	CONFLICT	UNP A0R1H7
A	994	UNK	ALA	CONFLICT	UNP A0R1H7
A	995	UNK	ARG	CONFLICT	UNP A0R1H7
A	996	UNK	LEU	CONFLICT	UNP A0R1H7
A	997	UNK	GLU	CONFLICT	UNP A0R1H7
A	998	UNK	VAL	CONFLICT	UNP A0R1H7
A	999	UNK	ALA	CONFLICT	UNP A0R1H7
A	1000	UNK	ASP	CONFLICT	UNP A0R1H7
A	1001	UNK	ASP	CONFLICT	UNP A0R1H7
A	1002	UNK	GLN	CONFLICT	UNP A0R1H7
A	1003	UNK	HIS	CONFLICT	UNP A0R1H7
A	1004	UNK	VAL	CONFLICT	UNP A0R1H7
A	1005	UNK	VAL	CONFLICT	UNP A0R1H7
A	1006	UNK	LEU	CONFLICT	UNP A0R1H7
A	1007	UNK	SER	CONFLICT	UNP A0R1H7
A	1008	UNK	VAL	CONFLICT	UNP A0R1H7
A	1009	UNK	PRO	CONFLICT	UNP A0R1H7
A	1010	UNK	LEU	CONFLICT	UNP A0R1H7
A	1011	UNK	SER	CONFLICT	UNP A0R1H7
A	1012	UNK	GLY	CONFLICT	UNP A0R1H7
A	1013	UNK	THR	CONFLICT	UNP A0R1H7
A	1014	UNK	TRP	CONFLICT	UNP A0R1H7
A	1196	UNK	GLY	CONFLICT	UNP A0R1H7
A	1197	UNK	ARG	CONFLICT	UNP A0R1H7
A	1198	UNK	THR	CONFLICT	UNP A0R1H7
A	1199	UNK	GLY	CONFLICT	UNP A0R1H7
A	1200	UNK	ALA	CONFLICT	UNP A0R1H7
A	1201	UNK	ALA	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1202	UNK	GLU	CONFLICT	UNP A0R1H7
A	1203	UNK	LEU	CONFLICT	UNP A0R1H7
A	1204	UNK	THR	CONFLICT	UNP A0R1H7
A	1205	UNK	ASP	CONFLICT	UNP A0R1H7
A	1206	UNK	PRO	CONFLICT	UNP A0R1H7
A	1207	UNK	VAL	CONFLICT	UNP A0R1H7
A	1208	UNK	ARG	CONFLICT	UNP A0R1H7
A	1209	UNK	ALA	CONFLICT	UNP A0R1H7
A	1210	UNK	GLY	CONFLICT	UNP A0R1H7
A	1211	UNK	GLY	CONFLICT	UNP A0R1H7
A	1212	UNK	ALA	CONFLICT	UNP A0R1H7
A	1213	UNK	ILE	CONFLICT	UNP A0R1H7
A	1214	UNK	SER	CONFLICT	UNP A0R1H7
A	1215	UNK	ASP	CONFLICT	UNP A0R1H7
A	1216	UNK	ASN	CONFLICT	UNP A0R1H7
A	1217	UNK	ALA	CONFLICT	UNP A0R1H7
A	1218	UNK	THR	CONFLICT	UNP A0R1H7
A	1219	UNK	ASP	CONFLICT	UNP A0R1H7
A	1220	UNK	THR	CONFLICT	UNP A0R1H7
A	1221	UNK	PRO	CONFLICT	UNP A0R1H7
A	1222	UNK	ARG	CONFLICT	UNP A0R1H7
A	1223	UNK	ARG	CONFLICT	UNP A0R1H7
A	1224	UNK	ARG	CONFLICT	UNP A0R1H7
A	1225	UNK	ARG	CONFLICT	UNP A0R1H7
A	1226	UNK	ARG	CONFLICT	UNP A0R1H7
A	1227	UNK	ASP	CONFLICT	UNP A0R1H7
A	2076	UNK	GLY	CONFLICT	UNP A0R1H7
A	2077	UNK	ASP	CONFLICT	UNP A0R1H7
A	2078	UNK	ILE	CONFLICT	UNP A0R1H7
A	2079	UNK	ASP	CONFLICT	UNP A0R1H7
A	2080	UNK	ALA	CONFLICT	UNP A0R1H7
A	2081	UNK	GLN	CONFLICT	UNP A0R1H7
A	2082	UNK	TRP	CONFLICT	UNP A0R1H7
A	2083	UNK	GLU	CONFLICT	UNP A0R1H7
A	2084	UNK	GLN	CONFLICT	UNP A0R1H7
A	2085	UNK	LEU	CONFLICT	UNP A0R1H7
A	2086	UNK	SER	CONFLICT	UNP A0R1H7
A	2087	UNK	GLN	CONFLICT	UNP A0R1H7
A	2088	UNK	ARG	CONFLICT	UNP A0R1H7
A	2089	UNK	PHE	CONFLICT	UNP A0R1H7
A	2090	UNK	GLU	CONFLICT	UNP A0R1H7
A	2091	UNK	GLY	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2092	UNK	THR	CONFLICT	UNP A0R1H7
A	2093	UNK	GLY	CONFLICT	UNP A0R1H7
A	2094	UNK	HIS	CONFLICT	UNP A0R1H7
A	2095	UNK	VAL	CONFLICT	UNP A0R1H7
A	2096	UNK	VAL	CONFLICT	UNP A0R1H7
A	2097	UNK	ALA	CONFLICT	UNP A0R1H7
A	2098	UNK	THR	CONFLICT	UNP A0R1H7
A	2099	UNK	GLN	CONFLICT	UNP A0R1H7
A	2100	UNK	ALA	CONFLICT	UNP A0R1H7
A	2101	UNK	ASN	CONFLICT	UNP A0R1H7
A	2102	UNK	TRP	CONFLICT	UNP A0R1H7
A	2103	UNK	TRP	CONFLICT	UNP A0R1H7
A	2104	UNK	GLN	CONFLICT	UNP A0R1H7
A	2105	UNK	GLY	CONFLICT	UNP A0R1H7
A	2106	UNK	LYS	CONFLICT	UNP A0R1H7
A	2107	UNK	ALA	CONFLICT	UNP A0R1H7
A	2108	UNK	LEU	CONFLICT	UNP A0R1H7
A	2109	UNK	ALA	CONFLICT	UNP A0R1H7
A	2110	UNK	ALA	CONFLICT	UNP A0R1H7
A	2111	UNK	GLY	CONFLICT	UNP A0R1H7
A	2112	UNK	ARG	CONFLICT	UNP A0R1H7
A	2113	UNK	ASN	CONFLICT	UNP A0R1H7
A	2114	UNK	VAL	CONFLICT	UNP A0R1H7
A	2115	UNK	HIS	CONFLICT	UNP A0R1H7
A	2116	UNK	ALA	CONFLICT	UNP A0R1H7
A	2117	UNK	SER	CONFLICT	UNP A0R1H7
A	2118	UNK	LEU	CONFLICT	UNP A0R1H7
A	2119	UNK	PHE	CONFLICT	UNP A0R1H7
A	2120	UNK	GLY	CONFLICT	UNP A0R1H7
A	2121	UNK	ARG	CONFLICT	UNP A0R1H7
A	2122	UNK	ILE	CONFLICT	UNP A0R1H7
A	2123	UNK	ALA	CONFLICT	UNP A0R1H7
A	2124	UNK	ALA	CONFLICT	UNP A0R1H7
A	2125	UNK	GLY	CONFLICT	UNP A0R1H7
A	2126	UNK	ALA	CONFLICT	UNP A0R1H7
A	2127	UNK	GLU	CONFLICT	UNP A0R1H7
A	2128	UNK	ASN	CONFLICT	UNP A0R1H7
A	2129	UNK	PRO	CONFLICT	UNP A0R1H7
A	2130	UNK	GLY	CONFLICT	UNP A0R1H7
A	2131	UNK	LYS	CONFLICT	UNP A0R1H7
A	2132	UNK	GLY	CONFLICT	UNP A0R1H7
A	2133	UNK	ARG	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2134	UNK	TYR	CONFLICT	UNP A0R1H7
A	2135	UNK	SER	CONFLICT	UNP A0R1H7
A	2422	UNK	GLU	CONFLICT	UNP A0R1H7
A	2423	UNK	SER	CONFLICT	UNP A0R1H7
A	2424	UNK	ASP	CONFLICT	UNP A0R1H7
A	2425	UNK	ASP	CONFLICT	UNP A0R1H7
A	2426	UNK	GLU	CONFLICT	UNP A0R1H7
A	2427	UNK	ALA	CONFLICT	UNP A0R1H7
A	2428	UNK	PRO	CONFLICT	UNP A0R1H7
A	2429	UNK	ALA	CONFLICT	UNP A0R1H7
A	2430	UNK	GLY	CONFLICT	UNP A0R1H7
A	2431	UNK	THR	CONFLICT	UNP A0R1H7
A	2432	UNK	ILE	CONFLICT	UNP A0R1H7
A	2433	UNK	ARG	CONFLICT	UNP A0R1H7
A	2434	UNK	ALA	CONFLICT	UNP A0R1H7
A	2435	UNK	LEU	CONFLICT	UNP A0R1H7
A	2436	UNK	PRO	CONFLICT	UNP A0R1H7
A	2437	UNK	SER	CONFLICT	UNP A0R1H7
A	2438	UNK	PRO	CONFLICT	UNP A0R1H7
A	2439	UNK	PRO	CONFLICT	UNP A0R1H7
A	2440	UNK	ARG	CONFLICT	UNP A0R1H7
A	2441	UNK	GLY	CONFLICT	UNP A0R1H7
A	2442	UNK	TYR	CONFLICT	UNP A0R1H7
A	2443	UNK	ASN	CONFLICT	UNP A0R1H7
A	2444	UNK	PRO	CONFLICT	UNP A0R1H7
A	2445	UNK	ALA	CONFLICT	UNP A0R1H7
A	2446	UNK	PRO	CONFLICT	UNP A0R1H7
A	2447	UNK	ALA	CONFLICT	UNP A0R1H7
A	2448	UNK	PRO	CONFLICT	UNP A0R1H7
A	2449	UNK	GLU	CONFLICT	UNP A0R1H7
A	2450	UNK	TRP	CONFLICT	UNP A0R1H7
A	2451	UNK	ASP	CONFLICT	UNP A0R1H7
A	2452	UNK	ASP	CONFLICT	UNP A0R1H7
A	2453	UNK	LEU	CONFLICT	UNP A0R1H7
B	929	UNK	GLU	CONFLICT	UNP A0R1H7
B	930	UNK	PRO	CONFLICT	UNP A0R1H7
B	931	UNK	VAL	CONFLICT	UNP A0R1H7
B	932	UNK	GLU	CONFLICT	UNP A0R1H7
B	933	UNK	VAL	CONFLICT	UNP A0R1H7
B	934	UNK	LEU	CONFLICT	UNP A0R1H7
B	935	UNK	SER	CONFLICT	UNP A0R1H7
B	936	UNK	ARG	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	937	UNK	ARG	CONFLICT	UNP A0R1H7
B	938	UNK	GLN	CONFLICT	UNP A0R1H7
B	939	UNK	ALA	CONFLICT	UNP A0R1H7
B	940	UNK	ARG	CONFLICT	UNP A0R1H7
B	941	UNK	ARG	CONFLICT	UNP A0R1H7
B	942	UNK	ASP	CONFLICT	UNP A0R1H7
B	943	UNK	ALA	CONFLICT	UNP A0R1H7
B	944	UNK	SER	CONFLICT	UNP A0R1H7
B	974	UNK	THR	CONFLICT	UNP A0R1H7
B	975	UNK	GLU	CONFLICT	UNP A0R1H7
B	976	UNK	TRP	CONFLICT	UNP A0R1H7
B	977	UNK	GLN	CONFLICT	UNP A0R1H7
B	978	UNK	VAL	CONFLICT	UNP A0R1H7
B	979	UNK	ARG	CONFLICT	UNP A0R1H7
B	980	UNK	GLU	CONFLICT	UNP A0R1H7
B	981	UNK	GLY	CONFLICT	UNP A0R1H7
B	982	UNK	SER	CONFLICT	UNP A0R1H7
B	983	UNK	ASP	CONFLICT	UNP A0R1H7
B	984	UNK	ASN	CONFLICT	UNP A0R1H7
B	985	UNK	ARG	CONFLICT	UNP A0R1H7
B	986	UNK	SER	CONFLICT	UNP A0R1H7
B	987	UNK	ALA	CONFLICT	UNP A0R1H7
B	988	UNK	SER	CONFLICT	UNP A0R1H7
B	989	UNK	HIS	CONFLICT	UNP A0R1H7
B	990	UNK	PRO	CONFLICT	UNP A0R1H7
B	991	UNK	SER	CONFLICT	UNP A0R1H7
B	992	UNK	THR	CONFLICT	UNP A0R1H7
B	993	UNK	GLY	CONFLICT	UNP A0R1H7
B	994	UNK	ALA	CONFLICT	UNP A0R1H7
B	995	UNK	ARG	CONFLICT	UNP A0R1H7
B	996	UNK	LEU	CONFLICT	UNP A0R1H7
B	997	UNK	GLU	CONFLICT	UNP A0R1H7
B	998	UNK	VAL	CONFLICT	UNP A0R1H7
B	999	UNK	ALA	CONFLICT	UNP A0R1H7
B	1000	UNK	ASP	CONFLICT	UNP A0R1H7
B	1001	UNK	ASP	CONFLICT	UNP A0R1H7
B	1002	UNK	GLN	CONFLICT	UNP A0R1H7
B	1003	UNK	HIS	CONFLICT	UNP A0R1H7
B	1004	UNK	VAL	CONFLICT	UNP A0R1H7
B	1005	UNK	VAL	CONFLICT	UNP A0R1H7
B	1006	UNK	LEU	CONFLICT	UNP A0R1H7
B	1007	UNK	SER	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1008	UNK	VAL	CONFLICT	UNP A0R1H7
B	1009	UNK	PRO	CONFLICT	UNP A0R1H7
B	1010	UNK	LEU	CONFLICT	UNP A0R1H7
B	1011	UNK	SER	CONFLICT	UNP A0R1H7
B	1012	UNK	GLY	CONFLICT	UNP A0R1H7
B	1013	UNK	THR	CONFLICT	UNP A0R1H7
B	1014	UNK	TRP	CONFLICT	UNP A0R1H7
B	1196	UNK	GLY	CONFLICT	UNP A0R1H7
B	1197	UNK	ARG	CONFLICT	UNP A0R1H7
B	1198	UNK	THR	CONFLICT	UNP A0R1H7
B	1199	UNK	GLY	CONFLICT	UNP A0R1H7
B	1200	UNK	ALA	CONFLICT	UNP A0R1H7
B	1201	UNK	ALA	CONFLICT	UNP A0R1H7
B	1202	UNK	GLU	CONFLICT	UNP A0R1H7
B	1203	UNK	LEU	CONFLICT	UNP A0R1H7
B	1204	UNK	THR	CONFLICT	UNP A0R1H7
B	1205	UNK	ASP	CONFLICT	UNP A0R1H7
B	1206	UNK	PRO	CONFLICT	UNP A0R1H7
B	1207	UNK	VAL	CONFLICT	UNP A0R1H7
B	1208	UNK	ARG	CONFLICT	UNP A0R1H7
B	1209	UNK	ALA	CONFLICT	UNP A0R1H7
B	1210	UNK	GLY	CONFLICT	UNP A0R1H7
B	1211	UNK	GLY	CONFLICT	UNP A0R1H7
B	1212	UNK	ALA	CONFLICT	UNP A0R1H7
B	1213	UNK	ILE	CONFLICT	UNP A0R1H7
B	1214	UNK	SER	CONFLICT	UNP A0R1H7
B	1215	UNK	ASP	CONFLICT	UNP A0R1H7
B	1216	UNK	ASN	CONFLICT	UNP A0R1H7
B	1217	UNK	ALA	CONFLICT	UNP A0R1H7
B	1218	UNK	THR	CONFLICT	UNP A0R1H7
B	1219	UNK	ASP	CONFLICT	UNP A0R1H7
B	1220	UNK	THR	CONFLICT	UNP A0R1H7
B	1221	UNK	PRO	CONFLICT	UNP A0R1H7
B	1222	UNK	ARG	CONFLICT	UNP A0R1H7
B	1223	UNK	ARG	CONFLICT	UNP A0R1H7
B	1224	UNK	ARG	CONFLICT	UNP A0R1H7
B	1225	UNK	ARG	CONFLICT	UNP A0R1H7
B	1226	UNK	ARG	CONFLICT	UNP A0R1H7
B	1227	UNK	ASP	CONFLICT	UNP A0R1H7
B	2076	UNK	GLY	CONFLICT	UNP A0R1H7
B	2077	UNK	ASP	CONFLICT	UNP A0R1H7
B	2078	UNK	ILE	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2079	UNK	ASP	CONFLICT	UNP A0R1H7
B	2080	UNK	ALA	CONFLICT	UNP A0R1H7
B	2081	UNK	GLN	CONFLICT	UNP A0R1H7
B	2082	UNK	TRP	CONFLICT	UNP A0R1H7
B	2083	UNK	GLU	CONFLICT	UNP A0R1H7
B	2084	UNK	GLN	CONFLICT	UNP A0R1H7
B	2085	UNK	LEU	CONFLICT	UNP A0R1H7
B	2086	UNK	SER	CONFLICT	UNP A0R1H7
B	2087	UNK	GLN	CONFLICT	UNP A0R1H7
B	2088	UNK	ARG	CONFLICT	UNP A0R1H7
B	2089	UNK	PHE	CONFLICT	UNP A0R1H7
B	2090	UNK	GLU	CONFLICT	UNP A0R1H7
B	2091	UNK	GLY	CONFLICT	UNP A0R1H7
B	2092	UNK	THR	CONFLICT	UNP A0R1H7
B	2093	UNK	GLY	CONFLICT	UNP A0R1H7
B	2094	UNK	HIS	CONFLICT	UNP A0R1H7
B	2095	UNK	VAL	CONFLICT	UNP A0R1H7
B	2096	UNK	VAL	CONFLICT	UNP A0R1H7
B	2097	UNK	ALA	CONFLICT	UNP A0R1H7
B	2098	UNK	THR	CONFLICT	UNP A0R1H7
B	2099	UNK	GLN	CONFLICT	UNP A0R1H7
B	2100	UNK	ALA	CONFLICT	UNP A0R1H7
B	2101	UNK	ASN	CONFLICT	UNP A0R1H7
B	2102	UNK	TRP	CONFLICT	UNP A0R1H7
B	2103	UNK	TRP	CONFLICT	UNP A0R1H7
B	2104	UNK	GLN	CONFLICT	UNP A0R1H7
B	2105	UNK	GLY	CONFLICT	UNP A0R1H7
B	2106	UNK	LYS	CONFLICT	UNP A0R1H7
B	2107	UNK	ALA	CONFLICT	UNP A0R1H7
B	2108	UNK	LEU	CONFLICT	UNP A0R1H7
B	2109	UNK	ALA	CONFLICT	UNP A0R1H7
B	2110	UNK	ALA	CONFLICT	UNP A0R1H7
B	2111	UNK	GLY	CONFLICT	UNP A0R1H7
B	2112	UNK	ARG	CONFLICT	UNP A0R1H7
B	2113	UNK	ASN	CONFLICT	UNP A0R1H7
B	2114	UNK	VAL	CONFLICT	UNP A0R1H7
B	2115	UNK	HIS	CONFLICT	UNP A0R1H7
B	2116	UNK	ALA	CONFLICT	UNP A0R1H7
B	2117	UNK	SER	CONFLICT	UNP A0R1H7
B	2118	UNK	LEU	CONFLICT	UNP A0R1H7
B	2119	UNK	PHE	CONFLICT	UNP A0R1H7
B	2120	UNK	GLY	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2121	UNK	ARG	CONFLICT	UNP A0R1H7
B	2122	UNK	ILE	CONFLICT	UNP A0R1H7
B	2123	UNK	ALA	CONFLICT	UNP A0R1H7
B	2124	UNK	ALA	CONFLICT	UNP A0R1H7
B	2125	UNK	GLY	CONFLICT	UNP A0R1H7
B	2126	UNK	ALA	CONFLICT	UNP A0R1H7
B	2127	UNK	GLU	CONFLICT	UNP A0R1H7
B	2128	UNK	ASN	CONFLICT	UNP A0R1H7
B	2129	UNK	PRO	CONFLICT	UNP A0R1H7
B	2130	UNK	GLY	CONFLICT	UNP A0R1H7
B	2131	UNK	LYS	CONFLICT	UNP A0R1H7
B	2132	UNK	GLY	CONFLICT	UNP A0R1H7
B	2133	UNK	ARG	CONFLICT	UNP A0R1H7
B	2134	UNK	TYR	CONFLICT	UNP A0R1H7
B	2135	UNK	SER	CONFLICT	UNP A0R1H7
B	2422	UNK	GLU	CONFLICT	UNP A0R1H7
B	2423	UNK	SER	CONFLICT	UNP A0R1H7
B	2424	UNK	ASP	CONFLICT	UNP A0R1H7
B	2425	UNK	ASP	CONFLICT	UNP A0R1H7
B	2426	UNK	GLU	CONFLICT	UNP A0R1H7
B	2427	UNK	ALA	CONFLICT	UNP A0R1H7
B	2428	UNK	PRO	CONFLICT	UNP A0R1H7
B	2429	UNK	ALA	CONFLICT	UNP A0R1H7
B	2430	UNK	GLY	CONFLICT	UNP A0R1H7
B	2431	UNK	THR	CONFLICT	UNP A0R1H7
B	2432	UNK	ILE	CONFLICT	UNP A0R1H7
B	2433	UNK	ARG	CONFLICT	UNP A0R1H7
B	2434	UNK	ALA	CONFLICT	UNP A0R1H7
B	2435	UNK	LEU	CONFLICT	UNP A0R1H7
B	2436	UNK	PRO	CONFLICT	UNP A0R1H7
B	2437	UNK	SER	CONFLICT	UNP A0R1H7
B	2438	UNK	PRO	CONFLICT	UNP A0R1H7
B	2439	UNK	PRO	CONFLICT	UNP A0R1H7
B	2440	UNK	ARG	CONFLICT	UNP A0R1H7
B	2441	UNK	GLY	CONFLICT	UNP A0R1H7
B	2442	UNK	TYR	CONFLICT	UNP A0R1H7
B	2443	UNK	ASN	CONFLICT	UNP A0R1H7
B	2444	UNK	PRO	CONFLICT	UNP A0R1H7
B	2445	UNK	ALA	CONFLICT	UNP A0R1H7
B	2446	UNK	PRO	CONFLICT	UNP A0R1H7
B	2447	UNK	ALA	CONFLICT	UNP A0R1H7
B	2448	UNK	PRO	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2449	UNK	GLU	CONFLICT	UNP A0R1H7
B	2450	UNK	TRP	CONFLICT	UNP A0R1H7
B	2451	UNK	ASP	CONFLICT	UNP A0R1H7
B	2452	UNK	ASP	CONFLICT	UNP A0R1H7
B	2453	UNK	LEU	CONFLICT	UNP A0R1H7
C	929	UNK	GLU	CONFLICT	UNP A0R1H7
C	930	UNK	PRO	CONFLICT	UNP A0R1H7
C	931	UNK	VAL	CONFLICT	UNP A0R1H7
C	932	UNK	GLU	CONFLICT	UNP A0R1H7
C	933	UNK	VAL	CONFLICT	UNP A0R1H7
C	934	UNK	LEU	CONFLICT	UNP A0R1H7
C	935	UNK	SER	CONFLICT	UNP A0R1H7
C	936	UNK	ARG	CONFLICT	UNP A0R1H7
C	937	UNK	ARG	CONFLICT	UNP A0R1H7
C	938	UNK	GLN	CONFLICT	UNP A0R1H7
C	939	UNK	ALA	CONFLICT	UNP A0R1H7
C	940	UNK	ARG	CONFLICT	UNP A0R1H7
C	941	UNK	ARG	CONFLICT	UNP A0R1H7
C	942	UNK	ASP	CONFLICT	UNP A0R1H7
C	943	UNK	ALA	CONFLICT	UNP A0R1H7
C	944	UNK	SER	CONFLICT	UNP A0R1H7
C	974	UNK	THR	CONFLICT	UNP A0R1H7
C	975	UNK	GLU	CONFLICT	UNP A0R1H7
C	976	UNK	TRP	CONFLICT	UNP A0R1H7
C	977	UNK	GLN	CONFLICT	UNP A0R1H7
C	978	UNK	VAL	CONFLICT	UNP A0R1H7
C	979	UNK	ARG	CONFLICT	UNP A0R1H7
C	980	UNK	GLU	CONFLICT	UNP A0R1H7
C	981	UNK	GLY	CONFLICT	UNP A0R1H7
C	982	UNK	SER	CONFLICT	UNP A0R1H7
C	983	UNK	ASP	CONFLICT	UNP A0R1H7
C	984	UNK	ASN	CONFLICT	UNP A0R1H7
C	985	UNK	ARG	CONFLICT	UNP A0R1H7
C	986	UNK	SER	CONFLICT	UNP A0R1H7
C	987	UNK	ALA	CONFLICT	UNP A0R1H7
C	988	UNK	SER	CONFLICT	UNP A0R1H7
C	989	UNK	HIS	CONFLICT	UNP A0R1H7
C	990	UNK	PRO	CONFLICT	UNP A0R1H7
C	991	UNK	SER	CONFLICT	UNP A0R1H7
C	992	UNK	THR	CONFLICT	UNP A0R1H7
C	993	UNK	GLY	CONFLICT	UNP A0R1H7
C	994	UNK	ALA	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	995	UNK	ARG	CONFLICT	UNP A0R1H7
C	996	UNK	LEU	CONFLICT	UNP A0R1H7
C	997	UNK	GLU	CONFLICT	UNP A0R1H7
C	998	UNK	VAL	CONFLICT	UNP A0R1H7
C	999	UNK	ALA	CONFLICT	UNP A0R1H7
C	1000	UNK	ASP	CONFLICT	UNP A0R1H7
C	1001	UNK	ASP	CONFLICT	UNP A0R1H7
C	1002	UNK	GLN	CONFLICT	UNP A0R1H7
C	1003	UNK	HIS	CONFLICT	UNP A0R1H7
C	1004	UNK	VAL	CONFLICT	UNP A0R1H7
C	1005	UNK	VAL	CONFLICT	UNP A0R1H7
C	1006	UNK	LEU	CONFLICT	UNP A0R1H7
C	1007	UNK	SER	CONFLICT	UNP A0R1H7
C	1008	UNK	VAL	CONFLICT	UNP A0R1H7
C	1009	UNK	PRO	CONFLICT	UNP A0R1H7
C	1010	UNK	LEU	CONFLICT	UNP A0R1H7
C	1011	UNK	SER	CONFLICT	UNP A0R1H7
C	1012	UNK	GLY	CONFLICT	UNP A0R1H7
C	1013	UNK	THR	CONFLICT	UNP A0R1H7
C	1014	UNK	TRP	CONFLICT	UNP A0R1H7
C	1196	UNK	GLY	CONFLICT	UNP A0R1H7
C	1197	UNK	ARG	CONFLICT	UNP A0R1H7
C	1198	UNK	THR	CONFLICT	UNP A0R1H7
C	1199	UNK	GLY	CONFLICT	UNP A0R1H7
C	1200	UNK	ALA	CONFLICT	UNP A0R1H7
C	1201	UNK	ALA	CONFLICT	UNP A0R1H7
C	1202	UNK	GLU	CONFLICT	UNP A0R1H7
C	1203	UNK	LEU	CONFLICT	UNP A0R1H7
C	1204	UNK	THR	CONFLICT	UNP A0R1H7
C	1205	UNK	ASP	CONFLICT	UNP A0R1H7
C	1206	UNK	PRO	CONFLICT	UNP A0R1H7
C	1207	UNK	VAL	CONFLICT	UNP A0R1H7
C	1208	UNK	ARG	CONFLICT	UNP A0R1H7
C	1209	UNK	ALA	CONFLICT	UNP A0R1H7
C	1210	UNK	GLY	CONFLICT	UNP A0R1H7
C	1211	UNK	GLY	CONFLICT	UNP A0R1H7
C	1212	UNK	ALA	CONFLICT	UNP A0R1H7
C	1213	UNK	ILE	CONFLICT	UNP A0R1H7
C	1214	UNK	SER	CONFLICT	UNP A0R1H7
C	1215	UNK	ASP	CONFLICT	UNP A0R1H7
C	1216	UNK	ASN	CONFLICT	UNP A0R1H7
C	1217	UNK	ALA	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1218	UNK	THR	CONFLICT	UNP A0R1H7
C	1219	UNK	ASP	CONFLICT	UNP A0R1H7
C	1220	UNK	THR	CONFLICT	UNP A0R1H7
C	1221	UNK	PRO	CONFLICT	UNP A0R1H7
C	1222	UNK	ARG	CONFLICT	UNP A0R1H7
C	1223	UNK	ARG	CONFLICT	UNP A0R1H7
C	1224	UNK	ARG	CONFLICT	UNP A0R1H7
C	1225	UNK	ARG	CONFLICT	UNP A0R1H7
C	1226	UNK	ARG	CONFLICT	UNP A0R1H7
C	1227	UNK	ASP	CONFLICT	UNP A0R1H7
C	2076	UNK	GLY	CONFLICT	UNP A0R1H7
C	2077	UNK	ASP	CONFLICT	UNP A0R1H7
C	2078	UNK	ILE	CONFLICT	UNP A0R1H7
C	2079	UNK	ASP	CONFLICT	UNP A0R1H7
C	2080	UNK	ALA	CONFLICT	UNP A0R1H7
C	2081	UNK	GLN	CONFLICT	UNP A0R1H7
C	2082	UNK	TRP	CONFLICT	UNP A0R1H7
C	2083	UNK	GLU	CONFLICT	UNP A0R1H7
C	2084	UNK	GLN	CONFLICT	UNP A0R1H7
C	2085	UNK	LEU	CONFLICT	UNP A0R1H7
C	2086	UNK	SER	CONFLICT	UNP A0R1H7
C	2087	UNK	GLN	CONFLICT	UNP A0R1H7
C	2088	UNK	ARG	CONFLICT	UNP A0R1H7
C	2089	UNK	PHE	CONFLICT	UNP A0R1H7
C	2090	UNK	GLU	CONFLICT	UNP A0R1H7
C	2091	UNK	GLY	CONFLICT	UNP A0R1H7
C	2092	UNK	THR	CONFLICT	UNP A0R1H7
C	2093	UNK	GLY	CONFLICT	UNP A0R1H7
C	2094	UNK	HIS	CONFLICT	UNP A0R1H7
C	2095	UNK	VAL	CONFLICT	UNP A0R1H7
C	2096	UNK	VAL	CONFLICT	UNP A0R1H7
C	2097	UNK	ALA	CONFLICT	UNP A0R1H7
C	2098	UNK	THR	CONFLICT	UNP A0R1H7
C	2099	UNK	GLN	CONFLICT	UNP A0R1H7
C	2100	UNK	ALA	CONFLICT	UNP A0R1H7
C	2101	UNK	ASN	CONFLICT	UNP A0R1H7
C	2102	UNK	TRP	CONFLICT	UNP A0R1H7
C	2103	UNK	TRP	CONFLICT	UNP A0R1H7
C	2104	UNK	GLN	CONFLICT	UNP A0R1H7
C	2105	UNK	GLY	CONFLICT	UNP A0R1H7
C	2106	UNK	LYS	CONFLICT	UNP A0R1H7
C	2107	UNK	ALA	CONFLICT	UNP A0R1H7

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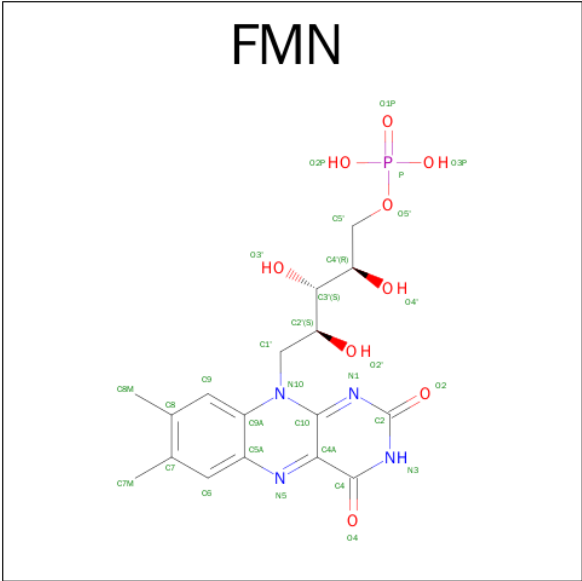
Chain	Residue	Modelled	Actual	Comment	Reference
C	2108	UNK	LEU	CONFLICT	UNP A0R1H7
C	2109	UNK	ALA	CONFLICT	UNP A0R1H7
C	2110	UNK	ALA	CONFLICT	UNP A0R1H7
C	2111	UNK	GLY	CONFLICT	UNP A0R1H7
C	2112	UNK	ARG	CONFLICT	UNP A0R1H7
C	2113	UNK	ASN	CONFLICT	UNP A0R1H7
C	2114	UNK	VAL	CONFLICT	UNP A0R1H7
C	2115	UNK	HIS	CONFLICT	UNP A0R1H7
C	2116	UNK	ALA	CONFLICT	UNP A0R1H7
C	2117	UNK	SER	CONFLICT	UNP A0R1H7
C	2118	UNK	LEU	CONFLICT	UNP A0R1H7
C	2119	UNK	PHE	CONFLICT	UNP A0R1H7
C	2120	UNK	GLY	CONFLICT	UNP A0R1H7
C	2121	UNK	ARG	CONFLICT	UNP A0R1H7
C	2122	UNK	ILE	CONFLICT	UNP A0R1H7
C	2123	UNK	ALA	CONFLICT	UNP A0R1H7
C	2124	UNK	ALA	CONFLICT	UNP A0R1H7
C	2125	UNK	GLY	CONFLICT	UNP A0R1H7
C	2126	UNK	ALA	CONFLICT	UNP A0R1H7
C	2127	UNK	GLU	CONFLICT	UNP A0R1H7
C	2128	UNK	ASN	CONFLICT	UNP A0R1H7
C	2129	UNK	PRO	CONFLICT	UNP A0R1H7
C	2130	UNK	GLY	CONFLICT	UNP A0R1H7
C	2131	UNK	LYS	CONFLICT	UNP A0R1H7
C	2132	UNK	GLY	CONFLICT	UNP A0R1H7
C	2133	UNK	ARG	CONFLICT	UNP A0R1H7
C	2134	UNK	TYR	CONFLICT	UNP A0R1H7
C	2135	UNK	SER	CONFLICT	UNP A0R1H7
C	2422	UNK	GLU	CONFLICT	UNP A0R1H7
C	2423	UNK	SER	CONFLICT	UNP A0R1H7
C	2424	UNK	ASP	CONFLICT	UNP A0R1H7
C	2425	UNK	ASP	CONFLICT	UNP A0R1H7
C	2426	UNK	GLU	CONFLICT	UNP A0R1H7
C	2427	UNK	ALA	CONFLICT	UNP A0R1H7
C	2428	UNK	PRO	CONFLICT	UNP A0R1H7
C	2429	UNK	ALA	CONFLICT	UNP A0R1H7
C	2430	UNK	GLY	CONFLICT	UNP A0R1H7
C	2431	UNK	THR	CONFLICT	UNP A0R1H7
C	2432	UNK	ILE	CONFLICT	UNP A0R1H7
C	2433	UNK	ARG	CONFLICT	UNP A0R1H7
C	2434	UNK	ALA	CONFLICT	UNP A0R1H7
C	2435	UNK	LEU	CONFLICT	UNP A0R1H7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2436	UNK	PRO	CONFLICT	UNP A0R1H7
C	2437	UNK	SER	CONFLICT	UNP A0R1H7
C	2438	UNK	PRO	CONFLICT	UNP A0R1H7
C	2439	UNK	PRO	CONFLICT	UNP A0R1H7
C	2440	UNK	ARG	CONFLICT	UNP A0R1H7
C	2441	UNK	GLY	CONFLICT	UNP A0R1H7
C	2442	UNK	TYR	CONFLICT	UNP A0R1H7
C	2443	UNK	ASN	CONFLICT	UNP A0R1H7
C	2444	UNK	PRO	CONFLICT	UNP A0R1H7
C	2445	UNK	ALA	CONFLICT	UNP A0R1H7
C	2446	UNK	PRO	CONFLICT	UNP A0R1H7
C	2447	UNK	ALA	CONFLICT	UNP A0R1H7
C	2448	UNK	PRO	CONFLICT	UNP A0R1H7
C	2449	UNK	GLU	CONFLICT	UNP A0R1H7
C	2450	UNK	TRP	CONFLICT	UNP A0R1H7
C	2451	UNK	ASP	CONFLICT	UNP A0R1H7
C	2452	UNK	ASP	CONFLICT	UNP A0R1H7
C	2453	UNK	LEU	CONFLICT	UNP A0R1H7

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	E	1	Total	C	N	O	P	0
			31	17	4	9	1	

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Mol	Chain	Residues	Atoms					AltConf
2	F	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	C	1	Total	C	N	O	P	0
			31	17	4	9	1	




GLU	ARG	ALA	E2074	D2136	W2265	L2398	M2481	R2610	L2709	D2805	P2901	L2989	GLU
LEU	VAL	ALA		E2137	W2268	L2401	E2482	V2611	L2710	R2806	P2902	G2992	THR
ASN	THR	ARG	X2077	V2140	Q2268	I2403	L2487	R2612	G2711	R2807	E2903	L2993	ILE
LEU	LYS	ARG	X2078	V2141	Q2274	L2403	L2487	R2613	E2712	R2808	E2903	L2993	TYR
GLY	THR	GLY	X2078	T2163	L2274	L2403	V2492	K2614	V2713	L2809	L2906	T2994	HIS
ILE	TRP	ILE	X2080	T2164	L2277	D2404	L2495	S2615	V2717	F2811	A2911	G2998	ASP
ASP	GLU	VAL	X2081	T2165	I2277	M2405	L2495	R2616	V2718	L2812	A2911	G2998	ASP
GLY	LEU	VAL	X2082	R2286	R2286	L2408	K2503	T2620	V2722	Q2815	R2916	H3001	VAL
ALA	PRO	GLY	X2083	A2166	L2287	L2408	K2503	V2621	V2722	Q2815	R2916	H3001	VAL
ALA	GLY	PRO	X2084	T2167	H2288	A2409	E2505	G2622	V2727	L2820	G2919	L3005	GLY
GLU	TRP	ALA	X2085	R2170	H2288	A2412	E2505	A2623	V2727	L2820	G2919	L3005	GLY
ALA	ALA	ALA	X2086				W2512	Q2624	V2730	L2821	G2920	V3009	ASP
ASP	LYS	GLY	X2087	D2173	L2291	M2416	W2512	L2625	P2736	L2822	G2921	V3009	ASP
LEU	HIS	GLY	X2088	D2174	S2294	S2417	Y2513	L2626	P2736	L2822	G2921	V3009	ASP
GLY	VAL	ALA	X2089	R2175	P2296	G2418	L2520	P2631	C2740	L2823	G2922	V3009	ASP
ALA	THR	SER	X2090	L2176	P2296	G2418	L2520	P2631	C2740	L2823	G2922	V3009	ASP
LEU	VAL	GLY	X2091	L2176	P2296	G2418	L2520	P2631	C2740	L2823	G2922	V3009	ASP
LYS	GLU	GLY	X2092	K2180	R2297	D2421	E2523	V2632	A2743	L2824	G2923	V3009	ASP
GLY	PHE	VAL	X2093	K2180	R2297	D2421	E2523	V2632	A2743	L2824	G2923	V3009	ASP
GLN	ALA	VAL	X2094	R2188	M2299	X2425	E2525	R2645	S2746	L2825	G2924	V3009	ASP
VAL	LEU	ASP	X2095	F2189	F2300	X2426	E2525	R2645	S2746	L2825	G2924	V3009	ASP
GLY	THR	ASP	X2096	F2189	F2300	X2426	E2525	R2645	S2746	L2825	G2924	V3009	ASP
THR	THR	THR	X2097	T2192	D2303	X2427	E2526	R2646	S2746	L2826	G2925	V3009	ASP
LYS	ARG	ARG	X2098	T2192	D2303	X2427	E2526	R2646	S2746	L2826	G2925	V3009	ASP
LEU	GLU	GLU	X2099	L2193	Y2306	X2428	E2528	R2647	S2746	L2827	G2926	V3009	ASP
ALA	GLY	GLY	X2100	W2194	Y2306	X2429	E2528	R2647	S2746	L2827	G2926	V3009	ASP
ARG	GLY	GLY	X2101	W2194	Y2306	X2429	E2528	R2647	S2746	L2827	G2926	V3009	ASP
THR	SER	SER	X2102	W2195	K2310	X2430	E2530	R2648	S2746	L2828	G2927	V3009	ASP
TYR	SER	SER	X2103	W2196	K2310	X2431	E2530	R2648	S2746	L2828	G2927	V3009	ASP
LYS	VAL	VAL	X2104	P2197	R2319	X2432	E2533	R2649	S2746	L2829	G2928	V3009	ASP
PRO	ARG	ARG	X2105	A2198	R2319	X2433	E2533	R2649	S2746	L2829	G2928	V3009	ASP
PHE	GLY	GLY	X2106	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
GLY	GLY	GLY	X2107	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
PRO	ASP	ASP	X2108	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
LEU	LEU	LEU	X2109	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
VAL	GLY	GLY	X2110	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
LEU	GLY	GLY	X2111	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
SER	GLY	GLY	X2112	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
ASP	LEU	LEU	X2113	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
ASP	LEU	LEU	X2114	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
ALA	HIS	HIS	X2115	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
ILE	ALA	ALA	X2116	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
ASN	GLY	GLY	X2117	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
ASP	ALA	ALA	X2118	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
GLN	LEU	LEU	X2119	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
LEU	ALA	ALA	X2120	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
ARG	SER	SER	X2121	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
THR	ALA	ALA	X2122	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
VAL	ALA	ALA	X2123	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
LEU	ASP	ASP	X2124	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
GLY	VAL	VAL	X2125	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
PRO	ASP	ASP	X2126	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
SER	LYS	LYS	X2127	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
GLY	VAL	VAL	X2128	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
LYS	ILE	ILE	X2129	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
ARG	ASP	ASP	X2130	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
PRO	GLY	GLY	X2131	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
ALA	ALA	ALA	X2132	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
THR	VAL	VAL	X2133	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
ILE	ALA	ALA	X2134	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP
THR	ALA	ALA	X2135	D2205	S2331	X2434	E2533	R2649	S2746	L2829	G2928	V3009	ASP

