



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:55 AM UTC

PDB ID : 4ZIW / pdb_00004ziw
Title : Crystal structure of AcrB deletion mutant in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-28
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

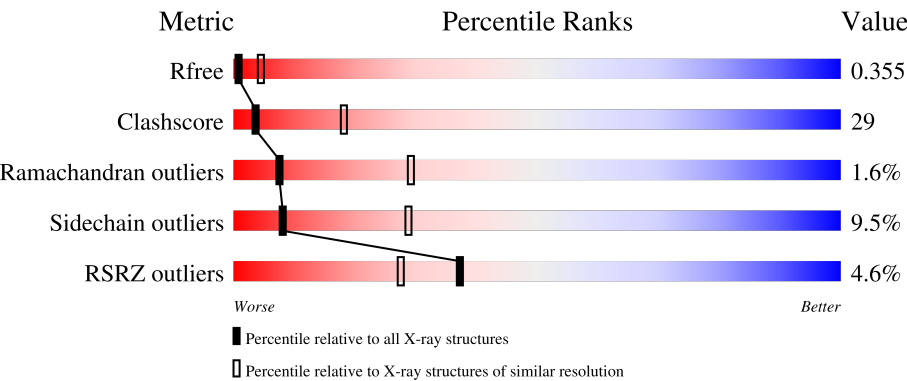
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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

Mol	Chain	Length	Quality of chain
1	A	1044	5% 43% 48% 8% .
1	B	1044	3% 47% 46% 6% .
1	C	1044	3% 42% 48% 9% ..
1	D	1044	4% 39% 51% 8% ..
1	E	1044	6% 45% 45% 9% ..

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Mol	Chain	Length	Quality of chain
1	F	1044	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	D	2000	X	-	-	-
2	LMT	E	1101	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47532 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	B	1039	Total	C	N	O	S	0	0	0
			7900	5076	1307	1474	43			
1	C	1035	Total	C	N	O	S	0	0	0
			7867	5057	1299	1468	43			
1	D	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	E	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			
1	F	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			

There are 36 discrepancies between the modelled and reference sequences:

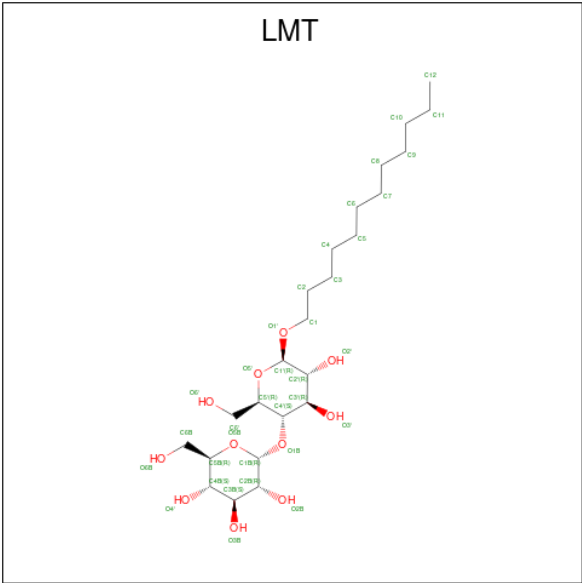
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	GLY	PHE	engineered mutation	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	PHE	deletion	UNP P31224
A	?	-	ALA	deletion	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	ARG	deletion	UNP P31224
B	615	GLY	PHE	engineered mutation	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	PHE	deletion	UNP P31224
B	?	-	ALA	deletion	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	ARG	deletion	UNP P31224
C	615	GLY	PHE	engineered mutation	UNP P31224
C	?	-	GLY	deletion	UNP P31224
C	?	-	PHE	deletion	UNP P31224
C	?	-	ALA	deletion	UNP P31224
C	?	-	GLY	deletion	UNP P31224

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P31224
D	615	GLY	PHE	engineered mutation	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	PHE	deletion	UNP P31224
D	?	-	ALA	deletion	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	ARG	deletion	UNP P31224
E	615	GLY	PHE	engineered mutation	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	PHE	deletion	UNP P31224
E	?	-	ALA	deletion	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	ARG	deletion	UNP P31224
F	615	GLY	PHE	engineered mutation	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	PHE	deletion	UNP P31224
F	?	-	ALA	deletion	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	ARG	deletion	UNP P31224

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		

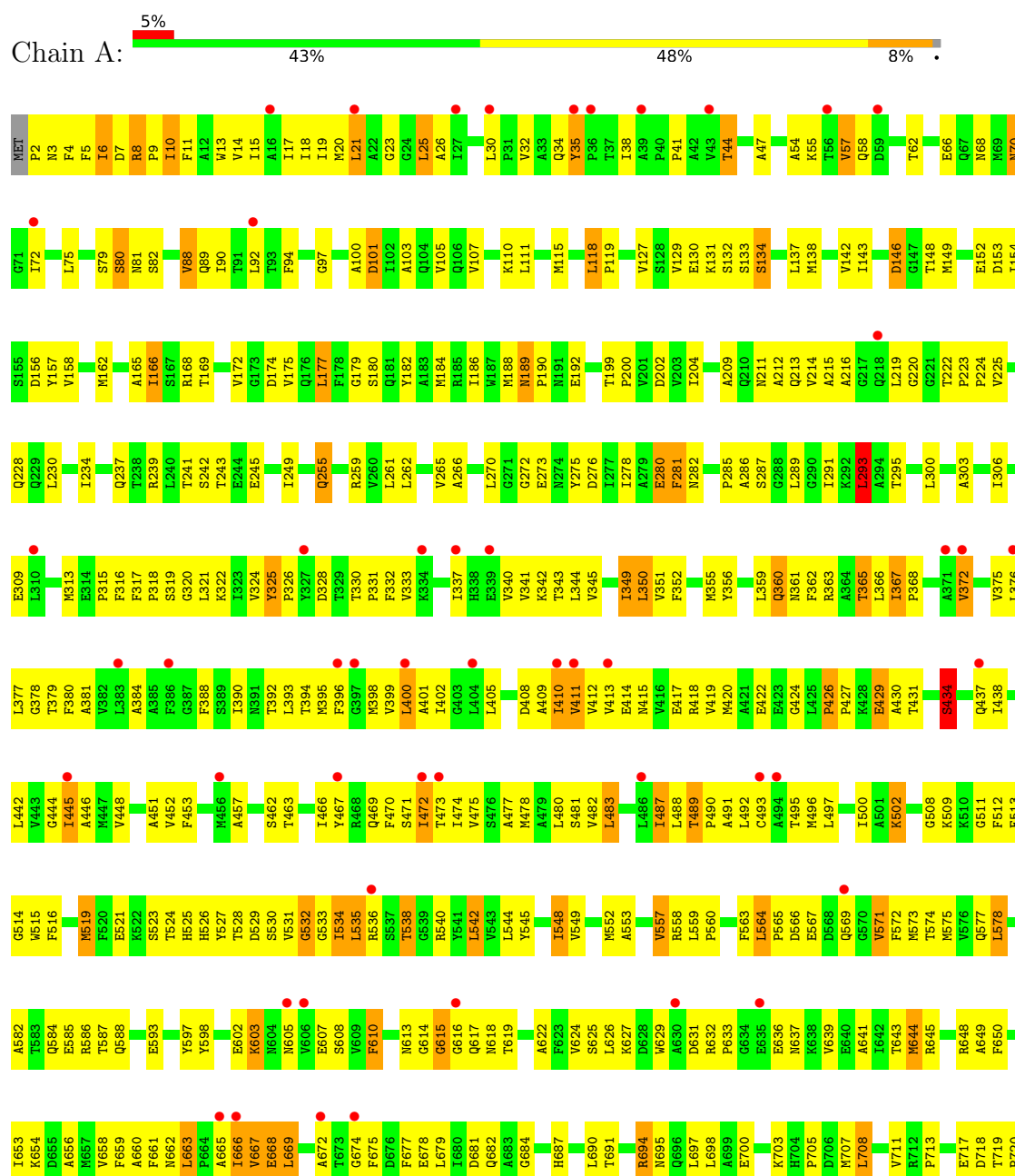
- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

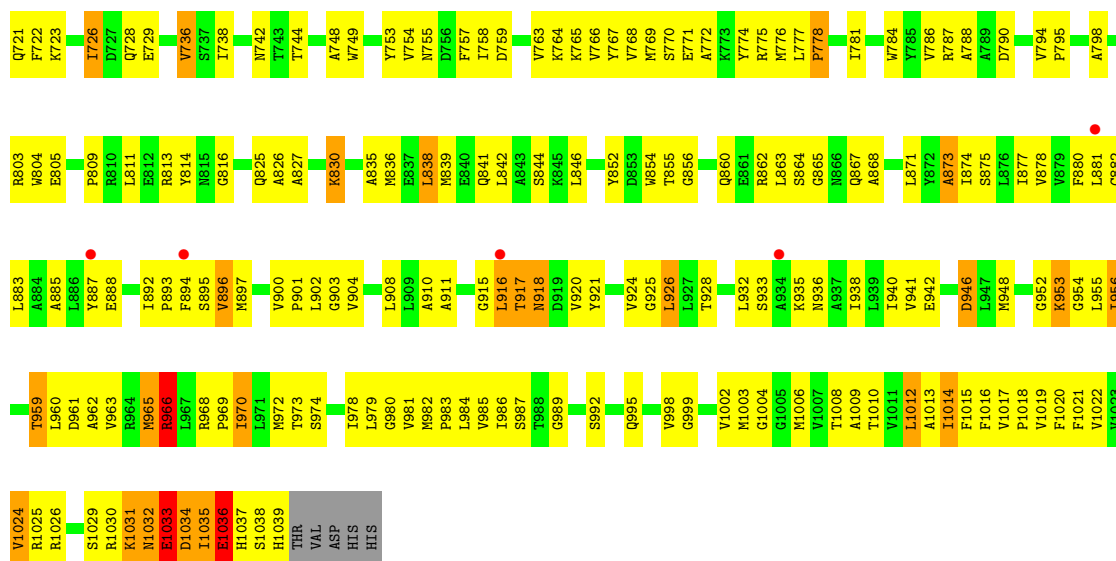
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		
3	E	1	Total	Ni	0	0
			1	1		

3 Residue-property plots

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

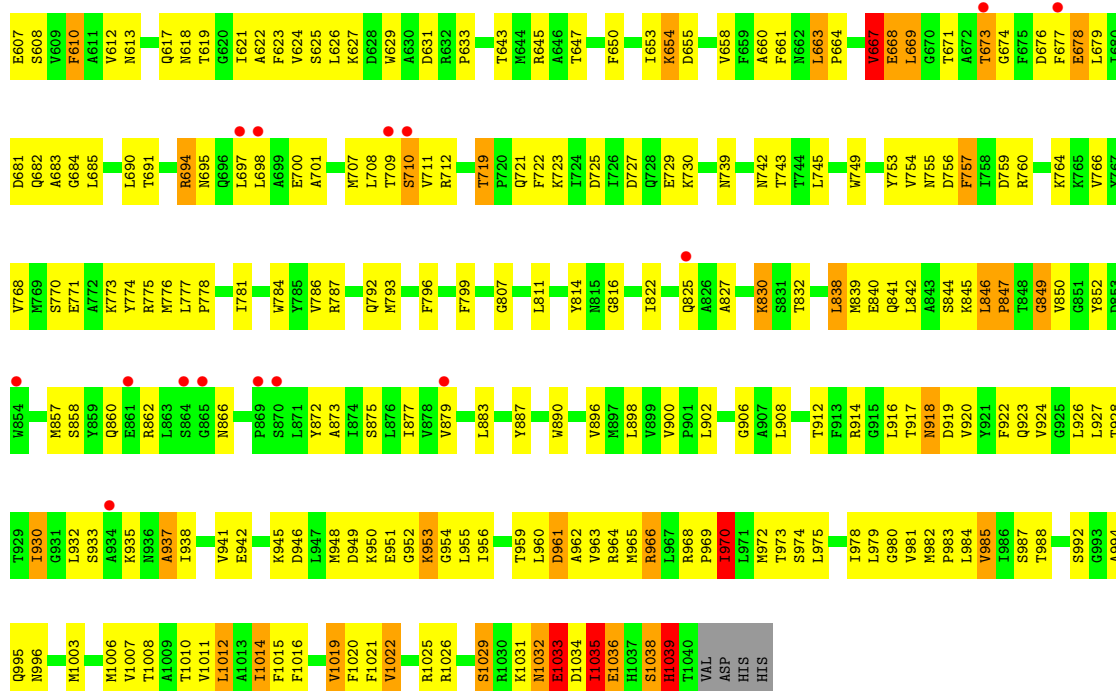
• Molecule 1: Multidrug efflux pump subunit AcrB



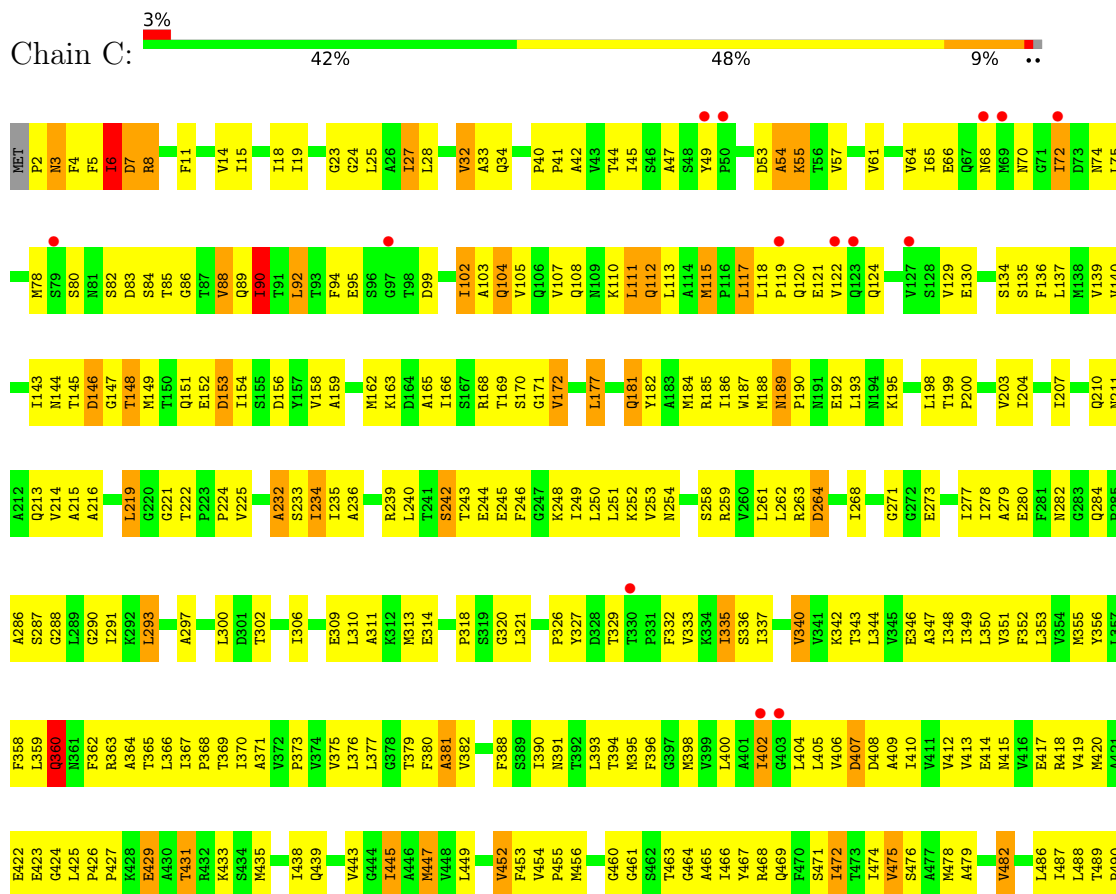


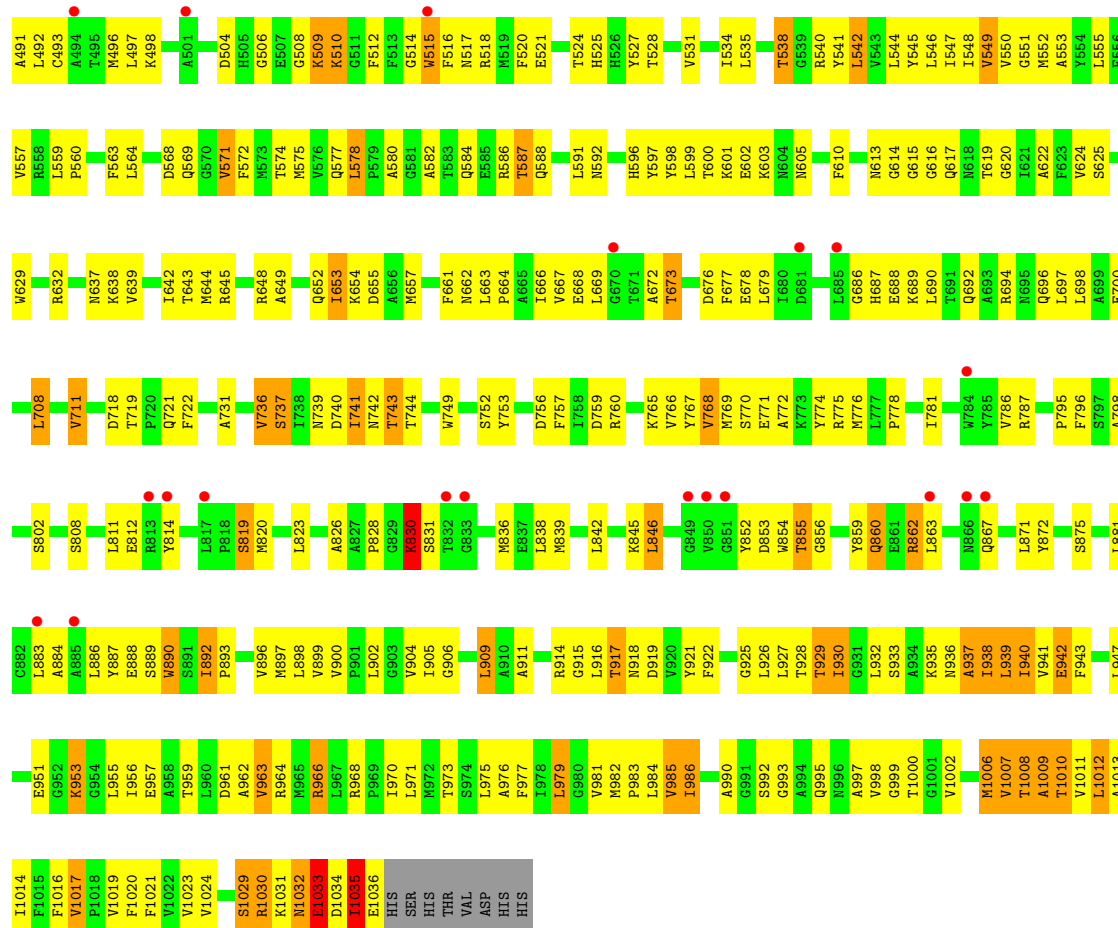
• Molecule 1: Multidrug efflux pump subunit AcrB



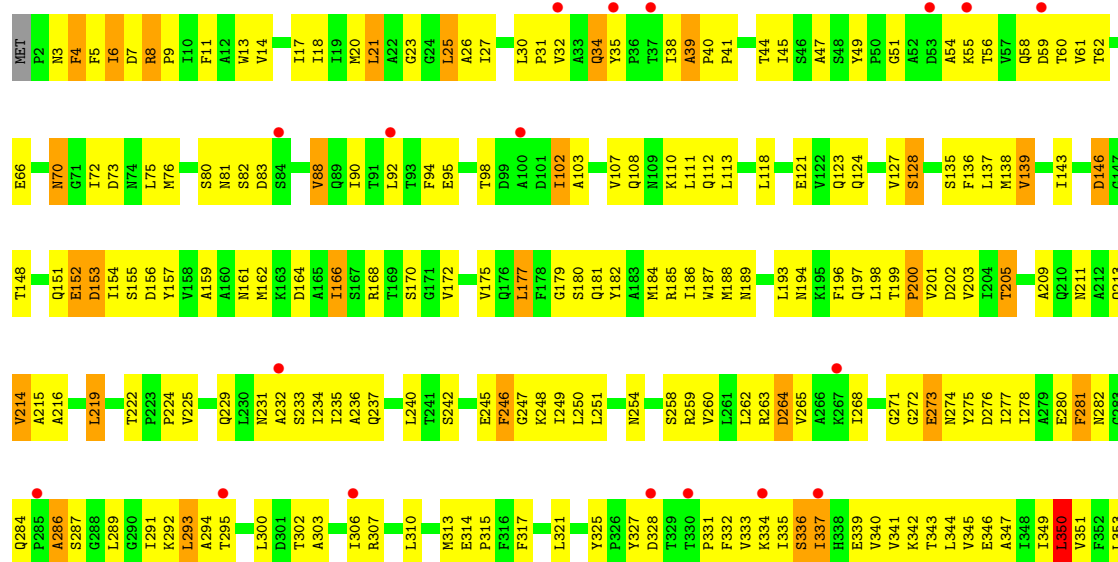


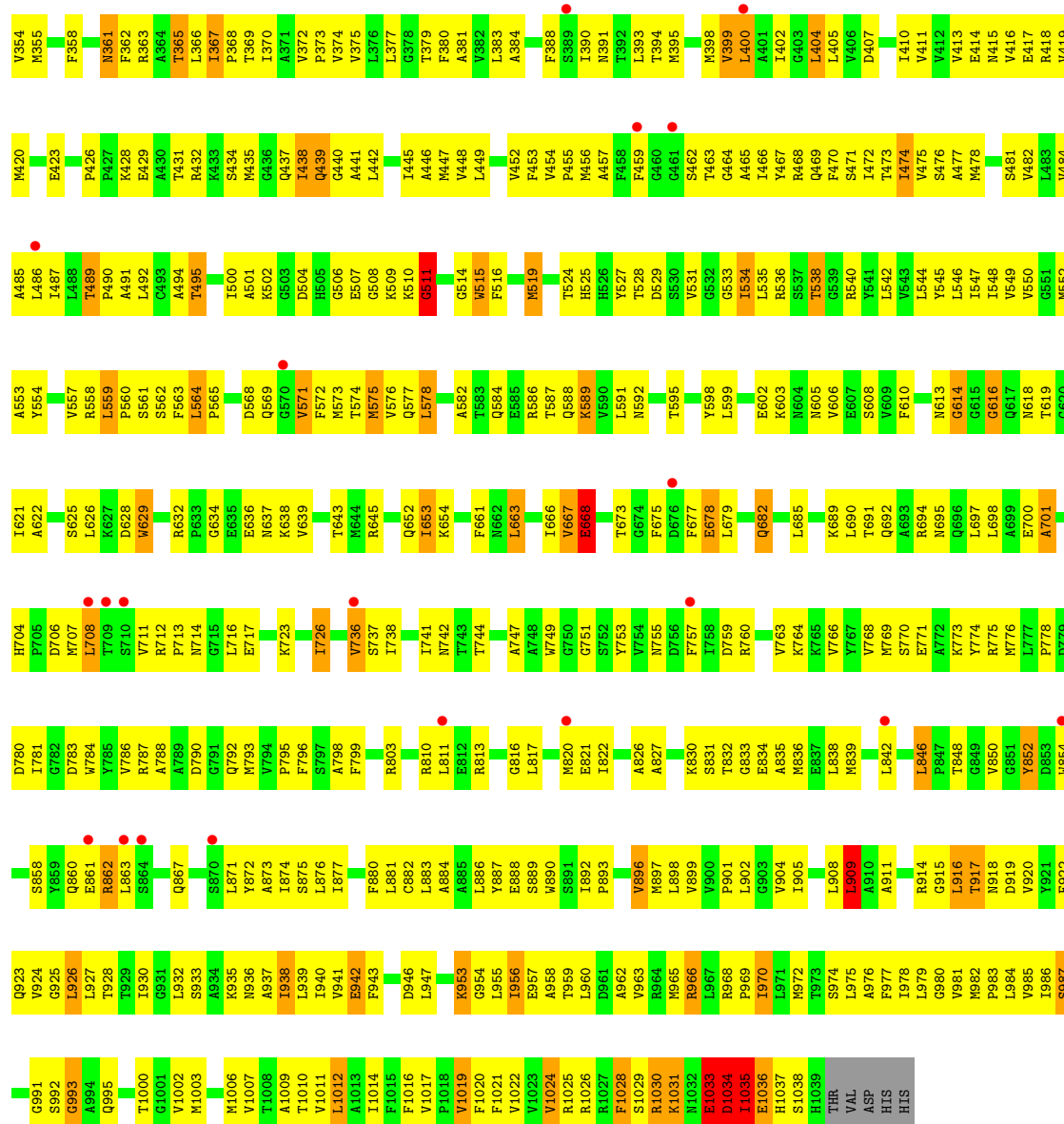
• Molecule 1: Multidrug efflux pump subunit AcrB



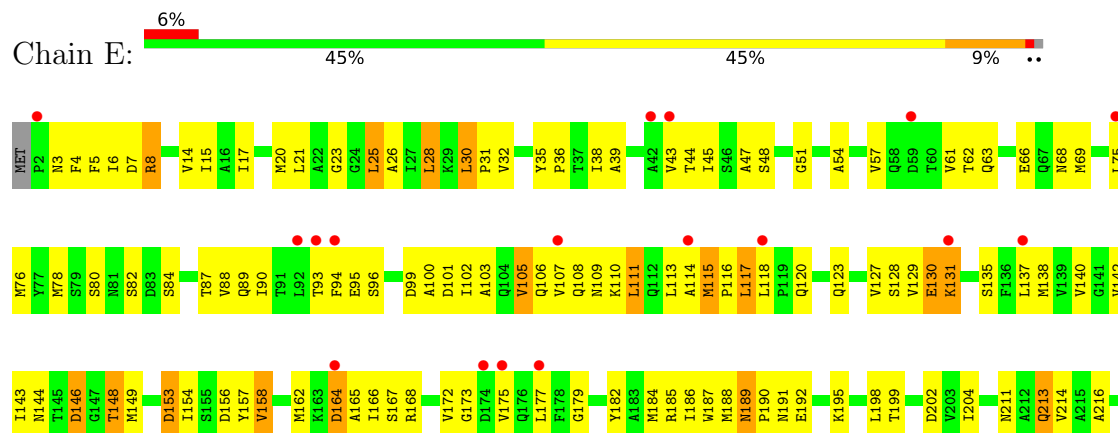


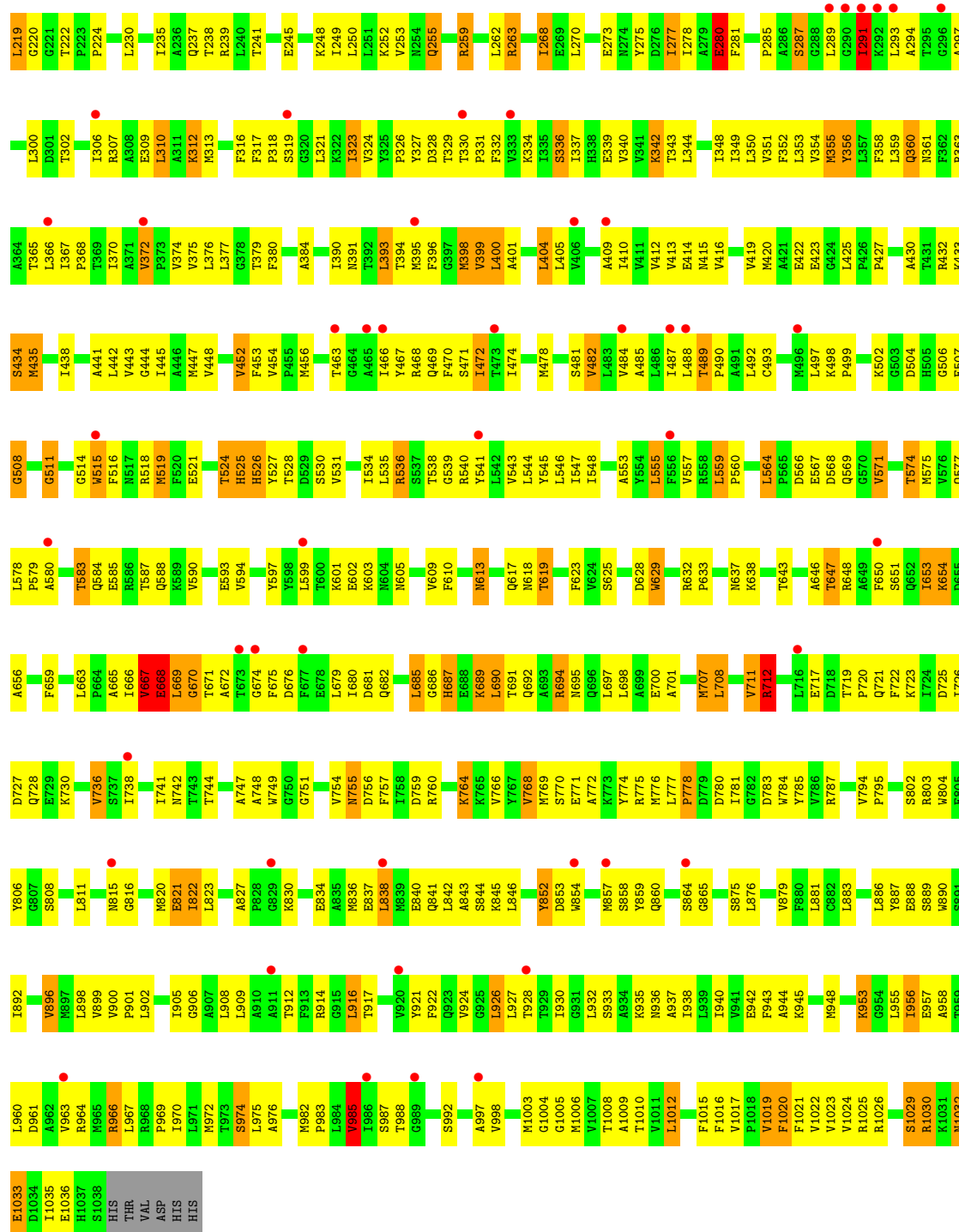
• Molecule 1: Multidrug efflux pump subunit AcrB





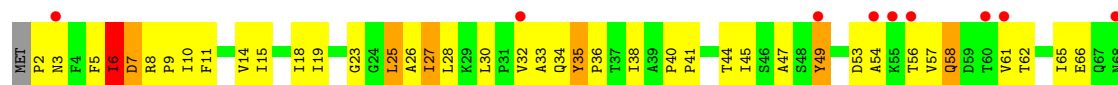
• Molecule 1: Multidrug efflux pump subunit AcrB





• Molecule 1: Multidrug efflux pump subunit AcrB

Chain F: 6% 42% 48% 9%



V1007	A834	R862	G791	A641	F563	A486	R432	R363	G218	S133	M69
T1008	K935	L863	Q792	I642	L564	L497	K453	A364	L219	S134	N70
A1009	N936	A868	T709	T643	D566	I500	M435	T365	T222	S135	G71
T1010	A937	A868	V794	M644	D566	A501	M435	L366	T222		T72
V1011	L938	L871	F795	R645	V571	K502	Q439	I367	P223	M138	D73
L1012	L939	Y872	F796	A646	V571	G503	G440	P368	P224	V139	N74
A1013	I940		T797	T647	V571	G504	A441	A371	V225	V140	L75
V1014	V941		N714	R648	T574	D504	L442		Q228		M76
F1015	K945	S875	G715	F650	M575	H505	V443	V375	Q229	T143	T77
F1016	D946	L876	D718		V576	G506	V444	L376	L230	T144	M78
P1018	L947	V878	T719	I653	V577	E507	G444	V376	L230	T145	
V1019	M948	E805	P720	I653	L578	G508	I445	T379	N231	D146	N81
F1020	F880	S808	Q721	D655	A582	K509	A446	F380	T234	G147	S82
F1021	L881	P809	F722	D655	T583	K510	M447	T379		T148	S83
G954	C882	R810	K723	M657	Q584	G511	V448	V382	Q237	M149	S84
L955	L883	L811	I724	V658	E585	F513	A451	T382	T238	T150	T85
V1023	A894	E812	D725	F659	E586	G514	V452	A384	E314	Q151	G86
V1024		R813	T587		T587	V515	P453		R239	E152	T87
			Q588		Q588	F516	V454	I380	L240	D153	V88
F1028	T959	Y887	D727	M662		F516	P454	I380	T243	T154	Q89
S1029	L960	E888	Q728	L663		N517	P455	N391			190
R1030	D961	G816	I738	P664	N592	R518	M456	T392	F246	V158	T91
A1031	A962	W890	I738	A665		M519		G320	T246		L92
N1032	V963	S891	I741	I666	T595	F520	F459	T394	G247	D164	T93
E1033	R964	S819	N742	V667		F521	G460	M395	K248	A165	F94
D1034	P893	M820	I742	E668	Y598	K522	G461		T249		E95
E1035	F894	E821	L745	L669	L599	S523	S462	M398	L250	S96	S96
R966	S895	L822	T745	G670	T600	T524	T463	V399	L251	R168	G97
R968	W896	L823	W749	A672	E601	H525	G464	L400	K252	T169	
P969	P869	L823	W749	A672	E601	H525	G464	L400	K252	G170	
S1038	N897			T673	K603	Y527	S471	I402		G171	
HIS	V900	A827	N755	G674	N604	V531	I473	G403	R259	S180	D101
THR	P901	K830	D756	F675	N605	N605	R468	L404	V260		I102
VAL	L902	S831	F757	D676	V606		Q469	L405	L261		A103
ASP	G903	T832	I758	F677			F470	S336	L262		V105
HIS	V904	G833	D759	E678	F610	L535	S471	D407	R263		Q106
HIS	I905	E334		T679	A611	R536	I473	I186			V107
		A835	R762	T680	V612	S537	T473	H338	A266		Q108
	L909	M836		D681	N613	T538	I474	A409	V267		M109
	A910	E937	V766	Q682	G614	G539	V475	I410	I268		K110
	A911	L838	Y767	A683	G615	R540	S476	V411	E289		L111
	M839	M839	V768	G684	G616	Y541	A477	V412	L270		Q112
	L842		M769	L485	G617	L542	M478	V413	G271		L113
	G915		S770	G686	N618	V543	A479	L344	G272		A114
	L916		E771	H687	T619	L544	L480	V345	E273		M115
	T917	K845	A772	E688	G620	Y545	V482	E346	N274		F116
	N918	L846	K773	K689	I621	L546	V482	A417	Y275		L117
	D919		Y774		A622	I547	V483	I349			L118
	V920	W850	R775	Q692	A622	T548	V484	M420	I278		P119
		G851	M776	A693	S626	Y549	V485	A421	A279		Q120
		Y852	L777	R694	N629	V550	L486	E422	E280		E121
	D853	Y854	P778	N695	W629	A553	L487	E423	F281		V122
	L927	T855	I781	L697	A630	A553	L488	G424	Q284		Q123
	T928	G856		L697	D631	V557	T489	L425			Q124
	T929	M857	E700		R632	R558	A491	P426	S287		V127
	I930	S858	Y785		P633	L559	L492	P427	Q288		S128
	G931	Y859	Y786		K638	P560	L492	K428	L289		V129
	L932	Q860	R787		V639	S561	G493	A429			E130
	S933	E861	D706		E640	S562	T495	A430	L293		K131
								T431	A294		S132

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	152.07Å 157.78Å 219.39Å 90.00° 93.14° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.40) 97.4 (20.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.275 , 0.349 0.288 , 0.355	Depositor DCC
R_{free} test set	7110 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	98.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	47532	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8623e-05.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.87	3/8043 (0.0%)	1.32	68/10922 (0.6%)
1	B	0.88	4/8050 (0.0%)	1.29	56/10932 (0.5%)
1	C	0.91	5/8015 (0.1%)	1.31	71/10884 (0.7%)
1	D	0.83	2/8043 (0.0%)	1.30	77/10922 (0.7%)
1	E	0.81	2/8032 (0.0%)	1.29	72/10907 (0.7%)
1	F	0.82	2/8032 (0.0%)	1.34	77/10907 (0.7%)
All	All	0.85	18/48215 (0.0%)	1.31	421/65474 (0.6%)

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	3
1	B	0	2
1	C	0	1
1	D	0	1
1	F	0	1
All	All	0	8

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	564	LEU	CA-C	-6.25	1.47	1.52
1	F	426	PRO	CA-C	5.90	1.55	1.51
1	A	513	PHE	CA-C	5.80	1.56	1.52
1	C	6	ILE	CA-C	5.76	1.60	1.52
1	B	534	ILE	CA-CB	5.75	1.61	1.54
1	D	399	VAL	CA-CB	-5.59	1.48	1.54
1	A	445	ILE	CA-CB	5.58	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	549	VAL	CA-CB	-5.47	1.48	1.54
1	E	926	LEU	CA-C	-5.45	1.45	1.52
1	D	1019	VAL	CA-CB	5.40	1.60	1.54
1	C	1007	VAL	CA-CB	-5.40	1.48	1.54
1	A	372	VAL	CA-C	5.37	1.58	1.52
1	B	887	TYR	CA-C	-5.36	1.45	1.53
1	C	929	THR	CA-CB	-5.31	1.45	1.53
1	E	1017	VAL	CA-CB	5.16	1.60	1.54
1	B	528	THR	CA-CB	5.13	1.61	1.53
1	B	1014	ILE	CA-CB	-5.12	1.47	1.54
1	C	937	ALA	CA-CB	-5.06	1.45	1.53

