



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 08:27 PM EDT

PDB ID : 4ZIV / pdb_00004ziv
Title : Crystal structure of AcrB triple mutant in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-28
Resolution : 3.16 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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

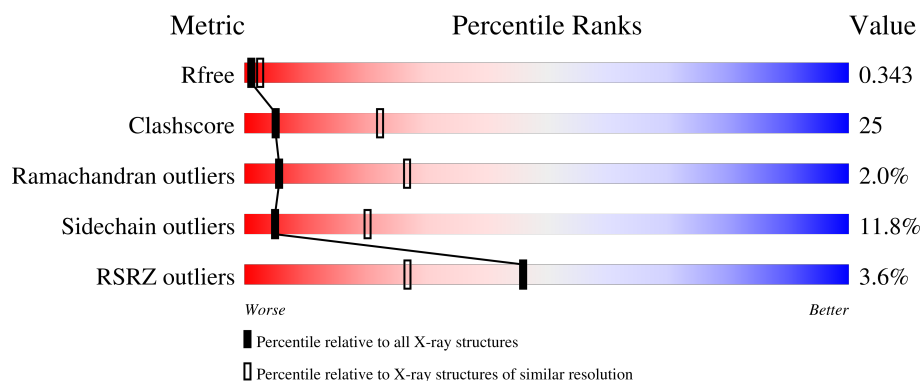
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	B	1101	X	-	-	-
2	LMT	C	1101	X	-	-	-

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	152.28Å 157.49Å 219.16Å 90.00° 92.74° 90.00°	Depositor
Resolution (Å)	19.98 – 3.16 19.98 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.98-3.16) 97.3 (19.98-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.270 , 0.335 0.282 , 0.343	Depositor DCC
R_{free} test set	8816 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	95.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.075 for -k,-h,-l 0.095 for k,h,-l 0.089 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	47736	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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 50.20 % 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 6.6875e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

3 Model quality

3.1 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	0.83	4/8056 (0.0%)	1.26	49/10940 (0.4%)
1	B	0.84	1/8089 (0.0%)	1.28	65/10986 (0.6%)
1	C	0.86	1/8074 (0.0%)	1.29	56/10965 (0.5%)
1	D	0.78	3/8056 (0.0%)	1.23	61/10940 (0.6%)
1	E	0.77	2/8056 (0.0%)	1.22	50/10940 (0.5%)
1	F	0.81	2/8089 (0.0%)	1.27	63/10986 (0.6%)
All	All	0.82	13/48420 (0.0%)	1.26	344/65757 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	2
1	F	0	2
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1022	VAL	CA-CB	11.56	1.59	1.54
1	A	1022	VAL	CA-CB	9.21	1.58	1.54
1	E	905	VAL	CA-CB	8.10	1.58	1.54
1	D	905	VAL	CA-CB	7.43	1.57	1.54
1	C	897	ILE	CA-CB	7.23	1.58	1.54
1	A	905	VAL	CA-CB	6.18	1.57	1.54
1	D	493	CYS	CA-C	-6.12	1.45	1.52
1	B	978	THR	CA-CB	5.73	1.62	1.53
1	F	897	ILE	CA-CB	5.45	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	PRO	CA-C	-5.38	1.49	1.51
1	D	978	THR	CA-C	-5.37	1.46	1.52
1	A	1040	ILE	CA-CB	5.34	1.61	1.54
1	F	216	ALA	CA-C	-5.08	1.50	1.53

All (344) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	TYR	CA-C-N	-12.51	108.13	120.52
1	A	35	TYR	C-N-CA	-12.51	108.13	120.52
1	C	1044	HIS	N-CA-C	12.51	119.04	108.78
1	E	515	TRP	N-CA-C	-10.77	99.32	111.82
1	A	39	ALA	CA-C-N	10.52	127.34	119.66
1	A	39	ALA	C-N-CA	10.52	127.34	119.66
1	D	673	GLU	N-CA-C	9.97	125.00	112.24
1	B	994	GLY	N-CA-C	-9.65	101.61	111.85
1	F	7	ASP	N-CA-C	-9.62	98.36	111.55
1	D	317	PHE	CA-C-N	9.48	131.69	119.84
1	D	317	PHE	C-N-CA	9.48	131.69	119.84
1	B	515	TRP	N-CA-C	-9.38	100.92	111.71
1	A	515	TRP	N-CA-C	-9.23	101.11	111.82
1	D	998	GLY	N-CA-C	-9.22	101.81	112.50
1	C	515	TRP	N-CA-C	-9.06	101.41	111.28
1	B	559	LEU	CA-C-N	9.06	129.61	119.92
1	B	559	LEU	C-N-CA	9.06	129.61	119.92
1	C	1033	PHE	CA-C-N	8.93	137.77	121.70
1	C	1033	PHE	C-N-CA	8.93	137.77	121.70
1	F	919	ARG	N-CA-C	-8.86	97.19	109.95
1	B	40	PRO	CA-C-N	8.55	130.53	119.84
1	B	40	PRO	C-N-CA	8.55	130.53	119.84
1	F	1041	GLU	CA-C-N	8.52	137.03	121.70
1	F	1041	GLU	C-N-CA	8.52	137.03	121.70
1	C	848	ALA	N-CA-C	8.49	122.90	112.54
1	C	7	ASP	CA-C-N	8.47	132.17	122.85
1	C	7	ASP	C-N-CA	8.47	132.17	122.85
1	E	1036	LYS	N-CA-C	8.41	120.53	110.44
1	B	287	SER	CA-C-N	-8.34	114.82	121.82
1	B	287	SER	C-N-CA	-8.34	114.82	121.82
1	E	1009	GLY	N-CA-C	-8.31	102.76	112.73
1	A	673	GLU	N-CA-C	8.28	122.84	112.24
1	E	4	PHE	N-CA-C	8.23	119.88	111.07
1	B	6	ILE	N-CA-C	-8.16	102.48	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ILE	N-CA-C	-8.14	105.25	113.47
1	B	1039	ASP	N-CA-C	8.10	125.98	113.19
1	B	147	GLY	N-CA-C	-8.09	103.35	115.00
1	D	1022	VAL	CA-C-N	-8.03	111.52	119.87
1	D	1022	VAL	C-N-CA	-8.03	111.52	119.87
1	A	1034	SER	CA-C-N	7.95	136.00	121.70
1	A	1034	SER	C-N-CA	7.95	136.00	121.70
1	B	854	GLY	N-CA-C	-7.84	104.21	115.27
1	B	659	LYS	N-CA-C	7.80	120.76	109.14
1	A	374	VAL	N-CA-C	7.79	117.86	110.30
1	B	367	ILE	CA-C-N	-7.77	111.71	119.56
1	B	367	ILE	C-N-CA	-7.77	111.71	119.56
1	C	973	ARG	CA-C-N	-7.74	110.98	119.19
1	C	973	ARG	C-N-CA	-7.74	110.98	119.19
1	B	799	VAL	CA-C-N	-7.74	112.78	120.21
1	B	799	VAL	C-N-CA	-7.74	112.78	120.21
1	B	85	THR	N-CA-C	-7.60	101.96	112.30
1	E	189	ASN	CA-C-N	7.55	127.08	118.85
1	E	189	ASN	C-N-CA	7.55	127.08	118.85
1	F	404	LEU	N-CA-C	7.45	120.86	111.69
1	D	374	VAL	N-CA-C	7.45	117.53	110.53
1	A	147	GLY	N-CA-C	-7.44	104.54	115.63
1	E	498	LYS	CA-C-N	7.43	127.19	119.76
1	E	498	LYS	C-N-CA	7.43	127.19	119.76
1	D	35	TYR	CA-C-N	7.39	128.89	120.98
1	D	35	TYR	C-N-CA	7.39	128.89	120.98
1	F	493	CYS	N-CA-C	-7.39	103.89	113.12
1	A	1024	VAL	N-CA-C	-7.36	103.69	110.82
1	E	213	GLN	N-CA-C	-7.35	99.03	110.42
1	A	493	CYS	N-CA-C	-7.34	103.95	113.12
1	C	1041	GLU	CA-C-N	7.32	134.88	121.70
1	C	1041	GLU	C-N-CA	7.32	134.88	121.70
1	F	325	TYR	CA-C-N	7.31	127.02	119.64
1	F	325	TYR	C-N-CA	7.31	127.02	119.64
1	D	515	TRP	N-CA-C	-7.29	103.64	112.54
1	D	367	ILE	CA-C-N	-7.23	112.25	119.56
1	D	367	ILE	C-N-CA	-7.23	112.25	119.56
1	E	1041	GLU	CA-C-N	7.22	134.69	121.70
1	E	1041	GLU	C-N-CA	7.22	134.69	121.70
1	D	671	ILE	N-CA-C	7.21	117.78	108.12
1	B	522	LYS	N-CA-C	-7.19	103.38	111.07
1	C	241	THR	N-CA-C	7.14	119.14	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	679	GLY	N-CA-C	7.11	123.14	111.27
1	C	758	TYR	N-CA-C	-7.11	99.14	109.59
1	F	559	LEU	CA-C-N	7.09	127.08	119.78
1	F	559	LEU	C-N-CA	7.09	127.08	119.78
1	C	1044	HIS	CA-C-O	7.09	122.05	117.94
1	A	679	GLY	N-CA-C	7.05	120.85	110.63
1	F	38	ILE	N-CA-C	-6.95	106.72	113.53
1	C	835	LYS	N-CA-C	6.94	120.77	109.59
1	A	758	TYR	N-CA-C	-6.91	99.44	109.59
1	D	671	ILE	CB-CA-C	-6.89	103.84	111.35
1	C	1044	HIS	CB-CA-C	-6.88	107.17	117.07
1	D	1034	SER	CA-C-N	6.88	134.07	121.70
1	D	1034	SER	C-N-CA	6.88	134.07	121.70
1	E	449	LEU	N-CA-C	-6.87	103.87	111.36
1	C	967	ALA	N-CA-C	-6.86	103.49	110.97
1	C	8	ARG	N-CA-C	-6.86	97.09	108.75
1	A	666	PHE	N-CA-C	6.85	119.28	108.79
1	B	1022	VAL	CA-C-N	-6.82	112.78	119.87
1	B	1022	VAL	C-N-CA	-6.82	112.78	119.87
1	D	317	PHE	N-CA-C	6.80	118.37	109.93
1	F	562	SER	N-CA-C	6.80	120.41	109.79
1	F	964	THR	N-CA-C	-6.80	103.86	111.28
1	B	493	CYS	N-CA-C	-6.79	104.63	113.12
1	C	1041	GLU	N-CA-C	-6.73	96.46	110.80
1	A	426	PRO	O-C-N	6.72	124.31	121.15
1	F	189	ASN	CA-C-N	6.72	126.31	119.19
1	F	189	ASN	C-N-CA	6.72	126.31	119.19
1	A	564	LEU	N-CA-C	6.72	116.78	108.11