• Molecule 1: FATTY ACID SYNTHASE

Chain B:  56% 33% 9%

MET	THR	ILE	TYR	GLU	HIS	ASP	ARG	VAL	PRO	ALA	GLY	TRP	ASN	ASP	GLU	SER	GLY	SER	ASP	ARG	THR	ALA	ASP	GLY	ALA	ALA	ASP	THR	A31	R32	A33	L34	V35	L36	R37	L38	G41	E42	P43	Y44	A45	V46	A47	G50	S53	L56	S70	E71	E78	E84	P85
	S88	E89	L90	R94	P95	A106	L107	E111	P112	V113	K117	L118	L119	V126	P127	G128	V129	Q133	V137	R138	A141	R142	Q143	G144	M145	D146	L147	T148	A149	T150	P151	P152	V153	A154	V155	Q160	L163	A164	A167	K171	G172	A173	K174	D175	V176	E177	L178				

ALA	I1703	I1611	R1495	V1408	K1304	A1193	T1096	X989	L787	G676	H584	L479	V376	D288	L179
ALA	G1704	G1612	S1496	H1412	D1307	I1194	V1097	X990	T895	A680	H585	R483	P377	P289	A180
PRO	V1705	R1613	S1496	H1412	D1307	R1195	P1098	X991	A896	A680	S586	R483	P377	P289	L181
ALA	S1707	R1614	R1503	P1413	Q1308	X1196	D1100	X992	A899	A681	E587	I485	R381	V292	L182
PRO	T1710	H1615	R1504	D1414	X1198	X1197	V1103	X993	G900	N682	D589	Q384	Q384	E293	Q183
SER	V1711	H1616	Q1507	C1415	D1310	X1199	G1104	X994	I901	N682	L590	I488	T389	V294	L184
GLY	V1712	H1617	T1508	V1416	F1311	X1204	C1104	X995	V904	N684	L593	I489	T390	L301	R195
PRO	G1713	L1618	T1508	L1417	R1312	X1205	C1106	X996	H795	S686	L594	I490	V390	I305	I198
ARG	L1714	P1620	D1511	T1420	V1314	X1206	F1110	X997	F915	S687	L595	I490	V393	E306	G202
PRO	P1722	R1621	D1514	Q1421	R1315	X1207	F1111	X1000	L824	R688	V598	Q500	P394	I307	D203
ASP	E1723	F1623	D1514	F1422	R1316	X1207	F1111	X1001	L824	D684	V598	V501	P395	I307	R204
ASP	T1725	L1625	V1519	T1423	G1317	X1212	A1117	X1002	A928	I695	R602	R504	W400	W311	P205
THR	S1726	L1625	V1519	Q1424	I1318	X1213	A1118	X1003	X929	H696	R602	R505	W400	T314	P206
PHE	E1730	R1634	L1530	V1425	V1320	X1214	T1119	X1004	X930	E697	N606	P405	P405	V315	N207
ASP	E1730	R1634	L1530	V1425	V1320	X1215	E1120	X1005	X931	E698	N606	Q508	T405	G316	V208
ALA	L1732	V1637	I1532	V1430	E1323	X1216	F1123	X1006	X932	E699	G613	R511	V407	L317	S209
ALA	L1732	V1637	I1532	A1431	X1324	X1217	F1124	X1007	X933	I700	G614	R511	V408	E327	V210
ASP	L1733	P1638	V1533	V1435	V1324	X1218	P1124	X1008	X934	A701	G614	R511	V408	E327	T211
ALA	A1639	A1639	F1535	V1327	E1326	X1219	T1126	X1009	X935	L709	P618	A515	L410	S328	L222
THR	E1735	N1536	N1536	Q1441	V1327	X1220	E1127	X1010	X936	L709	P618	A515	L410	S328	L222
VAL	R1736	T1651	L1537	Q1441	V1327	X1221	E1127	X1011	X936	L709	P618	A515	L410	S328	L222
ALA	D1737	W1652	R1538	V1445	X1328	X1224	G1128	X1012	X937	A713	S621	I517	D412	L330	L222
LEU	L1741	K1656	G1539	V1445	X1329	X1225	L1129	X1013	X938	A713	S621	I517	D412	L330	L222
ILE	L1741	K1656	G1539	V1445	X1329	X1225	L1129	X1013	X938	A713	S621	I517	D412	L330	L222
ALA	D1745	P1657	S1540	A1448	I1331	X1226	L1132	X1014	X939	A716	W624	V618	V415	W336	V232
LEU	D1745	P1657	S1540	A1448	I1331	X1226	L1132	X1014	X939	A716	W624	V618	V415	W336	V232
SER	ASP	E1659	Y1542	A1450	M1336	X1227	V1133	X1015	X940	W745	D641	E538	R427	A348	T251
ALA	ASP	E1659	A1543	A1450	M1336	X1227	V1133	X1015	X940	W745	D641	E538	R427	A348	T251
LYS	PRO	G1661	I1544	V1455	A1338	R1237	P1146	T1020	X941	W745	D641	E538	R427	A348	T251
NET	GLU	R1662	L1544	V1455	A1338	R1237	P1146	T1020	X941	W745	D641	E538	R427	A348	T251
ARG	PRO	K1663	L1544	V1455	A1338	R1237	P1146	T1020	X941	W745	D641	E538	R427	A348	T251
ILE	GLU	E1552	L1544	V1455	A1338	R1237	P1146	T1020	X941	W745	D641	E538	R427	A348	T251
ASP	PRO	E1553	L1544	V1455	A1338	R1237	P1146	T1020	X941	W745	D641	E538	R427	A348	T251
GLN	GLU	E1555	L1544	V1455	A1338	R1237	P1146	T1020	X941	W745	D641	E538	R427	A348	T251
ILE	ALA	E1556	L1544	V1455	A1338	R1237	P1146	T1020	X941	W745	D641	E538	R427	A348	T251
GLU	ASP	E1557	L1544	V1455	A1338	R1237	P1146	T1020	X941	W745	D641	E538	R427	A348	T251
ALA	GLU	W1671	R1560	V1464	Y1350	A1274	D1163	V1045	X967	W751	E654	S545	D441	G355	A266
LEU	PRO	Q1672	R1561	V1467	A1351	A1275	D1164	V1046	X967	W751	E654	S545	D441	G355	A266
ASP	THR	F1673	R1562	V1468	A1351	A1275	D1164	V1046	X967	W751	E654	S545	D441	G355	A266
SER	ALA	A1674	Q1563	E1469	P1353	H1277	D1164	V1046	X967	W751	E654	S545	D441	G355	A266
ILE	ASP	W1679	L1564	E1470	P1353	H1277	D1164	V1046	X967	W751	E654	S545	D441	G355	A266
GLU	PRO	D1684	L1564	E1471	Q1358	V1279	P1171	V1068	A971	S763	W657	F549	K443	D858	E267
ILE	ALA	D1684	L1564	E1471	Q1358	V1279	P1171	V1068	A971	S763	W657	F549	K443	D858	E267
THR	GLU	L1685	D1578	E1471	Q1358	V1279	P1171	V1068	A971	S763	W657	F549	K443	D858	E267
ASP	GLU	L1686	V1579	E1471	Q1358	V1279	P1171	V1068	A971	S763	W657	F549	K443	D858	E267
GLY	ALA	F1687	P1580	L1474	M1362	D1283	V1174	V1077	X976	D766	W661	P551	V445	L360	E270
ALA	ALA	F1687	F1581	R1480	V1376	G1284	R1177	T1084	X978	K768	K662	S559	N450	T361	A271
ALA	PRO	E1690	H1582	R1480	V1376	G1284	R1177	T1084	X978	K768	K662	S559	N450	T361	A271
SER	ALA	E1690	H1582	R1480	V1376	G1284	R1177	T1084	X978	K768	K662	S559	N450	T361	A271
SER	ALA	E1690	H1582	R1480	V1376	G1284	R1177	T1084	X978	K768	K662	S559	N450	T361	A271
ARG	ALA	G1694	L1586	M1484	D1381	P1286	G1088	F1087	X980	T776	W666	I563	G460	K276	K276
ASN	ALA	L1695	V1590	H1485	D1381	P1286	G1088	F1087	X980	T776	W666	I563	G460	K276	K276
ASN	ALA	L1695	V1590	H1485	D1381	P1286	G1088	F1087	X980	T776	W666	I563	G460	K276	K276
GLN	PRO	R1699	E1598	I1487	S1391	P1289	L1185	X1090	X983	W779	W669	I576	Q462	V367	G280
LEU	ALA	F1700	V1488	V1488	P1400	K1291	L1188	A1092	X985	D761	G670	E577	F468	R369	G281
LEU	PRO	V1701	R1490	R1490	T1401	L1292	L1188	A1092	X985	D761	G670	E577	F468	R369	G281
VAL	VAL	E1702	K1605	D1491	A1405	W1295	R1191	T1093	X986	F782	W671	R580	L475	I373	V286
							F1192	L1095	X988	E784	N674	G583	E476	I375	F287







4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON I	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.24	0/20319	0.48	0/27667
1	B	0.24	0/20319	0.48	0/27667
1	C	0.24	0/20319	0.48	0/27667
1	D	0.24	0/20319	0.48	0/27667
1	E	0.24	0/20319	0.48	0/27667
1	F	0.24	0/20319	0.48	0/27667
All	All	0.24	0/121914	0.48	0/166002

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	5
1	F	0	5
All	All	0	30

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1148	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	150	THR	Peptide
1	A	202	GLY	Peptide
1	A	2584	ASP	Peptide
1	A	357	GLY	Peptide
1	B	1148	GLU	Peptide
1	B	150	THR	Peptide
1	B	202	GLY	Peptide
1	B	2584	ASP	Peptide
1	B	357	GLY	Peptide
1	C	1148	GLU	Peptide
1	C	150	THR	Peptide
1	C	202	GLY	Peptide
1	C	2584	ASP	Peptide
1	C	357	GLY	Peptide
1	D	1148	GLU	Peptide
1	D	150	THR	Peptide
1	D	202	GLY	Peptide
1	D	2584	ASP	Peptide
1	D	357	GLY	Peptide
1	E	1148	GLU	Peptide
1	E	150	THR	Peptide
1	E	202	GLY	Peptide
1	E	2584	ASP	Peptide
1	E	357	GLY	Peptide
1	F	1148	GLU	Peptide
1	F	150	THR	Peptide
1	F	202	GLY	Peptide
1	F	2584	ASP	Peptide
1	F	357	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	21020	0	20990	1056	0
1	B	21020	0	20990	1067	0
1	C	21020	0	20990	1051	0
1	D	21020	0	20990	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	21020	0	20990	0	0
1	F	21020	0	20990	0	0
2	A	31	0	19	5	0
2	B	31	0	19	5	0
2	C	31	0	19	4	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	F	31	0	19	0	0
All	All	126306	0	126054	3117	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 25.