All (421) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	559	LEU	CA-C-N	12.63	132.78	119.78
1	B	559	LEU	C-N-CA	12.63	132.78	119.78
1	F	7	ASP	CA-C-N	12.36	133.86	122.37
1	F	7	ASP	C-N-CA	12.36	133.86	122.37
1	A	674	GLY	N-CA-C	12.30	126.13	110.38
1	F	35	TYR	CA-C-N	10.59	130.38	120.21
1	F	35	TYR	C-N-CA	10.59	130.38	120.21
1	F	559	LEU	CA-C-N	9.87	132.18	119.84
1	F	559	LEU	C-N-CA	9.87	132.18	119.84
1	E	189	ASN	CA-C-N	9.71	129.06	118.97
1	E	189	ASN	C-N-CA	9.71	129.06	118.97
1	C	7	ASP	N-CA-C	-9.29	98.95	110.65
1	B	887	TYR	N-CA-C	-9.02	98.37	110.55
1	D	374	VAL	N-CA-C	8.97	118.85	110.42
1	C	938	ILE	N-CA-C	8.77	118.84	110.42
1	A	1038	SER	N-CA-C	-8.73	100.43	112.30
1	F	7	ASP	N-CA-C	-8.73	99.65	110.65
1	F	40	PRO	CA-C-N	8.70	129.04	119.90
1	F	40	PRO	C-N-CA	8.70	129.04	119.90
1	F	663	LEU	CA-C-N	8.47	128.41	120.03
1	F	663	LEU	C-N-CA	8.47	128.41	120.03
1	A	345	VAL	N-CA-C	8.45	118.53	110.42
1	B	3	ASN	N-CA-C	-8.30	101.29	111.33
1	A	189	ASN	CA-C-N	8.29	127.60	118.97
1	A	189	ASN	C-N-CA	8.29	127.60	118.97
1	A	668	GLU	N-CA-C	8.23	122.49	111.30
1	C	7	ASP	CA-C-N	8.21	130.00	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	ASP	C-N-CA	8.21	130.00	122.37
1	E	515	TRP	N-CA-C	-8.16	103.08	112.87
1	B	849	GLY	N-CA-C	-8.05	104.08	115.43
1	E	559	LEU	CA-C-N	8.01	129.86	119.84
1	E	559	LEU	C-N-CA	8.01	129.86	119.84
1	E	434	SER	N-CA-C	7.98	119.76	111.14
1	C	1017	VAL	CA-C-N	-7.94	112.04	119.82
1	C	1017	VAL	C-N-CA	-7.94	112.04	119.82
1	D	232	ALA	N-CA-C	7.93	120.77	108.96
1	D	1017	VAL	CA-C-N	-7.91	111.57	119.56
1	D	1017	VAL	C-N-CA	-7.91	111.57	119.56
1	E	1032	ASN	CA-C-N	7.83	135.79	121.70
1	E	1032	ASN	C-N-CA	7.83	135.79	121.70
1	A	426	PRO	O-C-N	7.81	124.82	121.15
1	A	35	TYR	CA-C-N	-7.75	112.35	120.03
1	A	35	TYR	C-N-CA	-7.75	112.35	120.03
1	A	867	GLN	N-CA-C	-7.75	103.96	113.41
1	A	325	TYR	CA-C-N	7.71	129.48	119.84
1	A	325	TYR	C-N-CA	7.71	129.48	119.84
1	C	172	VAL	N-CA-C	7.58	119.06	107.99
1	A	965	MET	CA-C-N	-7.57	110.46	122.79
1	A	965	MET	C-N-CA	-7.57	110.46	122.79
1	B	1036	GLU	N-CA-C	7.57	121.20	110.68
1	D	489	THR	CA-C-N	-7.52	111.22	119.19
1	D	489	THR	C-N-CA	-7.52	111.22	119.19
1	D	166	ILE	N-CA-C	-7.47	103.00	110.62
1	D	663	LEU	CA-C-N	-7.42	112.36	119.85
1	D	663	LEU	C-N-CA	-7.42	112.36	119.85
1	B	17	ILE	CB-CA-C	-7.41	102.40	111.88
1	D	367	ILE	CA-C-N	-7.34	112.15	119.56
1	D	367	ILE	C-N-CA	-7.34	112.15	119.56
1	A	367	ILE	CA-C-N	-7.27	112.21	119.56
1	A	367	ILE	C-N-CA	-7.27	112.21	119.56
1	B	435	MET	N-CA-C	-7.25	103.41	111.82
1	A	777	LEU	CA-C-N	7.24	128.89	119.84
1	A	777	LEU	C-N-CA	7.24	128.89	119.84
1	C	8	ARG	N-CA-C	-7.21	98.38	108.76
1	B	669	LEU	N-CA-C	7.20	120.01	108.41
1	A	862	ARG	N-CA-C	7.20	121.82	112.89
1	E	287	SER	CA-C-N	-7.15	111.11	121.26
1	E	287	SER	C-N-CA	-7.15	111.11	121.26
1	F	484	VAL	N-CA-C	7.11	117.24	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1033	GLU	CA-C-N	7.10	134.47	121.70
1	D	1033	GLU	C-N-CA	7.10	134.47	121.70
1	E	777	LEU	CA-C-N	7.09	128.71	119.84
1	E	777	LEU	C-N-CA	7.09	128.71	119.84
1	E	974	SER	N-CA-C	-7.03	103.62	111.28
1	A	487	ILE	CB-CA-C	-6.98	105.78	111.71
1	B	667	VAL	N-CA-C	6.97	119.77	111.05
1	D	314	GLU	N-CA-C	6.97	122.32	113.25
1	E	268	ILE	N-CA-C	6.91	117.84	107.75
1	E	670	GLY	N-CA-C	6.89	129.51	113.18
1	B	314	GLU	CA-C-N	-6.88	112.72	119.87
1	B	314	GLU	C-N-CA	-6.88	112.72	119.87
1	B	970	ILE	N-CA-C	-6.86	103.62	110.62
1	A	115	MET	N-CA-C	6.84	122.88	113.16
1	F	758	ILE	N-CA-C	6.80	118.72	106.61
1	B	846	LEU	CA-C-N	6.80	127.72	120.11
1	B	846	LEU	C-N-CA	6.80	127.72	120.11
1	F	8	ARG	CA-C-N	6.78	126.74	119.28
1	F	8	ARG	C-N-CA	6.78	126.74	119.28
1	D	939	LEU	N-CA-C	6.77	118.66	111.28
1	B	937	ALA	CA-C-N	6.75	129.06	120.56
1	B	937	ALA	C-N-CA	6.75	129.06	120.56
1	D	668	GLU	N-CA-C	6.75	125.17	110.80
1	E	603	LYS	N-CA-C	6.74	118.63	111.28
1	C	489	THR	CA-C-N	-6.71	111.60	119.05
1	C	489	THR	C-N-CA	-6.71	111.60	119.05
1	D	197	GLN	N-CA-C	6.70	120.90	111.52
1	A	794	VAL	CA-C-N	6.70	126.66	120.03
1	A	794	VAL	C-N-CA	6.70	126.66	120.03
1	C	940	ILE	N-CA-C	6.70	116.72	110.42
1	E	3	ASN	N-CA-C	-6.68	104.02	111.71
1	C	221	GLY	N-CA-C	-6.65	104.28	111.93
1	E	8	ARG	N-CA-C	6.64	118.33	108.76
1	E	435	MET	N-CA-C	-6.61	104.10	111.71
1	C	89	GLN	N-CA-C	6.59	119.15	108.34
1	C	862	ARG	N-CA-C	-6.59	104.50	112.54
1	D	511	GLY	N-CA-C	6.59	128.79	113.18
1	F	1000	THR	N-CA-C	6.59	118.15	110.97
1	F	390	ILE	CB-CA-C	-6.57	104.84	111.80
1	C	181	GLN	N-CA-C	-6.56	101.88	110.53
1	F	482	VAL	CB-CA-C	-6.54	103.31	112.14
1	D	310	LEU	N-CA-C	6.53	118.19	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	564	LEU	CA-C-N	6.53	126.48	119.76
1	D	564	LEU	C-N-CA	6.53	126.48	119.76
1	B	317	PHE	N-CA-C	-6.51	101.10	110.08
1	F	148	THR	N-CA-C	6.50	119.66	110.23
1	D	34	GLN	N-CA-C	-6.50	104.12	111.14
1	F	777	LEU	CA-C-N	6.49	127.95	119.84
1	F	777	LEU	C-N-CA	6.49	127.95	119.84
1	C	521	GLU	N-CA-C	-6.49	104.13	111.14
1	F	489	THR	CA-C-N	-6.49	111.85	119.05
1	F	489	THR	C-N-CA	-6.49	111.85	119.05
1	B	887	TYR	CA-C-N	-6.48	112.19	122.95
1	B	887	TYR	C-N-CA	-6.48	112.19	122.95
1	F	531	VAL	N-CA-C	-6.48	104.20	110.42
1	F	524	THR	N-CA-C	-6.47	104.31	111.82
1	F	453	PHE	N-CA-C	-6.44	105.39	113.18
1	D	325	TYR	CA-C-N	6.44	127.89	119.84
1	D	325	TYR	C-N-CA	6.44	127.89	119.84
1	A	10	ILE	N-CA-C	-6.41	103.32	112.35
1	E	164	ASP	N-CA-C	6.40	119.21	111.40
1	E	712	ARG	CA-C-N	-6.38	113.40	119.85
1	E	712	ARG	C-N-CA	-6.38	113.40	119.85
1	E	158	VAL	N-CA-C	-6.36	104.13	110.62
1	A	434	SER	N-CA-C	-6.36	104.43	111.36
1	B	847	PRO	N-CA-C	6.36	120.42	111.33
1	F	85	THR	N-CA-C	-6.34	105.53	113.20
1	F	62	THR	N-CA-C	6.31	118.72	111.02
1	F	505	HIS	N-CA-C	-6.31	105.16	112.86
1	B	383	LEU	N-CA-C	-6.28	104.53	111.82
1	B	1019	VAL	N-CA-C	-6.27	104.52	110.42
1	F	654	LYS	N-CA-C	6.27	119.24	109.52
1	A	57	VAL	N-CA-C	6.27	117.05	110.72
1	F	819	SER	N-CA-C	6.26	118.58	109.07
1	E	827	ALA	CA-C-N	6.25	127.65	119.84
1	E	827	ALA	C-N-CA	6.25	127.65	119.84
1	E	671	THR	N-CA-C	-6.25	104.71	113.20
1	D	361	ASN	N-CA-C	6.24	118.23	107.93
1	B	710	SER	N-CA-C	6.23	120.24	111.52
1	D	273	GLU	N-CA-C	-6.18	104.62	111.36
1	D	447	MET	N-CA-C	6.18	119.29	111.69
1	E	821	GLU	N-CA-C	6.18	120.34	109.96
1	D	128	SER	N-CA-C	6.16	119.58	109.72
1	C	445	ILE	CB-CA-C	-6.16	104.11	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	115	MET	N-CA-C	6.16	122.01	113.45
1	B	777	LEU	CA-C-N	6.14	127.52	119.84
1	B	777	LEU	C-N-CA	6.14	127.52	119.84
1	E	525	HIS	N-CA-C	-6.07	104.75	111.36
1	B	287	SER	CA-C-N	-6.04	112.69	121.26
1	B	287	SER	C-N-CA	-6.04	112.69	121.26
1	B	890	TRP	N-CA-C	-6.03	105.41	112.89
1	A	341	VAL	N-CA-C	6.03	116.15	110.30
1	E	519	MET	CB-CG-SD	6.03	130.78	112.70
1	A	293	LEU	N-CA-C	6.01	118.98	110.50
1	F	8	ARG	N-CA-C	-6.01	100.11	108.76
1	F	404	LEU	N-CA-C	6.00	117.90	111.36
1	F	518	ARG	N-CA-C	-6.00	103.70	111.02
1	A	411	VAL	N-CA-C	-6.00	103.78	110.62
1	F	407	ASP	CA-C-N	5.99	128.56	120.65
1	F	407	ASP	C-N-CA	5.99	128.56	120.65
1	E	28	LEU	N-CA-C	5.99	117.81	111.28
1	F	968	ARG	CA-C-N	-5.97	112.42	119.05
1	F	968	ARG	C-N-CA	-5.97	112.42	119.05
1	C	232	ALA	N-CA-C	5.97	118.14	109.07
1	E	669	LEU	N-CA-C	5.96	117.86	107.49
1	A	472	ILE	N-CA-C	5.96	117.50	111.00
1	A	508	GLY	CA-C-N	-5.94	110.19	121.54
1	A	508	GLY	C-N-CA	-5.94	110.19	121.54
1	E	912	THR	N-CA-C	-5.93	104.21	112.45
1	D	284	GLN	CA-C-N	5.92	125.93	119.89
1	D	284	GLN	C-N-CA	5.92	125.93	119.89
1	F	243	THR	N-CA-C	-5.91	104.84	111.28
1	E	148	THR	N-CA-C	-5.89	104.76	111.07
1	E	30	LEU	CA-C-N	5.88	126.22	119.92
1	E	30	LEU	C-N-CA	5.88	126.22	119.92
1	F	94	PHE	N-CA-C	5.88	119.25	110.14
1	F	585	GLU	N-CA-C	5.88	117.77	111.36
1	F	673	THR	N-CA-C	5.87	118.22	109.59
1	C	512	PHE	CA-C-N	-5.87	115.46	122.44
1	C	512	PHE	C-N-CA	-5.87	115.46	122.44
1	B	519	MET	CB-CG-SD	5.86	130.28	112.70
1	B	149	MET	N-CA-C	5.86	119.13	110.46
1	C	1007	VAL	N-CA-C	5.86	115.98	110.30
1	F	49	TYR	CA-C-N	5.85	126.76	119.98
1	F	49	TYR	C-N-CA	5.85	126.76	119.98
1	F	122	VAL	N-CA-C	-5.83	104.83	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	971	LEU	O-C-N	5.83	128.32	122.03
1	E	864	SER	N-CA-C	5.83	119.73	110.70
1	C	917	THR	N-CA-C	5.82	118.13	108.99
1	C	930	ILE	CB-CA-C	-5.82	104.43	111.88
1	E	755	ASN	N-CA-C	5.82	118.25	109.41
1	E	900	VAL	CA-C-N	-5.82	112.59	119.05
1	E	900	VAL	C-N-CA	-5.82	112.59	119.05
1	F	989	GLY	N-CA-C	-5.80	103.72	112.60
1	F	688	GLU	CA-C-N	5.80	128.05	120.28
1	F	688	GLU	C-N-CA	5.80	128.05	120.28
1	E	1019	VAL	N-CA-C	-5.80	104.68	110.30
1	D	939	LEU	CA-CB-CG	-5.79	96.02	116.30
1	A	966	ARG	CB-CA-C	5.79	120.42	111.28
1	B	624	VAL	N-CA-C	5.78	116.21	108.11
1	E	130	GLU	N-CA-C	5.78	118.92	108.69
1	F	1036	GLU	CA-C-O	5.77	121.96	118.33
1	A	521	GLU	N-CA-C	-5.77	104.90	111.07
1	B	757	PHE	CA-C-N	-5.77	115.79	123.17
1	B	757	PHE	C-N-CA	-5.77	115.79	123.17
1	A	489	THR	CA-C-N	-5.76	112.94	119.28
1	A	489	THR	C-N-CA	-5.76	112.94	119.28
1	D	438	ILE	N-CA-C	5.75	120.29	113.22
1	E	489	THR	CA-C-N	-5.74	112.68	119.05
1	E	489	THR	C-N-CA	-5.74	112.68	119.05
1	D	993	GLY	N-CA-C	-5.73	105.85	112.50
1	D	439	GLN	N-CA-C	5.72	117.19	111.07
1	C	381	ALA	N-CA-C	-5.71	105.14	111.36
1	F	279	ALA	N-CA-C	5.71	118.20	108.90
1	D	426	PRO	O-C-N	5.70	123.93	121.31
1	A	474	ILE	N-CA-C	5.70	117.21	111.00
1	A	535	LEU	N-CA-C	-5.69	106.17	113.23
1	F	1036	GLU	CB-CA-C	-5.69	108.17	116.53
1	E	674	GLY	N-CA-C	5.68	126.65	113.18
1	D	139	VAL	N-CA-C	5.68	116.78	107.24
1	B	930	ILE	CB-CA-C	-5.67	104.62	111.88
1	F	361	ASN	N-CA-C	-5.67	97.75	107.61
1	A	8	ARG	CB-CG-CD	-5.67	98.27	111.30
1	F	791	GLY	N-CA-C	5.67	124.07	115.63
1	C	939	LEU	N-CA-C	-5.66	104.48	111.33
1	B	654	LYS	N-CA-C	5.65	118.78	109.85
1	B	712	ARG	N-CA-C	5.65	118.37	108.82
1	B	489	THR	CA-C-N	-5.65	112.78	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	THR	C-N-CA	-5.65	112.78	119.05
1	C	402	ILE	CB-CA-C	-5.65	104.64	112.04
1	A	18	ILE	N-CA-C	5.64	115.84	110.53
1	F	830	LYS	N-CA-C	5.63	118.86	110.52
1	C	971	LEU	CA-C-N	5.63	128.14	120.54
1	C	971	LEU	C-N-CA	5.63	128.14	120.54
1	D	49	TYR	CA-C-N	5.63	125.95	119.93
1	D	49	TYR	C-N-CA	5.63	125.95	119.93
1	C	234	ILE	N-CA-C	5.61	115.87	107.51
1	C	54	ALA	N-CA-C	5.61	117.20	111.14
1	E	794	VAL	CA-C-N	5.60	125.57	120.03
1	E	794	VAL	C-N-CA	5.60	125.57	120.03
1	A	118	LEU	CA-C-N	5.60	126.38	120.11
1	A	118	LEU	C-N-CA	5.60	126.38	120.11
1	D	716	LEU	N-CA-C	-5.60	100.58	109.59
1	C	90	ILE	N-CA-C	5.59	116.17	107.28
1	D	440	GLY	N-CA-C	-5.59	106.01	112.83
1	E	280	GLU	N-CA-C	5.59	118.58	109.24
1	F	540	ARG	N-CA-C	5.58	117.06	110.97
1	A	675	PHE	N-CA-C	5.58	117.32	108.79
1	B	367	ILE	CA-C-N	-5.57	113.88	119.56
1	B	367	ILE	C-N-CA	-5.57	113.88	119.56
1	F	517	ASN	N-CA-C	5.57	117.03	111.07
1	E	1004	GLY	N-CA-C	-5.57	106.05	112.73
1	A	873	ALA	N-CA-C	-5.55	105.14	111.14
1	B	296	GLY	N-CA-C	-5.54	107.55	115.64
1	D	315	PRO	N-CA-C	5.54	120.84	114.03
1	D	515	TRP	CA-C-N	5.53	130.03	120.58
1	D	515	TRP	C-N-CA	5.53	130.03	120.58
1	E	519	MET	N-CA-C	-5.52	104.65	111.33
1	C	993	GLY	N-CA-C	-5.52	106.11	112.73
1	D	495	THR	N-CA-C	5.52	119.59	111.04
1	C	242	SER	N-CA-C	5.52	118.69	110.14
1	E	1030	ARG	N-CA-C	5.52	117.42	108.26
1	C	846	LEU	CA-C-N	5.51	126.73	119.84
1	C	846	LEU	C-N-CA	5.51	126.73	119.84
1	E	454	VAL	CA-C-N	-5.51	112.94	119.05
1	E	454	VAL	C-N-CA	-5.51	112.94	119.05
1	A	529	ASP	N-CA-C	-5.50	104.67	111.33
1	A	134	SER	N-CA-C	-5.49	104.15	111.24
1	E	1017	VAL	CA-C-N	-5.49	113.96	119.56
1	E	1017	VAL	C-N-CA	-5.49	113.96	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	751	GLY	N-CA-C	-5.48	105.70	112.33
1	D	474	ILE	N-CA-C	5.46	115.67	110.53
1	D	678	GLU	N-CA-C	5.46	117.31	108.41
1	F	58	GLN	N-CA-C	5.46	118.15	111.82
1	A	614	GLY	N-CA-C	5.45	120.67	114.67
1	A	868	ALA	CA-C-N	-5.45	113.41	119.19
1	A	868	ALA	C-N-CA	-5.45	113.41	119.19
1	B	912	THR	N-CA-C	-5.45	104.88	112.45
1	A	315	PRO	N-CA-C	5.44	120.66	113.86
1	E	675	PHE	N-CA-C	5.44	117.53	108.99
1	A	319	SER	N-CA-C	5.44	118.06	109.96
1	A	1019	VAL	N-CA-C	-5.43	105.42	110.53
1	C	964	ARG	N-CA-C	5.43	117.00	111.14
1	A	863	LEU	N-CA-C	5.41	118.22	111.24
1	F	432	ARG	N-CA-C	-5.41	104.62	111.11
1	E	536	ARG	N-CA-C	-5.40	105.08	110.97
1	D	180	SER	N-CA-C	5.40	118.20	109.40
1	A	663	LEU	N-CA-C	-5.39	102.44	110.20
1	A	921	TYR	N-CA-C	5.39	117.15	111.28
1	C	85	THR	N-CA-C	-5.39	106.73	113.15
1	F	441	ALA	N-CA-C	5.39	116.83	111.07
1	A	320	GLY	N-CA-C	5.38	122.52	115.47
1	E	399	VAL	CB-CA-C	-5.38	105.00	111.88
1	B	866	ASN	N-CA-C	-5.37	106.32	112.92
1	D	334	LYS	N-CA-C	5.36	116.81	110.97
1	D	38	ILE	N-CA-C	-5.35	107.61	112.96
1	D	1026	ARG	N-CA-C	-5.35	107.30	112.97
1	F	231	ASN	N-CA-C	5.35	116.92	107.61
1	E	135	SER	N-CA-C	5.35	118.22	107.41
1	D	39	ALA	CA-C-N	5.34	125.88	120.38
1	D	39	ALA	C-N-CA	5.34	125.88	120.38
1	E	865	GLY	N-CA-C	-5.33	100.54	113.18
1	C	475	VAL	N-CA-CB	5.33	116.79	110.55
1	C	830	LYS	N-CA-C	5.33	118.41	110.52
1	D	605	ASN	N-CA-C	-5.32	105.85	112.93
1	D	189	ASN	CA-C-N	5.32	124.50	118.97
1	D	189	ASN	C-N-CA	5.32	124.50	118.97
1	F	872	TYR	N-CA-C	-5.32	106.75	113.18
1	F	562	SER	N-CA-C	5.31	118.09	109.86
1	C	170	SER	N-CA-C	5.31	117.87	109.96
1	D	639	VAL	N-CA-C	5.31	120.38	109.34
1	C	360	GLN	N-CA-C	5.30	122.10	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	139	VAL	CA-C-N	-5.30	115.53	122.37
1	F	139	VAL	C-N-CA	-5.30	115.53	122.37
1	F	317	PHE	CA-C-N	5.30	126.47	119.84
1	F	317	PHE	C-N-CA	5.30	126.47	119.84
1	E	653	ILE	N-CA-C	5.30	120.36	109.34
1	B	655	ASP	N-CA-C	-5.29	106.61	113.16
1	D	1034	ASP	CA-C-N	5.28	131.21	121.70
1	D	1034	ASP	C-N-CA	5.28	131.21	121.70
1	A	532	GLY	N-CA-C	-5.28	106.39	112.83
1	C	515	TRP	N-CA-C	-5.28	105.94	112.38
1	F	940	ILE	N-CA-C	5.26	115.48	110.53
1	D	701	ALA	N-CA-C	-5.26	106.71	113.23
1	E	277	ILE	CA-C-N	-5.25	115.53	122.98
1	E	277	ILE	C-N-CA	-5.25	115.53	122.98
1	F	993	GLY	N-CA-C	-5.24	106.42	112.50
1	B	719	THR	CA-C-N	-5.24	114.53	119.76
1	B	719	THR	C-N-CA	-5.24	114.53	119.76
1	C	117	LEU	N-CA-C	5.23	120.31	113.30
1	D	246	PHE	N-CA-C	-5.23	105.64	112.23
1	F	325	TYR	CA-C-N	5.23	126.37	119.84
1	F	325	TYR	C-N-CA	5.23	126.37	119.84
1	D	214	VAL	N-CA-C	5.22	116.17	108.45
1	E	393	LEU	N-CA-C	5.22	116.66	110.97
1	C	148	THR	N-CA-C	5.21	117.87	110.10
1	D	35	TYR	CA-C-N	-5.21	115.21	120.21
1	D	35	TYR	C-N-CA	-5.21	115.21	120.21
1	C	32	VAL	N-CA-C	5.21	116.16	108.45
1	B	474	ILE	N-CA-C	5.20	116.67	111.00
1	B	591	LEU	N-CA-C	5.20	116.64	111.07
1	C	938	ILE	CB-CA-C	-5.20	105.32	111.97
1	C	426	PRO	O-C-N	5.19	123.70	121.31
1	E	687	HIS	N-CA-C	-5.19	105.05	111.33
1	F	413	VAL	CB-CA-C	-5.19	105.24	111.88
1	A	729	GLU	N-CA-C	-5.18	105.53	111.07
1	C	1006	MET	CB-CG-SD	5.18	128.24	112.70
1	E	312	LYS	N-CA-C	5.18	116.93	111.28
1	C	655	ASP	N-CA-C	-5.18	106.55	112.92
1	A	266	ALA	N-CA-C	5.17	116.71	108.79
1	D	8	ARG	CA-C-N	5.17	124.96	119.28
1	D	8	ARG	C-N-CA	5.17	124.96	119.28
1	A	973	THR	CB-CA-C	-5.17	103.00	110.96
1	C	83	ASP	N-CA-C	5.16	118.16	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	MET	CA-C-N	-5.16	114.47	120.04
1	A	115	MET	C-N-CA	-5.16	114.47	120.04
1	E	291	ILE	N-CA-CB	5.15	116.14	110.53
1	C	189	ASN	CA-C-N	5.15	124.32	118.97
1	C	189	ASN	C-N-CA	5.15	124.32	118.97
1	B	406	VAL	N-CA-C	-5.15	105.48	110.42
1	A	719	THR	CA-C-N	-5.14	114.62	119.76
1	A	719	THR	C-N-CA	-5.14	114.62	119.76
1	B	1022	VAL	CA-C-N	-5.14	113.98	120.56
1	B	1022	VAL	C-N-CA	-5.14	113.98	120.56
1	C	999	GLY	N-CA-C	5.14	118.86	112.64
1	C	578	LEU	CA-C-N	5.13	125.41	119.92
1	C	578	LEU	C-N-CA	5.13	125.41	119.92
1	C	639	VAL	N-CA-C	5.13	120.00	109.34
1	A	933	SER	N-CA-C	5.12	116.55	111.07
1	A	365	THR	N-CA-C	-5.12	106.30	112.54
1	C	737	SER	N-CA-C	5.11	117.94	109.46
1	F	526	HIS	N-CA-C	-5.10	104.98	111.11
1	B	74	ASN	N-CA-C	5.10	118.66	111.52
1	A	80	SER	N-CA-C	5.10	117.71	109.40
1	C	743	THR	N-CA-C	5.10	117.73	111.82
1	D	652	GLN	N-CA-C	5.10	117.81	111.24
1	C	872	TYR	N-CA-C	-5.09	106.57	112.89
1	D	286	ALA	N-CA-C	5.09	116.26	108.42
1	B	970	ILE	N-CA-CB	5.09	117.46	110.54
1	D	336	SER	N-CA-C	5.09	116.52	111.07
1	F	482	VAL	N-CA-C	-5.07	105.44	110.62
1	C	819	SER	N-CA-C	5.07	116.52	108.96
1	E	628	ASP	N-CA-C	5.07	117.25	110.35
1	B	313	MET	CB-CG-SD	-5.07	97.49	112.70
1	E	1020	PHE	N-CA-C	5.07	117.19	111.11
1	D	1019	VAL	N-CA-C	-5.06	105.39	110.30
1	C	213	GLN	N-CA-C	-5.06	102.58	110.42
1	D	73	ASP	N-CA-C	5.06	117.77	110.28
1	E	985	VAL	N-CA-C	5.06	115.29	110.53
1	D	846	LEU	CA-C-N	5.06	126.16	119.84
1	D	846	LEU	C-N-CA	5.06	126.16	119.84
1	D	350	LEU	CA-CB-CG	-5.06	98.61	116.30
1	C	362	PHE	N-CA-C	5.05	117.44	111.33
1	E	764	LYS	N-CA-C	5.05	116.67	109.14
1	D	589	LYS	N-CA-C	5.05	116.47	110.97
1	F	223	PRO	CA-C-N	-5.04	113.54	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	223	PRO	C-N-CA	-5.04	113.54	119.84
1	D	986	ILE	N-CA-C	5.04	115.19	110.30
1	F	487	ILE	N-CA-C	5.04	116.22	111.48
1	C	40	PRO	CA-C-N	5.03	124.79	119.76
1	C	40	PRO	C-N-CA	5.03	124.79	119.76
1	B	100	ALA	N-CA-C	-5.03	105.49	110.97
1	C	454	VAL	CA-C-N	-5.03	113.47	119.05
1	C	454	VAL	C-N-CA	-5.03	113.47	119.05
1	C	979	LEU	N-CA-C	5.03	117.65	111.82
1	E	822	ILE	N-CA-C	5.03	115.87	107.18
1	C	4	PHE	N-CA-C	-5.02	105.26	111.33
1	C	1032	ASN	CA-C-N	5.01	130.73	121.70
1	C	1032	ASN	C-N-CA	5.01	130.73	121.70
1	F	451	ALA	N-CA-C	5.01	116.82	111.36
1	A	548	ILE	CB-CA-C	-5.00	105.38	112.14
1	D	987	SER	N-CA-C	5.00	121.46	110.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1033	GLU	Peptide
1	A	1034	ASP	Peptide
1	A	1036	GLU	Peptide
1	B	1033	GLU	Peptide
1	B	1035	ILE	Peptide
1	C	6	ILE	Peptide
1	D	1035	ILE	Peptide
1	F	6	ILE	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	7893	0	8034	484	0
1	B	7900	0	8041	407	0
1	C	7867	0	8015	480	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	7893	0	8034	546	0
1	E	7883	0	8027	484	0
1	F	7883	0	8027	503	0
2	A	35	0	46	4	0
2	B	35	0	46	3	0
2	C	35	0	46	2	0
2	D	35	0	46	3	0
2	E	35	0	46	8	0
2	F	35	0	46	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	47532	0	48454	2810	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 29.