1	C	117	LEU	N-CA-C	6.71	120.37	112.72
1	D	896	SER	CA-C-N	6.66	124.44	120.24
1	D	896	SER	C-N-CA	6.66	124.44	120.24
1	E	435	MET	N-CA-C	-6.66	104.02	111.28
1	D	716	VAL	N-CA-C	6.59	116.72	107.37
1	F	524	THR	N-CA-C	-6.57	104.20	111.82
1	C	90	ILE	N-CA-C	6.57	117.36	108.17
1	E	964	THR	N-CA-C	-6.55	104.18	111.71
1	C	460	GLY	N-CA-C	6.54	123.49	111.12
1	A	367	ILE	CA-C-N	-6.54	111.66	119.84
1	A	367	ILE	C-N-CA	-6.54	111.66	119.84
1	C	521	GLU	N-CA-C	-6.54	104.23	111.36
1	D	493	CYS	N-CA-C	-6.54	103.99	112.68
1	C	1022	VAL	CA-C-N	-6.51	113.10	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1022	VAL	C-N-CA	-6.51	113.10	119.87
1	F	1024	VAL	N-CA-C	-6.49	105.42	111.45
1	E	438	ILE	N-CA-C	6.45	121.16	113.22
1	D	666	PHE	N-CA-C	6.44	118.56	108.96
1	A	905	VAL	CB-CA-C	-6.43	107.59	113.70
1	D	447	MET	N-CA-C	6.40	121.17	113.23
1	C	524	THR	N-CA-C	-6.35	104.45	111.82
1	A	782	LEU	CA-C-N	6.33	127.76	119.84
1	A	782	LEU	C-N-CA	6.33	127.76	119.84
1	B	777	ALA	N-CA-C	6.31	117.82	111.07
1	F	531	VAL	N-CA-C	-6.30	104.19	110.62
1	F	482	VAL	CB-CA-C	-6.30	103.63	112.14
1	B	897	ILE	CB-CA-C	-6.27	107.71	114.35
1	D	214	VAL	N-CA-C	6.26	117.72	108.45
1	A	118	LEU	CA-C-N	6.26	126.61	119.92
1	A	118	LEU	C-N-CA	6.26	126.61	119.92
1	E	676	THR	N-CA-C	-6.25	100.58	109.96
1	F	100	ALA	N-CA-C	6.25	117.76	111.07
1	F	8	ARG	CA-C-N	6.25	126.16	119.28
1	F	8	ARG	C-N-CA	6.25	126.16	119.28
1	D	232	ALA	N-CA-C	6.25	117.72	108.60
1	A	180	SER	N-CA-C	6.24	118.79	108.99
1	C	426	PRO	O-C-N	6.23	124.08	121.15
1	D	8	ARG	CA-C-N	6.22	125.79	119.19
1	D	8	ARG	C-N-CA	6.22	125.79	119.19
1	B	100	ALA	N-CA-C	-6.22	104.41	111.07
1	F	7	ASP	CA-C-N	6.18	129.30	122.74
1	F	7	ASP	C-N-CA	6.18	129.30	122.74
1	D	563	PHE	N-CA-C	-6.15	105.68	113.43
1	B	39	ALA	CA-C-N	6.15	126.71	120.38
1	B	39	ALA	C-N-CA	6.15	126.71	120.38
1	B	403	GLY	N-CA-C	6.13	120.62	112.77
1	C	357	LEU	N-CA-C	-6.13	105.86	113.15
1	F	946	VAL	N-CA-C	6.10	116.27	110.42
1	C	5	PHE	N-CA-C	-6.09	104.55	112.23
1	A	83	ASP	N-CA-C	6.08	119.53	110.52
1	F	515	TRP	N-CA-C	-6.08	104.71	111.71
1	C	559	LEU	CA-C-N	6.08	126.04	119.78
1	C	559	LEU	C-N-CA	6.08	126.04	119.78
1	E	522	LYS	N-CA-C	-6.06	104.00	111.33
1	F	1003	VAL	CA-C-N	6.02	126.78	120.03
1	F	1003	VAL	C-N-CA	6.02	126.78	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	629	VAL	N-CA-C	6.02	116.52	107.80
1	D	49	TYR	CA-C-N	5.99	126.34	119.93
1	D	49	TYR	C-N-CA	5.99	126.34	119.93
1	D	288	GLY	N-CA-C	5.98	119.48	110.75
1	F	85	THR	N-CA-C	-5.97	104.65	112.41
1	C	623	ASN	N-CA-C	5.94	117.76	111.28
1	F	317	PHE	CA-C-N	5.92	127.23	119.84
1	F	317	PHE	C-N-CA	5.92	127.23	119.84
1	C	561	SER	N-CA-C	5.91	118.94	107.71
1	A	325	TYR	CA-C-N	5.91	127.22	119.84
1	A	325	TYR	C-N-CA	5.91	127.22	119.84
1	B	674	LEU	N-CA-C	5.90	118.18	109.69
1	D	272	GLY	N-CA-C	5.90	118.82	112.33
1	E	1034	SER	CB-CA-C	-5.88	108.79	115.79
1	A	680	PHE	N-CA-C	5.88	117.15	108.86
1	B	371	ALA	N-CA-C	5.88	117.48	111.14
1	F	691	GLY	N-CA-C	5.86	127.07	113.18
1	A	412	VAL	N-CA-C	5.86	115.98	110.30
1	E	356	TYR	N-CA-C	-5.81	105.08	111.82
1	F	922	THR	N-CA-C	5.80	118.22	109.23
1	B	1039	ASP	CA-C-N	5.79	132.13	121.70
1	B	1039	ASP	C-N-CA	5.79	132.13	121.70
1	F	904	VAL	N-CA-C	5.79	119.19	111.44
1	B	563	PHE	N-CA-C	-5.78	105.49	113.18
1	E	29	LYS	N-CA-C	5.78	116.69	108.54
1	F	333	VAL	N-CA-C	5.78	115.96	110.53
1	E	782	LEU	CA-C-N	5.77	127.06	119.84
1	E	782	LEU	C-N-CA	5.77	127.06	119.84
1	F	299	ALA	N-CA-C	5.77	117.25	110.97
1	E	233	SER	N-CA-C	5.76	118.04	108.20
1	D	440	GLY	N-CA-C	-5.75	105.81	112.83
1	C	897	ILE	N-CA-CB	5.75	114.93	110.45
1	F	44	THR	N-CA-C	5.75	118.27	108.90
1	D	1020	PHE	N-CA-C	-5.73	106.92	114.31
1	E	341	VAL	N-CA-C	-5.73	104.78	110.62
1	C	444	GLY	N-CA-C	5.72	119.56	112.64
1	B	489	THR	CA-C-N	-5.71	113.00	119.28
1	B	489	THR	C-N-CA	-5.71	113.00	119.28
1	C	278	ILE	N-CA-C	5.70	116.33	108.12
1	E	85	THR	N-CA-C	-5.69	105.01	112.41
1	E	39	ALA	CA-C-N	-5.68	114.53	120.38
1	E	39	ALA	C-N-CA	-5.68	114.53	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1037	ASN	CA-C-N	5.66	131.89	121.70
1	B	1037	ASN	C-N-CA	5.66	131.89	121.70
1	C	1043	SER	N-CA-C	5.66	116.04	108.23
1	D	314	GLU	N-CA-C	5.65	121.37	113.57
1	C	180	SER	N-CA-C	5.65	117.86	108.99
1	F	640	GLU	N-CA-C	-5.64	105.12	112.23
1	B	3	ASN	N-CA-C	-5.63	105.23	111.71
1	D	241	THR	N-CA-C	5.63	117.50	111.36
1	B	879	ILE	N-CA-C	-5.62	105.03	110.42
1	A	365	THR	N-CA-C	-5.61	105.70	112.54
1	E	511	GLY	N-CA-C	5.60	126.45	113.18
1	F	834	GLY	N-CA-C	-5.59	99.92	113.18
1	D	240	LEU	N-CA-C	5.57	117.78	109.25
1	E	1024	VAL	N-CA-C	-5.56	105.43	110.82
1	B	573	MET	N-CA-C	5.53	117.59	109.24
1	B	367	ILE	CB-CA-C	-5.52	106.76	114.00
1	C	240	LEU	N-CA-C	5.51	117.72	108.96
1	E	576	VAL	N-CA-C	5.50	115.81	108.11
1	B	724	THR	CA-C-N	-5.49	114.06	119.99
1	B	724	THR	C-N-CA	-5.49	114.06	119.99
1	E	434	SER	N-CA-C	5.47	117.05	111.14
1	E	851	LEU	CA-C-N	5.46	126.67	119.84
1	E	851	LEU	C-N-CA	5.46	126.67	119.84
1	B	314	GLU	CA-C-N	-5.46	114.39	120.45
1	B	314	GLU	C-N-CA	-5.46	114.39	120.45
1	A	80	SER	N-CA-C	5.45	117.98	108.76
1	D	4	PHE	CB-CA-C	-5.45	102.09	110.81
1	E	34	GLN	N-CA-C	-5.45	105.26	111.14
1	A	341	VAL	N-CA-C	5.44	115.65	110.53
1	C	381	ALA	N-CA-C	-5.44	105.43	111.36
1	D	511	GLY	N-CA-C	5.43	126.06	113.18
1	C	109	ASN	N-CA-C	5.43	118.11	111.82
1	F	319	SER	N-CA-C	5.42	117.56	109.59
1	F	4	PHE	N-CA-C	-5.42	105.47	111.71
1	C	108	GLN	N-CA-C	-5.42	105.48	111.71
1	B	929	VAL	N-CA-C	-5.42	104.44	110.62
1	E	839	GLU	N-CA-C	-5.41	105.28	111.07
1	A	320	GLY	N-CA-C	5.39	123.43	114.48
1	C	666	PHE	N-CA-C	5.39	117.27	109.07
1	F	952	LEU	N-CA-C	-5.38	105.33	111.14
1	B	293	LEU	N-CA-C	-5.37	102.44	110.23
1	B	644	VAL	N-CA-C	5.37	120.51	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	VAL	N-CA-C	5.36	115.80	107.28
1	A	671	ILE	CB-CA-C	-5.35	105.52	111.35
1	C	498	LYS	CA-C-N	-5.35	114.41	119.76
1	C	498	LYS	C-N-CA	-5.35	114.41	119.76
1	D	40	PRO	CA-C-N	-5.34	114.22	119.99
1	D	40	PRO	C-N-CA	-5.34	114.22	119.99
1	D	325	TYR	CA-C-N	5.34	125.03	119.64
1	D	325	TYR	C-N-CA	5.34	125.03	119.64
1	D	805	SER	N-CA-C	5.34	117.37	108.02
1	D	561	SER	N-CA-C	5.34	117.85	107.71
1	E	129	VAL	N-CA-C	5.34	115.54	107.80
1	F	277	ILE	N-CA-C	5.33	115.58	108.11
1	F	921	LEU	N-CA-C	5.33	118.63	110.36
1	B	498	LYS	N-CA-C	5.33	116.60	109.83
1	F	73	ASP	N-CA-C	5.33	118.17	110.28
1	F	390	ILE	CB-CA-C	-5.32	106.16	111.80
1	A	487	ILE	CB-CA-C	-5.32	107.19	111.71
1	C	978	THR	CB-CA-C	-5.31	102.79	110.96
1	C	360	GLN	N-CA-C	5.30	122.09	110.80
1	D	489	THR	CA-C-N	-5.29	113.58	119.19
1	D	489	THR	C-N-CA	-5.29	113.58	119.19