All (3117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ARG:O	1:A:2435:UNK:HG2	1.31	1.30
1:B:793:ARG:O	1:B:2435:UNK:HG2	1.31	1.28
1:B:2100:UNK:O	1:B:2103:UNK:HG3	1.36	1.26
1:A:2105:UNK:O	1:A:2108:UNK:HG3	1.34	1.25
1:B:2105:UNK:O	1:B:2108:UNK:HG3	1.34	1.25
1:C:2100:UNK:O	1:C:2103:UNK:HG3	1.36	1.23
1:C:793:ARG:O	1:C:2435:UNK:HG2	1.31	1.23
1:A:2093:UNK:HG1	1:A:2129:UNK:O	1.40	1.22
1:A:2100:UNK:O	1:A:2103:UNK:HG3	1.36	1.21
1:C:2093:UNK:HG1	1:C:2129:UNK:O	1.39	1.21
1:C:2105:UNK:O	1:C:2108:UNK:HG3	1.34	1.21
1:B:992:UNK:CG	1:B:996:UNK:HG3	1.72	1.20
1:C:992:UNK:CG	1:C:996:UNK:HG3	1.72	1.18
1:B:2093:UNK:HG1	1:B:2129:UNK:O	1.39	1.18
1:A:992:UNK:CG	1:A:996:UNK:HG3	1.72	1.18
1:B:2451:UNK:HG1	1:B:2454:ASP:OD2	1.44	1.17
1:C:2451:UNK:HG1	1:C:2454:ASP:OD2	1.44	1.16
1:A:2451:UNK:HG1	1:A:2454:ASP:OD2	1.44	1.15
1:C:2094:UNK:HG2	1:C:2096:UNK:HG3	1.32	1.12
1:C:2450:UNK:HG1	1:C:3016:ALA:HB1	1.23	1.11
1:A:2450:UNK:HG1	1:A:3016:ALA:HB1	1.23	1.11
1:B:2097:UNK:O	1:B:2100:UNK:HG3	1.51	1.10
1:B:2450:UNK:HG1	1:B:3016:ALA:HB1	1.23	1.09
1:A:2097:UNK:O	1:A:2100:UNK:HG3	1.51	1.09
1:C:2097:UNK:O	1:C:2100:UNK:HG3	1.51	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:975:UNK:HG3	1:B:993:UNK:CG	1.83	1.09
1:A:975:UNK:HG3	1:A:993:UNK:CG	1.82	1.08
1:A:2094:UNK:HG2	1:A:2096:UNK:HG3	1.32	1.08
1:C:975:UNK:HG3	1:C:993:UNK:CG	1.83	1.07
1:B:2094:UNK:HG2	1:B:2096:UNK:HG3	1.32	1.07
1:A:981:UNK:HG1	1:A:987:UNK:HG2	1.37	1.06
1:C:981:UNK:HG1	1:C:987:UNK:HG2	1.37	1.04
1:C:934:UNK:O	1:C:937:UNK:HG3	1.57	1.04
1:A:934:UNK:O	1:A:937:UNK:HG3	1.58	1.03
1:B:981:UNK:HG1	1:B:987:UNK:HG2	1.37	1.02
1:B:934:UNK:O	1:B:937:UNK:HG3	1.57	1.02
1:B:2094:UNK:CG	1:B:2096:UNK:HG3	1.90	1.02
1:C:975:UNK:CG	1:C:993:UNK:HG1	1.90	1.01
1:C:992:UNK:CG	1:C:996:UNK:CG	2.39	1.01
1:B:975:UNK:CG	1:B:993:UNK:HG1	1.90	1.01
1:C:2094:UNK:CG	1:C:2096:UNK:HG3	1.90	1.01
1:A:975:UNK:CG	1:A:993:UNK:HG1	1.89	1.01
1:A:2094:UNK:CG	1:A:2096:UNK:HG3	1.90	1.00
1:C:932:UNK:O	1:C:936:UNK:HG2	1.61	1.00
1:B:2088:UNK:O	1:B:2091:UNK:HG3	1.61	1.00
1:A:992:UNK:CG	1:A:996:UNK:CG	2.39	1.00
1:A:2113:UNK:O	1:A:2116:UNK:HG3	1.62	1.00
1:C:2113:UNK:O	1:C:2116:UNK:HG3	1.62	1.00
1:B:992:UNK:CG	1:B:996:UNK:CG	2.39	0.99
1:B:2433:UNK:HA	1:B:2524:CYS:HB3	1.44	0.99
1:B:1220:UNK:HG3	1:B:1221:UNK:N	1.78	0.99
1:A:2088:UNK:O	1:A:2091:UNK:HG3	1.61	0.99
1:B:976:UNK:HG3	1:B:993:UNK:HB1	1.43	0.99
1:C:2088:UNK:O	1:C:2091:UNK:HG3	1.61	0.99
1:B:932:UNK:O	1:B:936:UNK:HG2	1.61	0.99
1:B:792:ALA:O	1:B:2433:UNK:CG	2.12	0.98
1:A:992:UNK:HG1	1:A:996:UNK:HG3	1.41	0.98
1:A:932:UNK:O	1:A:936:UNK:HG2	1.61	0.98
1:A:792:ALA:O	1:A:2433:UNK:CG	2.12	0.98
1:B:2113:UNK:O	1:B:2116:UNK:HG3	1.62	0.98
1:C:1220:UNK:HG3	1:C:1221:UNK:N	1.78	0.98
1:C:792:ALA:O	1:C:2433:UNK:CG	2.12	0.98
1:C:992:UNK:HG1	1:C:996:UNK:HG3	1.41	0.98
1:A:976:UNK:HG3	1:A:993:UNK:HB1	1.43	0.98
1:B:992:UNK:HG1	1:B:996:UNK:HG3	1.41	0.97
1:C:975:UNK:HG3	1:C:993:UNK:HG1	0.99	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2096:UNK:O	1:B:2099:UNK:HG3	1.65	0.97
1:A:2433:UNK:HA	1:A:2524:CYS:HB3	1.44	0.97
1:C:1003:UNK:HG2	1:C:1004:UNK:N	1.78	0.97
1:B:975:UNK:HG3	1:B:993:UNK:HG1	0.99	0.97
1:C:407:VAL:HB	1:C:933:UNK:HG1	1.47	0.96
1:A:3080:ARG:HG3	1:A:3080:ARG:HH11	1.29	0.96
1:C:2096:UNK:O	1:C:2099:UNK:HG3	1.65	0.96
1:C:2433:UNK:HA	1:C:2524:CYS:HB3	1.44	0.96
1:B:1003:UNK:HG2	1:B:1004:UNK:N	1.78	0.96
1:A:2096:UNK:O	1:A:2099:UNK:HG3	1.65	0.96
1:B:407:VAL:HB	1:B:933:UNK:HG1	1.47	0.96
1:C:3080:ARG:HG3	1:C:3080:ARG:HH11	1.29	0.96
1:A:407:VAL:HB	1:A:933:UNK:HG1	1.47	0.96
1:A:1220:UNK:HG3	1:A:1221:UNK:N	1.78	0.95
1:A:793:ARG:HD3	1:A:2435:UNK:HG1	1.48	0.95
1:C:976:UNK:HG3	1:C:993:UNK:HB1	1.43	0.95
1:A:975:UNK:HG3	1:A:993:UNK:HG1	0.99	0.95
1:B:3080:ARG:HG3	1:B:3080:ARG:HH11	1.29	0.95
1:A:792:ALA:O	1:A:2433:UNK:HG1	1.67	0.94
1:C:792:ALA:O	1:C:2433:UNK:HG1	1.67	0.94
1:A:1003:UNK:HG2	1:A:1004:UNK:N	1.79	0.94
1:B:792:ALA:O	1:B:2433:UNK:HG1	1.67	0.94
1:B:793:ARG:HD3	1:B:2435:UNK:HG1	1.48	0.94
1:B:992:UNK:HG1	1:B:996:UNK:CG	1.97	0.93
1:C:793:ARG:HD3	1:C:2435:UNK:HG1	1.48	0.93
1:A:793:ARG:O	1:A:2435:UNK:CG	2.16	0.93
1:C:793:ARG:O	1:C:2435:UNK:CG	2.17	0.93
1:A:992:UNK:HG1	1:A:996:UNK:CG	1.97	0.93
1:B:793:ARG:O	1:B:2435:UNK:CG	2.17	0.93
1:C:1212:UNK:HG2	1:C:1342:ARG:HH21	1.32	0.93
1:A:929:UNK:O	1:A:930:UNK:HG3	1.69	0.93
1:A:2127:UNK:O	1:A:2130:UNK:HG3	1.69	0.93
1:B:2127:UNK:O	1:B:2130:UNK:HG3	1.70	0.92
1:B:929:UNK:O	1:B:930:UNK:HG3	1.69	0.92
1:C:992:UNK:HG1	1:C:996:UNK:CG	1.97	0.92
1:B:1225:UNK:HG1	1:B:1283:ASP:OD1	1.70	0.92
1:C:1225:UNK:HG1	1:C:1283:ASP:OD1	1.70	0.92
1:A:1013:UNK:HG2	1:A:1014:UNK:N	1.84	0.91
1:C:939:UNK:O	1:C:940:UNK:HG3	1.70	0.91
1:A:939:UNK:O	1:A:940:UNK:HG3	1.70	0.91
1:C:1012:UNK:O	1:C:1013:UNK:HG3	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1212:UNK:HG2	1:B:1342:ARG:HH21	1.32	0.91
1:A:1212:UNK:HG2	1:A:1342:ARG:HH21	1.32	0.91
1:A:1225:UNK:HG1	1:A:1283:ASP:OD1	1.70	0.91
1:C:2127:UNK:O	1:C:2130:UNK:HG3	1.69	0.91
1:B:1012:UNK:O	1:B:1013:UNK:HG3	1.69	0.91
1:B:2112:UNK:O	1:B:2115:UNK:HG3	1.70	0.91
1:A:2112:UNK:O	1:A:2115:UNK:HG3	1.70	0.91
1:C:929:UNK:O	1:C:930:UNK:HG3	1.69	0.91
1:A:943:UNK:O	1:A:944:UNK:HG3	1.71	0.91
1:C:1013:UNK:HG2	1:C:1014:UNK:N	1.84	0.90
1:C:943:UNK:O	1:C:944:UNK:HG3	1.71	0.90
1:C:2112:UNK:O	1:C:2115:UNK:HG3	1.70	0.90
1:A:1012:UNK:O	1:A:1013:UNK:HG3	1.69	0.90
1:B:939:UNK:O	1:B:940:UNK:HG3	1.70	0.90
1:B:943:UNK:O	1:B:944:UNK:HG3	1.71	0.90
1:C:2093:UNK:HA	1:C:2097:UNK:HG1	1.52	0.90
1:B:1013:UNK:HG2	1:B:1014:UNK:N	1.84	0.90
1:C:981:UNK:CG	1:C:987:UNK:HG2	2.02	0.89
1:B:2093:UNK:HA	1:B:2097:UNK:HG1	1.52	0.89
1:A:2093:UNK:HA	1:A:2097:UNK:HG1	1.52	0.89
1:A:981:UNK:CG	1:A:987:UNK:HG2	2.02	0.89
1:C:1002:UNK:O	1:C:1003:UNK:HG3	1.73	0.89
1:C:2434:UNK:HG3	1:C:2524:CYS:HA	1.54	0.89
1:B:1002:UNK:O	1:B:1003:UNK:HG3	1.73	0.89
1:B:2103:UNK:HG2	1:B:2104:UNK:N	1.89	0.88
1:B:981:UNK:CG	1:B:987:UNK:HG2	2.02	0.88
1:B:2100:UNK:O	1:B:2103:UNK:CG	2.22	0.88
1:C:2100:UNK:O	1:C:2103:UNK:CG	2.22	0.88
1:C:928:ALA:HB1	1:C:931:UNK:HB1	1.55	0.88
1:A:1002:UNK:O	1:A:1003:UNK:HG3	1.73	0.88
1:B:2112:UNK:H	1:B:2115:UNK:CG	1.87	0.88
1:A:2103:UNK:HG2	1:A:2104:UNK:N	1.89	0.87
1:B:2112:UNK:H	1:B:2115:UNK:HG1	1.40	0.87
1:A:2451:UNK:CG	1:A:2454:ASP:OD2	2.22	0.87
1:A:2434:UNK:HG3	1:A:2524:CYS:HA	1.54	0.87
1:B:2434:UNK:HG3	1:B:2524:CYS:HA	1.54	0.87
1:C:2112:UNK:H	1:C:2115:UNK:HG1	1.40	0.87
1:B:928:ALA:HB1	1:B:931:UNK:HB1	1.55	0.87
1:B:2086:UNK:O	1:B:2089:UNK:HG3	1.74	0.87
1:A:928:ALA:HB1	1:A:931:UNK:HB1	1.55	0.87
1:B:2126:UNK:O	1:B:2129:UNK:HG3	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2086:UNK:O	1:A:2089:UNK:HG3	1.74	0.86
1:A:2112:UNK:H	1:A:2115:UNK:CG	1.87	0.86
1:C:992:UNK:CG	1:C:994:UNK:HG3	2.05	0.86
1:A:2112:UNK:H	1:A:2115:UNK:HG1	1.40	0.86
1:C:2112:UNK:H	1:C:2115:UNK:CG	1.87	0.86
1:C:2451:UNK:CG	1:C:2454:ASP:OD2	2.22	0.86
1:A:2126:UNK:O	1:A:2129:UNK:HG3	1.75	0.86
1:C:2086:UNK:O	1:C:2089:UNK:HG3	1.74	0.86
1:A:992:UNK:CG	1:A:994:UNK:HG3	2.05	0.86
1:B:992:UNK:CG	1:B:994:UNK:CG	2.53	0.86
1:A:2100:UNK:O	1:A:2103:UNK:CG	2.22	0.86
1:B:2451:UNK:CG	1:B:2454:ASP:OD2	2.22	0.86
1:A:992:UNK:CG	1:A:994:UNK:CG	2.53	0.86
1:A:931:UNK:HG1	1:A:933:UNK:CG	2.06	0.86
1:C:2126:UNK:O	1:C:2129:UNK:HG3	1.75	0.86
1:C:992:UNK:CG	1:C:994:UNK:CG	2.53	0.85
1:A:2085:UNK:O	1:A:2088:UNK:HG3	1.76	0.85
1:B:2081:UNK:O	1:B:2084:UNK:HG3	1.76	0.85
1:B:992:UNK:CG	1:B:994:UNK:HG3	2.05	0.85
1:C:2103:UNK:HG2	1:C:2104:UNK:N	1.89	0.85
1:B:2085:UNK:O	1:B:2088:UNK:HG3	1.76	0.85
1:B:1218:UNK:HG2	1:B:1441:GLN:OE1	1.77	0.85
1:C:2081:UNK:O	1:C:2084:UNK:HG3	1.76	0.85
1:B:935:UNK:O	1:B:939:UNK:HG3	1.77	0.85
1:C:1218:UNK:HG2	1:C:1441:GLN:OE1	1.77	0.85
1:C:2085:UNK:O	1:C:2088:UNK:HG3	1.76	0.85
1:A:935:UNK:O	1:A:939:UNK:HG3	1.77	0.85
1:A:1218:UNK:HG2	1:A:1441:GLN:OE1	1.77	0.85
1:A:2118:UNK:O	1:A:2122:UNK:HG3	1.76	0.85
1:B:2118:UNK:O	1:B:2122:UNK:HG3	1.76	0.84
1:A:2081:UNK:O	1:A:2084:UNK:HG3	1.76	0.84
1:A:992:UNK:HG3	1:A:996:UNK:CG	2.07	0.84
1:B:931:UNK:HG1	1:B:933:UNK:CG	2.06	0.84
1:A:999:UNK:HG2	1:A:1007:UNK:CG	2.07	0.84
1:C:2118:UNK:O	1:C:2122:UNK:HG3	1.76	0.84
1:C:935:UNK:O	1:C:939:UNK:HG3	1.77	0.84
1:B:1538:ARG:HH11	1:B:1722:PRO:HB3	1.43	0.84
1:B:999:UNK:HG2	1:B:1007:UNK:CG	2.07	0.84
1:C:931:UNK:HG1	1:C:933:UNK:CG	2.06	0.83
1:A:43:PRO:HG2	1:A:348:ALA:HA	1.60	0.83
1:C:992:UNK:HG3	1:C:996:UNK:CG	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2105:UNK:O	1:B:2108:UNK:CG	2.24	0.83
1:A:992:UNK:HG1	1:A:994:UNK:CG	2.09	0.83
1:C:999:UNK:O	1:C:1007:UNK:HG3	1.80	0.82
1:C:1538:ARG:HH11	1:C:1722:PRO:HB3	1.43	0.82
1:C:2097:UNK:O	1:C:2100:UNK:CG	2.27	0.82
1:B:992:UNK:HG3	1:B:996:UNK:CG	2.07	0.82
1:B:992:UNK:HG1	1:B:994:UNK:CG	2.09	0.82
1:C:999:UNK:HG2	1:C:1007:UNK:CG	2.07	0.82
1:A:2097:UNK:O	1:A:2100:UNK:CG	2.27	0.82
1:C:992:UNK:HG1	1:C:994:UNK:CG	2.09	0.82
1:A:2016:VAL:HG13	1:A:2020:PRO:HG3	1.62	0.82
1:B:2097:UNK:O	1:B:2100:UNK:CG	2.27	0.82
1:C:2016:VAL:HG13	1:C:2020:PRO:HG3	1.62	0.82
1:A:2105:UNK:O	1:A:2108:UNK:CG	2.25	0.81
1:A:2093:UNK:CG	1:A:2129:UNK:O	2.27	0.81
1:B:999:UNK:O	1:B:1007:UNK:HG3	1.80	0.81
1:B:2730:TYR:OH	1:B:3059:ARG:NH1	2.14	0.81
1:B:43:PRO:HG2	1:B:348:ALA:HA	1.60	0.81
1:B:2016:VAL:HG13	1:B:2020:PRO:HG3	1.62	0.81
1:C:2091:UNK:O	1:C:2132:UNK:HG1	1.80	0.81
1:A:967:VAL:HA	1:A:970:ILE:HB	1.63	0.81
1:C:43:PRO:HG2	1:C:348:ALA:HA	1.60	0.81
1:C:138:ARG:NH2	1:C:175:ASP:OD2	2.14	0.81
1:B:2091:UNK:O	1:B:2132:UNK:HG1	1.80	0.81
1:A:2091:UNK:O	1:A:2132:UNK:HG1	1.80	0.81
1:A:2730:TYR:OH	1:A:3059:ARG:NH1	2.14	0.81
1:B:2093:UNK:CG	1:B:2129:UNK:O	2.27	0.80
1:A:138:ARG:NH2	1:A:175:ASP:OD2	2.14	0.80
1:C:46:VAL:HB	1:C:155:VAL:HG13	1.63	0.80
1:A:995:UNK:HB1	1:A:1011:UNK:HG3	1.63	0.80
1:C:2093:UNK:CG	1:C:2129:UNK:O	2.27	0.80
1:A:1538:ARG:HH11	1:A:1722:PRO:HB3	1.43	0.80
1:B:995:UNK:HB1	1:B:1011:UNK:HG3	1.63	0.80
1:C:2730:TYR:OH	1:C:3059:ARG:NH1	2.14	0.80
1:C:2123:UNK:O	1:C:2126:UNK:HG3	1.82	0.80
1:A:931:UNK:CG	1:A:933:UNK:CG	2.60	0.80
1:C:967:VAL:HA	1:C:970:ILE:HB	1.63	0.80
1:B:138:ARG:NH2	1:B:175:ASP:OD2	2.14	0.80
1:A:1001:UNK:HG1	1:A:1018:ARG:NH2	1.97	0.80
1:B:46:VAL:HB	1:B:155:VAL:HG13	1.63	0.80
1:A:999:UNK:O	1:A:1007:UNK:HG3	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ARG:HB2	1:C:282:VAL:H	1.47	0.80
1:C:1001:UNK:HG1	1:C:1018:ARG:NH2	1.97	0.79
1:B:931:UNK:CG	1:B:933:UNK:CG	2.60	0.79
1:A:46:VAL:HB	1:A:155:VAL:HG13	1.63	0.79
1:C:2105:UNK:O	1:C:2108:UNK:CG	2.24	0.79
1:C:1220:UNK:CG	1:C:1221:UNK:N	2.46	0.79
1:A:2098:UNK:O	1:A:2102:UNK:HG3	1.82	0.79
1:C:931:UNK:CG	1:C:933:UNK:CG	2.60	0.79
1:B:1001:UNK:HG1	1:B:1018:ARG:NH2	1.97	0.79
1:B:2610:ARG:HH12	1:B:2700:LEU:HD11	1.47	0.79
1:B:2084:UNK:O	1:B:2087:UNK:HG3	1.82	0.79
1:A:273:ARG:HB2	1:A:282:VAL:H	1.47	0.79
1:B:2098:UNK:O	1:B:2102:UNK:HG3	1.82	0.78
1:C:2077:UNK:HG2	1:C:2079:UNK:HG3	1.65	0.78
1:B:2123:UNK:O	1:B:2126:UNK:HG3	1.82	0.78
1:B:2077:UNK:HG2	1:B:2079:UNK:HG3	1.65	0.78
1:A:931:UNK:HG1	1:A:933:UNK:HG2	1.65	0.78
1:C:2610:ARG:HH12	1:C:2700:LEU:HD11	1.47	0.78
1:C:995:UNK:HB1	1:C:1011:UNK:HG3	1.63	0.78
1:A:2084:UNK:O	1:A:2087:UNK:HG3	1.82	0.78
1:B:967:VAL:HA	1:B:970:ILE:HB	1.63	0.78
1:B:930:UNK:O	1:B:930:UNK:HG2	1.83	0.78
1:B:273:ARG:HB2	1:B:282:VAL:H	1.47	0.78
1:C:2098:UNK:O	1:C:2102:UNK:HG3	1.82	0.78
1:C:930:UNK:HG2	1:C:930:UNK:O	1.83	0.78
1:A:2123:UNK:O	1:A:2126:UNK:HG3	1.82	0.78
1:C:2084:UNK:O	1:C:2087:UNK:HG3	1.82	0.78
1:A:971:ALA:O	1:A:974:UNK:HG3	1.84	0.78
1:A:2077:UNK:HG2	1:A:2079:UNK:HG3	1.65	0.78
1:C:971:ALA:O	1:C:974:UNK:HG3	1.84	0.77
1:B:2135:UNK:HG3	1:B:2136:ASP:N	1.99	0.77
1:B:1220:UNK:CG	1:B:1221:UNK:N	2.46	0.77
1:A:930:UNK:O	1:A:930:UNK:HG2	1.83	0.77
1:A:1329:ALA:HB3	1:A:1337:MET:H	1.48	0.77
1:B:1329:ALA:HB3	1:B:1337:MET:H	1.49	0.77
1:A:2135:UNK:HG3	1:A:2136:ASP:N	1.99	0.77
1:C:2135:UNK:HG3	1:C:2136:ASP:N	1.99	0.77
1:C:2100:UNK:HG2	1:C:2101:UNK:N	2.00	0.77
1:C:931:UNK:HG1	1:C:933:UNK:HG2	1.65	0.77
1:C:1329:ALA:HB3	1:C:1337:MET:H	1.49	0.77
1:B:971:ALA:O	1:B:974:UNK:HG3	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:931:UNK:CG	1:C:933:UNK:HG2	2.15	0.77
1:B:931:UNK:CG	1:B:933:UNK:HG2	2.15	0.77
1:A:257:ARG:HH12	1:C:1695:LEU:HD23	1.51	0.76
1:A:931:UNK:CG	1:A:933:UNK:HG2	2.15	0.76
1:B:1695:LEU:HD23	1:C:257:ARG:HH12	1.50	0.76
1:A:2610:ARG:HH12	1:A:2700:LEU:HD11	1.47	0.76
1:A:1695:LEU:HD23	1:B:257:ARG:HH12	1.51	0.76
1:A:2557:LEU:O	1:A:2613:ARG:N	2.18	0.76
1:C:934:UNK:O	1:C:937:UNK:CG	2.34	0.76
1:B:931:UNK:HG1	1:B:933:UNK:HG2	1.65	0.76
1:A:944:UNK:HG2	1:A:944:UNK:O	1.85	0.76
1:A:1097:VAL:HB	1:A:1146:PRO:HB2	1.68	0.76
1:B:1097:VAL:HB	1:B:1146:PRO:HB2	1.68	0.76
1:A:2100:UNK:HG2	1:A:2101:UNK:N	2.00	0.76
1:A:1220:UNK:CG	1:A:1221:UNK:N	2.46	0.76
1:B:2557:LEU:O	1:B:2613:ARG:N	2.18	0.76
1:A:995:UNK:HB1	1:A:1011:UNK:CG	2.17	0.75
1:B:2124:UNK:O	1:B:2127:UNK:HG3	1.86	0.75
1:C:2452:UNK:HG2	1:C:2453:UNK:N	2.01	0.75
1:A:940:UNK:O	1:A:940:UNK:HG2	1.86	0.75
1:B:2126:UNK:C	1:B:2129:UNK:HG3	2.16	0.75
1:B:2452:UNK:HG2	1:B:2453:UNK:N	2.00	0.75
1:B:944:UNK:O	1:B:944:UNK:HG2	1.85	0.75
1:B:2418:GLY:O	1:B:2422:UNK:HG3	1.87	0.75
1:C:2124:UNK:O	1:C:2127:UNK:HG3	1.87	0.75
1:A:2452:UNK:HG2	1:A:2453:UNK:N	2.00	0.75
1:B:2645:ASP:OD2	1:B:2691:SER:N	2.19	0.75
1:A:2418:GLY:O	1:A:2422:UNK:HG3	1.87	0.75
1:B:2088:UNK:O	1:B:2091:UNK:CG	2.35	0.75
1:B:2100:UNK:HG2	1:B:2101:UNK:N	2.00	0.75
1:C:2122:UNK:O	1:C:2125:UNK:HG3	1.87	0.75
1:A:1212:UNK:HG2	1:A:1342:ARG:NH2	2.02	0.75
1:B:995:UNK:HB1	1:B:1011:UNK:CG	2.17	0.75
1:A:2122:UNK:O	1:A:2125:UNK:HG3	1.87	0.74
1:C:944:UNK:HG2	1:C:944:UNK:O	1.85	0.74
1:C:995:UNK:HB1	1:C:1011:UNK:CG	2.17	0.74
1:C:445:VAL:HG13	1:C:475:LEU:HD21	1.69	0.74
1:C:2418:GLY:O	1:C:2422:UNK:HG3	1.87	0.74
1:C:2088:UNK:O	1:C:2091:UNK:CG	2.35	0.74
1:C:1097:VAL:HB	1:C:1146:PRO:HB2	1.68	0.74
1:B:1212:UNK:HG2	1:B:1342:ARG:NH2	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:VAL:HG13	1:B:475:LEU:HD21	1.69	0.74
1:A:2124:UNK:O	1:A:2127:UNK:HG3	1.86	0.74
1:C:33:ALA:HB2	1:C:390:VAL:HA	1.70	0.74
1:B:940:UNK:HG2	1:B:940:UNK:O	1.86	0.74
1:A:33:ALA:HB2	1:A:390:VAL:HA	1.70	0.74
1:A:1556:GLU:OE2	1:A:1560:ARG:NH2	2.20	0.74
1:A:934:UNK:O	1:A:937:UNK:CG	2.34	0.74
1:C:940:UNK:HG2	1:C:940:UNK:O	1.86	0.74
1:B:2122:UNK:O	1:B:2125:UNK:HG3	1.87	0.74
1:A:2087:UNK:HA	1:A:2090:UNK:HG3	1.70	0.74
1:A:2126:UNK:C	1:A:2129:UNK:HG3	2.17	0.74
1:A:994:UNK:HG2	1:A:996:UNK:HG3	1.70	0.74
1:C:1212:UNK:CG	1:C:1342:ARG:HE	2.01	0.74
1:A:2645:ASP:OD2	1:A:2691:SER:N	2.19	0.74
1:C:2557:LEU:O	1:C:2613:ARG:N	2.18	0.74
1:C:1212:UNK:HG2	1:C:1342:ARG:NH2	2.02	0.74
1:B:1212:UNK:CG	1:B:1342:ARG:HE	2.01	0.74
1:B:33:ALA:HB2	1:B:390:VAL:HA	1.69	0.74
1:A:799:PHE:CZ	1:A:2433:UNK:HG3	2.23	0.74
1:A:992:UNK:HG3	1:A:996:UNK:HG3	1.66	0.74
1:B:1001:UNK:O	1:B:1002:UNK:HG3	1.88	0.74
1:C:1556:GLU:OE2	1:C:1560:ARG:NH2	2.20	0.74
1:C:1168:ARG:N	1:C:1194:ILE:O	2.21	0.74
1:B:1556:GLU:OE2	1:B:1560:ARG:NH2	2.20	0.74
1:B:2087:UNK:HA	1:B:2090:UNK:HG3	1.70	0.73
1:C:2126:UNK:C	1:C:2129:UNK:HG3	2.17	0.73
1:B:934:UNK:O	1:B:937:UNK:CG	2.34	0.73
1:A:1212:UNK:CG	1:A:1342:ARG:HE	2.01	0.73
1:B:1226:UNK:HG3	1:B:1313:VAL:HG12	1.70	0.73
1:A:992:UNK:HG2	1:A:994:UNK:CG	2.17	0.73
1:A:1168:ARG:N	1:A:1194:ILE:O	2.21	0.73
1:B:992:UNK:HG2	1:B:994:UNK:CG	2.17	0.73
1:C:994:UNK:HG2	1:C:996:UNK:HG3	1.70	0.73
1:C:2096:UNK:O	1:C:2099:UNK:CG	2.37	0.73
1:B:3015:ILE:HG12	1:B:3023:ARG:HG3	1.69	0.73
1:B:799:PHE:CZ	1:B:2433:UNK:HG3	2.23	0.73
1:C:799:PHE:CZ	1:C:2433:UNK:HG3	2.23	0.73
1:B:994:UNK:HG2	1:B:996:UNK:HG3	1.70	0.73
1:C:3015:ILE:HG12	1:C:3023:ARG:HG3	1.69	0.73
1:B:2096:UNK:O	1:B:2099:UNK:CG	2.36	0.73
1:C:980:UNK:O	1:C:981:UNK:HG3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2053:ALA:O	1:B:2807:ARG:NH2	2.21	0.73
1:C:2053:ALA:O	1:C:2807:ARG:NH2	2.21	0.73
1:C:437:PRO:HG3	1:C:876:LEU:HB3	1.70	0.73
1:A:2883:ALA:O	1:A:2916:ARG:NH1	2.22	0.73
1:B:2093:UNK:HA	1:B:2097:UNK:CG	2.19	0.73
1:C:992:UNK:HG2	1:C:994:UNK:CG	2.17	0.73
1:C:1001:UNK:O	1:C:1002:UNK:HG3	1.88	0.73
1:C:976:UNK:HG3	1:C:993:UNK:CB	2.19	0.72
1:B:437:PRO:HG3	1:B:876:LEU:HB3	1.70	0.72
1:A:2053:ALA:O	1:A:2807:ARG:NH2	2.21	0.72
1:B:1168:ARG:N	1:B:1194:ILE:O	2.21	0.72
1:C:936:UNK:HB1	1:C:941:UNK:HB1	1.71	0.72
1:C:2883:ALA:O	1:C:2916:ARG:NH1	2.22	0.72
1:B:1253:ARG:HH11	1:B:1253:ARG:HG3	1.55	0.72
1:C:1253:ARG:HH11	1:C:1253:ARG:HG3	1.54	0.72
1:C:1226:UNK:HG3	1:C:1313:VAL:HG12	1.70	0.72
1:C:1400:PRO:HD2	1:C:1416:VAL:HG22	1.72	0.72
1:A:1226:UNK:HG3	1:A:1313:VAL:HG12	1.70	0.72
1:A:2093:UNK:HA	1:A:2097:UNK:CG	2.19	0.72
1:B:1400:PRO:HD2	1:B:1416:VAL:HG22	1.72	0.72
1:A:1001:UNK:O	1:A:1002:UNK:HG3	1.88	0.72
1:C:70:SER:OG	1:C:142:ARG:NH2	2.23	0.72
1:C:2645:ASP:OD2	1:C:2691:SER:N	2.19	0.72
1:B:2121:UNK:O	1:B:2124:UNK:HG3	1.90	0.72
1:A:2088:UNK:O	1:A:2091:UNK:CG	2.35	0.72
1:A:980:UNK:O	1:A:981:UNK:HG3	1.89	0.72
1:B:936:UNK:HB1	1:B:941:UNK:HB1	1.71	0.72
1:A:95:PRO:HB2	1:C:1237:ARG:NH1	2.05	0.72
1:A:2113:UNK:O	1:A:2116:UNK:CG	2.38	0.72
1:C:2093:UNK:HA	1:C:2097:UNK:CG	2.19	0.72
1:B:1218:UNK:CG	1:B:1441:GLN:OE1	2.38	0.72
1:A:70:SER:OG	1:A:142:ARG:NH2	2.23	0.72
1:A:3015:ILE:HG12	1:A:3023:ARG:HG3	1.69	0.72
1:A:445:VAL:HG13	1:A:475:LEU:HD21	1.69	0.72
1:A:992:UNK:HG2	1:A:994:UNK:HG3	1.72	0.72
1:B:980:UNK:O	1:B:981:UNK:HG3	1.89	0.72
1:C:992:UNK:HG2	1:C:994:UNK:HG3	1.72	0.72
1:A:1253:ARG:HH11	1:A:1253:ARG:HG3	1.55	0.72
1:A:1400:PRO:HD2	1:A:1416:VAL:HG22	1.72	0.72
1:B:2883:ALA:O	1:B:2916:ARG:NH1	2.22	0.72
1:C:2087:UNK:HA	1:C:2090:UNK:HG3	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2268:GLN:OE1	1:C:2319:ARG:NH1	2.23	0.71
1:A:2121:UNK:O	1:A:2124:UNK:HG3	1.90	0.71
1:B:70:SER:OG	1:B:142:ARG:NH2	2.23	0.71
1:A:1237:ARG:NH1	1:B:95:PRO:HB2	2.05	0.71
1:B:2268:GLN:OE1	1:B:2319:ARG:NH1	2.23	0.71
1:B:1237:ARG:NH1	1:C:95:PRO:HB2	2.05	0.71
1:C:2113:UNK:O	1:C:2116:UNK:CG	2.38	0.71
1:A:981:UNK:HG1	1:A:987:UNK:CG	2.19	0.71
1:C:1218:UNK:CG	1:C:1441:GLN:OE1	2.38	0.71
1:A:976:UNK:HG3	1:A:993:UNK:CB	2.19	0.71
1:A:982:UNK:HG2	1:A:983:UNK:N	2.05	0.71
1:B:976:UNK:HG3	1:B:993:UNK:CB	2.19	0.71
1:B:2998:GLY:N	1:B:3002:VAL:O	2.23	0.71
1:B:982:UNK:HG2	1:B:983:UNK:N	2.05	0.71
1:A:981:UNK:HB2	1:A:984:UNK:CG	2.21	0.71
1:A:936:UNK:HB1	1:A:941:UNK:HB1	1.71	0.71
1:C:2121:UNK:O	1:C:2124:UNK:HG3	1.90	0.71
1:C:1634:ARG:HH11	1:C:1639:ALA:H	1.39	0.71
1:A:2096:UNK:O	1:A:2099:UNK:CG	2.37	0.70
1:C:1507:GLN:O	1:C:1562:ARG:NH1	2.24	0.70
1:C:982:UNK:HG2	1:C:983:UNK:N	2.05	0.70
1:C:2112:UNK:O	1:C:2115:UNK:CG	2.38	0.70
1:A:437:PRO:HG3	1:A:876:LEU:HB3	1.70	0.70
1:A:1218:UNK:CG	1:A:1441:GLN:OE1	2.38	0.70
1:A:2558:LEU:HG	1:A:2612:PRO:HA	1.73	0.70
1:A:2268:GLN:OE1	1:A:2319:ARG:NH1	2.23	0.70
1:C:981:UNK:HG1	1:C:987:UNK:CG	2.19	0.70
1:B:981:UNK:HB2	1:B:984:UNK:CG	2.21	0.70
1:A:1507:GLN:O	1:A:1562:ARG:NH1	2.24	0.70
1:B:137:VAL:HG22	1:B:354:LEU:HD13	1.74	0.70
1:B:1634:ARG:HH11	1:B:1639:ALA:H	1.39	0.70
1:C:981:UNK:HB2	1:C:984:UNK:CG	2.21	0.70
1:A:2998:GLY:N	1:A:3002:VAL:O	2.23	0.70
1:A:2743:ALA:HB1	1:A:2940:VAL:HG23	1.73	0.70
1:C:2558:LEU:HG	1:C:2612:PRO:HA	1.73	0.70
1:C:974:UNK:HG1	1:C:977:UNK:HB1	1.74	0.70
1:B:580:ARG:HD2	1:B:614:GLY:HA3	1.73	0.70
1:B:2112:UNK:O	1:B:2115:UNK:CG	2.38	0.70
1:B:992:UNK:HG2	1:B:994:UNK:HG3	1.72	0.70
1:B:2743:ALA:HB1	1:B:2940:VAL:HG23	1.73	0.70
1:A:2112:UNK:O	1:A:2115:UNK:CG	2.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1634:ARG:HH11	1:A:1639:ALA:H	1.39	0.69
1:C:1035:VAL:HG12	1:C:1037:ASP:H	1.57	0.69
1:C:580:ARG:HD2	1:C:614:GLY:HA3	1.72	0.69
1:A:580:ARG:HD2	1:A:614:GLY:HA3	1.73	0.69
1:C:2860:ALA:HB3	1:C:2906:LEU:HD21	1.73	0.69
1:A:1035:VAL:HG12	1:A:1037:ASP:H	1.57	0.69
1:B:2860:ALA:HB3	1:B:2906:LEU:HD21	1.73	0.69
1:A:2860:ALA:HB3	1:A:2906:LEU:HD21	1.73	0.69
1:C:2085:UNK:O	1:C:2088:UNK:CG	2.41	0.69
1:B:2215:THR:HB	1:B:2229:LYS:HB2	1.74	0.69
1:A:1012:UNK:O	1:A:1013:UNK:CG	2.41	0.69
1:B:1177:ARG:HB2	1:B:1184:LEU:HD23	1.74	0.69
1:C:2122:UNK:HA	1:C:2125:UNK:HG3	1.75	0.69
1:B:2558:LEU:HG	1:B:2612:PRO:HA	1.74	0.69
1:A:137:VAL:HG22	1:A:354:LEU:HD13	1.74	0.69
1:B:1164:THR:N	1:B:1167:GLY:O	2.25	0.69
1:B:2122:UNK:HA	1:B:2125:UNK:HG3	1.75	0.69
1:C:2647:VAL:HG22	1:C:2769:ASP:HB2	1.75	0.69
1:A:2215:THR:HB	1:A:2229:LYS:HB2	1.74	0.69
1:C:2743:ALA:HB1	1:C:2940:VAL:HG23	1.73	0.69
1:B:1046:LEU:HD13	1:B:1129:LEU:HD22	1.75	0.69
1:C:1046:LEU:HD13	1:C:1129:LEU:HD22	1.75	0.69
1:B:1507:GLN:O	1:B:1562:ARG:NH1	2.24	0.69
1:C:2998:GLY:N	1:C:3002:VAL:O	2.23	0.69
1:C:2445:UNK:HG2	1:C:2985:GLY:O	1.93	0.69
1:A:1046:LEU:HD13	1:A:1129:LEU:HD22	1.75	0.69
1:C:2112:UNK:C	1:C:2115:UNK:HG3	2.22	0.69
1:B:2085:UNK:O	1:B:2088:UNK:CG	2.40	0.69
1:B:2946:LEU:HD11	1:B:2992:GLY:HA3	1.75	0.69
1:C:992:UNK:HG3	1:C:996:UNK:HG3	1.66	0.68
1:A:2445:UNK:HG2	1:A:2985:GLY:O	1.93	0.68
1:B:2113:UNK:C	1:B:2116:UNK:HG3	2.23	0.68
1:B:2112:UNK:C	1:B:2115:UNK:HG3	2.22	0.68
1:C:2093:UNK:CG	1:C:2132:UNK:HB1	2.24	0.68
1:B:2113:UNK:O	1:B:2116:UNK:CG	2.37	0.68
1:A:511:ARG:HD3	1:A:543:GLY:HA3	1.76	0.68
1:A:1177:ARG:HB2	1:A:1184:LEU:HD23	1.74	0.68
1:B:1035:VAL:HG12	1:B:1037:ASP:H	1.57	0.68
1:B:340:ILE:HD13	1:B:364:THR:HG21	1.75	0.68
1:C:1164:THR:N	1:C:1167:GLY:O	2.25	0.68
1:C:1177:ARG:HB2	1:C:1184:LEU:HD23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2112:UNK:C	1:A:2115:UNK:HG3	2.22	0.68
1:C:2113:UNK:C	1:C:2116:UNK:HG3	2.23	0.68
1:A:340:ILE:HD13	1:A:364:THR:HG21	1.75	0.68
1:C:511:ARG:HD3	1:C:543:GLY:HA3	1.76	0.68
1:B:2093:UNK:CG	1:B:2132:UNK:HB1	2.24	0.68
1:A:2093:UNK:CG	1:A:2132:UNK:HB1	2.24	0.68
1:B:2647:VAL:HG22	1:B:2769:ASP:HB2	1.75	0.68
1:C:2215:THR:HB	1:C:2229:LYS:HB2	1.74	0.68
1:C:137:VAL:HG22	1:C:354:LEU:HD13	1.74	0.68
1:A:2080:UNK:HB2	1:A:2082:UNK:HG3	1.75	0.68
1:C:269:GLU:HB3	1:C:282:VAL:HA	1.75	0.68
1:A:2946:LEU:HD11	1:A:2992:GLY:HA3	1.75	0.68
1:A:2085:UNK:O	1:A:2088:UNK:CG	2.40	0.68
1:C:2097:UNK:C	1:C:2100:UNK:HG3	2.24	0.68
1:C:1488:VAL:HG21	1:C:1580:PRO:HD2	1.76	0.68
1:B:2445:UNK:HG2	1:B:2985:GLY:O	1.93	0.68
1:C:2080:UNK:HB2	1:C:2082:UNK:HG3	1.75	0.68
1:A:992:UNK:HG3	1:A:996:UNK:HG2	1.76	0.68
1:B:511:ARG:HD3	1:B:543:GLY:HA3	1.76	0.68
1:A:1724:TYR:OH	1:B:267:GLU:OE2	2.08	0.68
1:A:2112:UNK:HG2	1:A:2114:UNK:HG3	1.77	0.67
1:A:2122:UNK:HA	1:A:2125:UNK:HG3	1.75	0.67
1:A:974:UNK:HG1	1:A:977:UNK:HB1	1.74	0.67
1:C:2946:LEU:HD11	1:C:2992:GLY:HA3	1.75	0.67
1:C:3080:ARG:HH11	1:C:3080:ARG:CG	2.07	0.67
1:A:2113:UNK:C	1:A:2116:UNK:HG3	2.23	0.67
1:B:974:UNK:HG1	1:B:977:UNK:HB1	1.74	0.67
1:B:1163:ASP:HB3	1:B:1199:UNK:HG3	1.76	0.67
1:B:2103:UNK:CG	1:B:2104:UNK:N	2.58	0.67
1:C:2112:UNK:HG2	1:C:2114:UNK:HG3	1.77	0.67
1:A:1164:THR:N	1:A:1167:GLY:O	2.25	0.67
1:B:792:ALA:HA	1:B:799:PHE:HE2	1.60	0.67
1:B:2086:UNK:C	1:B:2089:UNK:HG3	2.25	0.67
1:B:2093:UNK:HG3	1:B:2132:UNK:HB1	1.77	0.67
1:C:2103:UNK:CG	1:C:2104:UNK:N	2.58	0.67
1:C:2093:UNK:HG3	1:C:2132:UNK:HB1	1.77	0.67
1:B:3080:ARG:CG	1:B:3080:ARG:HH11	2.07	0.67
1:C:340:ILE:HD13	1:C:364:THR:HG21	1.75	0.67
1:B:2080:UNK:HB2	1:B:2082:UNK:HG3	1.75	0.67
1:A:2112:UNK:N	1:A:2115:UNK:CG	2.57	0.67
1:A:2126:UNK:O	1:A:2129:UNK:CG	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLU:HB3	1:B:282:VAL:HA	1.75	0.67
1:B:2080:UNK:O	1:B:2083:UNK:HG3	1.94	0.67
1:A:2081:UNK:O	1:A:2084:UNK:CG	2.43	0.67
1:A:2097:UNK:C	1:A:2100:UNK:HG3	2.24	0.67
1:B:931:UNK:CG	1:B:933:UNK:HG3	2.25	0.67
1:A:2103:UNK:CG	1:A:2104:UNK:N	2.58	0.67
1:B:1488:VAL:HG12	1:B:1490:ARG:NH1	2.10	0.67
1:A:1008:UNK:HG3	1:A:1019:PHE:HB3	1.76	0.67
1:A:2084:UNK:C	1:A:2087:UNK:HG3	2.25	0.66
1:C:970:ILE:HG12	1:C:996:UNK:HG1	1.76	0.66
1:A:269:GLU:HB3	1:A:282:VAL:HA	1.75	0.66
1:A:2647:VAL:HG22	1:A:2769:ASP:HB2	1.75	0.66
1:C:1008:UNK:HG3	1:C:1019:PHE:HB3	1.76	0.66
1:A:1488:VAL:HG21	1:A:1580:PRO:HD2	1.76	0.66
1:A:792:ALA:HA	1:A:799:PHE:HE2	1.60	0.66
1:B:2084:UNK:C	1:B:2087:UNK:HG3	2.25	0.66
1:A:2080:UNK:O	1:A:2083:UNK:HG3	1.95	0.66
1:A:2093:UNK:HG3	1:A:2132:UNK:HB1	1.77	0.66
1:C:992:UNK:HG3	1:C:996:UNK:HG2	1.76	0.66
1:C:981:UNK:O	1:C:981:UNK:HG2	1.95	0.66
1:B:1012:UNK:O	1:B:1013:UNK:CG	2.41	0.66
1:C:1163:ASP:HB3	1:C:1199:UNK:HG3	1.76	0.66
1:B:1168:ARG:HB2	1:B:1197:UNK:HB2	1.77	0.66
1:A:511:ARG:HB2	1:A:540:ASN:HB2	1.77	0.66
1:B:2097:UNK:C	1:B:2100:UNK:HG3	2.24	0.66
1:B:992:UNK:HG3	1:B:996:UNK:HG2	1.76	0.66
1:C:1358:GLN:HG2	1:C:1423:THR:HG23	1.78	0.66
1:B:2081:UNK:O	1:B:2084:UNK:CG	2.43	0.66
1:B:2126:UNK:O	1:B:2129:UNK:CG	2.43	0.66
1:C:2080:UNK:O	1:C:2083:UNK:HG3	1.94	0.66
1:C:511:ARG:HB2	1:C:540:ASN:HB2	1.78	0.66
1:C:2126:UNK:O	1:C:2129:UNK:CG	2.43	0.66
1:B:981:UNK:HG1	1:B:987:UNK:CG	2.19	0.66
1:A:1412:HIS:HD2	1:A:1413:PRO:HD2	1.61	0.66
1:B:511:ARG:HB2	1:B:540:ASN:HB2	1.77	0.66
1:C:683:GLY:HA2	1:C:700:ASN:HB2	1.78	0.66
1:C:1168:ARG:HB2	1:C:1197:UNK:HB2	1.77	0.66
1:A:1163:ASP:HB3	1:A:1199:UNK:HG3	1.76	0.66
1:B:1412:HIS:HD2	1:B:1413:PRO:HD2	1.61	0.66
1:B:1167:GLY:HA3	1:B:1195:ARG:HA	1.77	0.66
1:C:792:ALA:HA	1:C:799:PHE:HE2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:UNK:HG3	1:B:1019:PHE:HB3	1.76	0.66
1:A:2591:ARG:HH12	1:C:2012:GLY:C	1.99	0.66
1:B:2112:UNK:HG2	1:B:2114:UNK:HG3	1.77	0.66
1:C:931:UNK:CG	1:C:933:UNK:HG3	2.24	0.66
1:A:1358:GLN:HG2	1:A:1423:THR:HG23	1.78	0.66
1:B:35:VAL:HG11	1:B:147:LEU:HB3	1.78	0.66
1:C:1132:LEU:HD11	1:C:1192:PHE:HB3	1.78	0.66
1:A:1084:THR:HG21	1:A:1274:ALA:HA	1.78	0.66
1:C:2081:UNK:O	1:C:2084:UNK:CG	2.43	0.66
1:C:2112:UNK:N	1:C:2115:UNK:CG	2.57	0.66
1:A:931:UNK:CG	1:A:933:UNK:HG3	2.25	0.66
1:B:2012:GLY:C	1:C:2591:ARG:HH12	1.99	0.66
1:C:1084:THR:HG21	1:C:1274:ALA:HA	1.78	0.66
1:B:2112:UNK:N	1:B:2115:UNK:CG	2.57	0.66
1:A:2086:UNK:C	1:A:2089:UNK:HG3	2.25	0.66
1:B:1358:GLN:HG2	1:B:1423:THR:HG23	1.78	0.66
1:B:666:VAL:HG21	1:B:904:VAL:HB	1.78	0.66
1:C:997:UNK:O	1:C:1009:UNK:N	2.29	0.66
1:B:2123:UNK:C	1:B:2126:UNK:HG3	2.26	0.65
1:A:2112:UNK:N	1:A:2115:UNK:HG1	2.11	0.65
1:B:970:ILE:HG12	1:B:996:UNK:HG1	1.76	0.65
1:A:1167:GLY:HA3	1:A:1195:ARG:HA	1.78	0.65
1:B:1488:VAL:HG21	1:B:1580:PRO:HD2	1.77	0.65
1:A:2679:ALA:HB3	1:A:2762:VAL:HG12	1.78	0.65
1:A:997:UNK:O	1:A:1009:UNK:N	2.29	0.65
1:B:1534:ASN:HB2	1:B:1543:ALA:HB3	1.78	0.65
1:C:2123:UNK:C	1:C:2126:UNK:HG3	2.26	0.65
1:A:970:ILE:HG12	1:A:996:UNK:HG1	1.76	0.65
1:A:1488:VAL:HG12	1:A:1490:ARG:NH1	2.10	0.65
1:B:2706:PRO:HG2	1:B:2709:ILE:HG23	1.79	0.65
1:A:2123:UNK:C	1:A:2126:UNK:HG3	2.26	0.65
1:C:2084:UNK:C	1:C:2087:UNK:HG3	2.25	0.65
1:B:683:GLY:HA2	1:B:700:ASN:HB2	1.78	0.65
1:A:2012:GLY:C	1:B:2591:ARG:HH12	1.99	0.65
1:C:1534:ASN:HB2	1:C:1543:ALA:HB3	1.79	0.65
1:C:924:LEU:O	1:C:929:UNK:N	2.30	0.65
1:B:1417:LEU:O	1:B:1423:THR:OG1	2.14	0.65
1:C:2876:LEU:HD11	1:C:2886:ILE:HD11	1.79	0.65
1:C:203:ASP:OD1	1:C:204:ARG:N	2.29	0.65
1:B:2112:UNK:N	1:B:2115:UNK:HG1	2.11	0.65
1:C:2086:UNK:C	1:C:2089:UNK:HG3	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:UNK:HG2	1:A:981:UNK:O	1.95	0.65
1:C:1488:VAL:HG12	1:C:1490:ARG:NH1	2.10	0.65
1:B:2679:ALA:HB3	1:B:2762:VAL:HG12	1.78	0.65
1:B:3080:ARG:NH1	1:B:3080:ARG:HG3	2.09	0.65
1:C:1012:UNK:O	1:C:1013:UNK:CG	2.41	0.65
1:A:35:VAL:HG11	1:A:147:LEU:HB3	1.78	0.65
1:A:450:ASN:HA	1:A:483:ARG:HH11	1.62	0.65
1:C:1412:HIS:HD2	1:C:1413:PRO:HD2	1.61	0.65
1:C:1417:LEU:O	1:C:1423:THR:OG1	2.14	0.65
1:B:1132:LEU:HD11	1:B:1192:PHE:HB3	1.78	0.65
1:C:666:VAL:HG21	1:C:904:VAL:HB	1.78	0.65
1:A:2876:LEU:HD11	1:A:2886:ILE:HD11	1.79	0.65
1:A:1168:ARG:HB2	1:A:1197:UNK:HB2	1.77	0.65
1:B:2876:LEU:HD11	1:B:2886:ILE:HD11	1.79	0.65
1:B:500:GLN:O	1:B:504:LYS:N	2.24	0.65
1:A:666:VAL:HG21	1:A:904:VAL:HB	1.78	0.65
1:B:1084:THR:HG21	1:B:1274:ALA:HA	1.78	0.65
1:C:999:UNK:CG	1:C:1007:UNK:CG	2.75	0.65
1:A:3080:ARG:HH11	1:A:3080:ARG:CG	2.07	0.65
1:A:999:UNK:CG	1:A:1007:UNK:CG	2.75	0.65
1:A:943:UNK:O	1:A:944:UNK:CG	2.44	0.65
1:C:1167:GLY:HA3	1:C:1195:ARG:HA	1.78	0.65
1:A:1536:ASN:HA	1:A:1679:TRP:HB3	1.79	0.65
1:B:203:ASP:OD1	1:B:204:ARG:N	2.29	0.65
1:B:997:UNK:O	1:B:1009:UNK:N	2.29	0.65
1:B:943:UNK:O	1:B:944:UNK:CG	2.44	0.65
1:A:2652:ILE:HG12	1:A:2722:VAL:HG22	1.79	0.65
1:C:2706:PRO:HG2	1:C:2709:ILE:HG23	1.79	0.65
1:C:2652:ILE:HG12	1:C:2722:VAL:HG22	1.79	0.65
1:C:35:VAL:HG11	1:C:147:LEU:HB3	1.77	0.64
1:C:1536:ASN:HA	1:C:1679:TRP:HB3	1.78	0.64
1:B:981:UNK:O	1:B:981:UNK:HG2	1.95	0.64
1:A:408:VAL:HG13	1:A:943:UNK:HG1	1.80	0.64
1:A:1417:LEU:O	1:A:1423:THR:OG1	2.14	0.64
1:B:238:SER:HG	1:B:249:THR:HG1	1.42	0.64
1:A:56:LEU:HD22	1:A:119:LEU:HD13	1.79	0.64
1:A:2120:UNK:O	1:A:2123:UNK:HG3	1.97	0.64
1:A:924:LEU:O	1:A:929:UNK:N	2.30	0.64
1:A:2706:PRO:HG2	1:A:2709:ILE:HG23	1.78	0.64
1:B:924:LEU:O	1:B:929:UNK:N	2.30	0.64
1:C:943:UNK:O	1:C:944:UNK:CG	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1534:ASN:HB2	1:A:1543:ALA:HB3	1.78	0.64
1:C:450:ASN:HA	1:C:483:ARG:HH11	1.62	0.64
1:B:2120:UNK:O	1:B:2123:UNK:HG3	1.97	0.64
1:B:999:UNK:CG	1:B:1007:UNK:CG	2.75	0.64
1:B:42:GLU:HB3	1:B:349:ARG:HG3	1.79	0.64
1:C:2679:ALA:HB3	1:C:2762:VAL:HG12	1.78	0.64
1:B:2428:UNK:O	1:B:2428:UNK:HG2	1.98	0.64
1:C:2449:UNK:O	1:C:2449:UNK:HG2	1.98	0.64
1:A:643:ILE:HD12	1:A:915:PHE:HZ	1.62	0.64
1:A:34:LEU:O	1:A:38:LEU:N	2.25	0.64
1:C:408:VAL:HG13	1:C:943:UNK:HG1	1.79	0.64
1:A:792:ALA:O	1:A:2433:UNK:HG2	1.96	0.64
1:B:2080:UNK:HG2	1:B:2083:UNK:HG3	1.79	0.64
1:C:2120:UNK:O	1:C:2123:UNK:HG3	1.97	0.64
1:A:1132:LEU:HD11	1:A:1192:PHE:HB3	1.78	0.64
1:A:1214:UNK:HB1	1:A:1320:VAL:HB	1.80	0.64
1:A:683:GLY:HA2	1:A:700:ASN:HB2	1.78	0.64
1:B:56:LEU:HD22	1:B:119:LEU:HD13	1.79	0.64
1:B:1536:ASN:HA	1:B:1679:TRP:HB3	1.78	0.64
1:B:2252:VAL:HA	1:B:2255:ARG:HE	1.62	0.64
1:A:2252:VAL:HA	1:A:2255:ARG:HE	1.62	0.64
1:C:803:GLU:OE1	1:C:2431:UNK:HG3	1.98	0.64
1:A:203:ASP:OD1	1:A:204:ARG:N	2.30	0.64
1:B:2449:UNK:HG2	1:B:2449:UNK:O	1.98	0.64
1:C:2080:UNK:HG2	1:C:2083:UNK:HG3	1.79	0.63
1:C:42:GLU:HB3	1:C:349:ARG:HG3	1.79	0.63
1:A:42:GLU:HB3	1:A:349:ARG:HG3	1.79	0.63
1:A:974:UNK:CG	1:A:977:UNK:HB1	2.29	0.63
1:C:643:ILE:HD12	1:C:915:PHE:HZ	1.62	0.63
1:B:974:UNK:CG	1:B:977:UNK:HB1	2.29	0.63
1:A:2428:UNK:O	1:A:2428:UNK:HG2	1.98	0.63
1:B:2176:LEU:HG	1:B:2180:LYS:HE3	1.80	0.63
1:A:892:ILE:HG22	2:A:4000:FMN:HM82	1.80	0.63
1:B:643:ILE:HD12	1:B:915:PHE:HZ	1.62	0.63
1:B:450:ASN:HA	1:B:483:ARG:HH11	1.62	0.63
1:C:360:LEU:HD12	1:C:363:LEU:HD23	1.80	0.63
1:A:2080:UNK:HG2	1:A:2083:UNK:HG3	1.79	0.63
1:A:2422:UNK:HG2	1:A:2422:UNK:O	1.98	0.63
1:C:2428:UNK:HG2	1:C:2428:UNK:O	1.98	0.63
1:C:1214:UNK:HB1	1:C:1320:VAL:HB	1.80	0.63
1:C:2252:VAL:HA	1:C:2255:ARG:HE	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2094:UNK:CG	1:C:2096:UNK:CG	2.75	0.63
1:A:1072:TRP:NE1	1:A:1077:VAL:HG22	2.14	0.63
1:C:1072:TRP:NE1	1:C:1077:VAL:HG22	2.14	0.63
1:A:2092:UNK:HA	1:A:2189:PHE:HB2	1.81	0.63
1:B:2297:ARG:H	1:B:2297:ARG:HD3	1.64	0.63
1:B:2125:UNK:HA	1:B:2128:UNK:HG3	1.81	0.63
1:B:1212:UNK:HG2	1:B:1212:UNK:O	1.99	0.63
1:B:408:VAL:HG13	1:B:943:UNK:HG1	1.79	0.63
1:A:2135:UNK:HG3	1:A:2136:ASP:H	1.64	0.63
1:B:1072:TRP:NE1	1:B:1077:VAL:HG22	2.14	0.63
1:B:585:HIS:CD2	1:B:586:SER:H	2.17	0.63
1:B:2652:ILE:HG12	1:B:2722:VAL:HG22	1.79	0.63
1:C:1212:UNK:O	1:C:1212:UNK:HG2	1.99	0.63
1:B:1215:UNK:HG2	1:B:1216:UNK:N	2.14	0.63
1:C:2092:UNK:O	1:C:2092:UNK:HG2	1.99	0.63
1:A:2948:GLN:HG2	1:A:2951:ARG:HH21	1.64	0.63
1:B:2117:UNK:O	1:B:2121:UNK:HG3	1.98	0.63
1:A:2117:UNK:O	1:A:2121:UNK:HG3	1.98	0.63
1:A:980:UNK:C	1:A:981:UNK:HG3	2.29	0.63
1:A:1212:UNK:HG2	1:A:1212:UNK:O	1.99	0.63
1:B:360:LEU:HD12	1:B:363:LEU:HD23	1.80	0.63
1:A:2047:THR:OG1	1:A:2205:ASP:OD2	2.17	0.63
1:B:1212:UNK:HG2	1:B:1342:ARG:HE	1.64	0.63
1:A:2173:ASP:OD2	1:A:2799:LYS:NZ	2.32	0.63
1:B:803:GLU:OE1	1:B:2431:UNK:HG3	1.98	0.63
1:B:750:LEU:HD12	1:B:827:LEU:HD11	1.81	0.63
1:A:803:GLU:OE1	1:A:2431:UNK:HG3	1.98	0.63
1:A:2297:ARG:HD3	1:A:2297:ARG:H	1.64	0.63
1:A:360:LEU:HD12	1:A:363:LEU:HD23	1.80	0.63
1:B:2047:THR:OG1	1:B:2205:ASP:OD2	2.17	0.63
1:A:2125:UNK:HA	1:A:2128:UNK:HG3	1.81	0.62
1:C:974:UNK:CG	1:C:977:UNK:HB1	2.29	0.62
1:C:2422:UNK:HG2	1:C:2422:UNK:O	1.98	0.62
1:C:1126:ILE:HG22	1:C:1196:UNK:HG1	1.81	0.62
1:C:1412:HIS:ND1	1:C:1415:GLY:O	2.26	0.62
1:A:1412:HIS:ND1	1:A:1415:GLY:O	2.26	0.62
1:A:1315:ARG:HH21	1:A:1323:GLU:HG2	1.64	0.62
1:A:1215:UNK:HG2	1:A:1216:UNK:N	2.14	0.62
1:A:750:LEU:HD12	1:A:827:LEU:HD11	1.81	0.62
1:C:2117:UNK:O	1:C:2121:UNK:HG3	1.98	0.62
1:B:980:UNK:C	1:B:981:UNK:HG3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2422:UNK:HG2	1:B:2422:UNK:O	1.98	0.62
1:B:1126:ILE:HG22	1:B:1196:UNK:HG1	1.81	0.62
1:C:1376:VAL:HA	1:C:1470:LEU:HD13	1.81	0.62
1:B:34:LEU:O	1:B:38:LEU:N	2.25	0.62
1:A:664:LEU:HD13	1:A:701:ALA:HB1	1.81	0.62
1:B:1002:UNK:O	1:B:1003:UNK:CG	2.47	0.62
1:A:2092:UNK:O	1:A:2092:UNK:HG2	1.99	0.62
1:C:2176:LEU:HG	1:C:2180:LYS:HE3	1.80	0.62
1:B:1214:UNK:HB1	1:B:1320:VAL:HB	1.80	0.62
1:C:56:LEU:HD22	1:C:119:LEU:HD13	1.79	0.62
1:B:664:LEU:HD13	1:B:701:ALA:HB1	1.81	0.62
1:A:2449:UNK:O	1:A:2449:UNK:HG2	1.98	0.62
1:B:892:ILE:HG22	2:B:4000:FMN:HM82	1.80	0.62
1:C:1212:UNK:HG2	1:C:1342:ARG:HE	1.64	0.62
1:C:585:HIS:CD2	1:C:586:SER:H	2.17	0.62
1:B:1376:VAL:HA	1:B:1470:LEU:HD13	1.81	0.62
1:C:1095:LEU:HD12	1:C:1096:THR:H	1.64	0.62
1:C:992:UNK:CG	1:C:994:UNK:HG2	2.29	0.62
1:A:500:GLN:O	1:A:504:LYS:N	2.24	0.62
1:A:1376:VAL:HA	1:A:1470:LEU:HD13	1.81	0.62
1:C:792:ALA:O	1:C:2433:UNK:HG2	1.96	0.62
1:B:2765:GLY:HA2	1:B:2940:VAL:HG21	1.82	0.62
1:C:2765:GLY:HA2	1:C:2940:VAL:HG21	1.82	0.62
1:A:585:HIS:CD2	1:A:586:SER:H	2.17	0.62
1:A:1702:GLU:OE2	1:A:1711:VAL:HG13	1.99	0.62
1:B:2173:ASP:OD2	1:B:2799:LYS:NZ	2.32	0.62
1:B:1702:GLU:OE2	1:B:1711:VAL:HG13	1.99	0.62
1:A:1622:PRO:HD3	1:A:1685:LEU:HD11	1.81	0.62
1:B:792:ALA:O	1:B:2433:UNK:HG2	1.96	0.62
1:A:992:UNK:CG	1:A:994:UNK:HG2	2.29	0.62
1:B:975:UNK:HG3	1:B:993:UNK:CB	2.29	0.62
1:B:415:VAL:HG22	1:B:937:UNK:HG1	1.81	0.62
1:B:1353:PRO:HG3	1:B:1702:GLU:OE2	2.00	0.62
1:B:2237:LEU:HB2	1:B:2287:LEU:HD11	1.82	0.62
1:C:1215:UNK:HG2	1:C:1216:UNK:N	2.14	0.62
1:B:1725:SER:HB3	1:C:260:LEU:HD13	1.82	0.62
1:C:2096:UNK:HG2	1:C:2097:UNK:N	2.14	0.62
1:C:980:UNK:C	1:C:981:UNK:HG3	2.29	0.62
1:A:1002:UNK:O	1:A:1003:UNK:CG	2.47	0.62
1:B:2092:UNK:HA	1:B:2189:PHE:HB2	1.81	0.62
1:A:1095:LEU:HD12	1:A:1096:THR:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ALA:HA	1:C:178:LEU:HD13	1.82	0.62
1:B:2096:UNK:HG2	1:B:2097:UNK:N	2.14	0.62
1:B:992:UNK:HG3	1:B:996:UNK:HG3	1.66	0.62
1:C:415:VAL:HG22	1:C:937:UNK:HG1	1.81	0.62
1:A:1002:UNK:HG2	1:A:1002:UNK:O	1.99	0.62
1:A:238:SER:OG	1:A:249:THR:OG1	2.16	0.62
1:C:975:UNK:HG3	1:C:993:UNK:CB	2.29	0.61
1:C:203:ASP:O	1:C:205:PRO:HD3	2.00	0.61
1:C:2092:UNK:HA	1:C:2189:PHE:HB2	1.81	0.61
1:C:2047:THR:OG1	1:C:2205:ASP:OD2	2.17	0.61
1:C:2948:GLN:HG2	1:C:2951:ARG:HH21	1.64	0.61
1:C:2297:ARG:HD3	1:C:2297:ARG:H	1.64	0.61
1:C:664:LEU:HD13	1:C:701:ALA:HB1	1.81	0.61
1:C:1702:GLU:OE2	1:C:1711:VAL:HG13	1.99	0.61
1:B:2948:GLN:HG2	1:B:2951:ARG:HH21	1.64	0.61
1:C:1431:ALA:HB3	1:C:1459:THR:HG21	1.82	0.61
1:A:793:ARG:HD3	1:A:2435:UNK:CG	2.27	0.61
1:A:2122:UNK:C	1:A:2125:UNK:HG3	2.30	0.61
1:C:2125:UNK:HA	1:C:2128:UNK:HG3	1.81	0.61
1:B:971:ALA:O	1:B:974:UNK:CG	2.48	0.61
1:B:409:LYS:HD2	1:B:933:UNK:HA	1.82	0.61