All (2810) 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:E:536:ARG:NE	2:E:1101:LMT:O3B	1.81	1.13
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.38	1.04
1:D:954:GLY:HA2	1:D:1034:ASP:H	1.23	1.03
1:C:686:GLY:HA3	1:C:689:LYS:HD3	1.42	1.01
1:D:533:GLY:HA2	1:D:536:ARG:HD3	1.48	0.95
1:D:113:LEU:HD11	1:F:128:SER:HB3	1.46	0.94
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.50	0.92
1:E:214:VAL:HG11	1:F:742:ASN:HB3	1.51	0.91
1:F:340:VAL:HG11	1:F:395:MET:HB3	1.53	0.91
1:E:239:ARG:NH1	1:E:756:ASP:O	2.04	0.90
1:E:354:VAL:HG22	1:E:975:LEU:HD23	1.51	0.90
1:C:151:GLN:NE2	1:C:286:ALA:O	2.05	0.89
1:C:151:GLN:NE2	1:C:279:ALA:O	2.04	0.89
1:D:571:VAL:HG22	1:D:625:SER:HA	1.54	0.89
1:E:179:GLY:HA2	1:E:277:ILE:HD11	1.54	0.89
1:E:355:MET:HE1	1:E:410:ILE:HG12	1.52	0.89
1:E:355:MET:HG2	1:E:365:THR:HA	1.54	0.88
1:B:34:GLN:HG3	1:B:333:VAL:HG22	1.55	0.88
1:A:571:VAL:HG22	1:A:625:SER:HA	1.56	0.88
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.54	0.88
1:A:880:PHE:HD1	1:A:897:MET:HE1	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.56	0.87
1:E:211:ASN:O	1:E:755:ASN:ND2	2.07	0.87
1:E:680:ILE:HD11	1:E:853:ASP:HB2	1.56	0.87
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.56	0.87
1:D:776:MET:HE2	1:F:225:VAL:HG22	1.54	0.87
1:C:156:ASP:OD1	1:C:760:ARG:NH2	2.08	0.87
1:B:350:LEU:HD22	1:B:979:LEU:HB3	1.57	0.86
1:C:939:LEU:HB3	1:C:966:ARG:HD2	1.58	0.86
1:D:70:ASN:O	1:D:110:LYS:NZ	2.09	0.86
1:A:723:LYS:NZ	1:C:236:ALA:O	2.09	0.86
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.57	0.85
1:C:653:ILE:HG13	1:C:654:LYS:HE2	1.58	0.85
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.59	0.85
1:F:686:GLY:HA3	1:F:689:LYS:HD3	1.58	0.84
1:A:475:VAL:HA	1:A:478:MET:HE2	1.59	0.84
1:D:159:ALA:HB2	1:D:177:LEU:HD11	1.57	0.84
1:F:961:ASP:OD1	1:F:964:ARG:NH2	2.11	0.83
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.43	0.83
1:C:264:ASP:OD1	1:C:264:ASP:N	2.12	0.83
1:B:415:ASN:HD22	1:B:434:SER:HB2	1.42	0.83
1:D:457:ALA:O	1:D:468:ARG:NE	2.10	0.83
1:D:629:TRP:CD1	1:D:629:TRP:H	1.94	0.83
1:D:156:ASP:OD1	1:D:760:ARG:NH2	2.12	0.83
1:D:41:PRO:HG2	1:D:94:PHE:HB2	1.59	0.82
1:D:187:TRP:HB3	1:D:771:GLU:HA	1.59	0.82
1:B:664:PRO:HB3	1:B:669:LEU:HD12	1.61	0.82
1:D:706:ASP:O	1:D:830:LYS:NZ	2.11	0.82
1:D:225:VAL:HG22	1:E:776:MET:HE2	1.61	0.82
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.12	0.82
1:D:400:LEU:HD23	1:D:924:VAL:HG12	1.61	0.81
1:F:974:SER:HA	1:F:1006:MET:HE3	1.62	0.81
1:A:968:ARG:HG2	1:A:972:MET:HE2	1.61	0.81
1:E:629:TRP:CD1	1:E:629:TRP:H	1.96	0.81
1:D:60:THR:HG23	1:D:61:VAL:HG23	1.62	0.81
1:D:953:LYS:NZ	1:D:957:GLU:OE1	2.13	0.80
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.63	0.80
1:A:237:GLN:OE1	1:B:742:ASN:ND2	2.14	0.80
1:F:248:LYS:HA	1:F:261:LEU:HD13	1.63	0.80
1:D:453:PHE:O	1:D:471:SER:OG	1.99	0.80
1:A:158:VAL:HA	1:A:162:MET:HE3	1.61	0.79
1:A:691:THR:HG23	1:A:694:ARG:HH12	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:PRO:HG2	1:D:875:SER:HB2	1.62	0.79
1:E:1032:ASN:HB3	1:E:1033:GLU:HB3	1.64	0.79
1:A:966:ARG:HE	1:A:970:ILE:HD11	1.46	0.79
1:E:584:GLN:HB2	1:E:617:GLN:HG2	1.64	0.79
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.64	0.79
1:F:930:ILE:O	1:F:933:SER:OG	2.00	0.79
1:D:139:VAL:HB	1:D:327:TYR:HB3	1.65	0.79
1:D:222:THR:HA	1:D:224:PRO:HD3	1.63	0.79
1:A:153:ASP:OD2	1:A:182:TYR:OH	2.00	0.78
1:C:914:ARG:O	1:C:916:LEU:N	2.16	0.78
1:D:475:VAL:HA	1:D:478:MET:HE2	1.63	0.78
1:E:516:PHE:HA	1:E:519:MET:HG3	1.65	0.78
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.65	0.78
1:F:356:TYR:HA	1:F:365:THR:HG21	1.65	0.78
1:A:375:VAL:O	1:A:379:THR:OG1	2.01	0.78
1:A:955:LEU:O	1:A:959:THR:OG1	2.01	0.78
1:A:880:PHE:CD1	1:A:897:MET:HE1	2.19	0.78
1:A:1034:ASP:HB3	1:A:1035:ILE:HA	1.66	0.78
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.65	0.78
1:F:45:ILE:HG12	1:F:129:VAL:HG13	1.66	0.78
1:C:360:GLN:OE1	1:C:517:ASN:ND2	2.15	0.78
1:D:414:GLU:OE1	1:D:968:ARG:NH1	2.17	0.78
1:D:344:LEU:HD23	1:D:402:ILE:HD11	1.66	0.78
1:D:211:ASN:O	1:D:755:ASN:ND2	2.18	0.77
1:E:966:ARG:O	1:E:970:ILE:HG12	1.84	0.77
1:A:776:MET:HE2	1:C:225:VAL:HG22	1.65	0.77
1:C:3:ASN:N	1:C:3:ASN:OD1	2.16	0.77
1:B:327:TYR:HB2	1:B:623:PHE:HE2	1.47	0.77
1:F:82:SER:HB2	1:F:811:LEU:HB2	1.65	0.77
1:D:457:ALA:HA	1:D:468:ARG:HG3	1.67	0.77
1:E:156:ASP:OD1	1:E:760:ARG:NH2	2.18	0.77
1:E:708:LEU:HD21	1:E:838:LEU:HD12	1.67	0.77
1:B:602:GLU:HG3	1:B:605:ASN:HB2	1.66	0.77
1:D:632:ARG:HH12	1:D:638:LYS:HA	1.50	0.77
1:E:507:GLU:HG2	1:E:518:ARG:HA	1.66	0.76
1:F:662:ASN:O	1:F:673:THR:OG1	2.03	0.76
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.66	0.76
1:C:427:PRO:O	1:C:431:THR:OG1	2.03	0.76
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.67	0.76
1:C:588:GLN:NE2	1:C:592:ASN:OD1	2.17	0.76
1:C:940:ILE:HG12	1:C:966:ARG:CZ	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1036:GLU:HB3	1:D:1037:HIS:HB2	1.68	0.76
1:E:144:ASN:ND2	1:E:319:SER:O	2.15	0.76
1:A:225:VAL:HG22	1:B:776:MET:HE2	1.68	0.76
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.51	0.76
1:A:214:VAL:HG11	1:B:742:ASN:HB3	1.68	0.76
1:A:34:GLN:HE21	1:A:332:PHE:HE2	1.34	0.76
1:A:491:ALA:O	1:A:495:THR:OG1	2.04	0.76
1:A:605:ASN:HD21	1:A:637:ASN:HA	1.51	0.75
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.68	0.75
1:E:343:THR:HG21	1:E:399:VAL:HG13	1.65	0.75
1:C:932:LEU:HD13	1:C:1006:MET:HE2	1.68	0.75
1:E:241:THR:N	1:E:245:GLU:OE1	2.19	0.75
1:A:955:LEU:H	1:A:1033:GLU:HA	1.52	0.75
1:C:460:GLY:O	1:C:867:GLN:NE2	2.20	0.75
1:C:632:ARG:NH1	1:C:637:ASN:O	2.19	0.75
1:E:115:MET:O	1:E:123:GLN:NE2	2.18	0.75
1:A:687:HIS:NE2	1:A:718:ASP:OD1	2.19	0.75
1:B:17:ILE:HA	1:B:20:MET:HE3	1.68	0.75
1:A:639:VAL:HG11	1:A:662:ASN:HB2	1.67	0.75
1:D:11:PHE:N	1:E:888:GLU:OE1	2.17	0.75
1:C:418:ARG:O	1:C:422:GLU:HB2	1.87	0.75
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.67	0.75
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.68	0.74
1:C:198:LEU:HD11	1:C:252:LYS:HB2	1.67	0.74
1:C:708:LEU:HD23	1:C:711:VAL:HG21	1.69	0.74
1:D:770:SER:HB3	1:D:775:ARG:HD3	1.68	0.74
1:D:588:GLN:NE2	1:D:592:ASN:OD1	2.18	0.74
1:B:930:ILE:O	1:B:933:SER:OG	2.05	0.74
1:D:966:ARG:HE	1:D:970:ILE:HD11	1.50	0.74
1:F:715:GLY:HA3	1:F:812:GLU:OE1	1.88	0.74
1:A:955:LEU:HD21	1:A:1022:VAL:HG13	1.68	0.74
1:F:598:TYR:HB3	1:F:606:VAL:HG21	1.68	0.74
1:A:38:ILE:HD11	1:A:466:ILE:HD11	1.70	0.74
1:E:39:ALA:HB2	1:E:668:GLU:HG3	1.70	0.74
1:F:936:ASN:HD21	1:F:1010:THR:HG22	1.52	0.74
1:A:175:VAL:HG11	1:A:289:LEU:HD13	1.68	0.74
1:A:531:VAL:O	1:A:534:ILE:HG13	1.87	0.74
1:F:165:ALA:O	1:F:169:THR:OG1	2.03	0.74
1:A:707:MET:HG3	1:A:708:LEU:HD13	1.70	0.73
1:D:416:VAL:HG12	1:D:420:MET:HE2	1.70	0.73
1:D:448:VAL:HG22	1:D:882:CYS:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ARG:NH1	1:C:422:GLU:OE1	2.20	0.73
1:C:420:MET:O	1:C:424:GLY:N	2.20	0.73
1:F:887:TYR:O	1:F:889:SER:N	2.17	0.73
1:A:101:ASP:OD1	1:A:101:ASP:N	2.20	0.73
1:A:989:GLY:O	1:A:992:SER:OG	2.06	0.73
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.71	0.73
1:C:49:TYR:HD1	1:C:57:VAL:HG12	1.53	0.73
1:A:186:ILE:HB	1:A:768:VAL:HG22	1.68	0.73
1:D:587:THR:HB	1:D:613:ASN:ND2	2.02	0.73
1:D:587:THR:HB	1:D:613:ASN:HD21	1.53	0.73
1:E:101:ASP:OD1	1:E:131:LYS:NZ	2.20	0.73
1:E:759:ASP:OD2	1:E:764:LYS:NZ	2.21	0.73
1:A:966:ARG:HB3	1:A:966:ARG:HH11	1.53	0.73
1:A:584:GLN:HB2	1:A:617:GLN:HG2	1.71	0.73
1:B:166:ILE:HD11	1:B:310:LEU:HD11	1.69	0.73
1:C:187:TRP:HZ3	1:C:769:MET:HE2	1.53	0.72
1:D:56:THR:OG1	1:F:213:GLN:NE2	2.22	0.72
1:E:445:ILE:HG22	1:E:938:ILE:HD13	1.69	0.72
1:C:574:THR:HG21	1:C:598:TYR:HE2	1.53	0.72
1:D:61:VAL:HA	1:D:118:LEU:HD22	1.70	0.72
1:E:184:MET:HB3	1:E:766:VAL:HG13	1.71	0.72
1:F:65:ILE:HG21	1:F:90:ILE:HD13	1.70	0.72
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.25	0.72
1:D:351:VAL:HG22	1:D:976:ALA:HB1	1.71	0.72
1:E:448:VAL:HG13	1:E:879:VAL:HG13	1.72	0.72
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.72	0.72
1:C:853:ASP:OD2	1:C:862:ARG:NH2	2.23	0.72
1:B:896:VAL:HG21	1:B:938:ILE:HG13	1.68	0.72
1:E:375:VAL:O	1:E:379:THR:OG1	2.07	0.72
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.71	0.72
1:C:580:ALA:HB1	1:C:719:THR:HG22	1.69	0.71
1:A:5:PHE:O	1:A:8:ARG:N	2.15	0.71
1:D:137:LEU:HD23	1:D:291:ILE:HG22	1.69	0.71
1:D:598:TYR:HB3	1:D:606:VAL:HG11	1.71	0.71
1:D:602:GLU:OE2	1:D:645:ARG:NH1	2.23	0.71
1:B:540:ARG:HH22	2:B:2000:LMT:H6'1	1.54	0.71
1:E:351:VAL:HG22	1:E:976:ALA:HB1	1.72	0.71
1:F:61:VAL:HA	1:F:118:LEU:HD22	1.72	0.71
1:D:575:MET:HG2	1:D:661:PHE:HE1	1.54	0.71
1:B:350:LEU:HD13	1:B:980:GLY:HA2	1.70	0.71
1:B:985:VAL:O	1:B:996:ASN:ND2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:955:LEU:HD21	1:F:1022:VAL:HA	1.73	0.71
1:C:896:VAL:HG23	1:C:937:ALA:HB3	1.71	0.71
1:A:414:GLU:HG3	1:A:972:MET:HE1	1.72	0.71
1:B:174:ASP:HB3	1:B:292:LYS:HB2	1.72	0.71
1:C:629:TRP:CD1	1:C:629:TRP:H	2.08	0.71
1:B:375:VAL:O	1:B:379:THR:OG1	2.03	0.71
1:D:574:THR:HG23	1:D:622:ALA:HB3	1.71	0.71
1:C:2:PRO:O	1:C:6:ILE:HG12	1.90	0.71
1:B:61:VAL:HG21	1:B:122:VAL:HG21	1.72	0.70
1:C:61:VAL:HG13	1:C:118:LEU:HD13	1.71	0.70
1:A:723:LYS:HG2	1:A:803:ARG:NH1	2.06	0.70
1:B:448:VAL:HG13	1:B:879:VAL:HG13	1.72	0.70
1:D:32:VAL:HG22	1:D:390:ILE:HB	1.73	0.70
1:D:375:VAL:HB	1:D:405:LEU:HD13	1.72	0.70
1:D:880:PHE:CE1	1:D:893:PRO:HB2	2.26	0.70
1:F:629:TRP:H	1:F:629:TRP:CD1	2.08	0.70
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.73	0.70
1:F:45:ILE:HD11	1:F:107:VAL:HG12	1.72	0.70
1:C:940:ILE:HG12	1:C:966:ARG:NH2	2.06	0.70
1:F:544:LEU:HA	1:F:547:ILE:HD12	1.74	0.70
1:F:892:ILE:HG23	1:F:941:VAL:HG11	1.72	0.70
1:A:962:ALA:O	1:A:966:ARG:NH1	2.25	0.70
1:B:974:SER:OG	1:B:1010:THR:HG21	1.92	0.70
1:F:574:THR:HG23	1:F:622:ALA:HB3	1.73	0.70
1:F:945:LYS:HA	1:F:948:MET:HE3	1.74	0.70
1:D:941:VAL:HG13	1:D:1021:PHE:CE1	2.26	0.69
1:E:82:SER:HB2	1:E:811:LEU:HB2	1.73	0.69
1:A:424:GLY:O	1:A:502:LYS:NZ	2.25	0.69
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.25	0.69
1:A:653:ILE:HG13	1:A:654:LYS:HE2	1.75	0.69
1:B:149:MET:HG3	1:B:154:ILE:HG13	1.73	0.69
1:C:248:LYS:HA	1:C:261:LEU:HD13	1.73	0.69
1:D:6:ILE:HG22	1:D:490:PRO:HB2	1.75	0.69
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.74	0.69
1:F:714:ASN:HB3	1:F:821:GLU:HB3	1.73	0.69
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.75	0.69
1:A:1034:ASP:CB	1:A:1035:ILE:HA	2.22	0.69
1:B:239:ARG:NH1	1:B:756:ASP:HB2	2.08	0.69
1:F:531:VAL:O	1:F:535:LEU:HG	1.92	0.69
1:B:144:ASN:ND2	1:B:319:SER:O	2.23	0.69
1:B:184:MET:HB2	1:B:757:PHE:CE2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ASN:HB3	1:C:148:THR:HG23	1.75	0.69
1:B:422:GLU:OE2	1:B:964:ARG:NH1	2.26	0.68
1:B:969:PRO:HA	1:B:972:MET:HE3	1.73	0.68
1:C:326:PRO:O	1:C:625:SER:OG	2.11	0.68
1:C:587:THR:OG1	1:C:613:ASN:ND2	2.26	0.68
1:D:209:ALA:O	1:D:237:GLN:NE2	2.23	0.68
1:D:899:VAL:O	1:D:902:LEU:HB2	1.93	0.68
1:E:185:ARG:NH2	1:E:273:GLU:O	2.24	0.68
1:D:138:MET:HE1	1:D:303:ALA:HA	1.75	0.68
1:D:254:ASN:ND2	1:D:258:SER:OG	2.20	0.68
1:B:259:ARG:H	1:B:259:ARG:HD3	1.57	0.68
1:C:45:ILE:HB	1:C:90:ILE:HD12	1.75	0.68
1:D:274:ASN:ND2	1:D:276:ASP:OD2	2.26	0.68
1:E:192:GLU:HA	1:E:195:LYS:HE3	1.74	0.68
1:E:422:GLU:O	1:E:502:LYS:NZ	2.22	0.68
1:F:368:PRO:HG3	1:F:413:VAL:HG21	1.75	0.68
1:B:383:LEU:HD11	1:B:473:THR:HA	1.74	0.68
1:D:914:ARG:O	1:D:916:LEU:N	2.27	0.68
1:E:536:ARG:HE	2:E:1101:LMT:H3O1	1.38	0.68
1:F:149:MET:HG3	1:F:154:ILE:HG13	1.75	0.68
1:F:741:ILE:HG22	1:F:786:VAL:HG21	1.75	0.68
1:B:602:GLU:OE2	1:B:645:ARG:NH1	2.26	0.68
1:C:278:ILE:HG13	1:C:613:ASN:HB3	1.75	0.68
1:A:636:GLU:HB2	1:A:645:ARG:HH22	1.59	0.68
1:D:700:GLU:HB3	1:D:842:LEU:HD22	1.74	0.68
1:A:511:GLY:HA2	1:A:515:TRP:HD1	1.57	0.68
1:B:559:LEU:HD12	1:B:918:ASN:HB2	1.76	0.68
1:E:908:LEU:HD23	1:E:922:PHE:HZ	1.59	0.68
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.76	0.67
1:A:641:ALA:HA	1:A:644:MET:HE3	1.75	0.67
1:A:892:ILE:HG12	1:A:1025:ARG:HD3	1.75	0.67
1:C:3:ASN:ND2	1:C:486:LEU:O	2.28	0.67
1:D:250:LEU:HD13	1:D:259:ARG:HB3	1.75	0.67
1:D:707:MET:HG3	1:D:708:LEU:HD13	1.77	0.67
1:E:184:MET:HB2	1:E:757:PHE:CE2	2.29	0.67
1:C:5:PHE:O	1:C:7:ASP:N	2.27	0.67
1:B:219:LEU:HG	1:B:234:ILE:HD11	1.74	0.67
1:C:453:PHE:HD2	1:C:456:MET:CE	2.07	0.67
1:C:112:GLN:HG3	1:C:115:MET:HG3	1.77	0.67
1:C:696:GLN:HE21	1:C:845:LYS:HE3	1.59	0.67
1:D:884:ALA:HA	1:D:889:SER:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:ARG:HB2	1:F:758:ILE:HD12	1.75	0.67
1:A:697:LEU:HD12	1:A:846:LEU:HD21	1.75	0.67
1:C:942:GLU:HG3	1:C:943:PHE:N	2.09	0.67
1:D:47:ALA:HB2	1:D:127:VAL:HG13	1.76	0.67
1:E:906:GLY:HA3	1:E:1008:THR:HG21	1.76	0.67
1:A:129:VAL:HG23	1:B:113:LEU:HD11	1.77	0.67
1:A:1026:ARG:NH1	1:A:1033:GLU:OE1	2.27	0.67
1:D:375:VAL:O	1:D:379:THR:OG1	2.11	0.67
1:F:211:ASN:O	1:F:755:ASN:ND2	2.28	0.67
1:B:156:ASP:OD1	1:B:760:ARG:NH2	2.27	0.67
1:D:954:GLY:HA2	1:D:1034:ASP:N	2.05	0.67
1:E:1021:PHE:HE2	1:E:1025:ARG:HD3	1.58	0.67
1:B:770:SER:HB3	1:B:775:ARG:HD3	1.77	0.67
1:D:400:LEU:HD21	1:D:925:GLY:HA2	1.77	0.67
1:F:418:ARG:O	1:F:422:GLU:HB2	1.94	0.67
1:F:443:VAL:O	1:F:447:MET:HB3	1.95	0.67
1:B:309:GLU:HG3	1:B:313:MET:HE3	1.76	0.66
1:B:982:MET:HB3	1:B:983:PRO:HD3	1.77	0.66
1:C:855:THR:HA	1:C:859:TYR:HB2	1.77	0.66
1:D:452:VAL:HA	1:D:875:SER:OG	1.95	0.66
1:D:545:TYR:HD1	1:D:546:LEU:HD23	1.60	0.66
1:F:27:ILE:HG22	1:F:380:PHE:HB3	1.77	0.66
1:A:511:GLY:HA2	1:A:515:TRP:CD1	2.31	0.66
1:A:645:ARG:O	1:A:648:ARG:HB3	1.95	0.66
1:B:24:GLY:O	1:B:27:ILE:HG22	1.95	0.66
1:B:966:ARG:O	1:B:970:ILE:HG12	1.96	0.66
1:D:80:SER:HB3	1:D:90:ILE:HG23	1.76	0.66
1:D:343:THR:O	1:D:346:GLU:N	2.28	0.66
1:D:367:ILE:HG12	1:D:492:LEU:HB3	1.78	0.66
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.30	0.66
1:C:57:VAL:HG23	1:C:82:SER:HB3	1.76	0.66
1:C:688:GLU:HB3	1:C:689:LYS:HD2	1.77	0.66
1:D:442:LEU:O	1:D:445:ILE:HG13	1.95	0.66
1:F:144:ASN:O	1:F:148:THR:OG1	2.11	0.66
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.76	0.66
1:E:120:GLN:NE2	1:E:123:GLN:OE1	2.29	0.66
1:E:578:LEU:HD21	1:E:590:VAL:HG21	1.77	0.66
1:F:707:MET:O	1:F:827:ALA:N	2.26	0.66
1:A:9:PRO:HG2	1:A:10:ILE:HD12	1.76	0.66
1:D:400:LEU:HD11	1:D:1002:VAL:HG21	1.77	0.66
1:D:697:LEU:HD12	1:D:846:LEU:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:ILE:HG12	1:E:754:VAL:HG21	1.77	0.66
1:B:683:ALA:O	1:B:685:LEU:N	2.28	0.66
1:E:441:ALA:O	1:E:445:ILE:HG23	1.96	0.66
1:E:444:GLY:HA3	1:E:886:LEU:HD22	1.78	0.66
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.78	0.66
1:F:755:ASN:O	1:F:766:VAL:HB	1.94	0.66
1:A:398:MET:HE2	1:A:473:THR:HG23	1.78	0.66
1:B:453:PHE:O	1:B:471:SER:OG	2.11	0.66
1:A:960:LEU:O	1:A:963:VAL:HG12	1.95	0.66
1:E:559:LEU:HD23	1:E:560:PRO:HD2	1.78	0.66
1:D:194:ASN:HA	1:D:793:MET:HE2	1.79	0.65
1:E:774:TYR:O	1:E:784:TRP:NE1	2.25	0.65
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.78	0.65
1:F:902:LEU:HG	1:F:1012:LEU:HB3	1.78	0.65
1:F:939:LEU:HB3	1:F:966:ARG:HD2	1.78	0.65
1:A:626:LEU:HD11	1:A:639:VAL:HG23	1.76	0.65
1:C:400:LEU:HD23	1:C:474:ILE:HD11	1.78	0.65
1:F:880:PHE:HD2	1:F:881:LEU:HD22	1.62	0.65
1:F:1016:PHE:HB3	1:F:1020:PHE:CE1	2.32	0.65
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.77	0.65
1:D:375:VAL:HG11	1:D:405:LEU:HD22	1.78	0.65
1:D:509:LYS:HG2	1:D:510:LYS:HG3	1.77	0.65
1:F:213:GLN:HA	1:F:237:GLN:O	1.97	0.65
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.79	0.65
1:C:584:GLN:HB2	1:C:617:GLN:HG2	1.79	0.65
1:B:262:LEU:HG	1:B:268:ILE:HD11	1.77	0.65
1:B:567:GLU:OE2	1:B:994:ALA:N	2.29	0.65
1:C:146:ASP:O	1:C:148:THR:N	2.29	0.65
1:F:198:LEU:HD21	1:F:252:LYS:HB2	1.77	0.65
1:F:588:GLN:OE1	1:F:592:ASN:ND2	2.28	0.65
1:A:940:ILE:HG12	1:A:966:ARG:CZ	2.26	0.65
1:C:82:SER:HB2	1:C:811:LEU:HB2	1.79	0.65
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.79	0.65
1:F:527:TYR:CE1	1:F:1014:ILE:HD12	2.32	0.65
1:C:188:MET:HB3	1:C:193:LEU:HD11	1.78	0.65
1:D:1028:PHE:O	1:D:1030:ARG:N	2.29	0.65
1:E:156:ASP:OD2	1:E:764:LYS:NZ	2.26	0.65
1:F:197:GLN:HA	1:F:793:MET:SD	2.36	0.65
1:F:612:VAL:HB	1:F:621:ILE:HG22	1.78	0.65
1:B:573:MET:HG3	1:B:661:PHE:CE2	2.32	0.65
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:PHE:HA	1:E:8:ARG:HB2	1.78	0.65
1:F:278:ILE:HG13	1:F:613:ASN:HB3	1.79	0.65
1:F:966:ARG:HH21	1:F:970:ILE:HD11	1.60	0.65
1:A:527:TYR:OH	1:A:1014:ILE:O	2.06	0.65
1:D:694:ARG:NH2	1:D:717:GLU:OE1	2.29	0.65
1:A:143:ILE:O	1:A:321:LEU:HD22	1.96	0.64
1:A:883:LEU:HD22	1:A:887:TYR:CE2	2.32	0.64
1:B:350:LEU:CD2	1:B:979:LEU:HB3	2.27	0.64
1:E:326:PRO:O	1:E:625:SER:OG	2.15	0.64
1:A:538:THR:HG22	1:A:542:LEU:HD22	1.79	0.64
1:A:1037:HIS:HB3	1:A:1039:HIS:H	1.62	0.64
1:B:61:VAL:HG13	1:B:118:LEU:HD22	1.79	0.64
1:A:182:TYR:O	1:A:764:LYS:HD3	1.98	0.64
1:F:664:PRO:HG3	1:F:670:GLY:HA3	1.78	0.64
1:A:184:MET:HB2	1:A:757:PHE:CE2	2.32	0.64
1:B:197:GLN:HA	1:B:793:MET:SD	2.37	0.64
1:F:420:MET:HB3	1:F:500:ILE:HB	1.80	0.64
1:A:368:PRO:HB3	1:A:409:ALA:HB1	1.79	0.64
1:D:236:ALA:O	1:E:723:LYS:NZ	2.30	0.64
1:E:330:THR:HG22	1:E:334:LYS:HE2	1.80	0.64
1:B:139:VAL:O	1:B:326:PRO:HD2	1.98	0.64
1:C:32:VAL:HG22	1:C:390:ILE:HB	1.80	0.64
1:C:249:ILE:HB	1:C:262:LEU:HB2	1.80	0.64
1:D:414:GLU:CD	1:D:969:PRO:HG3	2.22	0.64
1:E:213:GLN:HA	1:E:237:GLN:O	1.97	0.64
1:E:687:HIS:NE2	1:E:808:SER:HB2	2.13	0.64
1:F:582:ALA:HB2	1:F:586:ARG:HH21	1.63	0.64
1:C:388:PHE:CZ	1:C:472:ILE:HG21	2.33	0.64
1:D:200:PRO:HA	1:D:203:VAL:HG23	1.79	0.64
1:E:610:PHE:N	1:E:623:PHE:O	2.26	0.64
1:A:643:THR:HB	1:A:660:ALA:O	1.98	0.64
1:A:827:ALA:HB3	1:A:830:LYS:HB2	1.78	0.64
1:E:605:ASN:OD1	1:E:637:ASN:ND2	2.31	0.64
1:F:164:ASP:HB3	1:F:168:ARG:NH2	2.13	0.64
1:B:572:PHE:HA	1:B:663:LEU:HD21	1.80	0.64
1:F:527:TYR:CE2	1:F:963:VAL:HG13	2.33	0.64
1:F:895:SER:HB3	1:F:1024:VAL:HG11	1.80	0.64
1:A:564:LEU:HB2	1:A:666:ILE:HD11	1.78	0.63
1:A:966:ARG:O	1:A:970:ILE:HG12	1.98	0.63
1:B:222:THR:HA	1:B:224:PRO:HD3	1.81	0.63
1:D:45:ILE:HA	1:D:128:SER:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:579:PRO:HD3	1:E:656:ALA:HB2	1.78	0.63
1:F:75:LEU:HD21	1:F:78:MET:HB2	1.81	0.63
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.33	0.63
1:A:94:PHE:CE1	1:A:103:ALA:HB1	2.34	0.63
1:E:94:PHE:CE1	1:E:103:ALA:HB1	2.34	0.63
1:F:914:ARG:O	1:F:916:LEU:N	2.28	0.63
1:B:201:VAL:O	1:B:205:THR:OG1	2.11	0.63
1:F:151:GLN:NE2	1:F:279:ALA:O	2.31	0.63
1:F:653:ILE:HD12	1:F:654:LYS:HE2	1.79	0.63
1:B:190:PRO:HG3	1:B:774:TYR:HB3	1.78	0.63
1:B:455:PRO:HG2	1:B:875:SER:OG	1.97	0.63
1:E:445:ILE:HG21	1:E:935:LYS:HD2	1.80	0.63
1:F:54:ALA:HB2	1:F:809:PRO:C	2.22	0.63
1:F:344:LEU:O	1:F:348:ILE:HG13	1.98	0.63
1:F:689:LYS:H	1:F:689:LYS:HD2	1.62	0.63
1:D:398:MET:HE2	1:D:473:THR:HG23	1.79	0.63
1:E:7:ASP:CG	1:E:432:ARG:HH21	2.07	0.63
1:E:778:PRO:O	1:E:781:ILE:HG12	1.98	0.63
1:F:45:ILE:HB	1:F:90:ILE:HD12	1.79	0.63
1:F:135:SER:HB3	1:F:668:GLU:HB3	1.80	0.63
1:C:892:ILE:HG23	1:C:941:VAL:HG11	1.80	0.63
1:D:632:ARG:NH1	1:D:637:ASN:O	2.32	0.63
1:D:677:PHE:HD2	1:D:822:ILE:HD12	1.61	0.63
1:E:189:ASN:HB3	1:E:192:GLU:HB2	1.80	0.63
1:E:840:GLU:HG2	1:E:852:TYR:CE1	2.33	0.63
1:F:890:TRP:CE3	1:F:890:TRP:HA	2.33	0.63
1:C:456:MET:HE3	1:C:467:TYR:O	1.99	0.63
1:C:464:GLY:O	1:C:468:ARG:HB2	1.98	0.63
1:D:198:LEU:HD11	1:D:251:LEU:O	1.98	0.63
1:D:394:THR:HG23	1:D:469:GLN:HB3	1.79	0.63
1:D:536:ARG:NH1	2:D:2000:LMT:O3B	2.32	0.63
1:F:54:ALA:HB2	1:F:809:PRO:O	1.99	0.63
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.80	0.63
1:A:241:THR:N	1:A:245:GLU:OE2	2.29	0.63
1:A:883:LEU:HD22	1:A:887:TYR:HE2	1.63	0.63
1:F:351:VAL:HG12	1:F:355:MET:HE2	1.81	0.63
1:E:14:VAL:HG22	1:F:881:LEU:HD12	1.79	0.63
1:F:44:THR:HA	1:F:90:ILE:O	1.99	0.63
1:F:66:GLU:OE1	1:F:816:GLY:HA2	1.99	0.63
1:B:527:TYR:OH	1:B:1014:ILE:O	2.11	0.62
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:953:LYS:HB3	1:E:958:ALA:HB2	1.81	0.62
1:F:663:LEU:HD23	1:F:663:LEU:H	1.64	0.62
1:B:978:ILE:HG23	1:B:1003:MET:HG3	1.81	0.62
1:D:361:ASN:O	1:D:365:THR:HG22	1.99	0.62
1:E:100:ALA:HB1	1:E:131:LYS:HE3	1.81	0.62
1:E:165:ALA:HB3	1:E:313:MET:CE	2.29	0.62
1:F:201:VAL:O	1:F:205:THR:OG1	2.14	0.62
1:B:189:ASN:HB3	1:B:192:GLU:HB2	1.79	0.62
1:D:216:ALA:N	1:E:51:GLY:O	2.30	0.62
1:D:871:LEU:HD23	1:D:874:ILE:HD12	1.80	0.62
1:A:309:GLU:HG3	1:A:313:MET:HE3	1.81	0.62
1:C:577:GLN:HG3	1:C:619:THR:HG22	1.82	0.62
1:E:525:HIS:HA	1:E:528:THR:HG22	1.81	0.62
1:A:137:LEU:HD22	1:A:293:LEU:HD23	1.81	0.62
1:C:757:PHE:CE1	1:C:759:ASP:HB2	2.35	0.62
1:F:146:ASP:O	1:F:148:THR:N	2.30	0.62
1:F:211:ASN:ND2	1:F:246:PHE:HZ	1.97	0.62
1:A:462:SER:O	1:A:466:ILE:HG12	1.99	0.62
1:B:24:GLY:O	1:B:28:LEU:HD23	1.99	0.62
1:C:396:PHE:O	1:C:400:LEU:HB2	2.00	0.62
1:D:445:ILE:O	1:D:449:LEU:HB2	2.00	0.62
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.82	0.62
1:A:966:ARG:HB3	1:A:966:ARG:NH1	2.15	0.62
1:B:842:LEU:O	1:B:845:LYS:HB2	2.00	0.62
1:C:453:PHE:HB3	1:C:471:SER:HA	1.82	0.62
1:C:939:LEU:C	1:C:966:ARG:HD2	2.24	0.62
1:C:947:LEU:HD23	1:C:951:GLU:HG3	1.81	0.62
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.81	0.62
1:F:164:ASP:CG	1:F:762:ARG:HH22	2.07	0.62
1:B:355:MET:HG3	1:B:359:LEU:HD12	1.81	0.62
1:C:545:TYR:CE2	1:C:1020:PHE:HZ	2.17	0.62
1:C:553:ALA:O	1:C:557:VAL:HG23	2.00	0.62
1:D:219:LEU:HG	1:D:234:ILE:HD11	1.81	0.62
1:E:679:LEU:HD22	1:E:822:ILE:HD11	1.81	0.62
1:F:645:ARG:O	1:F:648:ARG:HB3	2.00	0.62
1:A:326:PRO:O	1:A:625:SER:OG	2.17	0.61
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.82	0.61
1:B:435:MET:SD	1:B:490:PRO:HB3	2.40	0.61
1:D:4:PHE:HB2	1:D:5:PHE:CD1	2.35	0.61
1:E:908:LEU:HD23	1:E:922:PHE:CZ	2.34	0.61
1:E:945:LYS:HA	1:E:948:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:691:THR:HG23	1:E:694:ARG:HH12	1.65	0.61
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.82	0.61
1:A:901:PRO:O	1:A:904:VAL:N	2.33	0.61
1:F:522:LYS:O	1:F:525:HIS:N	2.32	0.61
1:A:142:VAL:HG11	1:A:162:MET:HE1	1.81	0.61
1:B:941:VAL:HG13	1:B:1021:PHE:HE1	1.64	0.61
1:A:974:SER:OG	1:A:1010:THR:HG21	2.01	0.61
1:B:204:ILE:HG12	1:B:754:VAL:HG21	1.83	0.61
1:D:219:LEU:HD23	1:E:749:TRP:CZ3	2.36	0.61
1:F:902:LEU:HD21	1:F:1016:PHE:HB2	1.82	0.61
1:A:75:LEU:HD13	1:A:92:LEU:HD23	1.81	0.61
1:D:445:ILE:HG21	1:D:935:LYS:HD2	1.81	0.61
1:B:80:SER:HB3	1:B:90:ILE:HG23	1.82	0.61
1:B:1006:MET:O	1:B:1010:THR:HG23	2.00	0.61
1:D:344:LEU:CD2	1:D:402:ILE:HD11	2.30	0.61
1:D:697:LEU:HD21	1:D:839:MET:HE1	1.82	0.61
1:E:280:GLU:HG3	1:E:285:PRO:HA	1.81	0.61
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.83	0.61
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.83	0.61
1:B:172:VAL:HG13	1:B:291:ILE:HG23	1.83	0.61
1:C:200:PRO:HB2	1:C:744:THR:HG22	1.83	0.61
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.83	0.61
1:E:531:VAL:O	1:E:534:ILE:HG13	2.01	0.61
1:C:254:ASN:ND2	1:C:258:SER:OG	2.22	0.61
1:C:1032:ASN:H	1:C:1033:GLU:HB2	1.65	0.61
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.36	0.61
1:F:57:VAL:HG23	1:F:82:SER:HB3	1.83	0.61
1:B:49:TYR:HD2	1:B:50:PRO:HD2	1.66	0.61
1:E:694:ARG:HB3	1:E:694:ARG:HH11	1.65	0.61
1:F:34:GLN:O	1:F:391:ASN:HB2	2.01	0.61
1:F:340:VAL:CG1	1:F:395:MET:HB3	2.28	0.61
1:F:121:GLU:O	1:F:124:GLN:HG2	2.00	0.60
1:A:525:HIS:HA	1:A:528:THR:HG22	1.82	0.60
1:B:395:MET:O	1:B:398:MET:HB2	2.00	0.60
1:B:697:LEU:HD22	1:B:846:LEU:HD11	1.83	0.60
1:C:697:LEU:HD12	1:C:846:LEU:HD11	1.82	0.60
1:D:695:ASN:HA	1:D:698:LEU:HD12	1.83	0.60
1:C:752:SER:O	1:C:767:TYR:HA	2.00	0.60
1:D:26:ALA:HB1	1:D:384:ALA:HB2	1.84	0.60
1:E:332:PHE:O	1:E:336:SER:OG	2.15	0.60
1:E:544:LEU:O	1:E:548:ILE:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:LEU:HD11	1:D:92:LEU:HD23	1.82	0.60
1:D:423:GLU:C	1:D:502:LYS:HB3	2.26	0.60
1:F:538:THR:HG23	1:F:542:LEU:HD13	1.83	0.60
1:A:448:VAL:HG22	1:A:882:CYS:HB3	1.84	0.60
1:A:514:GLY:C	1:A:516:PHE:H	2.10	0.60
1:A:723:LYS:HD2	1:C:235:ILE:O	2.01	0.60
1:C:925:GLY:HA2	1:C:1002:VAL:HG22	1.84	0.60
1:E:1006:MET:O	1:E:1010:THR:HG23	2.00	0.60
1:F:896:VAL:HG23	1:F:937:ALA:CB	2.32	0.60
1:A:281:PHE:CE1	1:A:324:VAL:HG21	2.36	0.60
1:A:605:ASN:OD1	1:A:637:ASN:ND2	2.34	0.60
1:C:515:TRP:HD1	1:C:518:ARG:HH12	1.49	0.60
1:C:689:LYS:HA	1:C:692:GLN:OE1	2.01	0.60
1:C:892:ILE:O	1:C:896:VAL:HG12	2.02	0.60
1:E:670:GLY:HA2	1:E:857:MET:SD	2.42	0.60
1:F:576:VAL:HG13	1:F:658:VAL:HG22	1.84	0.60
1:F:638:LYS:HE2	1:F:640:GLU:HG3	1.84	0.60
1:F:935:LYS:HE2	1:F:936:ASN:OD1	2.01	0.60
1:B:7:ASP:OD2	1:B:432:ARG:NH2	2.34	0.60
1:B:213:GLN:HA	1:B:237:GLN:O	2.02	0.60
1:C:676:ASP:HB3	1:C:823:LEU:HD23	1.82	0.60
1:E:57:VAL:HB	1:E:88:VAL:HG23	1.84	0.60
1:A:188:MET:O	1:A:771:GLU:HB2	2.02	0.60
1:B:778:PRO:O	1:B:781:ILE:HG12	2.02	0.60
1:D:3:ASN:O	1:D:6:ILE:N	2.35	0.60
1:E:1008:THR:O	1:E:1012:LEU:HB2	2.01	0.60
1:F:359:LEU:HB2	1:F:365:THR:HG22	1.84	0.60
1:C:171:GLY:HA3	1:C:302:THR:OG1	2.01	0.60
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.67	0.60
1:C:694:ARG:HD3	1:C:820:MET:SD	2.42	0.60
1:D:30:LEU:HD12	1:D:31:PRO:HD2	1.84	0.60
1:F:379:THR:HG23	1:F:476:SER:OG	2.02	0.60
1:B:757:PHE:HE1	1:B:759:ASP:HB2	1.65	0.59
1:C:884:ALA:HB1	1:C:890:TRP:CZ3	2.37	0.59
1:C:1030:ARG:HH21	1:C:1030:ARG:HB2	1.66	0.59
1:D:13:TRP:CZ2	1:D:492:LEU:HD21	2.36	0.59
1:E:396:PHE:O	1:E:400:LEU:HB2	2.02	0.59
1:F:239:ARG:NH1	1:F:756:ASP:HB2	2.17	0.59
1:A:549:VAL:O	1:A:552:MET:HB3	2.02	0.59
1:C:15:ILE:O	1:C:19:ILE:HG13	2.02	0.59
1:D:95:GLU:HB2	1:D:98:THR:OG1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:VAL:HG13	1:F:118:LEU:HD13	1.83	0.59
1:F:470:PHE:CD2	1:F:924:VAL:HG11	2.37	0.59
1:B:629:TRP:CD1	1:B:629:TRP:H	2.21	0.59
1:F:892:ILE:HD12	1:F:1021:PHE:HE1	1.67	0.59
1:A:216:ALA:HB1	1:A:234:ILE:O	2.02	0.59
1:A:602:GLU:HG3	1:A:605:ASN:HB2	1.84	0.59
1:A:771:GLU:HB3	1:A:774:TYR:HD1	1.68	0.59
1:B:187:TRP:HB3	1:B:771:GLU:HA	1.85	0.59
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.84	0.59
1:D:467:TYR:HE1	1:D:920:VAL:HG22	1.66	0.59
1:D:941:VAL:HG13	1:D:1021:PHE:HE1	1.68	0.59
1:D:1036:GLU:HB3	1:D:1037:HIS:CB	2.32	0.59
1:E:361:ASN:O	1:E:365:THR:HG22	2.01	0.59
1:A:523:SER:O	1:A:526:HIS:HB2	2.03	0.59
1:A:700:GLU:HB3	1:A:842:LEU:HD22	1.84	0.59
1:B:69:MET:HE1	1:B:107:VAL:HG13	1.84	0.59
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.37	0.59
1:B:327:TYR:HB2	1:B:623:PHE:CE2	2.34	0.59
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.82	0.59
1:E:613:ASN:HD22	1:E:613:ASN:C	2.10	0.59
1:F:15:ILE:O	1:F:19:ILE:HG13	2.01	0.59
1:A:721:GLN:HB3	1:C:233:SER:O	2.02	0.59
1:C:249:ILE:O	1:C:262:LEU:N	2.35	0.59
1:C:545:TYR:OH	1:C:898:LEU:O	2.13	0.59
1:E:1032:ASN:CB	1:E:1033:GLU:HB3	2.32	0.59
1:A:610:PHE:O	1:A:622:ALA:HA	2.03	0.59
1:B:143:ILE:HG12	1:B:322:LYS:O	2.02	0.59
1:B:631:ASP:C	1:B:633:PRO:HD3	2.28	0.59
1:B:945:LYS:HZ1	1:B:1025:ARG:HH21	1.50	0.59
1:E:545:TYR:OH	1:E:898:LEU:O	2.19	0.59
1:B:677:PHE:HE2	1:B:679:LEU:HB2	1.67	0.59
1:E:853:ASP:OD1	1:E:854:TRP:N	2.35	0.59
1:F:376:LEU:HD22	1:F:398:MET:HE1	1.84	0.59
1:D:26:ALA:HB1	1:D:384:ALA:CB	2.33	0.59
1:D:213:GLN:HA	1:D:237:GLN:O	2.02	0.59
1:E:140:VAL:HG13	1:E:324:VAL:O	2.02	0.59
1:F:631:ASP:C	1:F:633:PRO:HD3	2.27	0.59
1:B:492:LEU:O	1:B:496:MET:HG2	2.03	0.59
1:B:858:SER:O	1:B:862:ARG:HB2	2.02	0.59
1:D:737:SER:O	1:D:741:ILE:HG13	2.03	0.59
1:D:795:PRO:HG2	1:D:798:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:PRO:HD3	1:E:391:ASN:CG	2.28	0.59
1:E:76:MET:HE3	1:E:95:GLU:HA	1.84	0.59
1:A:920:VAL:O	1:A:924:VAL:HG23	2.03	0.58
1:C:455:PRO:HG2	1:C:875:SER:HA	1.85	0.58
1:D:694:ARG:NH1	1:D:820:MET:SD	2.76	0.58
1:F:595:THR:O	1:F:599:LEU:HG	2.03	0.58
1:A:593:GLU:OE2	1:A:654:LYS:NZ	2.34	0.58
1:E:599:LEU:HD21	1:E:609:VAL:HG23	1.84	0.58
1:E:955:LEU:HD21	1:E:1022:VAL:HA	1.85	0.58
1:F:689:LYS:H	1:F:689:LYS:CD	2.16	0.58
1:A:582:ALA:HB2	1:A:586:ARG:HH21	1.68	0.58
1:A:736:VAL:HG22	1:A:788:ALA:HB2	1.85	0.58
1:D:465:ALA:O	1:D:469:GLN:HG2	2.02	0.58
1:C:700:GLU:OE1	1:C:845:LYS:HE2	2.03	0.58
1:D:549:VAL:O	1:D:552:MET:HB3	2.03	0.58
1:D:887:TYR:CD2	1:D:892:ILE:HG22	2.38	0.58
1:E:540:ARG:HH22	2:E:1101:LMT:H6'2	1.68	0.58
1:F:133:SER:O	1:F:134:SER:HB2	2.02	0.58
1:F:184:MET:HB2	1:F:757:PHE:CE2	2.38	0.58
1:F:452:VAL:O	1:F:455:PRO:HD2	2.03	0.58
1:F:693:ALA:O	1:F:696:GLN:HB3	2.03	0.58
1:A:400:LEU:HD12	1:A:928:THR:HG21	1.85	0.58
1:A:574:THR:HG21	1:A:598:TYR:CE2	2.32	0.58
1:B:908:LEU:HD23	1:B:922:PHE:HZ	1.68	0.58
1:D:181:GLN:HG2	1:D:182:TYR:N	2.18	0.58
1:D:773:LYS:HB3	1:F:225:VAL:HG11	1.85	0.58
1:E:38:ILE:HD13	1:E:466:ILE:HG12	1.85	0.58
1:E:367:ILE:HD11	1:E:497:LEU:HD13	1.84	0.58
1:E:415:ASN:O	1:E:419:VAL:HG23	2.03	0.58
1:E:463:THR:O	1:E:467:TYR:HD1	1.86	0.58
1:F:571:VAL:HG22	1:F:625:SER:HA	1.86	0.58
1:F:616:GLY:O	1:F:618:ASN:N	2.37	0.58
1:F:884:ALA:HB2	1:F:893:PRO:HG2	1.85	0.58
1:C:597:TYR:HE1	1:C:601:LYS:HD2	1.68	0.58
1:E:166:ILE:HA	1:E:309:GLU:HG2	1.84	0.58
1:E:526:HIS:O	1:E:530:SER:HB2	2.03	0.58
1:A:770:SER:HB3	1:A:775:ARG:HD3	1.83	0.58
1:A:881:LEU:HB3	1:C:14:VAL:HG13	1.85	0.58
1:B:906:GLY:HA3	1:B:1008:THR:OG1	2.04	0.58
1:D:388:PHE:HE1	1:D:472:ILE:HG21	1.69	0.58
1:A:130:GLU:OE1	1:A:174:ASP:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:MET:HB2	1:B:153:ASP:HB2	1.86	0.58
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.86	0.58
1:C:336:SER:O	1:C:340:VAL:HG23	2.04	0.58
1:D:251:LEU:HD11	1:D:262:LEU:HD13	1.84	0.58
1:E:687:HIS:CE1	1:E:808:SER:HB2	2.38	0.58
1:F:563:PHE:CZ	1:F:564:LEU:HD13	2.39	0.58
1:A:728:GLN:HE22	1:A:738:ILE:HG21	1.69	0.58
1:A:1032:ASN:N	1:A:1035:ILE:HD11	2.18	0.58
1:B:545:TYR:CE2	1:B:1020:PHE:HZ	2.21	0.58
1:C:211:ASN:OD1	1:C:240:LEU:HG	2.04	0.58
1:B:602:GLU:OE1	1:B:645:ARG:HD2	2.04	0.58
1:C:222:THR:HA	1:C:224:PRO:HD3	1.85	0.58
1:D:438:ILE:O	1:D:441:ALA:HB3	2.03	0.58
1:F:185:ARG:NH2	1:F:273:GLU:O	2.28	0.58
1:F:536:ARG:HD2	2:F:2000:LMT:O4'	2.04	0.58
1:A:105:VAL:HG13	1:B:109:ASN:HD21	1.68	0.57
1:A:749:TRP:HZ3	1:C:219:LEU:HD23	1.67	0.57
1:B:559:LEU:HD22	1:B:560:PRO:HD2	1.85	0.57
1:E:239:ARG:NH1	1:E:755:ASN:OD1	2.37	0.57
1:E:653:ILE:HG13	1:E:654:LYS:HD2	1.86	0.57
1:E:686:GLY:H	1:E:689:LYS:HB2	1.68	0.57
1:C:216:ALA:HB1	1:C:234:ILE:O	2.05	0.57
1:C:356:TYR:CD1	1:C:365:THR:HG21	2.39	0.57
1:F:187:TRP:HB3	1:F:771:GLU:HA	1.85	0.57
1:A:531:VAL:O	1:A:535:LEU:HG	2.05	0.57
1:E:78:MET:N	1:E:815:ASN:OD1	2.33	0.57
1:E:354:VAL:HG21	1:E:976:ALA:HB2	1.86	0.57
1:E:670:GLY:C	1:E:672:ALA:H	2.12	0.57
1:E:982:MET:HA	1:E:1003:MET:HE3	1.87	0.57
1:F:982:MET:HB3	1:F:983:PRO:HD3	1.86	0.57
1:A:1022:VAL:O	1:A:1026:ARG:HG3	2.03	0.57
1:D:1035:ILE:O	1:D:1036:GLU:HG3	2.04	0.57
1:E:902:LEU:HG	1:E:1012:LEU:HB3	1.85	0.57
1:E:1029:SER:OG	1:E:1030:ARG:N	2.31	0.57
1:A:280:GLU:HG3	1:A:285:PRO:HA	1.85	0.57
1:B:677:PHE:CE2	1:B:822:ILE:HD12	2.39	0.57
1:D:525:HIS:HA	1:D:528:THR:HG22	1.86	0.57
1:A:350:LEU:HD13	1:A:980:GLY:HA2	1.86	0.57
1:B:415:ASN:O	1:B:419:VAL:HG23	2.05	0.57
1:C:756:ASP:OD1	1:C:765:LYS:HA	2.04	0.57
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:854:TRP:CE3	1:E:858:SER:HB3	2.40	0.57
1:F:452:VAL:C	1:F:455:PRO:HD2	2.30	0.57
1:B:676:ASP:N	1:B:858:SER:OG	2.33	0.57
1:C:75:LEU:HD11	1:C:92:LEU:HD12	1.86	0.57
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.39	0.57
1:D:527:TYR:O	1:D:531:VAL:HG23	2.05	0.57
1:E:889:SER:HB3	1:E:892:ILE:HG13	1.87	0.57
1:A:259:ARG:NH1	1:B:729:GLU:OE2	2.38	0.57
1:B:531:VAL:HA	1:B:534:ILE:HG12	1.87	0.57
1:C:563:PHE:O	1:C:919:ASP:HB2	2.05	0.57
1:C:884:ALA:HB2	1:C:893:PRO:HG2	1.85	0.57
1:D:405:LEU:HD22	1:D:481:SER:HB3	1.87	0.57
1:D:405:LEU:HD21	1:D:477:ALA:HB1	1.87	0.57
1:E:577:GLN:NE2	1:E:618:ASN:OD1	2.38	0.57
1:E:643:THR:O	1:E:647:THR:OG1	2.23	0.57
1:B:36:PRO:HD3	1:B:391:ASN:CG	2.30	0.57
1:B:484:VAL:O	1:B:489:THR:HG23	2.05	0.57
1:D:453:PHE:CE2	1:D:474:ILE:HG21	2.40	0.57
1:D:677:PHE:CD2	1:D:822:ILE:HD12	2.39	0.57
1:D:1030:ARG:HE	1:D:1031:LYS:HB2	1.69	0.57
1:E:154:ILE:HG22	1:E:287:SER:HB3	1.86	0.57
1:E:540:ARG:HH22	2:E:1101:LMT:C6B	2.18	0.57
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.86	0.57
1:F:771:GLU:HB2	1:F:774:TYR:CD1	2.39	0.57
1:A:916:LEU:HD13	1:A:917:THR:HG22	1.87	0.57
1:A:963:VAL:HA	1:A:966:ARG:HH22	1.69	0.57
1:E:697:LEU:HD11	1:E:842:LEU:HB3	1.86	0.57
1:F:23:GLY:HA2	1:F:381:ALA:HB2	1.86	0.57
1:A:133:SER:OG	1:A:134:SER:N	2.38	0.56
1:A:457:ALA:HB2	1:A:471:SER:OG	2.04	0.56
1:A:530:SER:HG	2:A:1101:LMT:H2O2	1.52	0.56
1:A:966:ARG:C	1:A:969:PRO:HD2	2.30	0.56
1:E:172:VAL:HG22	1:E:306:ILE:HD11	1.87	0.56
1:A:363:ARG:O	1:A:366:LEU:HB2	2.05	0.56
1:A:448:VAL:O	1:A:451:ALA:HB3	2.05	0.56
1:B:560:PRO:O	1:B:918:ASN:HB3	2.04	0.56
1:C:890:TRP:CE3	1:C:890:TRP:HA	2.41	0.56
1:D:247:GLY:O	1:D:263:ARG:N	2.33	0.56
1:D:393:LEU:HD22	1:D:470:PHE:HE1	1.69	0.56
1:D:516:PHE:HA	1:D:519:MET:HG3	1.86	0.56
1:D:564:LEU:HB2	1:D:666:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:966:ARG:HB3	1:D:966:ARG:HH11	1.70	0.56
1:E:597:TYR:OH	1:E:646:ALA:HA	2.05	0.56
1:A:418:ARG:O	1:A:422:GLU:HB2	2.05	0.56
1:B:968:ARG:HG2	1:B:972:MET:HE2	1.87	0.56
1:C:185:ARG:HH12	1:C:769:MET:HB2	1.70	0.56
1:C:188:MET:SD	1:C:200:PRO:HG3	2.45	0.56
1:C:352:PHE:HD1	1:C:369:THR:HG21	1.70	0.56
1:C:449:LEU:O	1:C:452:VAL:HG23	2.06	0.56
1:D:124:GLN:HA	1:E:117:LEU:HD12	1.87	0.56
1:D:858:SER:HA	1:D:861:GLU:CD	2.31	0.56
1:E:470:PHE:O	1:E:474:ILE:HG13	2.04	0.56
1:E:697:LEU:HD13	1:E:846:LEU:HD21	1.87	0.56
1:E:842:LEU:O	1:E:845:LYS:HB2	2.05	0.56
1:A:80:SER:HB3	1:A:90:ILE:HG23	1.88	0.56
1:A:399:VAL:HG11	1:A:984:LEU:HD11	1.86	0.56
1:A:534:ILE:HD12	1:A:535:LEU:HD23	1.87	0.56
1:C:154:ILE:HG22	1:C:287:SER:HB3	1.87	0.56
1:C:309:GLU:HG3	1:C:313:MET:HE3	1.86	0.56
1:C:355:MET:CG	1:C:410:ILE:HD11	2.36	0.56
1:A:978:ILE:HG23	1:A:1003:MET:HG3	1.88	0.56
1:B:525:HIS:NE2	1:B:529:ASP:OD1	2.38	0.56
1:D:393:LEU:HD11	1:D:466:ILE:HD13	1.86	0.56
1:E:35:TYR:HE2	1:E:393:LEU:HD21	1.71	0.56
1:E:1022:VAL:O	1:E:1026:ARG:HG3	2.06	0.56
1:F:514:GLY:HA2	1:F:517:ASN:OD1	2.06	0.56
1:A:10:ILE:O	1:A:14:VAL:HG23	2.04	0.56
1:A:776:MET:O	1:C:219:LEU:HB3	2.05	0.56
1:D:272:GLY:N	1:D:275:TYR:OH	2.35	0.56
1:D:966:ARG:C	1:D:969:PRO:HD2	2.30	0.56
1:E:280:GLU:O	1:E:610:PHE:HA	2.06	0.56
1:F:892:ILE:HD12	1:F:1021:PHE:CE1	2.40	0.56
1:A:795:PRO:HG2	1:A:798:ALA:HB2	1.87	0.56
1:C:925:GLY:O	1:C:929:THR:OG1	2.24	0.56
1:D:423:GLU:O	1:D:502:LYS:HB3	2.06	0.56
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.88	0.56
1:C:568:ASP:CG	1:C:632:ARG:HH22	2.13	0.56
1:C:602:GLU:OE2	1:C:645:ARG:NH1	2.39	0.56
1:E:840:GLU:HG2	1:E:852:TYR:HE1	1.71	0.56
1:B:412:VAL:O	1:B:416:VAL:HG23	2.05	0.56
1:D:455:PRO:HG2	1:D:875:SER:CB	2.35	0.56
1:E:380:PHE:O	1:E:384:ALA:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:LEU:O	1:E:445:ILE:HG13	2.06	0.56
1:C:149:MET:HG3	1:C:154:ILE:HG13	1.88	0.56
1:C:921:TYR:HD1	1:C:997:ALA:HB3	1.69	0.56
1:F:723:LYS:HG2	1:F:803:ARG:NH2	2.20	0.56
1:A:276:ASP:HA	1:C:222:THR:HG21	1.88	0.55
1:A:300:LEU:HD11	1:A:333:VAL:HG11	1.88	0.55
1:A:632:ARG:HB3	1:A:637:ASN:HB3	1.88	0.55
1:F:351:VAL:HG22	1:F:976:ALA:HB1	1.87	0.55
1:A:273:GLU:HG2	1:A:765:LYS:HD2	1.89	0.55
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.40	0.55
1:B:463:THR:HA	1:B:466:ILE:HD12	1.88	0.55
1:B:908:LEU:HD23	1:B:922:PHE:CZ	2.41	0.55
1:C:391:ASN:O	1:C:394:THR:OG1	2.21	0.55
1:D:185:ARG:HH12	1:D:769:MET:HB2	1.70	0.55
1:D:347:ALA:O	1:D:351:VAL:HG23	2.06	0.55
1:D:701:ALA:HB1	1:D:711:VAL:HG11	1.88	0.55
1:E:157:TYR:CZ	1:E:318:PRO:HD3	2.41	0.55
1:F:578:LEU:HD12	1:F:587:THR:HG22	1.88	0.55
1:A:544:LEU:O	1:A:548:ILE:HG13	2.07	0.55
1:D:170:SER:HB2	1:E:75:LEU:H	1.71	0.55
1:D:264:ASP:N	1:D:264:ASP:OD1	2.37	0.55
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.71	0.55
1:E:412:VAL:O	1:E:416:VAL:HG23	2.07	0.55
1:F:58:GLN:OE1	1:F:811:LEU:HB3	2.07	0.55
1:F:406:VAL:O	1:F:407:ASP:C	2.49	0.55
1:F:896:VAL:HG23	1:F:937:ALA:HB1	1.89	0.55
1:A:222:THR:HA	1:A:224:PRO:HD3	1.88	0.55
1:A:572:PHE:HB2	1:A:661:PHE:O	2.05	0.55
1:B:898:LEU:HB3	1:B:1020:PHE:CE2	2.42	0.55
1:C:184:MET:HB3	1:C:766:VAL:HG13	1.88	0.55
1:C:896:VAL:HG23	1:C:937:ALA:CB	2.36	0.55
1:D:59:ASP:OD2	1:F:758:ILE:HD13	2.07	0.55
1:D:888:GLU:OE1	1:F:11:PHE:HB2	2.07	0.55
1:E:953:LYS:HG3	1:E:957:GLU:CD	2.31	0.55
1:B:1031:LYS:H	1:B:1033:GLU:HG3	1.72	0.55
1:C:165:ALA:O	1:C:169:THR:OG1	2.09	0.55
1:C:391:ASN:OD1	1:C:393:LEU:HB2	2.07	0.55
1:D:470:PHE:CD2	1:D:924:VAL:HG21	2.42	0.55
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.88	0.55
1:E:281:PHE:HB2	1:E:610:PHE:CE1	2.41	0.55
1:F:135:SER:HB2	1:F:667:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1028:PHE:O	1:F:1030:ARG:N	2.40	0.55
1:A:146:ASP:OD2	1:A:146:ASP:N	2.36	0.55
1:A:841:GLN:O	1:A:844:SER:OG	2.25	0.55
1:C:68:ASN:HB3	1:C:110:LYS:O	2.07	0.55
1:D:448:VAL:HG22	1:D:882:CYS:CB	2.37	0.55
1:D:778:PRO:O	1:D:781:ILE:HG12	2.06	0.55
1:A:3:ASN:HA	1:A:6:ILE:HG23	1.89	0.55
1:B:184:MET:HB2	1:B:757:PHE:CD2	2.42	0.55
1:C:508:GLY:O	1:C:509:LYS:HB2	2.06	0.55
1:C:722:PHE:CE2	1:C:802:SER:HB2	2.42	0.55
1:C:942:GLU:HG3	1:C:943:PHE:HD1	1.71	0.55
1:D:449:LEU:HB3	1:D:478:MET:SD	2.46	0.55
1:D:836:MET:HG2	1:D:854:TRP:CZ2	2.42	0.55
1:E:105:VAL:HG21	1:F:105:VAL:HG13	1.89	0.55
1:F:143:ILE:O	1:F:321:LEU:HD22	2.06	0.55
1:F:298:ASN:HB3	1:F:301:ASP:OD2	2.07	0.55
1:F:412:VAL:O	1:F:416:VAL:HG23	2.06	0.55
1:F:728:GLN:OE1	1:F:738:ILE:HG12	2.07	0.55
1:F:887:TYR:C	1:F:889:SER:H	2.13	0.55
1:C:927:LEU:O	1:C:928:THR:C	2.50	0.55
1:D:501:ALA:O	1:D:504:ASP:HB2	2.06	0.55
1:D:723:LYS:HG2	1:D:803:ARG:CZ	2.37	0.55
1:E:569:GLN:NE2	1:E:665:ALA:HA	2.21	0.55
1:A:105:VAL:HG13	1:B:109:ASN:ND2	2.22	0.55
1:A:281:PHE:CD1	1:A:324:VAL:HG11	2.42	0.55
1:A:356:TYR:HD1	1:A:365:THR:HG21	1.72	0.55
1:D:143:ILE:O	1:D:321:LEU:HD22	2.07	0.55
1:E:149:MET:HG3	1:E:154:ILE:HG13	1.89	0.55
1:E:220:GLY:HA3	1:E:230:LEU:O	2.07	0.55
1:A:778:PRO:O	1:A:781:ILE:HG12	2.07	0.55
1:A:1002:VAL:O	1:A:1006:MET:HG2	2.07	0.55
1:B:757:PHE:CE1	1:B:759:ASP:HB2	2.41	0.55
1:C:200:PRO:HA	1:C:203:VAL:CG2	2.37	0.55
1:D:175:VAL:HG11	1:D:289:LEU:HD13	1.88	0.55
1:D:366:LEU:HD23	1:D:369:THR:HB	1.89	0.55
1:E:188:MET:O	1:E:771:GLU:HB2	2.06	0.55
1:E:712:ARG:HH21	1:E:823:LEU:HB3	1.71	0.55
1:F:688:GLU:HB3	1:F:689:LYS:HD2	1.89	0.55
1:A:396:PHE:HZ	1:A:995:GLN:HG2	1.70	0.54
1:B:425:LEU:HD12	1:B:430:ALA:HA	1.89	0.54
1:C:108:GLN:O	1:C:112:GLN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:VAL:HG12	1:C:472:ILE:HD11	1.89	0.54
1:C:531:VAL:HA	1:C:534:ILE:HG12	1.89	0.54
1:D:166:ILE:HD12	1:D:306:ILE:HG23	1.88	0.54
1:D:595:THR:O	1:D:599:LEU:HG	2.05	0.54
1:E:352:PHE:HE1	1:E:366:LEU:HD23	1.72	0.54
1:E:435:MET:SD	1:E:490:PRO:HB3	2.46	0.54
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.89	0.54
1:B:355:MET:HE2	1:B:972:MET:SD	2.48	0.54
1:B:404:LEU:HD12	1:B:932:LEU:HD21	1.89	0.54
1:C:568:ASP:O	1:C:629:TRP:CH2	2.61	0.54
1:C:795:PRO:HG2	1:C:798:ALA:HB2	1.90	0.54
1:D:449:LEU:O	1:D:452:VAL:HG22	2.07	0.54
1:E:355:MET:HB3	1:E:365:THR:OG1	2.06	0.54
1:E:514:GLY:C	1:E:516:PHE:H	2.15	0.54
1:E:613:ASN:ND2	1:E:619:THR:O	2.40	0.54
1:E:940:ILE:HD11	1:E:970:ILE:HD11	1.90	0.54
1:F:431:THR:O	1:F:435:MET:HE2	2.08	0.54
1:F:455:PRO:HG3	1:F:878:VAL:HG21	1.89	0.54
1:F:974:SER:OG	1:F:1010:THR:HG21	2.07	0.54
1:A:377:LEU:O	1:A:380:PHE:HB2	2.07	0.54
1:B:586:ARG:O	1:B:589:LYS:HB3	2.07	0.54
1:C:355:MET:HG2	1:C:410:ILE:HD11	1.88	0.54
1:D:188:MET:HB3	1:D:193:LEU:HD11	1.88	0.54
1:E:887:TYR:O	1:E:889:SER:N	2.40	0.54
1:A:202:ASP:OD1	1:A:787:ARG:NH2	2.38	0.54
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.87	0.54
1:B:739:ASN:O	1:B:743:THR:OG1	2.09	0.54
1:C:408:ASP:O	1:C:412:VAL:HG23	2.07	0.54
1:D:108:GLN:O	1:D:112:GLN:HG2	2.08	0.54
1:D:135:SER:O	1:D:292:LYS:HG2	2.07	0.54
1:D:242:SER:O	1:D:246:PHE:HD1	1.91	0.54
1:D:955:LEU:N	1:D:1033:GLU:O	2.37	0.54
1:A:420:MET:HB3	1:A:500:ILE:HB	1.90	0.54
1:B:423:GLU:O	1:B:502:LYS:HD2	2.06	0.54
1:D:54:ALA:HB1	1:D:811:LEU:HG	1.90	0.54
1:E:359:LEU:C	1:E:360:GLN:HG2	2.32	0.54
1:B:171:GLY:HA3	1:B:302:THR:OG1	2.07	0.54
1:C:883:LEU:HD21	1:C:938:ILE:HD11	1.89	0.54
1:D:880:PHE:HD1	1:D:897:MET:HE2	1.72	0.54
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.38	0.54
1:C:136:PHE:HB2	1:C:327:TYR:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:947:LEU:HB2	1:D:958:ALA:HB1	1.90	0.54
1:F:681:ASP:O	1:F:817:LEU:HD13	2.07	0.54
1:F:936:ASN:ND2	1:F:1010:THR:HG22	2.22	0.54
1:A:565:PRO:HG2	1:A:567:GLU:OE2	2.08	0.54
1:B:172:VAL:HG22	1:B:306:ILE:HD11	1.89	0.54
1:C:24:GLY:HA2	1:C:27:ILE:HG23	1.89	0.54
1:C:642:ILE:O	1:C:645:ARG:HG2	2.08	0.54
1:C:1006:MET:O	1:C:1010:THR:OG1	2.25	0.54
1:D:538:THR:HG23	1:D:542:LEU:HD13	1.90	0.54
1:D:904:VAL:HG22	1:D:926:LEU:HD21	1.89	0.54
1:D:962:ALA:O	1:D:965:MET:HG2	2.07	0.54
1:E:44:THR:HA	1:E:90:ILE:O	2.07	0.54
1:E:444:GLY:O	1:E:448:VAL:HG23	2.08	0.54
1:E:545:TYR:CE2	1:E:1020:PHE:HZ	2.25	0.54
1:E:663:LEU:HD23	1:E:663:LEU:H	1.72	0.54
1:F:677:PHE:HB2	1:F:854:TRP:CZ3	2.43	0.54
1:A:629:TRP:H	1:A:629:TRP:CD1	2.26	0.54
1:A:936:ASN:O	1:A:940:ILE:HG13	2.08	0.54
1:B:280:GLU:HG2	1:B:283:GLY:C	2.32	0.54
1:B:412:VAL:HG22	1:B:438:ILE:HD11	1.89	0.54
1:B:771:GLU:HB3	1:B:774:TYR:CD1	2.43	0.54
1:B:941:VAL:HG13	1:B:1021:PHE:CE1	2.42	0.54
1:C:395:MET:O	1:C:398:MET:HB2	2.07	0.54
1:D:692:GLN:HA	1:D:695:ASN:HB2	1.89	0.54
1:D:1033:GLU:HB3	1:D:1034:ASP:HB2	1.90	0.54
1:E:536:ARG:CZ	2:E:1101:LMT:O3B	2.55	0.54
1:E:770:SER:HB3	1:E:775:ARG:HD3	1.89	0.54
1:F:164:ASP:OD1	1:F:762:ARG:NH2	2.40	0.54
1:A:34:GLN:HE22	1:A:569:GLN:NE2	2.06	0.54
1:B:198:LEU:HD21	1:B:252:LYS:HB2	1.90	0.54
1:B:272:GLY:N	1:B:275:TYR:OH	2.21	0.54
1:C:520:PHE:CE2	1:C:968:ARG:HD2	2.43	0.54
1:D:559:LEU:HD23	1:D:560:PRO:HD2	1.90	0.54
1:D:776:MET:HE3	1:F:228:GLN:OE1	2.07	0.54
1:E:43:VAL:HG13	1:E:130:GLU:C	2.33	0.54
1:E:138:MET:HG3	1:E:327:TYR:O	2.08	0.54
1:E:356:TYR:C	1:E:358:PHE:H	2.16	0.54
1:E:593:GLU:OE1	1:E:654:LYS:NZ	2.34	0.54
1:F:114:ALA:O	1:F:118:LEU:HG	2.08	0.54