1	D	348	ILE	N-CA-C	5.29	115.73	110.23
1	E	115	MET	N-CA-C	5.28	120.79	113.45
1	E	452	VAL	N-CA-C	-5.28	107.27	111.81
1	C	945	ILE	N-CA-C	5.28	115.49	110.42
1	F	484	VAL	N-CA-C	5.27	116.04	110.72
1	C	1020	PHE	N-CA-C	-5.27	107.52	114.31
1	E	559	LEU	CA-C-N	5.27	125.55	119.92
1	E	559	LEU	C-N-CA	5.27	125.55	119.92
1	F	370	ILE	N-CA-C	-5.25	105.20	112.50
1	D	144	ASN	N-CA-C	5.24	117.62	108.76
1	F	115	MET	CA-C-N	-5.24	114.27	119.56
1	F	115	MET	C-N-CA	-5.24	114.27	119.56
1	A	223	PRO	CA-C-N	5.23	126.37	119.84
1	A	223	PRO	C-N-CA	5.23	126.37	119.84
1	F	49	TYR	CA-CB-CG	5.23	123.31	113.90
1	D	365	THR	N-CA-C	-5.22	105.76	111.82
1	F	468	ARG	N-CA-C	5.21	116.96	111.28
1	D	820	ASN	N-CA-C	5.21	118.77	111.74
1	A	292	LYS	CA-C-N	5.21	128.24	120.95
1	A	292	LYS	C-N-CA	5.21	128.24	120.95
1	A	919	ARG	N-CA-C	-5.21	102.07	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	497	LEU	N-CA-C	5.20	117.76	109.96
1	E	578	LEU	CA-C-N	-5.19	114.30	120.11
1	E	578	LEU	C-N-CA	-5.19	114.30	120.11
1	B	411	VAL	CA-C-N	5.18	127.04	120.72
1	B	411	VAL	C-N-CA	5.18	127.04	120.72
1	F	382	VAL	CB-CA-C	-5.17	105.16	112.14
1	B	519	MET	CB-CG-SD	5.17	128.20	112.70
1	B	761	ASP	N-CA-C	5.17	117.82	109.40
1	A	189	ASN	CA-C-N	5.16	124.47	118.85
1	A	189	ASN	C-N-CA	5.16	124.47	118.85
1	D	234	ILE	N-CA-C	5.16	115.65	108.84
1	B	893	GLU	N-CA-C	-5.15	99.82	110.80
1	D	162	MET	N-CA-C	5.15	119.01	111.34
1	E	486	LEU	N-CA-C	5.14	119.70	113.38
1	B	269	GLU	N-CA-C	5.14	116.88	108.76
1	B	260	VAL	N-CA-C	5.13	114.14	106.85
1	A	315	PRO	N-CA-C	5.13	120.76	114.35
1	E	303	ALA	N-CA-C	5.13	116.68	111.14
1	F	330	THR	CA-C-N	-5.13	113.64	119.28
1	F	330	THR	C-N-CA	-5.13	113.64	119.28
1	D	836	SER	N-CA-C	5.13	117.53	110.35
1	E	489	THR	CA-C-N	-5.13	113.64	119.28
1	E	489	THR	C-N-CA	-5.13	113.64	119.28
1	C	767	ARG	N-CA-C	5.12	116.76	108.41
1	D	992	SER	N-CA-C	5.12	121.70	110.80
1	F	998	GLY	N-CA-C	-5.12	106.56	112.50
1	F	172	VAL	N-CA-C	5.11	115.32	108.17
1	E	361	ASN	N-CA-C	5.10	117.03	107.99
1	D	495	THR	N-CA-C	5.10	120.89	114.31
1	D	644	VAL	N-CA-C	5.10	119.94	109.34
1	E	83	ASP	N-CA-C	5.09	118.06	110.52
1	B	531	VAL	N-CA-C	5.09	115.81	110.62
1	A	668	LEU	N-CA-C	-5.08	102.77	110.39
1	C	172	VAL	N-CA-C	5.08	115.62	108.36
1	A	327	TYR	N-CA-C	5.07	116.29	107.93
1	D	148	THR	N-CA-C	5.07	116.49	111.07
1	C	493	CYS	N-CA-C	-5.06	106.79	113.12
1	F	813	SER	N-CA-C	-5.06	103.39	109.72
1	B	39	ALA	N-CA-C	5.06	116.04	109.72
1	B	895	TRP	N-CA-C	-5.06	107.16	113.38
1	F	243	THR	N-CA-C	-5.06	105.95	111.82
1	C	1004	GLY	N-CA-C	5.04	118.74	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	658	ILE	CB-CA-C	-5.04	105.75	112.46
1	E	512	PHE	N-CA-C	5.04	118.89	112.34
1	B	240	LEU	N-CA-C	5.03	116.96	108.96
1	C	437	GLN	N-CA-C	5.03	116.57	111.14
1	F	420	MET	N-CA-C	5.03	116.84	111.36
1	B	973	ARG	N-CA-C	5.02	119.78	113.25
1	D	971	ARG	CB-CA-C	5.02	119.11	111.02
1	B	189	ASN	CA-C-N	5.01	124.32	118.85
1	B	189	ASN	C-N-CA	5.01	124.32	118.85
1	F	856	GLY	N-CA-C	5.01	118.54	111.42
1	F	89	GLN	CA-C-N	-5.01	116.97	123.19
1	F	89	GLN	C-N-CA	-5.01	116.97	123.19
1	A	329	THR	CA-C-N	5.01	125.39	119.83
1	A	329	THR	C-N-CA	5.01	125.39	119.83
1	C	189	ASN	CA-C-N	5.01	124.50	119.19
1	C	189	ASN	C-N-CA	5.01	124.50	119.19

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	6	ILE	Peptide
1	D	1034	SER	Peptide
1	D	992	SER	Peptide
1	F	1036	LYS	Peptide
1	F	1039	ASP	Peptide

3.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7907	0	8050	412	0
1	B	7939	0	8077	392	0
1	C	7924	0	8064	416	0
1	D	7907	0	8050	387	0
1	E	7907	0	8050	436	1
1	F	7939	0	8077	417	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	35	0	46	4	0
2	B	35	0	46	4	0
2	C	35	0	46	4	0
2	D	35	0	46	1	0
2	E	35	0	46	4	0
2	F	35	0	46	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	47736	0	48644	2373	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (2373) 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:D:446:ALA:HB2	1:D:482:VAL:HG21	1.39	0.99
1:A:957:GLY:HA2	1:A:1042:HIS:HB2	1.41	0.99
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.46	0.98
1:D:536:ARG:NH2	2:D:1101:LMT:O3B	1.97	0.97
1:F:578:LEU:HG	1:F:587:THR:HG22	1.46	0.95
1:F:135:SER:HB3	1:F:673:GLU:HB3	1.49	0.94
1:E:196:PHE:O	1:E:252:LYS:NZ	2.04	0.91
1:D:457:ALA:O	1:D:468:ARG:NE	2.03	0.90
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.54	0.90
1:F:35:TYR:HB3	1:F:38:ILE:HD12	1.54	0.89
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.54	0.89
1:E:159:ALA:O	1:E:767:ARG:NH2	2.07	0.88
1:E:354:VAL:HG11	1:E:980:LEU:HB3	1.55	0.88
1:C:1041:GLU:HB3	1:C:1042:HIS:HB2	1.53	0.88
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.54	0.88
1:F:1041:GLU:HB3	1:F:1042:HIS:HB3	1.56	0.88
1:F:452:VAL:HG12	1:F:880:SER:HB3	1.56	0.88
1:D:578:LEU:HD21	1:D:590:VAL:HG21	1.56	0.87
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.56	0.87
1:D:41:PRO:HG2	1:D:94:PHE:HB2	1.57	0.87
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.09	0.86
1:B:919:ARG:NH2	1:B:990:VAL:O	2.09	0.86
1:B:399:VAL:O	1:B:402:ILE:HG13	1.76	0.86
1:F:616:GLY:HA2	1:F:626:ILE:HD13	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:HD22	1:A:984:LEU:HB3	1.58	0.85
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.58	0.85
1:A:475:VAL:HA	1:A:478:MET:HE2	1.59	0.85
1:C:38:ILE:HG23	1:C:462:SER:HB2	1.57	0.85
1:A:400:LEU:HD23	1:A:929:VAL:HG12	1.59	0.84
1:E:56:THR:O	1:E:60:THR:OG1	1.95	0.84
1:A:619:GLY:HA3	1:A:815:ARG:HH22	1.40	0.84
1:F:559:LEU:HD22	1:F:560:PRO:HD2	1.60	0.84
1:C:112:GLN:HA	1:C:115:MET:HB2	1.60	0.83
1:B:992:SER:O	1:B:997:SER:OG	1.96	0.83
1:B:559:LEU:HD22	1:B:560:PRO:HD2	1.59	0.83
1:C:940:LYS:HZ1	1:C:978:THR:HG21	1.44	0.83
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.14	0.82
1:F:340:VAL:HG11	1:F:395:MET:HB3	1.59	0.82
1:D:416:VAL:HG12	1:D:420:MET:HE2	1.62	0.82
1:E:58:GLN:OE1	1:E:818:ARG:NH1	2.12	0.82
1:B:156:ASP:OD1	1:B:765:ARG:NH2	2.11	0.82
1:A:38:ILE:HG12	1:A:462:SER:HB2	1.62	0.81
1:E:692:HIS:NE2	1:E:813:SER:OG	2.13	0.81
1:D:170:SER:HB2	1:E:75:LEU:H	1.42	0.81
1:D:219:LEU:HD23	1:E:754:TRP:HZ3	1.45	0.81
1:E:702:LEU:HD11	1:E:847:LEU:HB3	1.60	0.81
1:E:508:GLY:HA3	1:E:518:ARG:HE	1.46	0.81
1:B:156:ASP:OD2	1:B:769:LYS:NZ	2.13	0.80
1:A:196:PHE:O	1:A:252:LYS:NZ	2.14	0.80
1:A:986:VAL:HG21	1:A:1007:VAL:HG11	1.63	0.80
1:C:536:ARG:NH2	2:C:1101:LMT:O3B	2.13	0.80
1:B:186:ILE:HG12	1:B:268:ILE:HG12	1.63	0.80
1:D:149:MET:HE3	1:D:153:ASP:HB3	1.64	0.80
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.62	0.80
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.62	0.80