1:B:939:UNK:O	1:B:940:UNK:CG	2.47	0.61
1:A:3080:ARG:HG3	1:A:3080:ARG:NH1	2.09	0.61
1:A:511:ARG:HH11	1:A:543:GLY:HA3	1.65	0.61
1:C:575:HIS:HD2	1:C:644:LEU:HD22	1.66	0.61
1:C:1622:PRO:HD3	1:C:1685:LEU:HD11	1.81	0.61
1:B:575:HIS:HD2	1:B:644:LEU:HD22	1.66	0.61
1:C:2103:UNK:HG1	1:C:2919:GLY:O	2.00	0.61
1:C:970:ILE:CG1	1:C:996:UNK:HG1	2.31	0.61
1:B:984:UNK:CG	1:B:987:UNK:CG	2.79	0.61
1:A:939:UNK:O	1:A:940:UNK:CG	2.47	0.61
1:B:511:ARG:HH11	1:B:543:GLY:HA3	1.66	0.61
1:B:2092:UNK:HG2	1:B:2092:UNK:O	1.99	0.61
1:C:34:LEU:H	1:C:393:VAL:HG21	1.65	0.61
1:C:2112:UNK:N	1:C:2115:UNK:HG1	2.11	0.61
1:C:2434:UNK:CG	1:C:2523:GLU:O	2.48	0.61
1:A:976:UNK:O	1:A:976:UNK:HG2	2.01	0.61
1:A:415:VAL:CG2	1:A:937:UNK:HG1	2.31	0.61
1:B:415:VAL:CG2	1:B:937:UNK:HG1	2.31	0.61
1:C:1002:UNK:O	1:C:1003:UNK:CG	2.47	0.61
1:C:892:ILE:HG22	2:C:4000:FMN:HM82	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1725:SER:HB3	1:B:260:LEU:HD13	1.82	0.61
1:B:929:UNK:O	1:B:930:UNK:CG	2.45	0.61
1:B:34:LEU:H	1:B:393:VAL:HG21	1.65	0.61
1:B:106:ALA:HB1	1:B:112:PRO:HB2	1.82	0.61
1:A:164:ALA:HA	1:A:178:LEU:HD13	1.82	0.61
1:B:1622:PRO:HD3	1:B:1685:LEU:HD11	1.81	0.61
1:C:971:ALA:O	1:C:974:UNK:CG	2.48	0.61
1:A:984:UNK:HG2	1:A:987:UNK:CG	2.31	0.61
1:C:984:UNK:HG2	1:C:987:UNK:CG	2.31	0.61
1:C:409:LYS:HD2	1:C:933:UNK:HA	1.82	0.61
1:A:409:LYS:HD2	1:A:933:UNK:HA	1.82	0.61
1:A:415:VAL:HG22	1:A:937:UNK:HG1	1.81	0.61
1:C:1227:UNK:O	1:C:1227:UNK:HG2	2.00	0.61
1:A:2176:LEU:HG	1:A:2180:LYS:HE3	1.80	0.61
1:A:2469:LEU:HD11	1:A:2653:VAL:HB	1.82	0.61
1:A:260:LEU:HD13	1:C:1725:SER:HB3	1.82	0.61
1:A:1431:ALA:HB3	1:A:1459:THR:HG21	1.82	0.61
1:B:2469:LEU:HD11	1:B:2653:VAL:HB	1.82	0.61
1:A:575:HIS:HD2	1:A:644:LEU:HD22	1.66	0.61
1:B:2122:UNK:C	1:B:2125:UNK:HG3	2.30	0.61
1:A:929:UNK:O	1:A:930:UNK:CG	2.45	0.61
1:B:2135:UNK:HG3	1:B:2136:ASP:H	1.64	0.61
1:A:1126:ILE:HG22	1:A:1196:UNK:HG1	1.81	0.61
1:C:511:ARG:HH11	1:C:543:GLY:HA3	1.66	0.61
1:A:1353:PRO:HG3	1:A:1702:GLU:OE2	2.00	0.61
1:C:34:LEU:O	1:C:38:LEU:N	2.25	0.61
1:C:2469:LEU:HD11	1:C:2653:VAL:HB	1.82	0.61
1:C:3058:ARG:HB2	1:C:3089:LEU:HB2	1.82	0.61
1:A:2103:UNK:HG1	1:A:2919:GLY:O	2.00	0.61
1:C:415:VAL:CG2	1:C:937:UNK:HG1	2.31	0.61
1:B:1007:UNK:HB2	1:B:1018:ARG:HE	1.66	0.61
1:A:1212:UNK:HG2	1:A:1342:ARG:HE	1.64	0.61
1:B:70:SER:HG	1:B:142:ARG:HH22	1.49	0.61
1:A:580:ARG:HG2	1:A:590:LEU:HD21	1.83	0.61
1:C:1353:PRO:HG3	1:C:1702:GLU:OE2	2.00	0.61
1:B:1227:UNK:HG2	1:B:1227:UNK:O	2.00	0.61
1:C:750:LEU:HD12	1:C:827:LEU:HD11	1.81	0.61
1:B:126:VAL:HG12	1:B:182:ALA:HB1	1.83	0.61
1:B:1431:ALA:HB3	1:B:1459:THR:HG21	1.82	0.61
1:A:106:ALA:HB1	1:A:112:PRO:HB2	1.82	0.61
1:B:2434:UNK:CG	1:B:2523:GLU:O	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:984:UNK:HG2	1:B:987:UNK:CG	2.31	0.61
1:C:1007:UNK:HG2	1:C:1007:UNK:O	2.01	0.61
1:B:2334:HIS:HD2	1:B:2391:LYS:HG3	1.66	0.61
1:B:979:UNK:HG2	1:B:979:UNK:O	2.01	0.61
1:C:488:ASN:HA	1:C:521:VAL:HB	1.83	0.61
1:B:970:ILE:CG1	1:B:996:UNK:HG1	2.31	0.61
1:A:984:UNK:CG	1:A:987:UNK:CG	2.79	0.61
1:A:1007:UNK:O	1:A:1007:UNK:HG2	2.01	0.61
1:A:1227:UNK:HG2	1:A:1227:UNK:O	2.00	0.61
1:C:1315:ARG:HH21	1:C:1323:GLU:HG2	1.64	0.61
1:B:3058:ARG:HB2	1:B:3089:LEU:HB2	1.82	0.61
1:A:680:ALA:HA	1:A:685:ALA:HB2	1.83	0.61
1:A:970:ILE:CG1	1:A:996:UNK:HG1	2.31	0.60
1:A:980:UNK:HB2	1:A:989:UNK:HB2	1.83	0.60
1:C:984:UNK:CG	1:C:987:UNK:CG	2.79	0.60
1:A:2765:GLY:HA2	1:A:2940:VAL:HG21	1.82	0.60
1:A:34:LEU:H	1:A:393:VAL:HG21	1.65	0.60
1:B:1095:LEU:HD12	1:B:1096:THR:H	1.64	0.60
1:B:438:THR:HA	1:B:880:HIS:HE1	1.66	0.60
1:C:2173:ASP:OD2	1:C:2799:LYS:NZ	2.32	0.60
1:A:2096:UNK:HG2	1:A:2097:UNK:N	2.14	0.60
1:C:980:UNK:HB2	1:C:989:UNK:HB2	1.83	0.60
1:A:1007:UNK:HB2	1:A:1018:ARG:HE	1.66	0.60
1:A:257:ARG:HH12	1:C:1695:LEU:CD2	2.13	0.60
1:A:2647:VAL:HA	1:A:2650:TRP:HD1	1.66	0.60
1:C:580:ARG:HG2	1:C:590:LEU:HD21	1.83	0.60
1:C:2237:LEU:HB2	1:C:2287:LEU:HD11	1.82	0.60
1:C:238:SER:OG	1:C:249:THR:OG1	2.15	0.60
1:B:1315:ARG:HH21	1:B:1323:GLU:HG2	1.64	0.60
1:B:488:ASN:HA	1:B:521:VAL:HB	1.83	0.60
1:C:1532:ILE:HA	1:C:1544:ILE:HG12	1.83	0.60
1:A:2434:UNK:CG	1:A:2523:GLU:O	2.48	0.60
1:A:2112:UNK:CG	1:A:2114:UNK:HG3	2.31	0.60
1:A:203:ASP:O	1:A:205:PRO:HD3	2.01	0.60
1:B:1098:VAL:HG12	1:B:1100:ASP:H	1.66	0.60
1:A:2372:MET:HB3	1:A:2394:LEU:HD22	1.83	0.60
1:A:2237:LEU:HB2	1:A:2287:LEU:HD11	1.82	0.60
1:A:1989:PHE:HD1	1:A:1992:LYS:HZ3	1.49	0.60
1:C:2800:PHE:HE1	1:C:2812:LEU:HD22	1.67	0.60
1:B:2121:UNK:C	1:B:2124:UNK:HG3	2.31	0.60
1:A:2121:UNK:C	1:A:2124:UNK:HG3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2112:UNK:CG	1:C:2114:UNK:HG3	2.31	0.60
1:A:971:ALA:O	1:A:974:UNK:CG	2.48	0.60
1:B:1002:UNK:O	1:B:1002:UNK:HG2	2.00	0.60
1:B:203:ASP:O	1:B:205:PRO:HD3	2.01	0.60
1:A:1537:LEU:HB2	1:A:1541:GLN:H	1.67	0.60
1:C:1537:LEU:HB2	1:C:1541:GLN:H	1.67	0.60
1:C:2686:MET:HE1	1:C:2935:LYS:HG3	1.83	0.60
1:A:979:UNK:O	1:A:979:UNK:HG2	2.01	0.60
1:B:680:ALA:HA	1:B:685:ALA:HB2	1.83	0.60
1:A:438:THR:HA	1:A:880:HIS:HE1	1.66	0.60
1:B:164:ALA:HA	1:B:178:LEU:HD13	1.82	0.60
1:B:2103:UNK:HG1	1:B:2919:GLY:O	2.00	0.60
1:A:2121:UNK:O	1:A:2124:UNK:CG	2.49	0.60
1:C:929:UNK:O	1:C:930:UNK:CG	2.45	0.60
1:B:1695:LEU:CD2	1:C:257:ARG:HH12	2.13	0.60
1:B:2212:TRP:HA	1:B:2229:LYS:HD3	1.83	0.60
1:C:2212:TRP:HA	1:C:2229:LYS:HD3	1.83	0.60
1:C:2962:ASP:N	1:C:2962:ASP:OD1	2.34	0.60
1:C:126:VAL:HG12	1:C:182:ALA:HB1	1.83	0.60
1:B:1012:UNK:C	1:B:1013:UNK:HG3	2.32	0.60
1:A:2651:ASN:HD22	1:A:2718:VAL:HG12	1.67	0.60
1:A:3058:ARG:HB2	1:A:3089:LEU:HB2	1.82	0.60
1:A:488:ASN:HA	1:A:521:VAL:HB	1.83	0.60
1:C:976:UNK:HG2	1:C:976:UNK:O	2.01	0.60
1:A:1309:VAL:HG22	1:A:1331:ILE:HG12	1.84	0.60
1:C:2135:UNK:HG3	1:C:2136:ASP:H	1.64	0.60
1:A:1695:LEU:CD2	1:B:257:ARG:HH12	2.13	0.60
1:A:2334:HIS:HD2	1:A:2391:LYS:HG3	1.66	0.60
1:B:688:ARG:O	1:B:872:ARG:NE	2.34	0.60
1:B:670:GLY:O	1:B:682:ASN:ND2	2.35	0.60
1:B:687:GLY:O	1:B:695:ILE:N	2.34	0.60
1:B:2651:ASN:HD22	1:B:2718:VAL:HG12	1.67	0.60
1:B:2112:UNK:CG	1:B:2114:UNK:HG3	2.31	0.60
1:C:2081:UNK:O	1:C:2085:UNK:HG2	2.02	0.60
1:A:975:UNK:HG3	1:A:993:UNK:CB	2.29	0.60
1:A:931:UNK:O	1:A:934:UNK:HG3	2.02	0.60
1:C:1002:UNK:O	1:C:1002:UNK:HG2	1.99	0.60
1:B:2647:VAL:HA	1:B:2650:TRP:HD1	1.66	0.60
1:B:580:ARG:HG2	1:B:590:LEU:HD21	1.83	0.60
1:C:1098:VAL:HG12	1:C:1100:ASP:H	1.66	0.60
1:C:2651:ASN:HD22	1:C:2718:VAL:HG12	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1435:VAL:HG11	1:B:1463:CYS:HB3	1.84	0.60
1:A:670:GLY:O	1:A:682:ASN:ND2	2.35	0.60
1:C:2461:VAL:HG11	1:C:2751:VAL:HG22	1.84	0.60
1:A:2081:UNK:O	1:A:2085:UNK:HG2	2.02	0.60
1:C:2121:UNK:O	1:C:2124:UNK:CG	2.49	0.60
1:C:2122:UNK:C	1:C:2125:UNK:HG3	2.30	0.60
1:B:931:UNK:O	1:B:934:UNK:HG3	2.02	0.60
1:C:939:UNK:O	1:C:940:UNK:CG	2.47	0.60
1:C:1007:UNK:HB2	1:C:1018:ARG:HE	1.66	0.60
1:B:1537:LEU:HB2	1:B:1541:GLN:H	1.67	0.60
1:C:2334:HIS:HD2	1:C:2391:LYS:HG3	1.66	0.60
1:C:670:GLY:O	1:C:682:ASN:ND2	2.35	0.60
1:C:688:ARG:O	1:C:872:ARG:NE	2.34	0.60
1:A:1532:ILE:HA	1:A:1544:ILE:HG12	1.83	0.60
1:A:126:VAL:HG12	1:A:182:ALA:HB1	1.83	0.60
1:C:2121:UNK:C	1:C:2124:UNK:HG3	2.31	0.59
1:A:1012:UNK:C	1:A:1013:UNK:HG3	2.32	0.59
1:C:1435:VAL:HG11	1:C:1463:CYS:HB3	1.84	0.59
1:C:410:LEU:HB3	1:C:1025:VAL:HG21	1.84	0.59
1:B:1532:ILE:HA	1:B:1544:ILE:HG12	1.83	0.59
1:B:2081:UNK:O	1:B:2085:UNK:HG2	2.02	0.59
1:B:2121:UNK:O	1:B:2124:UNK:CG	2.49	0.59
1:C:2056:PHE:HZ	1:C:2180:LYS:HE2	1.67	0.59
1:C:2429:UNK:O	1:C:2429:UNK:HG2	2.02	0.59
1:C:680:ALA:HA	1:C:685:ALA:HB2	1.83	0.59
1:B:1989:PHE:HD1	1:B:1992:LYS:HZ3	1.50	0.59
1:B:2372:MET:HB3	1:B:2394:LEU:HD22	1.83	0.59
1:B:1656:LYS:HG2	1:B:1660:LEU:HG	1.85	0.59
1:A:410:LEU:HB3	1:A:1025:VAL:HG21	1.84	0.59
1:B:795:HIS:HB3	1:B:799:PHE:CZ	2.37	0.59
1:C:2431:UNK:HG2	1:C:2431:UNK:O	2.01	0.59
1:A:2431:UNK:HG2	1:A:2431:UNK:O	2.01	0.59
1:C:106:ALA:HB1	1:C:112:PRO:HB2	1.82	0.59
1:C:2712:GLU:HA	1:C:2717:VAL:HG11	1.83	0.59
1:A:795:HIS:HB3	1:A:799:PHE:CZ	2.37	0.59
1:B:1002:UNK:C	1:B:1003:UNK:HG3	2.33	0.59
1:A:2820:ILE:HD13	1:A:2943:MET:HG2	1.84	0.59
1:A:2800:PHE:HE1	1:A:2812:LEU:HD22	1.67	0.59
1:A:1098:VAL:HG12	1:A:1100:ASP:H	1.66	0.59
1:C:1336:VAL:HG12	1:C:1337:MET:HG3	1.85	0.59
1:A:2056:PHE:HZ	1:A:2180:LYS:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2667:THR:HG21	1:B:3058:ARG:NH1	2.17	0.59
1:A:688:ARG:O	1:A:872:ARG:NE	2.34	0.59
1:C:2372:MET:HB3	1:C:2394:LEU:HD22	1.83	0.59
1:B:793:ARG:HD3	1:B:2435:UNK:CG	2.27	0.59
1:B:976:UNK:O	1:B:976:UNK:HG2	2.01	0.59
1:C:931:UNK:O	1:C:934:UNK:HG3	2.02	0.59
1:B:980:UNK:HB2	1:B:989:UNK:HB2	1.83	0.59
1:A:2212:TRP:HA	1:A:2229:LYS:HD3	1.83	0.59
1:C:2889:ILE:HG12	1:C:2922:LEU:HB3	1.84	0.59
1:B:2431:UNK:HG2	1:B:2431:UNK:O	2.01	0.59
1:B:992:UNK:CG	1:B:994:UNK:HG2	2.30	0.59
1:B:1007:UNK:HG2	1:B:1007:UNK:O	2.01	0.59
1:A:2667:THR:HG21	1:A:3058:ARG:NH1	2.17	0.59
1:A:2712:GLU:HA	1:A:2717:VAL:HG11	1.83	0.59
1:A:1656:LYS:HG2	1:A:1660:LEU:HG	1.85	0.59
1:A:2686:MET:HE1	1:A:2935:LYS:HG3	1.83	0.59
1:C:1701:VAL:HG22	1:C:1732:LEU:HB2	1.84	0.59
1:A:2693:GLN:O	1:A:2697:HIS:ND1	2.33	0.59
1:A:2094:UNK:CG	1:A:2096:UNK:CG	2.75	0.59
1:B:1336:VAL:HG12	1:B:1337:MET:HG3	1.85	0.59
1:C:2135:UNK:CG	1:C:2136:ASP:N	2.66	0.59
1:C:2647:VAL:HA	1:C:2650:TRP:HD1	1.66	0.59
1:B:2056:PHE:HZ	1:B:2180:LYS:HE2	1.67	0.59
1:B:2403:ILE:HG23	1:B:2408:LEU:HD12	1.85	0.59
1:B:2461:VAL:HG11	1:B:2751:VAL:HG22	1.84	0.59
1:C:1616:PRO:HG3	1:C:1668:LEU:HD13	1.85	0.59
1:B:934:UNK:C	1:B:937:UNK:HG3	2.32	0.59
1:A:943:UNK:C	1:A:944:UNK:HG3	2.32	0.59
1:C:1309:VAL:HG22	1:C:1331:ILE:HG12	1.84	0.59
1:A:150:THR:O	1:A:152:PRO:HD3	2.03	0.59
1:B:2800:PHE:HE1	1:B:2812:LEU:HD22	1.67	0.59
1:C:2124:UNK:O	1:C:2127:UNK:CG	2.51	0.58
1:C:836:VAL:HG12	1:C:837:VAL:H	1.67	0.58
1:C:979:UNK:O	1:C:979:UNK:HG2	2.01	0.58
1:B:2686:MET:HE1	1:B:2935:LYS:HG3	1.83	0.58
1:B:462:GLN:HG3	1:B:468:PHE:HD1	1.68	0.58
1:A:1001:UNK:C	1:A:1002:UNK:HG3	2.33	0.58
1:C:1012:UNK:C	1:C:1013:UNK:HG3	2.32	0.58
1:C:943:UNK:C	1:C:944:UNK:HG3	2.32	0.58
1:A:1336:VAL:HG12	1:A:1337:MET:HG3	1.85	0.58
1:C:438:THR:HA	1:C:880:HIS:HE1	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1616:PRO:HG3	1:A:1668:LEU:HD13	1.85	0.58
1:C:1001:UNK:C	1:C:1002:UNK:HG3	2.33	0.58
1:B:1001:UNK:C	1:B:1002:UNK:HG3	2.33	0.58
1:B:1008:UNK:CG	1:B:1019:PHE:HB3	2.33	0.58
1:C:621:SER:OG	1:C:643:ILE:HD13	2.04	0.58
1:A:2429:UNK:HG2	1:A:2429:UNK:O	2.02	0.58
1:A:2889:ILE:HG12	1:A:2922:LEU:HB3	1.84	0.58
1:B:1327:VAL:HB	1:B:1339:ALA:HB3	1.86	0.58
1:C:150:THR:O	1:C:152:PRO:HD3	2.03	0.58
1:B:1701:VAL:HG22	1:B:1732:LEU:HB2	1.84	0.58
1:C:795:HIS:HB3	1:C:799:PHE:CZ	2.37	0.58
1:B:1253:ARG:NH1	1:B:1253:ARG:HG3	2.18	0.58
1:A:1008:UNK:O	1:A:1008:UNK:HG2	2.03	0.58
1:B:2712:GLU:HA	1:B:2717:VAL:HG11	1.84	0.58
1:A:735:LYS:HD2	1:A:860:VAL:HG23	1.86	0.58
1:C:990:UNK:CG	1:C:998:UNK:HB2	2.34	0.58
1:C:1253:ARG:HG3	1:C:1253:ARG:NH1	2.18	0.58
1:A:1008:UNK:CG	1:A:1019:PHE:HB3	2.33	0.58
1:C:2667:THR:HG21	1:C:3058:ARG:NH1	2.17	0.58
1:A:1327:VAL:HB	1:A:1339:ALA:HB3	1.86	0.58
1:A:2461:VAL:HG11	1:A:2751:VAL:HG22	1.84	0.58
1:A:2124:UNK:C	1:A:2127:UNK:HG3	2.34	0.58
1:B:836:VAL:HG12	1:B:837:VAL:H	1.67	0.58
1:A:1701:VAL:HG22	1:A:1732:LEU:HB2	1.84	0.58
1:C:2521:VAL:HG13	1:C:2529:ARG:HH11	1.68	0.58
1:B:1008:UNK:O	1:B:1008:UNK:HG2	2.03	0.58
1:B:2876:LEU:HB3	1:B:2881:VAL:HG12	1.86	0.58
1:A:117:LYS:NZ	1:C:1087:PHE:HB3	2.18	0.58
1:B:2787:THR:HA	1:B:2790:MET:HG3	1.86	0.58
1:C:687:GLY:O	1:C:695:ILE:N	2.34	0.58
1:B:1616:PRO:HG3	1:B:1668:LEU:HD13	1.85	0.58
1:C:1989:PHE:HD1	1:C:1992:LYS:HZ3	1.51	0.58
1:A:836:VAL:HG12	1:A:837:VAL:H	1.67	0.58
1:B:2487:LEU:HD11	1:B:2495:LEU:HD12	1.86	0.58
1:A:2101:UNK:O	1:A:2105:UNK:HG3	2.04	0.58
1:B:970:ILE:CD1	1:B:996:UNK:HG1	2.34	0.58
1:C:970:ILE:CD1	1:C:996:UNK:HG1	2.34	0.58
1:A:511:ARG:HD2	1:A:517:ILE:O	2.04	0.58
1:C:1656:LYS:HG2	1:C:1660:LEU:HG	1.85	0.58
1:A:784:GLU:OE2	1:A:787:LEU:HD12	2.04	0.58
1:B:410:LEU:HB3	1:B:1025:VAL:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ASP:OD2	1:A:443:LYS:HB3	2.04	0.58
1:B:2820:ILE:HD13	1:B:2943:MET:HG2	1.84	0.58
1:B:2339:TRP:HB2	1:B:2398:LEU:HD11	1.86	0.58
1:B:776:ASP:O	1:B:779:TRP:N	2.31	0.58
1:B:990:UNK:CG	1:B:998:UNK:HB2	2.34	0.58
1:A:2487:LEU:HD11	1:A:2495:LEU:HD12	1.86	0.58
1:B:943:UNK:C	1:B:944:UNK:HG3	2.32	0.58
1:B:1309:VAL:HG22	1:B:1331:ILE:HG12	1.84	0.58
1:A:2787:THR:HA	1:A:2790:MET:HG3	1.86	0.58
1:A:2521:VAL:HG13	1:A:2529:ARG:HH11	1.68	0.58
1:B:784:GLU:OE2	1:B:787:LEU:HD12	2.03	0.58
1:A:2554:ALA:HB1	1:A:2614:LYS:NZ	2.19	0.58
1:B:1412:HIS:ND1	1:B:1415:GLY:O	2.26	0.57
1:C:1008:UNK:HG2	1:C:1008:UNK:O	2.03	0.57
1:C:2403:ILE:HG23	1:C:2408:LEU:HD12	1.85	0.57
1:A:1435:VAL:HG11	1:A:1463:CYS:HB3	1.84	0.57
1:A:1091:LEU:HD13	1:A:1281:ALA:HB3	1.86	0.57
1:A:462:GLN:HG3	1:A:468:PHE:HD1	1.68	0.57
1:C:441:ASP:OD2	1:C:443:LYS:HB3	2.04	0.57
1:B:2124:UNK:C	1:B:2127:UNK:HG3	2.34	0.57
1:C:2101:UNK:O	1:C:2105:UNK:HG3	2.04	0.57
1:A:924:LEU:HA	1:A:928:ALA:HB3	1.87	0.57
1:C:1002:UNK:C	1:C:1003:UNK:HG3	2.33	0.57
1:A:1002:UNK:C	1:A:1003:UNK:HG3	2.33	0.57
1:A:999:UNK:CG	1:A:1007:UNK:HG2	2.34	0.57
1:B:1226:UNK:HG3	1:B:1313:VAL:CG1	2.35	0.57
1:A:476:GLU:HA	1:A:479:LEU:HB2	1.86	0.57
1:A:1087:PHE:HB3	1:B:117:LYS:NZ	2.18	0.57
1:B:1009:UNK:HG2	1:B:1009:UNK:O	2.04	0.57
1:B:1095:LEU:HD22	1:B:1289:PRO:HA	1.85	0.57
1:C:2487:LEU:HD11	1:C:2495:LEU:HD12	1.86	0.57
1:B:2101:UNK:O	1:B:2105:UNK:HG3	2.04	0.57
1:C:934:UNK:C	1:C:937:UNK:HG3	2.32	0.57
1:B:621:SER:OG	1:B:643:ILE:HD13	2.04	0.57
1:A:1095:LEU:HD22	1:A:1289:PRO:HA	1.85	0.57
1:C:2339:TRP:HB2	1:C:2398:LEU:HD11	1.86	0.57
1:A:2339:TRP:HB2	1:A:2398:LEU:HD11	1.86	0.57
1:C:2554:ALA:HB1	1:C:2614:LYS:NZ	2.19	0.57
1:C:1017:ILE:HG23	1:C:1045:VAL:HG21	1.87	0.57
1:A:939:UNK:C	1:A:940:UNK:HG3	2.33	0.57
1:C:511:ARG:HD2	1:C:517:ILE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1087:PHE:HB3	1:C:117:LYS:NZ	2.19	0.57
1:A:621:SER:OG	1:A:643:ILE:HD13	2.04	0.57
1:A:1405:ALA:HB3	1:A:1408:VAL:HG23	1.86	0.57
1:C:129:VAL:HG13	1:C:356:PRO:HG2	1.85	0.57
1:A:990:UNK:CG	1:A:998:UNK:HB2	2.34	0.57
1:A:2124:UNK:O	1:A:2127:UNK:CG	2.51	0.57
1:C:2086:UNK:HA	1:C:2089:UNK:HG3	1.86	0.57
1:C:2124:UNK:C	1:C:2127:UNK:HG3	2.34	0.57
1:A:970:ILE:CD1	1:A:996:UNK:HG1	2.34	0.57
1:C:924:LEU:HA	1:C:928:ALA:HB3	1.87	0.57
1:B:924:LEU:HA	1:B:928:ALA:HB3	1.86	0.57
1:C:999:UNK:CG	1:C:1007:UNK:HG2	2.34	0.57
1:C:476:GLU:HA	1:C:479:LEU:HB2	1.86	0.57
1:B:129:VAL:HG13	1:B:356:PRO:HG2	1.85	0.57
1:C:2820:ILE:HD13	1:C:2943:MET:HG2	1.84	0.57
1:B:2889:ILE:HG12	1:B:2922:LEU:HB3	1.84	0.57
1:B:2983:LEU:HB3	1:B:2987:PHE:O	2.05	0.57
1:B:2521:VAL:HG13	1:B:2529:ARG:HH11	1.68	0.57
1:C:490:LEU:HD23	1:C:523:SER:HB2	1.87	0.57
1:C:1445:VAL:HG23	1:C:1448:ALA:HB2	1.87	0.57
1:C:2846:ALA:HA	1:C:3001:HIS:O	2.05	0.57
1:B:975:UNK:HG2	1:B:976:UNK:N	2.20	0.57
1:C:939:UNK:C	1:C:940:UNK:HG3	2.33	0.57
1:C:1008:UNK:CG	1:C:1019:PHE:HB3	2.33	0.57
1:C:1009:UNK:O	1:C:1009:UNK:HG2	2.04	0.57
1:A:1009:UNK:HG2	1:A:1009:UNK:O	2.03	0.57
1:A:2709:ILE:O	1:A:2713:VAL:HG13	2.05	0.57
1:C:1095:LEU:HD22	1:C:1289:PRO:HA	1.85	0.57
1:C:2622:GLY:HA2	1:C:2812:LEU:HD11	1.87	0.57
1:B:2429:UNK:HG2	1:B:2429:UNK:O	2.02	0.57
1:C:2876:LEU:HB3	1:C:2881:VAL:HG12	1.86	0.57
1:A:2403:ILE:HG23	1:A:2408:LEU:HD12	1.85	0.57
1:B:2846:ALA:HA	1:B:3001:HIS:O	2.05	0.57
1:C:784:GLU:OE2	1:C:787:LEU:HD12	2.03	0.57
1:A:2846:ALA:HA	1:A:3001:HIS:O	2.05	0.57
1:B:1445:VAL:HG23	1:B:1448:ALA:HB2	1.87	0.57
1:B:2084:UNK:O	1:B:2087:UNK:CG	2.52	0.57
1:A:980:UNK:O	1:A:981:UNK:CG	2.53	0.57
1:C:929:UNK:C	1:C:930:UNK:HG3	2.35	0.57
1:A:2876:LEU:HB3	1:A:2881:VAL:HG12	1.86	0.57
1:A:1537:LEU:HD11	1:A:1714:LEU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:735:LYS:HD2	1:B:860:VAL:HG23	1.85	0.57
1:C:127:PRO:HG3	1:C:183:GLN:HA	1.86	0.57
1:B:978:UNK:HB2	1:B:991:UNK:HG2	1.87	0.57
1:B:441:ASP:OD2	1:B:443:LYS:HB3	2.04	0.57
1:C:1091:LEU:HD13	1:C:1281:ALA:HB3	1.86	0.57
1:B:2100:UNK:CG	1:B:2101:UNK:N	2.68	0.57
1:B:511:ARG:NH1	1:B:543:GLY:HA3	2.19	0.57
1:B:127:PRO:HG3	1:B:183:GLN:HA	1.86	0.57
1:C:462:GLN:HG3	1:C:468:PHE:HD1	1.68	0.57
1:B:2124:UNK:O	1:B:2127:UNK:CG	2.51	0.57
1:C:980:UNK:O	1:C:981:UNK:CG	2.53	0.57
1:C:2787:THR:HA	1:C:2790:MET:HG3	1.86	0.57
1:B:868:ARG:HB3	1:B:872:ARG:HH11	1.70	0.57
1:C:2521:VAL:HG13	1:C:2529:ARG:NH1	2.20	0.57
1:B:1126:ILE:O	1:B:1197:UNK:CG	2.53	0.56
1:A:511:ARG:NH1	1:A:543:GLY:HA3	2.19	0.56
1:C:868:ARG:HB3	1:C:872:ARG:HH11	1.70	0.56
1:A:868:ARG:HB3	1:A:872:ARG:HH11	1.70	0.56
1:B:2961:LEU:HD23	1:B:2978:ARG:HB3	1.87	0.56
1:A:129:VAL:HG13	1:A:356:PRO:HG2	1.85	0.56
1:A:127:PRO:HG3	1:A:183:GLN:HA	1.85	0.56
1:C:793:ARG:HD3	1:C:2435:UNK:CG	2.27	0.56
1:A:490:LEU:HD23	1:A:523:SER:HB2	1.87	0.56
1:C:735:LYS:HD2	1:C:860:VAL:HG23	1.85	0.56
1:A:2086:UNK:HA	1:A:2089:UNK:HG3	1.86	0.56
1:A:976:UNK:CG	1:A:993:UNK:HB1	2.29	0.56
1:B:939:UNK:C	1:B:940:UNK:HG3	2.33	0.56
1:B:999:UNK:CG	1:B:1007:UNK:HG2	2.34	0.56
1:B:1001:UNK:O	1:B:1002:UNK:CG	2.53	0.56
1:B:476:GLU:HA	1:B:479:LEU:HB2	1.86	0.56
1:A:37:ARG:O	1:A:41:GLY:N	2.38	0.56
1:B:1637:VAL:HG21	1:B:1671:TRP:CG	2.40	0.56
1:B:511:ARG:HD2	1:B:517:ILE:O	2.04	0.56
1:B:2709:ILE:O	1:B:2713:VAL:HG13	2.05	0.56
1:C:1537:LEU:HD11	1:C:1714:LEU:HB3	1.86	0.56
1:B:2521:VAL:HG13	1:B:2529:ARG:NH1	2.20	0.56
1:C:1420:THR:OG1	1:C:1485:HIS:NE2	2.38	0.56
1:A:745:THR:OG1	1:A:834:GLU:O	2.19	0.56
1:C:177:GLU:HB3	1:C:317:LEU:HD13	1.87	0.56
1:B:150:THR:O	1:B:152:PRO:HD3	2.03	0.56
1:B:2554:ALA:HB1	1:B:2614:LYS:NZ	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2481:MET:O	1:B:2959:ARG:NH2	2.39	0.56
1:A:1017:ILE:HG23	1:A:1045:VAL:HG21	1.87	0.56
1:C:1126:ILE:O	1:C:1197:UNK:CG	2.53	0.56
1:A:1253:ARG:NH1	1:A:1253:ARG:HG3	2.18	0.56
1:C:511:ARG:NH1	1:C:543:GLY:HA3	2.19	0.56
1:A:2881:VAL:HG13	1:A:2885:ASP:HB2	1.88	0.56
1:A:2521:VAL:HG13	1:A:2529:ARG:NH1	2.20	0.56
1:C:2957:PRO:HD3	1:C:2980:PRO:HB3	1.88	0.56
1:B:177:GLU:HB3	1:B:317:LEU:HD13	1.87	0.56
1:A:978:UNK:HB2	1:A:991:UNK:HG2	1.87	0.56
1:A:776:ASP:O	1:A:779:TRP:N	2.31	0.56
1:B:1091:LEU:HD13	1:B:1281:ALA:HB3	1.86	0.56
1:A:975:UNK:HG2	1:A:976:UNK:N	2.20	0.56
1:B:2622:GLY:HA2	1:B:2812:LEU:HD11	1.87	0.56
1:A:990:UNK:O	1:A:990:UNK:HG2	2.05	0.56
1:C:2693:GLN:O	1:C:2697:HIS:ND1	2.33	0.56
1:C:475:LEU:O	1:C:479:LEU:N	2.37	0.56
1:B:2962:ASP:OD1	1:B:2962:ASP:N	2.34	0.56
1:B:1511:ASP:H	1:B:1514:ASP:HB2	1.71	0.56
1:A:2983:LEU:HB3	1:A:2987:PHE:O	2.05	0.56
1:C:1327:VAL:HB	1:C:1339:ALA:HB3	1.86	0.56
1:C:1511:ASP:H	1:C:1514:ASP:HB2	1.71	0.56
1:C:1226:UNK:HG3	1:C:1313:VAL:CG1	2.35	0.56
1:C:1637:VAL:HG21	1:C:1671:TRP:CG	2.40	0.56
1:A:1637:VAL:HG21	1:A:1671:TRP:CG	2.40	0.56
1:C:2478:ARG:NH1	1:C:2482:GLU:OE1	2.39	0.56
1:B:2478:ARG:NH1	1:B:2482:GLU:OE1	2.39	0.56
1:B:2086:UNK:HA	1:B:2089:UNK:HG3	1.86	0.56
1:B:2094:UNK:CG	1:B:2096:UNK:CG	2.75	0.56
1:C:2084:UNK:O	1:C:2087:UNK:CG	2.52	0.56
1:C:992:UNK:CG	1:C:996:UNK:HG2	2.32	0.56
1:A:1126:ILE:O	1:A:1197:UNK:CG	2.53	0.56
1:A:1226:UNK:HG3	1:A:1313:VAL:CG1	2.35	0.56
1:C:2709:ILE:O	1:C:2713:VAL:HG13	2.05	0.56
1:B:1537:LEU:HD11	1:B:1714:LEU:HB3	1.87	0.56
1:C:2961:LEU:HD23	1:C:2978:ARG:HB3	1.87	0.56
1:A:1511:ASP:H	1:A:1514:ASP:HB2	1.71	0.56
1:C:2983:LEU:HB3	1:C:2987:PHE:O	2.05	0.56
1:C:978:UNK:HB2	1:C:991:UNK:HG2	1.87	0.56
1:A:2478:ARG:NH1	1:A:2482:GLU:OE1	2.39	0.56
1:A:2961:LEU:HD23	1:A:2978:ARG:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2102:UNK:C	1:A:2105:UNK:HG3	2.36	0.56
1:C:2102:UNK:C	1:C:2105:UNK:HG3	2.36	0.56
1:B:1017:ILE:HG23	1:B:1045:VAL:HG21	1.87	0.56
1:B:490:LEU:HD23	1:B:523:SER:HB2	1.87	0.56
1:C:1618:LEU:HG	1:C:1619:VAL:HG23	1.88	0.56
1:B:1618:LEU:HG	1:B:1619:VAL:HG23	1.88	0.56
1:A:687:GLY:O	1:A:695:ILE:N	2.34	0.56
1:A:2084:UNK:O	1:A:2087:UNK:CG	2.52	0.56
1:C:975:UNK:HG2	1:C:976:UNK:N	2.20	0.56
1:C:37:ARG:O	1:C:41:GLY:N	2.39	0.56
1:C:990:UNK:O	1:C:990:UNK:HG2	2.05	0.56
1:B:990:UNK:HG2	1:B:990:UNK:O	2.05	0.56
1:B:2303:ASP:OD1	1:B:2303:ASP:N	2.39	0.56
1:C:1405:ALA:HB3	1:C:1408:VAL:HG23	1.86	0.56
1:A:1445:VAL:HG23	1:A:1448:ALA:HB2	1.87	0.56
1:B:1420:THR:OG1	1:B:1485:HIS:NE2	2.38	0.56
1:A:934:UNK:C	1:A:937:UNK:HG3	2.32	0.55
1:B:929:UNK:C	1:B:930:UNK:HG3	2.35	0.55
1:B:2743:ALA:HB3	1:B:2939:ALA:HB3	1.88	0.55
1:B:540:ASN:HD21	1:B:544:ILE:HG13	1.71	0.55
1:A:2743:ALA:HB3	1:A:2939:ALA:HB3	1.88	0.55
1:B:1405:ALA:HB3	1:B:1408:VAL:HG23	1.87	0.55
1:A:2481:MET:O	1:A:2959:ARG:NH2	2.39	0.55
1:B:2102:UNK:C	1:B:2105:UNK:HG3	2.36	0.55
1:A:929:UNK:C	1:A:930:UNK:HG3	2.35	0.55
1:B:931:UNK:HG2	1:B:934:UNK:N	2.21	0.55
1:B:475:LEU:O	1:B:479:LEU:N	2.37	0.55
1:B:737:TYR:HE1	1:B:862:VAL:HA	1.72	0.55
1:A:1618:LEU:HG	1:A:1619:VAL:HG23	1.88	0.55
1:B:975:UNK:CG	1:B:976:UNK:N	2.70	0.55
1:B:980:UNK:O	1:B:981:UNK:CG	2.53	0.55
1:A:2135:UNK:CG	1:A:2136:ASP:N	2.66	0.55
1:A:2622:GLY:HA2	1:A:2812:LEU:HD11	1.87	0.55
1:C:2442:UNK:HG2	1:C:2442:UNK:O	2.07	0.55
1:C:1496:SER:HB3	1:C:1578:ASP:HB3	1.89	0.55
1:C:2481:MET:O	1:C:2959:ARG:NH2	2.39	0.55
1:B:1010:UNK:O	1:B:1017:ILE:N	2.29	0.55
1:C:1010:UNK:O	1:C:1017:ILE:N	2.29	0.55
1:A:540:ASN:HD21	1:A:544:ILE:HG13	1.71	0.55
1:C:2881:VAL:HG13	1:C:2885:ASP:HB2	1.88	0.55
1:B:551:PRO:HG3	1:B:560:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HB3	1:A:317:LEU:HD13	1.87	0.55
1:B:2704:ALA:O	1:B:2705:LYS:HD3	2.07	0.55
1:A:931:UNK:HG2	1:A:933:UNK:CG	2.37	0.55
1:A:1690:GLU:O	1:A:1694:GLY:N	2.40	0.55
1:C:2810:GLY:HA2	1:C:2896:THR:HA	1.89	0.55
1:B:2458:ALA:HA	1:B:2824:ARG:HD2	1.89	0.55
1:A:1734:SER:HA	1:A:1741:LEU:HD11	1.89	0.55
1:A:931:UNK:HG2	1:A:934:UNK:N	2.21	0.55
1:B:2135:UNK:CG	1:B:2136:ASP:N	2.66	0.55
1:B:238:SER:OG	1:B:249:THR:OG1	2.15	0.55
1:B:2957:PRO:HD3	1:B:2980:PRO:HB3	1.88	0.55
1:C:737:TYR:HE1	1:C:862:VAL:HA	1.72	0.55
1:C:1690:GLU:O	1:C:1694:GLY:N	2.40	0.55
1:B:1496:SER:HB3	1:B:1578:ASP:HB3	1.88	0.55
1:A:737:TYR:HE1	1:A:862:VAL:HA	1.72	0.55
1:A:2087:UNK:CA	1:A:2090:UNK:HG3	2.37	0.55
1:C:994:UNK:CG	1:C:996:UNK:HG3	2.37	0.55
1:C:1001:UNK:O	1:C:1002:UNK:CG	2.53	0.55
1:B:2418:GLY:O	1:B:2422:UNK:N	2.40	0.55
1:A:2704:ALA:O	1:A:2705:LYS:HD3	2.07	0.55
1:A:2458:ALA:HA	1:A:2824:ARG:HD2	1.89	0.55
1:C:144:GLY:O	1:C:148:THR:N	2.34	0.55
1:B:1724:TYR:OH	1:C:267:GLU:OE2	2.07	0.55
1:A:1001:UNK:O	1:A:1002:UNK:CG	2.53	0.55
1:A:2418:GLY:O	1:A:2422:UNK:N	2.40	0.54
1:B:1163:ASP:CB	1:B:1199:UNK:HG3	2.37	0.54
1:B:2442:UNK:O	1:B:2442:UNK:HG2	2.07	0.54
1:B:763:SER:O	1:B:766:ASP:N	2.41	0.54
1:B:1690:GLU:O	1:B:1694:GLY:N	2.40	0.54
1:A:975:UNK:CG	1:A:976:UNK:N	2.70	0.54
1:C:975:UNK:CG	1:C:976:UNK:N	2.70	0.54
1:A:33:ALA:O	1:A:37:ARG:N	2.35	0.54
1:C:540:ASN:HD21	1:C:544:ILE:HG13	1.71	0.54
1:C:978:UNK:HB2	1:C:991:UNK:CG	2.37	0.54
1:A:2303:ASP:N	1:A:2303:ASP:OD1	2.39	0.54
1:A:2810:GLY:HA2	1:A:2896:THR:HA	1.89	0.54
1:B:2810:GLY:HA2	1:B:2896:THR:HA	1.89	0.54
1:C:931:UNK:HG2	1:C:934:UNK:N	2.21	0.54
1:A:2957:PRO:HD3	1:A:2980:PRO:HB3	1.88	0.54
1:C:2704:ALA:O	1:C:2705:LYS:HD3	2.07	0.54
1:B:2115:UNK:HA	1:B:2118:UNK:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:UNK:O	1:A:1017:ILE:N	2.29	0.54
1:C:931:UNK:HG2	1:C:933:UNK:CG	2.37	0.54
1:C:2743:ALA:HB3	1:C:2939:ALA:HB3	1.88	0.54
1:B:2881:VAL:HG13	1:B:2885:ASP:HB2	1.88	0.54
1:A:2417:SER:O	1:A:2421:ASP:N	2.40	0.54
1:C:763:SER:O	1:C:766:ASP:N	2.41	0.54
1:C:2103:UNK:O	1:C:2106:UNK:HG3	2.08	0.54
1:C:2860:ALA:HB1	1:C:3005:LEU:HD13	1.90	0.54
1:A:668:THR:OG1	1:A:698:ILE:HD11	2.08	0.54
1:A:3018:LEU:O	1:A:3022:GLU:HB2	2.08	0.54
1:B:2693:GLN:O	1:B:2697:HIS:ND1	2.33	0.54
1:C:2458:ALA:HA	1:C:2824:ARG:HD2	1.89	0.54
1:C:273:ARG:HD2	1:C:282:VAL:HG12	1.90	0.54
1:B:580:ARG:HH11	1:B:614:GLY:HA3	1.72	0.54
1:C:580:ARG:HH11	1:C:614:GLY:HA3	1.73	0.54
1:A:1496:SER:HB3	1:A:1578:ASP:HB3	1.89	0.54
1:C:716:ALA:HA	1:C:719:VAL:HG23	1.90	0.54
1:A:2122:UNK:CA	1:A:2125:UNK:HG3	2.38	0.54
1:C:2100:UNK:CG	1:C:2101:UNK:N	2.68	0.54
1:C:2115:UNK:HA	1:C:2118:UNK:HG3	1.90	0.54
1:C:2127:UNK:O	1:C:2130:UNK:CG	2.52	0.54
1:C:1003:UNK:CG	1:C:1004:UNK:N	2.53	0.54
1:C:2418:GLY:O	1:C:2422:UNK:N	2.40	0.54
1:B:37:ARG:O	1:B:41:GLY:N	2.39	0.54
1:C:1163:ASP:CB	1:C:1199:UNK:HG3	2.38	0.54
1:A:2246:ALA:C	1:A:2255:ARG:HH12	2.11	0.54
1:A:763:SER:O	1:A:766:ASP:N	2.41	0.54
1:B:2768:ASP:OD2	1:B:2936:GLY:N	2.41	0.54
1:C:1357:ILE:HG13	1:C:1710:THR:HG21	1.89	0.54
1:A:456:GLU:HG2	1:A:486:GLN:HE21	1.73	0.54
1:A:2112:UNK:N	1:A:2115:UNK:HG3	2.23	0.54
1:B:273:ARG:HD2	1:B:282:VAL:HG12	1.90	0.54
1:B:668:THR:OG1	1:B:698:ILE:HD11	2.08	0.54
1:B:978:UNK:HB2	1:B:991:UNK:CG	2.37	0.54
1:A:978:UNK:HB2	1:A:991:UNK:CG	2.37	0.54
1:A:2492:VAL:HG21	1:A:2527:VAL:HG22	1.90	0.54
1:C:456:GLU:HG2	1:C:486:GLN:HE21	1.73	0.54
1:A:1357:ILE:HG13	1:A:1710:THR:HG21	1.89	0.54
1:B:2104:UNK:HA	1:B:2107:UNK:HG3	1.90	0.54
1:C:33:ALA:O	1:C:37:ARG:N	2.35	0.54
1:C:3018:LEU:O	1:C:3022:GLU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2100:UNK:C	1:B:2103:UNK:HG3	2.31	0.54
1:C:2087:UNK:CA	1:C:2090:UNK:HG3	2.37	0.54
1:A:994:UNK:CG	1:A:996:UNK:HG3	2.37	0.54
1:A:980:UNK:N	1:A:989:UNK:O	2.41	0.54
1:B:2860:ALA:HB1	1:B:3005:LEU:HD13	1.90	0.54
1:A:2012:GLY:C	1:B:2591:ARG:NH1	2.61	0.54
1:B:624:TYR:HA	1:B:629:TRP:CD1	2.43	0.54
1:C:624:TYR:HA	1:C:629:TRP:CD1	2.43	0.54
1:B:1734:SER:HA	1:B:1741:LEU:HD11	1.89	0.54
1:A:2100:UNK:CG	1:A:2101:UNK:N	2.68	0.53
1:A:475:LEU:O	1:A:479:LEU:N	2.37	0.53
1:C:2653:VAL:HA	1:C:3051:MET:HE3	1.90	0.53
1:C:1323:GLU:N	1:C:1343:LEU:O	2.41	0.53
1:B:1089:ALA:O	1:B:1091:LEU:N	2.41	0.53
1:A:2442:UNK:O	1:A:2442:UNK:HG2	2.07	0.53
1:A:267:GLU:OE2	1:C:1724:TYR:OH	2.07	0.53
1:A:368:ILE:HG21	1:A:373:ILE:HG13	1.90	0.53
1:B:456:GLU:HG2	1:B:486:GLN:HE21	1.73	0.53
1:C:2551:PRO:O	1:C:2617:LEU:HB2	2.08	0.53
1:B:2417:SER:O	1:B:2421:ASP:N	2.40	0.53
1:B:2103:UNK:O	1:B:2106:UNK:HG3	2.08	0.53
1:C:2104:UNK:HA	1:C:2107:UNK:HG3	1.90	0.53
1:C:992:UNK:HG2	1:C:994:UNK:HG2	1.87	0.53
1:C:999:UNK:HG3	1:C:1007:UNK:HG2	1.90	0.53
1:C:33:ALA:O	1:C:37:ARG:HG2	2.08	0.53
1:A:1089:ALA:O	1:A:1091:LEU:N	2.42	0.53
1:C:1734:SER:HA	1:C:1741:LEU:HD11	1.89	0.53
1:C:2303:ASP:OD1	1:C:2303:ASP:N	2.39	0.53
1:B:2425:UNK:O	1:B:2425:UNK:HG2	2.09	0.53
1:C:551:PRO:HG3	1:C:560:VAL:HG21	1.89	0.53
1:A:624:TYR:HA	1:A:629:TRP:CD1	2.43	0.53
1:B:2492:VAL:HG21	1:B:2527:VAL:HG22	1.90	0.53
1:B:2088:UNK:HG2	1:B:2188:ARG:HH12	1.73	0.53
1:B:992:UNK:HG2	1:B:994:UNK:HG2	1.87	0.53
1:B:994:UNK:CG	1:B:996:UNK:HG3	2.37	0.53
1:A:1163:ASP:CB	1:A:1199:UNK:HG3	2.38	0.53
1:A:580:ARG:HH11	1:A:614:GLY:HA3	1.72	0.53
1:C:2768:ASP:OD2	1:C:2936:GLY:N	2.41	0.53
1:A:2088:UNK:HG2	1:A:2188:ARG:HH12	1.74	0.53
1:C:2122:UNK:CA	1:C:2125:UNK:HG3	2.38	0.53
1:C:970:ILE:HD13	1:C:996:UNK:HG1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:668:THR:OG1	1:C:698:ILE:HD11	2.08	0.53
1:A:1323:GLU:N	1:A:1343:LEU:O	2.41	0.53
1:C:836:VAL:HG21	1:C:2437:UNK:HB2	1.90	0.53
1:A:2425:UNK:O	1:A:2425:UNK:HG2	2.09	0.53
1:A:526:ILE:HD12	1:A:549:PHE:HB3	1.90	0.53
1:A:2768:ASP:OD2	1:A:2936:GLY:N	2.41	0.53
1:A:792:ALA:HA	1:A:799:PHE:CE2	2.43	0.53
1:A:2085:UNK:C	1:A:2088:UNK:HG3	2.38	0.53
1:A:2104:UNK:HA	1:A:2107:UNK:HG3	1.90	0.53
1:A:992:UNK:CG	1:A:996:UNK:HG2	2.32	0.53
1:C:980:UNK:N	1:C:989:UNK:O	2.41	0.53
1:C:1089:ALA:O	1:C:1091:LEU:N	2.42	0.53
1:B:3018:LEU:O	1:B:3022:GLU:HB2	2.08	0.53
1:C:500:GLN:O	1:C:504:LYS:N	2.24	0.53
1:B:2551:PRO:O	1:B:2617:LEU:HB2	2.08	0.53
1:A:1425:VAL:HG13	1:A:1474:LEU:HD13	1.91	0.53
1:C:2492:VAL:HG21	1:C:2527:VAL:HG22	1.90	0.53
1:B:2086:UNK:O	1:B:2089:UNK:CG	2.52	0.53
1:A:2081:UNK:C	1:A:2084:UNK:HG3	2.39	0.53
1:C:2123:UNK:O	1:C:2126:UNK:CG	2.55	0.53
1:B:980:UNK:N	1:B:989:UNK:O	2.41	0.53
1:B:1538:ARG:NH1	1:B:1722:PRO:HB3	2.18	0.53
1:A:2591:ARG:NH1	1:C:2012:GLY:C	2.61	0.53
1:B:411:PRO:HD2	1:B:1025:VAL:HG11	1.91	0.53
1:C:1425:VAL:HG13	1:C:1474:LEU:HD13	1.91	0.53
1:C:745:THR:HG23	1:C:834:GLU:HA	1.90	0.53
1:B:1148:GLU:O	1:B:1150:ALA:N	2.42	0.53
1:A:716:ALA:HA	1:A:719:VAL:HG23	1.90	0.53
1:C:2631:PRO:HG3	1:C:2649:LEU:HD13	1.90	0.53
1:A:551:PRO:HG3	1:A:560:VAL:HG21	1.89	0.53
1:C:2082:UNK:O	1:C:2086:UNK:HG3	2.09	0.53
1:B:992:UNK:HG1	1:B:994:UNK:HG3	1.81	0.53
1:A:970:ILE:HD13	1:A:996:UNK:HG1	1.91	0.53
1:A:999:UNK:HG3	1:A:1007:UNK:HG2	1.90	0.53
1:B:33:ALA:O	1:B:37:ARG:HG2	2.08	0.53
1:C:1226:UNK:HB1	1:C:1282:THR:HG21	1.90	0.53
1:A:1087:PHE:HB3	1:B:117:LYS:HZ1	1.74	0.53
1:A:836:VAL:HG21	1:A:2437:UNK:HB2	1.90	0.53
1:B:526:ILE:HD12	1:B:549:PHE:HB3	1.90	0.53
1:A:2088:UNK:C	1:A:2188:ARG:NH1	2.72	0.53
1:B:931:UNK:HG2	1:B:933:UNK:CG	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2135:UNK:CG	1:B:2136:ASP:H	2.22	0.53
1:A:2135:UNK:CG	1:A:2136:ASP:H	2.22	0.53
1:A:961:ARG:NH2	1:A:1196:UNK:O	2.42	0.53
1:C:1634:ARG:HD2	1:C:1638:PRO:HA	1.91	0.53
1:B:1488:VAL:HG12	1:B:1490:ARG:HH11	1.73	0.53
1:B:2012:GLY:C	1:C:2591:ARG:NH1	2.61	0.53
1:B:2246:ALA:C	1:B:2255:ARG:HH12	2.11	0.53
1:B:836:VAL:HG21	1:B:2437:UNK:HB2	1.90	0.53
1:B:1151:GLU:HB2	1:B:1179:ALA:HB3	1.90	0.53
1:A:588:GLU:HB3	1:A:593:LEU:HD11	1.91	0.53
1:C:1174:VAL:HB	1:C:1188:LEU:HB3	1.91	0.53
1:A:1420:THR:OG1	1:A:1485:HIS:NE2	2.38	0.53
1:B:970:ILE:HD13	1:B:996:UNK:HG1	1.91	0.53
1:B:2740:CYS:HB2	1:B:2998:GLY:HA2	1.91	0.53
1:C:2246:ALA:C	1:C:2255:ARG:HH12	2.11	0.53
1:C:2425:UNK:HG2	1:C:2425:UNK:O	2.09	0.53
1:A:1148:GLU:O	1:A:1150:ALA:N	2.42	0.53
1:A:1151:GLU:HB2	1:A:1179:ALA:HB3	1.90	0.53
1:B:2631:PRO:HG3	1:B:2649:LEU:HD13	1.90	0.53
1:B:2087:UNK:CA	1:B:2090:UNK:HG3	2.37	0.53
1:C:2088:UNK:C	1:C:2188:ARG:NH1	2.72	0.53
1:C:2094:UNK:H	1:C:2097:UNK:HG3	1.74	0.53
1:C:2112:UNK:N	1:C:2115:UNK:HG3	2.23	0.53
1:A:992:UNK:HG2	1:A:994:UNK:HG2	1.87	0.53
1:A:33:ALA:O	1:A:37:ARG:HG2	2.08	0.53
1:B:33:ALA:O	1:B:37:ARG:N	2.35	0.53
1:A:2860:ALA:HB1	1:A:3005:LEU:HD13	1.90	0.53
1:B:1323:GLU:N	1:B:1343:LEU:O	2.42	0.53
1:B:2081:UNK:C	1:B:2084:UNK:HG3	2.39	0.52
1:A:2103:UNK:O	1:A:2106:UNK:HG3	2.08	0.52
1:A:2115:UNK:HA	1:A:2118:UNK:HG3	1.90	0.52
1:B:961:ARG:NH2	1:B:1196:UNK:O	2.42	0.52
1:A:1634:ARG:HD2	1:A:1638:PRO:HA	1.91	0.52
1:C:2740:CYS:HB2	1:C:2998:GLY:HA2	1.92	0.52
1:C:2215:THR:HG22	1:C:2216:GLU:HG3	1.91	0.52
1:C:368:ILE:HG21	1:C:373:ILE:HG13	1.90	0.52
1:A:2551:PRO:O	1:A:2617:LEU:HB2	2.08	0.52
1:C:1530:LEU:HD21	1:C:1554:LEU:HD22	1.91	0.52
1:B:2085:UNK:C	1:B:2088:UNK:HG3	2.38	0.52
1:B:2112:UNK:N	1:B:2115:UNK:HG3	2.23	0.52
1:C:2085:UNK:C	1:C:2088:UNK:HG3	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:PRO:HD2	1:C:1025:VAL:HG11	1.91	0.52
1:C:2554:ALA:HB1	1:C:2614:LYS:HZ2	1.74	0.52
1:A:208:VAL:HG12	1:A:248:ILE:HG12	1.92	0.52
1:B:1001:UNK:HG1	1:B:1018:ARG:HH22	1.74	0.52
1:C:71:GLU:HG2	1:C:142:ARG:NH2	2.24	0.52
1:A:1174:VAL:HB	1:A:1188:LEU:HB3	1.91	0.52
1:B:716:ALA:HA	1:B:719:VAL:HG23	1.90	0.52
1:B:2094:UNK:HG2	1:B:2096:UNK:CG	2.23	0.52
1:A:2089:UNK:HA	1:A:2188:ARG:HH11	1.74	0.52
1:A:931:UNK:HG2	1:A:933:UNK:HG2	1.91	0.52
1:C:1538:ARG:NH1	1:C:1722:PRO:HB3	2.18	0.52
1:A:71:GLU:HG2	1:A:142:ARG:NH2	2.24	0.52
1:B:71:GLU:HG2	1:B:142:ARG:NH2	2.24	0.52
1:A:745:THR:HG23	1:A:834:GLU:HA	1.90	0.52
1:A:2808:ARG:HB2	1:A:2895:SER:O	2.10	0.52
1:A:1530:LEU:HD21	1:A:1554:LEU:HD22	1.91	0.52
1:A:1733:ASN:HD22	1:A:1736:ARG:HD2	1.74	0.52
1:C:1151:GLU:HB2	1:C:1179:ALA:HB3	1.90	0.52
1:B:2089:UNK:HA	1:B:2188:ARG:HH11	1.74	0.52
1:B:2094:UNK:H	1:B:2097:UNK:HG3	1.75	0.52
1:C:2135:UNK:CG	1:C:2136:ASP:H	2.22	0.52
1:B:2236:LEU:HD23	1:B:2288:HIS:HB2	1.92	0.52
1:B:368:ILE:HG21	1:B:373:ILE:HG13	1.90	0.52
1:A:400:TRP:CZ3	1:A:636:PRO:HB2	2.45	0.52
1:B:1357:ILE:HG13	1:B:1710:THR:HG21	1.89	0.52
1:C:1148:GLU:O	1:C:1150:ALA:N	2.42	0.52
1:B:1287:VAL:O	1:B:1291:LYS:HG3	2.10	0.52
1:B:2087:UNK:HA	1:B:2090:UNK:CG	2.39	0.52
1:C:2081:UNK:C	1:C:2084:UNK:HG3	2.39	0.52
1:B:999:UNK:HG3	1:B:1007:UNK:HG2	1.90	0.52
1:A:411:PRO:HD2	1:A:1025:VAL:HG11	1.91	0.52
1:B:2808:ARG:HB2	1:B:2895:SER:O	2.10	0.52
1:B:745:THR:HG23	1:B:834:GLU:HA	1.90	0.52
1:A:2631:PRO:HG3	1:A:2649:LEU:HD13	1.90	0.52
1:C:526:ILE:HD12	1:C:549:PHE:HB3	1.90	0.52
1:B:1093:PRO:HB3	1:B:1277:HIS:HE1	1.75	0.52
1:A:1287:VAL:O	1:A:1291:LYS:HG3	2.10	0.52
1:A:1110:VAL:HG13	1:A:1172:VAL:HG11	1.92	0.52
1:A:2094:UNK:H	1:A:2097:UNK:HG3	1.75	0.52
1:C:2122:UNK:HA	1:C:2125:UNK:CG	2.40	0.52
1:A:273:ARG:HD2	1:A:282:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:961:ARG:NH2	1:C:1196:UNK:O	2.42	0.52
1:B:1226:UNK:HB1	1:B:1282:THR:HG21	1.90	0.52
1:A:1164:THR:HA	1:A:1204:UNK:O	2.10	0.52
1:B:1110:VAL:HG13	1:B:1172:VAL:HG11	1.92	0.52
1:C:208:VAL:HB	1:C:255:LEU:HD13	1.92	0.52
1:A:1093:PRO:HB3	1:A:1277:HIS:HE1	1.75	0.52
1:C:1287:VAL:O	1:C:1291:LYS:HG3	2.10	0.52
1:C:1110:VAL:HG13	1:C:1172:VAL:HG11	1.92	0.52
1:B:2122:UNK:CA	1:B:2125:UNK:HG3	2.38	0.52
1:C:577:GLU:OE2	2:C:4000:FMN:O3'	2.28	0.52
1:C:2087:UNK:C	1:C:2090:UNK:HG3	2.40	0.52
1:C:2088:UNK:HG2	1:C:2188:ARG:HH12	1.73	0.52
1:A:2740:CYS:HB2	1:A:2998:GLY:HA2	1.92	0.52
1:A:2215:THR:HG22	1:A:2216:GLU:HG3	1.92	0.52
1:A:577:GLU:OE2	2:A:4000:FMN:O3'	2.28	0.52
1:B:1622:PRO:HD3	1:B:1685:LEU:HD21	1.92	0.52
1:C:208:VAL:HG12	1:C:248:ILE:HG12	1.92	0.52
1:C:400:TRP:CZ3	1:C:636:PRO:HB2	2.45	0.52
1:B:1425:VAL:HG13	1:B:1474:LEU:HD13	1.91	0.52
1:B:2087:UNK:C	1:B:2090:UNK:HG3	2.40	0.52
1:B:2122:UNK:HA	1:B:2125:UNK:CG	2.40	0.52
1:C:2094:UNK:HG2	1:C:2096:UNK:CG	2.23	0.52
1:B:106:ALA:O	1:B:112:PRO:HD2	2.10	0.52
1:C:106:ALA:O	1:C:112:PRO:HD2	2.10	0.52
1:B:2698:GLY:HA3	1:B:2705:LYS:HG3	1.92	0.52
1:B:588:GLU:HB3	1:B:593:LEU:HD11	1.91	0.52
1:B:1174:VAL:HB	1:B:1188:LEU:HB3	1.91	0.52
1:C:1119:THR:O	1:C:1123:PHE:HB2	2.10	0.52
1:B:144:GLY:O	1:B:148:THR:N	2.34	0.52
1:A:542:VAL:HG11	1:A:964:VAL:HB	1.92	0.52
1:C:2236:LEU:HD23	1:C:2288:HIS:HB2	1.92	0.52
1:B:2088:UNK:C	1:B:2188:ARG:NH1	2.72	0.51
1:A:2094:UNK:HG2	1:A:2096:UNK:CG	2.23	0.51
1:C:984:UNK:HG2	1:C:987:UNK:HG2	1.92	0.51
1:C:932:UNK:O	1:C:936:UNK:CG	2.48	0.51
1:B:336:TRP:CE2	1:B:360:LEU:HD11	2.45	0.51
1:A:336:TRP:CE2	1:A:360:LEU:HD11	2.45	0.51
1:C:420:LYS:HB3	1:C:641:ASP:OD2	2.10	0.51
1:A:2552:ASP:OD1	1:A:2552:ASP:N	2.43	0.51
1:B:1530:LEU:HD21	1:B:1554:LEU:HD22	1.91	0.51
1:B:405:PRO:HG3	1:B:625:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:VAL:O	1:B:180:ALA:N	2.36	0.51
1:B:2082:UNK:O	1:B:2086:UNK:HG3	2.09	0.51
1:A:1226:UNK:HB1	1:A:1282:THR:HG21	1.90	0.51
1:C:1164:THR:HA	1:C:1204:UNK:O	2.10	0.51
1:A:1488:VAL:HG12	1:A:1490:ARG:HH11	1.73	0.51
1:B:1598:GLU:HG2	1:B:1666:ILE:HD13	1.93	0.51
1:A:2082:UNK:O	1:A:2086:UNK:HG3	2.09	0.51
1:A:2087:UNK:HA	1:A:2090:UNK:CG	2.39	0.51
1:B:2215:THR:HG22	1:B:2216:GLU:HG3	1.91	0.51
1:C:2790:MET:HG2	1:C:2809:LEU:HD11	1.93	0.51
1:C:588:GLU:HB3	1:C:593:LEU:HD11	1.91	0.51
1:B:2434:UNK:O	1:B:2434:UNK:HG2	2.11	0.51
1:B:2123:UNK:O	1:B:2126:UNK:CG	2.56	0.51
1:A:2086:UNK:O	1:A:2089:UNK:CG	2.52	0.51
1:A:2087:UNK:C	1:A:2090:UNK:HG3	2.40	0.51
1:C:508:GLN:HA	1:C:540:ASN:HB3	1.92	0.51
1:A:2690:THR:O	1:A:2693:GLN:HG2	2.11	0.51
1:A:2401:ILE:HG23	1:A:2403:ILE:H	1.75	0.51
1:B:400:TRP:CZ3	1:B:636:PRO:HB2	2.45	0.51
1:B:542:VAL:HG11	1:B:964:VAL:HB	1.92	0.51
1:B:1733:ASN:HD22	1:B:1736:ARG:HD2	1.74	0.51
1:B:420:LYS:HB3	1:B:641:ASP:OD2	2.10	0.51
1:A:1119:THR:O	1:A:1123:PHE:HB2	2.10	0.51
1:B:1634:ARG:HD2	1:B:1638:PRO:HA	1.91	0.51