1:F:435:MET:O	1:F:439:GLN:HB2	2.08	0.54
1:F:488:LEU:O	1:F:491:ALA:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ILE:HD11	1:A:306:ILE:HG23	1.90	0.53
1:A:220:GLY:HA3	1:A:230:LEU:O	2.08	0.53
1:A:545:TYR:O	1:A:549:VAL:HG23	2.08	0.53
1:A:577:GLN:OE1	1:A:619:THR:HG23	2.08	0.53
1:A:769:MET:HG2	1:A:770:SER:H	1.72	0.53
1:B:468:ARG:HG2	1:B:472:ILE:HD13	1.89	0.53
1:B:1038:SER:OG	1:B:1039:HIS:N	2.31	0.53
1:C:351:VAL:HG12	1:C:355:MET:HE2	1.89	0.53
1:D:694:ARG:HD2	1:D:713:PRO:HB3	1.90	0.53
1:E:1019:VAL:O	1:E:1023:VAL:HG23	2.08	0.53
1:F:38:ILE:HD13	1:F:466:ILE:HD13	1.90	0.53
1:F:772:ALA:O	1:F:776:MET:HE3	2.07	0.53
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.90	0.53
1:A:896:VAL:HG21	1:A:938:ILE:HG13	1.90	0.53
1:B:945:LYS:NZ	1:B:1025:ARG:HH21	2.07	0.53
1:B:1034:ASP:N	1:B:1035:ILE:HG22	2.24	0.53
1:D:21:LEU:O	1:D:25:LEU:HB2	2.08	0.53
1:D:185:ARG:HB2	1:D:271:GLY:HA3	1.89	0.53
1:D:186:ILE:HB	1:D:768:VAL:HG22	1.91	0.53
1:D:908:LEU:HD23	1:D:922:PHE:CZ	2.43	0.53
1:A:451:ALA:HB1	1:A:878:VAL:HG12	1.91	0.53
1:A:492:LEU:O	1:A:496:MET:HG2	2.08	0.53
1:A:728:GLN:NE2	1:A:738:ILE:HG21	2.23	0.53
1:A:940:ILE:HG12	1:A:966:ARG:NE	2.23	0.53
1:C:893:PRO:HA	1:C:896:VAL:HG12	1.89	0.53
1:C:935:LYS:NZ	1:C:973:THR:HG21	2.24	0.53
1:D:491:ALA:O	1:D:495:THR:OG1	2.24	0.53
1:A:143:ILE:HG22	1:A:286:ALA:HB1	1.91	0.53
1:A:157:TYR:CZ	1:A:318:PRO:HD3	2.44	0.53
1:A:281:PHE:HB2	1:A:610:PHE:CE1	2.43	0.53
1:B:902:LEU:HD11	1:B:1016:PHE:HD2	1.73	0.53
1:C:23:GLY:HA2	1:C:381:ALA:HB2	1.91	0.53
1:C:366:LEU:O	1:C:370:ILE:HG13	2.08	0.53
1:C:525:HIS:HA	1:C:528:THR:HG22	1.91	0.53
1:C:935:LYS:HE2	1:C:936:ASN:OD1	2.09	0.53
1:D:418:ARG:CZ	1:D:965:MET:HE2	2.39	0.53
1:D:873:ALA:O	1:D:877:ILE:HG12	2.08	0.53
1:E:553:ALA:O	1:E:557:VAL:HG23	2.08	0.53
1:F:184:MET:HB2	1:F:757:PHE:CD2	2.42	0.53
1:F:446:ALA:HB3	1:F:482:VAL:HG22	1.89	0.53
1:B:108:GLN:HA	1:B:129:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:THR:HG21	1:C:598:TYR:CE2	2.40	0.53
1:D:428:LYS:O	1:D:431:THR:N	2.42	0.53
1:D:559:LEU:HD12	1:D:908:LEU:HD22	1.90	0.53
1:D:578:LEU:HB2	1:D:618:ASN:O	2.09	0.53
1:E:482:VAL:O	1:E:485:ALA:HB3	2.09	0.53
1:E:926:LEU:O	1:E:930:ILE:HG13	2.09	0.53
1:E:942:GLU:O	1:E:945:LYS:N	2.42	0.53
1:F:197:GLN:HG3	1:F:793:MET:SD	2.49	0.53
1:A:954:GLY:HA2	1:A:1034:ASP:H	1.74	0.53
1:B:952:GLY:O	1:B:1036:GLU:HA	2.08	0.53
1:C:184:MET:HB3	1:C:766:VAL:HG22	1.91	0.53
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.90	0.53
1:D:219:LEU:HD23	1:E:749:TRP:HZ3	1.73	0.53
1:D:723:LYS:HG2	1:D:803:ARG:NH1	2.23	0.53
1:E:26:ALA:O	1:E:30:LEU:HB2	2.09	0.53
1:E:80:SER:HB3	1:E:90:ILE:HG23	1.90	0.53
1:E:974:SER:OG	1:E:1010:THR:HG21	2.09	0.53
1:A:953:LYS:O	1:A:1035:ILE:HB	2.09	0.53
1:C:479:ALA:O	1:C:482:VAL:HG23	2.09	0.53
1:D:233:SER:HB2	1:E:721:GLN:HB3	1.91	0.53
1:D:428:LYS:HG2	1:D:494:ALA:HB1	1.91	0.53
1:E:20:MET:HG3	1:E:374:VAL:HG22	1.91	0.53
1:E:140:VAL:HA	1:E:326:PRO:HD2	1.91	0.53
1:E:468:ARG:HG2	1:E:472:ILE:CD1	2.39	0.53
1:A:888:GLU:OE1	1:C:11:PHE:HB2	2.09	0.53
1:B:902:LEU:HD21	1:B:1016:PHE:HB2	1.90	0.53
1:C:544:LEU:O	1:C:547:ILE:HB	2.08	0.53
1:C:770:SER:HB3	1:C:775:ARG:HD3	1.91	0.53
1:D:335:ILE:O	1:D:339:GLU:HG2	2.09	0.53
1:D:769:MET:HE2	1:D:775:ARG:CZ	2.39	0.53
1:D:968:ARG:HG2	1:D:972:MET:HE2	1.91	0.53
1:E:1005:GLY:O	1:E:1009:ALA:HB2	2.08	0.53
1:F:700:GLU:HA	1:F:703:LYS:NZ	2.24	0.53
1:A:13:TRP:HE1	1:A:492:LEU:HD21	1.73	0.53
1:A:21:LEU:O	1:A:25:LEU:HB2	2.09	0.53
1:A:44:THR:HA	1:A:90:ILE:O	2.09	0.53
1:A:626:LEU:HD11	1:A:639:VAL:CG2	2.39	0.53
1:B:82:SER:HA	1:B:88:VAL:HG22	1.89	0.53
1:B:154:ILE:O	1:B:158:VAL:HG23	2.09	0.53
1:C:65:ILE:HG23	1:C:111:LEU:HD23	1.90	0.53
1:C:571:VAL:HG22	1:C:625:SER:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:899:VAL:O	1:C:902:LEU:HB2	2.09	0.53
1:A:234:ILE:HD11	1:B:749:TRP:CE3	2.44	0.52
1:A:475:VAL:O	1:A:478:MET:HB3	2.08	0.52
1:A:763:VAL:HG12	1:B:63:GLN:HE21	1.73	0.52
1:C:144:ASN:O	1:C:148:THR:OG1	2.22	0.52
1:C:415:ASN:O	1:C:419:VAL:HG23	2.10	0.52
1:E:514:GLY:C	1:E:516:PHE:N	2.63	0.52
1:E:701:ALA:HB1	1:E:711:VAL:HG11	1.90	0.52
1:F:3:ASN:ND2	1:F:435:MET:SD	2.77	0.52
1:F:45:ILE:HD13	1:F:111:LEU:HG	1.89	0.52
1:F:75:LEU:HD11	1:F:92:LEU:HD12	1.91	0.52
1:F:676:ASP:HB3	1:F:823:LEU:HD23	1.91	0.52
1:F:966:ARG:O	1:F:966:ARG:NE	2.40	0.52
1:A:527:TYR:CE1	1:A:1014:ILE:HD12	2.44	0.52
1:A:536:ARG:NH1	2:A:1101:LMT:O4'	2.41	0.52
1:A:910:ALA:HB2	1:A:1004:GLY:HA3	1.90	0.52
1:B:377:LEU:O	1:B:380:PHE:HB2	2.09	0.52
1:B:841:GLN:O	1:B:844:SER:OG	2.26	0.52
1:C:151:GLN:HE22	1:C:286:ALA:H	1.56	0.52
1:C:663:LEU:HA	1:C:672:ALA:HA	1.91	0.52
1:C:917:THR:O	1:C:919:ASP:N	2.43	0.52
1:C:977:PHE:HE2	1:C:1002:VAL:HG12	1.75	0.52
1:D:137:LEU:HD13	1:D:293:LEU:HB2	1.91	0.52
1:D:211:ASN:OD1	1:D:240:LEU:HG	2.09	0.52
1:D:514:GLY:C	1:D:516:PHE:H	2.16	0.52
1:D:991:GLY:O	1:D:993:GLY:N	2.42	0.52
1:E:15:ILE:HD12	1:E:487:ILE:HG21	1.91	0.52
1:E:355:MET:SD	1:E:368:PRO:HG2	2.48	0.52
1:E:854:TRP:HE3	1:E:858:SER:HB3	1.72	0.52
1:A:8:ARG:O	1:A:11:PHE:N	2.42	0.52
1:A:940:ILE:HD12	1:A:1017:VAL:HG11	1.90	0.52
1:B:677:PHE:CD2	1:B:822:ILE:HD12	2.45	0.52
1:C:371:ALA:O	1:C:375:VAL:HG23	2.10	0.52
1:D:366:LEU:HA	1:D:369:THR:HB	1.90	0.52
1:D:896:VAL:HG21	1:D:938:ILE:HG13	1.90	0.52
1:E:445:ILE:HG22	1:E:938:ILE:CD1	2.38	0.52
1:E:961:ASP:O	1:E:964:ARG:HB3	2.09	0.52
1:F:47:ALA:HB2	1:F:127:VAL:HG13	1.92	0.52
1:F:154:ILE:HG22	1:F:287:SER:HB3	1.90	0.52
1:F:446:ALA:CB	1:F:482:VAL:HG22	2.40	0.52
1:A:272:GLY:N	1:A:275:TYR:OH	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:GLU:HG2	1:C:248:LYS:HE3	1.90	0.52
1:C:600:THR:O	1:C:603:LYS:HG3	2.09	0.52
1:D:278:ILE:CG1	1:D:613:ASN:HB3	2.40	0.52
1:D:434:SER:O	1:D:438:ILE:HG12	2.09	0.52
1:E:887:TYR:C	1:E:889:SER:H	2.17	0.52
1:A:452:VAL:HA	1:A:875:SER:OG	2.09	0.52
1:C:190:PRO:HG3	1:C:774:TYR:CG	2.44	0.52
1:C:940:ILE:HA	1:C:966:ARG:NH1	2.25	0.52
1:D:121:GLU:O	1:D:124:GLN:HG2	2.10	0.52
1:D:546:LEU:O	1:D:550:VAL:HG23	2.10	0.52
1:D:673:THR:HA	1:D:832:THR:OG1	2.10	0.52
1:E:707:MET:HE3	1:E:834:GLU:HB3	1.92	0.52
1:E:982:MET:HB3	1:E:983:PRO:HD3	1.91	0.52
1:F:329:THR:O	1:F:333:VAL:HG23	2.09	0.52
1:F:456:MET:HA	1:F:459:PHE:CD1	2.45	0.52
1:F:914:ARG:C	1:F:916:LEU:H	2.16	0.52
1:B:796:PHE:HA	1:B:799:PHE:CZ	2.45	0.52
1:B:953:LYS:O	1:B:1035:ILE:HG12	2.09	0.52
1:C:11:PHE:O	1:C:15:ILE:HG13	2.10	0.52
1:C:355:MET:SD	1:C:368:PRO:HB2	2.50	0.52
1:D:153:ASP:OD2	1:D:153:ASP:N	2.42	0.52
1:F:184:MET:HB3	1:F:766:VAL:HG22	1.91	0.52
1:A:4:PHE:HB3	1:A:8:ARG:CZ	2.39	0.52
1:B:510:LYS:HB3	1:B:513:PHE:HB3	1.92	0.52
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.91	0.52
1:C:662:ASN:O	1:C:673:THR:N	2.37	0.52
1:D:278:ILE:HD13	1:D:584:GLN:OE1	2.09	0.52
1:E:199:THR:HG21	1:E:787:ARG:H	1.73	0.52
1:E:524:THR:O	1:E:527:TYR:HB3	2.09	0.52
1:F:356:TYR:C	1:F:358:PHE:H	2.16	0.52
1:F:408:ASP:O	1:F:412:VAL:HG23	2.09	0.52
1:A:708:LEU:HD21	1:A:838:LEU:HD12	1.90	0.52
1:C:211:ASN:CG	1:C:240:LEU:HG	2.35	0.52
1:C:251:LEU:HD11	1:C:262:LEU:HD13	1.92	0.52
1:C:549:VAL:O	1:C:552:MET:HB3	2.10	0.52
1:D:478:MET:O	1:D:482:VAL:HG23	2.09	0.52
1:D:653:ILE:HG13	1:D:654:LYS:HE2	1.92	0.52
1:D:771:GLU:HB3	1:D:774:TYR:HD1	1.75	0.52
1:D:940:ILE:HG12	1:D:966:ARG:CZ	2.39	0.52
1:E:47:ALA:O	1:E:87:THR:HA	2.10	0.52
1:F:94:PHE:CE1	1:F:103:ALA:HB1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:314:GLU:HB2	1:F:315:PRO:HD3	1.92	0.52
1:F:352:PHE:HA	1:F:355:MET:HE3	1.91	0.52
1:F:559:LEU:HD11	1:F:911:ALA:HB1	1.92	0.52
1:C:545:TYR:CE2	1:C:1020:PHE:CZ	2.98	0.52
1:C:884:ALA:HB1	1:C:890:TRP:HZ3	1.74	0.52
1:D:17:ILE:HA	1:D:20:MET:CE	2.40	0.52
1:D:542:LEU:O	1:D:546:LEU:HG	2.09	0.52
1:F:757:PHE:HE1	1:F:759:ASP:HB2	1.74	0.52
1:A:415:ASN:HD22	1:A:434:SER:HB2	1.74	0.52
1:A:902:LEU:HD21	1:A:1016:PHE:CD1	2.44	0.52
1:B:58:GLN:O	1:B:63:GLN:HG3	2.09	0.52
1:B:340:VAL:HG11	1:B:395:MET:HB3	1.91	0.52
1:D:23:GLY:HA2	1:D:381:ALA:HB2	1.90	0.52
1:D:27:ILE:HG23	1:D:390:ILE:HD11	1.91	0.52
1:D:137:LEU:HB3	1:D:291:ILE:O	2.10	0.52
1:D:276:ASP:O	1:D:614:GLY:HA2	2.10	0.52
1:D:361:ASN:HD21	1:D:363:ARG:HG2	1.74	0.52
1:D:936:ASN:ND2	1:D:970:ILE:HG23	2.25	0.52
1:E:695:ASN:O	1:E:698:LEU:HB2	2.10	0.52
1:F:453:PHE:HB2	1:F:475:VAL:HG23	1.90	0.52
1:F:778:PRO:O	1:F:781:ILE:HG12	2.10	0.52
1:F:986:ILE:HG23	1:F:986:ILE:O	2.10	0.52
1:A:442:LEU:O	1:A:445:ILE:HG13	2.10	0.51
1:A:553:ALA:O	1:A:557:VAL:HG23	2.10	0.51
1:A:969:PRO:HA	1:A:972:MET:HE3	1.91	0.51
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.92	0.51
1:B:413:VAL:O	1:B:417:GLU:HG2	2.11	0.51
1:C:493:CYS:O	1:C:497:LEU:HB2	2.11	0.51
1:D:225:VAL:H	1:E:776:MET:CE	2.22	0.51
1:E:757:PHE:HD2	1:E:766:VAL:HG22	1.75	0.51
1:F:872:TYR:O	1:F:876:LEU:HD12	2.09	0.51
1:F:905:ILE:O	1:F:909:LEU:HB2	2.10	0.51
1:A:694:ARG:NH2	1:A:717:GLU:OE1	2.43	0.51
1:B:549:VAL:O	1:B:552:MET:HB3	2.10	0.51
1:B:578:LEU:HB2	1:B:618:ASN:O	2.10	0.51
1:D:201:VAL:O	1:D:205:THR:OG1	2.26	0.51
1:D:974:SER:OG	1:D:1010:THR:HG21	2.10	0.51
1:E:32:VAL:HG21	1:E:300:LEU:HD13	1.90	0.51
1:E:76:MET:HB2	1:E:93:THR:O	2.09	0.51
1:F:431:THR:HG22	1:F:435:MET:HE1	1.91	0.51
1:A:13:TRP:O	1:A:17:ILE:HG13	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LEU:HD12	1:C:232:ALA:HB3	1.92	0.51
1:C:906:GLY:HA3	1:C:1008:THR:OG1	2.10	0.51
1:D:636:GLU:HB2	1:D:645:ARG:NH2	2.25	0.51
1:D:881:LEU:HD13	1:F:18:ILE:HG13	1.92	0.51
1:E:534:ILE:HG21	2:E:1101:LMT:H12	1.92	0.51
1:F:382:VAL:HG21	1:F:476:SER:HB2	1.92	0.51
1:F:506:GLY:C	1:F:508:GLY:H	2.18	0.51
1:A:58:GLN:HA	1:A:62:THR:HB	1.92	0.51
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.45	0.51
1:B:52:ALA:HB1	1:B:56:THR:HB	1.93	0.51
1:B:700:GLU:HB3	1:B:842:LEU:HD22	1.92	0.51
1:B:950:LYS:O	1:B:951:GLU:HG2	2.10	0.51
1:C:110:LYS:O	1:C:113:LEU:HB2	2.10	0.51
1:C:781:ILE:O	1:C:796:PHE:HB2	2.11	0.51
1:C:985:VAL:HG13	1:C:1000:THR:OG1	2.10	0.51
1:D:56:THR:O	1:D:60:THR:HG22	2.10	0.51
1:D:575:MET:HG2	1:D:661:PHE:CE1	2.42	0.51
1:D:757:PHE:CE1	1:D:759:ASP:HB2	2.45	0.51
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.92	0.51
1:F:375:VAL:O	1:F:379:THR:OG1	2.09	0.51
1:A:417:GLU:HG2	1:A:497:LEU:HD21	1.92	0.51
1:A:632:ARG:NH1	1:A:637:ASN:O	2.44	0.51
1:B:515:TRP:O	1:B:519:MET:HG3	2.11	0.51
1:B:560:PRO:HG2	1:B:917:THR:HA	1.93	0.51
1:B:673:THR:HA	1:B:832:THR:OG1	2.11	0.51
1:C:445:ILE:HG12	1:C:935:LYS:HG3	1.91	0.51
1:D:113:LEU:HD11	1:F:128:SER:CB	2.30	0.51
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.92	0.51
1:D:363:ARG:O	1:D:366:LEU:HB2	2.10	0.51
1:F:110:LYS:O	1:F:113:LEU:HB2	2.10	0.51
1:F:395:MET:O	1:F:398:MET:HB2	2.11	0.51
1:F:422:GLU:HB3	1:F:423:GLU:HG3	1.93	0.51
1:F:666:ILE:HD12	1:F:857:MET:SD	2.51	0.51
1:F:667:VAL:HB	1:F:668:GLU:OE2	2.10	0.51
1:B:44:THR:HA	1:B:90:ILE:O	2.10	0.51
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.92	0.51
1:C:80:SER:HB3	1:C:90:ILE:HG23	1.92	0.51
1:C:538:THR:CG2	1:C:542:LEU:HD13	2.41	0.51
1:C:568:ASP:O	1:C:629:TRP:HH2	1.94	0.51
1:C:982:MET:O	1:C:985:VAL:N	2.44	0.51
1:D:225:VAL:HG12	1:E:772:ALA:HB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:ALA:CA	1:D:468:ARG:HG3	2.37	0.51
1:D:899:VAL:HA	1:D:902:LEU:HD22	1.92	0.51
1:E:653:ILE:C	1:E:654:LYS:HD2	2.36	0.51
1:E:1016:PHE:O	1:E:1019:VAL:HB	2.10	0.51
1:F:639:VAL:HA	1:F:642:ILE:HD12	1.92	0.51
1:F:892:ILE:CG2	1:F:941:VAL:HG11	2.40	0.51
1:A:355:MET:HE2	1:A:368:PRO:HG2	1.93	0.51
1:A:359:LEU:C	1:A:360:GLN:HG2	2.34	0.51
1:A:400:LEU:HD11	1:A:925:GLY:HA2	1.92	0.51
1:B:393:LEU:HD22	1:B:470:PHE:HE1	1.76	0.51
1:B:544:LEU:HA	1:B:547:ILE:HD12	1.92	0.51
1:C:778:PRO:O	1:C:781:ILE:HG12	2.10	0.51
1:E:438:ILE:O	1:E:441:ALA:HB3	2.11	0.51
1:E:456:MET:HE1	1:E:924:VAL:HG13	1.93	0.51
1:E:511:GLY:HA2	1:E:515:TRP:HD1	1.76	0.51
1:F:36:PRO:HD3	1:F:391:ASN:CG	2.35	0.51
1:F:144:ASN:O	1:F:284:GLN:NE2	2.42	0.51
1:F:375:VAL:HA	1:F:480:LEU:HD13	1.91	0.51
1:F:455:PRO:HG2	1:F:875:SER:HA	1.91	0.51
1:F:770:SER:HB2	1:F:784:TRP:CZ2	2.46	0.51
1:A:166:ILE:HG22	1:A:175:VAL:HG21	1.93	0.51
1:D:573:MET:HG3	1:D:661:PHE:CE2	2.45	0.51
1:E:68:ASN:HB3	1:E:114:ALA:HB2	1.92	0.51
1:A:209:ALA:O	1:A:237:GLN:NE2	2.43	0.51
1:A:219:LEU:HD13	1:A:230:LEU:HD21	1.93	0.51
1:B:143:ILE:O	1:B:321:LEU:HG	2.11	0.51
1:B:415:ASN:OD1	1:B:418:ARG:NH1	2.44	0.51
1:B:678:GLU:HG2	1:B:814:TYR:CG	2.46	0.51
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.93	0.51
1:C:329:THR:O	1:C:332:PHE:HB3	2.11	0.51
1:C:616:GLY:N	1:C:619:THR:OG1	2.43	0.51
1:C:966:ARG:O	1:C:970:ILE:HG13	2.11	0.51
1:C:982:MET:HB3	1:C:983:PRO:HD3	1.93	0.51
1:D:562:SER:N	1:D:917:THR:OG1	2.39	0.51
1:E:7:ASP:OD1	1:E:432:ARG:NH2	2.44	0.51
1:E:109:ASN:OD1	1:E:110:LYS:N	2.44	0.51
1:E:237:GLN:OE1	1:F:742:ASN:ND2	2.44	0.51
1:F:409:ALA:O	1:F:413:VAL:HG23	2.11	0.51
1:F:542:LEU:O	1:F:546:LEU:HG	2.11	0.51
1:F:664:PRO:HD3	1:F:672:ALA:C	2.36	0.51
1:F:687:HIS:NE2	1:F:718:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:VAL:CG2	1:A:625:SER:HA	2.35	0.51
1:B:372:VAL:O	1:B:376:LEU:HG	2.10	0.51
1:B:501:ALA:O	1:B:504:ASP:HB2	2.10	0.51
1:C:287:SER:OG	1:C:288:GLY:N	2.42	0.51
1:D:168:ARG:NH2	1:E:816:GLY:HA3	2.26	0.51
1:D:216:ALA:HB1	1:D:234:ILE:O	2.10	0.51
1:D:577:GLN:OE1	1:D:619:THR:HG22	2.11	0.51
1:D:678:GLU:OE1	1:D:678:GLU:HA	2.11	0.51
1:F:465:ALA:HA	1:F:468:ARG:NH1	2.25	0.51
1:A:228:GLN:NE2	1:A:230:LEU:H	2.09	0.50
1:A:607:GLU:OE1	1:A:627:LYS:HA	2.12	0.50
1:B:181:GLN:HG2	1:B:182:TYR:N	2.25	0.50
1:B:352:PHE:C	1:B:352:PHE:CD2	2.88	0.50
1:B:574:THR:HA	1:B:660:ALA:HA	1.92	0.50
1:E:281:PHE:CZ	1:E:324:VAL:HG21	2.46	0.50
1:E:423:GLU:O	1:E:502:LYS:HB2	2.11	0.50
1:F:445:ILE:HG12	1:F:935:LYS:HG3	1.93	0.50
1:F:830:LYS:HG3	1:F:831:SER:N	2.26	0.50
1:A:605:ASN:ND2	1:A:637:ASN:HA	2.24	0.50
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.44	0.50
1:B:375:VAL:HG11	1:B:481:SER:HB3	1.92	0.50
1:C:393:LEU:HD11	1:C:466:ILE:HD13	1.92	0.50
1:D:368:PRO:HD3	1:D:413:VAL:HG21	1.94	0.50
1:F:836:MET:HG2	1:F:854:TRP:CH2	2.46	0.50
1:A:511:GLY:CA	1:A:515:TRP:CD1	2.94	0.50
1:A:908:LEU:O	1:A:911:ALA:HB3	2.10	0.50
1:B:493:CYS:O	1:B:497:LEU:HB2	2.11	0.50
1:B:667:VAL:HB	1:B:668:GLU:CD	2.36	0.50
1:C:129:VAL:O	1:C:130:GLU:HG3	2.10	0.50
1:C:377:LEU:O	1:C:380:PHE:HB2	2.12	0.50
1:C:666:ILE:HD13	1:C:669:LEU:HD12	1.94	0.50
1:C:939:LEU:HB3	1:C:966:ARG:CD	2.37	0.50
1:D:200:PRO:HA	1:D:203:VAL:CG2	2.41	0.50
1:D:899:VAL:HG21	1:D:937:ALA:HB2	1.93	0.50
1:E:583:THR:HG23	1:E:585:GLU:H	1.77	0.50
1:F:49:TYR:N	1:F:86:GLY:O	2.40	0.50
1:F:262:LEU:HG	1:F:268:ILE:HD11	1.93	0.50
1:F:508:GLY:O	1:F:509:LYS:HB2	2.09	0.50
1:F:947:LEU:HD22	1:F:953:LYS:CE	2.42	0.50
1:A:372:VAL:HG13	1:A:405:LEU:HD12	1.94	0.50
1:A:567:GLU:HG2	1:A:665:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:PHE:HD1	1:A:897:MET:CE	2.15	0.50
1:B:917:THR:O	1:B:919:ASP:N	2.45	0.50
1:C:737:SER:O	1:C:741:ILE:HG22	2.10	0.50
1:C:927:LEU:O	1:C:930:ILE:HB	2.11	0.50
1:D:83:ASP:OD2	1:D:810:ARG:NH1	2.44	0.50
1:D:691:THR:HG23	1:D:694:ARG:NH2	2.26	0.50
1:E:115:MET:SD	1:E:123:GLN:HG2	2.52	0.50
1:F:3:ASN:OD1	1:F:486:LEU:HB3	2.11	0.50
1:F:338:HIS:O	1:F:341:VAL:HB	2.12	0.50
1:F:566:ASP:CG	1:F:673:THR:HG23	2.36	0.50
1:F:918:ASN:O	1:F:918:ASN:ND2	2.39	0.50
1:C:11:PHE:O	1:C:11:PHE:HD2	1.93	0.50
1:C:456:MET:HB3	1:C:871:LEU:HD21	1.94	0.50
1:C:860:GLN:O	1:C:863:LEU:HB3	2.11	0.50
1:C:887:TYR:O	1:C:889:SER:N	2.42	0.50
1:C:953:LYS:HG2	1:C:957:GLU:OE2	2.11	0.50
1:D:616:GLY:N	1:D:619:THR:OG1	2.44	0.50
1:E:45:ILE:O	1:E:89:GLN:HA	2.12	0.50
1:E:355:MET:HB3	1:E:365:THR:CB	2.41	0.50
1:E:700:GLU:HB3	1:E:842:LEU:HD22	1.93	0.50
1:A:375:VAL:HG13	1:A:480:LEU:CB	2.42	0.50
1:A:649:ALA:O	1:A:653:ILE:HG12	2.12	0.50
1:A:989:GLY:N	1:A:992:SER:OG	2.44	0.50
1:B:80:SER:HB3	1:B:90:ILE:HG12	1.94	0.50
1:B:573:MET:HG3	1:B:661:PHE:HE2	1.77	0.50
1:C:68:ASN:O	1:C:110:LYS:HB3	2.11	0.50
1:C:453:PHE:HB3	1:C:456:MET:HE2	1.94	0.50
1:C:963:VAL:HA	1:C:966:ARG:HH22	1.77	0.50
1:D:172:VAL:HG22	1:D:302:THR:HG23	1.93	0.50
1:D:355:MET:HE2	1:D:368:PRO:HG2	1.94	0.50
1:D:917:THR:O	1:D:919:ASP:N	2.45	0.50
1:F:406:VAL:O	1:F:408:ASP:N	2.45	0.50
1:F:773:LYS:HG3	1:F:774:TYR:CZ	2.47	0.50
1:A:394:THR:HG22	1:A:473:THR:OG1	2.12	0.50
1:B:27:ILE:HD13	1:B:380:PHE:CG	2.47	0.50
1:B:376:LEU:HD22	1:B:398:MET:HE1	1.94	0.50
1:C:311:ALA:O	1:C:314:GLU:HB2	2.12	0.50
1:D:3:ASN:O	1:D:4:PHE:C	2.55	0.50
1:D:242:SER:OG	1:D:245:GLU:HG2	2.11	0.50
1:D:545:TYR:HB2	1:D:1016:PHE:HE2	1.76	0.50
1:D:747:ALA:O	1:D:769:MET:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:697:LEU:HD12	1:E:700:GLU:HB2	1.94	0.50
1:F:355:MET:SD	1:F:368:PRO:HB2	2.52	0.50
1:F:893:PRO:O	1:F:897:MET:HG2	2.11	0.50
1:B:595:THR:O	1:B:599:LEU:HG	2.12	0.50
2:B:2000:LMT:H6E	2:B:2000:LMT:O5B	2.11	0.50
1:C:162:MET:O	1:C:166:ILE:N	2.41	0.50
1:D:188:MET:HB3	1:D:193:LEU:CD1	2.42	0.50
1:D:222:THR:HA	1:D:224:PRO:CD	2.38	0.50
1:D:249:ILE:O	1:D:262:LEU:N	2.45	0.50
1:D:525:HIS:NE2	1:D:529:ASP:OD1	2.45	0.50
1:D:854:TRP:CE3	1:D:858:SER:HB2	2.46	0.50
1:E:468:ARG:HG2	1:E:472:ILE:HD13	1.94	0.50
1:E:632:ARG:NH1	1:E:637:ASN:O	2.45	0.50
1:F:1016:PHE:HB3	1:F:1020:PHE:CZ	2.46	0.50
1:B:771:GLU:HB3	1:B:774:TYR:HD1	1.76	0.50
1:D:168:ARG:HB3	1:E:75:LEU:HD22	1.93	0.50
1:D:248:LYS:HG2	1:D:263:ARG:HH21	1.76	0.50
1:E:76:MET:SD	1:E:859:TYR:HE2	2.35	0.50
1:F:112:GLN:HG3	1:F:115:MET:HG3	1.93	0.50
1:F:219:LEU:H	1:F:219:LEU:HD12	1.76	0.50
1:F:966:ARG:NH2	1:F:970:ILE:HD11	2.25	0.50
1:A:408:ASP:O	1:A:412:VAL:HG23	2.12	0.49
1:A:431:THR:HG21	1:A:490:PRO:O	2.12	0.49
1:B:709:THR:HB	1:B:827:ALA:HA	1.94	0.49
1:B:962:ALA:O	1:B:965:MET:HG2	2.12	0.49
1:C:602:GLU:OE1	1:C:645:ARG:HD2	2.12	0.49
1:C:740:ASP:O	1:C:744:THR:OG1	2.22	0.49
1:D:51:GLY:O	1:F:217:GLY:N	2.44	0.49
1:D:337:ILE:HA	1:D:340:VAL:HG23	1.94	0.49
1:D:632:ARG:NH1	1:D:638:LYS:HA	2.23	0.49
1:D:889:SER:HB3	1:D:892:ILE:HB	1.92	0.49
1:D:920:VAL:HA	1:D:923:GLN:OE1	2.11	0.49
1:E:452:VAL:HA	1:E:875:SER:OG	2.12	0.49
1:F:5:PHE:O	1:F:7:ASP:N	2.42	0.49
1:F:484:VAL:O	1:F:487:ILE:N	2.38	0.49
1:C:687:HIS:NE2	1:C:718:ASP:OD2	2.35	0.49
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.94	0.49
1:D:836:MET:HE1	1:D:862:ARG:HD2	1.93	0.49
1:E:281:PHE:HB2	1:E:610:PHE:HE1	1.77	0.49
1:E:969:PRO:HA	1:E:972:MET:HE3	1.94	0.49
1:A:753:TYR:HB2	1:A:767:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:VAL:HG22	1:B:438:ILE:CD1	2.41	0.49
1:B:414:GLU:HG3	1:B:972:MET:HE1	1.94	0.49
1:C:465:ALA:O	1:C:469:GLN:HG2	2.12	0.49
1:D:1006:MET:O	1:D:1009:ALA:HB3	2.11	0.49
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.95	0.49
1:E:356:TYR:HD1	1:E:365:THR:HG21	1.76	0.49
1:E:478:MET:O	1:E:482:VAL:HG12	2.12	0.49
1:E:748:ALA:O	1:E:770:SER:HB3	2.12	0.49
1:E:769:MET:HG2	1:E:770:SER:H	1.77	0.49
1:F:479:ALA:O	1:F:483:LEU:HG	2.12	0.49
1:F:893:PRO:HA	1:F:896:VAL:HG12	1.93	0.49
1:A:212:ALA:HA	1:A:239:ARG:HE	1.78	0.49
1:B:57:VAL:HG11	1:B:86:GLY:O	2.11	0.49
1:C:425:LEU:HB3	1:C:429:GLU:CG	2.42	0.49
1:C:569:GLN:OE1	1:C:663:LEU:HD11	2.12	0.49
1:D:18:ILE:HG13	1:E:881:LEU:HD23	1.93	0.49
1:D:76:MET:HE3	1:D:95:GLU:OE1	2.13	0.49
1:D:695:ASN:O	1:D:698:LEU:HB2	2.12	0.49
1:E:108:GLN:CD	1:F:112:GLN:HG2	2.37	0.49
1:E:146:ASP:OD2	1:E:146:ASP:N	2.45	0.49
1:E:987:SER:O	1:E:992:SER:HB2	2.12	0.49
1:F:836:MET:HE3	1:F:854:TRP:CE2	2.46	0.49
1:F:887:TYR:C	1:F:889:SER:N	2.70	0.49
1:A:177:LEU:HD13	1:A:179:GLY:O	2.11	0.49
1:A:948:MET:HE1	1:A:1021:PHE:HE2	1.77	0.49
1:B:770:SER:HG	1:B:775:ARG:HG2	1.76	0.49
1:D:249:ILE:HB	1:D:262:LEU:HB2	1.94	0.49
1:D:393:LEU:HD12	1:D:469:GLN:HG3	1.94	0.49
1:D:415:ASN:O	1:D:419:VAL:HG23	2.13	0.49
1:D:691:THR:HG23	1:D:694:ARG:HH22	1.77	0.49
1:D:826:ALA:HB2	1:D:835:ALA:HB2	1.93	0.49
1:E:484:VAL:HG13	1:E:488:LEU:HB3	1.95	0.49
1:F:272:GLY:N	1:F:275:TYR:OH	2.22	0.49
1:A:695:ASN:HA	1:A:698:LEU:HD12	1.94	0.49
1:B:355:MET:HE1	1:B:410:ILE:HG12	1.93	0.49
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.95	0.49
1:B:574:THR:HG23	1:B:622:ALA:HB3	1.92	0.49
1:B:906:GLY:HA3	1:B:1008:THR:HG21	1.95	0.49
1:B:961:ASP:O	1:B:964:ARG:HB3	2.11	0.49
1:D:214:VAL:HG11	1:E:742:ASN:CG	2.38	0.49
1:E:434:SER:O	1:E:438:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:747:ALA:O	1:E:769:MET:HA	2.13	0.49
1:A:952:GLY:HA2	1:A:1035:ILE:HG22	1.93	0.49
1:B:174:ASP:HB3	1:B:292:LYS:HD2	1.94	0.49
1:B:362:PHE:HA	1:B:365:THR:CG2	2.42	0.49
1:E:527:TYR:O	1:E:531:VAL:HG23	2.13	0.49
1:F:365:THR:O	1:F:368:PRO:HD2	2.13	0.49
1:A:156:ASP:OD2	1:A:182:TYR:HB2	2.12	0.49
1:A:968:ARG:HG2	1:A:972:MET:CE	2.40	0.49
1:B:896:VAL:HG23	1:B:937:ALA:HB3	1.93	0.49
1:D:278:ILE:HG13	1:D:613:ASN:HB3	1.93	0.49
1:E:375:VAL:HG11	1:E:481:SER:HB3	1.95	0.49
1:F:81:ASN:HB2	1:F:89:GLN:HB2	1.95	0.49
1:F:213:GLN:OE1	1:F:238:THR:HA	2.13	0.49
1:F:406:VAL:O	1:F:409:ALA:N	2.45	0.49
1:A:199:THR:HG21	1:A:786:VAL:HA	1.95	0.49
1:A:636:GLU:HA	1:A:641:ALA:CB	2.42	0.49
1:B:418:ARG:CZ	1:B:965:MET:HE3	2.42	0.49
1:B:988:THR:HA	1:B:992:SER:OG	2.13	0.49
1:C:184:MET:HE3	1:C:185:ARG:N	2.28	0.49
1:C:599:LEU:O	1:C:603:LYS:HG2	2.12	0.49
1:D:151:GLN:HG3	1:D:152:GLU:N	2.28	0.49
1:F:75:LEU:CD1	1:F:92:LEU:HD12	2.43	0.49
1:F:144:ASN:ND2	1:F:319:SER:O	2.40	0.49
1:F:927:LEU:O	1:F:928:THR:C	2.55	0.49
1:A:330:THR:HB	1:A:331:PRO:HD3	1.95	0.49
1:A:453:PHE:O	1:A:471:SER:OG	2.23	0.49
1:A:574:THR:HG23	1:A:622:ALA:HB3	1.94	0.49
1:A:1016:PHE:HB3	1:A:1020:PHE:CE1	2.48	0.49
1:C:492:LEU:O	1:C:496:MET:HG2	2.12	0.49
1:C:678:GLU:HG2	1:C:814:TYR:CG	2.48	0.49
1:C:708:LEU:HD21	1:C:839:MET:HG2	1.95	0.49
1:D:281:PHE:CZ	1:D:608:SER:HB2	2.47	0.49
1:D:375:VAL:HG22	1:D:484:VAL:HG21	1.95	0.49
1:F:133:SER:OG	1:F:293:LEU:O	2.14	0.49
1:F:375:VAL:HB	1:F:405:LEU:HD22	1.95	0.49
1:A:225:VAL:HG11	1:B:773:LYS:HA	1.95	0.48
1:A:645:ARG:HA	1:A:648:ARG:HB3	1.95	0.48
1:C:975:LEU:O	1:C:976:ALA:C	2.55	0.48
1:D:462:SER:O	1:D:466:ILE:HG12	2.13	0.48
1:D:514:GLY:C	1:D:516:PHE:N	2.71	0.48
1:D:527:TYR:CE1	1:D:1014:ILE:HD12	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:860:GLN:O	1:D:863:LEU:HB2	2.13	0.48
1:F:311:ALA:HA	1:F:314:GLU:HG3	1.95	0.48
1:F:700:GLU:HA	1:F:703:LYS:HZ2	1.78	0.48
1:F:900:VAL:O	1:F:904:VAL:HG23	2.12	0.48
1:B:272:GLY:H	1:B:275:TYR:HH	1.53	0.48
1:B:508:GLY:O	1:B:510:LYS:N	2.42	0.48
1:C:686:GLY:O	1:C:690:LEU:N	2.37	0.48
1:D:155:SER:OG	1:D:179:GLY:HA3	2.13	0.48
1:D:413:VAL:O	1:D:417:GLU:HG2	2.13	0.48
1:D:749:TRP:HZ3	1:F:219:LEU:HG	1.78	0.48
1:F:484:VAL:C	1:F:486:LEU:N	2.71	0.48
1:A:138:MET:HE2	1:A:328:ASP:OD1	2.14	0.48
1:A:378:GLY:O	1:A:381:ALA:HB3	2.14	0.48
1:A:401:ALA:O	1:A:405:LEU:HG	2.13	0.48
1:A:948:MET:O	1:A:1035:ILE:HG21	2.13	0.48
1:B:441:ALA:HB2	1:B:942:GLU:OE1	2.13	0.48
1:B:721:GLN:CD	1:B:807:GLY:HA3	2.38	0.48
1:C:520:PHE:HE2	1:C:968:ARG:HD2	1.76	0.48
1:C:538:THR:HG23	1:C:542:LEU:HD13	1.94	0.48
1:D:184:MET:HB3	1:D:766:VAL:HG22	1.95	0.48
1:D:966:ARG:HB3	1:D:966:ARG:NH1	2.28	0.48
1:E:187:TRP:CZ3	1:E:769:MET:HB3	2.48	0.48
1:F:2:PRO:O	1:F:5:PHE:HB3	2.13	0.48
1:A:47:ALA:HB3	1:A:88:VAL:HG13	1.94	0.48
1:A:573:MET:HG3	1:A:661:PHE:CE2	2.48	0.48
1:A:795:PRO:O	1:A:798:ALA:HB3	2.13	0.48
1:A:1013:ALA:C	1:A:1015:PHE:H	2.21	0.48
1:B:175:VAL:HG23	1:C:70:ASN:HD22	1.78	0.48
1:C:72:ILE:HD13	1:C:107:VAL:HG22	1.95	0.48
1:C:356:TYR:HD1	1:C:365:THR:HG21	1.77	0.48
1:C:370:ILE:C	1:C:373:PRO:HD2	2.39	0.48
1:C:645:ARG:O	1:C:648:ARG:HB3	2.13	0.48
1:D:7:ASP:OD2	1:D:432:ARG:NH2	2.41	0.48
1:D:66:GLU:OE2	1:D:80:SER:OG	2.31	0.48
1:D:354:VAL:HG22	1:D:975:LEU:HD23	1.96	0.48
1:D:375:VAL:HG11	1:D:481:SER:HB3	1.96	0.48
1:D:391:ASN:O	1:D:395:MET:HG2	2.13	0.48
1:D:568:ASP:OD1	1:D:632:ARG:NH2	2.43	0.48
1:E:137:LEU:HD12	1:E:329:THR:HG22	1.94	0.48
1:F:36:PRO:HD3	1:F:391:ASN:ND2	2.29	0.48
1:F:189:ASN:HB3	1:F:192:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:GLN:O	1:A:656:ALA:HB1	2.14	0.48
1:B:277:ILE:H	1:B:277:ILE:HG13	1.44	0.48
1:C:185:ARG:HB2	1:C:271:GLY:HA3	1.95	0.48
1:D:17:ILE:HA	1:D:20:MET:HE3	1.96	0.48
1:D:32:VAL:HB	1:D:300:LEU:HD22	1.94	0.48
1:D:343:THR:O	1:D:344:LEU:C	2.55	0.48
1:E:43:VAL:HG22	1:E:131:LYS:HG3	1.94	0.48
1:E:372:VAL:O	1:E:376:LEU:HG	2.12	0.48
1:E:757:PHE:CD2	1:E:766:VAL:HG22	2.49	0.48
1:F:9:PRO:HB3	1:F:495:THR:HG21	1.96	0.48
1:F:361:ASN:ND2	1:F:364:ALA:HB2	2.28	0.48
1:F:574:THR:OG1	1:F:659:PHE:O	2.30	0.48
1:B:344:LEU:HD23	1:B:402:ILE:HG12	1.96	0.48
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.45	0.48
1:C:6:ILE:HG12	1:C:6:ILE:H	1.43	0.48
1:C:54:ALA:HB3	1:C:808:SER:O	2.14	0.48
1:D:830:LYS:HG2	1:D:834:GLU:OE2	2.13	0.48
1:D:896:VAL:HG23	1:D:937:ALA:HB3	1.95	0.48
1:D:936:ASN:O	1:D:940:ILE:HG13	2.14	0.48
1:E:239:ARG:HH12	1:E:756:ASP:H	1.60	0.48
1:F:400:LEU:O	1:F:404:LEU:HD22	2.14	0.48
1:F:587:THR:HG21	1:F:617:GLN:O	2.13	0.48
1:F:940:ILE:HA	1:F:966:ARG:NH1	2.28	0.48
1:A:607:GLU:HB2	1:A:627:LYS:N	2.28	0.48
1:B:156:ASP:OD2	1:B:764:LYS:NZ	2.45	0.48
1:B:349:ILE:O	1:B:352:PHE:HB3	2.13	0.48
1:B:872:TYR:HA	1:B:875:SER:HB2	1.95	0.48
1:B:954:GLY:HA2	1:B:1035:ILE:HG23	1.96	0.48
1:C:318:PRO:HG2	1:C:321:LEU:HB2	1.94	0.48
1:D:75:LEU:HD23	1:F:168:ARG:HB3	1.96	0.48
1:D:393:LEU:HB3	1:D:470:PHE:CE1	2.49	0.48
1:D:571:VAL:CG2	1:D:625:SER:HA	2.35	0.48
1:E:317:PHE:CZ	1:E:323:ILE:HG12	2.49	0.48
1:E:422:GLU:O	1:E:502:LYS:HG3	2.13	0.48
1:F:362:PHE:H	1:F:363:ARG:NH2	2.12	0.48
1:F:414:GLU:OE1	1:F:968:ARG:NH1	2.43	0.48
1:F:900:VAL:HG22	1:F:930:ILE:HG23	1.95	0.48
1:B:535:LEU:HD21	1:B:1019:VAL:HA	1.96	0.48
1:C:769:MET:HE3	1:C:775:ARG:NH2	2.28	0.48
1:C:902:LEU:HG	1:C:1012:LEU:HB3	1.95	0.48
1:C:1031:LYS:HD2	1:C:1033:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:GLN:OE1	1:F:813:ARG:HD2	2.14	0.48
1:F:152:GLU:HG2	1:F:275:TYR:HE2	1.79	0.48
1:F:853:ASP:OD2	1:F:854:TRP:N	2.46	0.48
1:A:3:ASN:O	1:A:4:PHE:C	2.57	0.48
1:A:70:ASN:OD1	1:A:110:LYS:HD2	2.14	0.48
1:A:361:ASN:O	1:A:365:THR:HG22	2.14	0.48
1:A:532:GLY:O	1:A:536:ARG:HG2	2.14	0.48
1:A:723:LYS:HB2	1:A:805:GLU:OE2	2.14	0.48
1:A:946:ASP:C	1:A:946:ASP:OD1	2.56	0.48
1:B:952:GLY:HA2	1:B:1035:ILE:HD11	1.95	0.48
1:B:981:VAL:O	1:B:982:MET:C	2.57	0.48
1:C:278:ILE:HD13	1:C:584:GLN:OE1	2.14	0.48
1:C:654:LYS:HA	1:C:654:LYS:HD3	1.51	0.48
1:C:893:PRO:O	1:C:897:MET:HG2	2.14	0.48
1:D:956:ILE:HD12	1:D:957:GLU:H	1.79	0.48
1:E:78:MET:O	1:E:815:ASN:N	2.35	0.48
1:E:143:ILE:O	1:E:321:LEU:HG	2.13	0.48
1:E:887:TYR:HB3	1:E:892:ILE:HD12	1.95	0.48
1:E:906:GLY:HA3	1:E:1008:THR:CG2	2.41	0.48
1:F:459:PHE:CE1	1:F:871:LEU:HG	2.48	0.48
1:B:535:LEU:HD13	1:B:1022:VAL:HG21	1.96	0.48
1:C:110:LYS:HA	1:C:110:LYS:HD3	1.68	0.48
1:D:61:VAL:HG13	1:D:118:LEU:HD13	1.95	0.48
1:E:401:ALA:HB2	1:E:474:ILE:HG23	1.96	0.48
1:E:414:GLU:HG3	1:E:969:PRO:HB3	1.96	0.48
1:F:194:ASN:OD1	1:F:793:MET:HE2	2.13	0.48
1:F:901:PRO:O	1:F:904:VAL:N	2.47	0.48
1:F:956:ILE:H	1:F:956:ILE:HD12	1.79	0.48
1:A:157:TYR:OH	1:A:316:PHE:O	2.32	0.47
1:B:277:ILE:HD12	1:B:277:ILE:O	2.14	0.47
1:B:708:LEU:HG	1:B:838:LEU:HD12	1.95	0.47
1:B:753:TYR:OH	1:B:756:ASP:OD1	2.23	0.47
1:C:1032:ASN:OD1	1:C:1033:GLU:HA	2.14	0.47
1:D:164:ASP:HB3	1:D:168:ARG:NH2	2.28	0.47
1:D:890:TRP:NE1	1:F:10:ILE:HG12	2.29	0.47
1:D:908:LEU:HD23	1:D:922:PHE:HZ	1.79	0.47
1:E:339:GLU:HA	1:E:342:LYS:HB2	1.95	0.47
1:E:906:GLY:CA	1:E:1008:THR:HG21	2.44	0.47
1:F:54:ALA:HB3	1:F:808:SER:O	2.13	0.47
1:F:103:ALA:O	1:F:107:VAL:HG23	2.14	0.47
1:F:120:GLN:HG3	1:F:123:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:681:ASP:CG	1:F:682:GLN:N	2.71	0.47
1:F:692:GLN:HA	1:F:695:ASN:HB2	1.96	0.47
1:F:770:SER:HB3	1:F:775:ARG:HD3	1.95	0.47
1:F:983:PRO:HA	1:F:986:ILE:HG22	1.94	0.47
1:A:225:VAL:H	1:B:776:MET:HE2	1.79	0.47
1:A:278:ILE:CG1	1:A:613:ASN:HB3	2.44	0.47
1:B:352:PHE:HZ	1:B:362:PHE:CE1	2.32	0.47
1:B:422:GLU:O	1:B:502:LYS:NZ	2.47	0.47
1:C:409:ALA:O	1:C:413:VAL:HG23	2.13	0.47
1:C:551:GLY:O	1:C:555:LEU:HB2	2.14	0.47
1:D:233:SER:O	1:E:721:GLN:HB2	2.14	0.47
1:E:57:VAL:HG23	1:E:82:SER:HB3	1.96	0.47
1:E:99:ASP:HB3	1:E:102:ILE:HB	1.96	0.47
1:F:917:THR:O	1:F:919:ASP:N	2.47	0.47
1:A:165:ALA:HB3	1:A:313:MET:CE	2.44	0.47
1:A:241:THR:HG23	1:A:758:ILE:O	2.14	0.47
1:A:514:GLY:C	1:A:516:PHE:N	2.69	0.47
1:A:669:LEU:HD23	1:A:669:LEU:HA	1.61	0.47
1:B:45:ILE:HA	1:B:128:SER:O	2.14	0.47
1:D:137:LEU:HD22	1:D:293:LEU:HB2	1.96	0.47
1:D:776:MET:HE1	1:F:225:VAL:H	1.79	0.47
1:E:20:MET:CG	1:E:374:VAL:HG22	2.44	0.47
1:E:638:LYS:NZ	1:E:988:THR:HG23	2.29	0.47
1:E:948:MET:HE3	1:E:948:MET:HB2	1.55	0.47
1:F:959:THR:O	1:F:963:VAL:HB	2.14	0.47
1:A:2:PRO:HB2	1:A:3:ASN:H	1.45	0.47
1:A:127:VAL:O	1:B:113:LEU:HD13	2.15	0.47
1:A:143:ILE:HG12	1:A:322:LYS:O	2.15	0.47
1:A:317:PHE:CD2	1:A:321:LEU:HD12	2.49	0.47
1:B:625:SER:O	1:B:626:LEU:HD23	2.14	0.47
1:B:773:LYS:HG3	1:B:774:TYR:CZ	2.49	0.47
1:C:242:SER:HB2	1:C:245:GLU:H	1.78	0.47
1:C:826:ALA:HB3	1:C:830:LYS:HG3	1.96	0.47
1:D:574:THR:HG21	1:D:598:TYR:CE2	2.49	0.47
1:D:872:TYR:O	1:D:876:LEU:HB2	2.14	0.47
1:E:309:GLU:OE2	1:E:313:MET:HE3	2.14	0.47
1:A:169:THR:HB	1:A:172:VAL:CG2	2.45	0.47
1:C:544:LEU:HD12	1:C:547:ILE:HD12	1.97	0.47
1:D:137:LEU:HG	1:D:138:MET:HE3	1.97	0.47
1:D:400:LEU:HA	1:D:400:LEU:HD12	1.52	0.47
1:E:35:TYR:CE2	1:E:393:LEU:HD21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:THR:HG21	1:E:319:SER:HB2	1.96	0.47
1:E:356:TYR:O	1:E:358:PHE:N	2.47	0.47
1:E:543:VAL:HA	1:E:546:LEU:HG	1.95	0.47
1:A:864:SER:OG	1:A:865:GLY:N	2.47	0.47
1:B:167:SER:HB3	1:B:175:VAL:HG21	1.97	0.47
1:B:364:ALA:O	1:B:368:PRO:HD3	2.14	0.47
1:C:119:PRO:O	1:C:122:VAL:HB	2.15	0.47
1:C:203:VAL:O	1:C:207:ILE:HG13	2.14	0.47
1:C:352:PHE:C	1:C:352:PHE:CD2	2.93	0.47
1:C:395:MET:HA	1:C:398:MET:HG3	1.97	0.47
1:C:966:ARG:HE	1:C:970:ILE:HD11	1.79	0.47
1:D:235:ILE:O	1:E:723:LYS:HD2	2.14	0.47
1:D:282:ASN:HD21	1:D:608:SER:HA	1.78	0.47
1:D:531:VAL:HG13	1:D:534:ILE:HD11	1.96	0.47
1:D:675:PHE:HB2	1:D:854:TRP:CZ3	2.49	0.47
1:E:518:ARG:O	1:E:521:GLU:N	2.47	0.47
1:E:749:TRP:CZ2	1:E:781:ILE:HD13	2.50	0.47
1:F:144:ASN:HB3	1:F:148:THR:HG23	1.95	0.47
1:F:248:LYS:O	1:F:261:LEU:HD22	2.14	0.47
1:A:157:TYR:HE2	1:A:317:PHE:CD1	2.33	0.47
1:A:587:THR:HB	1:A:613:ASN:ND2	2.30	0.47
1:A:602:GLU:OE1	1:A:645:ARG:HD2	2.14	0.47
1:A:749:TRP:C	1:A:769:MET:HE3	2.40	0.47
1:B:49:TYR:HB3	1:B:57:VAL:HG12	1.97	0.47
1:B:418:ARG:O	1:B:422:GLU:HB2	2.15	0.47
1:B:513:PHE:O	1:B:515:TRP:N	2.48	0.47
1:B:525:HIS:O	1:B:526:HIS:C	2.58	0.47
1:B:653:ILE:O	1:B:654:LYS:HD2	2.15	0.47
1:B:770:SER:HB2	1:B:784:TRP:CZ2	2.50	0.47
1:B:1035:ILE:H	1:B:1036:GLU:HG3	1.79	0.47
1:C:203:VAL:HG12	1:C:207:ILE:HD11	1.97	0.47
1:C:351:VAL:HG11	1:C:406:VAL:HG21	1.97	0.47
1:C:1008:THR:C	1:C:1010:THR:H	2.23	0.47
1:D:188:MET:SD	1:D:200:PRO:HG3	2.55	0.47
1:D:582:ALA:HA	1:D:586:ARG:HH21	1.79	0.47
1:D:736:VAL:HG21	1:D:799:PHE:CE1	2.50	0.47
1:D:905:ILE:O	1:D:909:LEU:HB2	2.15	0.47
1:D:1030:ARG:HE	1:D:1031:LYS:N	2.13	0.47
1:E:182:TYR:O	1:E:764:LYS:HD3	2.15	0.47
1:E:351:VAL:O	1:E:354:VAL:HB	2.13	0.47
1:E:508:GLY:HA2	1:E:514:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:571:VAL:HG13	1:E:623:PHE:HE1	1.80	0.47
1:E:578:LEU:O	1:E:618:ASN:ND2	2.38	0.47
1:E:780:ASP:O	1:E:783:ASP:HB2	2.14	0.47
1:E:836:MET:O	1:E:840:GLU:HG3	2.13	0.47
1:F:228:GLN:NE2	1:F:230:LEU:O	2.45	0.47
1:F:480:LEU:O	1:F:484:VAL:HG23	2.15	0.47
1:F:600:THR:C	1:F:602:GLU:H	2.22	0.47
1:F:689:LYS:HD2	1:F:689:LYS:N	2.29	0.47
1:F:1008:THR:O	1:F:1012:LEU:HB2	2.15	0.47
1:B:5:PHE:C	1:B:8:ARG:H	2.22	0.47
1:B:960:LEU:O	1:B:963:VAL:HG12	2.15	0.47
1:B:1007:VAL:O	1:B:1011:VAL:HG23	2.14	0.47
1:C:204:ILE:O	1:C:207:ILE:HB	2.15	0.47
1:C:402:ILE:O	1:C:406:VAL:HG22	2.15	0.47
1:D:103:ALA:O	1:D:107:VAL:HG23	2.15	0.47
1:D:199:THR:O	1:D:202:ASP:N	2.47	0.47
1:D:770:SER:HB2	1:D:784:TRP:CZ2	2.49	0.47
1:E:356:TYR:C	1:E:358:PHE:N	2.71	0.47
1:E:944:ALA:HB3	1:E:1021:PHE:HE1	1.78	0.47
1:F:407:ASP:O	1:F:411:VAL:HG23	2.15	0.47
1:F:516:PHE:O	1:F:520:PHE:N	2.43	0.47
1:F:1006:MET:O	1:F:1010:THR:HG23	2.15	0.47
1:A:23:GLY:HA3	1:A:377:LEU:O	2.14	0.47
1:A:41:PRO:HD3	1:A:97:GLY:H	1.79	0.47
1:A:300:LEU:O	1:A:303:ALA:HB3	2.15	0.47
1:A:826:ALA:HB2	1:A:835:ALA:HB2	1.97	0.47
1:E:410:ILE:HD13	1:E:972:MET:HB3	1.97	0.47
1:E:466:ILE:HD13	1:E:564:LEU:HD11	1.97	0.47
1:F:76:MET:HE2	1:F:859:TYR:CZ	2.49	0.47
1:F:154:ILE:O	1:F:158:VAL:HG23	2.15	0.47
1:F:222:THR:HA	1:F:224:PRO:HD3	1.97	0.47
1:A:68:ASN:O	1:A:110:LYS:HB3	2.16	0.47
1:A:190:PRO:HG3	1:A:784:TRP:CH2	2.50	0.47
1:A:559:LEU:HD13	1:A:918:ASN:HB2	1.96	0.47
1:A:1032:ASN:O	1:A:1033:GLU:HB2	2.13	0.47
1:B:1008:THR:O	1:B:1012:LEU:HB2	2.15	0.47
1:C:413:VAL:O	1:C:417:GLU:HG2	2.15	0.47
1:C:422:GLU:HB3	1:C:423:GLU:HG3	1.96	0.47
1:C:669:LEU:HD23	1:C:669:LEU:HA	1.61	0.47
1:D:404:LEU:HD21	1:D:449:LEU:HD13	1.96	0.47
1:E:61:VAL:HG22	1:E:118:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:594:VAL:HG22	1:E:650:PHE:CE2	2.50	0.47
1:E:932:LEU:HA	1:E:932:LEU:HD23	1.72	0.47
1:F:69:MET:SD	1:F:72:ILE:HD11	2.55	0.47
1:F:371:ALA:O	1:F:375:VAL:HG23	2.15	0.47
1:F:471:SER:O	1:F:475:VAL:HB	2.14	0.47
1:F:559:LEU:HA	1:F:560:PRO:HD2	1.49	0.47
1:B:480:LEU:HD23	1:B:480:LEU:HA	1.68	0.46
1:B:583:THR:HG23	1:B:585:GLU:H	1.80	0.46
1:B:959:THR:HG21	1:B:1022:VAL:HG23	1.97	0.46
1:C:104:GLN:HG3	1:C:105:VAL:N	2.29	0.46
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.43	0.46
1:D:742:ASN:ND2	1:F:214:VAL:HG21	2.30	0.46
1:E:69:MET:HE1	1:E:107:VAL:HG13	1.97	0.46
1:E:318:PRO:HG2	1:E:321:LEU:HB2	1.97	0.46
1:E:356:TYR:CD1	1:E:365:THR:HG21	2.50	0.46
1:E:728:GLN:NE2	1:E:738:ILE:HG21	2.30	0.46
1:E:785:TYR:CZ	1:E:795:PRO:HB3	2.50	0.46
1:F:510:LYS:O	1:F:512:PHE:N	2.40	0.46
1:F:697:LEU:HD12	1:F:846:LEU:HD11	1.97	0.46
1:F:723:LYS:HG2	1:F:803:ARG:CZ	2.45	0.46
1:A:166:ILE:HD13	1:A:166:ILE:HA	1.59	0.46
1:A:340:VAL:O	1:A:343:THR:HB	2.15	0.46
1:B:393:LEU:HD22	1:B:470:PHE:CE1	2.50	0.46
1:C:527:TYR:HE2	1:C:963:VAL:HG13	1.80	0.46
1:D:880:PHE:HA	1:D:883:LEU:HD12	1.97	0.46
1:F:486:LEU:O	1:F:490:PRO:HG2	2.15	0.46
1:F:563:PHE:CE2	1:F:564:LEU:HD13	2.50	0.46
1:A:157:TYR:HD2	1:A:162:MET:HE2	1.80	0.46
1:A:190:PRO:HG2	1:A:774:TYR:CG	2.51	0.46
1:A:200:PRO:HB2	1:A:744:THR:HG22	1.98	0.46
1:A:281:PHE:HB2	1:A:610:PHE:HE1	1.80	0.46
1:A:772:ALA:HB1	1:C:225:VAL:HG12	1.97	0.46
1:A:932:LEU:HD23	1:A:932:LEU:HA	1.51	0.46
1:B:366:LEU:O	1:B:369:THR:HB	2.15	0.46
1:C:572:PHE:CE1	1:C:643:THR:HG22	2.51	0.46
1:C:587:THR:HG21	1:C:617:GLN:O	2.15	0.46
1:C:899:VAL:CG2	1:C:1017:VAL:HG22	2.45	0.46
1:D:23:GLY:O	1:D:27:ILE:HG13	2.15	0.46
1:D:152:GLU:CD	1:D:152:GLU:H	2.24	0.46
1:D:544:LEU:O	1:D:548:ILE:HG13	2.16	0.46
1:E:101:ASP:HA	1:E:131:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:356:TYR:C	1:F:358:PHE:N	2.73	0.46
1:F:419:VAL:HG21	1:F:434:SER:HB3	1.96	0.46
1:F:859:TYR:HD2	1:F:859:TYR:O	1.98	0.46
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.96	0.46
1:A:412:VAL:HG22	1:A:438:ILE:HD11	1.96	0.46
1:A:574:THR:HG22	1:A:624:VAL:CG2	2.45	0.46
1:A:836:MET:HG2	1:A:854:TRP:CH2	2.49	0.46
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.97	0.46
1:B:507:GLU:O	1:B:509:LYS:HG3	2.16	0.46
1:C:45:ILE:HG21	1:C:111:LEU:HG	1.96	0.46
1:C:293:LEU:HD22	1:C:297:ALA:HB3	1.96	0.46
1:C:1007:VAL:O	1:C:1011:VAL:HG23	2.16	0.46
1:D:55:LYS:HB3	1:D:55:LYS:HE2	1.71	0.46
1:D:749:TRP:CZ3	1:F:219:LEU:HG	2.51	0.46
1:E:394:THR:HG23	1:E:469:GLN:HB3	1.98	0.46
1:E:841:GLN:O	1:E:844:SER:OG	2.33	0.46
1:F:288:GLY:O	1:F:289:LEU:HD23	2.16	0.46
1:F:795:PRO:HG2	1:F:798:ALA:HB2	1.97	0.46
1:A:379:THR:HG21	1:A:477:ALA:HB2	1.96	0.46
1:B:462:SER:O	1:B:466:ILE:HG13	2.15	0.46
1:B:525:HIS:HA	1:B:528:THR:HG22	1.97	0.46
1:B:527:TYR:CE1	1:B:1014:ILE:HD12	2.51	0.46
1:B:932:LEU:HD23	1:B:932:LEU:HA	1.78	0.46
1:D:621:ILE:HD12	1:D:622:ALA:H	1.79	0.46
1:D:698:LEU:HD21	1:D:713:PRO:HD3	1.96	0.46
1:E:453:PHE:O	1:E:471:SER:OG	2.32	0.46
1:E:484:VAL:O	1:E:489:THR:HG23	2.15	0.46
1:E:720:PRO:HA	1:E:806:TYR:HA	1.96	0.46
1:F:6:ILE:H	1:F:6:ILE:HG12	1.40	0.46
1:F:96:SER:HB3	1:F:461:GLY:HA2	1.98	0.46
1:F:139:VAL:O	1:F:326:PRO:HD2	2.15	0.46
1:F:293:LEU:HD13	1:F:294:ALA:O	2.15	0.46
1:F:504:ASP:C	1:F:506:GLY:N	2.72	0.46
1:A:21:LEU:HA	1:A:21:LEU:HD13	1.74	0.46
1:A:211:ASN:O	1:A:755:ASN:ND2	2.46	0.46
1:A:375:VAL:HG13	1:A:480:LEU:HB2	1.97	0.46
1:A:749:TRP:CZ3	1:C:219:LEU:HD23	2.49	0.46
1:B:76:MET:HB2	1:B:93:THR:O	2.16	0.46
1:B:394:THR:HG23	1:B:469:GLN:OE1	2.15	0.46
1:B:840:GLU:HG2	1:B:852:TYR:CE1	2.51	0.46
1:C:47:ALA:HB3	1:C:88:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:SER:O	1:C:246:PHE:HD1	1.99	0.46
1:C:855:THR:HG23	1:C:856:GLY:N	2.31	0.46
1:D:21:LEU:HA	1:D:21:LEU:HD13	1.57	0.46
1:D:30:LEU:CD1	1:D:384:ALA:HA	2.46	0.46
1:D:420:MET:HB3	1:D:500:ILE:HB	1.98	0.46
1:D:749:TRP:CE3	1:F:234:ILE:HD11	2.51	0.46
1:E:222:THR:HA	1:E:224:PRO:HD3	1.98	0.46
1:E:896:VAL:HG23	1:E:937:ALA:HB3	1.98	0.46
1:F:967:LEU:HA	1:F:970:ILE:HD12	1.98	0.46
1:A:645:ARG:C	1:A:648:ARG:HB3	2.41	0.46
1:A:1006:MET:O	1:A:1010:THR:HG23	2.16	0.46
1:C:135:SER:HB3	1:C:668:GLU:HA	1.98	0.46
1:C:210:GLN:OE1	1:C:249:ILE:HG23	2.15	0.46
1:C:900:VAL:O	1:C:904:VAL:HG23	2.16	0.46
1:D:136:PHE:CE2	1:D:292:LYS:HE3	2.50	0.46
1:D:277:ILE:HG12	1:D:614:GLY:HA3	1.98	0.46
1:D:787:ARG:HA	1:D:792:GLN:O	2.15	0.46
1:A:100:ALA:HB1	1:A:131:LYS:HD2	1.98	0.46
1:A:212:ALA:HA	1:A:239:ARG:NE	2.30	0.46
1:A:249:ILE:HB	1:A:262:LEU:HB2	1.97	0.46
1:A:255:GLN:H	1:A:255:GLN:HG3	1.57	0.46
1:A:375:VAL:HG21	1:A:481:SER:HA	1.97	0.46
1:A:636:GLU:HA	1:A:641:ALA:HB3	1.98	0.46
1:B:727:ASP:OD1	1:B:730:LYS:HG3	2.16	0.46
1:B:906:GLY:HA3	1:B:1008:THR:CG2	2.46	0.46
1:C:144:ASN:HA	1:C:320:GLY:O	2.16	0.46
1:C:250:LEU:CD1	1:C:259:ARG:HB3	2.45	0.46
1:C:277:ILE:HA	1:C:614:GLY:HA2	1.98	0.46
1:C:534:ILE:HG21	1:C:534:ILE:HD13	1.67	0.46
1:C:739:ASN:O	1:C:743:THR:OG1	2.18	0.46
1:D:757:PHE:HE1	1:D:759:ASP:HB2	1.81	0.46
1:E:648:ARG:O	1:E:651:SER:OG	2.34	0.46
1:F:10:ILE:O	1:F:14:VAL:HG23	2.16	0.46
1:F:105:VAL:HA	1:F:108:GLN:HE21	1.80	0.46
1:F:138:MET:HE2	1:F:140:VAL:HG22	1.98	0.46
1:F:340:VAL:HG12	1:F:395:MET:HE3	1.97	0.46
1:F:421:ALA:O	1:F:503:GLY:N	2.30	0.46
1:F:757:PHE:CE1	1:F:759:ASP:HB2	2.50	0.46
1:A:325:TYR:HA	1:A:326:PRO:HD2	1.86	0.46
1:A:438:ILE:O	1:A:442:LEU:HG	2.16	0.46
1:B:677:PHE:HB3	1:B:822:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:900:VAL:HG22	1:B:930:ILE:HG23	1.98	0.46
1:C:731:ALA:HA	1:C:736:VAL:HG23	1.97	0.46
1:C:902:LEU:HD23	1:C:1013:ALA:HA	1.97	0.46
1:D:30:LEU:HD13	1:D:384:ALA:HA	1.98	0.46
1:E:694:ARG:NH1	1:E:820:MET:HE1	2.31	0.46
1:F:425:LEU:HB3	1:F:429:GLU:HG2	1.98	0.46
1:F:738:ILE:O	1:F:741:ILE:HG13	2.16	0.46
1:A:72:ILE:HD13	1:A:107:VAL:HG22	1.98	0.46
1:B:68:ASN:CB	1:B:114:ALA:HB2	2.46	0.46
1:B:457:ALA:HB2	1:B:471:SER:OG	2.16	0.46
1:B:544:LEU:O	1:B:547:ILE:HB	2.16	0.46
1:B:787:ARG:HA	1:B:792:GLN:O	2.15	0.46
1:C:2:PRO:HB2	1:C:3:ASN:OD1	2.15	0.46
1:C:836:MET:HA	1:C:854:TRP:CH2	2.51	0.46
1:E:4:PHE:O	1:E:8:ARG:HD2	2.15	0.46
1:E:190:PRO:HB3	1:E:784:TRP:CE2	2.51	0.46
1:E:691:THR:HA	1:E:694:ARG:NH1	2.31	0.46
1:E:748:ALA:O	1:E:769:MET:HG2	2.16	0.46
1:F:26:ALA:HB1	1:F:384:ALA:CB	2.45	0.46
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.98	0.46
1:F:352:PHE:HA	1:F:355:MET:CE	2.46	0.46
1:F:945:LYS:O	1:F:948:MET:N	2.49	0.46
1:A:488:LEU:O	1:A:491:ALA:HB3	2.15	0.45
1:A:516:PHE:HA	1:A:519:MET:HG3	1.98	0.45
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.51	0.45
1:B:427:PRO:O	1:B:430:ALA:HB3	2.17	0.45
1:B:455:PRO:HG2	1:B:875:SER:HG	1.81	0.45
1:C:423:GLU:HB2	1:C:425:LEU:HG	1.98	0.45
1:C:986:ILE:O	1:C:986:ILE:HD13	2.16	0.45
1:D:136:PHE:HD2	1:D:292:LYS:HG3	1.81	0.45
1:D:250:LEU:CD1	1:D:259:ARG:HB3	2.44	0.45
1:D:332:PHE:CD1	1:D:569:GLN:HG2	2.50	0.45
1:D:456:MET:HE3	1:D:471:SER:CA	2.46	0.45
1:D:559:LEU:HD13	1:D:918:ASN:HB2	1.96	0.45
1:E:748:ALA:HB3	1:E:749:TRP:HD1	1.81	0.45
1:F:110:LYS:HD3	1:F:110:LYS:HA	1.61	0.45
1:F:344:LEU:HD13	1:F:402:ILE:HD11	1.98	0.45
1:F:654:LYS:HB3	1:F:656:ALA:H	1.81	0.45
1:A:424:GLY:C	1:A:502:LYS:HZ2	2.19	0.45
1:A:681:ASP:OD1	1:A:684:GLY:N	2.47	0.45
1:B:470:PHE:O	1:B:474:ILE:HG13	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ALA:O	1:C:391:ASN:HA	2.16	0.45
1:C:200:PRO:HA	1:C:203:VAL:HG23	1.98	0.45
1:C:343:THR:HG23	1:C:983:PRO:HB2	1.98	0.45
1:C:542:LEU:O	1:C:546:LEU:HG	2.16	0.45
1:C:890:TRP:HA	1:C:890:TRP:HE3	1.81	0.45
1:D:3:ASN:O	1:D:5:PHE:N	2.49	0.45
1:D:184:MET:HB3	1:D:766:VAL:HG13	1.97	0.45
1:E:106:GLN:HA	1:E:109:ASN:ND2	2.31	0.45
1:E:172:VAL:CG2	1:E:306:ILE:HD11	2.46	0.45
1:E:445:ILE:HG21	1:E:935:LYS:CD	2.46	0.45
1:E:955:LEU:HD13	1:E:1025:ARG:HG2	1.98	0.45
1:F:101:ASP:OD1	1:F:131:LYS:NZ	2.46	0.45
1:F:171:GLY:HA3	1:F:302:THR:OG1	2.15	0.45
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.97	0.45
1:A:363:ARG:O	1:A:366:LEU:N	2.49	0.45
1:B:23:GLY:HA3	1:B:377:LEU:HB3	1.99	0.45
1:B:119:PRO:HG2	1:B:122:VAL:CG2	2.46	0.45
1:B:363:ARG:HD2	1:B:498:LYS:HD2	1.97	0.45
1:B:510:LYS:HB2	1:B:514:GLY:H	1.82	0.45
1:C:514:GLY:O	1:C:518:ARG:HD3	2.16	0.45
1:C:541:TYR:OH	2:C:1101:LMT:O6'	2.34	0.45
1:C:1006:MET:HA	1:C:1009:ALA:HB3	1.97	0.45
1:D:72:ILE:HD13	1:D:107:VAL:HG22	1.99	0.45
1:D:470:PHE:CE2	1:D:924:VAL:HG21	2.51	0.45
1:D:974:SER:CB	1:D:1010:THR:HG21	2.47	0.45
1:E:186:ILE:O	1:E:768:VAL:HA	2.16	0.45
1:F:65:ILE:HD13	1:F:90:ILE:HD11	1.97	0.45
1:F:77:TYR:CE1	1:F:93:THR:HG21	2.52	0.45
1:F:676:ASP:HB3	1:F:823:LEU:CD2	2.46	0.45
1:F:941:VAL:HG13	1:F:1021:PHE:CZ	2.52	0.45
1:F:1003:MET:O	1:F:1007:VAL:HG23	2.16	0.45
1:A:349:ILE:O	1:A:352:PHE:HB3	2.17	0.45
1:A:654:LYS:HD3	1:A:654:LYS:HA	1.62	0.45
1:B:347:ALA:O	1:B:351:VAL:HG23	2.16	0.45
1:B:418:ARG:HD2	1:B:965:MET:HB2	1.98	0.45
1:C:662:ASN:OD1	1:C:663:LEU:HD23	2.16	0.45
1:D:456:MET:HE3	1:D:471:SER:HA	1.99	0.45
1:D:776:MET:CE	1:F:225:VAL:H	2.30	0.45
1:E:54:ALA:N	1:E:84:SER:HA	2.31	0.45
1:E:166:ILE:HG23	1:E:306:ILE:HG12	1.99	0.45
1:E:876:LEU:HD23	1:E:876:LEU:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:982:MET:O	1:E:985:VAL:HG23	2.16	0.45
1:F:459:PHE:CZ	1:F:871:LEU:HG	2.52	0.45