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.64	0.80
1:C:3:ASN:OD1	1:C:3:ASN:N	2.13	0.80
1:E:156:ASP:OD1	1:E:769:LYS:NZ	2.15	0.80
1:E:261:LEU:HD12	1:E:263:ARG:HH12	1.46	0.79
1:E:236:ALA:O	1:F:728:LYS:NZ	2.15	0.79
1:A:146:ASP:OD2	1:A:146:ASP:N	2.16	0.79
1:A:248:LYS:HA	1:A:261:LEU:HD13	1.64	0.79
1:B:508:GLY:HA2	1:B:518:ARG:HH21	1.47	0.79
1:F:510:LYS:HA	1:F:518:ARG:HH12	1.45	0.79
1:A:564:LEU:HD13	1:A:671:ILE:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.63	0.79
1:A:56:THR:O	1:A:60:THR:OG1	1.98	0.79
1:B:1013:THR:O	1:B:1017:LEU:HB2	1.83	0.79
1:F:986:VAL:HG21	1:F:1007:VAL:HG11	1.63	0.78
1:C:452:VAL:HG12	1:C:880:SER:HB3	1.65	0.78
1:E:42:ALA:HB2	1:E:93:THR:HG23	1.64	0.78
1:F:509:LYS:O	1:F:518:ARG:NH1	2.16	0.78
1:E:555:LEU:HD22	1:E:913:LEU:HB3	1.64	0.78
1:C:435:MET:HE3	1:C:490:PRO:HB3	1.66	0.78
1:C:881:LEU:HD22	1:C:902:MET:HE1	1.65	0.78
1:F:944:LEU:HB3	1:F:971:ARG:HE	1.49	0.78
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.66	0.78
1:C:356:TYR:HA	1:C:365:THR:HG21	1.65	0.78
1:A:818:ARG:HH12	1:A:823:PRO:HG3	1.46	0.78
1:B:350:LEU:HD22	1:B:984:LEU:HB3	1.64	0.78
1:C:940:LYS:NZ	1:C:978:THR:HG21	1.98	0.78
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.66	0.77
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.66	0.77
1:E:559:LEU:HD22	1:E:560:PRO:HD2	1.65	0.77
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.64	0.77
1:D:58:GLN:O	1:D:63:GLN:HG3	1.85	0.77
1:E:326:PRO:O	1:E:630:SER:OG	2.01	0.77
1:F:536:ARG:NH1	2:F:1101:LMT:O4'	2.16	0.77
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.66	0.77
1:B:602:GLU:OE2	1:B:650:ARG:NH1	2.17	0.77
1:B:957:GLY:O	1:B:1041:GLU:HA	1.83	0.77
1:A:149:MET:HE3	1:A:153:ASP:HB3	1.67	0.77
1:B:6:ILE:O	1:B:428:LYS:NZ	2.17	0.77
1:D:426:PRO:HD2	1:D:429:GLU:HG3	1.67	0.77
1:A:108:GLN:NE2	1:B:109:ASN:O	2.17	0.77
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.67	0.77
1:D:183:ALA:HB2	1:D:273:GLU:HG3	1.66	0.77
1:B:196:PHE:O	1:B:252:LYS:NZ	2.17	0.77
1:F:298:ASN:ND2	1:F:301:ASP:OD2	2.17	0.77
1:B:362:PHE:O	1:B:365:THR:HG22	1.84	0.77
1:C:602:GLU:OE2	1:C:650:ARG:NH1	2.18	0.77
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.51	0.76
1:B:9:PRO:HB3	1:B:495:THR:HG21	1.68	0.76
1:D:448:VAL:HG22	1:D:887:CYS:HB3	1.67	0.76
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.68	0.76
1:E:841:MET:HE1	1:E:867:ARG:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.66	0.75
1:A:634:TRP:CD1	1:A:634:TRP:H	2.01	0.75
1:D:507:GLU:O	1:D:509:LYS:N	2.19	0.75
1:E:634:TRP:H	1:E:634:TRP:CD1	2.01	0.75
1:D:61:VAL:HG21	1:D:122:VAL:HG21	1.68	0.75
1:E:907:LEU:HG	1:E:1017:LEU:HB3	1.68	0.75
1:F:705:GLU:HA	1:F:708:LYS:HE3	1.68	0.75
1:C:527:TYR:OH	1:C:1019:ILE:O	2.03	0.75
1:A:236:ALA:O	1:B:728:LYS:NZ	2.18	0.74
1:A:405:LEU:HD22	1:A:481:SER:HB2	1.69	0.74
1:C:671:ILE:HD13	1:C:674:LEU:HD12	1.68	0.74
1:F:525:HIS:HA	1:F:528:THR:HG22	1.69	0.74
1:D:375:VAL:HB	1:D:405:LEU:HD13	1.67	0.74
1:E:1026:PHE:O	1:E:1030:ARG:HB2	1.88	0.74
1:F:23:GLY:HA2	1:F:381:ALA:HB2	1.69	0.74
1:B:108:GLN:HE22	1:C:112:GLN:HB3	1.53	0.74
1:C:591:LEU:HD13	1:C:611:ALA:HB1	1.69	0.74
1:F:588:GLN:O	1:F:592:ASN:ND2	2.18	0.74
1:D:72:ILE:HD13	1:D:107:VAL:HG22	1.68	0.74
1:F:944:LEU:HB3	1:F:971:ARG:NE	2.03	0.74
1:A:1039:ASP:OD1	1:A:1039:ASP:N	2.20	0.74
1:B:163:LYS:HA	1:B:289:LEU:HD11	1.70	0.74
1:E:637:ARG:HB3	1:E:642:ASN:HB3	1.68	0.74
1:A:712:MET:HB3	1:A:713:LEU:HD22	1.69	0.73
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.69	0.73
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.51	0.73
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.70	0.73
1:D:248:LYS:HA	1:D:261:LEU:HD13	1.70	0.73
1:E:146:ASP:OD2	1:E:146:ASP:N	2.19	0.73
1:A:362:PHE:O	1:A:365:THR:HG22	1.88	0.73
1:E:61:VAL:HA	1:E:118:LEU:HD22	1.70	0.73
1:F:344:LEU:HD22	1:F:402:ILE:HD11	1.69	0.73
1:E:602:GLU:OE2	1:E:650:ARG:NH1	2.21	0.73
1:B:139:VAL:O	1:B:326:PRO:HD2	1.87	0.73
1:B:345:VAL:O	1:B:348:ILE:HG22	1.89	0.73
1:B:699:ARG:HH11	1:B:825:MET:HE1	1.54	0.73
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.69	0.73
1:B:634:TRP:H	1:B:634:TRP:CD1	2.02	0.73
1:D:144:ASN:HA	1:D:320:GLY:O	1.89	0.73
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.71	0.73
1:E:986:VAL:HG21	1:E:1007:VAL:HG11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ALA:O	1:C:728:LYS:NZ	2.19	0.72
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.71	0.72
1:E:157:TYR:OH	1:E:316:PHE:O	2.05	0.72
1:F:733:GLN:HE22	1:F:743:ILE:HG21	1.55	0.72
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.70	0.72
1:F:380:PHE:HD2	1:F:383:LEU:HD12	1.54	0.72
1:A:26:ALA:O	1:A:30:LEU:HB2	1.90	0.72
1:B:58:GLN:O	1:B:63:GLN:HG3	1.88	0.72
1:E:162:MET:O	1:E:164:ASP:N	2.17	0.72
1:D:151:GLN:CD	1:D:151:GLN:H	1.97	0.72
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.72	0.72
1:B:508:GLY:O	1:B:510:LYS:N	2.22	0.72
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.71	0.72
1:D:455:PRO:HG2	1:D:880:SER:HB2	1.70	0.72
1:E:520:PHE:O	1:E:523:SER:OG	2.05	0.72
1:E:578:LEU:HD21	1:E:590:VAL:HG21	1.71	0.72
1:E:189:ASN:HB3	1:E:192:GLU:HB2	1.72	0.72
1:C:240:LEU:HB2	1:C:246:PHE:HE1	1.54	0.72
1:F:971:ARG:HH21	1:F:975:ILE:HD11	1.55	0.72
1:F:972:LEU:HA	1:F:975:ILE:HD12	1.71	0.71
1:A:417:GLU:O	1:A:420:MET:N	2.24	0.71
1:B:26:ALA:O	1:B:30:LEU:HB2	1.89	0.71
1:B:871:ASN:OD1	1:B:871:ASN:N	2.23	0.71
1:C:278:ILE:HG13	1:C:613:ASN:HB3	1.72	0.71
1:D:375:VAL:HG22	1:D:484:VAL:HG21	1.72	0.71
1:D:435:MET:HE3	1:D:439:GLN:HG3	1.71	0.71
1:E:353:LEU:O	1:E:355:MET:N	2.21	0.71
1:B:428:LYS:HD3	1:B:494:ALA:HB1	1.70	0.71
1:B:907:LEU:HG	1:B:1017:LEU:HD23	1.72	0.71
1:A:25:LEU:HA	1:A:28:LEU:HD12	1.72	0.71
1:D:971:ARG:H	1:D:971:ARG:NH1	1.88	0.71
1:F:1041:GLU:CB	1:F:1042:HIS:HB3	2.21	0.71
1:D:555:LEU:HD22	1:D:913:LEU:HB3	1.73	0.71
1:E:185:ARG:HH12	1:E:774:MET:HE3	1.55	0.71
1:F:634:TRP:CD1	1:F:634:TRP:H	2.07	0.71
1:E:658:ILE:O	1:E:659:LYS:NZ	2.22	0.71
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.55	0.70
1:A:555:LEU:HD22	1:A:913:LEU:HB3	1.74	0.70
1:E:508:GLY:HA3	1:E:518:ARG:NE	2.06	0.70
1:B:1037:ASN:H	1:B:1038:GLU:HB3	1.55	0.70
1:B:527:TYR:O	1:B:531:VAL:HG23	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LEU:HD13	1:C:200:PRO:HD3	1.73	0.70
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.27	0.70
1:E:291:ILE:HD13	1:E:306:ILE:HD13	1.73	0.70
1:C:578:LEU:HD13	1:C:579:PRO:HD2	1.73	0.70
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.73	0.70
1:C:682:PHE:CE1	1:C:857:TYR:HB2	2.26	0.70
1:D:18:ILE:HG13	1:E:886:LEU:HD23	1.74	0.70