1:A:1622:PRO:HD3	1:A:1685:LEU:HD21	1.92	0.51
1:B:745:THR:OG1	1:B:834:GLU:O	2.19	0.51
1:C:2417:SER:O	1:C:2421:ASP:N	2.40	0.51
1:A:206:PRO:HG2	1:A:294:VAL:HA	1.92	0.51
1:A:2122:UNK:HA	1:A:2125:UNK:CG	2.40	0.51
1:B:984:UNK:HG2	1:B:987:UNK:HG2	1.93	0.51
1:B:2690:THR:O	1:B:2693:GLN:HG2	2.11	0.51
1:C:2089:UNK:HA	1:C:2188:ARG:HH11	1.74	0.51
1:A:937:UNK:HG2	1:A:938:UNK:N	2.26	0.51
1:A:2790:MET:HG2	1:A:2809:LEU:HD11	1.93	0.51
1:C:2401:ILE:HG23	1:C:2403:ILE:H	1.76	0.51
1:C:746:TYR:HA	1:C:749:TRP:HD1	1.76	0.51
1:A:420:LYS:HB3	1:A:641:ASP:OD2	2.10	0.51
1:B:206:PRO:HG2	1:B:294:VAL:HA	1.92	0.51
1:A:2434:UNK:HG2	1:A:2434:UNK:O	2.11	0.51
1:C:792:ALA:HA	1:C:799:PHE:CE2	2.43	0.51
1:B:1164:THR:HA	1:B:1204:UNK:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1488:VAL:HG12	1:C:1490:ARG:HH11	1.73	0.51
1:B:2401:ILE:HG23	1:B:2403:ILE:H	1.76	0.51
1:B:208:VAL:HB	1:B:255:LEU:HD13	1.92	0.51
1:C:1598:GLU:HG2	1:C:1666:ILE:HD13	1.92	0.51
1:C:1733:ASN:HD22	1:C:1736:ARG:HD2	1.74	0.51
1:A:2105:UNK:HG2	1:A:2106:UNK:N	2.26	0.51
1:A:2123:UNK:O	1:A:2126:UNK:CG	2.56	0.51
1:B:981:UNK:HG1	1:B:987:UNK:C	2.41	0.51
1:B:937:UNK:HG2	1:B:938:UNK:N	2.25	0.51
1:A:2653:VAL:HA	1:A:3051:MET:HE3	1.92	0.51
1:A:106:ALA:O	1:A:112:PRO:HD2	2.10	0.51
1:A:2667:THR:HG21	1:A:3058:ARG:HH11	1.76	0.51
1:B:1119:THR:O	1:B:1123:PHE:HB2	2.10	0.51
1:C:2754:ILE:HA	1:C:2759:ALA:O	2.11	0.51
1:C:2086:UNK:O	1:C:2089:UNK:CG	2.52	0.51
1:C:937:UNK:HG2	1:C:938:UNK:N	2.25	0.51
1:C:936:UNK:O	1:C:941:UNK:N	2.44	0.51
1:C:1001:UNK:HG1	1:C:1018:ARG:HH22	1.74	0.51
1:C:2698:GLY:HA3	1:C:2705:LYS:HG3	1.92	0.51
1:B:42:GLU:CD	1:B:42:GLU:H	2.14	0.50
1:C:2452:UNK:CG	1:C:2453:UNK:N	2.73	0.50
1:A:42:GLU:H	1:A:42:GLU:CD	2.14	0.50
1:C:2056:PHE:CZ	1:C:2180:LYS:HE2	2.47	0.50
1:C:1986:LEU:HA	1:C:1989:PHE:HD2	1.76	0.50
1:A:2554:ALA:HB1	1:A:2614:LYS:HZ2	1.74	0.50
1:B:1317:GLY:H	1:B:1324:VAL:HG12	1.76	0.50
1:A:2236:LEU:HD23	1:A:2288:HIS:HB2	1.92	0.50
1:A:272:GLU:HB3	1:A:280:GLY:O	2.11	0.50
1:C:2104:UNK:C	1:C:2107:UNK:HG3	2.42	0.50
1:C:2434:UNK:HG2	1:C:2434:UNK:O	2.11	0.50
1:A:1331:ILE:HG13	1:A:1336:VAL:HG21	1.94	0.50
1:A:1634:ARG:HH11	1:A:1639:ALA:N	2.08	0.50
1:C:42:GLU:H	1:C:42:GLU:CD	2.14	0.50
1:C:336:TRP:CE2	1:C:360:LEU:HD11	2.45	0.50
1:C:1622:PRO:HD3	1:C:1685:LEU:HD21	1.92	0.50
1:C:2361:VAL:HG11	1:C:2398:LEU:HD23	1.93	0.50
1:B:746:TYR:HA	1:B:749:TRP:HD1	1.76	0.50
1:B:2104:UNK:C	1:B:2107:UNK:HG3	2.42	0.50
1:C:1212:UNK:HG1	1:C:1342:ARG:HE	1.76	0.50
1:B:1590:VAL:HG11	1:B:1671:TRP:CD2	2.47	0.50
1:A:2245:VAL:HG13	1:A:2255:ARG:CZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2245:VAL:HG13	1:C:2255:ARG:CZ	2.41	0.50
1:A:2180:LYS:HZ1	1:A:2962:ASP:HB3	1.75	0.50
1:B:2653:VAL:HA	1:B:3051:MET:HE3	1.93	0.50
1:A:780:ARG:HD2	1:A:816:LEU:HB3	1.93	0.50
1:C:2808:ARG:HB2	1:C:2895:SER:O	2.10	0.50
1:A:2662:SER:HB2	1:A:2833:LEU:HD22	1.93	0.50
1:A:1598:GLU:HG2	1:A:1666:ILE:HD13	1.93	0.50
1:C:1093:PRO:HB3	1:C:1277:HIS:HE1	1.75	0.50
1:A:257:ARG:NH1	1:C:1695:LEU:HD23	2.23	0.50
1:C:1590:VAL:HG11	1:C:1671:TRP:CD2	2.47	0.50
1:C:780:ARG:HD2	1:C:816:LEU:HB3	1.93	0.50
1:A:1380:ALA:HB1	1:A:1474:LEU:HD12	1.93	0.50
1:A:1317:GLY:H	1:A:1324:VAL:HG12	1.76	0.50
1:A:2261:LYS:HA	1:A:2265:TRP:HB2	1.94	0.50
1:C:272:GLU:HB3	1:C:280:GLY:O	2.11	0.50
1:B:2127:UNK:O	1:B:2130:UNK:CG	2.52	0.50
1:A:1538:ARG:NH1	1:A:1722:PRO:HB3	2.18	0.50
1:A:2698:GLY:HA3	1:A:2705:LYS:HG3	1.92	0.50
1:C:2140:VAL:HG22	1:C:2165:ILE:HD12	1.93	0.50
1:C:1010:UNK:CG	1:C:1017:ILE:HB	2.42	0.50
1:B:1331:ILE:HG13	1:B:1336:VAL:HG21	1.94	0.50
1:A:1590:VAL:HG11	1:A:1671:TRP:CD2	2.47	0.50
1:B:936:UNK:O	1:B:941:UNK:N	2.44	0.50
1:A:932:UNK:O	1:A:936:UNK:CG	2.48	0.50
1:A:936:UNK:O	1:A:941:UNK:N	2.45	0.50
1:B:133:GLN:HG2	1:B:355:GLY:HA2	1.94	0.50
1:B:207:MET:HA	1:B:249:THR:HG22	1.94	0.50
1:B:1711:VAL:HA	1:B:1714:LEU:HG	1.93	0.50
1:A:208:VAL:HB	1:A:255:LEU:HD13	1.92	0.50
1:B:208:VAL:HG12	1:B:248:ILE:HG12	1.92	0.50
1:C:1207:UNK:HG2	1:C:1207:UNK:O	2.12	0.50
1:C:2552:ASP:N	1:C:2552:ASP:OD1	2.43	0.50
1:C:405:PRO:HG3	1:C:625:LEU:HG	1.93	0.50
1:A:2754:ILE:HA	1:A:2759:ALA:O	2.11	0.50
1:B:272:GLU:HB3	1:B:280:GLY:O	2.11	0.50
1:A:981:UNK:HG1	1:A:987:UNK:C	2.41	0.50
1:C:981:UNK:HG1	1:C:987:UNK:C	2.41	0.50
1:A:1212:UNK:HG1	1:A:1342:ARG:HE	1.75	0.50
1:A:1212:UNK:O	1:A:1342:ARG:NH2	2.45	0.50
1:A:505:ARG:HA	1:A:508:GLN:HB2	1.94	0.50
1:A:1986:LEU:HA	1:A:1989:PHE:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2623:ALA:HB2	1:A:2812:LEU:HD21	1.94	0.50
1:C:2690:THR:O	1:C:2693:GLN:HG2	2.11	0.50
1:A:405:PRO:HG3	1:A:625:LEU:HG	1.93	0.50
1:C:206:PRO:HG2	1:C:294:VAL:HA	1.92	0.50
1:C:542:VAL:HG11	1:C:964:VAL:HB	1.92	0.50
1:A:2811:PHE:HB3	1:A:2894:THR:HG22	1.94	0.50
1:C:2274:LEU:HD23	1:C:2277:ILE:HD12	1.94	0.50
1:C:981:UNK:HG1	1:C:987:UNK:O	2.12	0.50
1:C:981:UNK:CG	1:C:987:UNK:O	2.60	0.50
1:A:1212:UNK:HG2	1:A:1342:ARG:NE	2.26	0.50
1:A:133:GLN:HG2	1:A:355:GLY:HA2	1.94	0.50
1:B:2334:HIS:HB3	1:B:2391:LYS:HA	1.94	0.50
1:C:1331:ILE:HG13	1:C:1336:VAL:HG21	1.94	0.49
1:B:2557:LEU:HD22	1:B:2613:ARG:HB2	1.94	0.49
1:C:2557:LEU:HD22	1:C:2613:ARG:HB2	1.94	0.49
1:A:2334:HIS:HB3	1:A:2391:LYS:HA	1.94	0.49
1:C:1711:VAL:HA	1:C:1714:LEU:HG	1.94	0.49
1:B:2667:THR:HG21	1:B:3058:ARG:HH11	1.76	0.49
1:B:990:UNK:HG3	1:B:998:UNK:HB2	1.94	0.49
1:A:990:UNK:HG3	1:A:998:UNK:HB2	1.94	0.49
1:B:2829:LEU:HD21	1:B:3014:PHE:HE2	1.76	0.49
1:C:2261:LYS:HA	1:C:2265:TRP:HB2	1.94	0.49
1:A:2104:UNK:C	1:A:2107:UNK:HG3	2.42	0.49
1:A:2127:UNK:O	1:A:2130:UNK:CG	2.52	0.49
1:A:984:UNK:HG2	1:A:987:UNK:HG2	1.93	0.49
1:A:1001:UNK:HG1	1:A:1018:ARG:HH22	1.74	0.49
1:B:2056:PHE:CZ	1:B:2180:LYS:HE2	2.47	0.49
1:B:1986:LEU:HA	1:B:1989:PHE:HD2	1.76	0.49
1:B:2361:VAL:HG11	1:B:2398:LEU:HD23	1.93	0.49
1:B:2140:VAL:HG22	1:B:2165:ILE:HD12	1.93	0.49
1:C:2811:PHE:HB3	1:C:2894:THR:HG22	1.94	0.49
1:C:1317:GLY:H	1:C:1324:VAL:HG12	1.76	0.49
1:B:2754:ILE:HA	1:B:2759:ALA:O	2.11	0.49
1:A:981:UNK:CG	1:A:987:UNK:O	2.60	0.49
1:C:1212:UNK:O	1:C:1342:ARG:NH2	2.45	0.49
1:B:1212:UNK:HG1	1:B:1342:ARG:HE	1.75	0.49
1:B:1212:UNK:O	1:B:1342:ARG:NH2	2.45	0.49
1:A:508:GLN:HA	1:A:540:ASN:HB3	1.92	0.49
1:A:647:THR:OG1	2:A:4000:FMN:O3P	2.27	0.49
1:A:2056:PHE:CZ	1:A:2180:LYS:HE2	2.47	0.49
1:A:1207:UNK:HG2	1:A:1207:UNK:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2140:VAL:HG22	1:A:2165:ILE:HD12	1.93	0.49
1:C:1178:ASN:HB2	1:C:1185:LEU:HD11	1.94	0.49
1:C:1637:VAL:HG21	1:C:1671:TRP:CD2	2.48	0.49
1:B:577:GLU:OE2	2:B:4000:FMN:O3'	2.28	0.49
1:A:2361:VAL:HG11	1:A:2398:LEU:HD23	1.93	0.49
1:C:1119:THR:HA	1:C:1123:PHE:CD1	2.48	0.49
1:B:1119:THR:HA	1:B:1123:PHE:CD1	2.47	0.49
1:C:776:ASP:O	1:C:779:TRP:N	2.31	0.49
1:C:2662:SER:HB2	1:C:2833:LEU:HD22	1.93	0.49
1:B:2105:UNK:HG2	1:B:2106:UNK:N	2.26	0.49
1:B:981:UNK:HG1	1:B:987:UNK:O	2.12	0.49
1:A:3080:ARG:NH1	1:A:3080:ARG:CG	2.72	0.49
1:A:2557:LEU:HD22	1:A:2613:ARG:HB2	1.94	0.49
1:B:1637:VAL:HG21	1:B:1671:TRP:CD2	2.48	0.49
1:B:2245:VAL:HG13	1:B:2255:ARG:CZ	2.41	0.49
1:C:1380:ALA:HB1	1:C:1474:LEU:HD12	1.94	0.49
1:A:2274:LEU:HD23	1:A:2277:ILE:HD12	1.94	0.49
1:C:184:LEU:HB3	1:C:311:TRP:HE3	1.78	0.49
1:B:976:UNK:CG	1:B:993:UNK:HB1	2.29	0.49
1:A:981:UNK:HG1	1:A:987:UNK:O	2.12	0.49
1:B:1212:UNK:HG2	1:B:1342:ARG:NE	2.26	0.49
1:B:505:ARG:HA	1:B:508:GLN:HB2	1.94	0.49
1:B:508:GLN:HA	1:B:540:ASN:HB3	1.92	0.49
1:C:207:MET:HA	1:C:249:THR:HG22	1.94	0.49
1:B:2662:SER:HB2	1:B:2833:LEU:HD22	1.94	0.49
1:C:2087:UNK:HA	1:C:2090:UNK:CG	2.39	0.49
1:C:2105:UNK:HG2	1:C:2106:UNK:N	2.26	0.49
1:B:932:UNK:HA	1:B:935:UNK:HG3	1.94	0.49
1:C:3080:ARG:NH1	1:C:3080:ARG:HG3	2.09	0.49
1:B:2790:MET:HG2	1:B:2809:LEU:HD11	1.93	0.49
1:A:1119:THR:HA	1:A:1123:PHE:CD1	2.47	0.49
1:A:184:LEU:HB3	1:A:311:TRP:HE3	1.78	0.49
1:A:2503:LYS:HE3	1:A:2505:GLU:OE2	2.13	0.49
1:B:1010:UNK:CG	1:B:1017:ILE:HB	2.42	0.49
1:A:1010:UNK:CG	1:A:1017:ILE:HB	2.42	0.49
1:B:981:UNK:CG	1:B:987:UNK:O	2.60	0.49
1:A:117:LYS:HZ1	1:C:1087:PHE:HB3	1.78	0.49
1:A:207:MET:HA	1:A:249:THR:HG22	1.94	0.49
1:B:1291:LYS:HA	1:B:1344:ALA:HB3	1.95	0.49
1:B:2261:LYS:HA	1:B:2265:TRP:HB2	1.93	0.49
1:A:2829:LEU:HD21	1:A:3014:PHE:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ILE:HD13	1:C:327:GLU:HG2	1.95	0.49
1:C:1362:MET:HG3	1:C:1430:VAL:HG21	1.95	0.49
1:B:792:ALA:HA	1:B:799:PHE:CE2	2.43	0.49
1:B:2087:UNK:O	1:B:2090:UNK:HG3	2.13	0.49
1:C:2094:UNK:O	1:C:2098:UNK:HG3	2.13	0.49
1:C:992:UNK:HG1	1:C:994:UNK:HG3	1.81	0.49
1:C:932:UNK:HA	1:C:935:UNK:HG3	1.94	0.49
1:C:999:UNK:O	1:C:1007:UNK:N	2.46	0.49
1:A:1695:LEU:HD23	1:B:257:ARG:NH1	2.23	0.49
1:A:2962:ASP:N	1:A:2962:ASP:OD1	2.34	0.49
1:B:780:ARG:HD2	1:B:816:LEU:HB3	1.93	0.49
1:B:1380:ALA:HB1	1:B:1474:LEU:HD12	1.93	0.49
1:A:2291:LEU:HD21	1:A:2332:LEU:HD22	1.95	0.49
1:B:184:LEU:HB3	1:B:311:TRP:HE3	1.78	0.49
1:A:790:ALA:HB3	1:A:826:LEU:HD21	1.95	0.49
1:A:444:ILE:HD12	1:A:655:ALA:HA	1.95	0.49
1:B:2274:LEU:HD23	1:B:2277:ILE:HD12	1.94	0.49
1:B:999:UNK:O	1:B:1007:UNK:N	2.46	0.49
1:C:997:UNK:HB1	1:C:1009:UNK:HG2	1.95	0.49
1:C:2334:HIS:HB3	1:C:2391:LYS:HA	1.94	0.49
1:A:746:TYR:HA	1:A:749:TRP:HD1	1.76	0.49
1:B:2094:UNK:O	1:B:2098:UNK:HG3	2.13	0.48
1:B:2120:UNK:HG2	1:B:2121:UNK:N	2.28	0.48
1:A:2087:UNK:O	1:A:2090:UNK:HG3	2.13	0.48
1:C:2100:UNK:C	1:C:2103:UNK:HG3	2.31	0.48
1:C:2118:UNK:HG2	1:C:2119:UNK:N	2.28	0.48
1:A:1012:UNK:HG2	1:A:1012:UNK:O	2.13	0.48
1:A:1111:PHE:HE1	1:A:1129:LEU:HD11	1.78	0.48
1:C:2667:THR:HG21	1:C:3058:ARG:HH11	1.76	0.48
1:A:868:ARG:HB3	1:A:872:ARG:NH1	2.28	0.48
1:A:1637:VAL:HG21	1:A:1671:TRP:CD2	2.48	0.48
1:B:1207:UNK:HG2	1:B:1207:UNK:O	2.12	0.48
1:C:2829:LEU:HD21	1:C:3014:PHE:HE2	1.76	0.48
1:B:444:ILE:HD12	1:B:655:ALA:HA	1.95	0.48
1:B:361:THR:HG21	1:B:377:PRO:HG3	1.95	0.48
1:B:2086:UNK:CA	1:B:2089:UNK:HG3	2.43	0.48
1:A:999:UNK:O	1:A:1007:UNK:N	2.46	0.48
1:A:1225:UNK:HG1	1:A:1283:ASP:CG	2.34	0.48
1:C:1533:VAL:HG13	1:C:1582:HIS:HB2	1.95	0.48
1:A:1651:THR:HB	1:A:1656:LYS:HD2	1.95	0.48
1:A:2926:SER:HB3	1:A:2976:TRP:HH2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2115:UNK:O	1:B:2119:UNK:HG3	2.13	0.48
1:A:2086:UNK:CA	1:A:2089:UNK:HG3	2.43	0.48
1:C:996:UNK:O	1:C:996:UNK:HG2	2.13	0.48
1:A:932:UNK:HA	1:A:935:UNK:HG3	1.94	0.48
1:B:1003:UNK:CG	1:B:1004:UNK:N	2.53	0.48
1:C:133:GLN:HG2	1:C:355:GLY:HA2	1.94	0.48
1:B:1533:VAL:HG13	1:B:1582:HIS:HB2	1.95	0.48
1:B:2820:ILE:HD12	1:B:2822:LEU:HD21	1.95	0.48
1:B:501:VAL:HA	1:B:504:LYS:HE2	1.96	0.48
1:C:2623:ALA:HB2	1:C:2812:LEU:HD21	1.94	0.48
1:C:2503:LYS:HE3	1:C:2505:GLU:OE2	2.13	0.48
1:C:361:THR:HG21	1:C:377:PRO:HG3	1.95	0.48
1:B:2291:LEU:HD21	1:B:2332:LEU:HD22	1.95	0.48
1:B:790:ALA:HB3	1:B:826:LEU:HD21	1.95	0.48
1:A:2103:UNK:CG	1:A:2919:GLY:O	2.62	0.48
1:C:2667:THR:HB	1:C:3081:LEU:HD11	1.95	0.48
1:B:2623:ALA:HB2	1:B:2812:LEU:HD21	1.94	0.48
1:A:1435:VAL:HG22	1:A:1703:ILE:HD12	1.95	0.48
1:C:2848:GLY:H	1:C:3001:HIS:CD2	2.31	0.48
1:A:2167:THR:HB	1:A:2198:ALA:HB3	1.96	0.48
1:C:976:UNK:CG	1:C:993:UNK:HB1	2.29	0.48
1:C:505:ARG:HA	1:C:508:GLN:HB2	1.94	0.48
1:B:1087:PHE:HB3	1:C:117:LYS:HZ3	1.77	0.48
1:A:1711:VAL:HA	1:A:1714:LEU:HG	1.93	0.48
1:B:2667:THR:HB	1:B:3081:LEU:HD11	1.96	0.48
1:B:1435:VAL:HG22	1:B:1703:ILE:HD12	1.95	0.48
1:C:1381:ASP:OD1	1:C:1391:SER:OG	2.22	0.48
1:B:1103:VAL:HG21	1:B:1269:MET:SD	2.54	0.48
1:A:2170:ARG:HB2	1:A:2175:ARG:HG3	1.95	0.48
1:A:1996:PRO:O	1:A:2000:LEU:N	2.41	0.48
1:B:2167:THR:HB	1:B:2198:ALA:HB3	1.96	0.48
1:C:2736:PRO:HG2	1:C:2746:SER:HA	1.96	0.48
1:A:2060:TRP:HZ2	1:A:2966:ASP:HA	1.79	0.48
1:C:2087:UNK:O	1:C:2090:UNK:HG3	2.13	0.48
1:C:2088:UNK:O	1:C:2188:ARG:NH1	2.47	0.48
1:C:1012:UNK:HG2	1:C:1012:UNK:O	2.13	0.48
1:B:1695:LEU:HD23	1:C:257:ARG:NH1	2.23	0.48
1:B:2645:ASP:OD1	1:B:2647:VAL:HG23	2.14	0.48
1:C:2645:ASP:OD1	1:C:2647:VAL:HG23	2.13	0.48
1:B:982:UNK:CG	1:B:983:UNK:N	2.76	0.48
1:C:2820:ILE:HD12	1:C:2822:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2648:ALA:HA	1:C:2718:VAL:HG13	1.96	0.48
1:A:2848:GLY:H	1:A:3001:HIS:CD2	2.31	0.48
1:C:1291:LYS:HA	1:C:1344:ALA:HB3	1.95	0.48
1:A:184:LEU:HD13	1:A:311:TRP:HB3	1.96	0.48
1:B:2060:TRP:HZ2	1:B:2966:ASP:HA	1.79	0.48
1:C:1103:VAL:HG21	1:C:1269:MET:SD	2.54	0.48
1:B:2811:PHE:HB3	1:B:2894:THR:HG22	1.94	0.48
1:C:444:ILE:HD12	1:C:655:ALA:HA	1.95	0.48
1:B:1133:VAL:O	1:B:1193:ALA:N	2.42	0.48
1:B:2103:UNK:CG	1:B:2919:GLY:O	2.62	0.48
1:A:2115:UNK:O	1:A:2119:UNK:HG3	2.13	0.48
1:B:931:UNK:CG	1:B:934:UNK:HG3	2.44	0.48
1:C:1634:ARG:HH11	1:C:1639:ALA:N	2.08	0.48
1:B:1508:ILE:HB	1:B:1562:ARG:HD3	1.96	0.48
1:B:803:GLU:OE1	1:B:2431:UNK:CG	2.62	0.48
1:C:2060:TRP:HZ2	1:C:2966:ASP:HA	1.79	0.48
1:A:1178:ASN:HB2	1:A:1185:LEU:HD11	1.94	0.48
1:B:1362:MET:HG3	1:B:1430:VAL:HG21	1.95	0.48
1:A:2088:UNK:O	1:A:2188:ARG:NH1	2.47	0.48
1:C:2094:UNK:HG1	1:C:2096:UNK:HG3	1.90	0.48
1:C:2115:UNK:O	1:C:2119:UNK:HG3	2.13	0.48
1:A:985:UNK:HG2	1:A:986:UNK:N	2.29	0.48
1:A:931:UNK:CG	1:A:934:UNK:HG3	2.44	0.48
1:C:1212:UNK:HG2	1:C:1342:ARG:NE	2.26	0.48
1:A:1163:ASP:CG	1:A:1199:UNK:HG3	2.34	0.48
1:A:2180:LYS:NZ	1:A:2962:ASP:HB3	2.29	0.48
1:C:868:ARG:HB3	1:C:872:ARG:NH1	2.28	0.48
1:C:990:UNK:HG3	1:C:998:UNK:HB2	1.94	0.48
1:A:1291:LYS:HA	1:A:1344:ALA:HB3	1.95	0.48
1:B:305:ILE:HD13	1:B:327:GLU:HG2	1.95	0.48
1:A:144:GLY:O	1:A:148:THR:N	2.34	0.48
1:A:1103:VAL:HG21	1:A:1269:MET:SD	2.54	0.48
1:A:2666:PRO:CB	1:A:2727:VAL:HA	2.44	0.48
1:A:1362:MET:HG3	1:A:1430:VAL:HG21	1.95	0.48
1:C:2666:PRO:CB	1:C:2727:VAL:HA	2.44	0.48
1:C:2167:THR:HB	1:C:2198:ALA:HB3	1.96	0.48
1:A:2592:PRO:HA	1:A:2599:TRP:CD1	2.49	0.48
1:B:2088:UNK:O	1:B:2188:ARG:NH1	2.47	0.48
1:A:2094:UNK:O	1:A:2098:UNK:HG3	2.13	0.48
1:A:2120:UNK:HG2	1:A:2121:UNK:N	2.28	0.48
1:A:2645:ASP:OD1	1:A:2647:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:997:UNK:N	1:C:1009:UNK:O	2.47	0.48
1:A:997:UNK:N	1:A:1009:UNK:O	2.47	0.48
1:B:647:THR:HG22	1:B:901:ILE:HD11	1.96	0.48
1:A:2667:THR:HB	1:A:3081:LEU:HD11	1.96	0.48
1:C:2926:SER:HB3	1:C:2976:TRP:HH2	1.78	0.48
1:C:1467:VAL:HA	1:C:1605:LYS:HD2	1.96	0.48
1:A:305:ILE:HD13	1:A:327:GLU:HG2	1.95	0.48
1:B:171:LYS:HE3	1:B:173:ALA:HB3	1.96	0.48
1:C:2592:PRO:HA	1:C:2599:TRP:CD1	2.49	0.48
1:A:2762:VAL:HG22	1:A:2822:LEU:HB2	1.96	0.48
1:A:2820:ILE:HD12	1:A:2822:LEU:HD21	1.95	0.48
1:B:997:UNK:N	1:B:1009:UNK:O	2.47	0.48
1:C:575:HIS:CD2	1:C:644:LEU:HD22	2.48	0.48
1:B:575:HIS:CD2	1:B:644:LEU:HD22	2.49	0.48
1:C:1651:THR:HB	1:C:1656:LYS:HD2	1.95	0.48
1:C:641:ASP:OD1	1:C:641:ASP:N	2.47	0.48
1:C:2448:UNK:HG2	1:C:2448:UNK:O	2.13	0.48
1:C:301:LEU:HD13	1:C:330:LEU:HD22	1.96	0.48
1:B:2352:ILE:HG12	1:B:2412:ALA:HB1	1.96	0.48
1:B:808:ALA:HB3	1:B:811:ASP:HB2	1.96	0.48
1:C:171:LYS:HE3	1:C:173:ALA:HB3	1.96	0.48
1:A:996:UNK:O	1:A:996:UNK:HG2	2.13	0.47
1:C:1013:UNK:CG	1:C:1014:UNK:N	2.58	0.47
1:C:2843:GLN:HG2	1:C:2845:PHE:CZ	2.49	0.47
1:B:2180:LYS:NZ	1:B:2962:ASP:HB3	2.29	0.47
1:B:670:GLY:HA3	1:B:899:ALA:HB2	1.96	0.47
1:C:1435:VAL:HG22	1:C:1703:ILE:HD12	1.95	0.47
1:A:176:VAL:O	1:A:180:ALA:N	2.36	0.47
1:B:2448:UNK:HG2	1:B:2448:UNK:O	2.13	0.47
1:A:2736:PRO:HG2	1:A:2746:SER:HA	1.96	0.47
1:B:2666:PRO:CB	1:B:2727:VAL:HA	2.44	0.47
1:B:674:TRP:CD1	1:B:895:THR:HG21	2.49	0.47
1:B:2434:UNK:HG3	1:B:2523:GLU:O	2.14	0.47
1:B:2101:UNK:HG2	1:B:2102:UNK:N	2.29	0.47
1:C:1010:UNK:HG2	1:C:1017:ILE:HB	1.96	0.47
1:B:1012:UNK:HG2	1:B:1012:UNK:O	2.14	0.47
1:B:2884:ASP:HA	1:B:2916:ARG:NH1	2.30	0.47
1:B:1111:PHE:HE1	1:B:1129:LEU:HD11	1.78	0.47
1:C:2180:LYS:NZ	1:C:2962:ASP:HB3	2.29	0.47
1:C:647:THR:HG22	1:C:901:ILE:HD11	1.96	0.47
1:B:1651:THR:HB	1:B:1656:LYS:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2554:ALA:HB1	1:A:2614:LYS:HD2	1.95	0.47
1:C:2554:ALA:HB1	1:C:2614:LYS:HD2	1.95	0.47
1:B:2848:GLY:H	1:B:3001:HIS:CD2	2.31	0.47
1:C:184:LEU:HD13	1:C:311:TRP:HB3	1.96	0.47
1:C:606:ASN:H	1:C:606:ASN:HD22	1.62	0.47
1:A:2348:GLN:O	1:A:2416:MET:HG3	2.15	0.47
1:B:2503:LYS:HE3	1:B:2505:GLU:OE2	2.13	0.47
1:B:2592:PRO:HA	1:B:2599:TRP:CD1	2.49	0.47
1:A:2434:UNK:HG3	1:A:2523:GLU:O	2.14	0.47
1:C:1225:UNK:HG1	1:C:1283:ASP:CG	2.34	0.47
1:B:1072:TRP:HE1	1:B:1077:VAL:HG22	1.80	0.47
1:C:1163:ASP:CG	1:C:1199:UNK:HG3	2.34	0.47
1:B:1625:LEU:HD11	1:B:1660:LEU:HB3	1.95	0.47
1:C:176:VAL:O	1:C:180:ALA:N	2.36	0.47
1:A:1533:VAL:HG13	1:A:1582:HIS:HB2	1.95	0.47
1:B:2927:GLN:HE22	1:B:2941:PHE:C	2.17	0.47
1:C:790:ALA:HB3	1:C:826:LEU:HD21	1.95	0.47
1:B:1178:ASN:HB2	1:B:1185:LEU:HD11	1.94	0.47
1:C:1450:ALA:N	1:C:1613:ARG:O	2.48	0.47
1:B:365:ALA:O	1:B:369:ARG:N	2.42	0.47
1:B:2123:UNK:HA	1:B:2126:UNK:HG3	1.97	0.47
1:B:2093:UNK:HG1	1:B:2132:UNK:HB1	1.95	0.47
1:B:2252:VAL:HG22	1:B:2255:ARG:NH2	2.30	0.47
1:B:2648:ALA:HA	1:B:2718:VAL:HG13	1.96	0.47
1:B:2461:VAL:HG21	1:B:2751:VAL:HG13	1.96	0.47
1:A:674:TRP:CD1	1:A:895:THR:HG21	2.50	0.47
1:C:2170:ARG:HB2	1:C:2175:ARG:HG3	1.95	0.47
1:A:365:ALA:HB3	1:A:366:PRO:HD3	1.96	0.47
1:C:985:UNK:HG2	1:C:986:UNK:N	2.29	0.47
1:C:674:TRP:CD1	1:C:895:THR:HG21	2.49	0.47
1:C:808:ALA:HB3	1:C:811:ASP:HB2	1.96	0.47
1:C:365:ALA:HB3	1:C:366:PRO:HD3	1.96	0.47
1:A:2118:UNK:HG2	1:A:2119:UNK:N	2.28	0.47
1:C:2103:UNK:CG	1:C:2919:GLY:O	2.62	0.47
1:C:2123:UNK:HA	1:C:2126:UNK:HG3	1.97	0.47
1:B:985:UNK:HG2	1:B:986:UNK:N	2.29	0.47
1:A:1508:ILE:HB	1:A:1562:ARG:HD3	1.97	0.47
1:A:2843:GLN:HG2	1:A:2845:PHE:CZ	2.49	0.47
1:A:997:UNK:HB1	1:A:1009:UNK:CG	2.44	0.47
1:B:997:UNK:HB1	1:B:1009:UNK:HG2	1.95	0.47
1:A:2648:ALA:HA	1:A:2718:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2461:VAL:HG21	1:C:2751:VAL:HG13	1.96	0.47
1:B:832:ASP:O	1:B:836:VAL:HG23	2.14	0.47
1:C:1455:VAL:HB	1:C:1480:ARG:HH12	1.80	0.47
1:B:2170:ARG:HB2	1:B:2175:ARG:HG3	1.96	0.47
1:A:2927:GLN:HE22	1:A:2941:PHE:C	2.17	0.47
1:A:2093:UNK:HG1	1:A:2132:UNK:HB1	1.95	0.47
1:B:996:UNK:O	1:B:996:UNK:HG2	2.13	0.47
1:C:966:PRO:O	1:C:970:ILE:N	2.48	0.47
1:B:932:UNK:O	1:B:936:UNK:CG	2.47	0.47
1:B:1590:VAL:HG11	1:B:1671:TRP:CE2	2.50	0.47
1:C:997:UNK:HB1	1:C:1009:UNK:CG	2.45	0.47
1:A:997:UNK:HB1	1:A:1009:UNK:HG2	1.95	0.47
1:B:683:GLY:CA	1:B:700:ASN:HB2	2.44	0.47
1:C:1723:GLU:C	1:C:1725:SER:H	2.18	0.47
1:B:641:ASP:OD1	1:B:641:ASP:N	2.47	0.47
1:C:2927:GLN:HE22	1:C:2941:PHE:C	2.17	0.47
1:A:2448:UNK:O	1:A:2448:UNK:HG2	2.13	0.47
1:A:606:ASN:HD22	1:A:606:ASN:H	1.63	0.47
1:B:2376:LEU:HD22	1:B:2392:VAL:HG21	1.97	0.47
1:B:2681:THR:O	1:B:2764:ALA:HA	2.15	0.47
1:A:2101:UNK:HG2	1:A:2102:UNK:N	2.29	0.47
1:C:2120:UNK:HG2	1:C:2121:UNK:N	2.28	0.47
1:C:941:UNK:HG3	1:C:942:UNK:N	2.30	0.47
1:A:2884:ASP:HA	1:A:2916:ARG:NH1	2.29	0.47
1:B:1163:ASP:CG	1:B:1199:UNK:HG3	2.34	0.47
1:C:2762:VAL:HG22	1:C:2822:LEU:HB2	1.96	0.47
1:A:1723:GLU:C	1:A:1725:SER:H	2.18	0.47
1:C:670:GLY:HA3	1:C:899:ALA:HB2	1.96	0.47
1:A:2800:PHE:CE1	1:A:2812:LEU:HD22	2.50	0.47
1:A:713:ALA:O	1:A:868:ARG:NH2	2.48	0.47
1:A:1625:LEU:HD11	1:A:1660:LEU:HB3	1.96	0.47
1:C:832:ASP:O	1:C:836:VAL:HG23	2.14	0.47
1:C:1625:LEU:HD11	1:C:1660:LEU:HB3	1.96	0.47
1:B:2926:SER:HB3	1:B:2976:TRP:HH2	1.79	0.47
1:B:745:THR:HG22	1:B:747:LEU:H	1.80	0.47
1:B:184:LEU:HD13	1:B:311:TRP:HB3	1.96	0.47
1:B:365:ALA:HB3	1:B:366:PRO:HD3	1.96	0.47
1:A:1672:GLN:HE21	1:A:1672:GLN:HB3	1.58	0.47
1:B:1455:VAL:HB	1:B:1480:ARG:HH12	1.80	0.47
1:C:2773:GLU:HA	1:C:2776:ILE:HG22	1.97	0.47
1:B:1672:GLN:HB3	1:B:1672:GLN:HE21	1.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:VAL:HG22	1:C:287:PHE:CD1	2.50	0.47
1:B:2630:ASP:HB3	1:B:2633:VAL:HG23	1.97	0.47
1:A:1381:ASP:OD1	1:A:1391:SER:OG	2.22	0.47
1:A:782:ARG:HD3	1:A:853:LEU:HD22	1.97	0.47
1:B:2125:UNK:HA	1:B:2128:UNK:CG	2.45	0.47
1:C:2086:UNK:CA	1:C:2089:UNK:HG3	2.43	0.47
1:A:1010:UNK:HG2	1:A:1017:ILE:HB	1.96	0.47
1:A:966:PRO:O	1:A:970:ILE:N	2.48	0.47
1:B:2450:UNK:HG1	1:B:3016:ALA:CB	2.17	0.47
1:C:931:UNK:CG	1:C:934:UNK:HG3	2.44	0.47
1:B:931:UNK:HG2	1:B:933:UNK:HG2	1.92	0.47
1:B:2762:VAL:HG22	1:B:2822:LEU:HB2	1.96	0.47
1:C:803:GLU:OE1	1:C:2431:UNK:CG	2.62	0.47
1:B:868:ARG:HB3	1:B:872:ARG:NH1	2.28	0.47
1:A:2210:VAL:HB	1:A:2277:ILE:HD11	1.96	0.47
1:B:778:THR:HG21	1:B:854:GLY:HA3	1.97	0.47
1:A:1467:VAL:HA	1:A:1605:LYS:HD2	1.96	0.47
1:A:301:LEU:HD13	1:A:330:LEU:HD22	1.96	0.47
1:C:2376:LEU:HD22	1:C:2392:VAL:HG21	1.97	0.47
1:C:2681:THR:O	1:C:2764:ALA:HA	2.15	0.47
1:C:1276:GLN:HE21	1:C:1292:LEU:HD13	1.79	0.47
1:B:1010:UNK:HG2	1:B:1017:ILE:HB	1.96	0.47
1:B:941:UNK:HG3	1:B:942:UNK:N	2.30	0.47
1:A:198:ILE:HG12	1:C:1087:PHE:CE1	2.50	0.47
1:B:585:HIS:HD2	1:B:586:SER:H	1.62	0.47
1:A:803:GLU:OE1	1:A:2431:UNK:CG	2.62	0.47
1:B:713:ALA:O	1:B:868:ARG:NH2	2.48	0.47
1:A:2785:ALA:HB1	1:A:2809:LEU:HG	1.97	0.47
1:A:832:ASP:O	1:A:836:VAL:HG23	2.14	0.47
1:B:2554:ALA:HB1	1:B:2614:LYS:HD2	1.96	0.47
1:B:782:ARG:HD3	1:B:853:LEU:HD22	1.97	0.47
1:B:210:VAL:HG22	1:B:287:PHE:CD1	2.50	0.47
1:A:808:ALA:HB3	1:A:811:ASP:HB2	1.96	0.47
1:B:1457:GLU:OE2	1:B:1614:TYR:OH	2.30	0.47
1:C:2291:LEU:HD21	1:C:2332:LEU:HD22	1.95	0.47
1:C:2101:UNK:HG2	1:C:2102:UNK:N	2.29	0.47
1:C:2125:UNK:HA	1:C:2128:UNK:CG	2.44	0.47
1:B:992:UNK:CG	1:B:996:UNK:HG2	2.32	0.47
1:C:3080:ARG:NH1	1:C:3080:ARG:CG	2.72	0.47
1:B:2843:GLN:HG2	1:B:2845:PHE:CZ	2.49	0.47
1:C:1111:PHE:HE1	1:C:1129:LEU:HD11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1723:GLU:C	1:B:1725:SER:H	2.18	0.47
1:C:836:VAL:HG12	1:C:837:VAL:N	2.29	0.47
1:A:2482:GLU:HG2	1:A:2956:PRO:HB3	1.97	0.47
1:C:2427:UNK:O	1:C:2427:UNK:HG2	2.15	0.47
1:B:301:LEU:HD13	1:B:330:LEU:HD22	1.96	0.47
1:A:141:ALA:O	1:A:145:MET:HB2	2.15	0.47
1:C:2104:UNK:HA	1:C:2107:UNK:CG	2.46	0.46
1:B:966:PRO:O	1:B:970:ILE:N	2.48	0.46
1:A:1237:ARG:CZ	1:B:95:PRO:HB2	2.46	0.46
1:B:94:ARG:HG3	1:B:95:PRO:HD3	1.98	0.46
1:C:1590:VAL:HG11	1:C:1671:TRP:CE2	2.50	0.46
1:B:997:UNK:HB1	1:B:1009:UNK:CG	2.44	0.46
1:C:2252:VAL:HG13	1:C:2255:ARG:HH21	1.81	0.46
1:B:836:VAL:HG12	1:B:837:VAL:N	2.29	0.46
1:A:836:VAL:HG12	1:A:837:VAL:N	2.29	0.46
1:C:222:LEU:HD21	1:C:236:VAL:HA	1.97	0.46
1:C:2210:VAL:HB	1:C:2277:ILE:HD11	1.97	0.46
1:A:2058:ASP:N	1:A:2058:ASP:OD1	2.46	0.46
1:B:1467:VAL:HA	1:B:1605:LYS:HD2	1.96	0.46
1:A:2096:UNK:C	1:A:2099:UNK:HG3	2.43	0.46
1:C:2096:UNK:C	1:C:2099:UNK:HG3	2.43	0.46
1:C:931:UNK:HG2	1:C:933:UNK:HG2	1.92	0.46
1:A:941:UNK:HG3	1:A:942:UNK:N	2.30	0.46
1:A:2077:UNK:CG	1:A:2079:UNK:HG3	2.41	0.46
1:C:1508:ILE:HB	1:C:1562:ARG:HD3	1.97	0.46
1:B:518:ASP:HA	1:B:543:GLY:O	2.15	0.46
1:A:670:GLY:HA3	1:A:899:ALA:HB2	1.96	0.46
1:C:713:ALA:O	1:C:868:ARG:NH2	2.48	0.46
1:C:656:THR:HG1	1:C:880:HIS:CE1	2.30	0.46
1:B:2961:LEU:HD22	1:B:2976:TRP:CD1	2.51	0.46
1:C:501:VAL:HA	1:C:504:LYS:HE2	1.96	0.46
1:C:2352:ILE:HG12	1:C:2412:ALA:HB1	1.96	0.46
1:C:84:GLU:HB2	1:C:85:PRO:HD3	1.97	0.46
1:A:778:THR:HG21	1:A:854:GLY:HA3	1.97	0.46
1:B:2118:UNK:HG2	1:B:2119:UNK:N	2.28	0.46
1:C:2434:UNK:HG3	1:C:2523:GLU:O	2.14	0.46
1:B:996:UNK:HA	1:B:1010:UNK:HA	1.97	0.46
1:B:1001:UNK:O	1:B:1005:UNK:HB2	2.16	0.46
1:B:1319:ASP:HB2	1:B:1342:ARG:NH1	2.31	0.46
1:C:2884:ASP:HA	1:C:2916:ARG:NH1	2.29	0.46
1:C:982:UNK:CG	1:C:983:UNK:N	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:PRO:CD	1:B:289:PRO:HB3	2.46	0.46
1:A:2252:VAL:HG13	1:A:2255:ARG:HH21	1.80	0.46
1:A:2978:ARG:NH1	1:A:2979:GLU:OE2	2.49	0.46
1:A:365:ALA:O	1:A:369:ARG:N	2.42	0.46
1:A:171:LYS:HE3	1:A:173:ALA:HB3	1.96	0.46
1:A:361:THR:HG21	1:A:377:PRO:HG3	1.95	0.46
1:A:210:VAL:HG22	1:A:287:PHE:CD1	2.50	0.46
1:A:2681:THR:O	1:A:2764:ALA:HA	2.15	0.46
1:A:2352:ILE:HG12	1:A:2412:ALA:HB1	1.96	0.46
1:B:1634:ARG:HH11	1:B:1639:ALA:N	2.08	0.46
1:A:518:ASP:HA	1:A:543:GLY:O	2.15	0.46
1:C:518:ASP:HA	1:C:543:GLY:O	2.15	0.46
1:A:683:GLY:CA	1:A:700:ASN:HB2	2.44	0.46
1:B:2252:VAL:HG13	1:B:2255:ARG:HH21	1.81	0.46
1:A:2461:VAL:HG21	1:A:2751:VAL:HG13	1.96	0.46
1:A:84:GLU:HB2	1:A:85:PRO:HD3	1.98	0.46
1:C:2348:GLN:O	1:C:2416:MET:HG3	2.15	0.46
1:A:1612:GLY:N	1:A:1623:PHE:O	2.48	0.46
1:B:2736:PRO:HG2	1:B:2746:SER:HA	1.95	0.46
1:A:1699:ARG:HG3	1:A:1730:GLU:HB3	1.97	0.46
1:B:1237:ARG:CZ	1:C:95:PRO:HB2	2.46	0.46
1:C:2252:VAL:HG22	1:C:2255:ARG:NH2	2.30	0.46
1:A:1325:LEU:HD11	1:A:1343:LEU:HD22	1.98	0.46
1:B:2554:ALA:HB1	1:B:2614:LYS:HZ2	1.78	0.46
1:A:2961:LEU:HD22	1:A:2976:TRP:CD1	2.51	0.46
1:C:745:THR:HG22	1:C:747:LEU:H	1.80	0.46
1:A:1346:PRO:HG2	1:A:1699:ARG:HD3	1.98	0.46
1:B:768:LYS:HA	1:B:775:LEU:HD11	1.97	0.46
1:B:1699:ARG:HG3	1:B:1730:GLU:HB3	1.97	0.46
1:B:2543:PHE:HA	1:B:2624:GLN:HE22	1.81	0.46
1:C:782:ARG:HD3	1:C:853:LEU:HD22	1.97	0.46
1:B:1276:GLN:HE21	1:B:1292:LEU:HD13	1.79	0.46
1:B:2104:UNK:HA	1:B:2107:UNK:CG	2.46	0.46
1:C:406:THR:OG1	1:C:418:GLU:OE1	2.34	0.46
1:C:1325:LEU:HD11	1:C:1343:LEU:HD22	1.98	0.46
1:C:2361:VAL:HG21	1:C:2401:ILE:HD11	1.98	0.46
1:C:778:THR:HG21	1:C:854:GLY:HA3	1.97	0.46
1:C:1699:ARG:HG3	1:C:1730:GLU:HB3	1.97	0.46
1:C:141:ALA:O	1:C:145:MET:HB2	2.15	0.46
1:C:534:ASP:O	1:C:538:GLU:HG3	2.16	0.46
1:C:1001:UNK:O	1:C:1005:UNK:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1319:ASP:HB2	1:C:1342:ARG:NH1	2.31	0.46
1:A:1072:TRP:CD1	1:A:1097:VAL:HG22	2.51	0.46
1:B:1072:TRP:CD1	1:B:1097:VAL:HG22	2.51	0.46
1:B:540:ASN:ND2	1:B:544:ILE:HG13	2.30	0.46
1:A:575:HIS:CD2	1:A:644:LEU:HD22	2.49	0.46
1:C:2957:PRO:HB3	1:C:2979:GLU:C	2.36	0.46
1:A:1590:VAL:HG11	1:A:1671:TRP:CE2	2.50	0.46
1:C:2482:GLU:HG2	1:C:2956:PRO:HB3	1.97	0.46
1:B:2210:VAL:HB	1:B:2277:ILE:HD11	1.96	0.46
1:C:1346:PRO:HG2	1:C:1699:ARG:HD3	1.98	0.46
1:B:606:ASN:H	1:B:606:ASN:HD22	1.62	0.46
1:B:84:GLU:HB2	1:B:85:PRO:HD3	1.97	0.46
1:B:2348:GLN:O	1:B:2416:MET:HG3	2.15	0.46
1:B:406:THR:OG1	1:B:418:GLU:OE1	2.34	0.46
1:B:141:ALA:O	1:B:145:MET:HB2	2.15	0.46
1:C:1094:THR:O	1:C:1288:PRO:HG2	2.15	0.46
1:A:3065:PRO:O	1:A:3069:GLN:N	2.42	0.46
1:A:2104:UNK:HA	1:A:2107:UNK:CG	2.46	0.46
1:C:996:UNK:HA	1:C:1010:UNK:HA	1.97	0.46
1:A:1212:UNK:CG	1:A:1342:ARG:HH21	2.17	0.46
1:C:94:ARG:HG3	1:C:95:PRO:HD3	1.98	0.46
1:A:501:VAL:HA	1:A:504:LYS:HE2	1.96	0.46
1:A:167:ALA:HB3	1:A:178:LEU:HD21	1.98	0.46
1:B:2957:PRO:HB3	1:B:2979:GLU:C	2.36	0.46
1:B:2978:ARG:NH1	1:B:2979:GLU:OE2	2.49	0.46
1:A:2957:PRO:HB3	1:A:2979:GLU:C	2.36	0.46
1:A:277:LEU:HD22	1:A:676:GLY:O	2.16	0.46
1:A:2630:ASP:HB3	1:A:2633:VAL:HG23	1.97	0.46
1:A:2376:LEU:HD22	1:A:2392:VAL:HG21	1.97	0.46
1:A:1276:GLN:HE21	1:A:1292:LEU:HD13	1.79	0.46
1:A:1205:UNK:HG2	1:A:1206:UNK:N	2.30	0.46
1:B:984:UNK:HG1	1:B:987:UNK:CG	2.46	0.46
1:A:2610:ARG:NH1	1:A:2700:LEU:HD21	2.31	0.46
1:A:95:PRO:HB2	1:C:1237:ARG:CZ	2.45	0.46
1:A:2212:TRP:HA	1:A:2229:LYS:HB3	1.98	0.46
1:C:2946:LEU:HD22	1:C:2994:VAL:HG23	1.98	0.46
1:A:2252:VAL:HG22	1:A:2255:ARG:NH2	2.30	0.46
1:A:647:THR:HG22	1:A:901:ILE:HD11	1.96	0.46
1:B:111:GLU:HB2	1:B:112:PRO:HD3	1.98	0.46
1:C:111:GLU:HB2	1:C:112:PRO:HD3	1.98	0.46
1:A:2790:MET:SD	1:A:2800:PHE:HB2	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1205:UNK:HG2	1:B:1206:UNK:N	2.31	0.46
1:B:1304:LYS:O	1:B:1307:ASP:HB2	2.16	0.46
1:B:2619:ARG:NH1	1:B:2779:GLY:HA2	2.31	0.46
1:C:1205:UNK:HG2	1:C:1206:UNK:N	2.30	0.46
1:C:2619:ARG:NH1	1:C:2779:GLY:HA2	2.31	0.46
1:A:2773:GLU:HA	1:A:2776:ILE:HG22	1.97	0.46
1:A:1455:VAL:HB	1:A:1480:ARG:HH12	1.80	0.46
1:A:2125:UNK:HA	1:A:2128:UNK:CG	2.45	0.46
1:A:2123:UNK:HA	1:A:2126:UNK:HG3	1.97	0.46
1:C:408:VAL:CG1	1:C:943:UNK:HG1	2.46	0.46
1:B:2770:LEU:HB3	1:B:2815:GLN:HB3	1.97	0.46
1:C:1072:TRP:CD1	1:C:1097:VAL:HG22	2.51	0.46
1:B:1087:PHE:CE1	1:C:198:ILE:HG12	2.51	0.46
1:A:1087:PHE:CE1	1:B:198:ILE:HG12	2.51	0.46
1:A:205:PRO:CD	1:A:289:PRO:HB3	2.46	0.46
1:C:2234:PRO:HB2	1:C:2287:LEU:HD13	1.98	0.46
1:A:868:ARG:HD3	1:A:872:ARG:HH12	1.81	0.46
1:A:745:THR:HG22	1:A:747:LEU:H	1.80	0.46
1:C:1304:LYS:O	1:C:1307:ASP:HB2	2.16	0.46
1:C:2879:LEU:HD13	1:C:3009:VAL:HG11	1.98	0.46
1:A:2879:LEU:HD13	1:A:3009:VAL:HG11	1.98	0.46
1:B:793:ARG:HA	1:B:2435:UNK:HG1	1.97	0.45
1:B:2094:UNK:HG1	1:B:2096:UNK:HG3	1.90	0.45
1:A:2100:UNK:C	1:A:2103:UNK:HG3	2.31	0.45
1:A:111:GLU:HB2	1:A:112:PRO:HD3	1.98	0.45
1:B:1325:LEU:HD11	1:B:1343:LEU:HD22	1.98	0.45
1:A:2891:LYS:HG3	1:A:2924:ILE:HD13	1.98	0.45
1:B:2889:ILE:HD11	1:B:2922:LEU:HD22	1.98	0.45
1:B:2672:TRP:CD1	1:B:2831:MET:HG2	2.52	0.45
1:A:2137:GLU:O	1:A:2163:THR:N	2.30	0.45
1:B:1094:THR:O	1:B:1288:PRO:HG2	2.15	0.45
1:B:2773:GLU:HA	1:B:2776:ILE:HG22	1.97	0.45
1:A:793:ARG:HA	1:A:2435:UNK:HG1	1.98	0.45
1:A:996:UNK:HA	1:A:1010:UNK:HA	1.97	0.45
1:A:1003:UNK:CG	1:A:1004:UNK:N	2.53	0.45
1:A:1319:ASP:HB2	1:A:1342:ARG:NH1	2.31	0.45
1:B:2946:LEU:HD22	1:B:2994:VAL:HG23	1.98	0.45
1:C:540:ASN:ND2	1:C:544:ILE:HG13	2.30	0.45
1:C:2212:TRP:HA	1:C:2229:LYS:HB3	1.98	0.45
1:C:683:GLY:CA	1:C:700:ASN:HB2	2.44	0.45
1:B:1702:GLU:OE1	1:B:1712:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2234:PRO:HB2	1:B:2287:LEU:HD13	1.98	0.45
1:C:2961:LEU:HD22	1:C:2976:TRP:CD1	2.51	0.45
1:B:2482:GLU:HG2	1:B:2956:PRO:HB3	1.97	0.45
1:A:2543:PHE:HA	1:A:2624:GLN:HE22	1.81	0.45
1:C:1462:ALA:HB2	1:C:1468:TYR:HE1	1.81	0.45
1:C:277:LEU:HD22	1:C:676:GLY:O	2.16	0.45
1:A:1450:ALA:N	1:A:1613:ARG:O	2.48	0.45
1:A:1094:THR:O	1:A:1288:PRO:HG2	2.15	0.45
1:C:47:ALA:O	1:C:353:ASP:HA	2.17	0.45
1:C:984:UNK:HG1	1:C:987:UNK:CG	2.46	0.45
1:A:944:UNK:O	1:A:944:UNK:CG	2.59	0.45
1:A:94:ARG:HG3	1:A:95:PRO:HD3	1.98	0.45
1:B:351:ILE:HB	1:B:375:ILE:HG12	1.99	0.45
1:C:205:PRO:CD	1:C:289:PRO:HB3	2.46	0.45
1:B:1352:PHE:HA	1:B:1353:PRO:HD3	1.72	0.45
1:B:2891:LYS:HG3	1:B:2924:ILE:HD13	1.99	0.45
1:C:746:TYR:HB2	1:C:833:ALA:HB1	1.99	0.45
1:A:2619:ARG:NH1	1:A:2779:GLY:HA2	2.31	0.45
1:C:381:ARG:O	1:C:384:GLN:HG2	2.17	0.45
1:A:1133:VAL:O	1:A:1193:ALA:N	2.42	0.45
1:C:2070:LEU:O	1:C:2074:GLU:HG3	2.16	0.45
1:A:1462:ALA:HB2	1:A:1468:TYR:HE1	1.81	0.45
1:C:2472:TYR:CZ	1:C:2930:LEU:HD22	2.52	0.45
1:B:1462:ALA:HB2	1:B:1468:TYR:HE1	1.81	0.45
1:A:1483:LYS:O	1:A:1487:ILE:HG23	2.17	0.45
1:B:2096:UNK:C	1:B:2099:UNK:HG3	2.43	0.45
1:B:1001:UNK:HG1	1:B:1018:ARG:HH21	1.80	0.45
1:C:1212:UNK:HG2	1:C:1342:ARG:CZ	2.47	0.45
1:B:2769:ASP:OD1	1:B:2770:LEU:N	2.49	0.45
1:A:2845:PHE:HD2	1:A:2860:ALA:HA	1.82	0.45
1:A:2246:ALA:N	1:A:2255:ARG:NH1	2.64	0.45
1:C:585:HIS:CB	1:C:694:ASP:HB2	2.47	0.45
1:B:2785:ALA:HB1	1:B:2809:LEU:HG	1.97	0.45
1:A:2889:ILE:HD11	1:A:2922:LEU:HD22	1.98	0.45
1:A:784:GLU:OE2	1:A:816:LEU:HD21	2.16	0.45
1:A:747:LEU:HD22	1:A:751:ARG:CZ	2.47	0.45
1:A:222:LEU:HD21	1:A:236:VAL:HA	1.97	0.45
1:C:684:MET:HG3	1:C:895:THR:HA	1.98	0.45
1:B:1346:PRO:HG2	1:B:1699:ARG:HD3	1.98	0.45
1:C:1483:LYS:O	1:C:1487:ILE:HG23	2.17	0.45
1:B:2879:LEU:HD13	1:B:3009:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2672:TRP:CD1	1:A:2831:MET:HG2	2.52	0.45
1:B:47:ALA:O	1:B:353:ASP:HA	2.17	0.45
1:A:2770:LEU:HB3	1:A:2815:GLN:HB3	1.97	0.45
1:A:544:ILE:O	1:A:546:HIS:N	2.41	0.45
1:C:511:ARG:CB	1:C:540:ASN:HB2	2.46	0.45
1:C:351:ILE:HB	1:C:375:ILE:HG12	1.99	0.45
1:B:207:MET:HG3	1:B:292:VAL:HB	1.98	0.45
1:B:2246:ALA:N	1:B:2255:ARG:NH1	2.64	0.45
1:C:2790:MET:SD	1:C:2800:PHE:HB2	2.56	0.45
1:C:2785:ALA:HB1	1:C:2809:LEU:HG	1.97	0.45
1:B:868:ARG:HD3	1:B:872:ARG:HH12	1.81	0.45
1:A:222:LEU:HD13	1:A:248:ILE:HD12	1.99	0.45
1:B:746:TYR:HB2	1:B:833:ALA:HB1	1.99	0.45
1:A:684:MET:HG3	1:A:895:THR:HA	1.98	0.45
1:A:2427:UNK:HG2	1:A:2427:UNK:O	2.15	0.45
1:C:768:LYS:HA	1:C:775:LEU:HD11	1.97	0.45
1:A:381:ARG:O	1:A:384:GLN:HG2	2.17	0.45
1:A:1001:UNK:O	1:A:1005:UNK:HB2	2.15	0.45
1:A:408:VAL:CG1	1:A:943:UNK:HG1	2.46	0.45
1:A:540:ASN:ND2	1:A:544:ILE:HG13	2.30	0.45
1:C:1488:VAL:HB	1:C:1579:VAL:HG22	1.99	0.45
1:B:195:ARG:NH1	1:B:198:ILE:HD12	2.31	0.45
1:B:585:HIS:CB	1:B:694:ASP:HB2	2.47	0.45
1:A:1702:GLU:OE1	1:A:1712:ALA:N	2.49	0.45
1:C:167:ALA:HB3	1:C:178:LEU:HD21	1.98	0.45
1:B:1519:VAL:HG13	1:B:1530:LEU:HD23	1.98	0.45
1:A:2070:LEU:O	1:A:2074:GLU:HG3	2.16	0.45
1:C:1553:ALA:O	1:C:1557:GLU:HG2	2.17	0.45
1:A:534:ASP:O	1:A:538:GLU:HG3	2.16	0.45
1:B:1450:ALA:N	1:B:1613:ARG:O	2.48	0.45
1:C:2630:ASP:HB3	1:C:2633:VAL:HG23	1.97	0.45
1:A:2080:UNK:HG2	1:A:2083:UNK:CG	2.45	0.45
1:B:3080:ARG:CG	1:B:3080:ARG:NH1	2.72	0.45
1:A:1072:TRP:HE1	1:A:1077:VAL:HG22	1.80	0.45
1:B:2452:UNK:CG	1:B:2453:UNK:N	2.73	0.45
1:B:2452:UNK:HA	1:B:3017:ALA:HA	1.99	0.45
1:B:2212:TRP:HA	1:B:2229:LYS:HB3	1.98	0.45
1:B:1488:VAL:HB	1:B:1579:VAL:HG22	1.99	0.45
1:C:1684:ASP:HA	1:C:1687:PHE:HD2	1.82	0.45
1:B:2790:MET:SD	1:B:2800:PHE:HB2	2.56	0.45
1:A:2361:VAL:HG21	1:A:2401:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:763:SER:HB3	1:C:766:ASP:HB2	1.99	0.45
1:C:747:LEU:HD22	1:C:751:ARG:CZ	2.47	0.45
1:B:1605:LYS:H	1:B:1658:LYS:HE2	1.82	0.45
1:A:768:LYS:HA	1:A:775:LEU:HD11	1.98	0.45
1:B:2137:GLU:O	1:B:2163:THR:N	2.30	0.45
1:A:406:THR:OG1	1:A:418:GLU:OE1	2.34	0.45
1:B:1996:PRO:O	1:B:2000:LEU:N	2.41	0.45
1:B:534:ASP:O	1:B:538:GLU:HG3	2.16	0.45
1:C:2093:UNK:HG1	1:C:2132:UNK:HB1	1.95	0.45
1:C:2114:UNK:HA	1:C:2117:UNK:HG3	1.99	0.45
1:B:1212:UNK:HG2	1:B:1342:ARG:CZ	2.47	0.45
1:C:2610:ARG:NH1	1:C:2700:LEU:HD21	2.31	0.45
1:C:2769:ASP:OD1	1:C:2770:LEU:N	2.49	0.45
1:C:2770:LEU:HB3	1:C:2815:GLN:HB3	1.97	0.45
1:C:2845:PHE:HD2	1:C:2860:ALA:HA	1.81	0.45
1:B:2845:PHE:HD2	1:B:2860:ALA:HA	1.81	0.45
1:C:195:ARG:NH1	1:C:198:ILE:HD12	2.31	0.45
1:A:195:ARG:NH1	1:A:198:ILE:HD12	2.31	0.45
1:B:2361:VAL:HG21	1:B:2401:ILE:HD11	1.98	0.45
1:C:784:GLU:OE2	1:C:816:LEU:HD21	2.16	0.45
1:B:763:SER:HB3	1:B:766:ASP:HB2	1.99	0.45
1:C:222:LEU:HD13	1:C:248:ILE:HD12	1.99	0.45
1:C:1996:PRO:O	1:C:2000:LEU:N	2.41	0.45
1:B:2610:ARG:NH1	1:B:2700:LEU:HD21	2.31	0.45
1:C:1072:TRP:HE1	1:C:1077:VAL:HG22	1.80	0.45
1:C:1634:ARG:NH1	1:C:1639:ALA:N	2.65	0.45
1:C:2845:PHE:CD2	1:C:2860:ALA:HA	2.52	0.45
1:B:336:TRP:CH2	1:B:360:LEU:HD21	2.52	0.45
1:A:351:ILE:HB	1:A:375:ILE:HG12	1.99	0.45
1:C:544:ILE:O	1:C:546:HIS:N	2.40	0.45
1:A:2591:ARG:HH12	1:C:2014:SER:H	1.65	0.45
1:B:997:UNK:O	1:B:1009:UNK:HG3	2.17	0.45
1:B:1284:GLY:HA2	1:B:1343:LEU:HD11	1.99	0.45
1:B:167:ALA:HB3	1:B:178:LEU:HD21	1.98	0.45
1:B:784:GLU:OE2	1:B:816:LEU:HD21	2.16	0.45
1:B:222:LEU:HD21	1:B:236:VAL:HA	1.97	0.45
1:A:1605:LYS:H	1:A:1658:LYS:HE2	1.82	0.45
1:C:2672:TRP:CD1	1:C:2831:MET:HG2	2.52	0.45
1:B:1171:PRO:HA	1:B:1191:ARG:HG2	1.99	0.45
1:C:2296:ASN:HB3	1:C:2299:MET:SD	2.57	0.45
1:A:799:PHE:CZ	1:A:2433:UNK:CG	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1001:UNK:HG1	1:C:1018:ARG:HH21	1.80	0.45
1:A:2946:LEU:HD22	1:A:2994:VAL:HG23	1.98	0.45
1:B:544:ILE:O	1:B:546:HIS:N	2.41	0.45
1:A:1488:VAL:HB	1:A:1579:VAL:HG22	1.99	0.45
1:A:997:UNK:O	1:A:1009:UNK:HG3	2.17	0.45
1:A:2014:SER:H	1:B:2591:ARG:HH12	1.65	0.45
1:C:2246:ALA:N	1:C:2255:ARG:NH1	2.64	0.45
1:C:2246:ALA:N	1:C:2255:ARG:HH12	2.15	0.45
1:C:2800:PHE:CE1	1:C:2812:LEU:HD22	2.50	0.45
1:C:868:ARG:HD3	1:C:872:ARG:HH12	1.81	0.45
1:C:2978:ARG:NH1	1:C:2979:GLU:OE2	2.49	0.45
1:A:746:TYR:HB2	1:A:833:ALA:HB1	1.99	0.45
1:B:2619:ARG:HH12	1:B:2779:GLY:HA2	1.81	0.45
1:C:1581:PHE:HB2	1:C:1586:LEU:HD22	1.99	0.45
1:B:381:ARG:O	1:B:384:GLN:HG2	2.17	0.45
1:B:799:PHE:CZ	1:B:2433:UNK:CG	2.99	0.44
1:A:984:UNK:HG1	1:A:987:UNK:CG	2.46	0.44
1:A:999:UNK:C	1:A:1007:UNK:HG3	2.46	0.44
1:A:1212:UNK:HG2	1:A:1342:ARG:CZ	2.47	0.44
1:A:2845:PHE:CD2	1:A:2860:ALA:HA	2.52	0.44
1:C:997:UNK:O	1:C:1009:UNK:HG3	2.18	0.44
1:B:664:LEU:HB3	1:B:701:ALA:HB1	1.99	0.44
1:C:664:LEU:HB3	1:C:701:ALA:HB1	1.99	0.44
1:C:1702:GLU:OE1	1:C:1712:ALA:N	2.49	0.44