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.78	0.45
1:A:981:VAL:O	1:A:984:LEU:N	2.46	0.45
1:C:527:TYR:CE2	1:C:963:VAL:HG13	2.52	0.45
1:C:812:GLU:HB2	1:C:819:SER:O	2.16	0.45
1:C:892:ILE:HD12	1:C:1021:PHE:HE1	1.81	0.45
1:D:293:LEU:HD13	1:D:294:ALA:O	2.16	0.45
1:D:414:GLU:OE2	1:D:969:PRO:HG3	2.16	0.45
1:D:572:PHE:CE1	1:D:643:THR:HG22	2.50	0.45
1:E:331:PRO:HA	1:E:334:LYS:HD2	1.98	0.45
1:E:697:LEU:HD12	1:E:697:LEU:HA	1.75	0.45
1:F:694:ARG:HD3	1:F:820:MET:SD	2.57	0.45
1:A:30:LEU:HD11	1:A:384:ALA:HA	1.98	0.45
1:A:168:ARG:NE	1:B:78:MET:HE1	2.32	0.45
1:A:708:LEU:HA	1:A:825:GLN:O	2.16	0.45
1:A:900:VAL:O	1:A:904:VAL:HG23	2.17	0.45
1:A:948:MET:HG3	1:A:954:GLY:O	2.17	0.45
1:B:373:PRO:O	1:B:376:LEU:HB2	2.17	0.45
1:B:442:LEU:O	1:B:445:ILE:HG13	2.16	0.45
1:B:961:ASP:OD2	1:B:964:ARG:NH2	2.50	0.45
1:C:121:GLU:O	1:C:124:GLN:HG2	2.15	0.45
1:C:152:GLU:CD	1:C:152:GLU:H	2.24	0.45
1:C:786:VAL:HG23	1:C:796:PHE:CE2	2.51	0.45
1:D:222:THR:OG1	1:E:275:TYR:O	2.31	0.45
1:D:225:VAL:H	1:E:776:MET:HE2	1.81	0.45
1:D:251:LEU:HD12	1:D:265:VAL:HG21	1.99	0.45
1:E:377:LEU:O	1:E:380:PHE:HB2	2.17	0.45
1:E:415:ASN:HD22	1:E:434:SER:CB	2.27	0.45
1:F:138:MET:HE3	1:F:138:MET:HB2	1.68	0.45
1:F:250:LEU:HD13	1:F:259:ARG:HB3	1.98	0.45
1:F:525:HIS:O	1:F:526:HIS:C	2.60	0.45
1:F:642:ILE:O	1:F:645:ARG:HG2	2.17	0.45
1:F:980:GLY:O	1:F:983:PRO:HD2	2.17	0.45
1:A:839:MET:HE2	1:A:842:LEU:HD12	1.97	0.45
1:A:941:VAL:HG22	1:A:1021:PHE:CD1	2.52	0.45
1:B:580:ALA:HB1	1:B:719:THR:HG22	1.99	0.45
1:B:647:THR:CG2	1:B:660:ALA:H	2.29	0.45
1:C:153:ASP:OD2	1:C:153:ASP:N	2.47	0.45
1:C:394:THR:O	1:C:398:MET:HG2	2.17	0.45
1:C:407:ASP:OD1	1:C:407:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:PHE:C	1:D:281:PHE:CD2	2.95	0.45
1:D:383:LEU:HD22	1:D:388:PHE:CD1	2.52	0.45
1:D:383:LEU:HD22	1:D:388:PHE:HD1	1.81	0.45
1:D:618:ASN:N	1:D:618:ASN:OD1	2.50	0.45
1:D:977:PHE:HD2	1:D:1006:MET:HG3	1.82	0.45
1:D:1016:PHE:O	1:D:1019:VAL:HB	2.17	0.45
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.98	0.45
1:E:354:VAL:CG1	1:E:972:MET:HG2	2.46	0.45
1:E:708:LEU:H	1:E:708:LEU:HG	1.42	0.45
1:F:5:PHE:HD2	1:F:6:ILE:HG12	1.82	0.45
1:F:361:ASN:HD22	1:F:364:ALA:HB2	1.80	0.45
1:F:932:LEU:O	1:F:935:LYS:HB3	2.17	0.45
1:A:184:MET:HB3	1:A:766:VAL:HG13	1.98	0.45
1:A:597:TYR:CD2	1:A:650:PHE:CZ	3.05	0.45
1:A:873:ALA:O	1:A:877:ILE:HG12	2.16	0.45
1:A:956:ILE:H	1:A:956:ILE:HG13	1.38	0.45
1:B:139:VAL:HA	1:B:289:LEU:O	2.16	0.45
1:B:293:LEU:HD11	1:B:297:ALA:O	2.17	0.45
1:B:428:LYS:O	1:B:431:THR:N	2.49	0.45
1:C:376:LEU:HD22	1:C:398:MET:CE	2.47	0.45
1:C:379:THR:HG23	1:C:476:SER:OG	2.17	0.45
1:C:453:PHE:CD2	1:C:456:MET:CE	2.95	0.45
1:D:7:ASP:O	1:D:8:ARG:HG3	2.16	0.45
1:D:240:LEU:HD22	1:D:245:GLU:OE1	2.16	0.45
1:D:763:VAL:HG12	1:E:63:GLN:OE1	2.17	0.45
1:D:880:PHE:O	1:D:883:LEU:HB2	2.17	0.45
1:D:979:LEU:HA	1:D:979:LEU:HD23	1.34	0.45
1:E:425:LEU:HD12	1:E:430:ALA:HA	1.99	0.45
1:E:564:LEU:CD1	1:E:666:ILE:HD12	2.47	0.45
1:E:564:LEU:HD13	1:E:666:ILE:HD12	1.98	0.45
1:F:414:GLU:HB2	1:F:972:MET:HE1	1.98	0.45
1:F:521:GLU:O	1:F:524:THR:HB	2.16	0.45
1:F:787:ARG:HA	1:F:792:GLN:O	2.17	0.45
1:A:882:CYS:O	1:A:885:ALA:HB3	2.16	0.45
1:B:445:ILE:HG21	1:B:935:LYS:HD2	1.98	0.45
1:C:181:GLN:HG2	1:C:182:TYR:N	2.31	0.45
1:D:441:ALA:HB2	1:D:942:GLU:OE2	2.17	0.45
1:A:75:LEU:CD1	1:A:92:LEU:HD23	2.47	0.45
1:A:414:GLU:CG	1:A:972:MET:HE1	2.46	0.45
1:A:444:GLY:O	1:A:448:VAL:HG23	2.17	0.45
1:A:720:PRO:HA	1:A:805:GLU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:ASP:OD2	1:A:764:LYS:NZ	2.40	0.45
1:A:1013:ALA:C	1:A:1015:PHE:N	2.75	0.45
1:B:354:VAL:HG22	1:B:975:LEU:HD23	1.99	0.45
1:B:383:LEU:HD22	1:B:472:ILE:HG22	1.99	0.45
1:B:528:THR:O	1:B:529:ASP:C	2.60	0.45
1:B:650:PHE:HB3	1:B:658:VAL:HB	1.99	0.45
1:C:461:GLY:HA3	1:C:863:LEU:HD21	1.99	0.45
1:D:685:LEU:O	1:D:689:LYS:HD2	2.16	0.45
1:D:776:MET:HE3	1:F:228:GLN:CD	2.42	0.45
1:E:367:ILE:CD1	1:E:497:LEU:HD13	2.47	0.45
1:E:427:PRO:O	1:E:430:ALA:HB3	2.16	0.45
1:F:363:ARG:CZ	1:F:363:ARG:H	2.29	0.45
1:A:35:TYR:CE2	1:A:564:LEU:HD21	2.52	0.44
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.52	0.44
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.83	0.44
1:B:525:HIS:O	1:B:528:THR:HG22	2.17	0.44
1:B:674:GLY:HA2	1:B:825:GLN:HA	1.98	0.44
1:B:723:LYS:HE3	1:B:725:ASP:OD2	2.17	0.44
1:B:873:ALA:O	1:B:877:ILE:HG13	2.17	0.44
1:C:163:LYS:HE3	1:C:177:LEU:HB2	1.99	0.44
1:C:694:ARG:HG2	1:C:698:LEU:HD12	1.98	0.44
1:C:845:LYS:HD2	1:C:845:LYS:O	2.17	0.44
1:D:214:VAL:HG21	1:E:742:ASN:ND2	2.32	0.44
1:D:262:LEU:HG	1:D:268:ILE:HD11	1.99	0.44
1:D:685:LEU:HD21	1:D:848:THR:O	2.18	0.44
1:D:831:SER:OG	1:D:832:THR:N	2.49	0.44
1:E:7:ASP:C	1:E:8:ARG:HG3	2.42	0.44
1:E:108:GLN:HA	1:E:129:VAL:HG21	1.98	0.44
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.98	0.44
1:E:162:MET:HA	1:E:313:MET:HE1	1.99	0.44
1:E:571:VAL:HG22	1:E:625:SER:HA	1.98	0.44
1:F:187:TRP:O	1:F:266:ALA:HB1	2.17	0.44
1:F:614:GLY:O	1:F:616:GLY:HA3	2.16	0.44
1:A:388:PHE:CE2	1:A:472:ILE:HD13	2.53	0.44
1:A:470:PHE:CD2	1:A:924:VAL:HG11	2.52	0.44
1:A:722:PHE:CD1	1:A:804:TRP:CE2	3.05	0.44
1:A:904:VAL:HA	1:A:926:LEU:HD21	1.99	0.44
1:B:329:THR:O	1:B:333:VAL:HG23	2.16	0.44
1:B:576:VAL:HG22	1:B:658:VAL:HG22	1.99	0.44
1:D:307:ARG:HD3	1:D:307:ARG:HA	1.88	0.44
1:D:336:SER:O	1:D:340:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:723:LYS:HB3	1:D:803:ARG:HG2	2.00	0.44
1:D:1033:GLU:H	1:D:1034:ASP:C	2.25	0.44
1:E:102:ILE:O	1:E:106:GLN:HG3	2.17	0.44
1:E:255:GLN:H	1:E:255:GLN:HG3	1.38	0.44
1:E:329:THR:O	1:E:332:PHE:HB3	2.18	0.44
1:E:409:ALA:O	1:E:413:VAL:HG23	2.17	0.44
1:E:568:ASP:O	1:E:629:TRP:CZ3	2.70	0.44
1:E:770:SER:OG	1:E:775:ARG:HG2	2.18	0.44
1:F:65:ILE:O	1:F:69:MET:HG2	2.17	0.44
1:F:940:ILE:HG12	1:F:966:ARG:NH2	2.32	0.44
1:A:213:GLN:HA	1:A:237:GLN:O	2.17	0.44
1:A:663:LEU:HD12	1:A:667:VAL:HG13	1.98	0.44
1:A:871:LEU:O	1:A:874:ILE:HB	2.17	0.44
1:B:65:ILE:O	1:B:69:MET:HG2	2.17	0.44
1:B:235:ILE:HD11	1:C:721:GLN:OE1	2.17	0.44
1:B:330:THR:HB	1:B:331:PRO:HD3	1.98	0.44
1:B:984:LEU:HB3	1:B:995:GLN:O	2.17	0.44
1:C:615:GLY:HA2	1:C:616:GLY:HA3	1.69	0.44
1:D:123:GLN:HB3	1:E:116:PRO:HB3	1.99	0.44
1:D:463:THR:HG22	1:D:467:TYR:CE2	2.51	0.44
1:D:827:ALA:O	1:D:830:LYS:N	2.39	0.44
1:A:34:GLN:O	1:A:392:THR:OG1	2.16	0.44
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.45	0.44
1:A:376:LEU:HD22	1:A:398:MET:SD	2.57	0.44
1:A:650:PHE:HD1	1:A:653:ILE:HD11	1.83	0.44
1:B:573:MET:HE3	1:B:621:ILE:HD11	2.00	0.44
1:D:531:VAL:O	1:D:535:LEU:HG	2.17	0.44
1:D:833:GLY:O	1:D:836:MET:HB2	2.17	0.44
1:D:871:LEU:HD23	1:D:871:LEU:HA	1.66	0.44
1:D:911:ALA:HB2	1:D:922:PHE:CE1	2.53	0.44
1:E:344:LEU:O	1:E:348:ILE:HG13	2.18	0.44
1:E:632:ARG:HB3	1:E:637:ASN:HB3	1.99	0.44
1:E:837:GLU:O	1:E:840:GLU:HB2	2.18	0.44
1:F:247:GLY:O	1:F:261:LEU:HB3	2.18	0.44
1:F:312:LYS:O	1:F:312:LYS:HD3	2.17	0.44
1:A:631:ASP:C	1:A:633:PRO:HD3	2.42	0.44
1:A:892:ILE:HG12	1:A:1025:ARG:CD	2.46	0.44
1:A:998:VAL:O	1:A:999:GLY:C	2.61	0.44
1:C:53:ASP:HA	1:C:84:SER:HB2	1.99	0.44
1:C:103:ALA:O	1:C:107:VAL:HG23	2.18	0.44
1:C:343:THR:HA	1:C:346:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:ASP:O	1:D:331:PRO:HD2	2.18	0.44
1:D:366:LEU:HD22	1:D:370:ILE:HG13	2.00	0.44
1:D:982:MET:HB3	1:D:983:PRO:HD3	2.00	0.44
1:E:545:TYR:O	1:E:546:LEU:C	2.61	0.44
1:E:568:ASP:O	1:E:629:TRP:HZ3	2.00	0.44
1:E:685:LEU:HD11	1:E:690:LEU:HG	1.99	0.44
1:E:776:MET:HE3	1:E:776:MET:HB3	1.69	0.44
1:F:400:LEU:HD11	1:F:1002:VAL:HG21	1.99	0.44
1:F:728:GLN:HE22	1:F:738:ILE:HG21	1.83	0.44
1:F:919:ASP:C	1:F:919:ASP:OD1	2.60	0.44
1:A:413:VAL:HA	1:A:493:CYS:SG	2.57	0.44
1:A:691:THR:HG23	1:A:694:ARG:NH1	2.25	0.44
1:A:742:ASN:CG	1:C:214:VAL:HG11	2.43	0.44
1:A:769:MET:HG2	1:A:770:SER:N	2.33	0.44
1:A:959:THR:HG21	1:A:1022:VAL:HG23	1.99	0.44
1:B:61:VAL:HG22	1:B:119:PRO:HD2	1.99	0.44
1:B:399:VAL:HA	1:B:402:ILE:HG13	2.00	0.44
1:B:707:MET:SD	1:B:830:LYS:HG2	2.58	0.44
1:C:6:ILE:HG22	1:C:8:ARG:O	2.17	0.44
1:C:84:SER:C	1:C:86:GLY:H	2.23	0.44
1:C:506:GLY:C	1:C:508:GLY:N	2.75	0.44
1:C:538:THR:HG21	1:C:1023:VAL:CG2	2.48	0.44
1:D:345:VAL:O	1:D:349:ILE:HD12	2.18	0.44
1:D:400:LEU:HG	1:D:928:THR:OG1	2.18	0.44
1:D:682:GLN:HG3	1:D:817:LEU:HD13	2.00	0.44
1:E:198:LEU:HD21	1:E:252:LYS:HB2	1.99	0.44
1:E:420:MET:SD	1:E:499:PRO:HA	2.58	0.44
1:E:610:PHE:HB2	1:E:623:PHE:HB3	2.00	0.44
1:E:728:GLN:HE22	1:E:738:ILE:HG21	1.82	0.44
1:E:942:GLU:O	1:E:943:PHE:C	2.59	0.44
1:F:647:THR:HG23	1:F:659:PHE:CE1	2.53	0.44
1:F:1018:PRO:O	1:F:1022:VAL:HG23	2.18	0.44
1:A:180:SER:HG	1:A:273:GLU:H	1.65	0.44
1:A:363:ARG:O	1:A:496:MET:HE2	2.18	0.44
1:A:415:ASN:O	1:A:419:VAL:HG23	2.17	0.44
1:B:478:MET:O	1:B:482:VAL:HG12	2.17	0.44
1:C:65:ILE:HD11	1:C:118:LEU:HD11	1.99	0.44
1:C:158:VAL:HG13	1:C:162:MET:HE3	1.99	0.44
1:C:574:THR:HG23	1:C:622:ALA:HB3	1.98	0.44
1:C:955:LEU:O	1:C:959:THR:HG23	2.17	0.44
1:D:346:GLU:O	1:D:350:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:MET:O	1:D:399:VAL:HG23	2.17	0.44
1:D:975:LEU:HD12	1:D:975:LEU:HA	1.82	0.44
1:E:21:LEU:O	1:E:25:LEU:HB2	2.18	0.44
1:E:694:ARG:NH2	1:E:717:GLU:OE1	2.50	0.44
1:F:101:ASP:O	1:F:105:VAL:HG23	2.17	0.44
1:F:345:VAL:O	1:F:349:ILE:HD12	2.18	0.44
1:F:468:ARG:HA	1:F:471:SER:OG	2.18	0.44
1:F:677:PHE:C	1:F:677:PHE:CD2	2.95	0.44
1:F:687:HIS:HE2	1:F:718:ASP:CG	2.25	0.44
1:B:13:TRP:O	1:B:17:ILE:HG13	2.17	0.44
1:B:72:ILE:HG12	1:B:106:GLN:HB3	1.99	0.44
1:D:164:ASP:HB3	1:D:168:ARG:HH21	1.82	0.44
1:D:927:LEU:O	1:D:928:THR:C	2.61	0.44
1:D:956:ILE:H	1:D:956:ILE:HG13	1.16	0.44
1:E:165:ALA:HB3	1:E:313:MET:HE2	2.00	0.44
1:F:602:GLU:HB3	1:F:606:VAL:HG23	1.99	0.44
1:F:644:MET:HE2	1:F:709:THR:HG21	2.00	0.44
1:F:916:LEU:HD23	1:F:916:LEU:HA	1.76	0.44
1:A:130:GLU:HB3	1:A:132:SER:HB2	2.00	0.44
1:A:324:VAL:HG22	1:A:325:TYR:H	1.82	0.44
1:A:483:LEU:HD13	1:A:487:ILE:HD12	1.99	0.44
1:A:636:GLU:HB2	1:A:645:ARG:NH2	2.30	0.44
1:A:895:SER:HB2	1:A:1021:PHE:HA	1.99	0.44
1:B:399:VAL:O	1:B:402:ILE:HG13	2.18	0.44
1:B:445:ILE:HD12	1:B:449:LEU:HD12	2.00	0.44
1:B:975:LEU:O	1:B:979:LEU:HB2	2.18	0.44
1:C:429:GLU:O	1:C:433:LYS:HB2	2.18	0.44
1:C:435:MET:HE2	1:C:435:MET:HB2	1.65	0.44
1:C:453:PHE:HD2	1:C:456:MET:HE1	1.80	0.44
1:C:541:TYR:HH	2:C:1101:LMT:H6'	1.64	0.44
1:C:663:LEU:HD23	1:C:663:LEU:H	1.83	0.44
1:D:563:PHE:O	1:D:564:LEU:HD12	2.18	0.44
2:D:2000:LMT:H6E	2:D:2000:LMT:O5B	2.18	0.44
1:E:172:VAL:HG22	1:E:302:THR:HG23	2.00	0.44
1:E:515:TRP:O	1:E:519:MET:HG3	2.18	0.44
1:E:905:ILE:HG23	1:E:906:GLY:N	2.33	0.44
1:F:669:LEU:HD22	1:F:856:GLY:HA2	1.98	0.44
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.85	0.43
1:A:451:ALA:CB	1:A:878:VAL:HG12	2.48	0.43
1:B:214:VAL:HG21	1:C:742:ASN:ND2	2.32	0.43
1:B:902:LEU:HD11	1:B:1016:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:959:THR:HG21	1:B:1022:VAL:CG2	2.48	0.43
1:C:282:ASN:C	1:C:284:GLN:H	2.26	0.43
1:C:722:PHE:CZ	1:C:802:SER:HB2	2.53	0.43
1:D:196:PHE:CG	1:D:260:VAL:HG11	2.53	0.43
1:D:377:LEU:O	1:D:380:PHE:HB2	2.17	0.43
1:D:712:ARG:O	1:D:822:ILE:HG23	2.17	0.43
1:E:110:LYS:HD3	1:E:110:LYS:HA	1.60	0.43
1:E:149:MET:HB2	1:E:153:ASP:CB	2.43	0.43
1:F:35:TYR:HB3	1:F:38:ILE:HD12	2.00	0.43
1:F:49:TYR:CD1	1:F:57:VAL:HA	2.52	0.43
1:F:146:ASP:OD2	1:F:147:GLY:N	2.49	0.43
1:F:281:PHE:HB2	1:F:610:PHE:CE1	2.53	0.43
1:F:343:THR:O	1:F:346:GLU:N	2.51	0.43
1:F:425:LEU:HB3	1:F:429:GLU:HB3	2.00	0.43
1:F:770:SER:OG	1:F:775:ARG:HG2	2.18	0.43
1:A:788:ALA:HB3	1:A:790:ASP:OD2	2.18	0.43
1:A:961:ASP:O	1:A:962:ALA:C	2.61	0.43
1:A:1035:ILE:O	1:A:1036:GLU:HB2	2.18	0.43
1:B:424:GLY:HA3	1:B:502:LYS:HB2	2.00	0.43
1:B:526:HIS:O	1:B:529:ASP:HB2	2.18	0.43
1:B:691:THR:HG23	1:B:694:ARG:NH1	2.33	0.43
1:B:755:ASN:O	1:B:766:VAL:HB	2.18	0.43
1:C:129:VAL:C	1:C:130:GLU:HG3	2.42	0.43
1:D:34:GLN:HB2	1:D:333:VAL:HG22	2.00	0.43
1:D:960:LEU:HD23	1:D:960:LEU:HA	1.75	0.43
1:D:991:GLY:C	1:D:993:GLY:H	2.26	0.43
1:D:1020:PHE:O	1:D:1024:VAL:HB	2.18	0.43
1:E:187:TRP:HZ3	1:E:769:MET:HB3	1.82	0.43
1:E:370:ILE:HD12	1:E:492:LEU:HD13	2.00	0.43
1:E:676:ASP:HA	1:E:823:LEU:HD23	1.99	0.43
1:E:821:GLU:HG2	1:E:822:ILE:N	2.33	0.43
1:F:309:GLU:OE2	1:F:313:MET:HE3	2.18	0.43
1:F:343:THR:HA	1:F:346:GLU:OE1	2.18	0.43
1:F:610:PHE:O	1:F:622:ALA:HA	2.18	0.43
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.78	0.43
1:A:527:TYR:O	1:A:530:SER:HB3	2.18	0.43
1:A:667:VAL:HG12	1:A:668:GLU:OE1	2.19	0.43
1:A:770:SER:OG	1:A:775:ARG:HG2	2.18	0.43
1:A:962:ALA:O	1:A:965:MET:HG2	2.18	0.43
1:B:108:GLN:CD	1:C:112:GLN:HG2	2.44	0.43
1:B:544:LEU:O	1:B:548:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:LEU:HD12	1:C:406:VAL:N	2.34	0.43
1:C:679:LEU:O	1:C:819:SER:HB2	2.18	0.43
1:C:905:ILE:HG13	1:C:909:LEU:HD23	2.00	0.43
1:C:911:ALA:HB2	1:C:922:PHE:CE1	2.52	0.43
1:D:246:PHE:O	1:D:262:LEU:HD23	2.18	0.43
1:D:281:PHE:C	1:D:281:PHE:HD2	2.26	0.43
1:D:343:THR:HG21	1:D:984:LEU:HD21	2.00	0.43
1:D:415:ASN:ND2	1:D:943:PHE:HZ	2.15	0.43
1:D:559:LEU:HA	1:D:560:PRO:HD2	1.68	0.43
1:D:588:GLN:NE2	1:D:588:GLN:O	2.51	0.43
1:D:691:THR:HA	1:D:694:ARG:NH1	2.33	0.43
1:D:981:VAL:O	1:D:982:MET:C	2.61	0.43
1:E:238:THR:HG22	1:E:239:ARG:O	2.17	0.43
1:E:559:LEU:CD2	1:E:560:PRO:HD2	2.46	0.43
1:E:574:THR:OG1	1:E:659:PHE:O	2.27	0.43
1:F:143:ILE:HG12	1:F:322:LYS:O	2.19	0.43
1:F:348:ILE:HG12	1:F:402:ILE:HD13	2.00	0.43
1:F:650:PHE:HB2	1:F:658:VAL:O	2.18	0.43
1:F:707:MET:HB2	1:F:708:LEU:HD12	2.00	0.43
1:A:154:ILE:HG22	1:A:287:SER:HB3	2.01	0.43
1:A:615:GLY:HA2	1:A:617:GLN:H	1.82	0.43
1:A:695:ASN:O	1:A:698:LEU:HB2	2.18	0.43
1:A:722:PHE:HD1	1:A:804:TRP:CE2	2.37	0.43
1:A:932:LEU:O	1:A:935:LYS:HB3	2.18	0.43
1:B:452:VAL:HG23	1:B:453:PHE:CD2	2.53	0.43
1:B:574:THR:HG21	1:B:598:TYR:HE2	1.83	0.43
1:B:594:VAL:HG22	1:B:650:PHE:CZ	2.53	0.43
1:B:1031:LYS:HA	1:B:1032:ASN:HA	1.68	0.43
1:C:143:ILE:HG22	1:C:286:ALA:CB	2.48	0.43
1:C:146:ASP:O	1:C:148:THR:OG1	2.36	0.43
1:C:356:TYR:C	1:C:358:PHE:H	2.25	0.43
1:C:363:ARG:NH2	1:C:498:LYS:HD2	2.33	0.43
1:C:1031:LYS:HD2	1:C:1033:GLU:CB	2.49	0.43
1:D:81:ASN:O	1:D:88:VAL:HG23	2.19	0.43
1:D:124:GLN:NE2	1:D:753:TYR:HD2	2.16	0.43
1:D:372:VAL:O	1:D:373:PRO:C	2.62	0.43
1:D:454:VAL:O	1:D:457:ALA:HB3	2.19	0.43
1:D:771:GLU:HB3	1:D:774:TYR:CD1	2.53	0.43
1:D:786:VAL:HG23	1:D:796:PHE:CE2	2.53	0.43
1:D:1007:VAL:O	1:D:1011:VAL:HG23	2.18	0.43
1:E:17:ILE:HA	1:E:20:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:GLY:O	1:F:71:GLY:HA3	2.18	0.43
1:F:54:ALA:HB1	1:F:811:LEU:HG	2.00	0.43
1:F:84:SER:HB3	1:F:809:PRO:O	2.17	0.43
1:F:144:ASN:OD1	1:F:148:THR:HA	2.18	0.43
1:A:137:LEU:HD13	1:A:293:LEU:HG	1.99	0.43
1:A:189:ASN:HA	1:A:190:PRO:HD3	1.74	0.43
1:A:225:VAL:H	1:B:776:MET:CE	2.31	0.43
1:B:681:ASP:HA	1:B:849:GLY:O	2.18	0.43
1:C:546:LEU:O	1:C:550:VAL:HG23	2.18	0.43
1:D:199:THR:HG21	1:D:787:ARG:H	1.82	0.43
1:D:959:THR:HG21	1:D:1022:VAL:CG2	2.49	0.43
1:E:30:LEU:HA	1:E:30:LEU:HD12	1.78	0.43
1:E:597:TYR:O	1:E:601:LYS:HB2	2.18	0.43
1:F:196:PHE:CD2	1:F:260:VAL:HG21	2.54	0.43
1:F:544:LEU:O	1:F:547:ILE:HB	2.18	0.43
1:F:771:GLU:HB2	1:F:774:TYR:HD1	1.82	0.43
1:A:79:SER:HA	1:A:813:ARG:O	2.19	0.43
1:A:530:SER:O	1:A:533:GLY:N	2.51	0.43
1:A:639:VAL:CG1	1:A:662:ASN:HB2	2.42	0.43
1:A:814:TYR:OH	1:A:854:TRP:O	2.29	0.43
1:B:281:PHE:HB2	1:B:610:PHE:CE1	2.53	0.43
1:B:398:MET:HE3	1:B:398:MET:HB3	1.63	0.43
1:B:407:ASP:OD1	1:B:973:THR:HG21	2.19	0.43
1:B:422:GLU:C	1:B:423:GLU:HG3	2.44	0.43
1:B:949:ASP:O	1:B:951:GLU:N	2.52	0.43
1:B:1033:GLU:OE2	1:B:1034:ASP:HB2	2.18	0.43
1:C:487:ILE:C	1:C:490:PRO:HD2	2.43	0.43
1:C:514:GLY:C	1:C:516:PHE:N	2.74	0.43
1:C:531:VAL:O	1:C:535:LEU:HG	2.19	0.43
1:C:836:MET:HG2	1:C:854:TRP:CZ3	2.53	0.43
1:C:927:LEU:O	1:C:930:ILE:N	2.51	0.43
1:C:963:VAL:HA	1:C:966:ARG:HH12	1.82	0.43
1:D:852:TYR:CD2	1:D:852:TYR:N	2.86	0.43
1:D:966:ARG:O	1:D:970:ILE:HG12	2.18	0.43
1:E:250:LEU:HD21	1:E:253:VAL:HG22	2.00	0.43
1:F:38:ILE:HD13	1:F:466:ILE:CD1	2.49	0.43
1:F:462:SER:O	1:F:466:ILE:HG12	2.19	0.43
1:F:602:GLU:HG3	1:F:605:ASN:HB2	2.01	0.43
1:A:142:VAL:O	1:A:286:ALA:HB1	2.18	0.43
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.79	0.43
1:A:540:ARG:HH22	2:A:1101:LMT:H6'2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:GLN:OE1	1:A:738:ILE:HG12	2.19	0.43
1:B:26:ALA:HB1	1:B:384:ALA:CB	2.49	0.43
1:B:535:LEU:CD2	1:B:1019:VAL:HA	2.49	0.43
1:B:709:THR:O	1:B:710:SER:OG	2.31	0.43
1:C:188:MET:HB3	1:C:193:LEU:CD1	2.46	0.43
1:C:506:GLY:C	1:C:508:GLY:H	2.25	0.43
1:C:677:PHE:CE1	1:C:852:TYR:HB2	2.53	0.43
1:C:966:ARG:O	1:C:966:ARG:HG2	2.19	0.43
1:D:102:ILE:HD12	1:F:101:ASP:HB3	2.01	0.43
1:D:978:ILE:HG23	1:D:1003:MET:HE2	2.00	0.43
1:E:324:VAL:O	1:E:326:PRO:HD3	2.19	0.43
1:E:518:ARG:O	1:E:519:MET:C	2.62	0.43
1:E:602:GLU:HG3	1:E:602:GLU:O	2.19	0.43
1:F:49:TYR:CE1	1:F:57:VAL:HA	2.53	0.43
1:F:49:TYR:CG	1:F:57:VAL:HG12	2.54	0.43
1:F:343:THR:O	1:F:344:LEU:C	2.62	0.43
1:F:344:LEU:CD2	1:F:402:ILE:HD11	2.48	0.43
1:F:376:LEU:HD22	1:F:398:MET:CE	2.49	0.43
1:F:489:THR:O	1:F:490:PRO:C	2.59	0.43
1:F:706:ASP:OD1	1:F:706:ASP:N	2.49	0.43
1:A:242:SER:OG	1:A:245:GLU:HG2	2.19	0.43
1:A:722:PHE:HB2	1:A:804:TRP:CZ3	2.52	0.43
1:A:893:PRO:O	1:A:896:VAL:HG13	2.18	0.43
1:C:66:GLU:HG2	1:C:78:MET:SD	2.59	0.43
1:C:139:VAL:HG22	1:C:290:GLY:HA2	1.99	0.43
1:C:166:ILE:HG23	1:C:172:VAL:HG11	2.01	0.43
1:C:211:ASN:OD1	1:C:239:ARG:HA	2.18	0.43
1:C:979:LEU:HD23	1:C:979:LEU:HA	1.51	0.43
1:C:986:ILE:HD13	1:C:986:ILE:C	2.44	0.43
1:D:14:VAL:HG13	1:E:881:LEU:HB3	2.01	0.43
1:D:339:GLU:HA	1:D:342:LYS:HB2	2.00	0.43
1:D:464:GLY:O	1:D:468:ARG:HB2	2.18	0.43
1:D:470:PHE:HD2	1:D:924:VAL:HG11	1.84	0.43
1:D:507:GLU:O	1:D:509:LYS:N	2.52	0.43
1:D:531:VAL:HA	1:D:534:ILE:CG1	2.49	0.43
1:D:553:ALA:O	1:D:557:VAL:HG23	2.18	0.43
1:D:663:LEU:HD23	1:D:663:LEU:H	1.83	0.43
1:E:45:ILE:HA	1:E:128:SER:O	2.19	0.43
1:E:248:LYS:HG2	1:E:263:ARG:NH2	2.33	0.43
1:E:350:LEU:O	1:E:353:LEU:HB2	2.19	0.43
1:E:525:HIS:O	1:E:526:HIS:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:PHE:C	1:F:11:PHE:CD2	2.97	0.43
1:F:180:SER:CB	1:F:274:ASN:H	2.31	0.43
1:F:836:MET:HE3	1:F:854:TRP:NE1	2.34	0.43
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.99	0.43
1:A:748:ALA:HB3	1:A:749:TRP:HD1	1.83	0.43
1:A:966:ARG:NE	1:A:970:ILE:HD11	2.25	0.43
1:B:352:PHE:HD2	1:B:353:LEU:HD23	1.84	0.43
1:C:393:LEU:HD13	1:C:466:ILE:HA	2.00	0.43
1:C:548:ILE:CD1	1:C:1016:PHE:HE1	2.32	0.43
1:C:992:SER:HA	1:C:995:GLN:HG3	2.00	0.43
1:D:83:ASP:OD1	1:D:810:ARG:HD3	2.18	0.43
1:D:293:LEU:HD22	1:D:294:ALA:H	1.83	0.43
1:D:485:ALA:O	1:D:490:PRO:HD3	2.18	0.43
1:D:867:GLN:HB3	1:D:871:LEU:HD12	2.00	0.43
1:D:1035:ILE:HG22	1:D:1036:GLU:O	2.19	0.43
1:E:32:VAL:HA	1:E:390:ILE:O	2.19	0.43
1:E:899:VAL:CG1	1:E:933:SER:HB2	2.48	0.43
1:F:344:LEU:CD1	1:F:402:ILE:HD11	2.48	0.43
1:F:871:LEU:HD22	1:F:927:LEU:HD21	2.01	0.43
1:A:763:VAL:HG12	1:B:63:GLN:NE2	2.33	0.43
1:A:969:PRO:HA	1:A:972:MET:CE	2.49	0.43
1:C:291:ILE:HD13	1:C:306:ILE:HD13	2.01	0.43
1:C:544:LEU:O	1:C:548:ILE:HG13	2.19	0.43
1:C:559:LEU:HA	1:C:560:PRO:HD2	1.77	0.43
1:D:5:PHE:CD2	1:D:487:ILE:HG23	2.53	0.43
1:D:402:ILE:HD13	1:D:402:ILE:HG21	1.81	0.43
1:D:575:MET:HE2	1:D:575:MET:HB2	1.89	0.43
1:D:992:SER:HA	1:D:995:GLN:HG3	2.00	0.43
1:E:219:LEU:HD23	1:F:749:TRP:CZ3	2.53	0.43
1:E:580:ALA:HB1	1:E:719:THR:HG21	2.00	0.43
1:E:685:LEU:HD12	1:E:686:GLY:O	2.18	0.43
1:E:723:LYS:HE3	1:E:725:ASP:HB2	2.01	0.43
1:F:53:ASP:O	1:F:57:VAL:HG13	2.19	0.43
1:F:355:MET:CG	1:F:410:ILE:HD11	2.49	0.43
1:A:26:ALA:O	1:A:30:LEU:HB2	2.19	0.42
1:A:726:ILE:H	1:A:726:ILE:HG12	1.13	0.42
1:B:612:VAL:HB	1:B:621:ILE:HG23	2.01	0.42
1:B:695:ASN:O	1:B:698:LEU:HB2	2.18	0.42
1:B:948:MET:HB2	1:B:948:MET:HE3	1.51	0.42
1:B:982:MET:HB3	1:B:983:PRO:CD	2.48	0.42
1:C:356:TYR:HA	1:C:365:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASN:ND2	1:C:438:ILE:HG21	2.34	0.42
1:C:447:MET:SD	1:C:886:LEU:HD22	2.59	0.42
1:C:1034:ASP:O	1:C:1035:ILE:HG12	2.19	0.42
1:D:25:LEU:HA	1:D:25:LEU:HD12	1.64	0.42
1:D:82:SER:HB2	1:D:811:LEU:HB2	2.00	0.42
1:D:157:TYR:O	1:D:161:ASN:ND2	2.46	0.42
1:D:341:VAL:O	1:D:342:LYS:C	2.62	0.42
1:D:504:ASP:C	1:D:506:GLY:H	2.27	0.42
1:E:164:ASP:O	1:E:168:ARG:HG3	2.19	0.42
1:E:190:PRO:HG3	1:E:774:TYR:CG	2.54	0.42
1:E:191:ASN:O	1:E:195:LYS:HB2	2.19	0.42
1:F:114:ALA:HA	1:F:117:LEU:HD12	2.00	0.42
1:F:344:LEU:HD11	1:F:376:LEU:HD11	2.01	0.42
1:A:603:LYS:C	1:A:603:LYS:HE2	2.44	0.42
1:A:1008:THR:O	1:A:1012:LEU:HB2	2.20	0.42
1:B:9:PRO:O	1:B:12:ALA:HB3	2.18	0.42
1:B:478:MET:HE3	1:B:478:MET:HB3	1.87	0.42
1:C:435:MET:HE3	1:C:490:PRO:HB3	2.01	0.42
1:C:474:ILE:O	1:C:475:VAL:C	2.61	0.42
1:C:649:ALA:O	1:C:653:ILE:HG12	2.19	0.42
1:D:564:LEU:HA	1:D:565:PRO:HD2	1.84	0.42
1:D:959:THR:HG21	1:D:1022:VAL:HG22	2.01	0.42
1:E:670:GLY:C	1:E:672:ALA:N	2.77	0.42
1:F:686:GLY:CA	1:F:689:LYS:HD3	2.40	0.42
1:F:920:VAL:HA	1:F:923:GLN:OE1	2.19	0.42
1:A:5:PHE:C	1:A:7:ASP:N	2.73	0.42
1:A:410:ILE:O	1:A:411:VAL:C	2.62	0.42
1:B:5:PHE:CE1	1:B:487:ILE:HG12	2.53	0.42
1:B:219:LEU:HD23	1:C:749:TRP:HZ3	1.84	0.42
1:B:514:GLY:C	1:B:516:PHE:H	2.26	0.42
1:B:984:LEU:HD23	1:B:984:LEU:HA	1.77	0.42
1:C:504:ASP:C	1:C:506:GLY:N	2.77	0.42
1:D:13:TRP:HB3	1:E:890:TRP:HZ2	1.84	0.42
1:D:576:VAL:HG21	1:D:591:LEU:HD21	2.00	0.42
1:D:1012:LEU:O	1:D:1016:PHE:HB2	2.19	0.42
1:E:430:ALA:O	1:E:433:LYS:HB3	2.19	0.42
1:E:751:GLY:HA3	1:E:769:MET:HE2	2.01	0.42
1:F:464:GLY:HA2	1:F:467:TYR:CD1	2.53	0.42
1:F:483:LEU:O	1:F:486:LEU:HB2	2.19	0.42
1:F:514:GLY:C	1:F:516:PHE:N	2.77	0.42
1:A:34:GLN:HB2	1:A:333:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:SER:HA	1:A:89:GLN:O	2.18	0.42
1:A:776:MET:HB3	1:A:776:MET:HE3	1.78	0.42
1:B:2:PRO:HB2	1:B:439:GLN:OE1	2.19	0.42
1:B:78:MET:HE3	1:B:816:GLY:N	2.34	0.42
1:B:456:MET:HE1	1:B:924:VAL:HG13	2.00	0.42
1:B:667:VAL:HB	1:B:668:GLU:OE2	2.20	0.42
1:B:847:PRO:O	1:B:850:VAL:HB	2.20	0.42
1:C:42:ALA:HA	1:C:92:LEU:O	2.19	0.42
1:C:192:GLU:O	1:C:195:LYS:HB3	2.19	0.42
1:C:347:ALA:HB3	1:C:402:ILE:HD12	2.01	0.42
1:C:510:LYS:C	1:C:510:LYS:HD3	2.44	0.42
1:C:836:MET:HG2	1:C:854:TRP:CH2	2.54	0.42
1:D:39:ALA:HA	1:D:40:PRO:HD2	1.76	0.42
1:D:626:LEU:HB3	1:D:632:ARG:HD3	2.01	0.42
1:D:883:LEU:CB	1:D:893:PRO:HB3	2.49	0.42
1:D:976:ALA:O	1:D:980:GLY:N	2.52	0.42
1:E:310:LEU:CD2	1:E:323:ILE:HG21	2.49	0.42
1:E:404:LEU:HA	1:E:404:LEU:HD12	1.84	0.42
1:E:588:GLN:NE2	1:E:588:GLN:O	2.52	0.42
1:E:898:LEU:O	1:E:901:PRO:HD2	2.19	0.42
1:F:32:VAL:HG22	1:F:390:ILE:HB	2.01	0.42
1:F:603:LYS:HB3	1:F:603:LYS:HE2	1.65	0.42
1:A:219:LEU:HD11	1:B:722:PHE:HB2	2.01	0.42
1:A:368:PRO:HB3	1:A:409:ALA:CB	2.47	0.42
1:A:677:PHE:CZ	1:A:852:TYR:HB2	2.54	0.42
1:A:916:LEU:HB3	1:A:917:THR:H	1.66	0.42
1:A:1030:ARG:O	1:A:1031:LYS:HG2	2.20	0.42
1:B:514:GLY:C	1:B:516:PHE:N	2.77	0.42
1:B:574:THR:HG21	1:B:598:TYR:CE2	2.55	0.42
1:C:249:ILE:HB	1:C:262:LEU:CB	2.49	0.42
1:C:418:ARG:HH11	1:C:422:GLU:CD	2.22	0.42
1:C:423:GLU:OE1	1:C:425:LEU:HD11	2.19	0.42
1:D:30:LEU:HD12	1:D:31:PRO:CD	2.48	0.42
1:D:182:TYR:O	1:D:764:LYS:HD3	2.20	0.42
1:D:586:ARG:O	1:D:589:LYS:HB3	2.19	0.42
1:D:813:ARG:NH2	1:D:816:GLY:O	2.53	0.42
1:D:1021:PHE:O	1:D:1025:ARG:HG2	2.19	0.42
1:E:692:GLN:O	1:E:695:ASN:HB2	2.20	0.42
1:E:695:ASN:HA	1:E:698:LEU:HD12	2.01	0.42
1:F:307:ARG:NH2	1:F:311:ALA:HB2	2.35	0.42
1:F:484:VAL:C	1:F:486:LEU:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:638:LYS:HE2	1:F:640:GLU:CG	2.48	0.42
1:F:723:LYS:HG3	1:F:725:ASP:OD1	2.20	0.42
1:A:142:VAL:O	1:A:287:SER:N	2.51	0.42
1:A:679:LEU:HA	1:A:679:LEU:HD12	1.76	0.42
1:A:895:SER:HB3	1:A:1024:VAL:HB	2.02	0.42
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.54	0.42
1:C:300:LEU:HD11	1:C:333:VAL:HG11	2.02	0.42
1:C:353:LEU:HD23	1:C:353:LEU:HA	1.79	0.42
1:C:360:GLN:HE21	1:C:360:GLN:HB3	1.66	0.42
1:C:425:LEU:HB3	1:C:429:GLU:HG3	1.99	0.42
1:C:506:GLY:O	1:C:508:GLY:N	2.48	0.42
1:C:941:VAL:O	1:C:942:GLU:C	2.61	0.42
1:D:251:LEU:CD1	1:D:265:VAL:HG21	2.50	0.42
1:D:370:ILE:C	1:D:373:PRO:HD2	2.45	0.42
1:E:188:MET:HE3	1:E:188:MET:HB2	1.73	0.42
1:E:443:VAL:O	1:E:447:MET:HG2	2.20	0.42
1:E:534:ILE:CG2	2:E:1101:LMT:H12	2.49	0.42
1:E:633:PRO:HD2	1:E:637:ASN:OD1	2.19	0.42
1:E:690:LEU:HB3	1:E:820:MET:SD	2.59	0.42
1:E:883:LEU:HD23	1:E:883:LEU:HA	1.85	0.42
1:E:944:ALA:HB3	1:E:1021:PHE:CE1	2.54	0.42
1:F:152:GLU:HG2	1:F:275:TYR:CE2	2.55	0.42
1:F:831:SER:HB3	1:F:834:GLU:HG3	2.01	0.42
1:F:1010:THR:O	1:F:1014:ILE:HG23	2.20	0.42
1:A:81:ASN:O	1:A:88:VAL:HA	2.20	0.42
1:A:409:ALA:O	1:A:413:VAL:HG23	2.20	0.42
1:A:855:THR:OG1	1:A:856:GLY:N	2.52	0.42
1:A:982:MET:HB3	1:A:983:PRO:HD3	2.01	0.42
1:B:345:VAL:O	1:B:348:ILE:HB	2.20	0.42
1:B:375:VAL:HG22	1:B:484:VAL:HG21	2.01	0.42
1:B:553:ALA:O	1:B:557:VAL:HG23	2.20	0.42
1:B:927:LEU:O	1:B:928:THR:C	2.62	0.42
1:B:1022:VAL:O	1:B:1026:ARG:HG3	2.19	0.42
1:C:102:ILE:HA	1:C:102:ILE:HD13	1.78	0.42
1:C:186:ILE:O	1:C:768:VAL:HG23	2.19	0.42
1:C:488:LEU:O	1:C:491:ALA:HB3	2.20	0.42
1:C:571:VAL:HG22	1:C:624:VAL:O	2.19	0.42
1:C:657:MET:HE2	1:C:657:MET:HB2	1.87	0.42
1:C:855:THR:O	1:C:856:GLY:C	2.61	0.42
1:D:146:ASP:OD2	1:D:146:ASP:N	2.52	0.42
1:D:200:PRO:HB2	1:D:744:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:MET:O	1:D:439:GLN:HB2	2.20	0.42
1:D:578:LEU:HD11	1:D:587:THR:N	2.35	0.42
1:D:914:ARG:HD2	1:D:1000:THR:HG21	2.02	0.42
1:D:932:LEU:O	1:D:933:SER:C	2.62	0.42
1:E:432:ARG:O	1:E:433:LYS:C	2.62	0.42
1:E:463:THR:O	1:E:467:TYR:CD1	2.69	0.42
1:F:211:ASN:OD1	1:F:240:LEU:HG	2.19	0.42
1:F:304:ALA:O	1:F:307:ARG:HB3	2.19	0.42
1:F:932:LEU:HD11	1:F:977:PHE:CE2	2.55	0.42
1:A:13:TRP:NE1	1:A:492:LEU:HD21	2.35	0.42
1:A:166:ILE:HG23	1:A:166:ILE:HD12	1.74	0.42
1:A:948:MET:SD	1:A:955:LEU:HA	2.58	0.42
1:B:26:ALA:O	1:B:30:LEU:HB2	2.20	0.42
1:B:409:ALA:O	1:B:413:VAL:HG23	2.20	0.42
1:B:607:GLU:OE1	1:B:627:LYS:HG2	2.20	0.42
1:B:701:ALA:HB3	1:B:711:VAL:HG11	2.01	0.42
1:D:475:VAL:O	1:D:478:MET:HB3	2.20	0.42
1:D:886:LEU:HD12	1:D:886:LEU:HA	1.76	0.42
1:F:399:VAL:HG11	1:F:984:LEU:HD21	2.02	0.42
1:F:509:LYS:HA	1:F:509:LYS:HD2	1.83	0.42
1:F:981:VAL:O	1:F:982:MET:C	2.61	0.42
1:A:199:THR:HG21	1:A:787:ARG:H	1.85	0.42
1:A:352:PHE:CD2	1:A:352:PHE:C	2.98	0.42
1:B:3:ASN:O	1:B:6:ILE:HB	2.20	0.42
1:B:359:LEU:C	1:B:360:GLN:HG2	2.44	0.42
1:B:513:PHE:C	1:B:515:TRP:H	2.28	0.42
1:B:671:THR:O	1:B:671:THR:OG1	2.35	0.42
1:B:898:LEU:HB3	1:B:1020:PHE:CZ	2.54	0.42
1:C:55:LYS:HB3	1:C:55:LYS:HE2	1.72	0.42
1:C:343:THR:HG21	1:C:984:LEU:HD23	2.02	0.42
1:C:926:LEU:HA	1:C:926:LEU:HD23	1.82	0.42
1:D:852:TYR:N	1:D:852:TYR:HD2	2.18	0.42
1:E:30:LEU:HA	1:E:31:PRO:HD3	1.82	0.42
1:E:113:LEU:HA	1:E:113:LEU:HD23	1.80	0.42
1:E:235:ILE:HD11	1:F:721:GLN:OE1	2.20	0.42
1:E:294:ALA:HB3	1:E:297:ALA:HB2	2.01	0.42
1:E:544:LEU:O	1:E:547:ILE:HB	2.19	0.42
1:E:843:ALA:O	1:E:846:LEU:HG	2.20	0.42
1:E:921:TYR:HB3	1:E:998:VAL:HG23	2.02	0.42
1:F:25:LEU:HD12	1:F:25:LEU:HA	1.62	0.42
1:F:41:PRO:O	1:F:94:PHE:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:883:LEU:HD11	1:F:938:ILE:HD11	2.00	0.42
1:A:282:ASN:HD21	1:A:608:SER:CB	2.33	0.42
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.84	0.42
1:A:563:PHE:O	1:A:564:LEU:HD12	2.20	0.42
1:A:694:ARG:HB3	1:A:694:ARG:HH11	1.85	0.42
1:B:955:LEU:O	1:B:959:THR:HG23	2.20	0.42
1:C:159:ALA:HB2	1:C:177:LEU:HD11	2.02	0.42
1:C:335:ILE:HG12	1:C:990:ALA:HB2	2.02	0.42
1:C:753:TYR:HD1	1:C:767:TYR:HE2	1.66	0.42
1:D:193:LEU:CD2	1:D:265:VAL:HB	2.50	0.42
1:D:836:MET:CE	1:D:862:ARG:HD2	2.49	0.42
1:D:941:VAL:HG22	1:D:1021:PHE:CD1	2.55	0.42
1:E:43:VAL:HG13	1:E:130:GLU:O	2.20	0.42
1:E:722:PHE:CZ	1:E:802:SER:HB2	2.55	0.42
1:E:722:PHE:CD1	1:E:804:TRP:CE2	3.08	0.42
1:E:960:LEU:O	1:E:963:VAL:HG12	2.20	0.42
1:E:1029:SER:HG	1:E:1030:ARG:H	1.61	0.42
1:F:364:ALA:O	1:F:368:PRO:HD3	2.19	0.42
1:F:786:VAL:HG23	1:F:796:PHE:CE2	2.55	0.42
1:F:932:LEU:HD22	1:F:1006:MET:HE2	2.01	0.42
1:F:960:LEU:HD23	1:F:960:LEU:HA	1.89	0.42
1:A:585:GLU:O	1:A:588:GLN:HB3	2.20	0.41
1:B:15:ILE:HD13	1:B:15:ILE:HG21	1.86	0.41
1:C:24:GLY:CA	1:C:27:ILE:HG23	2.50	0.41
1:C:148:THR:HG22	1:C:149:MET:O	2.20	0.41
1:C:278:ILE:CG1	1:C:613:ASN:HB3	2.48	0.41
1:C:514:GLY:C	1:C:516:PHE:H	2.27	0.41
1:C:855:THR:CA	1:C:859:TYR:HB2	2.47	0.41
1:C:899:VAL:HG12	1:C:933:SER:HB2	2.02	0.41
1:C:977:PHE:HE2	1:C:1002:VAL:CG1	2.32	0.41
1:D:235:ILE:HG23	1:D:235:ILE:HD12	1.74	0.41
1:D:393:LEU:HD13	1:D:466:ILE:HA	2.02	0.41
1:D:470:PHE:CD2	1:D:924:VAL:HG11	2.54	0.41
1:E:579:PRO:HD3	1:E:656:ALA:CB	2.48	0.41
1:E:727:ASP:OD1	1:E:730:LYS:HG3	2.20	0.41
1:E:741:ILE:O	1:E:744:THR:OG1	2.34	0.41
1:F:3:ASN:HD21	1:F:486:LEU:HA	1.85	0.41
1:F:355:MET:HG2	1:F:410:ILE:HD11	2.01	0.41
1:F:587:THR:HG21	1:F:618:ASN:HA	2.02	0.41
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.76	0.41
1:A:149:MET:HG3	1:A:154:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:PRO:O	1:A:430:ALA:HB3	2.19	0.41
1:A:901:PRO:HA	1:A:904:VAL:HB	2.02	0.41
1:B:4:PHE:CZ	1:B:8:ARG:HD3	2.55	0.41
1:B:248:LYS:O	1:B:261:LEU:HD22	2.20	0.41
1:B:368:PRO:HG3	1:B:413:VAL:HG21	2.02	0.41
1:B:486:LEU:HA	1:B:486:LEU:HD23	1.77	0.41
1:B:914:ARG:NH1	1:B:985:VAL:HG12	2.35	0.41
1:B:1015:PHE:CZ	2:B:2000:LMT:H52	2.55	0.41
1:C:187:TRP:HB3	1:C:771:GLU:HA	2.02	0.41
1:C:443:VAL:O	1:C:447:MET:HB3	2.20	0.41
1:C:504:ASP:C	1:C:506:GLY:H	2.26	0.41
1:C:584:GLN:N	1:C:617:GLN:HB3	2.34	0.41
1:E:363:ARG:CZ	1:E:498:LYS:HE3	2.49	0.41
1:E:493:CYS:O	1:E:497:LEU:HB2	2.19	0.41
1:F:344:LEU:HD22	1:F:402:ILE:HD11	2.02	0.41
1:A:169:THR:HB	1:A:172:VAL:HG23	2.02	0.41
1:A:894:PHE:HD2	1:A:897:MET:HE3	1.86	0.41
1:B:363:ARG:NH1	1:B:498:LYS:HG3	2.35	0.41
1:B:463:THR:O	1:B:466:ILE:HB	2.20	0.41
1:B:480:LEU:O	1:B:484:VAL:HG23	2.20	0.41
1:B:482:VAL:O	1:B:485:ALA:HB3	2.20	0.41
1:B:527:TYR:O	1:B:531:VAL:HG23	2.20	0.41
1:B:701:ALA:CB	1:B:711:VAL:HG11	2.50	0.41
1:C:443:VAL:HG12	1:C:886:LEU:HD21	2.01	0.41
1:C:453:PHE:HD2	1:C:456:MET:HE2	1.84	0.41
1:C:753:TYR:HD1	1:C:767:TYR:CE2	2.38	0.41
1:C:772:ALA:O	1:C:776:MET:HE3	2.20	0.41
1:C:966:ARG:HH21	1:C:970:ILE:HD11	1.85	0.41
1:C:981:VAL:O	1:C:982:MET:C	2.64	0.41
1:D:459:PHE:O	1:D:468:ARG:NH2	2.54	0.41
1:D:482:VAL:O	1:D:486:LEU:HG	2.20	0.41
1:D:515:TRP:O	1:D:519:MET:HE2	2.20	0.41
1:E:62:THR:O	1:E:66:GLU:HG3	2.21	0.41
1:E:158:VAL:HG11	1:E:289:LEU:HG	2.01	0.41
1:E:202:ASP:OD2	1:E:787:ARG:NH2	2.46	0.41
1:E:306:ILE:O	1:E:309:GLU:HB3	2.20	0.41
1:E:927:LEU:HA	1:E:930:ILE:HD12	2.02	0.41
1:F:356:TYR:HD1	1:F:365:THR:HG21	1.84	0.41
1:F:578:LEU:HA	1:F:656:ALA:HB1	2.02	0.41
1:A:54:ALA:HB2	1:A:809:PRO:O	2.20	0.41
1:A:273:GLU:CG	1:A:765:LYS:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:MET:CE	1:C:225:VAL:H	2.33	0.41
1:A:1017:VAL:HB	1:A:1018:PRO:HD3	2.02	0.41
1:B:27:ILE:HD12	1:B:27:ILE:HA	1.86	0.41
1:B:576:VAL:HG13	1:B:658:VAL:HG22	2.01	0.41
1:C:614:GLY:O	1:C:616:GLY:HA3	2.20	0.41
1:C:664:PRO:HG2	1:C:666:ILE:O	2.20	0.41
1:D:5:PHE:CE1	1:D:487:ILE:HG12	2.55	0.41
1:D:234:ILE:HA	1:E:722:PHE:O	2.20	0.41
1:D:432:ARG:HH11	1:D:432:ARG:HD2	1.68	0.41
1:D:531:VAL:O	1:D:534:ILE:HG13	2.20	0.41
1:D:544:LEU:O	1:D:547:ILE:HB	2.20	0.41
1:D:679:LEU:HD11	1:D:850:VAL:HG12	2.02	0.41
1:D:726:ILE:H	1:D:726:ILE:HG12	1.24	0.41
1:D:898:LEU:O	1:D:901:PRO:HD2	2.20	0.41
1:D:941:VAL:HG13	1:D:1021:PHE:CD1	2.56	0.41
1:E:7:ASP:O	1:E:8:ARG:HG3	2.20	0.41
1:E:448:VAL:HG13	1:E:879:VAL:CG1	2.47	0.41
1:E:1015:PHE:O	1:E:1019:VAL:HG23	2.21	0.41
1:E:1021:PHE:O	1:E:1022:VAL:C	2.61	0.41
1:F:53:ASP:OD1	1:F:56:THR:OG1	2.28	0.41
1:F:578:LEU:CD1	1:F:587:THR:HG22	2.50	0.41
1:A:165:ALA:HA	1:A:168:ARG:NH1	2.35	0.41
1:A:446:ALA:CB	1:A:482:VAL:HG21	2.51	0.41
1:B:572:PHE:CE1	1:B:643:THR:HG22	2.56	0.41
1:C:527:TYR:OH	1:C:1014:ILE:O	2.24	0.41
1:D:9:PRO:O	1:D:13:TRP:CD1	2.74	0.41
1:D:473:THR:O	1:D:476:SER:OG	2.38	0.41
1:D:531:VAL:HA	1:D:534:ILE:HD11	2.01	0.41
1:D:573:MET:HE2	1:D:661:PHE:CE2	2.55	0.41
1:D:634:GLY:O	1:D:638:LYS:HG3	2.20	0.41
1:E:165:ALA:HB3	1:E:313:MET:HE3	2.02	0.41
1:E:504:ASP:C	1:E:506:GLY:H	2.29	0.41
1:E:697:LEU:HA	1:E:700:GLU:HB2	2.02	0.41
1:E:927:LEU:O	1:E:928:THR:C	2.63	0.41
1:F:149:MET:HB2	1:F:153:ASP:HB3	2.03	0.41
1:F:199:THR:HG22	1:F:785:TYR:O	2.20	0.41
1:F:620:GLY:O	1:F:621:ILE:HD12	2.20	0.41
1:F:666:ILE:HD13	1:F:669:LEU:HD12	2.03	0.41
1:F:694:ARG:HE	1:F:713:PRO:HB3	1.85	0.41
1:F:720:PRO:HA	1:F:805:GLU:O	2.20	0.41
1:A:118:LEU:HA	1:A:119:PRO:HD3	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ILE:HG12	1:A:754:VAL:HG21	2.02	0.41
1:A:578:LEU:HB2	1:A:618:ASN:HA	2.02	0.41
1:A:650:PHE:HB3	1:A:658:VAL:HB	2.02	0.41
1:B:7:ASP:C	1:B:8:ARG:HG3	2.46	0.41
1:B:121:GLU:O	1:B:125:GLN:HB2	2.21	0.41
1:B:149:MET:H	1:B:149:MET:HG2	1.75	0.41
1:B:167:SER:HB2	1:C:70:ASN:HB3	2.02	0.41
1:C:836:MET:O	1:C:854:TRP:HZ2	2.03	0.41
1:D:44:THR:HA	1:D:90:ILE:O	2.20	0.41
1:D:58:GLN:HA	1:D:62:THR:HB	2.03	0.41
1:D:138:MET:CG	1:D:291:ILE:HB	2.51	0.41
1:D:418:ARG:HH21	1:D:943:PHE:HE2	1.69	0.41
1:E:175:VAL:HG11	1:E:289:LEU:HD13	2.02	0.41
1:E:189:ASN:O	1:E:192:GLU:HB2	2.21	0.41
1:E:262:LEU:HG	1:E:268:ILE:HD11	2.02	0.41
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.55	0.41
1:E:585:GLU:O	1:E:588:GLN:HB3	2.20	0.41
1:E:914:ARG:NH1	1:E:985:VAL:HG12	2.36	0.41
1:E:927:LEU:O	1:E:930:ILE:HB	2.21	0.41
1:F:540:ARG:O	1:F:543:VAL:HB	2.20	0.41
1:F:679:LEU:HD23	1:F:820:MET:HB2	2.03	0.41
1:F:970:ILE:H	1:F:970:ILE:HG13	1.64	0.41
1:A:66:GLU:OE1	1:A:816:GLY:HA2	2.20	0.41
1:A:367:ILE:HG21	1:A:367:ILE:HD13	1.84	0.41
1:B:144:ASN:HA	1:B:321:LEU:HA	2.02	0.41
1:C:370:ILE:O	1:C:373:PRO:HD2	2.20	0.41
1:C:591:LEU:HD11	1:C:620:GLY:HA3	2.01	0.41
1:C:689:LYS:H	1:C:689:LYS:CD	2.33	0.41
1:C:1012:LEU:HD12	1:C:1012:LEU:HA	1.85	0.41
1:D:366:LEU:HD23	1:D:366:LEU:HA	1.74	0.41
1:D:452:VAL:C	1:D:455:PRO:HD2	2.45	0.41
1:D:572:PHE:CD1	1:D:643:THR:HG22	2.56	0.41
1:D:667:VAL:HG12	1:D:668:GLU:OE1	2.20	0.41
1:D:788:ALA:HB3	1:D:790:ASP:OD2	2.20	0.41
1:E:250:LEU:HD13	1:E:259:ARG:HB2	2.02	0.41
1:F:510:LYS:HA	1:F:518:ARG:HH12	1.86	0.41
1:F:914:ARG:NH1	1:F:996:ASN:HB3	2.36	0.41
1:A:11:PHE:CE1	1:A:15:ILE:HD11	2.56	0.41
1:A:17:ILE:HA	1:A:20:MET:HE3	2.02	0.41
1:A:57:VAL:CG1	1:A:88:VAL:HB	2.50	0.41
1:A:82:SER:HB2	1:A:811:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:THR:HG21	1:A:984:LEU:HD21	2.02	0.41
1:A:574:THR:OG1	1:A:659:PHE:O	2.22	0.41
1:A:694:ARG:HD2	1:A:713:PRO:HB3	2.03	0.41
1:A:948:MET:HE3	1:A:948:MET:HB2	1.84	0.41
1:A:979:LEU:HD23	1:A:979:LEU:HA	1.80	0.41
2:A:1101:LMT:H81	2:A:1101:LMT:H51	1.51	0.41
1:B:82:SER:HB2	1:B:811:LEU:HB2	2.03	0.41
1:B:469:GLN:O	1:B:473:THR:OG1	2.14	0.41
1:B:539:GLY:O	1:B:540:ARG:C	2.64	0.41
1:B:883:LEU:HD23	1:B:883:LEU:HA	1.88	0.41
1:B:923:GLN:O	1:B:926:LEU:HB2	2.21	0.41
1:C:153:ASP:HA	1:C:182:TYR:OH	2.20	0.41
1:E:186:ILE:HG12	1:E:268:ILE:HG12	2.02	0.41
1:E:219:LEU:HD23	1:F:749:TRP:HZ3	1.85	0.41
1:E:224:PRO:HD2	1:F:584:GLN:NE2	2.35	0.41
1:E:555:LEU:HB3	1:E:908:LEU:HD13	2.03	0.41
1:E:916:LEU:HD11	1:E:997:ALA:HA	2.03	0.41
1:F:61:VAL:O	1:F:65:ILE:HG13	2.19	0.41
1:F:120:GLN:O	1:F:123:GLN:HB2	2.21	0.41
1:F:345:VAL:HA	1:F:348:ILE:HD12	2.03	0.41
1:F:356:TYR:O	1:F:358:PHE:N	2.53	0.41
1:F:407:ASP:HB3	1:F:445:ILE:HD13	2.03	0.41
1:F:649:ALA:O	1:F:653:ILE:HG12	2.20	0.41
1:F:741:ILE:HG22	1:F:786:VAL:HG11	2.03	0.41
1:F:803:ARG:NH1	1:F:805:GLU:OE2	2.54	0.41
1:A:75:LEU:HD23	1:C:168:ARG:HB3	2.03	0.41
1:A:189:ASN:O	1:A:192:GLU:HB2	2.20	0.41
1:A:223:PRO:HD2	1:B:775:ARG:NH2	2.36	0.41
1:A:261:LEU:O	1:A:265:VAL:HG22	2.21	0.41
1:A:492:LEU:HD22	1:A:496:MET:SD	2.61	0.41
1:B:40:PRO:HA	1:B:41:PRO:HD3	1.82	0.41
1:B:80:SER:CB	1:B:90:ILE:HG12	2.51	0.41
1:B:105:VAL:HG21	1:C:105:VAL:HG13	2.03	0.41
1:B:361:ASN:O	1:B:365:THR:HG22	2.21	0.41
1:C:64:VAL:HG11	1:C:117:LEU:HB2	2.01	0.41
1:C:605:ASN:HD21	1:C:637:ASN:HA	1.85	0.41
1:C:930:ILE:HG21	1:C:930:ILE:HD13	1.87	0.41
1:C:961:ASP:O	1:C:962:ALA:C	2.63	0.41
1:D:11:PHE:HB2	1:E:888:GLU:OE2	2.21	0.41
1:D:166:ILE:HD13	1:D:166:ILE:HA	1.91	0.41
1:D:293:LEU:HD22	1:D:294:ALA:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:562:SER:H	1:D:917:THR:HG1	1.62	0.41
1:D:770:SER:OG	1:D:775:ARG:HG2	2.20	0.41
1:D:963:VAL:HA	1:D:966:ARG:HH12	1.85	0.41
1:E:103:ALA:O	1:E:107:VAL:HG23	2.21	0.41
1:E:313:MET:HA	1:E:316:PHE:HD2	1.86	0.41
1:E:327:TYR:CD2	1:E:327:TYR:C	2.98	0.41
1:E:527:TYR:CE2	1:E:967:LEU:HG	2.56	0.41
1:E:535:LEU:HD13	1:E:1022:VAL:HG21	2.02	0.41
1:E:559:LEU:HD22	1:E:917:THR:HA	2.03	0.41
1:E:685:LEU:HD13	1:E:689:LYS:HB3	2.02	0.41
1:F:33:ALA:HB2	1:F:298:ASN:OD1	2.21	0.41
1:F:379:THR:N	1:F:480:LEU:HD11	2.35	0.41
1:F:398:MET:HB3	1:F:398:MET:HE3	1.42	0.41
1:F:406:VAL:C	1:F:408:ASP:N	2.79	0.41
1:F:510:LYS:HA	1:F:518:ARG:NH1	2.35	0.41
1:F:545:TYR:O	1:F:549:VAL:HG23	2.21	0.41
1:F:553:ALA:O	1:F:557:VAL:HG23	2.20	0.41
1:F:932:LEU:HD11	1:F:977:PHE:HE2	1.85	0.41
1:A:757:PHE:CE1	1:A:759:ASP:HB2	2.55	0.41
1:A:893:PRO:C	1:A:897:MET:HE2	2.46	0.41
1:A:903:GLY:HA2	1:A:1009:ALA:HB2	2.03	0.41
1:B:407:ASP:O	1:B:411:VAL:HG23	2.21	0.41
1:B:914:ARG:HH12	1:B:985:VAL:HG12	1.86	0.41
1:B:914:ARG:NH2	1:B:996:ASN:HB3	2.36	0.41
1:B:926:LEU:HA	1:B:926:LEU:HD23	1.69	0.41
1:C:65:ILE:HG21	1:C:90:ILE:HD13	2.03	0.41
1:C:199:THR:HG21	1:C:787:ARG:H	1.86	0.41
1:C:404:LEU:HB3	1:C:478:MET:SD	2.61	0.41
1:C:509:LYS:HD2	1:C:509:LYS:HA	1.83	0.41
1:D:317:PHE:CD1	1:D:321:LEU:HD12	2.56	0.41
1:D:339:GLU:OE1	1:D:342:LYS:HD3	2.21	0.41
1:D:780:ASP:O	1:D:783:ASP:HB2	2.20	0.41
1:E:142:VAL:O	1:E:154:ILE:HD13	2.21	0.41
1:E:235:ILE:HB	1:F:723:LYS:HA	2.01	0.41
1:E:567:GLU:O	1:E:569:GLN:HG3	2.21	0.41
1:E:838:LEU:HD22	1:E:841:GLN:HB2	2.02	0.41
1:F:726:ILE:H	1:F:726:ILE:HG13	1.65	0.41
1:F:979:LEU:HD23	1:F:979:LEU:HA	1.75	0.41
1:A:66:GLU:OE2	1:A:80:SER:OG	2.34	0.40
1:A:678:GLU:HG2	1:A:814:TYR:CG	2.56	0.40
1:A:723:LYS:HB2	1:A:805:GLU:CD	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:LYS:HG3	1:B:774:TYR:CE2	2.56	0.40
1:C:5:PHE:C	1:C:7:ASP:H	2.28	0.40
1:C:497:LEU:HD12	1:C:497:LEU:HA	1.82	0.40
1:C:632:ARG:HH12	1:C:638:LYS:HA	1.86	0.40
1:C:1010:THR:O	1:C:1014:ILE:HG23	2.21	0.40
1:D:143:ILE:HG22	1:D:286:ALA:HB2	2.02	0.40
1:D:442:LEU:HD23	1:D:442:LEU:HA	1.70	0.40
1:D:591:LEU:HD23	1:D:591:LEU:HA	1.71	0.40
1:D:654:LYS:HA	1:D:654:LYS:HD3	1.77	0.40
1:D:940:ILE:HG12	1:D:966:ARG:NH2	2.36	0.40
1:E:343:THR:HG21	1:E:399:VAL:CG1	2.43	0.40
1:E:723:LYS:HG2	1:E:803:ARG:NH1	2.36	0.40
1:E:736:VAL:HB	1:E:741:ILE:HD11	2.03	0.40
1:F:104:GLN:OE1	1:F:108:GLN:NE2	2.54	0.40
1:F:217:GLY:O	1:F:234:ILE:HB	2.22	0.40
1:C:527:TYR:O	1:C:531:VAL:HG23	2.21	0.40
1:C:963:VAL:HA	1:C:966:ARG:NH2	2.37	0.40
1:C:984:LEU:HB3	1:C:995:GLN:O	2.21	0.40
1:D:162:MET:HA	1:D:313:MET:SD	2.62	0.40
1:D:404:LEU:HD21	1:D:449:LEU:HD22	2.02	0.40
1:D:540:ARG:NH2	2:D:2000:LMT:H6'2	2.36	0.40
1:D:564:LEU:HD22	1:D:666:ILE:HG12	2.04	0.40
1:D:564:LEU:CD2	1:D:666:ILE:HG12	2.51	0.40
1:E:69:MET:HE3	1:E:69:MET:HB3	1.97	0.40
1:E:330:THR:HB	1:E:331:PRO:HD3	2.03	0.40
1:E:516:PHE:HA	1:E:519:MET:CG	2.45	0.40
1:E:541:TYR:HH	2:E:1101:LMT:H6'	1.54	0.40
1:E:956:ILE:H	1:E:956:ILE:HG13	1.27	0.40
1:F:489:THR:HA	1:F:492:LEU:HB2	2.03	0.40
1:F:538:THR:O	1:F:539:GLY:C	2.64	0.40
1:F:868:ALA:HB2	1:F:923:GLN:NE2	2.36	0.40
1:F:941:VAL:HG13	1:F:1021:PHE:CE1	2.56	0.40
1:A:697:LEU:HA	1:A:700:GLU:HB2	2.03	0.40
1:A:722:PHE:HB2	1:A:804:TRP:CH2	2.56	0.40
1:B:233:SER:HB2	1:C:721:GLN:HG2	2.03	0.40
1:B:786:VAL:HG23	1:B:796:PHE:CE2	2.55	0.40
1:B:983:PRO:O	1:B:987:SER:HB2	2.22	0.40
1:C:364:ALA:O	1:C:368:PRO:HD3	2.21	0.40
1:C:414:GLU:O	1:C:415:ASN:C	2.61	0.40
1:C:584:GLN:N	1:C:617:GLN:OE1	2.31	0.40
1:D:231:ASN:ND2	1:E:617:GLN:HE22	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:511:GLY:CA	1:D:515:TRP:CD1	3.01	0.40
1:D:714:ASN:HD22	1:D:821:GLU:CD	2.29	0.40
1:E:667:VAL:H	1:E:667:VAL:HG23	1.58	0.40
1:A:19:ILE:HD13	1:A:19:ILE:HG21	1.83	0.40
1:A:351:VAL:O	1:A:355:MET:HG2	2.22	0.40
1:A:467:TYR:CE2	1:A:920:VAL:HG22	2.55	0.40
1:C:55:LYS:HA	1:C:811:LEU:HD11	2.03	0.40
1:C:137:LEU:HB2	1:C:293:LEU:HB2	2.03	0.40
1:C:188:MET:O	1:C:771:GLU:HG3	2.20	0.40
1:C:252:LYS:HE2	1:C:253:VAL:O	2.21	0.40
1:C:431:THR:HG21	1:C:490:PRO:O	2.22	0.40
1:E:587:THR:HB	1:E:613:ASN:OD1	2.21	0.40
1:E:681:ASP:HB2	1:E:690:LEU:HG	2.04	0.40
1:E:722:PHE:HD1	1:E:804:TRP:CE2	2.40	0.40
1:F:180:SER:HB3	1:F:273:GLU:CB	2.51	0.40
1:F:546:LEU:O	1:F:550:VAL:HG23	2.21	0.40
1:A:142:VAL:N	1:A:287:SER:O	2.44	0.40
1:A:615:GLY:HA2	1:A:616:GLY:HA2	1.75	0.40
1:A:703:LYS:C	1:A:705:PRO:HD3	2.46	0.40
1:A:778:PRO:HG3	1:A:804:TRP:HZ2	1.87	0.40
1:A:885:ALA:O	1:A:888:GLU:CD	2.64	0.40
1:B:58:GLN:OE1	1:B:811:LEU:HB3	2.21	0.40
1:B:356:TYR:C	1:B:358:PHE:H	2.29	0.40
1:B:534:ILE:HD13	1:B:534:ILE:HG21	1.91	0.40
1:C:44:THR:HA	1:C:90:ILE:O	2.21	0.40
1:C:359:LEU:HB2	1:C:365:THR:HG22	2.03	0.40
1:C:1029:SER:OG	1:C:1030:ARG:N	2.48	0.40
1:C:1031:LYS:HA	1:C:1031:LYS:HD3	1.86	0.40
1:D:188:MET:HE3	1:D:784:TRP:HH2	1.86	0.40
1:D:407:ASP:O	1:D:411:VAL:HG23	2.22	0.40
1:D:554:TYR:CE2	1:D:558:ARG:HG3	2.56	0.40
1:D:704:HIS:CE1	1:D:842:LEU:HD21	2.56	0.40
1:D:916:LEU:HB3	1:D:917:THR:H	1.68	0.40
1:D:984:LEU:HB3	1:D:995:GLN:O	2.21	0.40
1:E:376:LEU:HD22	1:E:398:MET:HE3	2.04	0.40
1:E:936:ASN:ND2	1:E:970:ILE:HG23	2.36	0.40
1:F:337:ILE:HD11	1:F:391:ASN:HA	2.04	0.40
1:F:343:THR:HG21	1:F:984:LEU:HD23	2.03	0.40
1:F:348:ILE:HG13	1:F:348:ILE:H	1.68	0.40
1:F:478:MET:O	1:F:482:VAL:HG23	2.21	0.40
1:F:497:LEU:HD12	1:F:497:LEU:HA	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:527:TYR:O	1:F:531:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1036/1044 (99%)	942 (91%)	79 (8%)	15 (1%)	9	31
1	B	1037/1044 (99%)	942 (91%)	85 (8%)	10 (1%)	12	40
1	C	1033/1044 (99%)	931 (90%)	84 (8%)	18 (2%)	7	28
1	D	1036/1044 (99%)	934 (90%)	83 (8%)	19 (2%)	6	26
1	E	1035/1044 (99%)	937 (90%)	87 (8%)	11 (1%)	11	38
1	F	1035/1044 (99%)	926 (90%)	84 (8%)	25 (2%)	4	22
All	All	6212/6264 (99%)	5612 (90%)	502 (8%)	98 (2%)	7	29