1:A:186:ILE:HG12	1:A:268:ILE:HG12	1.74	0.70
1:B:60:THR:HG22	1:B:119:PRO:HD3	1.74	0.70
1:C:1033:PHE:H	1:C:1034:SER:CB	2.03	0.70
1:E:45:ILE:HG23	1:E:129:VAL:HG22	1.73	0.70
1:F:211:ASN:O	1:F:760:ASN:ND2	2.24	0.70
1:F:278:ILE:HG13	1:F:613:ASN:HB3	1.73	0.70
1:F:317:PHE:HE2	1:F:323:ILE:HD11	1.57	0.70
1:F:668:LEU:HD23	1:F:668:LEU:H	1.56	0.70
1:B:383:LEU:HD13	1:B:388:PHE:HD1	1.57	0.69
1:B:845:GLU:OE2	1:B:867:ARG:NH1	2.24	0.69
1:D:318:PRO:HD2	1:D:321:LEU:HD12	1.71	0.69
1:E:422:GLU:O	1:E:502:LYS:NZ	2.25	0.69
1:E:463:THR:O	1:E:467:TYR:HD1	1.75	0.69
1:F:284:GLN:HG3	1:F:285:PRO:HD2	1.74	0.69
1:F:971:ARG:NH2	1:F:975:ILE:HD11	2.07	0.69
1:A:519:MET:O	1:A:523:SER:OG	2.09	0.69
1:C:340:VAL:HG12	1:C:395:MET:HE3	1.75	0.69
1:E:203:VAL:O	1:E:207:ILE:HG13	1.92	0.69
1:E:983:ILE:HG23	1:E:1008:MET:HE2	1.74	0.69
1:A:35:TYR:CE2	1:A:564:LEU:HD21	2.27	0.69
1:D:243:THR:HG23	1:D:268:ILE:HG22	1.73	0.69
1:E:211:ASN:OD1	1:E:760:ASN:ND2	2.26	0.69
1:E:441:ALA:HA	1:E:891:LEU:HD21	1.74	0.69
1:A:527:TYR:OH	1:A:1019:ILE:O	2.09	0.69
1:E:971:ARG:O	1:E:975:ILE:HG12	1.91	0.69
1:A:129:VAL:O	1:B:110:LYS:NZ	2.22	0.69
1:A:721:LEU:HB3	1:A:814:PRO:HG2	1.75	0.69
1:F:383:LEU:HD23	1:F:472:ILE:HD13	1.75	0.69
1:F:731:ILE:HD13	1:F:746:ILE:HD11	1.74	0.69
1:E:534:ILE:HG22	2:E:1101:LMT:HI'	1.74	0.68
1:F:971:ARG:HB3	1:F:971:ARG:NH1	2.08	0.68
1:C:556:PHE:HD1	1:C:913:LEU:HD21	1.59	0.68
1:E:169:THR:HG21	1:E:306:ILE:HG13	1.73	0.68
1:F:420:MET:HB3	1:F:500:ILE:HB	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:604:ASN:OD1	1:F:604:ASN:N	2.26	0.68
1:D:298:ASN:HB3	1:D:301:ASP:HB2	1.74	0.68
1:D:564:LEU:HD13	1:D:671:ILE:HD13	1.76	0.68
1:D:189:ASN:HB3	1:D:192:GLU:HB2	1.75	0.68
1:D:225:VAL:HG22	1:E:781:MET:HE2	1.75	0.68
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.75	0.68
1:C:201:VAL:HA	1:C:204:ILE:HD12	1.74	0.68
1:E:157:TYR:CZ	1:E:318:PRO:HD3	2.29	0.67
1:A:411:VAL:HG22	1:A:971:ARG:HH22	1.60	0.67
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.76	0.67
1:E:613:ASN:HD22	1:E:614:GLY:N	1.92	0.67
1:A:1034:SER:OG	1:A:1035:ARG:O	2.12	0.67
1:B:225:VAL:HG12	1:C:777:ALA:HB1	1.75	0.67
1:F:186:ILE:HG12	1:F:268:ILE:HG12	1.76	0.67
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.75	0.67
1:C:298:ASN:ND2	1:C:301:ASP:OD2	2.23	0.67
1:D:967:ALA:O	1:D:971:ARG:NH1	2.27	0.67
1:A:696:THR:HG23	1:A:699:ARG:HH12	1.57	0.67
1:C:249:ILE:HB	1:C:262:LEU:HB2	1.77	0.67
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.76	0.67
1:C:944:LEU:HB3	1:C:971:ARG:HD2	1.77	0.67
1:A:203:VAL:O	1:A:207:ILE:HG13	1.95	0.67
1:D:979:SER:OG	1:D:1015:THR:HG21	1.94	0.67
1:A:646:ALA:HA	1:A:649:MET:HE3	1.77	0.67
1:A:909:VAL:HA	1:A:931:LEU:HD21	1.77	0.67
1:B:986:VAL:HG21	1:B:1007:VAL:HG11	1.75	0.67
1:D:191:ASN:O	1:D:194:ASN:N	2.27	0.67
1:D:393:LEU:HD11	1:D:466:ILE:HD13	1.75	0.67
1:E:445:ILE:HG12	1:E:940:LYS:HE3	1.76	0.67
1:E:756:GLY:HA3	1:E:774:MET:HE2	1.76	0.67
1:F:146:ASP:O	1:F:148:THR:N	2.27	0.67
1:A:564:LEU:HD23	1:A:565:PRO:HD2	1.75	0.67
1:A:953:MET:HE2	1:A:963:ALA:HB3	1.77	0.67
1:C:987:MET:O	1:C:990:VAL:N	2.26	0.67
1:E:166:ILE:HD11	1:E:310:LEU:HD13	1.76	0.67
1:E:451:ALA:HB1	1:E:883:VAL:HG13	1.75	0.67
1:E:546:LEU:O	1:E:550:VAL:HG23	1.94	0.67
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.77	0.67
1:C:587:THR:HG21	1:C:622:GLN:O	1.93	0.67
1:D:344:LEU:HD13	1:D:376:LEU:HD13	1.77	0.66
1:D:982:PHE:O	1:D:985:GLY:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:VAL:HG12	1:B:420:MET:HE2	1.77	0.66
1:F:34:GLN:HG2	1:F:333:VAL:HG22	1.76	0.66
1:B:469:GLN:O	1:B:473:THR:OG1	2.14	0.66
1:F:139:VAL:HG22	1:F:290:GLY:HA2	1.78	0.66
1:B:108:GLN:OE1	1:C:112:GLN:HG3	1.96	0.66
1:B:249:ILE:HD11	1:B:262:LEU:HD22	1.78	0.66
1:B:396:PHE:O	1:B:400:LEU:HB2	1.95	0.66
1:D:190:PRO:HB3	1:D:789:TRP:CE2	2.30	0.66
1:C:531:VAL:O	1:C:534:ILE:HG13	1.95	0.66
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.78	0.66
1:E:525:HIS:HA	1:E:528:THR:HG22	1.77	0.66
1:A:1030:ARG:HH12	1:A:1033:PHE:HB3	1.61	0.66
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.76	0.66
1:E:653:ARG:O	1:E:656:SER:OG	2.14	0.66
1:A:251:LEU:HD11	1:A:262:LEU:HA	1.78	0.65
1:B:176:GLN:O	1:B:289:LEU:HD23	1.95	0.65
1:D:82:SER:HB2	1:D:816:LEU:HB2	1.77	0.65
1:F:329:THR:O	1:F:333:VAL:HG23	1.96	0.65
1:F:401:ALA:HB2	1:F:474:ILE:HG12	1.78	0.65
1:F:38:ILE:HG23	1:F:462:SER:HB2	1.78	0.65
1:C:11:PHE:O	1:C:11:PHE:HD2	1.78	0.65
1:F:400:LEU:HB3	1:F:474:ILE:HD11	1.79	0.65
1:F:1040:ILE:HA	1:F:1041:GLU:HB2	1.77	0.65
1:E:376:LEU:HD22	1:E:398:MET:HE3	1.77	0.65
1:F:948:PHE:HD2	1:F:970:MET:HE3	1.60	0.65
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.78	0.65
1:B:558:ARG:HA	1:B:558:ARG:HE	1.62	0.65
1:F:24:GLY:O	1:F:27:ILE:HG12	1.96	0.65
1:F:534:ILE:HD11	1:F:1024:VAL:HG22	1.77	0.65
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.27	0.65
1:C:947:GLU:HG3	1:C:948:PHE:HD1	1.61	0.65
1:A:455:PRO:HG2	1:A:880:SER:HB2	1.79	0.65
1:A:979:SER:OG	1:A:1015:THR:HG21	1.96	0.65
1:B:578:LEU:HD21	1:B:590:VAL:HG21	1.78	0.65
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.78	0.65
1:D:584:GLN:HB2	1:D:622:GLN:HG2	1.78	0.65
1:E:641:GLU:HA	1:E:646:ALA:HB3	1.80	0.65
1:F:58:GLN:HA	1:F:62:THR:HB	1.79	0.65
1:E:120:GLN:OE1	1:E:123:GLN:NE2	2.30	0.64
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.79	0.64
1:C:146:ASP:O	1:C:148:THR:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:VAL:HG12	1:B:946:VAL:HG21	1.78	0.64
1:C:66:GLU:OE1	1:C:821:GLY:HA2	1.97	0.64
1:D:332:PHE:O	1:D:336:SER:HB3	1.98	0.64
1:B:576:VAL:HG22	1:B:663:VAL:HG22	1.79	0.64
1:E:703:LEU:HD11	1:E:718:PRO:HG3	1.78	0.64
1:E:1013:THR:O	1:E:1017:LEU:HB2	1.97	0.64
1:C:248:LYS:HA	1:C:261:LEU:HD13	1.79	0.64
1:E:733:GLN:NE2	1:E:743:ILE:HG21	2.13	0.64
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.80	0.64
1:C:420:MET:HB3	1:C:500:ILE:HB	1.80	0.64
1:D:699:ARG:HG3	1:D:827:ILE:HD11	1.79	0.64
1:E:353:LEU:C	1:E:355:MET:H	2.06	0.64
1:C:23:GLY:HA2	1:C:381:ALA:HB2	1.80	0.64
1:C:27:ILE:HA	1:C:30:LEU:HD22	1.80	0.63
1:A:158:VAL:HA	1:A:162:MET:HE2	1.79	0.63
1:C:555:LEU:HD22	1:C:913:LEU:HB3	1.79	0.63
1:D:388:PHE:HE2	1:D:472:ILE:HG21	1.64	0.63
1:F:57:VAL:HG23	1:F:82:SER:HB3	1.81	0.63
1:F:509:LYS:HG2	1:F:513:PHE:HB2	1.79	0.63
1:B:272:GLY:N	1:B:275:TYR:OH	2.30	0.63
1:E:184:MET:HB3	1:E:771:VAL:HG13	1.81	0.63
1:F:291:ILE:HD13	1:F:306:ILE:HD13	1.79	0.63
1:B:171:GLY:O	1:B:294:ALA:N	2.30	0.63
1:F:935:ILE:O	1:F:938:SER:OG	2.16	0.63
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.27	0.63
1:D:568:ASP:O	1:D:634:TRP:HZ3	1.82	0.63
1:F:1021:PHE:HB3	1:F:1025:PHE:CE1	2.32	0.63