1:C:2891:LYS:HG3	1:C:2924:ILE:HD13	1.98	0.44
1:B:2300:PHE:CZ	1:B:2398:LEU:HB3	2.52	0.44
1:B:2891:LYS:HZ2	1:B:2903:GLU:HG2	1.82	0.44
1:C:365:ALA:O	1:C:369:ARG:N	2.42	0.44
1:A:210:VAL:HG22	1:A:287:PHE:HD1	1.83	0.44
1:B:2427:UNK:O	1:B:2427:UNK:HG2	2.15	0.44
1:B:1285:LYS:HB3	1:B:1286:PRO:HD2	1.99	0.44
1:B:999:UNK:HG2	1:B:1007:UNK:HG1	1.96	0.44
1:C:2452:UNK:HA	1:C:3017:ALA:HA	1.98	0.44
1:A:1634:ARG:NH1	1:A:1639:ALA:N	2.65	0.44
1:B:550:LYS:HD3	1:B:577:GLU:OE2	2.17	0.44
1:A:207:MET:HG3	1:A:292:VAL:HB	1.98	0.44
1:C:207:MET:HG3	1:C:292:VAL:HB	1.98	0.44
1:C:671:THR:HB	1:C:682:ASN:CG	2.38	0.44
1:C:2300:PHE:CZ	1:C:2398:LEU:HB3	2.52	0.44
1:C:210:VAL:HG22	1:C:287:PHE:HD1	1.83	0.44
1:B:210:VAL:HG22	1:B:287:PHE:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2619:ARG:HH12	1:C:2779:GLY:HA2	1.81	0.44
1:C:2831:MET:HB3	1:C:2831:MET:HE2	1.88	0.44
1:B:277:LEU:HD22	1:B:676:GLY:O	2.16	0.44
1:A:1304:LYS:O	1:A:1307:ASP:HB2	2.16	0.44
1:C:2543:PHE:HA	1:C:2624:GLN:HE22	1.81	0.44
1:B:1612:GLY:N	1:B:1623:PHE:O	2.48	0.44
1:B:2299:MET:H	1:B:2299:MET:HG2	1.68	0.44
1:B:2080:UNK:HG2	1:B:2083:UNK:CG	2.45	0.44
1:A:2120:UNK:O	1:A:2123:UNK:CG	2.66	0.44
1:A:2452:UNK:CG	1:A:2453:UNK:N	2.73	0.44
1:A:511:ARG:CB	1:A:540:ASN:HB2	2.46	0.44
1:A:2246:ALA:N	1:A:2255:ARG:HH12	2.15	0.44
1:C:336:TRP:CH2	1:C:360:LEU:HD21	2.52	0.44
1:A:664:LEU:HB3	1:A:701:ALA:HB1	1.99	0.44
1:B:1350:TYR:CD1	1:B:1703:ILE:HD11	2.53	0.44
1:C:2891:LYS:HZ2	1:C:2903:GLU:HG2	1.83	0.44
1:A:2300:PHE:CZ	1:A:2398:LEU:HB3	2.52	0.44
1:B:747:LEU:HD22	1:B:751:ARG:CZ	2.47	0.44
1:B:684:MET:HG3	1:B:895:THR:HA	1.98	0.44
1:C:2209:LEU:O	1:C:2213:VAL:HG23	2.18	0.44
1:A:2555:SER:HA	1:A:2556:PRO:HD2	1.84	0.44
1:C:1171:PRO:HA	1:C:1191:ARG:HG2	1.99	0.44
1:B:2472:TYR:CZ	1:B:2930:LEU:HD22	2.52	0.44
1:A:47:ALA:O	1:A:353:ASP:HA	2.17	0.44
1:B:2083:UNK:HA	1:B:2086:UNK:HG3	2.00	0.44
1:C:2080:UNK:HG2	1:C:2083:UNK:CG	2.45	0.44
1:B:999:UNK:C	1:B:1007:UNK:HG3	2.47	0.44
1:A:583:GLY:HA2	1:A:892:ILE:HD13	2.00	0.44
1:C:583:GLY:HA2	1:C:892:ILE:HD13	2.00	0.44
1:C:2889:ILE:HD11	1:C:2922:LEU:HD22	1.98	0.44
1:A:1519:VAL:HG13	1:A:1530:LEU:HD23	1.99	0.44
1:B:222:LEU:HD13	1:B:248:ILE:HD12	1.99	0.44
1:C:1605:LYS:H	1:C:1658:LYS:HE2	1.82	0.44
1:B:1553:ALA:O	1:B:1557:GLU:HG2	2.17	0.44
1:B:44:TYR:O	1:B:153:VAL:N	2.44	0.44
1:C:970:ILE:HG23	1:C:992:UNK:HG1	2.00	0.44
1:B:1225:UNK:HG1	1:B:1283:ASP:CG	2.34	0.44
1:A:2452:UNK:HA	1:A:3017:ALA:HA	1.98	0.44
1:A:475:LEU:HD23	1:A:475:LEU:HA	1.79	0.44
1:A:2591:ARG:NH1	1:C:2014:SER:N	2.66	0.44
1:A:2014:SER:N	1:B:2591:ARG:NH1	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2334:HIS:CD2	1:B:2391:LYS:HG3	2.50	0.44
1:A:1284:GLY:HA2	1:A:1343:LEU:HD11	1.99	0.44
1:A:671:THR:HB	1:A:682:ASN:CG	2.38	0.44
1:A:1350:TYR:CD1	1:A:1703:ILE:HD11	2.53	0.44
1:C:1093:PRO:HB3	1:C:1277:HIS:CE1	2.52	0.44
1:A:2619:ARG:HH12	1:A:2779:GLY:HA2	1.81	0.44
1:B:2296:ASN:HB3	1:B:2299:MET:SD	2.57	0.44
1:B:515:ALA:HA	1:B:516:PRO:HD3	1.84	0.44
1:A:2472:TYR:CZ	1:A:2930:LEU:HD22	2.52	0.44
1:B:1503:ILE:HB	1:B:1542:TYR:HB2	2.00	0.44
1:B:2114:UNK:HA	1:B:2117:UNK:HG3	1.99	0.44
1:C:2119:UNK:HG2	1:C:2120:UNK:N	2.33	0.44
1:C:793:ARG:HA	1:C:2435:UNK:HG1	1.97	0.44
1:A:2769:ASP:OD1	1:A:2770:LEU:N	2.49	0.44
1:B:1634:ARG:NH1	1:B:1639:ALA:N	2.65	0.44
1:B:2246:ALA:N	1:B:2255:ARG:HH12	2.15	0.44
1:B:1684:ASP:HA	1:B:1687:PHE:HD2	1.82	0.44
1:B:1723:GLU:O	1:B:1725:SER:N	2.51	0.44
1:C:1723:GLU:O	1:C:1725:SER:N	2.51	0.44
1:A:2234:PRO:HB2	1:A:2287:LEU:HD13	1.98	0.44
1:C:1350:TYR:CD1	1:C:1703:ILE:HD11	2.53	0.44
1:C:2580:PHE:HE1	1:C:2603:ARG:HH21	1.66	0.44
1:C:2471:PRO:HA	1:C:2625:ILE:HA	2.00	0.44
1:B:944:UNK:CG	1:B:944:UNK:O	2.59	0.44
1:B:2014:SER:H	1:C:2591:ARG:HH12	1.65	0.44
1:C:1582:HIS:HA	1:C:1674:ALA:O	2.18	0.44
1:A:550:LYS:HD3	1:A:577:GLU:OE2	2.17	0.44
1:B:2297:ARG:HH22	1:B:2391:LYS:HZ3	1.65	0.44
1:B:2209:LEU:O	1:B:2213:VAL:HG23	2.18	0.44
1:A:585:HIS:CB	1:A:694:ASP:HB2	2.47	0.44
1:B:1537:LEU:HD13	1:B:1541:GLN:HB2	2.00	0.44
1:C:1537:LEU:HD13	1:C:1541:GLN:HB2	2.00	0.44
1:C:1284:GLY:HA2	1:C:1343:LEU:HD11	1.99	0.44
1:B:671:THR:HB	1:B:682:ASN:CG	2.38	0.44
1:A:412:ASP:H	1:A:1025:VAL:CG2	2.31	0.44
1:C:745:THR:OG1	1:C:834:GLU:O	2.19	0.44
1:B:782:ARG:NH1	1:B:857:VAL:HG22	2.33	0.44
1:C:782:ARG:NH1	1:C:857:VAL:HG22	2.33	0.44
1:A:88:SER:HB3	1:A:314:THR:OG1	2.18	0.44
1:A:1705:VAL:O	1:A:1735:GLU:HB2	2.18	0.44
1:A:2296:ASN:HB3	1:A:2299:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:THR:HB	1:A:662:LYS:HE3	2.00	0.44
1:C:2122:UNK:O	1:C:2125:UNK:CG	2.63	0.44
1:B:408:VAL:CG1	1:B:943:UNK:HG1	2.46	0.44
1:B:2845:PHE:CD2	1:B:2860:ALA:HA	2.52	0.44
1:A:2252:VAL:HG22	1:A:2255:ARG:HH21	1.82	0.44
1:C:2334:HIS:CD2	1:C:2391:LYS:HG3	2.50	0.44
1:C:393:VAL:HG12	1:C:394:PRO:N	2.32	0.44
1:C:2958:ASN:HD22	1:C:2976:TRP:HE1	1.65	0.44
1:A:763:SER:HB3	1:A:766:ASP:HB2	1.99	0.44
1:A:1581:PHE:HB2	1:A:1586:LEU:HD22	1.99	0.44
1:A:2013:LEU:HA	1:A:2013:LEU:HD23	1.87	0.44
1:A:163:LEU:HD13	1:A:181:LEU:HD23	2.00	0.44
1:A:1171:PRO:HA	1:A:1191:ARG:HG2	1.99	0.44
1:B:2119:UNK:HG2	1:B:2120:UNK:N	2.33	0.44
1:A:2094:UNK:HG1	1:A:2096:UNK:HG3	1.90	0.44
1:B:995:UNK:HB1	1:B:1011:UNK:HG2	1.99	0.44
1:B:647:THR:OG1	2:B:4000:FMN:O3P	2.27	0.44
1:C:550:LYS:HD3	1:C:577:GLU:OE2	2.17	0.44
1:A:1684:ASP:HA	1:A:1687:PHE:HD2	1.82	0.44
1:B:2958:ASN:HD22	1:B:2976:TRP:HE1	1.65	0.44
1:C:1733:ASN:H	1:C:1737:ASP:HB2	1.83	0.44
1:C:857:VAL:HG13	1:C:859:PHE:H	1.83	0.44
1:B:2753:LYS:HA	1:B:2753:LYS:HD3	1.83	0.44
1:C:1285:LYS:HB3	1:C:1286:PRO:HD2	1.99	0.44
1:B:2462:VAL:HG13	1:B:2835:VAL:HG13	2.00	0.44
1:B:1483:LYS:O	1:B:1487:ILE:HG23	2.17	0.44
1:A:1553:ALA:O	1:A:1557:GLU:HG2	2.17	0.44
1:A:2083:UNK:HA	1:A:2086:UNK:HG3	2.00	0.43
1:C:2120:UNK:O	1:C:2123:UNK:CG	2.65	0.43
1:A:981:UNK:CG	1:A:987:UNK:C	2.96	0.43
1:C:931:UNK:HG3	1:C:934:UNK:HG3	2.00	0.43
1:C:2710:LEU:O	1:C:2713:VAL:HG22	2.18	0.43
1:A:2297:ARG:HH22	1:A:2391:LYS:HZ3	1.66	0.43
1:B:583:GLY:HA2	1:B:892:ILE:HD13	2.00	0.43
1:B:2903:GLU:OE2	1:B:2995:THR:OG1	2.36	0.43
1:A:1733:ASN:H	1:A:1737:ASP:HB2	1.83	0.43
1:B:344:HIS:CD2	1:B:373:ILE:HG13	2.53	0.43
1:B:1093:PRO:HB3	1:B:1277:HIS:CE1	2.52	0.43
1:A:1093:PRO:HB3	1:A:1277:HIS:CE1	2.52	0.43
1:B:602:ARG:NH2	1:B:641:ASP:OD1	2.27	0.43
1:A:782:ARG:NH1	1:A:857:VAL:HG22	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:VAL:N	1:A:1193:ALA:O	2.48	0.43
1:A:2989:LEU:HA	1:A:2989:LEU:HD12	1.77	0.43
1:A:1268:GLY:HA2	1:A:1271:LEU:HD12	1.99	0.43
1:A:1285:LYS:HB3	1:A:1286:PRO:HD2	1.99	0.43
1:B:657:THR:HB	1:B:662:LYS:HE3	2.00	0.43
1:B:2120:UNK:O	1:B:2123:UNK:CG	2.66	0.43
1:A:999:UNK:HG2	1:A:1007:UNK:HG1	1.96	0.43
1:C:1163:ASP:HA	1:C:1168:ARG:HA	2.01	0.43
1:A:982:UNK:CG	1:A:983:UNK:N	2.76	0.43
1:B:340:ILE:HD11	1:B:351:ILE:HD13	2.01	0.43
1:A:336:TRP:CH2	1:A:360:LEU:HD21	2.52	0.43
1:C:34:LEU:O	1:C:38:LEU:HG	2.18	0.43
1:A:695:ILE:HG22	1:A:697:GLU:HG3	2.01	0.43
1:A:602:ARG:NH2	1:A:641:ASP:OD1	2.27	0.43
1:B:2070:LEU:O	1:B:2074:GLU:HG3	2.16	0.43
1:C:1133:VAL:O	1:C:1193:ALA:N	2.42	0.43
1:C:874:ASP:OD2	1:C:877:TRP:CD1	2.72	0.43
1:A:3044:ALA:HB1	1:A:3050:PRO:HB3	2.00	0.43
1:A:2114:UNK:HA	1:A:2117:UNK:HG3	1.99	0.43
1:B:970:ILE:HG23	1:B:992:UNK:HG1	2.00	0.43
1:C:981:UNK:HG2	1:C:988:UNK:HA	2.01	0.43
1:A:393:VAL:HG12	1:A:394:PRO:N	2.32	0.43
1:C:2180:LYS:HZ1	1:C:2962:ASP:HB3	1.82	0.43
1:A:641:ASP:N	1:A:641:ASP:OD1	2.48	0.43
1:B:1705:VAL:O	1:B:1735:GLU:HB2	2.18	0.43
1:C:2462:VAL:HG13	1:C:2835:VAL:HG13	2.00	0.43
1:C:1612:GLY:N	1:C:1623:PHE:O	2.48	0.43
1:C:1268:GLY:HA2	1:C:1271:LEU:HD12	2.00	0.43
1:C:2115:UNK:HA	1:C:2118:UNK:CG	2.49	0.43
1:B:981:UNK:CG	1:B:987:UNK:C	2.96	0.43
1:A:580:ARG:HD3	1:A:896:ALA:HB3	2.01	0.43
1:B:2710:LEU:O	1:B:2713:VAL:HG22	2.18	0.43
1:B:393:VAL:HG12	1:B:394:PRO:N	2.32	0.43
1:A:341:THR:HG23	1:A:344:HIS:ND1	2.34	0.43
1:A:1582:HIS:HA	1:A:1674:ALA:O	2.18	0.43
1:B:857:VAL:HG13	1:B:859:PHE:H	1.83	0.43
1:C:657:THR:HB	1:C:662:LYS:HE3	2.00	0.43
1:B:2580:PHE:HE1	1:B:2603:ARG:HH21	1.66	0.43
1:A:2541:ARG:O	1:A:2621:VAL:HG13	2.18	0.43
1:B:2541:ARG:O	1:B:2621:VAL:HG13	2.18	0.43
1:C:2095:UNK:C	1:C:2098:UNK:HG3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:ASP:HA	1:A:1168:ARG:HA	2.01	0.43
1:C:2706:PRO:O	1:C:2709:ILE:HG12	2.19	0.43
1:A:2209:LEU:O	1:A:2213:VAL:HG23	2.18	0.43
1:B:2092:UNK:CG	1:B:2092:UNK:O	2.64	0.43
1:C:647:THR:N	2:C:4000:FMN:O3P	2.51	0.43
1:A:1723:GLU:O	1:A:1725:SER:N	2.51	0.43
1:A:344:HIS:CD2	1:A:373:ILE:HG13	2.53	0.43
1:C:1519:VAL:HG13	1:C:1530:LEU:HD23	1.99	0.43
1:B:516:PRO:HA	1:B:962:MET:SD	2.58	0.43
1:C:3044:ALA:HB1	1:C:3050:PRO:HB3	2.00	0.43
1:B:2512:TRP:O	1:B:2520:LEU:HD12	2.19	0.43
1:C:276:LYS:HB3	1:C:587:TRP:CH2	2.53	0.43
1:B:2471:PRO:HA	1:B:2625:ILE:HA	2.00	0.43
1:B:1268:GLY:HA2	1:B:1271:LEU:HD12	1.99	0.43
1:C:2083:UNK:HA	1:C:2086:UNK:HG3	2.00	0.43
1:C:999:UNK:C	1:C:1007:UNK:HG3	2.47	0.43
1:B:2610:ARG:NH1	1:B:2700:LEU:HD11	2.25	0.43
1:C:580:ARG:HD3	1:C:896:ALA:HB3	2.01	0.43
1:C:340:ILE:HD11	1:C:351:ILE:HD13	2.01	0.43
1:A:2591:ARG:HH12	1:C:2014:SER:N	2.16	0.43
1:B:276:LYS:HB3	1:B:587:TRP:CH2	2.53	0.43
1:A:2297:ARG:HH12	1:A:2391:LYS:NZ	2.17	0.43
1:C:695:ILE:HG22	1:C:697:GLU:HG3	2.00	0.43
1:B:412:ASP:H	1:B:1025:VAL:CG2	2.31	0.43
1:B:315:VAL:C	1:B:317:LEU:H	2.22	0.43
1:A:315:VAL:C	1:A:317:LEU:H	2.22	0.43
1:C:344:HIS:CD2	1:C:373:ILE:HG13	2.53	0.43
1:C:782:ARG:HH11	1:C:857:VAL:HG22	1.83	0.43
1:B:2426:UNK:HG2	1:B:2426:UNK:O	2.18	0.43
1:B:1581:PHE:HB2	1:B:1586:LEU:HD22	1.99	0.43
1:A:2462:VAL:HG13	1:A:2835:VAL:HG13	2.00	0.43
1:C:163:LEU:HD13	1:C:181:LEU:HD23	2.00	0.43
1:A:874:ASP:OD2	1:A:877:TRP:CD1	2.71	0.43
1:A:931:UNK:HG3	1:A:934:UNK:HG3	2.01	0.43
1:B:940:UNK:O	1:B:940:UNK:CG	2.60	0.43
1:B:1582:HIS:HA	1:B:1674:ALA:O	2.18	0.43
1:C:2903:GLU:OE2	1:C:2995:THR:OG1	2.36	0.43
1:A:2891:LYS:HZ2	1:A:2903:GLU:HG2	1.83	0.43
1:A:857:VAL:HG13	1:A:859:PHE:H	1.83	0.43
1:A:2471:PRO:HA	1:A:2625:ILE:HA	2.00	0.43
1:B:2786:ASP:OD2	1:B:2789:MET:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:SER:HB3	1:C:314:THR:OG1	2.18	0.43
1:C:1705:VAL:O	1:C:1735:GLU:HB2	2.18	0.43
1:B:658:SER:HB2	1:B:661:VAL:HG23	2.01	0.43
1:C:2064:ARG:HG2	1:C:2100:UNK:HG1	2.01	0.43
1:B:981:UNK:HG2	1:B:988:UNK:HA	2.00	0.43
1:B:931:UNK:HG3	1:B:934:UNK:HG3	2.01	0.43
1:A:408:VAL:HG13	1:A:943:UNK:CG	2.48	0.43
1:B:2014:SER:N	1:C:2591:ARG:NH1	2.66	0.43
1:A:2710:LEU:O	1:A:2713:VAL:HG22	2.18	0.43
1:B:34:LEU:O	1:B:38:LEU:HG	2.18	0.43
1:B:647:THR:N	2:B:4000:FMN:O3P	2.51	0.43
1:A:276:LYS:HB3	1:A:587:TRP:CH2	2.53	0.43
1:C:613:GLY:HA2	2:C:4000:FMN:O5'	2.19	0.43
1:B:488:ASN:OD1	1:B:523:SER:OG	2.34	0.43
1:A:2903:GLU:OE2	1:A:2995:THR:OG1	2.36	0.43
1:B:1619:VAL:HA	1:B:1620:PRO:HD2	1.80	0.43
1:A:2958:ASN:HD22	1:A:2976:TRP:HE1	1.65	0.43
1:C:2810:GLY:HA2	1:C:2896:THR:HG22	2.01	0.43
1:B:1021:LEU:HB3	1:B:1034:GLU:HG2	2.01	0.43
1:B:88:SER:HB3	1:B:314:THR:OG1	2.18	0.43
1:B:856:PRO:HG2	1:B:874:ASP:HB2	2.00	0.43
1:A:1070:VAL:N	1:A:1152:PHE:O	2.52	0.43
1:A:2119:UNK:HG2	1:A:2120:UNK:N	2.34	0.43
1:A:2122:UNK:O	1:A:2125:UNK:CG	2.63	0.43
1:A:981:UNK:HG2	1:A:988:UNK:HA	2.01	0.43
1:C:475:LEU:HA	1:C:475:LEU:HD23	1.79	0.43
1:A:340:ILE:HD11	1:A:351:ILE:HD13	2.01	0.43
1:B:511:ARG:CB	1:B:540:ASN:HB2	2.46	0.43
1:A:2706:PRO:O	1:A:2709:ILE:HG12	2.19	0.43
1:A:34:LEU:O	1:A:38:LEU:HG	2.19	0.43
1:A:1352:PHE:HA	1:A:1353:PRO:HD3	1.72	0.43
1:A:709:LEU:HD21	1:A:872:ARG:NE	2.34	0.43
1:B:780:ARG:NH1	1:B:817:GLU:OE2	2.52	0.43
1:B:1317:GLY:O	1:B:1324:VAL:HG12	2.19	0.43
1:B:307:ILE:HG22	1:B:311:TRP:CE2	2.54	0.43
1:B:1133:VAL:N	1:B:1193:ALA:O	2.48	0.43
1:B:2665:THR:HA	1:B:2666:PRO:HD3	1.86	0.43
1:B:782:ARG:HH11	1:B:857:VAL:HG22	1.83	0.43
1:A:2299:MET:HG2	1:A:2299:MET:H	1.68	0.43
1:C:856:PRO:HG2	1:C:874:ASP:HB2	2.00	0.43
1:A:2530:TYR:O	1:A:2533:ALA:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1503:ILE:HB	1:A:1542:TYR:HB2	2.00	0.43
1:C:2530:TYR:O	1:C:2533:ALA:N	2.52	0.43
1:B:3044:ALA:HB1	1:B:3050:PRO:HB3	2.00	0.43
1:B:163:LEU:HD13	1:B:181:LEU:HD23	2.00	0.43
1:A:2786:ASP:OD2	1:A:2789:MET:HG2	2.19	0.43
1:C:2096:UNK:CG	1:C:2097:UNK:N	2.82	0.43
1:A:999:UNK:HG2	1:A:1007:UNK:HG3	1.96	0.43
1:C:2557:LEU:HB3	1:C:2613:ARG:HB2	2.01	0.43
1:A:1084:THR:CG2	1:A:1274:ALA:HA	2.48	0.43
1:A:2244:ARG:HG2	1:A:2245:VAL:N	2.34	0.43
1:A:2092:UNK:O	1:A:2092:UNK:CG	2.64	0.43
1:B:393:VAL:O	1:B:395:GLU:N	2.52	0.43
1:B:695:ILE:HG22	1:B:697:GLU:HG3	2.00	0.43
1:A:780:ARG:NH1	1:A:817:GLU:OE2	2.52	0.43
1:B:2810:GLY:HA2	1:B:2896:THR:HG22	2.01	0.43
1:C:2058:ASP:N	1:C:2058:ASP:OD1	2.46	0.43
1:C:2137:GLU:O	1:C:2163:THR:N	2.30	0.43
1:A:885:GLU:HG2	1:A:887:ASP:H	1.84	0.43
1:C:1117:ALA:HA	1:C:1120:GLU:HB2	2.01	0.43
1:A:2580:PHE:HE1	1:A:2603:ARG:HH21	1.66	0.43
1:A:2695:MET:HG3	1:A:2696:TYR:N	2.34	0.43
1:B:2014:SER:N	1:C:2591:ARG:HH12	2.16	0.42
1:C:1084:THR:CG2	1:C:1274:ALA:HA	2.49	0.42
1:B:1087:PHE:CZ	1:C:203:ASP:OD2	2.72	0.42
1:A:1087:PHE:HD2	1:B:117:LYS:HZ1	1.67	0.42
1:B:2244:ARG:HG2	1:B:2245:VAL:N	2.34	0.42
1:C:2889:ILE:HB	1:C:2924:ILE:HG12	2.01	0.42
1:C:1660:LEU:HA	1:C:1660:LEU:HD23	1.86	0.42
1:B:2957:PRO:HB3	1:B:2980:PRO:N	2.34	0.42
1:B:1733:ASN:H	1:B:1737:ASP:HB2	1.83	0.42
1:C:1317:GLY:O	1:C:1324:VAL:HG12	2.19	0.42
1:C:78:GLU:HB2	1:C:176:VAL:HG21	2.01	0.42
1:A:782:ARG:HH11	1:A:857:VAL:HG22	1.83	0.42
1:B:874:ASP:OD2	1:B:877:TRP:CD1	2.72	0.42
1:A:2426:UNK:O	1:A:2426:UNK:HG2	2.18	0.42
1:C:2426:UNK:HG2	1:C:2426:UNK:O	2.18	0.42
1:C:2541:ARG:O	1:C:2621:VAL:HG13	2.18	0.42
1:B:2115:UNK:HA	1:B:2118:UNK:CG	2.48	0.42
1:C:2077:UNK:CG	1:C:2079:UNK:HG3	2.41	0.42
1:B:355:GLY:HA2	1:B:356:PRO:HD3	1.86	0.42
1:B:2706:PRO:O	1:B:2709:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1533:VAL:N	1:C:1543:ALA:O	2.52	0.42
1:B:2180:LYS:HZ1	1:B:2962:ASP:HB3	1.82	0.42
1:C:709:LEU:HD21	1:C:872:ARG:NE	2.34	0.42
1:B:2800:PHE:CE1	1:B:2812:LEU:HD22	2.50	0.42
1:B:2891:LYS:HZ1	1:B:2904:THR:N	2.17	0.42
1:A:2810:GLY:HA2	1:A:2896:THR:HG22	2.01	0.42
1:C:341:THR:HG23	1:C:344:HIS:ND1	2.34	0.42
1:B:2296:ASN:ND2	1:B:2395:THR:HG21	2.34	0.42
1:B:1551:LEU:HA	1:B:1551:LEU:HD13	1.80	0.42
1:C:1662:ARG:HG3	1:C:1663:LYS:N	2.34	0.42
1:B:1117:ALA:HA	1:B:1120:GLU:HB2	2.01	0.42
1:C:2141:VAL:HG22	1:C:2238:PHE:HD2	1.85	0.42
1:C:516:PRO:HA	1:C:962:MET:SD	2.58	0.42
1:A:1662:ARG:HG3	1:A:1663:LYS:N	2.34	0.42
1:B:2122:UNK:O	1:B:2125:UNK:CG	2.63	0.42
1:A:2095:UNK:C	1:A:2098:UNK:HG3	2.49	0.42
1:C:999:UNK:HG2	1:C:1007:UNK:HG1	1.96	0.42
1:B:2911:ALA:O	1:B:2916:ARG:HB2	2.19	0.42
1:B:45:ALA:O	1:B:351:ILE:HA	2.20	0.42
1:B:2252:VAL:HG22	1:B:2255:ARG:HH21	1.82	0.42
1:A:613:GLY:HA2	2:A:4000:FMN:O5'	2.19	0.42
1:C:438:THR:HA	1:C:880:HIS:CE1	2.51	0.42
1:A:2957:PRO:HB3	1:A:2980:PRO:N	2.34	0.42
1:A:2808:ARG:HH21	1:A:2901:PRO:HD3	1.85	0.42
1:C:307:ILE:HG22	1:C:311:TRP:CE2	2.54	0.42
1:A:211:THR:HB	1:A:286:VAL:HB	2.02	0.42
1:A:1504:ARG:HA	1:A:1540:SER:O	2.19	0.42
1:C:1275:ALA:HB2	1:C:1311:PHE:CE2	2.55	0.42
1:A:2141:VAL:HG22	1:A:2238:PHE:HD2	1.85	0.42
1:B:2095:UNK:C	1:B:2098:UNK:HG3	2.49	0.42
1:A:2105:UNK:C	1:A:2108:UNK:HG3	2.34	0.42
1:A:970:ILE:HG23	1:A:992:UNK:HG1	2.00	0.42
1:B:1163:ASP:HA	1:B:1168:ARG:HA	2.01	0.42
1:C:2252:VAL:HG22	1:C:2255:ARG:HH21	1.82	0.42
1:A:1106:CYS:SG	1:A:1174:VAL:HG11	2.60	0.42
1:A:1317:GLY:O	1:A:1324:VAL:HG12	2.19	0.42
1:B:53:SER:HA	1:B:359:ILE:HG13	2.01	0.42
1:A:516:PRO:HA	1:A:962:MET:SD	2.58	0.42
1:C:2584:ASP:O	1:C:2586:GLU:N	2.53	0.42
1:C:981:UNK:CG	1:C:987:UNK:C	2.96	0.42
1:C:999:UNK:HG2	1:C:1007:UNK:HG3	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2911:ALA:O	1:C:2916:ARG:HB2	2.19	0.42
1:A:1399:ASN:HA	1:A:1400:PRO:HD3	1.86	0.42
1:A:1087:PHE:CZ	1:B:203:ASP:OD2	2.72	0.42
1:C:2244:ARG:HG2	1:C:2245:VAL:N	2.34	0.42
1:A:1537:LEU:HD13	1:A:1541:GLN:HB2	2.00	0.42
1:B:1660:LEU:HD23	1:B:1660:LEU:HA	1.85	0.42
1:C:2961:LEU:HD22	1:C:2976:TRP:HD1	1.85	0.42
1:C:1106:CYS:SG	1:C:1174:VAL:HG11	2.60	0.42
1:B:341:THR:HG23	1:B:344:HIS:ND1	2.34	0.42
1:B:1280:THR:O	1:B:1288:PRO:HB3	2.20	0.42
1:A:1280:THR:O	1:A:1288:PRO:HB3	2.20	0.42
1:B:2836:LEU:HA	1:B:2836:LEU:HD23	1.87	0.42
1:A:2512:TRP:O	1:A:2520:LEU:HD12	2.19	0.42
1:B:211:THR:HB	1:B:286:VAL:HB	2.01	0.42
1:B:2695:MET:HG3	1:B:2696:TYR:N	2.34	0.42
1:C:2444:UNK:HB2	1:C:2988:PRO:HB3	2.01	0.42
1:B:2444:UNK:HB2	1:B:2988:PRO:HB3	2.01	0.42
1:C:2512:TRP:O	1:C:2520:LEU:HD12	2.19	0.42
1:C:2620:THR:OG1	1:C:2791:ARG:NH2	2.53	0.42
1:A:1021:LEU:HB3	1:A:1034:GLU:HG2	2.01	0.42
1:A:107:LEU:HD13	1:A:113:VAL:HB	2.02	0.42
1:C:970:ILE:O	1:C:974:UNK:HG3	2.20	0.42
1:B:42:GLU:HA	1:B:43:PRO:HD3	1.91	0.42
1:A:2610:ARG:NH1	1:A:2700:LEU:HD11	2.25	0.42
1:A:2805:ASP:OD2	1:A:2807:ARG:HB2	2.20	0.42
1:C:1637:VAL:HA	1:C:1638:PRO:HD2	1.91	0.42
1:C:45:ALA:O	1:C:351:ILE:HA	2.20	0.42
1:B:2297:ARG:HH12	1:B:2391:LYS:NZ	2.17	0.42
1:B:613:GLY:HA2	2:B:4000:FMN:O5'	2.19	0.42
1:C:2297:ARG:HH12	1:C:2391:LYS:NZ	2.17	0.42
1:B:2889:ILE:HB	1:B:2924:ILE:HG12	2.01	0.42
1:C:2846:ALA:O	1:C:2859:GLY:HA3	2.19	0.42
1:B:2294:SER:HB3	1:B:2310:LYS:HB2	2.02	0.42
1:B:107:LEU:HD13	1:B:113:VAL:HB	2.01	0.42
1:C:3065:PRO:O	1:C:3069:GLN:N	2.42	0.42
1:C:1504:ARG:HA	1:C:1540:SER:O	2.19	0.42
1:A:2115:UNK:HA	1:A:2118:UNK:CG	2.49	0.42
1:C:2120:UNK:C	1:C:2123:UNK:HG3	2.50	0.42
1:C:2125:UNK:CA	1:C:2128:UNK:HG3	2.49	0.42
1:C:795:HIS:NE2	1:C:797:GLN:HB2	2.35	0.42
1:B:479:LEU:HD21	1:B:485:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2911:ALA:O	1:A:2916:ARG:HB2	2.19	0.42
1:B:668:THR:HG23	1:B:683:GLY:HA3	2.02	0.42
1:A:647:THR:N	2:A:4000:FMN:O3P	2.51	0.42
1:C:2297:ARG:HH22	1:C:2391:LYS:HZ3	1.67	0.42
1:B:1703:ILE:HG22	1:B:1704:GLY:H	1.85	0.42
1:B:1656:LYS:N	1:B:1657:PRO:HD2	2.35	0.42
1:C:2891:LYS:NZ	1:C:2903:GLU:HB3	2.35	0.42
1:A:2889:ILE:HG13	1:A:2922:LEU:HD13	2.02	0.42
1:C:780:ARG:NH1	1:C:817:GLU:OE2	2.52	0.42
1:A:307:ILE:HG22	1:A:311:TRP:CE2	2.54	0.42
1:A:856:PRO:HG2	1:A:874:ASP:HB2	2.00	0.42
1:C:1120:GLU:HA	1:C:1125:VAL:CG2	2.50	0.42
1:C:658:SER:HB2	1:C:661:VAL:HG23	2.01	0.42
1:A:1275:ALA:O	1:A:1279:VAL:HG23	2.20	0.42
1:C:50:GLY:O	1:C:53:SER:OG	2.36	0.42
1:B:1275:ALA:HB2	1:B:1311:PHE:CE2	2.55	0.42
1:B:885:GLU:HG2	1:B:887:ASP:H	1.84	0.42
1:B:1504:ARG:HA	1:B:1540:SER:O	2.19	0.42
1:C:2113:UNK:HG2	1:C:2114:UNK:N	2.35	0.42
1:B:999:UNK:O	1:B:1007:UNK:CG	2.61	0.42
1:C:479:LEU:HD21	1:C:485:ILE:HD11	2.02	0.42
1:B:436:THR:OG1	1:B:437:PRO:HD3	2.19	0.42
1:C:336:TRP:HE3	1:C:339:GLU:OE2	2.03	0.42
1:A:336:TRP:HE3	1:A:339:GLU:OE2	2.03	0.42
1:A:1687:PHE:CE1	1:A:1723:GLU:HG2	2.55	0.42
1:A:488:ASN:OD1	1:A:523:SER:OG	2.34	0.42
1:C:412:ASP:H	1:C:1025:VAL:CG2	2.31	0.42
1:B:2300:PHE:HZ	1:B:2398:LEU:HB3	1.85	0.42
1:C:1656:LYS:N	1:C:1657:PRO:HD2	2.35	0.42
1:B:2846:ALA:O	1:B:2859:GLY:HA3	2.19	0.42
1:B:2961:LEU:HD22	1:B:2976:TRP:HD1	1.85	0.42
1:C:315:VAL:C	1:C:317:LEU:H	2.22	0.42
1:A:2296:ASN:ND2	1:A:2395:THR:HG21	2.34	0.42
1:B:2620:THR:OG1	1:B:2791:ARG:NH2	2.53	0.42
1:C:1021:LEU:HB3	1:C:1034:GLU:HG2	2.01	0.42
1:C:957:LEU:O	1:C:1034:GLU:HB2	2.20	0.42
1:C:1503:ILE:HB	1:C:1542:TYR:HB2	2.00	0.42
1:A:2064:ARG:HG2	1:A:2100:UNK:HG1	2.01	0.42
1:B:408:VAL:HG13	1:B:943:UNK:CG	2.48	0.42
1:B:2557:LEU:HB3	1:B:2613:ARG:HB2	2.01	0.42
1:C:436:THR:OG1	1:C:437:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2800:PHE:CZ	1:B:2812:LEU:HD13	2.55	0.42
1:A:2846:ALA:O	1:A:2859:GLY:HA3	2.20	0.42
1:A:1380:ALA:HB1	1:A:1474:LEU:CD1	2.50	0.42
1:A:78:GLU:HB2	1:A:176:VAL:HG21	2.01	0.42
1:C:1280:THR:O	1:C:1288:PRO:HB3	2.20	0.42
1:C:1275:ALA:O	1:C:1279:VAL:HG23	2.20	0.42
1:A:1228:VAL:HB	1:A:1311:PHE:HB2	2.02	0.42
1:C:53:SER:HA	1:C:359:ILE:HG13	2.01	0.42
1:A:2753:LYS:HA	1:A:2753:LYS:HD3	1.83	0.42
1:A:2620:THR:OG1	1:A:2791:ARG:NH2	2.53	0.42
1:B:2530:TYR:O	1:B:2533:ALA:N	2.52	0.42
1:A:2584:ASP:O	1:A:2586:GLU:N	2.53	0.42
1:A:658:SER:HB2	1:A:661:VAL:HG23	2.01	0.42
1:C:2294:SER:HB3	1:C:2310:LYS:HB2	2.02	0.42
1:A:2055:VAL:HG22	1:A:2194:TRP:CD1	2.55	0.42
1:A:2123:UNK:CA	1:A:2126:UNK:HG3	2.50	0.42
1:A:2125:UNK:CA	1:A:2128:UNK:HG3	2.49	0.42
1:B:970:ILE:O	1:B:974:UNK:HG3	2.20	0.42
1:A:436:THR:OG1	1:A:437:PRO:HD3	2.19	0.42
1:A:1008:UNK:CG	1:A:1008:UNK:O	2.67	0.42
1:C:668:THR:HG23	1:C:683:GLY:HA3	2.02	0.42
1:A:668:THR:HG23	1:A:683:GLY:HA3	2.02	0.42
1:A:2800:PHE:CZ	1:A:2812:LEU:HD13	2.55	0.42
1:C:2957:PRO:HB3	1:C:2980:PRO:N	2.34	0.42
1:C:1228:VAL:HB	1:C:1311:PHE:HB2	2.02	0.42
1:A:1275:ALA:HB2	1:A:1311:PHE:CE2	2.55	0.42
1:C:2354:SER:O	1:C:2358:GLU:HG3	2.20	0.42
1:B:2055:VAL:HG22	1:B:2194:TRP:CD1	2.55	0.42
1:A:1460:ALA:O	1:A:1464:VAL:HG22	2.20	0.42
1:B:2892:HIS:HA	1:B:2942:GLN:HE22	1.85	0.42
1:B:2584:ASP:O	1:B:2586:GLU:N	2.53	0.42
1:B:2125:UNK:CA	1:B:2128:UNK:HG3	2.49	0.41
1:A:2096:UNK:CG	1:A:2097:UNK:N	2.82	0.41
1:C:2450:UNK:HG1	1:C:3016:ALA:CB	2.17	0.41
1:A:976:UNK:CG	1:A:976:UNK:O	2.68	0.41
1:B:2077:UNK:CG	1:B:2079:UNK:HG3	2.41	0.41
1:A:2014:SER:N	1:B:2591:ARG:HH12	2.16	0.41
1:A:203:ASP:OD2	1:C:1087:PHE:CZ	2.72	0.41
1:C:1352:PHE:HA	1:C:1353:PRO:HD3	1.72	0.41
1:B:709:LEU:HD21	1:B:872:ARG:NE	2.34	0.41
1:C:1703:ILE:HG22	1:C:1704:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1656:LYS:N	1:A:1657:PRO:HD2	2.35	0.41
1:A:2891:LYS:NZ	1:A:2903:GLU:HB3	2.35	0.41
1:A:2300:PHE:HZ	1:A:2398:LEU:HB3	1.85	0.41
1:B:2889:ILE:HG13	1:B:2922:LEU:HD13	2.02	0.41
1:B:2808:ARG:HH21	1:B:2901:PRO:HD3	1.85	0.41
1:C:2299:MET:HG2	1:C:2299:MET:H	1.68	0.41
1:B:1120:GLU:HA	1:B:1125:VAL:CG2	2.50	0.41
1:B:2141:VAL:HG22	1:B:2238:PHE:HD2	1.85	0.41
1:B:2354:SER:O	1:B:2358:GLU:HG3	2.20	0.41
1:B:2405:MET:HA	1:B:2405:MET:HE2	2.02	0.41
1:A:1117:ALA:HA	1:A:1120:GLU:HB2	2.01	0.41
1:B:1611:ILE:HG23	1:B:1624:THR:HA	2.02	0.41
1:C:160:GLN:HA	1:C:329:ILE:HD13	2.02	0.41
1:A:53:SER:HA	1:A:359:ILE:HG13	2.01	0.41
1:A:970:ILE:O	1:A:974:UNK:HG3	2.20	0.41
1:A:984:UNK:HG2	1:A:984:UNK:O	2.20	0.41
1:A:2591:ARG:NH1	1:C:2014:SER:H	2.19	0.41
1:C:618:PRO:HB3	1:C:915:PHE:HA	2.02	0.41
1:C:360:LEU:HA	1:C:363:LEU:HB3	2.02	0.41
1:C:2800:PHE:CZ	1:C:2812:LEU:HD13	2.55	0.41
1:A:438:THR:HA	1:A:880:HIS:CE1	2.51	0.41
1:A:669:LYS:O	1:A:682:ASN:HB3	2.20	0.41
1:B:78:GLU:HB2	1:B:176:VAL:HG21	2.01	0.41
1:C:2808:ARG:HH21	1:C:2901:PRO:HD3	1.85	0.41
1:C:2503:LYS:HG3	1:C:2513:TYR:HB2	2.02	0.41
1:C:756:LEU:HD13	1:C:859:PHE:CD2	2.55	0.41
1:B:50:GLY:O	1:B:53:SER:OG	2.36	0.41
1:C:2200:MET:HE3	1:C:2200:MET:HB3	1.95	0.41
1:C:559:SER:O	1:C:563:ILE:HG12	2.20	0.41
1:C:2786:ASP:OD2	1:C:2789:MET:HG2	2.19	0.41
1:A:266:ALA:O	1:A:270:GLU:HG3	2.20	0.41
1:B:266:ALA:O	1:B:270:GLU:HG3	2.20	0.41
1:C:1611:ILE:HG23	1:C:1624:THR:HA	2.02	0.41
1:A:2294:SER:HB3	1:A:2310:LYS:HB2	2.02	0.41
1:A:795:HIS:NE2	1:A:797:GLN:HB2	2.35	0.41
1:B:2064:ARG:HG2	1:B:2100:UNK:HG1	2.01	0.41
1:A:2919:GLY:O	1:A:2921:PRO:HD3	2.21	0.41
1:C:2123:UNK:CA	1:C:2126:UNK:HG3	2.50	0.41
1:B:2805:ASP:OD2	1:B:2807:ARG:HB2	2.20	0.41
1:A:70:SER:HG	1:A:142:ARG:HH22	1.65	0.41
1:B:336:TRP:HE3	1:B:339:GLU:OE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:LEU:HA	1:A:363:LEU:HB3	2.02	0.41
1:C:1095:LEU:HD23	1:C:1098:VAL:HA	2.03	0.41
1:B:487:PHE:O	1:B:521:VAL:N	2.51	0.41
1:C:369:ARG:HD2	1:C:369:ARG:HA	1.85	0.41
1:B:1706:LYS:HA	1:B:1735:GLU:HG3	2.02	0.41
1:B:1228:VAL:HB	1:B:1311:PHE:HB2	2.02	0.41
1:C:2695:MET:HG3	1:C:2696:TYR:N	2.34	0.41
1:A:2444:UNK:HB2	1:A:2988:PRO:HB3	2.01	0.41
1:A:1611:ILE:HG23	1:A:1624:THR:HA	2.02	0.41
1:C:211:THR:HB	1:C:286:VAL:HB	2.01	0.41
1:A:2563:LEU:HD21	1:A:2567:PHE:HB2	2.02	0.41
1:A:559:SER:O	1:A:563:ILE:HG12	2.20	0.41
1:B:980:UNK:C	1:B:981:UNK:CG	2.96	0.41
1:A:2557:LEU:HB3	1:A:2613:ARG:HB2	2.01	0.41
1:B:436:THR:HG22	1:B:460:GLY:HA3	2.03	0.41
1:B:580:ARG:HD3	1:B:896:ALA:HB3	2.01	0.41
1:B:1095:LEU:HD23	1:B:1098:VAL:HA	2.02	0.41
1:C:669:LYS:O	1:C:682:ASN:HB3	2.20	0.41
1:B:2891:LYS:NZ	1:B:2903:GLU:HB3	2.35	0.41
1:B:1106:CYS:SG	1:B:1174:VAL:HG11	2.60	0.41
1:C:2296:ASN:ND2	1:C:2395:THR:HG21	2.34	0.41
1:B:1224:UNK:HG2	1:B:1224:UNK:O	2.20	0.41
1:C:2055:VAL:HG22	1:C:2194:TRP:CD1	2.55	0.41
1:B:1662:ARG:HG3	1:B:1663:LYS:N	2.34	0.41
1:A:2892:HIS:HA	1:A:2942:GLN:HE22	1.85	0.41
1:C:266:ALA:O	1:C:270:GLU:HG3	2.20	0.41
1:B:793:ARG:HH12	1:B:2523:GLU:CD	2.24	0.41
1:B:2096:UNK:CG	1:B:2097:UNK:N	2.82	0.41
1:B:2123:UNK:CA	1:B:2126:UNK:HG3	2.50	0.41
1:C:2104:UNK:CA	1:C:2107:UNK:HG3	2.50	0.41
1:C:1399:ASN:HA	1:C:1400:PRO:HD3	1.86	0.41
1:C:374:GLY:C	1:C:375:ILE:HG13	2.41	0.41
1:A:117:LYS:HZ1	1:C:1087:PHE:HD2	1.68	0.41
1:A:2134:UNK:HB1	1:A:2189:PHE:HD2	1.85	0.41
1:C:2092:UNK:O	1:C:2092:UNK:CG	2.64	0.41
1:B:2205:ASP:O	1:B:2209:LEU:HB2	2.21	0.41
1:C:1687:PHE:CE1	1:C:1723:GLU:HG2	2.55	0.41
1:B:669:LYS:O	1:B:682:ASN:HB3	2.20	0.41
1:C:2889:ILE:HG13	1:C:2922:LEU:HD13	2.02	0.41
1:A:2889:ILE:HB	1:A:2924:ILE:HG12	2.01	0.41
1:A:1703:ILE:HG22	1:A:1704:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2492:VAL:HG12	1:A:2526:ILE:HG22	2.02	0.41
1:C:417:LEU:HD21	1:C:625:LEU:HD21	2.02	0.41
1:B:2503:LYS:HG3	1:B:2513:TYR:HB2	2.02	0.41
1:C:1672:GLN:HE21	1:C:1672:GLN:HB3	1.58	0.41
1:A:2354:SER:O	1:A:2358:GLU:HG3	2.20	0.41
1:A:233:LEU:HB3	1:A:251:THR:OG1	2.21	0.41
1:C:885:GLU:HG2	1:C:887:ASP:H	1.84	0.41
1:B:2563:LEU:HD21	1:B:2567:PHE:HB2	2.02	0.41
1:B:1460:ALA:O	1:B:1464:VAL:HG22	2.20	0.41
1:A:2113:UNK:HG2	1:A:2114:UNK:N	2.35	0.41
1:A:2113:UNK:HA	1:A:2116:UNK:HG3	2.03	0.41
1:C:2113:UNK:HA	1:C:2116:UNK:HG3	2.03	0.41
1:B:936:UNK:HA	1:B:939:UNK:CG	2.51	0.41
1:C:1634:ARG:NH1	1:C:1639:ALA:H	2.11	0.41
1:A:2014:SER:H	1:B:2591:ARG:NH1	2.18	0.41
1:A:202:GLY:O	1:A:289:PRO:HD2	2.21	0.41
1:C:585:HIS:HB3	1:C:694:ASP:HB2	2.03	0.41
1:A:587:TRP:CZ2	1:A:694:ASP:OD2	2.74	0.41
1:C:2468:GLU:OE2	1:C:2478:ARG:NH2	2.48	0.41
1:A:756:LEU:HD13	1:A:859:PHE:CD2	2.55	0.41
1:C:1706:LYS:HA	1:C:1735:GLU:HG3	2.03	0.41
1:A:1491:ASP:HB2	1:A:1495:ARG:HB2	2.02	0.41
1:B:2058:ASP:OD1	1:B:2058:ASP:N	2.46	0.41
1:B:2483:VAL:HG13	1:B:2954:VAL:HG11	2.03	0.41
1:B:2120:UNK:C	1:B:2123:UNK:HG3	2.50	0.41
1:C:2919:GLY:O	1:C:2921:PRO:HD3	2.21	0.41
1:B:2770:LEU:CB	1:B:2815:GLN:HB3	2.51	0.41
1:A:2770:LEU:CB	1:A:2815:GLN:HB3	2.51	0.41
1:C:2805:ASP:OD2	1:C:2807:ARG:HB2	2.20	0.41
1:B:1400:PRO:O	1:B:1415:GLY:HA2	2.21	0.41
1:A:1400:PRO:O	1:A:1415:GLY:HA2	2.21	0.41
1:A:1535:PHE:O	1:A:1679:TRP:N	2.48	0.41
1:B:202:GLY:O	1:B:289:PRO:HD2	2.21	0.41
1:C:2710:LEU:HD12	1:C:2713:VAL:HG21	2.03	0.41
1:A:393:VAL:O	1:A:395:GLU:N	2.52	0.41
1:B:709:LEU:HD11	1:B:872:ARG:CZ	2.51	0.41
1:C:515:ALA:HA	1:C:516:PRO:HD3	1.84	0.41
1:A:2141:VAL:HG22	1:A:2238:PHE:CD2	2.56	0.41
1:A:957:LEU:O	1:A:1034:GLU:HB2	2.20	0.41
1:B:1275:ALA:O	1:B:1279:VAL:HG23	2.20	0.41
1:B:1491:ASP:HB2	1:B:1495:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1460:ALA:O	1:C:1464:VAL:HG22	2.20	0.41
1:A:160:GLN:HA	1:A:329:ILE:HD13	2.02	0.41
1:C:2286:ARG:HD3	1:C:2331:SER:OG	2.20	0.41
1:B:233:LEU:HB3	1:B:251:THR:OG1	2.21	0.41
1:B:2286:ARG:HD3	1:B:2331:SER:OG	2.20	0.41
1:C:2114:UNK:O	1:C:2118:UNK:HG3	2.21	0.41
1:B:2113:UNK:HA	1:B:2116:UNK:HG3	2.03	0.41
1:B:1695:LEU:HD12	1:B:1695:LEU:HA	1.71	0.41
1:A:479:LEU:HD21	1:A:485:ILE:HD11	2.02	0.41
1:B:1164:THR:HG22	1:B:1204:UNK:HB2	2.03	0.41
1:B:374:GLY:C	1:B:375:ILE:HG13	2.41	0.41
1:C:2428:UNK:O	1:C:2428:UNK:CG	2.67	0.41
1:B:2891:LYS:HZ2	1:B:2903:GLU:CG	2.34	0.41
1:A:2831:MET:HB3	1:A:2831:MET:HE2	1.87	0.41
1:B:957:LEU:O	1:B:1034:GLU:HB2	2.20	0.41
1:C:107:LEU:HD13	1:C:113:VAL:HB	2.01	0.41
1:B:160:GLN:HA	1:B:329:ILE:HD13	2.02	0.41
1:A:1099:PRO:HB2	1:A:1295:TRP:HE1	1.86	0.41
1:C:3062:HIS:H	1:C:3066:GLU:HG3	1.86	0.41
1:B:3065:PRO:O	1:B:3069:GLN:N	2.42	0.41
1:B:559:SER:O	1:B:563:ILE:HG12	2.20	0.41
1:A:795:HIS:HE2	1:A:797:GLN:HB2	1.86	0.41
1:B:795:HIS:NE2	1:B:797:GLN:HB2	2.35	0.41
1:B:2104:UNK:CA	1:B:2107:UNK:HG3	2.50	0.41
1:A:2104:UNK:CA	1:A:2107:UNK:HG3	2.50	0.41
1:A:2114:UNK:O	1:A:2118:UNK:HG3	2.21	0.41
1:B:1017:ILE:HG12	1:B:1045:VAL:HG11	2.03	0.41
1:A:985:UNK:O	1:A:988:UNK:HG3	2.21	0.41
1:C:936:UNK:HA	1:C:939:UNK:CG	2.51	0.41
1:A:936:UNK:HA	1:A:939:UNK:CG	2.51	0.41
1:C:1002:UNK:CG	1:C:1005:UNK:HB2	2.51	0.41
1:C:436:THR:HG22	1:C:460:GLY:HA3	2.03	0.41
1:B:1637:VAL:HA	1:B:1638:PRO:HD2	1.90	0.41
1:A:1634:ARG:NH1	1:A:1639:ALA:H	2.11	0.41
1:B:2212:TRP:O	1:B:2229:LYS:HB3	2.21	0.41
1:A:133:GLN:O	1:A:137:VAL:HG23	2.21	0.41
1:B:360:LEU:HA	1:B:363:LEU:HB3	2.03	0.41
1:A:45:ALA:O	1:A:351:ILE:HA	2.20	0.41
1:B:618:PRO:HB3	1:B:915:PHE:HA	2.02	0.41
1:A:585:HIS:HB3	1:A:694:ASP:HB2	2.03	0.41
1:B:1687:PHE:CE1	1:B:1723:GLU:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2889:ILE:HD12	1:C:2993:LEU:HD23	2.03	0.41
1:C:1986:LEU:HA	1:C:1989:PHE:CD2	2.56	0.41
1:C:2978:ARG:HG3	1:C:2979:GLU:HG3	2.03	0.41
1:A:2961:LEU:HD22	1:A:2976:TRP:HD1	1.85	0.41
1:C:2492:VAL:HG12	1:C:2526:ILE:HG22	2.02	0.41
1:B:369:ARG:HD2	1:B:369:ARG:HA	1.85	0.41
1:A:278:ARG:HD2	1:A:674:TRP:CE3	2.56	0.41
1:B:2405:MET:O	1:B:2409:ALA:HB3	2.21	0.41
1:B:2989:LEU:HD12	1:B:2989:LEU:HA	1.77	0.41
1:C:3057:ASP:N	1:C:3057:ASP:OD1	2.54	0.41
1:C:1491:ASP:HB2	1:C:1495:ARG:HB2	2.02	0.41
1:A:594:LEU:O	1:A:598:TYR:HB2	2.21	0.41
1:A:1224:UNK:O	1:A:1224:UNK:HG2	2.20	0.41
1:A:3057:ASP:N	1:A:3057:ASP:OD1	2.54	0.41
1:B:3057:ASP:N	1:B:3057:ASP:OD1	2.54	0.41
1:C:1099:PRO:HB2	1:C:1295:TRP:HE1	1.86	0.41
1:C:233:LEU:HB3	1:C:251:THR:OG1	2.21	0.41
1:C:2010:GLN:OE1	1:C:2013:LEU:HD11	2.21	0.41
1:B:3062:HIS:H	1:B:3066:GLU:HG3	1.86	0.41
1:A:793:ARG:HH12	1:A:2523:GLU:CD	2.24	0.41
1:B:2919:GLY:O	1:B:2921:PRO:HD3	2.21	0.41
1:A:2098:UNK:HG2	1:A:2099:UNK:N	2.36	0.41
1:A:2212:TRP:O	1:A:2229:LYS:HB3	2.21	0.41
1:A:2334:HIS:CD2	1:A:2391:LYS:HG3	2.50	0.41
1:C:709:LEU:HD11	1:C:872:ARG:CZ	2.51	0.41
1:B:2927:GLN:HE21	1:B:2927:GLN:HB3	1.70	0.41
1:C:278:ARG:HD2	1:C:674:TRP:CE3	2.56	0.41
1:B:1462:ALA:HB2	1:B:1468:TYR:CE1	2.56	0.41
1:C:2989:LEU:HD12	1:C:2989:LEU:HA	1.77	0.41
1:B:594:LEU:O	1:B:598:TYR:HB2	2.21	0.41
1:C:594:LEU:O	1:C:598:TYR:HB2	2.21	0.41
1:C:2483:VAL:HG13	1:C:2954:VAL:HG11	2.03	0.41
1:A:2086:UNK:HA	1:A:2089:UNK:CG	2.51	0.40
1:A:2093:UNK:HB2	1:A:2129:UNK:HB2	2.03	0.40
1:C:984:UNK:HG2	1:C:984:UNK:O	2.20	0.40
1:C:273:ARG:HD2	1:C:282:VAL:CG1	2.51	0.40
1:A:1087:PHE:CD1	1:B:198:ILE:HG23	2.56	0.40
1:A:1095:LEU:HD13	1:A:1289:PRO:CB	2.52	0.40
1:C:2300:PHE:HZ	1:C:2398:LEU:HB3	1.85	0.40
1:C:602:ARG:NH2	1:C:641:ASP:OD1	2.27	0.40
1:C:180:ALA:O	1:C:184:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ASP:OD2	1:B:361:THR:HB	2.21	0.40
1:C:1133:VAL:N	1:C:1193:ALA:O	2.48	0.40
1:A:1120:GLU:HA	1:A:1125:VAL:CG2	2.50	0.40
1:C:1224:UNK:O	1:C:1224:UNK:HG2	2.20	0.40
1:A:2120:UNK:C	1:A:2123:UNK:HG3	2.50	0.40
1:C:2114:UNK:O	1:C:2117:UNK:HG3	2.21	0.40
1:B:999:UNK:HG2	1:B:1007:UNK:HG3	1.96	0.40
1:A:1695:LEU:HD12	1:A:1695:LEU:HA	1.71	0.40
1:C:1400:PRO:O	1:C:1415:GLY:HA2	2.21	0.40
1:B:1237:ARG:HG2	1:B:1237:ARG:HH11	1.86	0.40
1:B:133:GLN:O	1:B:137:VAL:HG23	2.21	0.40
1:C:544:ILE:C	1:C:546:HIS:H	2.22	0.40
1:C:133:GLN:O	1:C:137:VAL:HG23	2.21	0.40
1:B:1533:VAL:N	1:B:1543:ALA:O	2.52	0.40
1:B:1087:PHE:CD1	1:C:198:ILE:HG23	2.56	0.40
1:A:2710:LEU:HD12	1:A:2713:VAL:HG21	2.03	0.40
1:C:2449:UNK:O	1:C:2449:UNK:CG	2.68	0.40
1:A:1702:GLU:OE1	1:A:1711:VAL:HG22	2.22	0.40
1:C:1215:UNK:CG	1:C:1216:UNK:N	2.84	0.40
1:C:393:VAL:O	1:C:395:GLU:N	2.52	0.40
1:A:709:LEU:HD11	1:A:872:ARG:CZ	2.51	0.40
1:B:2978:ARG:HG3	1:B:2979:GLU:HG3	2.03	0.40
1:B:417:LEU:HD21	1:B:625:LEU:HD21	2.02	0.40
1:A:278:ARG:HD2	1:A:674:TRP:HE3	1.87	0.40
1:B:756:LEU:HD13	1:B:859:PHE:CD2	2.55	0.40
1:A:1462:ALA:HB2	1:A:1468:TYR:CE1	2.56	0.40
1:A:2010:GLN:OE1	1:A:2013:LEU:HD11	2.21	0.40
1:C:2892:HIS:HA	1:C:2942:GLN:HE22	1.85	0.40
1:A:1604:ASP:N	1:A:1604:ASP:OD1	2.55	0.40
1:B:1604:ASP:OD1	1:B:1604:ASP:N	2.55	0.40
1:B:2400:ASP:N	1:B:2400:ASP:OD1	2.45	0.40
1:A:2405:MET:HA	1:A:2405:MET:HE2	2.03	0.40
1:B:1381:ASP:OD1	1:B:1391:SER:OG	2.22	0.40
1:B:2114:UNK:O	1:B:2117:UNK:HG3	2.21	0.40
1:B:2093:UNK:HB2	1:B:2129:UNK:HB2	2.03	0.40
1:C:793:ARG:HH12	1:C:2523:GLU:CD	2.24	0.40
1:C:799:PHE:CZ	1:C:2433:UNK:CG	2.99	0.40
1:C:976:UNK:CG	1:C:976:UNK:O	2.68	0.40
1:B:984:UNK:HG2	1:B:984:UNK:O	2.20	0.40
1:C:995:UNK:HB1	1:C:1011:UNK:HG2	1.99	0.40
1:C:2770:LEU:CB	1:C:2815:GLN:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1237:ARG:HH11	1:C:1237:ARG:HG2	1.86	0.40
1:B:2014:SER:H	1:C:2591:ARG:NH1	2.19	0.40
1:A:618:PRO:HB3	1:A:915:PHE:HA	2.02	0.40
1:A:198:ILE:HG23	1:C:1087:PHE:CD1	2.56	0.40
1:B:1095:LEU:HD13	1:B:1289:PRO:CB	2.52	0.40
1:A:487:PHE:O	1:A:521:VAL:N	2.51	0.40
1:B:1616:PRO:HG2	1:B:1619:VAL:HB	2.04	0.40
1:C:745:THR:HG22	1:C:747:LEU:N	2.37	0.40
1:C:2574:GLU:HG3	1:C:2599:TRP:CE2	2.57	0.40
1:B:2672:TRP:CZ3	1:B:2830:LYS:HG2	2.56	0.40
1:C:2672:TRP:CZ3	1:C:2830:LYS:HG2	2.56	0.40
1:C:2141:VAL:HG22	1:C:2238:PHE:CD2	2.56	0.40
1:A:2346:MET:O	1:A:2349:ASN:N	2.55	0.40
1:C:2405:MET:O	1:C:2409:ALA:HB3	2.21	0.40
1:A:2286:ARG:HD3	1:A:2331:SER:OG	2.20	0.40
1:C:794:LEU:HD12	1:C:830:TYR:HB3	2.04	0.40
1:C:2093:UNK:HB2	1:C:2129:UNK:HB2	2.03	0.40
1:B:1002:UNK:CG	1:B:1005:UNK:HB2	2.51	0.40
1:B:142:ARG:HA	1:B:142:ARG:HD3	1.91	0.40
1:A:2611:VAL:HA	1:A:2612:PRO:HD3	1.86	0.40
1:B:336:TRP:HE1	1:B:364:THR:HG22	1.86	0.40
1:B:544:ILE:C	1:B:546:HIS:H	2.22	0.40
1:B:1087:PHE:HZ	1:C:203:ASP:OD2	2.05	0.40
1:C:1535:PHE:O	1:C:1679:TRP:N	2.48	0.40
1:B:587:TRP:CZ2	1:B:694:ASP:OD2	2.74	0.40
1:C:1095:LEU:HD12	1:C:1096:THR:N	2.35	0.40
1:B:1353:PRO:HB2	1:B:1707:SER:HB2	2.04	0.40
1:C:1616:PRO:HG2	1:C:1619:VAL:HB	2.04	0.40
1:C:1619:VAL:HA	1:C:1620:PRO:HD2	1.80	0.40
1:A:745:THR:HG22	1:A:747:LEU:N	2.37	0.40
1:B:1380:ALA:HB1	1:B:1474:LEU:CD1	2.50	0.40
1:A:417:LEU:HD21	1:A:625:LEU:HD21	2.02	0.40
1:A:180:ALA:O	1:A:184:LEU:HG	2.21	0.40
1:A:2672:TRP:CZ3	1:A:2830:LYS:HG2	2.56	0.40
1:A:1706:LYS:HA	1:A:1735:GLU:HG3	2.03	0.40
1:A:2618:SER:HB3	1:A:2786:ASP:OD1	2.21	0.40
1:B:2907:HIS:HA	1:B:2910:ILE:HG12	2.04	0.40
1:A:2114:UNK:O	1:A:2117:UNK:HG3	2.22	0.40
1:B:985:UNK:O	1:B:988:UNK:HG3	2.21	0.40
1:A:1013:UNK:CG	1:A:1014:UNK:N	2.58	0.40
1:C:408:VAL:HG23	1:C:418:GLU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ARG:HD2	1:B:282:VAL:CG1	2.51	0.40
1:B:2557:LEU:HD23	1:B:2558:LEU:N	2.37	0.40
1:B:2611:VAL:HA	1:B:2612:PRO:HD3	1.86	0.40
1:A:544:ILE:C	1:A:546:HIS:H	2.22	0.40
1:A:374:GLY:C	1:A:375:ILE:HG13	2.41	0.40
1:B:585:HIS:HB3	1:B:694:ASP:HB2	2.03	0.40
1:A:2205:ASP:O	1:A:2209:LEU:HB2	2.21	0.40
1:B:2492:VAL:HG12	1:B:2526:ILE:HG22	2.02	0.40
1:B:541:GLU:HG3	1:B:542:VAL:N	2.37	0.40
1:A:2503:LYS:HG3	1:A:2513:TYR:HB2	2.02	0.40
1:A:358:ASP:OD2	1:A:361:THR:HB	2.21	0.40
1:C:2930:LEU:HD23	1:C:2930:LEU:HA	1.93	0.40
1:A:2405:MET:O	1:A:2409:ALA:HB3	2.21	0.40
1:A:2836:LEU:HD23	1:A:2836:LEU:HA	1.87	0.40
1:B:2346:MET:O	1:B:2349:ASN:N	2.55	0.40
1:A:1629:PHE:O	1:A:1633:ILE:HG13	2.22	0.40
1:B:1099:PRO:HB2	1:B:1295:TRP:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	2637/3089 (85%)	2489 (94%)	140 (5%)	8 (0%)	46	83
1	B	2637/3089 (85%)	2489 (94%)	140 (5%)	8 (0%)	46	83
1	C	2637/3089 (85%)	2489 (94%)	139 (5%)	9 (0%)	46	83
1	D	2637/3089 (85%)	2488 (94%)	140 (5%)	9 (0%)	46	83
1	E	2637/3089 (85%)	2488 (94%)	141 (5%)	8 (0%)	46	83
1	F	2637/3089 (85%)	2488 (94%)	140 (5%)	9 (0%)	46	83
All	All	15822/18534 (85%)	14931 (94%)	840 (5%)	51 (0%)	50	83