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	672	ALA
1	A	986	ILE
1	A	1029	SER
1	A	1033	GLU
1	B	617	GLN
1	B	1029	SER
1	B	1038	SER
1	C	509	LYS
1	C	915	GLY
1	C	1009	ALA
1	C	1029	SER

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Mol	Chain	Res	Type
1	C	1035	ILE
1	D	508	GLY
1	D	511	GLY
1	D	668	GLU
1	D	915	GLY
1	D	1029	SER
1	D	1034	ASP
1	D	1035	ILE
1	D	1036	GLU
1	D	1038	SER
1	E	667	VAL
1	E	1029	SER
1	E	1033	GLU
1	E	1036	GLU
1	F	134	SER
1	F	145	THR
1	F	509	LYS
1	F	617	GLN
1	F	888	GLU
1	F	1029	SER
1	F	1032	ASN
1	F	1035	ILE
1	A	915	GLY
1	A	987	SER
1	A	1032	ASN
1	B	514	GLY
1	B	684	GLY
1	B	1035	ILE
1	C	147	GLY
1	C	831	SER
1	D	4	PHE
1	D	987	SER
1	D	1028	PHE
1	D	1031	LYS
1	E	668	GLU
1	F	6	ILE
1	F	146	ASP
1	F	147	GLY
1	F	511	GLY
1	F	684	GLY
1	F	918	ASN
1	F	1028	PHE