1:A:400:LEU:HD21	1:A:930:GLY:HA2	1.78	0.63
1:A:885:PHE:HD1	1:A:902:MET:HE1	1.63	0.63
1:A:941:ASN:HB3	1:A:975:ILE:HD13	1.80	0.63
1:C:404:LEU:HB3	1:C:478:MET:SD	2.39	0.63
1:D:452:VAL:HA	1:D:880:SER:OG	1.99	0.63
1:A:183:ALA:HB2	1:A:273:GLU:HG3	1.81	0.63
1:B:13:TRP:CH2	1:B:492:LEU:HD21	2.33	0.63
1:A:832:ALA:HB3	1:A:835:LYS:HD3	1.81	0.63
1:B:459:PHE:CE1	1:B:876:LEU:HD12	2.34	0.63
1:D:567:GLU:OE1	1:D:996:GLY:HA2	1.99	0.63
1:D:971:ARG:C	1:D:974:PRO:HD2	2.23	0.63
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.81	0.62
1:E:144:ASN:ND2	1:E:319:SER:O	2.30	0.62
1:D:591:LEU:HD13	1:D:611:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:945:ILE:HD12	1:E:971:ARG:HD3	1.81	0.62
1:E:949:ALA:HB3	1:E:1026:PHE:HE2	1.64	0.62
1:A:445:ILE:HD13	1:A:940:LYS:HE2	1.82	0.62
1:A:531:VAL:O	1:A:535:LEU:HG	1.99	0.62
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.80	0.62
1:C:535:LEU:HD13	1:C:1027:VAL:HG21	1.81	0.62
1:D:358:PHE:CD1	1:D:977:MET:HG2	2.35	0.62
1:F:187:TRP:HA	1:F:774:MET:O	1.99	0.62
1:F:979:SER:HA	1:F:1011:MET:HE3	1.80	0.62
1:B:185:ARG:HH12	1:B:774:MET:HE3	1.65	0.62
1:F:203:VAL:O	1:F:207:ILE:HG13	1.99	0.62
1:A:449:LEU:HD22	1:A:453:PHE:HE1	1.64	0.62
1:E:471:SER:O	1:E:475:VAL:HG23	2.00	0.62
1:F:120:GLN:HG3	1:F:123:GLN:HB2	1.81	0.62
1:C:536:ARG:HH21	2:C:1101:LMT:H3O1	1.43	0.62
1:D:280:GLU:OE2	1:D:588:GLN:NE2	2.32	0.62
1:D:360:GLN:NE2	1:D:513:PHE:O	2.31	0.62
1:E:162:MET:C	1:E:164:ASP:H	2.04	0.62
1:A:246:PHE:HB3	1:A:268:ILE:HD13	1.80	0.62
1:A:359:LEU:O	1:A:361:ASN:N	2.32	0.62
1:A:492:LEU:O	1:A:496:MET:HG2	1.99	0.62
1:C:450:SER:O	1:C:454:VAL:HG23	2.00	0.62
1:D:445:ILE:O	1:D:449:LEU:HB2	1.98	0.62
1:F:602:GLU:OE2	1:F:650:ARG:NH1	2.32	0.62
1:B:298:ASN:HB3	1:B:301:ASP:HB2	1.81	0.62
1:B:442:LEU:O	1:B:445:ILE:HG13	2.00	0.62
1:C:950:LYS:HG3	1:C:951:ASP:N	2.14	0.62
1:D:634:TRP:CD1	1:D:634:TRP:H	2.16	0.62
1:B:531:VAL:HA	1:B:534:ILE:HG23	1.82	0.62
1:C:712:MET:HB3	1:C:713:LEU:HD12	1.82	0.62
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.82	0.62
1:F:698:ALA:O	1:F:701:GLN:HB3	1.99	0.62
1:A:971:ARG:C	1:A:974:PRO:HD2	2.25	0.62
1:C:144:ASN:HA	1:C:320:GLY:O	1.99	0.62
1:C:162:MET:O	1:C:164:ASP:N	2.33	0.62
1:E:751:GLY:O	1:E:753:ALA:N	2.33	0.62
1:F:733:GLN:NE2	1:F:743:ILE:HG21	2.14	0.62
1:A:216:ALA:HB1	1:A:234:ILE:HG22	1.82	0.61
1:C:380:PHE:HD2	1:C:383:LEU:HD12	1.64	0.61
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.35	0.61
1:F:5:PHE:O	1:F:7:ASP:N	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ILE:HD13	1:A:940:LYS:CE	2.30	0.61
1:B:219:LEU:HD23	1:C:754:TRP:HZ3	1.64	0.61
1:B:658:ILE:O	1:B:659:LYS:HD2	1.99	0.61
1:E:186:ILE:HD13	1:E:262:LEU:HD21	1.80	0.61
1:E:717:ARG:HH21	1:E:828:LEU:HB3	1.63	0.61
1:F:365:THR:O	1:F:368:PRO:HD2	1.98	0.61
1:A:375:VAL:HG11	1:A:481:SER:HB2	1.82	0.61
1:B:919:ARG:HB3	1:B:921:LEU:HD23	1.82	0.61
1:C:584:GLN:HB2	1:C:622:GLN:HG2	1.82	0.61
1:C:960:LEU:O	1:C:964:THR:HG23	2.00	0.61
1:F:919:ARG:NH2	1:F:990:VAL:O	2.33	0.61
1:F:1039:ASP:HB3	1:F:1040:ILE:HA	1.83	0.61
1:D:281:PHE:CZ	1:D:608:SER:HB2	2.34	0.61
1:E:441:ALA:O	1:E:445:ILE:HG23	1.99	0.61
1:E:960:LEU:HD13	1:E:1030:ARG:HG2	1.81	0.61
1:E:986:VAL:HG12	1:E:1008:MET:HE3	1.82	0.61
1:F:187:TRP:HB3	1:F:776:GLU:HG2	1.81	0.61
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.82	0.61
1:C:47:ALA:HB3	1:C:88:VAL:HG13	1.81	0.61
1:F:340:VAL:CG1	1:F:395:MET:HB3	2.31	0.61
1:C:252:LYS:NZ	1:C:254:ASN:OD1	2.33	0.61
1:C:746:ILE:HG13	1:C:747:ASN:N	2.14	0.61
1:D:388:PHE:CE2	1:D:472:ILE:HG21	2.34	0.61
1:E:692:HIS:CD2	1:E:813:SER:HG	2.16	0.61
1:A:703:LEU:HD21	1:A:718:PRO:HD3	1.83	0.61
1:C:897:ILE:HD12	1:C:946:VAL:CG1	2.31	0.61
1:C:731:ILE:HD13	1:C:746:ILE:HD11	1.81	0.61
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.82	0.61
1:F:66:GLU:OE2	1:F:80:SER:OG	2.13	0.61
1:F:470:PHE:CD1	1:F:929:VAL:HG11	2.36	0.61
1:C:482:VAL:O	1:C:486:LEU:HG	2.01	0.61
1:D:158:VAL:HA	1:D:162:MET:HE2	1.81	0.61
1:D:507:GLU:C	1:D:509:LYS:H	2.09	0.61
1:F:559:LEU:HD12	1:F:923:ASN:HB2	1.83	0.61
1:B:706:ALA:HB3	1:B:716:VAL:HG11	1.81	0.60
1:C:115:MET:HB3	1:C:116:PRO:HD3	1.81	0.60
1:E:354:VAL:O	1:E:354:VAL:HG12	2.00	0.60
1:F:649:MET:HE1	1:F:833:PRO:HD3	1.82	0.60
1:A:58:GLN:HE21	1:A:63:GLN:HE21	1.49	0.60
1:A:154:ILE:O	1:A:157:TYR:N	2.34	0.60
1:C:578:LEU:HG	1:C:587:THR:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:623:ASN:N	1:C:623:ASN:OD1	2.34	0.60
1:C:668:LEU:HD23	1:C:668:LEU:H	1.65	0.60
1:F:149:MET:HE3	1:F:153:ASP:HB3	1.83	0.60
1:A:157:TYR:OH	1:A:316:PHE:O	2.20	0.60
1:A:326:PRO:HA	1:A:630:SER:OG	2.01	0.60
1:F:375:VAL:HB	1:F:405:LEU:HD22	1.82	0.60
1:C:309:GLU:HG3	1:C:313:MET:HE3	1.83	0.60
1:C:817:GLU:HB2	1:C:824:SER:O	2.01	0.60
1:E:251:LEU:HD11	1:E:262:LEU:HA	1.83	0.60
1:F:350:LEU:HD23	1:F:984:LEU:HB3	1.84	0.60
1:F:456:MET:HE3	1:F:932:LEU:HD12	1.82	0.60
1:E:216:ALA:HB1	1:E:234:ILE:HG22	1.83	0.60
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.02	0.60
1:C:634:TRP:CD1	1:C:634:TRP:H	2.14	0.60
1:D:519:MET:O	1:D:523:SER:OG	2.17	0.60
1:F:248:LYS:HA	1:F:261:LEU:HD13	1.84	0.60
1:B:171:GLY:HA3	1:B:302:THR:OG1	2.00	0.60
1:D:278:ILE:HG13	1:D:613:ASN:HB3	1.83	0.60
1:D:904:VAL:HG21	1:D:942:ALA:HB2	1.83	0.60
1:D:228:GLN:HB3	1:E:583:THR:HG21	1.83	0.60
1:D:475:VAL:HA	1:D:478:MET:HE2	1.83	0.60
1:F:527:TYR:O	1:F:531:VAL:HG23	2.02	0.60
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.84	0.60
1:C:559:LEU:HD23	1:C:560:PRO:HD2	1.84	0.60
1:C:563:PHE:CE2	1:C:564:LEU:HD22	2.36	0.60
1:E:140:VAL:N	1:E:289:LEU:O	2.35	0.60
1:F:542:LEU:O	1:F:546:LEU:HG	2.02	0.60
1:C:38:ILE:CG2	1:C:462:SER:HB2	2.29	0.59
1:C:1040:ILE:HG12	1:C:1041:GLU:N	2.16	0.59
1:D:70:ASN:O	1:D:110:LYS:NZ	2.36	0.59
1:E:111:LEU:HD11	1:E:127:VAL:HB	1.84	0.59
1:A:379:THR:HG23	1:A:476:SER:OG	2.02	0.59
1:A:943:ILE:O	1:A:947:GLU:HB3	2.02	0.59
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.84	0.59
1:D:958:LYS:HB3	1:D:963:ALA:HB2	1.83	0.59
1:F:45:ILE:HG23	1:F:129:VAL:HG22	1.82	0.59
1:F:429:GLU:O	1:F:433:LYS:HB2	2.02	0.59
1:A:906:PRO:O	1:A:908:GLY:N	2.35	0.59
1:B:203:VAL:O	1:B:207:ILE:HG13	2.02	0.59
1:F:58:GLN:OE1	1:F:818:ARG:NH1	2.33	0.59
1:A:518:ARG:O	1:A:522:LYS:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.84	0.59
1:C:1043:SER:OG	1:C:1044:HIS:N	2.21	0.59
1:F:82:SER:HB2	1:F:816:LEU:HB2	1.83	0.59
1:A:203:VAL:HG12	1:A:207:ILE:HD11	1.83	0.59
1:B:682:PHE:O	1:B:827:ILE:N	2.22	0.59
1:E:211:ASN:ND2	1:E:240:LEU:H	2.00	0.59
1:F:61:VAL:HA	1:F:118:LEU:HD22	1.85	0.59
1:F:455:PRO:HG2	1:F:880:SER:HA	1.83	0.59
1:A:960:LEU:O	1:A:964:THR:HG23	2.02	0.59