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1148	GLU
1	E	1148	GLU
1	F	1148	GLU
1	A	1148	GLU
1	B	1148	GLU
1	C	1148	GLU
1	D	1724	TYR
1	E	1724	TYR
1	F	1724	TYR
1	A	1724	TYR
1	B	1724	TYR
1	C	1724	TYR
1	D	149	ALA
1	D	1652	TRP
1	D	1705	VAL
1	E	149	ALA
1	E	1652	TRP
1	E	1705	VAL
1	F	149	ALA
1	F	1652	TRP
1	F	1705	VAL
1	A	149	ALA
1	A	1652	TRP
1	A	1705	VAL
1	B	149	ALA
1	B	1652	TRP
1	B	1705	VAL
1	C	149	ALA
1	C	1652	TRP
1	C	1705	VAL
1	D	89	GLU
1	E	89	GLU
1	F	89	GLU
1	A	89	GLU
1	B	89	GLU
1	C	89	GLU
1	D	1068	VAL
1	D	1285	LYS
1	E	1068	VAL
1	E	1285	LYS
1	F	1068	VAL
1	F	1285	LYS

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Mol	Chain	Res	Type
1	A	1068	VAL
1	A	1285	LYS
1	B	1068	VAL
1	B	1285	LYS
1	C	1068	VAL
1	C	1285	LYS
1	D	2585	PRO
1	F	2585	PRO
1	C	2585	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 PDB entries followed by that with respect to all EM entries.