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Mol	Chain	Res	Type
1	A	615	GLY
1	A	1031	LYS
1	B	918	ASN
1	C	134	SER
1	C	146	ASP
1	C	360	GLN
1	C	888	GLU
1	F	407	ASP
1	F	507	GLU
1	F	831	SER
1	F	1034	ASP
1	A	215	ALA
1	B	215	ALA
1	C	6	ILE
1	C	1033	GLU
1	D	614	GLY
1	D	653	ILE
1	D	909	LEU
1	F	360	GLN
1	A	918	ASN
1	A	1036	GLU
1	B	1039	HIS
1	C	215	ALA
1	C	918	ASN
1	D	215	ALA
1	E	216	ALA
1	F	150	THR
1	F	215	ALA
1	A	509	LYS
1	E	778	PRO
1	F	773	LYS
1	F	915	GLY
1	A	666	ILE
1	A	778	PRO
1	C	998	VAL
1	E	511	GLY
1	E	1035	ILE
1	D	616	GLY
1	C	828	PRO
1	E	508	GLY
1	E	539	GLY
1	F	778	PRO

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Mol	Chain	Res	Type
1	B	318	PRO
1	C	653	ILE
1	D	200	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	846/852 (99%)	768 (91%)	78 (9%)	8	29
1	B	847/852 (99%)	766 (90%)	81 (10%)	8	28
1	C	843/852 (99%)	753 (89%)	90 (11%)	6	23
1	D	846/852 (99%)	771 (91%)	75 (9%)	9	31
1	E	845/852 (99%)	763 (90%)	82 (10%)	8	28
1	F	845/852 (99%)	767 (91%)	78 (9%)	8	29
All	All	5072/5112 (99%)	4588 (90%)	484 (10%)	8	29

All (484) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	21	LEU
1	A	25	LEU
1	A	44	THR
1	A	70	ASN
1	A	88	VAL
1	A	101	ASP
1	A	111	LEU
1	A	146	ASP
1	A	148	THR
1	A	152	GLU
1	A	166	ILE
1	A	177	LEU
1	A	243	THR
1	A	255	GLN

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Mol	Chain	Res	Type
1	A	280	GLU
1	A	281	PHE
1	A	293	LEU
1	A	295	THR
1	A	337	ILE
1	A	342	LYS
1	A	349	ILE
1	A	350	LEU
1	A	360	GLN
1	A	362	PHE
1	A	400	LEU
1	A	410	ILE
1	A	429	GLU
1	A	434	SER
1	A	437	GLN
1	A	463	THR
1	A	483	LEU
1	A	489	THR
1	A	502	LYS
1	A	512	PHE
1	A	519	MET
1	A	524	THR
1	A	534	ILE
1	A	538	THR
1	A	542	LEU
1	A	557	VAL
1	A	558	ARG
1	A	564	LEU
1	A	566	ASP
1	A	571	VAL
1	A	575	MET
1	A	578	LEU
1	A	603	LYS
1	A	610	PHE
1	A	644	MET
1	A	667	VAL
1	A	669	LEU
1	A	682	GLN
1	A	690	LEU
1	A	694	ARG
1	A	708	LEU
1	A	711	VAL

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Mol	Chain	Res	Type
1	A	726	ILE
1	A	736	VAL
1	A	830	LYS
1	A	838	LEU
1	A	860	GLN
1	A	896	VAL
1	A	916	LEU
1	A	917	THR
1	A	926	LEU
1	A	942	GLU
1	A	946	ASP
1	A	953	LYS
1	A	956	ILE
1	A	959	THR
1	A	966	ARG
1	A	970	ILE
1	A	985	VAL
1	A	1012	LEU
1	A	1014	ILE
1	A	1024	VAL
1	A	1035	ILE
1	B	6	ILE
1	B	10	ILE
1	B	29	LYS
1	B	34	GLN
1	B	48	SER
1	B	96	SER
1	B	102	ILE
1	B	111	LEU
1	B	117	LEU
1	B	129	VAL
1	B	131	LYS
1	B	153	ASP
1	B	177	LEU
1	B	185	ARG
1	B	213	GLN
1	B	243	THR
1	B	255	GLN
1	B	259	ARG
1	B	264	ASP
1	B	277	ILE
1	B	280	GLU

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Mol	Chain	Res	Type
1	B	293	LEU
1	B	295	THR
1	B	323	ILE
1	B	349	ILE
1	B	350	LEU
1	B	355	MET
1	B	358	PHE
1	B	360	GLN
1	B	365	THR
1	B	372	VAL
1	B	389	SER
1	B	400	LEU
1	B	404	LEU
1	B	422	GLU
1	B	445	ILE
1	B	472	ILE
1	B	482	VAL
1	B	489	THR
1	B	524	THR
1	B	538	THR
1	B	542	LEU
1	B	555	LEU
1	B	559	LEU
1	B	571	VAL
1	B	575	MET
1	B	578	LEU
1	B	583	THR
1	B	587	THR
1	B	610	PHE
1	B	619	THR
1	B	663	LEU
1	B	667	VAL
1	B	668	GLU
1	B	673	THR
1	B	678	GLU
1	B	682	GLN
1	B	690	LEU
1	B	694	ARG
1	B	745	LEU
1	B	768	VAL
1	B	830	LYS
1	B	838	LEU

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Mol	Chain	Res	Type
1	B	839	MET
1	B	857	MET
1	B	860	GLN
1	B	916	LEU
1	B	920	VAL
1	B	946	ASP
1	B	953	LYS
1	B	956	ILE
1	B	961	ASP
1	B	966	ARG
1	B	970	ILE
1	B	985	VAL
1	B	1012	LEU
1	B	1029	SER
1	B	1032	ASN
1	B	1033	GLU
1	B	1035	ILE
1	B	1039	HIS
1	C	3	ASN
1	C	6	ILE
1	C	18	ILE
1	C	25	LEU
1	C	27	ILE
1	C	28	LEU
1	C	55	LYS
1	C	72	ILE
1	C	88	VAL
1	C	90	ILE
1	C	92	LEU
1	C	102	ILE
1	C	104	GLN
1	C	111	LEU
1	C	112	GLN
1	C	115	MET
1	C	120	GLN
1	C	145	THR
1	C	153	ASP
1	C	177	LEU
1	C	219	LEU
1	C	243	THR
1	C	263	ARG
1	C	264	ASP

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Mol	Chain	Res	Type
1	C	273	GLU
1	C	280	GLU
1	C	293	LEU
1	C	335	ILE
1	C	337	ILE
1	C	340	VAL
1	C	342	LYS
1	C	349	ILE
1	C	350	LEU
1	C	360	GLN
1	C	407	ASP
1	C	429	GLU
1	C	431	THR
1	C	439	GLN
1	C	447	MET
1	C	452	VAL
1	C	463	THR
1	C	472	ILE
1	C	482	VAL
1	C	510	LYS
1	C	524	THR
1	C	538	THR
1	C	540	ARG
1	C	542	LEU
1	C	564	LEU
1	C	571	VAL
1	C	575	MET
1	C	578	LEU
1	C	587	THR
1	C	596	HIS
1	C	610	PHE
1	C	644	MET
1	C	652	GLN
1	C	661	PHE
1	C	667	VAL
1	C	673	THR
1	C	708	LEU
1	C	711	VAL
1	C	736	VAL
1	C	741	ILE
1	C	768	VAL
1	C	830	LYS

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Mol	Chain	Res	Type
1	C	838	LEU
1	C	842	LEU
1	C	855	THR
1	C	860	GLN
1	C	881	LEU
1	C	890	TRP
1	C	892	ILE
1	C	909	LEU
1	C	942	GLU
1	C	953	LYS
1	C	956	ILE
1	C	963	VAL
1	C	966	ARG
1	C	985	VAL
1	C	986	ILE
1	C	1008	THR
1	C	1010	THR
1	C	1012	LEU
1	C	1019	VAL
1	C	1024	VAL
1	C	1030	ARG
1	C	1033	GLU
1	C	1035	ILE
1	C	1036	GLU
1	D	6	ILE
1	D	21	LEU
1	D	25	LEU
1	D	70	ASN
1	D	88	VAL
1	D	102	ILE
1	D	111	LEU
1	D	146	ASP
1	D	148	THR
1	D	152	GLU
1	D	153	ASP
1	D	177	LEU
1	D	205	THR
1	D	219	LEU
1	D	229	GLN
1	D	264	ASP
1	D	273	GLU
1	D	280	GLU

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Mol	Chain	Res	Type
1	D	281	PHE
1	D	293	LEU
1	D	295	THR
1	D	337	ILE
1	D	350	LEU
1	D	353	LEU
1	D	358	PHE
1	D	362	PHE
1	D	365	THR
1	D	400	LEU
1	D	404	LEU
1	D	410	ILE
1	D	429	GLU
1	D	437	GLN
1	D	489	THR
1	D	519	MET
1	D	524	THR
1	D	534	ILE
1	D	538	THR
1	D	559	LEU
1	D	561	SER
1	D	571	VAL
1	D	575	MET
1	D	578	LEU
1	D	603	LYS
1	D	610	PHE
1	D	628	ASP
1	D	629	TRP
1	D	667	VAL
1	D	682	GLN
1	D	690	LEU
1	D	708	LEU
1	D	726	ILE
1	D	736	VAL
1	D	738	ILE
1	D	838	LEU
1	D	852	TYR
1	D	862	ARG
1	D	896	VAL
1	D	909	LEU
1	D	916	LEU
1	D	917	THR

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Mol	Chain	Res	Type
1	D	926	LEU
1	D	930	ILE
1	D	938	ILE
1	D	942	GLU
1	D	946	ASP
1	D	953	LYS
1	D	956	ILE
1	D	966	ARG
1	D	970	ILE
1	D	985	VAL
1	D	1012	LEU
1	D	1024	VAL
1	D	1030	ARG
1	D	1033	GLU
1	D	1035	ILE
1	E	6	ILE
1	E	25	LEU
1	E	28	LEU
1	E	48	SER
1	E	96	SER
1	E	105	VAL
1	E	111	LEU
1	E	117	LEU
1	E	131	LYS
1	E	146	ASP
1	E	153	ASP
1	E	177	LEU
1	E	213	GLN
1	E	219	LEU
1	E	249	ILE
1	E	255	GLN
1	E	259	ARG
1	E	263	ARG
1	E	270	LEU
1	E	280	GLU
1	E	291	ILE
1	E	293	LEU
1	E	310	LEU
1	E	312	LYS
1	E	323	ILE
1	E	336	SER
1	E	337	ILE

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Mol	Chain	Res	Type
1	E	342	LYS
1	E	349	ILE
1	E	355	MET
1	E	356	TYR
1	E	360	GLN
1	E	372	VAL
1	E	398	MET
1	E	400	LEU
1	E	404	LEU
1	E	452	VAL
1	E	472	ILE
1	E	482	VAL
1	E	524	THR
1	E	526	HIS
1	E	538	THR
1	E	555	LEU
1	E	564	LEU
1	E	566	ASP
1	E	571	VAL
1	E	574	THR
1	E	575	MET
1	E	583	THR
1	E	613	ASN
1	E	619	THR
1	E	629	TRP
1	E	647	THR
1	E	654	LYS
1	E	667	VAL
1	E	668	GLU
1	E	669	LEU
1	E	682	GLN
1	E	685	LEU
1	E	689	LYS
1	E	690	LEU
1	E	694	ARG
1	E	707	MET
1	E	708	LEU
1	E	711	VAL
1	E	712	ARG
1	E	726	ILE
1	E	736	VAL
1	E	768	VAL

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Mol	Chain	Res	Type
1	E	830	LYS
1	E	838	LEU
1	E	852	TYR
1	E	860	GLN
1	E	896	VAL
1	E	909	LEU
1	E	916	LEU
1	E	953	LYS
1	E	956	ILE
1	E	966	ARG
1	E	985	VAL
1	E	1012	LEU
1	E	1024	VAL
1	F	6	ILE
1	F	25	LEU
1	F	27	ILE
1	F	28	LEU
1	F	70	ASN
1	F	88	VAL
1	F	92	LEU
1	F	102	ILE
1	F	104	GLN
1	F	108	GLN
1	F	111	LEU
1	F	112	GLN
1	F	115	MET
1	F	129	VAL
1	F	153	ASP
1	F	197	GLN
1	F	205	THR
1	F	243	THR
1	F	263	ARG
1	F	280	GLU
1	F	293	LEU
1	F	312	LYS
1	F	335	ILE
1	F	337	ILE
1	F	340	VAL
1	F	349	ILE
1	F	350	LEU
1	F	360	GLN
1	F	363	ARG

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Mol	Chain	Res	Type
1	F	404	LEU
1	F	407	ASP
1	F	431	THR
1	F	447	MET
1	F	448	VAL
1	F	475	VAL
1	F	515	TRP
1	F	518	ARG
1	F	519	MET
1	F	534	ILE
1	F	538	THR
1	F	542	LEU
1	F	571	VAL
1	F	575	MET
1	F	578	LEU
1	F	587	THR
1	F	603	LYS
1	F	610	PHE
1	F	621	ILE
1	F	644	MET
1	F	653	ILE
1	F	657	MET
1	F	667	VAL
1	F	681	ASP
1	F	694	ARG
1	F	711	VAL
1	F	714	ASN
1	F	726	ILE
1	F	745	LEU
1	F	768	VAL
1	F	838	LEU
1	F	842	LEU
1	F	845	LYS
1	F	860	GLN
1	F	881	LEU
1	F	909	LEU
1	F	918	ASN
1	F	953	LYS
1	F	961	ASP
1	F	963	VAL
1	F	966	ARG
1	F	985	VAL

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Mol	Chain	Res	Type
1	F	986	ILE
1	F	1010	THR
1	F	1012	LEU
1	F	1021	PHE
1	F	1033	GLU
1	F	1034	ASP
1	F	1035	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	228	GLN
1	A	231	ASN
1	A	274	ASN
1	A	437	GLN
1	A	569	GLN
1	A	732	GLN
1	B	63	GLN
1	B	112	GLN
1	B	161	ASN
1	B	569	GLN
1	B	662	ASN
1	B	742	ASN
1	B	1039	HIS
1	C	151	GLN
1	C	161	ASN
1	C	189	ASN
1	C	254	ASN
1	C	274	ASN
1	C	577	GLN
1	C	732	GLN
1	C	755	ASN
1	D	74	ASN
1	D	109	ASN
1	D	231	ASN
1	D	254	ASN
1	D	437	GLN
1	D	742	ASN
1	D	867	GLN
1	D	918	ASN
1	E	34	GLN