1:B:369:THR:O	1:B:373:PRO:HG2	2.03	0.59
1:C:959:GLY:HA2	1:C:1041:GLU:O	2.03	0.59
1:F:462:SER:OG	1:F:865:GLN:HG2	2.03	0.59
1:A:680:PHE:HB2	1:A:859:TRP:HZ3	1.67	0.59
1:B:354:VAL:O	1:B:358:PHE:HB2	2.03	0.59
1:D:699:ARG:NE	1:D:718:PRO:HB3	2.18	0.59
1:C:634:TRP:CD1	1:C:634:TRP:N	2.71	0.59
1:E:562:SER:OG	1:E:563:PHE:N	2.33	0.59
1:E:979:SER:HB3	1:E:1015:THR:HG21	1.85	0.59
1:F:587:THR:HG21	1:F:622:GLN:O	2.03	0.59
1:A:577:GLN:O	1:A:661:ALA:HB1	2.03	0.59
1:A:696:THR:HG23	1:A:699:ARG:NH1	2.18	0.59
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.84	0.59
1:C:443:VAL:O	1:C:447:MET:HB3	2.02	0.59
1:C:573:MET:HE3	1:C:626:ILE:HD11	1.85	0.59
1:A:394:THR:HG23	1:A:469:GLN:HB3	1.84	0.58
1:B:162:MET:O	1:B:164:ASP:N	2.36	0.58
1:B:213:GLN:HE22	1:C:52:ALA:HA	1.68	0.58
1:C:66:GLU:OE2	1:C:80:SER:OG	2.15	0.58
1:C:518:ARG:O	1:C:522:LYS:HG3	2.02	0.58
1:B:744:ASN:O	1:B:748:THR:HG23	2.03	0.58
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.34	0.58
1:E:703:LEU:HD21	1:E:718:PRO:HD3	1.85	0.58
1:E:752:ALA:O	1:E:774:MET:HA	2.04	0.58
1:F:982:PHE:HD2	1:F:1011:MET:HG2	1.67	0.58
1:A:904:VAL:HG12	1:A:938:SER:HB2	1.84	0.58
1:C:669:PRO:HD3	1:C:677:ALA:C	2.28	0.58
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.03	0.58
1:B:104:GLN:HG2	1:C:109:ASN:ND2	2.18	0.58
1:B:173:GLY:HA2	1:C:71:GLY:HA3	1.85	0.58
1:B:351:VAL:HG22	1:B:981:ALA:HB1	1.85	0.58
1:C:751:GLY:O	1:C:753:ALA:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:751:GLY:O	1:D:753:ALA:N	2.36	0.58
1:E:166:ILE:HG13	1:E:309:GLU:HB3	1.86	0.58
1:E:394:THR:HG23	1:E:469:GLN:HB3	1.86	0.58
1:F:13:TRP:HH2	1:F:370:ILE:HD13	1.69	0.58
1:F:368:PRO:HG3	1:F:413:VAL:HG21	1.85	0.58
1:F:492:LEU:HA	1:F:495:THR:OG1	2.03	0.58
1:F:551:GLY:O	1:F:555:LEU:HB2	2.03	0.58
1:A:459:PHE:CZ	1:A:876:LEU:HD12	2.39	0.58
1:A:733:GLN:NE2	1:A:743:ILE:HG21	2.18	0.58
1:B:511:GLY:HA2	1:B:515:TRP:HE1	1.69	0.58
1:C:371:ALA:O	1:C:375:VAL:HG23	2.04	0.58
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.85	0.58
1:D:696:THR:HG23	1:D:699:ARG:HH12	1.68	0.58
1:B:685:ILE:HD11	1:B:819:TYR:HD2	1.68	0.58
1:E:14:VAL:HG22	1:F:886:LEU:HD12	1.84	0.58
1:E:871:ASN:OD1	1:E:871:ASN:N	2.37	0.58
1:F:351:VAL:HG11	1:F:406:VAL:HG11	1.85	0.58
1:A:906:PRO:O	1:A:909:VAL:N	2.37	0.58
1:F:380:PHE:HA	1:F:383:LEU:HD12	1.85	0.58
1:A:140:VAL:HG11	1:A:310:LEU:HD21	1.86	0.58
1:A:146:ASP:HB2	1:A:148:THR:HG23	1.85	0.58
1:A:960:LEU:HD23	1:A:1031:ARG:CZ	2.34	0.58
1:B:189:ASN:HB3	1:B:192:GLU:HB2	1.86	0.58
1:D:113:LEU:HD11	1:F:128:SER:HB3	1.84	0.58
1:D:230:LEU:HD21	1:E:809:TRP:HH2	1.68	0.58
1:D:897:ILE:HG12	1:D:1030:ARG:HD2	1.85	0.58
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.67	0.58
1:F:1040:ILE:CA	1:F:1041:GLU:HB2	2.33	0.58
1:A:94:PHE:CE1	1:A:103:ALA:HB1	2.39	0.58
1:A:137:LEU:HB2	1:A:293:LEU:HB2	1.85	0.58
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.85	0.58
1:F:164:ASP:O	1:F:168:ARG:NH1	2.36	0.58
1:A:400:LEU:CD2	1:A:929:VAL:HG12	2.33	0.57
1:A:435:MET:HE3	1:A:439:GLN:HB2	1.85	0.57
1:B:167:SER:OG	1:C:70:ASN:ND2	2.37	0.57
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.85	0.57
1:C:414:GLU:OE1	1:C:973:ARG:NH1	2.36	0.57
1:C:1039:ASP:HB3	1:C:1040:ILE:HA	1.85	0.57
1:D:383:LEU:HD22	1:D:388:PHE:HD2	1.69	0.57
1:D:674:LEU:HD23	1:D:675:GLY:N	2.19	0.57
1:D:726:GLN:CD	1:D:812:GLY:HA3	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:LEU:CD1	1:C:579:PRO:HD2	2.33	0.57
1:D:420:MET:HB3	1:D:500:ILE:HB	1.85	0.57
1:E:166:ILE:HG23	1:E:306:ILE:HG12	1.87	0.57
1:E:869:SER:O	1:E:869:SER:OG	2.21	0.57
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.38	0.57
1:F:66:GLU:OE1	1:F:821:GLY:HA2	2.04	0.57
1:F:81:ASN:HD21	1:F:815:ARG:HH22	1.52	0.57
1:A:590:VAL:O	1:A:593:GLU:HB2	2.04	0.57
1:D:448:VAL:HG22	1:D:887:CYS:CB	2.34	0.57
1:E:115:MET:HE1	1:E:123:GLN:HA	1.86	0.57
1:F:1043:SER:OG	1:F:1044:HIS:N	2.32	0.57
1:A:13:TRP:O	1:A:17:ILE:HG13	2.04	0.57
1:C:326:PRO:O	1:C:630:SER:HB2	2.04	0.57
1:C:521:GLU:O	1:C:524:THR:HG22	2.03	0.57
1:C:525:HIS:HA	1:C:528:THR:HG22	1.87	0.57
1:D:989:LEU:HB3	1:D:1000:GLN:O	2.04	0.57
1:E:931:LEU:O	1:E:935:ILE:HG13	2.03	0.57
1:F:426:PRO:HD2	1:F:429:GLU:HG2	1.85	0.57
1:A:165:ALA:HB3	1:A:313:MET:HE1	1.85	0.57
1:A:832:ALA:O	1:A:835:LYS:HB2	2.05	0.57
1:A:947:GLU:HG3	1:A:948:PHE:HD1	1.69	0.57
1:D:154:ILE:O	1:D:157:TYR:N	2.37	0.57
1:D:781:MET:HE2	1:F:225:VAL:HG22	1.85	0.57
1:D:52:ALA:HB1	1:D:56:THR:HB	1.86	0.57
1:D:165:ALA:HB3	1:D:313:MET:HE1	1.86	0.57
1:D:728:LYS:HG2	1:D:808:ARG:NH1	2.19	0.57
1:F:612:VAL:HB	1:F:626:ILE:HG22	1.85	0.57
1:E:535:LEU:O	1:E:537:SER:N	2.38	0.57
1:A:465:ALA:O	1:A:469:GLN:HG2	2.04	0.57
1:B:172:VAL:HG22	1:B:306:ILE:HD11	1.86	0.57
1:E:359:LEU:O	1:E:361:ASN:N	2.37	0.57
1:E:911:GLY:HA3	1:E:1013:THR:OG1	2.05	0.57
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.87	0.57
1:F:744:ASN:O	1:F:748:THR:HG23	2.04	0.57
1:A:254:ASN:HB2	1:A:258:SER:O	2.05	0.57
1:A:515:TRP:O	1:A:519:MET:HG3	2.05	0.57
1:A:744:ASN:O	1:A:748:THR:HG23	2.04	0.57
1:C:418:ARG:O	1:C:422:GLU:HB2	2.05	0.57
1:E:987:MET:O	1:E:990:VAL:N	2.35	0.57
1:A:344:LEU:HD11	1:A:398:MET:HB3	1.85	0.57
1:C:171:GLY:HA3	1:C:302:THR:OG1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:LEU:CD2	1:D:402:ILE:HD11	2.34	0.57
1:E:344:LEU:HD23	1:E:402:ILE:HD11	1.86	0.57
1:E:634:TRP:CD1	1:E:634:TRP:N	2.71	0.57
1:E:699:ARG:NH2	1:E:722:GLU:OE2	2.38	0.57
1:A:4:PHE:O	1:A:8:ARG:HD2	2.04	0.56
1:A:411:VAL:HG22	1:A:971:ARG:NH2	2.20	0.56
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.87	0.56
1:B:540:ARG:O	1:B:543:VAL:HB	2.05	0.56
1:C:6:ILE:CG2	1:C:12:ALA:HB2	2.35	0.56
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.87	0.56
1:F:694:LYS:H	1:F:694:LYS:HD2	1.70	0.56
1:B:181:GLN:NE2	1:B:769:LYS:HG2	2.19	0.56
1:B:535:LEU:HD13	1:B:1027:VAL:HG21	1.86	0.56
1:B:686:ASP:HB2	1:B:695:LEU:HD23	1.88	0.56
1:D:350:LEU:HD13	1:D:984:LEU:O	2.05	0.56
1:E:399:VAL:O	1:E:402:ILE:HG13	2.05	0.56
1:F:336:SER:O	1:F:340:VAL:HG23	2.04	0.56
1:A:69:MET:SD	1:A:72:ILE:HD11	2.45	0.56
1:A:947:GLU:HG3	1:A:948:PHE:N	2.19	0.56
1:B:400:LEU:HG	1:B:929:VAL:HG12	1.87	0.56
1:D:350:LEU:HD22	1:D:984:LEU:HB3	1.88	0.56
1:D:485:ALA:O	1:D:490:PRO:HD3	2.04	0.56
1:D:527:TYR:O	1:D:531:VAL:HG23	2.05	0.56
1:E:355:MET:SD	1:E:365:THR:HA	2.44	0.56
1:E:418:ARG:NH1	1:E:970:MET:HE3	2.19	0.56
1:E:542:LEU:O	1:E:546:LEU:HG	2.05	0.56
1:F:5:PHE:C	1:F:7:ASP:H	2.13	0.56
1:F:713:LEU:HD11	1:F:843:LEU:HD12	1.87	0.56
1:F:987:MET:HG3	1:F:1008:MET:HE1	1.86	0.56
1:F:1039:ASP:OD2	1:F:1041:GLU:HG3	2.05	0.56
1:B:713:LEU:HD11	1:B:843:LEU:HD12	1.86	0.56