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	2076/2264 (92%)	1987 (96%)	89 (4%)	35	70
1	B	2076/2264 (92%)	1986 (96%)	90 (4%)	35	70
1	C	2076/2264 (92%)	1987 (96%)	89 (4%)	35	70
1	D	2076/2264 (92%)	1987 (96%)	89 (4%)	35	70
1	E	2076/2264 (92%)	1987 (96%)	89 (4%)	35	70
1	F	2076/2264 (92%)	1987 (96%)	89 (4%)	35	70
All	All	12456/13584 (92%)	11921 (96%)	535 (4%)	40	70

All (535) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	90	LEU
1	D	208	VAL
1	D	209	SER
1	D	232	VAL
1	D	233	LEU
1	D	248	ILE
1	D	251	THR
1	D	342	GLU
1	D	344	HIS

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Mol	Chain	Res	Type
1	D	358	ASP
1	D	361	THR
1	D	389	THR
1	D	390	VAL
1	D	400	TRP
1	D	409	LYS
1	D	424	LEU
1	D	427	ARG
1	D	439	THR
1	D	456	GLU
1	D	517	ILE
1	D	544	ILE
1	D	580	ARG
1	D	584	HIS
1	D	595	LEU
1	D	606	ASN
1	D	621	SER
1	D	638	MET
1	D	644	LEU
1	D	654	GLU
1	D	694	ASP
1	D	696	HIS
1	D	699	ASP
1	D	791	GLU
1	D	857	VAL
1	D	1021	LEU
1	D	1096	THR
1	D	1105	ARG
1	D	1127	GLU
1	D	1162	THR
1	D	1253	ARG
1	D	1358	GLN
1	D	1421	GLN
1	D	1468	TYR
1	D	1471	GLU
1	D	1488	VAL
1	D	1508	ILE
1	D	1544	ILE
1	D	1551	LEU
1	D	1564	ILE
1	D	1618	LEU
1	D	1651	THR

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Mol	Chain	Res	Type
1	D	1662	ARG
1	D	1672	GLN
1	D	1673	PHE
1	D	1745	ASP
1	D	2059	ARG
1	D	2067	LEU
1	D	2070	LEU
1	D	2192	THR
1	D	2196	VAL
1	D	2209	LEU
1	D	2294	SER
1	D	2297	ARG
1	D	2299	MET
1	D	2303	ASP
1	D	2306	TYR
1	D	2395	THR
1	D	2401	ILE
1	D	2620	THR
1	D	2692	MET
1	D	2742	THR
1	D	2784	THR
1	D	2800	PHE
1	D	2802	ARG
1	D	2809	LEU
1	D	2827	LEU
1	D	2861	LEU
1	D	2871	THR
1	D	2879	LEU
1	D	2894	THR
1	D	2916	ARG
1	D	2930	LEU
1	D	2935	LYS
1	D	2962	ASP
1	D	3001	HIS
1	D	3019	ASP
1	D	3076	SER
1	D	3077	THR
1	D	3080	ARG
1	E	90	LEU
1	E	208	VAL
1	E	209	SER
1	E	232	VAL

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Mol	Chain	Res	Type
1	E	233	LEU
1	E	248	ILE
1	E	251	THR
1	E	342	GLU
1	E	344	HIS
1	E	358	ASP
1	E	361	THR
1	E	389	THR
1	E	390	VAL
1	E	400	TRP
1	E	409	LYS
1	E	424	LEU
1	E	427	ARG
1	E	439	THR
1	E	456	GLU
1	E	517	ILE
1	E	544	ILE
1	E	580	ARG
1	E	584	HIS
1	E	595	LEU
1	E	606	ASN
1	E	621	SER
1	E	638	MET
1	E	644	LEU
1	E	654	GLU
1	E	694	ASP
1	E	696	HIS
1	E	699	ASP
1	E	791	GLU
1	E	857	VAL
1	E	1021	LEU
1	E	1096	THR
1	E	1105	ARG
1	E	1127	GLU
1	E	1162	THR
1	E	1253	ARG
1	E	1358	GLN
1	E	1421	GLN
1	E	1468	TYR
1	E	1471	GLU
1	E	1488	VAL
1	E	1508	ILE

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Mol	Chain	Res	Type
1	E	1544	ILE
1	E	1551	LEU
1	E	1564	ILE
1	E	1618	LEU
1	E	1651	THR
1	E	1662	ARG
1	E	1672	GLN
1	E	1673	PHE
1	E	1745	ASP
1	E	2059	ARG
1	E	2067	LEU
1	E	2070	LEU
1	E	2192	THR
1	E	2196	VAL
1	E	2209	LEU
1	E	2294	SER
1	E	2297	ARG
1	E	2299	MET
1	E	2303	ASP
1	E	2306	TYR
1	E	2395	THR
1	E	2401	ILE
1	E	2620	THR
1	E	2692	MET
1	E	2742	THR
1	E	2784	THR
1	E	2800	PHE
1	E	2802	ARG
1	E	2809	LEU
1	E	2827	LEU
1	E	2861	LEU
1	E	2871	THR
1	E	2879	LEU
1	E	2894	THR
1	E	2916	ARG
1	E	2930	LEU
1	E	2935	LYS
1	E	2962	ASP
1	E	3001	HIS
1	E	3019	ASP
1	E	3076	SER
1	E	3077	THR

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Mol	Chain	Res	Type
1	E	3080	ARG
1	F	90	LEU
1	F	208	VAL
1	F	209	SER
1	F	232	VAL
1	F	233	LEU
1	F	248	ILE
1	F	251	THR
1	F	342	GLU
1	F	344	HIS
1	F	358	ASP
1	F	361	THR
1	F	389	THR
1	F	390	VAL
1	F	400	TRP
1	F	409	LYS
1	F	424	LEU
1	F	427	ARG
1	F	439	THR
1	F	456	GLU
1	F	517	ILE
1	F	544	ILE
1	F	580	ARG
1	F	584	HIS
1	F	595	LEU
1	F	606	ASN
1	F	621	SER
1	F	638	MET
1	F	644	LEU
1	F	654	GLU
1	F	694	ASP
1	F	696	HIS
1	F	699	ASP
1	F	791	GLU
1	F	857	VAL
1	F	1021	LEU
1	F	1096	THR
1	F	1105	ARG
1	F	1127	GLU
1	F	1162	THR
1	F	1253	ARG
1	F	1358	GLN

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Mol	Chain	Res	Type
1	F	1421	GLN
1	F	1468	TYR
1	F	1471	GLU
1	F	1488	VAL
1	F	1508	ILE
1	F	1544	ILE
1	F	1551	LEU
1	F	1564	ILE
1	F	1618	LEU
1	F	1651	THR
1	F	1662	ARG
1	F	1672	GLN
1	F	1673	PHE
1	F	1745	ASP
1	F	2059	ARG
1	F	2067	LEU
1	F	2070	LEU
1	F	2192	THR
1	F	2196	VAL
1	F	2209	LEU
1	F	2294	SER
1	F	2297	ARG
1	F	2299	MET
1	F	2303	ASP
1	F	2306	TYR
1	F	2395	THR
1	F	2401	ILE
1	F	2620	THR
1	F	2692	MET
1	F	2742	THR
1	F	2784	THR
1	F	2800	PHE
1	F	2802	ARG
1	F	2809	LEU
1	F	2827	LEU
1	F	2861	LEU
1	F	2871	THR
1	F	2879	LEU
1	F	2894	THR
1	F	2916	ARG
1	F	2930	LEU
1	F	2935	LYS

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Mol	Chain	Res	Type
1	F	2962	ASP
1	F	3001	HIS
1	F	3019	ASP
1	F	3076	SER
1	F	3077	THR
1	F	3080	ARG
1	A	90	LEU
1	A	208	VAL
1	A	209	SER
1	A	232	VAL
1	A	233	LEU
1	A	248	ILE
1	A	251	THR
1	A	342	GLU
1	A	344	HIS
1	A	358	ASP
1	A	361	THR
1	A	389	THR
1	A	390	VAL
1	A	400	TRP
1	A	409	LYS
1	A	424	LEU
1	A	427	ARG
1	A	439	THR
1	A	456	GLU
1	A	517	ILE
1	A	544	ILE
1	A	580	ARG
1	A	584	HIS
1	A	595	LEU
1	A	606	ASN
1	A	621	SER
1	A	638	MET
1	A	644	LEU
1	A	654	GLU
1	A	694	ASP
1	A	696	HIS
1	A	699	ASP
1	A	791	GLU
1	A	857	VAL
1	A	1021	LEU
1	A	1096	THR

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Mol	Chain	Res	Type
1	A	1105	ARG
1	A	1127	GLU
1	A	1162	THR
1	A	1253	ARG
1	A	1358	GLN
1	A	1421	GLN
1	A	1468	TYR
1	A	1471	GLU
1	A	1488	VAL
1	A	1508	ILE
1	A	1544	ILE
1	A	1551	LEU
1	A	1564	ILE
1	A	1618	LEU
1	A	1651	THR
1	A	1662	ARG
1	A	1672	GLN
1	A	1673	PHE
1	A	1745	ASP
1	A	2059	ARG
1	A	2067	LEU
1	A	2070	LEU
1	A	2192	THR
1	A	2196	VAL
1	A	2209	LEU
1	A	2294	SER
1	A	2297	ARG
1	A	2299	MET
1	A	2303	ASP
1	A	2306	TYR
1	A	2395	THR
1	A	2401	ILE
1	A	2620	THR
1	A	2692	MET
1	A	2742	THR
1	A	2784	THR
1	A	2800	PHE
1	A	2802	ARG
1	A	2809	LEU
1	A	2827	LEU
1	A	2861	LEU
1	A	2871	THR

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Mol	Chain	Res	Type
1	A	2879	LEU
1	A	2894	THR
1	A	2916	ARG
1	A	2930	LEU
1	A	2935	LYS
1	A	2962	ASP
1	A	3001	HIS
1	A	3019	ASP
1	A	3076	SER
1	A	3077	THR
1	A	3080	ARG
1	B	90	LEU
1	B	208	VAL
1	B	209	SER
1	B	232	VAL
1	B	233	LEU
1	B	248	ILE
1	B	251	THR
1	B	342	GLU
1	B	344	HIS
1	B	358	ASP
1	B	361	THR
1	B	389	THR
1	B	390	VAL
1	B	400	TRP
1	B	409	LYS
1	B	424	LEU
1	B	427	ARG
1	B	439	THR
1	B	456	GLU
1	B	517	ILE
1	B	544	ILE
1	B	580	ARG
1	B	584	HIS
1	B	595	LEU
1	B	606	ASN
1	B	621	SER
1	B	638	MET
1	B	644	LEU
1	B	654	GLU
1	B	694	ASP
1	B	696	HIS

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Mol	Chain	Res	Type
1	B	699	ASP
1	B	791	GLU
1	B	857	VAL
1	B	1021	LEU
1	B	1096	THR
1	B	1105	ARG
1	B	1127	GLU
1	B	1162	THR
1	B	1253	ARG
1	B	1358	GLN
1	B	1401	THR
1	B	1421	GLN
1	B	1468	TYR
1	B	1471	GLU
1	B	1488	VAL
1	B	1508	ILE
1	B	1544	ILE
1	B	1551	LEU
1	B	1564	ILE
1	B	1618	LEU
1	B	1651	THR
1	B	1662	ARG
1	B	1672	GLN
1	B	1673	PHE
1	B	1745	ASP
1	B	2059	ARG
1	B	2067	LEU
1	B	2070	LEU
1	B	2192	THR
1	B	2196	VAL
1	B	2209	LEU
1	B	2294	SER
1	B	2297	ARG
1	B	2299	MET
1	B	2303	ASP
1	B	2306	TYR
1	B	2395	THR
1	B	2401	ILE
1	B	2620	THR
1	B	2692	MET
1	B	2742	THR
1	B	2784	THR

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Mol	Chain	Res	Type
1	B	2800	PHE
1	B	2802	ARG
1	B	2809	LEU
1	B	2827	LEU
1	B	2861	LEU
1	B	2871	THR
1	B	2879	LEU
1	B	2894	THR
1	B	2916	ARG
1	B	2930	LEU
1	B	2935	LYS
1	B	2962	ASP
1	B	3001	HIS
1	B	3019	ASP
1	B	3076	SER
1	B	3077	THR
1	B	3080	ARG
1	C	90	LEU
1	C	208	VAL
1	C	209	SER
1	C	232	VAL
1	C	233	LEU
1	C	248	ILE
1	C	251	THR
1	C	342	GLU
1	C	344	HIS
1	C	358	ASP
1	C	361	THR
1	C	389	THR
1	C	390	VAL
1	C	400	TRP
1	C	409	LYS
1	C	424	LEU
1	C	427	ARG
1	C	439	THR
1	C	456	GLU
1	C	517	ILE
1	C	544	ILE
1	C	580	ARG
1	C	584	HIS
1	C	595	LEU
1	C	606	ASN

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Mol	Chain	Res	Type
1	C	621	SER
1	C	638	MET
1	C	644	LEU
1	C	654	GLU
1	C	694	ASP
1	C	696	HIS
1	C	699	ASP
1	C	791	GLU
1	C	857	VAL
1	C	1021	LEU
1	C	1096	THR
1	C	1105	ARG
1	C	1127	GLU
1	C	1162	THR
1	C	1253	ARG
1	C	1358	GLN
1	C	1421	GLN
1	C	1468	TYR
1	C	1471	GLU
1	C	1488	VAL
1	C	1508	ILE
1	C	1544	ILE
1	C	1551	LEU
1	C	1564	ILE
1	C	1618	LEU
1	C	1651	THR
1	C	1662	ARG
1	C	1672	GLN
1	C	1673	PHE
1	C	1745	ASP
1	C	2059	ARG
1	C	2067	LEU
1	C	2070	LEU
1	C	2192	THR
1	C	2196	VAL
1	C	2209	LEU
1	C	2294	SER
1	C	2297	ARG
1	C	2299	MET
1	C	2303	ASP
1	C	2306	TYR
1	C	2395	THR

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Mol	Chain	Res	Type
1	C	2401	ILE
1	C	2620	THR
1	C	2692	MET
1	C	2742	THR
1	C	2784	THR
1	C	2800	PHE
1	C	2802	ARG
1	C	2809	LEU
1	C	2827	LEU
1	C	2861	LEU
1	C	2871	THR
1	C	2879	LEU
1	C	2894	THR
1	C	2916	ARG
1	C	2930	LEU
1	C	2935	LYS
1	C	2962	ASP
1	C	3001	HIS
1	C	3019	ASP
1	C	3076	SER
1	C	3077	THR
1	C	3080	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	ASN
1	A	486	GLN
1	A	540	ASN
1	A	585	HIS
1	A	606	ASN
1	A	1057	ASN
1	A	1134	HIS
1	A	1276	GLN
1	A	1277	HIS
1	A	1355	GLN
1	A	1582	HIS
1	A	1617	ASN
1	A	1672	GLN
1	A	2288	HIS
1	A	2334	HIS
1	A	2349	ASN

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Mol	Chain	Res	Type
1	A	2651	ASN
1	A	2699	ASN
1	A	2815	GLN
1	A	2850	HIS
1	A	2927	GLN
1	A	2942	GLN
1	A	2973	HIS
1	B	386	ASN
1	B	486	GLN
1	B	540	ASN
1	B	575	HIS
1	B	585	HIS
1	B	1057	ASN
1	B	1134	HIS
1	B	1276	GLN
1	B	1277	HIS
1	B	1355	GLN
1	B	1582	HIS
1	B	1617	ASN
1	B	1672	GLN
1	B	2288	HIS
1	B	2296	ASN
1	B	2334	HIS
1	B	2349	ASN
1	B	2651	ASN
1	B	2699	ASN
1	B	2815	GLN
1	B	2850	HIS
1	B	2927	GLN
1	B	2942	GLN
1	B	2973	HIS
1	C	386	ASN
1	C	486	GLN
1	C	540	ASN
1	C	575	HIS
1	C	585	HIS
1	C	1057	ASN
1	C	1134	HIS
1	C	1276	GLN
1	C	1277	HIS
1	C	1355	GLN
1	C	1582	HIS

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Mol	Chain	Res	Type
1	C	1617	ASN
1	C	1672	GLN
1	C	2288	HIS
1	C	2296	ASN
1	C	2334	HIS
1	C	2349	ASN
1	C	2651	ASN
1	C	2699	ASN
1	C	2815	GLN
1	C	2850	HIS
1	C	2927	GLN
1	C	2942	GLN
1	C	2973	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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	$\# Z > 2$
2	FMN	A	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.72	7 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	B	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.71	7 (20%)
2	FMN	C	4000	-	32,33,33	1.22	3 (9%)	34,50,50	1.70	7 (20%)
2	FMN	D	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.72	7 (20%)
2	FMN	E	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.71	7 (20%)
2	FMN	F	4000	-	32,33,33	1.21	3 (9%)	34,50,50	1.70	7 (20%)

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
2	FMN	A	4000	-	-	0/18/18/18	0/3/3/3
2	FMN	B	4000	-	-	0/18/18/18	0/3/3/3
2	FMN	C	4000	-	-	0/18/18/18	0/3/3/3
2	FMN	D	4000	-	-	0/18/18/18	0/3/3/3
2	FMN	E	4000	-	-	0/18/18/18	0/3/3/3
2	FMN	F	4000	-	-	0/18/18/18	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4000	FMN	C5A-N5	2.23	1.38	1.35
2	A	4000	FMN	C5A-N5	2.24	1.38	1.35
2	B	4000	FMN	C5A-N5	2.25	1.38	1.35
2	D	4000	FMN	C5A-N5	2.30	1.38	1.35
2	C	4000	FMN	C5A-N5	2.31	1.38	1.35
2	F	4000	FMN	C5A-N5	2.31	1.38	1.35
2	B	4000	FMN	C4-N3	3.14	1.38	1.33
2	A	4000	FMN	C4-N3	3.16	1.38	1.33
2	F	4000	FMN	C4-N3	3.16	1.38	1.33
2	D	4000	FMN	C4-N3	3.16	1.38	1.33
2	E	4000	FMN	C4-N3	3.16	1.38	1.33
2	C	4000	FMN	C4-N3	3.22	1.38	1.33
2	A	4000	FMN	C4A-N5	3.47	1.38	1.33
2	D	4000	FMN	C4A-N5	3.47	1.38	1.33
2	C	4000	FMN	C4A-N5	3.48	1.38	1.33
2	F	4000	FMN	C4A-N5	3.48	1.38	1.33
2	E	4000	FMN	C4A-N5	3.52	1.38	1.33
2	B	4000	FMN	C4A-N5	3.55	1.38	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	FMN	N3-C2-N1	-4.47	120.16	127.69
2	B	4000	FMN	N3-C2-N1	-4.46	120.19	127.69
2	D	4000	FMN	N3-C2-N1	-4.45	120.19	127.69
2	E	4000	FMN	N3-C2-N1	-4.45	120.20	127.69
2	C	4000	FMN	N3-C2-N1	-4.44	120.22	127.69
2	F	4000	FMN	N3-C2-N1	-4.44	120.22	127.69
2	A	4000	FMN	C4A-C4-N3	-2.85	119.80	123.52
2	D	4000	FMN	C4A-C4-N3	-2.85	119.80	123.52
2	F	4000	FMN	C4A-C4-N3	-2.84	119.81	123.52
2	C	4000	FMN	C4A-C4-N3	-2.84	119.81	123.52
2	E	4000	FMN	C4A-C4-N3	-2.84	119.82	123.52
2	B	4000	FMN	C4A-C4-N3	-2.82	119.84	123.52
2	F	4000	FMN	C1'-N10-C9A	2.03	121.18	118.83
2	B	4000	FMN	C1'-N10-C9A	2.06	121.22	118.83
2	E	4000	FMN	C1'-N10-C9A	2.06	121.22	118.83
2	D	4000	FMN	C1'-N10-C9A	2.06	121.22	118.83
2	C	4000	FMN	C1'-N10-C9A	2.07	121.23	118.83
2	A	4000	FMN	C1'-N10-C9A	2.08	121.24	118.83
2	C	4000	FMN	C4-C4A-N5	2.21	121.39	118.70
2	F	4000	FMN	C4-C4A-N5	2.22	121.39	118.70
2	A	4000	FMN	C4-C4A-N5	2.26	121.45	118.70
2	D	4000	FMN	C4-C4A-N5	2.26	121.45	118.70
2	B	4000	FMN	C4-C4A-N5	2.26	121.45	118.70
2	E	4000	FMN	C4-C4A-N5	2.28	121.47	118.70
2	C	4000	FMN	C4A-N5-C5A	2.70	119.90	116.72
2	F	4000	FMN	C4A-N5-C5A	2.70	119.90	116.72
2	B	4000	FMN	C4A-N5-C5A	2.70	119.90	116.72
2	D	4000	FMN	C4A-N5-C5A	2.72	119.93	116.72
2	A	4000	FMN	C4A-N5-C5A	2.73	119.94	116.72
2	E	4000	FMN	C4A-N5-C5A	2.74	119.95	116.72
2	E	4000	FMN	C5A-C9A-N10	2.88	119.74	117.58
2	F	4000	FMN	C5A-C9A-N10	2.94	119.78	117.58
2	A	4000	FMN	C5A-C9A-N10	2.95	119.79	117.58
2	D	4000	FMN	C5A-C9A-N10	2.96	119.80	117.58
2	C	4000	FMN	C5A-C9A-N10	2.96	119.80	117.58
2	B	4000	FMN	C5A-C9A-N10	2.98	119.81	117.58
2	C	4000	FMN	C4-N3-C2	5.91	120.08	115.16
2	F	4000	FMN	C4-N3-C2	5.92	120.09	115.16
2	E	4000	FMN	C4-N3-C2	5.94	120.11	115.16
2	B	4000	FMN	C4-N3-C2	5.96	120.13	115.16
2	A	4000	FMN	C4-N3-C2	5.99	120.15	115.16
2	D	4000	FMN	C4-N3-C2	5.99	120.15	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4000	FMN	5	0
2	B	4000	FMN	5	0
2	C	4000	FMN	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.