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Mol	Chain	Res	Type
1	E	67	GLN
1	E	231	ASN
1	E	274	ASN
1	E	569	GLN
1	E	605	ASN
1	E	613	ASN
1	E	637	ASN
1	E	704	HIS
1	E	732	GLN
1	F	108	GLN
1	F	125	GLN
1	F	161	ASN
1	F	191	ASN
1	F	213	GLN
1	F	237	GLN
1	F	569	GLN
1	F	584	GLN
1	F	605	ASN
1	F	613	ASN
1	F	704	HIS
1	F	732	GLN
1	F	755	ASN
1	F	996	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LMT	E	1101	-	36,36,36	1.84	10 (27%)	47,47,47	1.95	9 (19%)
2	LMT	C	1101	-	36,36,36	1.85	10 (27%)	47,47,47	1.43	7 (14%)
2	LMT	A	1101	-	36,36,36	1.80	12 (33%)	47,47,47	1.38	6 (12%)
2	LMT	D	2000	-	36,36,36	1.87	11 (30%)	47,47,47	1.72	8 (17%)
2	LMT	F	2000	-	36,36,36	1.86	8 (22%)	47,47,47	1.15	4 (8%)
2	LMT	B	2000	-	36,36,36	1.81	9 (25%)	47,47,47	1.52	8 (17%)

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	LMT	E	1101	-	1/1/10/10	12/21/61/61	0/2/2/2
2	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	8/21/61/61	0/2/2/2
2	LMT	D	2000	-	1/1/10/10	12/21/61/61	0/2/2/2
2	LMT	F	2000	-	-	15/21/61/61	0/2/2/2
2	LMT	B	2000	-	-	13/21/61/61	0/2/2/2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	LMT	O1'-C1'	4.30	1.47	1.40
2	C	1101	LMT	O5'-C5'	4.06	1.54	1.44
2	F	2000	LMT	O1'-C1'	4.05	1.46	1.40
2	D	2000	LMT	O1'-C1'	4.03	1.46	1.40
2	F	2000	LMT	O5'-C1'	4.03	1.52	1.41
2	B	2000	LMT	O5'-C5'	3.93	1.54	1.44
2	F	2000	LMT	O5'-C5'	3.93	1.54	1.44
2	A	1101	LMT	O5'-C5'	3.87	1.53	1.44
2	D	2000	LMT	O5'-C5'	3.81	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	LMT	O1'-C1'	3.74	1.46	1.40
2	E	1101	LMT	O5'-C5'	3.56	1.53	1.44
2	D	2000	LMT	O5B-C1B	3.48	1.50	1.41
2	C	1101	LMT	C6'-C5'	-3.45	1.40	1.51
2	E	1101	LMT	O5'-C1'	3.44	1.50	1.41
2	A	1101	LMT	O1'-C1'	3.42	1.45	1.40
2	F	2000	LMT	C6'-C5'	-3.41	1.40	1.51
2	F	2000	LMT	O5B-C1B	3.37	1.50	1.41
2	E	1101	LMT	C6'-C5'	-3.34	1.40	1.51
2	A	1101	LMT	O5B-C1B	3.33	1.50	1.41
2	C	1101	LMT	O5'-C1'	3.30	1.50	1.41
2	B	2000	LMT	C6'-C5'	-3.24	1.40	1.51
2	A	1101	LMT	C6'-C5'	-3.19	1.41	1.51
2	C	1101	LMT	O5B-C1B	3.18	1.50	1.41
2	B	2000	LMT	O5B-C1B	3.16	1.50	1.41
2	B	2000	LMT	O1'-C1'	3.14	1.45	1.40
2	E	1101	LMT	O5B-C1B	3.09	1.49	1.41
2	D	2000	LMT	C3'-C2'	-3.09	1.44	1.52
2	D	2000	LMT	C6'-C5'	-3.04	1.41	1.51
2	B	2000	LMT	O5'-C1'	2.94	1.49	1.41
2	C	1101	LMT	O3B-C3B	2.91	1.50	1.43
2	B	2000	LMT	C3'-C2'	-2.89	1.44	1.52
2	D	2000	LMT	O5'-C1'	2.84	1.49	1.41
2	B	2000	LMT	C3B-C2B	-2.83	1.45	1.52
2	E	1101	LMT	C3'-C2'	-2.78	1.45	1.52
2	F	2000	LMT	C3'-C2'	-2.75	1.45	1.52
2	D	2000	LMT	O3B-C3B	2.73	1.49	1.43
2	E	1101	LMT	O1B-C1B	-2.65	1.34	1.41
2	A	1101	LMT	O5'-C1'	2.62	1.48	1.41
2	D	2000	LMT	C3B-C2B	-2.61	1.45	1.52
2	A	1101	LMT	C3'-C2'	-2.59	1.45	1.52
2	E	1101	LMT	O3B-C3B	2.56	1.49	1.43
2	D	2000	LMT	O2'-C2'	2.40	1.48	1.43
2	B	2000	LMT	C5-C4	2.33	1.63	1.51
2	C	1101	LMT	C3'-C2'	-2.29	1.46	1.52
2	F	2000	LMT	C5-C4	2.28	1.63	1.51
2	F	2000	LMT	O3B-C3B	2.27	1.48	1.43
2	A	1101	LMT	C1'-C2'	-2.25	1.45	1.52
2	A	1101	LMT	O2'-C2'	2.24	1.48	1.43
2	C	1101	LMT	C5-C4	2.23	1.62	1.51
2	C	1101	LMT	O2'-C2'	2.21	1.48	1.43
2	E	1101	LMT	O1B-C4'	-2.21	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	LMT	C3B-C2B	-2.20	1.46	1.52
2	A	1101	LMT	O3B-C3B	2.16	1.48	1.43
2	C	1101	LMT	C8-C7	2.15	1.62	1.51
2	D	2000	LMT	C5-C4	2.14	1.62	1.51
2	A	1101	LMT	C5-C4	2.14	1.62	1.51
2	B	2000	LMT	O3B-C3B	2.13	1.48	1.43
2	E	1101	LMT	C5-C4	2.12	1.62	1.51
2	A	1101	LMT	O1B-C1B	-2.03	1.36	1.41
2	D	2000	LMT	C2-C1	2.00	1.59	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1101	LMT	O1B-C4'-C5'	-5.45	95.18	109.48
2	D	2000	LMT	O1'-C1'-C2'	5.27	116.28	108.27
2	C	1101	LMT	O1'-C1'-C2'	5.03	115.91	108.27
2	E	1101	LMT	C4B-C3B-C2B	4.79	119.23	110.83
2	D	2000	LMT	C1-O1'-C1'	4.66	121.63	113.68
2	E	1101	LMT	C3B-C4B-C5B	4.63	118.63	110.23
2	A	1101	LMT	C1B-O5B-C5B	4.43	122.37	113.72
2	E	1101	LMT	O1'-C1'-C2'	4.29	114.78	108.27
2	A	1101	LMT	O5B-C5B-C4B	4.05	116.99	109.70
2	B	2000	LMT	C1B-O1B-C4'	-4.05	108.39	117.98
2	B	2000	LMT	O5B-C5B-C4B	3.74	116.44	109.70
2	D	2000	LMT	O2'-C2'-C1'	3.68	118.84	110.08
2	E	1101	LMT	O4'-C4B-C3B	-3.61	101.86	110.38
2	B	2000	LMT	C1'-C2'-C3'	-3.54	102.57	110.01
2	D	2000	LMT	C1B-O1B-C4'	-3.48	109.73	117.98
2	E	1101	LMT	O5'-C5'-C6'	3.06	114.03	106.44
2	B	2000	LMT	O3B-C3B-C2B	-2.98	103.34	110.38
2	D	2000	LMT	C1'-O5'-C5'	2.96	119.49	113.72
2	F	2000	LMT	C1B-O5B-C5B	-2.84	108.17	113.72
2	E	1101	LMT	O1B-C1B-C2B	-2.83	101.11	108.09
2	D	2000	LMT	C1'-C2'-C3'	-2.80	104.11	110.01
2	E	1101	LMT	O5B-C5B-C4B	2.78	114.70	109.70
2	B	2000	LMT	O1'-C1'-C2'	2.71	112.38	108.27
2	C	1101	LMT	C1'-C2'-C3'	-2.67	104.40	110.01
2	C	1101	LMT	C3'-C4'-C5'	-2.64	105.07	110.93
2	B	2000	LMT	O1B-C1B-C2B	2.59	114.46	108.09
2	C	1101	LMT	O3'-C3'-C4'	2.58	116.54	109.94
2	C	1101	LMT	C1B-O1B-C4'	-2.55	111.94	117.98
2	D	2000	LMT	O3'-C3'-C4'	2.51	116.37	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2000	LMT	C1B-O5B-C5B	2.45	118.51	113.72
2	F	2000	LMT	O5B-C5B-C4B	2.39	114.00	109.70
2	A	1101	LMT	C1B-C2B-C3B	2.35	114.96	110.01
2	F	2000	LMT	C1'-O5'-C5'	2.31	118.23	113.72
2	B	2000	LMT	C1'-O5'-C5'	-2.31	109.21	113.72
2	D	2000	LMT	C4B-C3B-C2B	2.27	114.81	110.83
2	A	1101	LMT	O3B-C3B-C4B	-2.26	105.06	110.38
2	E	1101	LMT	O2'-C2'-C1'	2.25	115.44	110.08
2	A	1101	LMT	O5B-C1B-C2B	2.19	114.86	110.37
2	F	2000	LMT	O5B-C5B-C6B	2.17	111.82	106.44
2	C	1101	LMT	C1B-C2B-C3B	2.12	114.46	110.01
2	C	1101	LMT	O1B-C4'-C3'	2.04	112.42	107.23
2	A	1101	LMT	C6B-C5B-C4B	-2.01	108.09	113.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2000	LMT	C3B
2	E	1101	LMT	C2B

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2000	LMT	C2'-C1'-O1'-C1
2	E	1101	LMT	C4B-C5B-C6B-O6B
2	A	1101	LMT	O5'-C5'-C6'-O6'
2	F	2000	LMT	O5'-C5'-C6'-O6'
2	C	1101	LMT	O5B-C5B-C6B-O6B
2	E	1101	LMT	O5B-C5B-C6B-O6B
2	E	1101	LMT	O5'-C5'-C6'-O6'
2	D	2000	LMT	O5'-C5'-C6'-O6'
2	A	1101	LMT	C4'-C5'-C6'-O6'
2	E	1101	LMT	C4'-C5'-C6'-O6'
2	D	2000	LMT	C4'-C5'-C6'-O6'
2	C	1101	LMT	O5'-C5'-C6'-O6'
2	F	2000	LMT	C4'-C5'-C6'-O6'
2	C	1101	LMT	O5'-C1'-O1'-C1
2	F	2000	LMT	O5B-C5B-C6B-O6B
2	B	2000	LMT	C2-C3-C4-C5
2	C	1101	LMT	C4-C5-C6-C7
2	F	2000	LMT	C4B-C5B-C6B-O6B
2	A	1101	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	B	2000	LMT	C4'-C5'-C6'-O6'
2	C	1101	LMT	C4B-C5B-C6B-O6B
2	C	1101	LMT	C2'-C1'-O1'-C1
2	C	1101	LMT	C4'-C5'-C6'-O6'
2	A	1101	LMT	O5B-C5B-C6B-O6B
2	A	1101	LMT	C5-C6-C7-C8
2	D	2000	LMT	O5'-C1'-O1'-C1
2	A	1101	LMT	O1'-C1-C2-C3
2	B	2000	LMT	O5'-C5'-C6'-O6'
2	C	1101	LMT	C6-C7-C8-C9
2	D	2000	LMT	C2'-C1'-O1'-C1
2	B	2000	LMT	O1'-C1-C2-C3
2	F	2000	LMT	O5'-C1'-O1'-C1
2	B	2000	LMT	C1-C2-C3-C4
2	C	1101	LMT	C2-C3-C4-C5
2	E	1101	LMT	C11-C10-C9-C8
2	E	1101	LMT	C2-C1-O1'-C1'
2	E	1101	LMT	C5-C6-C7-C8
2	A	1101	LMT	C4-C5-C6-C7
2	F	2000	LMT	C11-C10-C9-C8
2	B	2000	LMT	C11-C10-C9-C8
2	B	2000	LMT	C5-C6-C7-C8
2	D	2000	LMT	O5B-C5B-C6B-O6B
2	C	1101	LMT	C5-C6-C7-C8
2	F	2000	LMT	C6-C7-C8-C9
2	F	2000	LMT	C1-C2-C3-C4
2	C	1101	LMT	C1-C2-C3-C4
2	E	1101	LMT	C3-C4-C5-C6
2	F	2000	LMT	C7-C8-C9-C10
2	D	2000	LMT	C1-C2-C3-C4
2	E	1101	LMT	C5'-C4'-O1B-C1B
2	B	2000	LMT	C9-C10-C11-C12
2	E	1101	LMT	C2-C3-C4-C5
2	F	2000	LMT	C2-C3-C4-C5
2	F	2000	LMT	C9-C10-C11-C12
2	E	1101	LMT	C3'-C4'-O1B-C1B
2	B	2000	LMT	C7-C8-C9-C10
2	D	2000	LMT	C6-C7-C8-C9
2	B	2000	LMT	O5B-C5B-C6B-O6B
2	B	2000	LMT	O5'-C1'-O1'-C1
2	F	2000	LMT	C4-C5-C6-C7
2	D	2000	LMT	C5-C6-C7-C8

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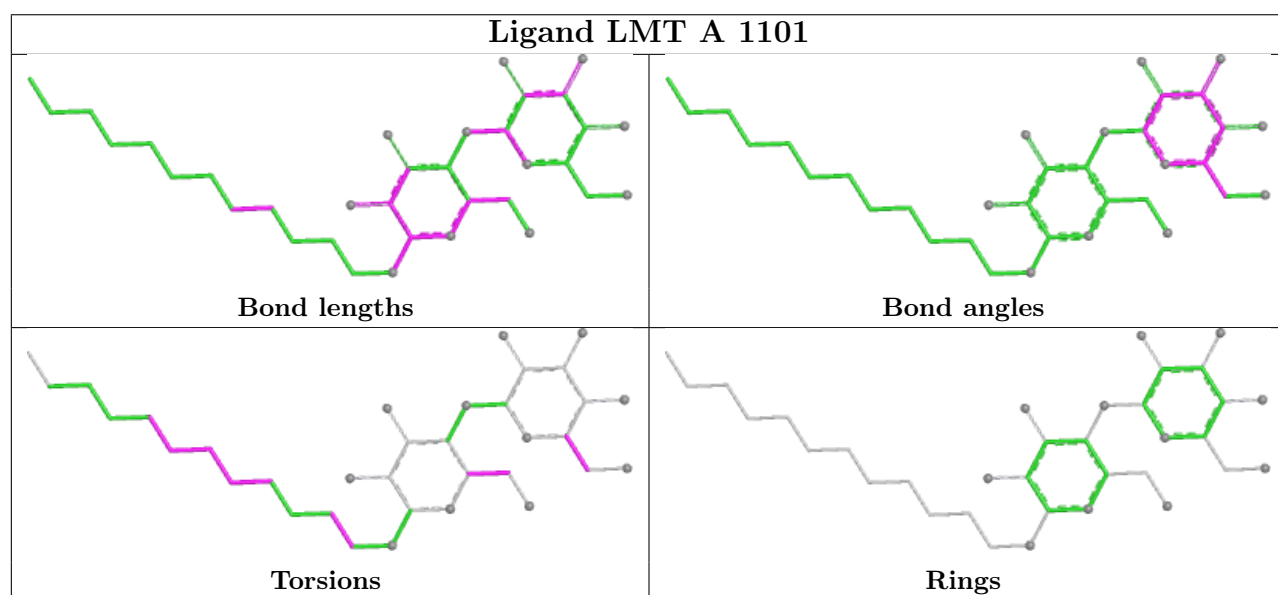
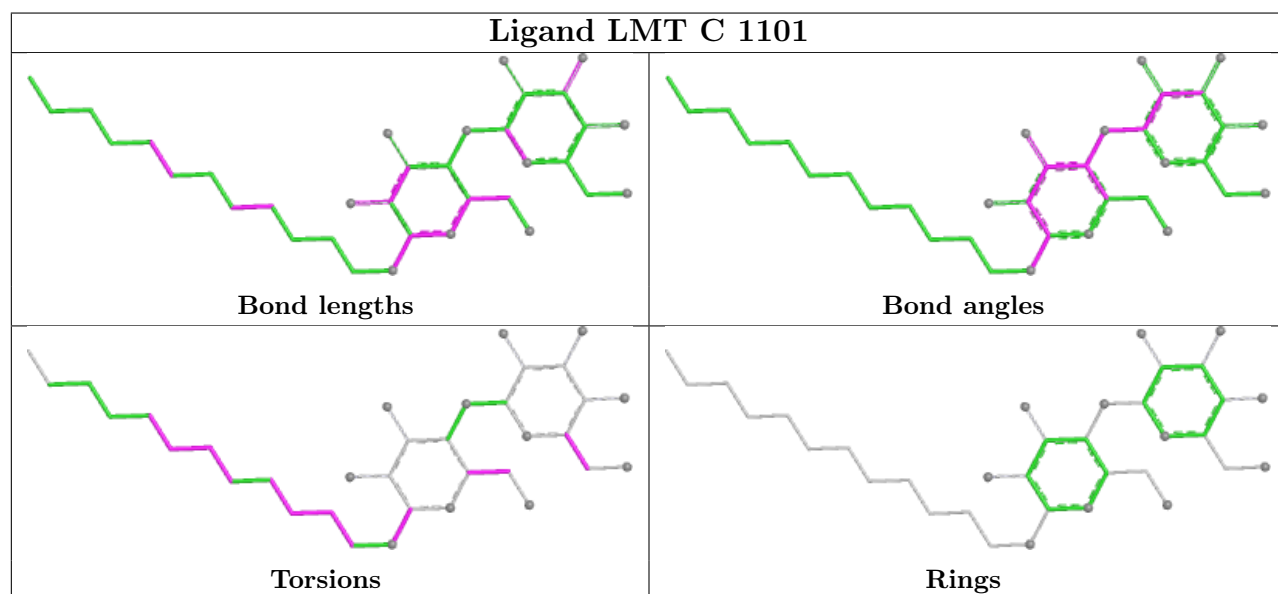
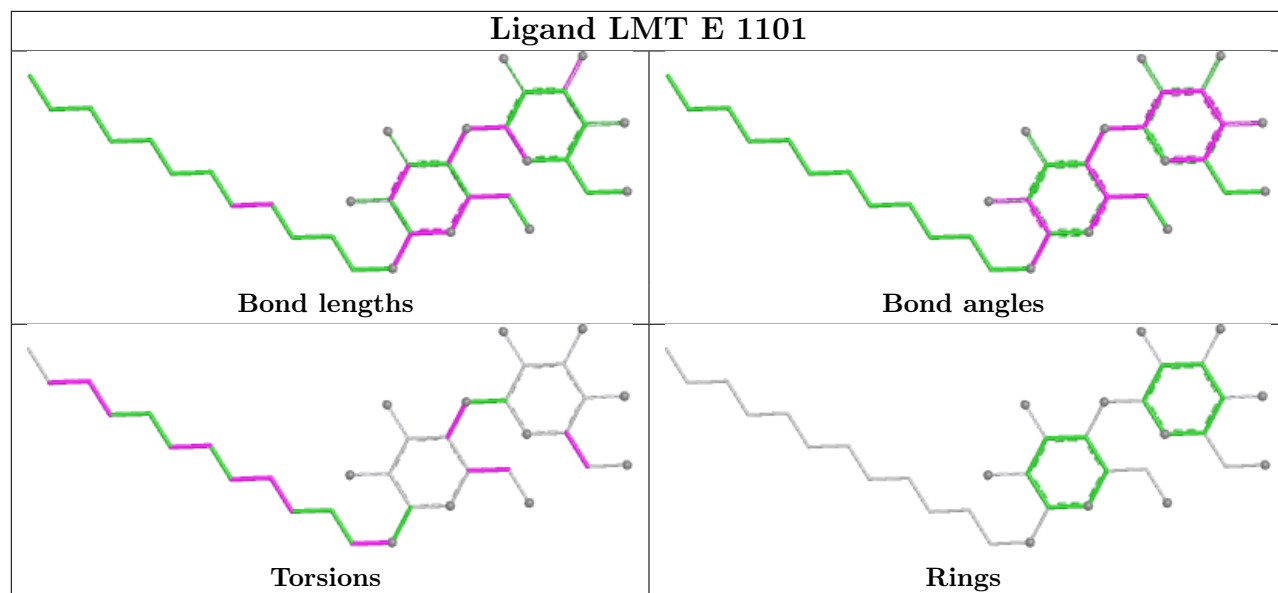
Mol	Chain	Res	Type	Atoms
2	D	2000	LMT	C11-C10-C9-C8
2	B	2000	LMT	C4-C5-C6-C7
2	D	2000	LMT	C7-C8-C9-C10
2	D	2000	LMT	C4-C5-C6-C7
2	F	2000	LMT	C3-C4-C5-C6
2	F	2000	LMT	O1'-C1-C2-C3
2	D	2000	LMT	C9-C10-C11-C12
2	A	1101	LMT	C6-C7-C8-C9
2	E	1101	LMT	C9-C10-C11-C12
2	B	2000	LMT	C2-C1-O1'-C1'
2	C	1101	LMT	O1'-C1-C2-C3

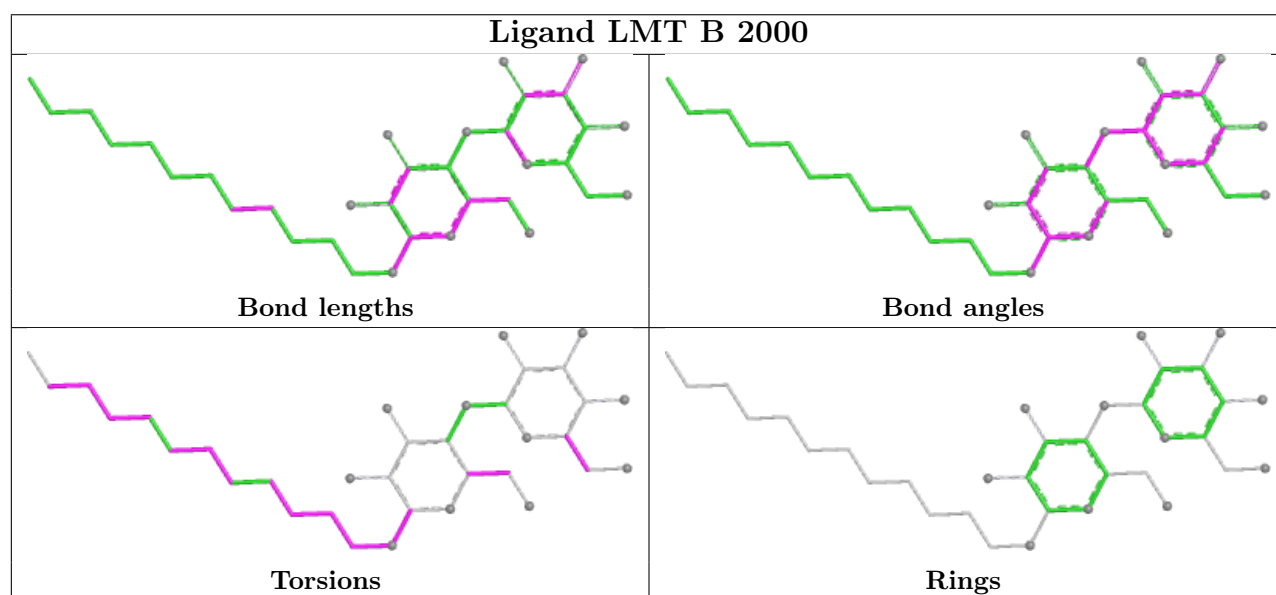
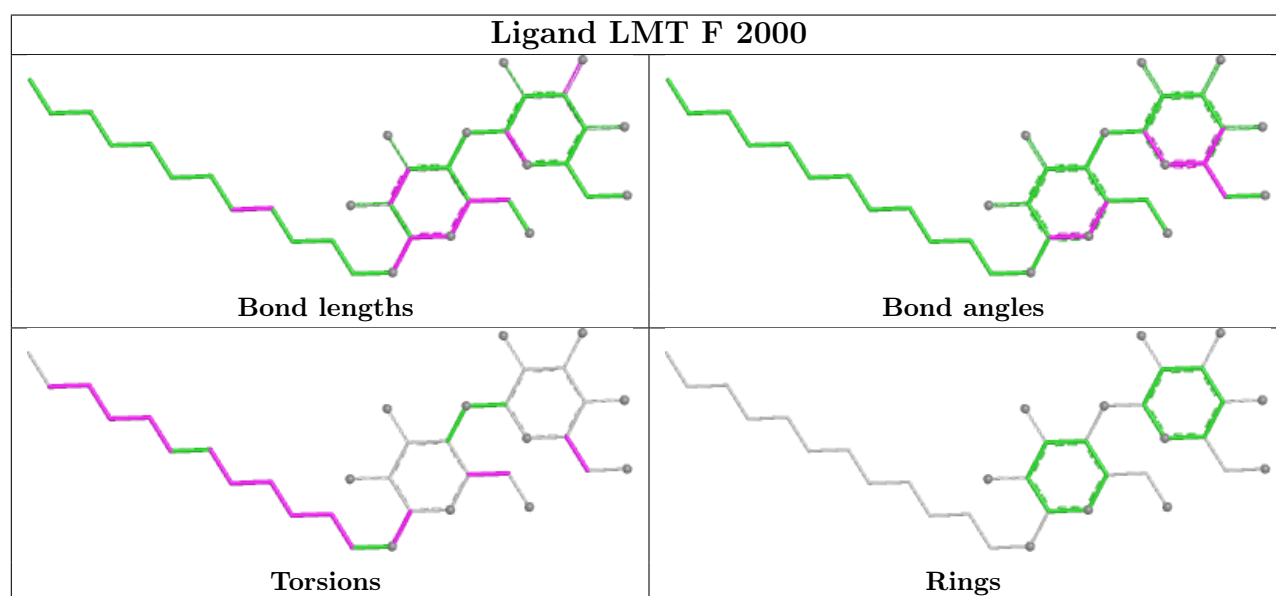
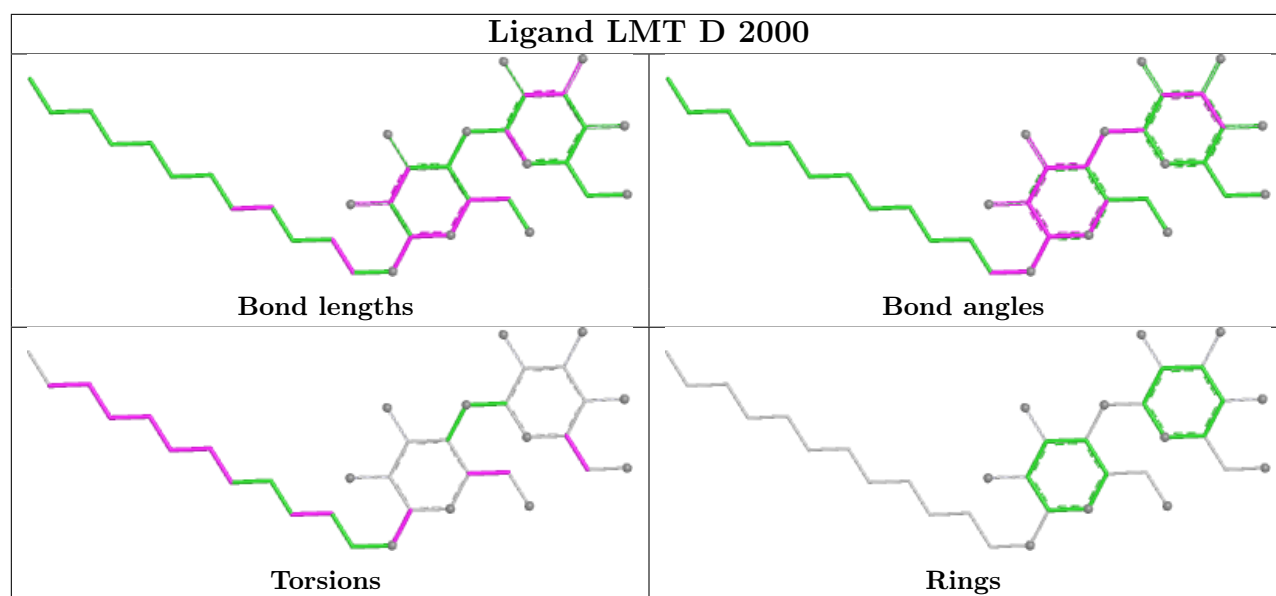
There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1101	LMT	8	0
2	C	1101	LMT	2	0
2	A	1101	LMT	4	0
2	D	2000	LMT	3	0
2	F	2000	LMT	1	0
2	B	2000	LMT	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1038/1044 (99%)	0.27	55 (5%)	32	24	27, 75, 109, 132	0
1	B	1039/1044 (99%)	0.04	27 (2%)	57	42	18, 68, 104, 130	0
1	C	1035/1044 (99%)	0.10	34 (3%)	49	36	17, 69, 104, 126	0
1	D	1038/1044 (99%)	0.29	38 (3%)	45	32	16, 90, 130, 173	0
1	E	1037/1044 (99%)	0.44	64 (6%)	26	21	40, 91, 115, 134	0
1	F	1037/1044 (99%)	0.42	67 (6%)	25	20	24, 84, 118, 142	0
All	All	6224/6264 (99%)	0.26	285 (4%)	37	27	16, 80, 115, 173	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	291	ILE	8.1
1	D	59	ASP	7.6
1	B	710	SER	6.6
1	A	383	LEU	6.3
1	E	864	SER	6.2
1	C	851	GLY	6.0
1	F	851	GLY	6.0
1	F	832	THR	5.9
1	F	501	ALA	5.7
1	E	290	GLY	5.4
1	C	69	MET	4.9
1	B	864	SER	4.8
1	F	442	LEU	4.7
1	A	35	TYR	4.7
1	F	883	LEU	4.6
1	A	666	ILE	4.6
1	E	164	ASP	4.5
1	D	864	SER	4.5
1	F	503	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	605	ASN	4.4
1	E	366	LEU	4.4
1	C	833	GLY	4.3
1	A	445	ILE	4.3
1	D	330	THR	4.3
1	D	709	THR	4.3
1	F	500	ILE	4.2
1	C	866	ASN	4.1
1	F	410	ILE	4.1
1	C	850	VAL	4.0
1	F	107	VAL	4.0
1	E	488	LEU	4.0
1	F	861	GLU	4.0
1	A	372	VAL	4.0
1	E	59	ASP	4.0
1	C	685	LEU	4.0
1	A	59	ASP	4.0
1	F	872	TYR	3.8
1	B	290	GLY	3.8
1	E	997	ALA	3.7
1	F	833	GLY	3.7
1	C	49	TYR	3.7
1	B	697	LEU	3.7
1	E	406	VAL	3.7
1	E	496	MET	3.7
1	F	49	TYR	3.6
1	F	481	SER	3.6
1	C	681	ASP	3.6
1	C	330	THR	3.6
1	D	337	ILE	3.6
1	E	911	ALA	3.6
1	B	164	ASP	3.6
1	A	376	LEU	3.6
1	A	400	LEU	3.6
1	C	817	LEU	3.6
1	A	887	TYR	3.5
1	E	292	LYS	3.5
1	D	708	LEU	3.5
1	A	339	GLU	3.5
1	A	606	VAL	3.5
1	C	79	SER	3.5
1	F	879	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	486	LEU	3.4
1	D	811	LEU	3.4
1	F	3	ASN	3.4
1	C	494	ALA	3.4
1	F	441	ALA	3.4
1	E	330	THR	3.4
1	B	698	LEU	3.3
1	B	300	LEU	3.3
1	E	838	LEU	3.3
1	A	310	LEU	3.3
1	A	396	PHE	3.3
1	F	822	ILE	3.3
1	E	989	GLY	3.3
1	A	327	TYR	3.3
1	E	541	TYR	3.2
1	C	883	LEU	3.2
1	F	831	SER	3.2
1	A	386	PHE	3.2
1	A	493	CYS	3.2
1	C	127	VAL	3.2
1	C	68	ASN	3.2
1	E	92	LEU	3.2
1	C	50	PRO	3.2
1	A	16	ALA	3.2
1	D	459	PHE	3.1
1	B	291	ILE	3.1
1	E	289	LEU	3.1
1	F	670	GLY	3.1
1	B	472	ILE	3.1
1	F	306	ILE	3.1
1	E	293	LEU	3.1
1	E	920	VAL	3.1
1	C	832	THR	3.1
1	A	43	VAL	3.1
1	D	389	SER	3.1
1	D	854	TRP	3.1
1	D	334	LYS	3.0
1	F	708	LEU	3.0
1	F	406	VAL	3.0
1	B	870	SER	3.0
1	E	466	ILE	3.0
1	E	2	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	868	ALA	3.0
1	C	122	VAL	3.0
1	E	986	ILE	3.0
1	F	56	THR	3.0
1	C	863	LEU	2.9
1	F	473	THR	2.9
1	A	92	LEU	2.9
1	B	315	PRO	2.9
1	F	887	TYR	2.9
1	F	863	LEU	2.9
1	A	467	TYR	2.9
1	F	852	TYR	2.9
1	B	515	TRP	2.9
1	C	403	GLY	2.9
1	E	174	ASP	2.8
1	E	487	ILE	2.8
1	B	854	TRP	2.8
1	E	556	PHE	2.8
1	E	42	ALA	2.8
1	F	60	THR	2.8
1	A	916	LEU	2.8
1	E	857	MET	2.8
1	A	630	ALA	2.8
1	D	32	VAL	2.8
1	F	117	LEU	2.8
1	F	678	GLU	2.8
1	F	54	ALA	2.7
1	E	333	VAL	2.7
1	A	881	LEU	2.7
1	F	61	VAL	2.7
1	A	21	LEU	2.7
1	A	72	ILE	2.7
1	A	894	PHE	2.7
1	F	674	GLY	2.7
1	B	825	GLN	2.7
1	A	494	ALA	2.7
1	F	685	LEU	2.7
1	A	569	GLN	2.6
1	E	674	GLY	2.6
1	E	673	THR	2.6
1	B	934	ALA	2.6
1	D	84	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	35	TYR	2.6
1	E	473	THR	2.6
1	B	677	PHE	2.6
1	A	218	GLN	2.6
1	D	92	LEU	2.6
1	F	109	ASN	2.6
1	F	193	LEU	2.6
1	B	865	GLY	2.6
1	D	461	GLY	2.6
1	D	676	ASP	2.6
1	E	928	THR	2.6
1	B	174	ASP	2.5
1	A	665	ALA	2.5
1	F	417	GLU	2.5
1	A	472	ILE	2.5
1	E	319	SER	2.5
1	F	359	LEU	2.5
1	E	43	VAL	2.5
1	E	580	ALA	2.5
1	B	673	THR	2.5
1	D	295	THR	2.5
1	E	94	PHE	2.5
1	E	463	THR	2.5
1	B	869	PRO	2.5
1	B	861	GLU	2.5
1	F	335	ILE	2.5
1	F	415	ASN	2.5
1	F	675	PHE	2.5
1	E	677	PHE	2.4
1	F	68	ASN	2.4
1	A	616	GLY	2.4
1	D	736	VAL	2.4
1	D	400	LEU	2.4
1	E	137	LEU	2.4
1	B	879	VAL	2.4
1	F	32	VAL	2.4
1	A	410	ILE	2.4
1	F	434	SER	2.4
1	F	669	LEU	2.4
1	E	107	VAL	2.4
1	C	813	ARG	2.4
1	B	314	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	409	ALA	2.4
1	A	486	LEU	2.4
1	E	599	LEU	2.4
1	E	716	LEU	2.4
1	F	111	LEU	2.4
1	F	357	LEU	2.4
1	A	473	THR	2.3
1	E	296	GLY	2.3
1	C	402	ILE	2.3
1	A	411	VAL	2.3
1	E	372	VAL	2.3
1	E	963	VAL	2.3
1	D	37	THR	2.3
1	E	131	LYS	2.3
1	A	674	GLY	2.3
1	F	97	GLY	2.3
1	F	55	LYS	2.3
1	D	100	ALA	2.3
1	F	890	TRP	2.3
1	D	267	LYS	2.3
1	C	119	PRO	2.3
1	E	738	ILE	2.3
1	A	934	ALA	2.3
1	D	863	LEU	2.3
1	C	867	GLN	2.3
1	A	334	LYS	2.2
1	F	127	VAL	2.2
1	A	337	ILE	2.2
1	C	72	ILE	2.2
1	D	232	ALA	2.2
1	C	784	TRP	2.2
1	C	814	TYR	2.2
1	A	413	VAL	2.2
1	F	695	ASN	2.2
1	E	177	LEU	2.2
1	C	515	TRP	2.2
1	A	56	THR	2.2
1	A	437	GLN	2.2
1	B	487	ILE	2.2
1	E	75	LEU	2.2
1	F	494	ALA	2.2
1	A	397	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	829	GLY	2.2
1	E	650	PHE	2.2
1	E	515	TRP	2.2
1	F	392	THR	2.1
1	D	842	LEU	2.1
1	D	55	LYS	2.1
1	D	710	SER	2.1
1	E	395	MET	2.1
1	E	465	ALA	2.1
1	E	815	ASN	2.1
1	E	118	LEU	2.1
1	A	456	MET	2.1
1	F	839	MET	2.1
1	E	114	ALA	2.1
1	A	635	GLU	2.1
1	C	97	GLY	2.1
1	E	484	VAL	2.1
1	A	39	ALA	2.1
1	A	36	PRO	2.1
1	D	870	SER	2.1
1	E	175	VAL	2.1
1	A	536	ARG	2.1
1	D	820	MET	2.1
1	C	885	ALA	2.1
1	C	123	GLN	2.1
1	D	757	PHE	2.1
1	F	1016	PHE	2.1
1	A	27	ILE	2.1
1	A	404	LEU	2.1
1	B	6	ILE	2.1
1	D	306	ILE	2.1
1	F	270	LEU	2.1
1	D	53	ASP	2.1
1	B	709	THR	2.1
1	F	537	SER	2.0
1	A	30	LEU	2.0
1	E	306	ILE	2.0
1	F	118	LEU	2.0
1	A	371	ALA	2.0
1	D	328	ASP	2.0
1	E	93	THR	2.0
1	B	556	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	670	GLY	2.0
1	C	849	GLY	2.0
1	D	570	GLY	2.0
1	F	516	PHE	2.0
1	F	502	LYS	2.0
1	E	854	TRP	2.0
1	A	672	ALA	2.0
1	C	501	ALA	2.0
1	F	169	THR	2.0
1	F	814	TYR	2.0
1	D	285	PRO	2.0
1	F	119	PRO	2.0
1	D	861	GLU	2.0
1	F	850	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

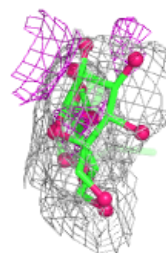
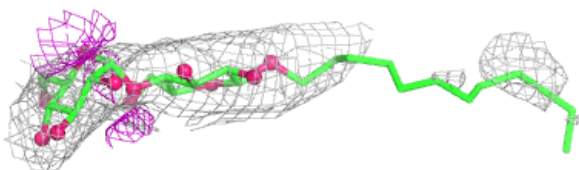
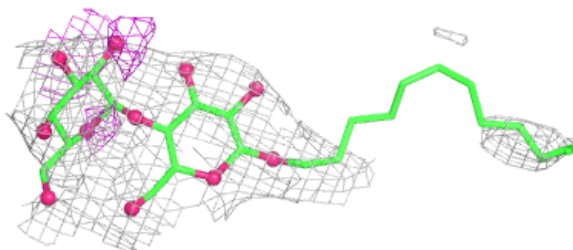
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LMT	F	2000	35/35	0.79	0.13	40,64,89,94	0
2	LMT	B	2000	35/35	0.84	0.15	31,50,60,69	0
2	LMT	E	1101	35/35	0.85	0.11	41,74,104,107	0
2	LMT	D	2000	35/35	0.90	0.09	21,41,56,63	0
2	LMT	C	1101	35/35	0.91	0.07	12,41,56,72	0
2	LMT	A	1101	35/35	0.92	0.09	31,41,90,99	0
3	NI	E	1102	1/1	0.95	0.06	170,170,170,170	0
3	NI	A	1102	1/1	0.96	0.06	154,154,154,154	0
3	NI	C	1102	1/1	1.00	0.05	41,41,41,41	0

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

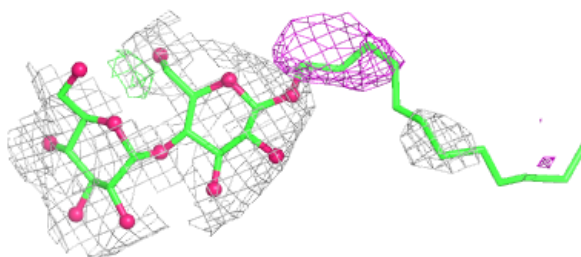
Electron density around LMT F 2000:

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

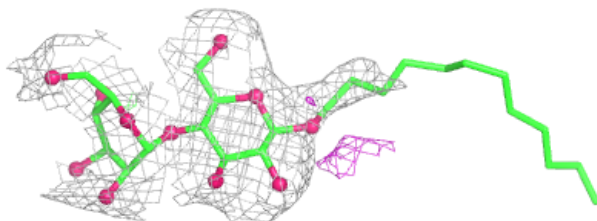


Electron density around LMT B 2000:

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

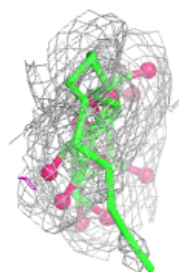
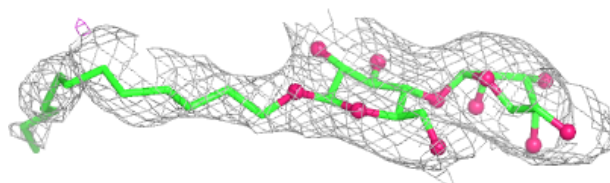
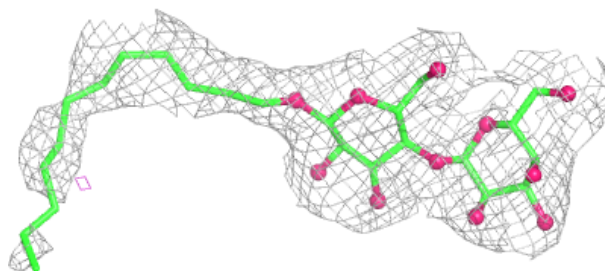
**Electron density around LMT E 1101:**

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

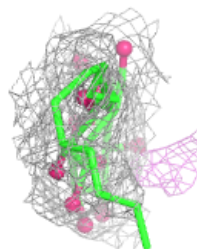
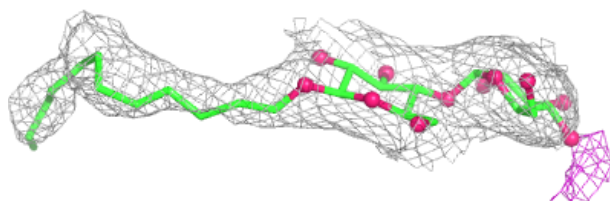
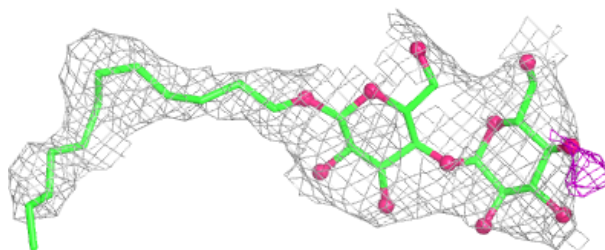


Electron density around LMT D 2000:

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

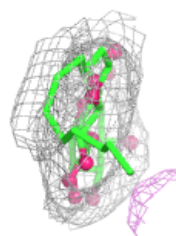
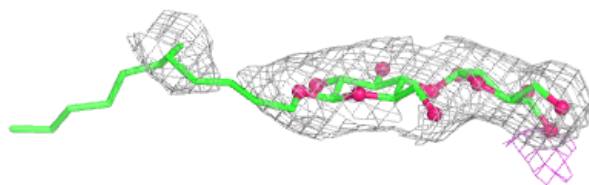
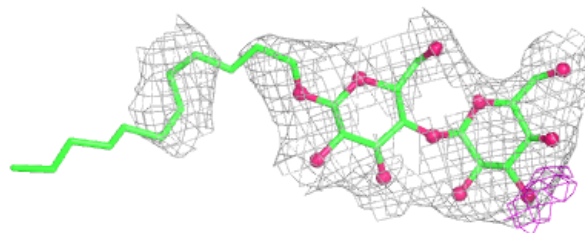
**Electron density around LMT C 1101:**

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



Electron density around LMT A 1101:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.