1:C:958:LYS:HB3	1:C:963:ALA:HB2	1.88	0.56
1:D:1013:THR:O	1:D:1017:LEU:HB2	2.05	0.56
1:F:420:MET:HG2	1:F:425:LEU:O	2.06	0.56
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.87	0.56
1:A:157:TYR:CZ	1:A:318:PRO:HD3	2.40	0.56
1:A:395:MET:O	1:A:398:MET:HB2	2.06	0.56
1:A:564:LEU:HD22	1:A:671:ILE:HG13	1.87	0.56
1:D:184:MET:HB3	1:D:771:VAL:HG13	1.87	0.56
1:D:932:LEU:HD23	1:D:935:ILE:HD12	1.87	0.56
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:LEU:HB2	1:F:293:LEU:HB2	1.87	0.56
1:F:156:ASP:OD1	1:F:765:ARG:NH2	2.38	0.56
1:F:414:GLU:OE1	1:F:973:ARG:HD3	2.06	0.56
1:F:455:PRO:HG3	1:F:883:VAL:HG21	1.87	0.56
1:A:512:PHE:HB3	1:A:513:PHE:CD1	2.40	0.56
1:B:356:TYR:C	1:B:358:PHE:H	2.13	0.56
1:C:356:TYR:HE1	1:C:362:PHE:HA	1.70	0.56
1:C:979:SER:HB3	1:C:1015:THR:HG21	1.87	0.56
1:D:391:ASN:O	1:D:395:MET:HG2	2.05	0.56
1:D:393:LEU:HD13	1:D:466:ILE:HA	1.88	0.56
1:F:99:ASP:O	1:F:102:ILE:HB	2.05	0.56
1:F:504:ASP:C	1:F:506:GLY:H	2.12	0.56
1:A:332:PHE:O	1:A:336:SER:HB3	2.05	0.56
1:A:549:VAL:O	1:A:552:MET:HB3	2.04	0.56
1:A:623:ASN:N	1:A:623:ASN:OD1	2.36	0.56
1:B:231:ASN:HD22	1:C:622:GLN:CD	2.13	0.56
1:D:375:VAL:HG11	1:D:405:LEU:HD22	1.88	0.56
1:E:347:ALA:HB1	1:E:402:ILE:HG21	1.88	0.56
1:E:367:ILE:HG12	1:E:496:MET:SD	2.45	0.56
1:A:751:GLY:O	1:A:753:ALA:N	2.39	0.56
1:B:652:THR:CG2	1:B:665:ALA:H	2.19	0.56
1:C:968:VAL:HA	1:C:971:ARG:HH12	1.71	0.56
1:B:184:MET:HE1	1:B:243:THR:HG22	1.87	0.56
1:C:6:ILE:HG21	1:C:12:ALA:HB2	1.87	0.56
1:C:40:PRO:HD2	1:C:674:LEU:HD11	1.88	0.56
1:D:955:LYS:O	1:D:956:GLU:HG2	2.06	0.56
1:E:459:PHE:CB	1:E:464:GLY:HA2	2.36	0.56
1:E:589:LYS:HA	1:E:592:ASN:HD22	1.70	0.56
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.71	0.56
1:E:699:ARG:O	1:E:703:LEU:HB2	2.05	0.56
1:F:566:ASP:CG	1:F:678:THR:HG23	2.31	0.56
1:F:743:ILE:O	1:F:746:ILE:HG13	2.06	0.56
1:D:66:GLU:OE2	1:D:80:SER:OG	2.14	0.56
1:D:251:LEU:HD11	1:D:265:VAL:HG21	1.88	0.56
1:D:643:LYS:NZ	1:D:993:THR:HG23	2.21	0.56
1:E:42:ALA:HB3	1:E:132:SER:HB3	1.87	0.56
1:E:524:THR:O	1:E:527:TYR:HB3	2.06	0.56
1:F:409:ALA:O	1:F:413:VAL:HG23	2.06	0.56
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.41	0.55
1:B:399:VAL:HG13	1:B:402:ILE:HD11	1.88	0.55
1:B:456:MET:HG3	1:B:471:SER:OG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:947:GLU:HG3	1:C:948:PHE:CD1	2.41	0.55
1:D:699:ARG:HE	1:D:703:LEU:HD11	1.70	0.55
1:E:751:GLY:O	1:E:754:TRP:N	2.39	0.55
1:F:350:LEU:HD23	1:F:984:LEU:HD22	1.88	0.55
1:F:671:ILE:HG21	1:F:674:LEU:HB2	1.87	0.55
1:B:142:VAL:HG21	1:B:162:MET:HE1	1.88	0.55
1:C:187:TRP:HA	1:C:774:MET:O	2.05	0.55
1:D:38:ILE:HG23	1:D:462:SER:OG	2.06	0.55
1:A:736:ALA:HB1	1:A:741:VAL:HG23	1.88	0.55
1:C:108:GLN:O	1:C:112:GLN:HG2	2.06	0.55
1:C:121:GLU:O	1:C:124:GLN:HG2	2.06	0.55
1:D:185:ARG:NE	1:D:272:GLY:O	2.39	0.55
1:D:366:LEU:HA	1:D:369:THR:HB	1.87	0.55
1:B:861:GLY:O	1:B:864:TYR:HB3	2.07	0.55
1:B:1011:MET:O	1:B:1015:THR:HG23	2.05	0.55
1:F:358:PHE:HB3	1:F:977:MET:HE2	1.88	0.55
1:F:359:LEU:O	1:F:361:ASN:N	2.39	0.55
1:A:166:ILE:HD12	1:A:306:ILE:HG12	1.87	0.55
1:C:441:ALA:HB2	1:C:948:PHE:HE1	1.72	0.55
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.72	0.55
1:C:775:SER:HB2	1:C:789:TRP:CZ2	2.42	0.55
1:D:456:MET:HG3	1:D:471:SER:HB2	1.89	0.55
1:E:534:ILE:CG2	2:E:1101:LMT:H1'	2.36	0.55
1:E:668:LEU:HD23	1:E:668:LEU:H	1.71	0.55
1:E:692:HIS:CE1	1:E:813:SER:HG	2.15	0.55
1:F:135:SER:HB3	1:F:673:GLU:CB	2.31	0.55
1:B:230:LEU:HD21	1:C:809:TRP:HH2	1.71	0.55
1:B:352:PHE:C	1:B:352:PHE:CD2	2.85	0.55
1:C:355:MET:SD	1:C:368:PRO:HB2	2.46	0.55
1:C:363:ARG:HB3	1:C:363:ARG:HH11	1.71	0.55
1:C:654:ALA:O	1:C:658:ILE:HG12	2.07	0.55
1:D:449:LEU:HB3	1:D:478:MET:SD	2.47	0.55
1:F:703:LEU:HD11	1:F:718:PRO:HD3	1.87	0.55
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.42	0.55
1:B:377:LEU:O	1:B:380:PHE:HB2	2.06	0.55
1:C:375:VAL:HA	1:C:480:LEU:HD13	1.89	0.55
1:C:568:ASP:O	1:C:634:TRP:HZ3	1.89	0.55
1:C:758:TYR:HB2	1:C:772:TYR:CZ	2.41	0.55
1:D:75:LEU:HD11	1:D:92:LEU:HD23	1.88	0.55
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.89	0.55
1:B:375:VAL:O	1:B:379:THR:OG1	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:775:SER:HB2	1:E:789:TRP:CZ2	2.42	0.55
1:A:453:PHE:O	1:A:471:SER:OG	2.13	0.55
1:C:279:ALA:HB3	1:C:286:ALA:O	2.07	0.55
1:C:464:GLY:O	1:C:468:ARG:HB2	2.06	0.55
1:C:590:VAL:HA	1:C:593:GLU:OE1	2.07	0.55
1:D:4:PHE:HB2	1:D:5:PHE:CD1	2.42	0.55
1:D:253:VAL:HG12	1:D:259:ARG:HG2	1.88	0.55
1:D:668:LEU:H	1:D:668:LEU:HD23	1.70	0.55
1:F:948:PHE:CD2	1:F:970:MET:HE3	2.41	0.55
1:A:318:PRO:HD2	1:A:321:LEU:HD12	1.89	0.55
1:B:456:MET:O	1:B:467:TYR:HB3	2.07	0.55
1:D:480:LEU:O	1:D:484:VAL:HG23	2.06	0.55
1:D:987:MET:HB3	1:D:988:PRO:HD3	1.89	0.55
1:E:254:ASN:HB2	1:E:258:SER:O	2.06	0.55
1:A:136:PHE:HE2	1:A:290:GLY:HA3	1.72	0.54
1:A:144:ASN:OD1	1:A:148:THR:OG1	2.25	0.54
1:A:244:GLU:O	1:A:247:GLY:N	2.36	0.54
1:A:327:TYR:HA	1:A:571:VAL:HG11	1.89	0.54
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.88	0.54
1:A:521:GLU:O	1:A:524:THR:HG22	2.07	0.54
1:B:616:GLY:HA3	1:B:624:THR:HB	1.87	0.54
1:D:563:PHE:C	1:D:564:LEU:HD12	2.32	0.54
1:E:140:VAL:O	1:E:289:LEU:N	2.39	0.54
1:E:669:PRO:HB3	1:E:674:LEU:HD12	1.89	0.54
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.88	0.54
1:F:623:ASN:OD1	1:F:623:ASN:N	2.40	0.54
1:B:1037:ASN:N	1:B:1038:GLU:HB3	2.23	0.54
1:D:169:THR:HG21	1:D:306:ILE:HG13	1.90	0.54
1:D:647:ILE:HG12	1:D:650:ARG:HH12	1.72	0.54
1:E:376:LEU:O	1:E:379:THR:N	2.39	0.54
1:E:568:ASP:O	1:E:634:TRP:HZ3	1.90	0.54
1:A:573:MET:HE2	1:A:666:PHE:HE2	1.71	0.54
1:A:692:HIS:HE2	1:A:723:ASP:CG	2.15	0.54
1:B:317:PHE:CE2	1:B:323:ILE:HD11	2.43	0.54
1:C:730:ASP:CG	1:C:808:ARG:HH21	2.15	0.54
1:C:983:ILE:HG23	1:C:1008:MET:HE3	1.88	0.54
1:E:139:VAL:O	1:E:326:PRO:HD2	2.06	0.54
1:E:459:PHE:HB2	1:E:464:GLY:HA2	1.89	0.54
1:F:145:THR:HA	1:F:284:GLN:HE22	1.73	0.54
1:A:531:VAL:O	1:A:534:ILE:HG13	2.07	0.54
1:B:685:ILE:HD11	1:B:819:TYR:CD2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:THR:HG22	1:D:473:THR:OG1	2.07	0.54
1:F:189:ASN:HB3	1:F:192:GLU:HB2	1.88	0.54
1:F:940:LYS:NZ	1:F:978:THR:HG21	2.23	0.54
1:B:545:TYR:CE2	1:B:1025:PHE:HZ	2.26	0.54
1:C:850:LYS:O	1:C:850:LYS:NZ	2.33	0.54
1:E:104:GLN:HB2	1:E:131:LYS:HD2	1.90	0.54
1:E:165:ALA:HB3	1:E:313:MET:HE3	1.89	0.54
1:E:181:GLN:HG2	1:E:182:TYR:N	2.23	0.54
1:E:201:VAL:HG21	1:E:745:ASP:HB3	1.90	0.54
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.90	0.54
1:F:184:MET:HB3	1:F:771:VAL:HG13	1.88	0.54
1:C:412:VAL:HG22	1:C:438:ILE:HD12	1.89	0.54
1:C:504:ASP:OD1	1:C:506:GLY:N	2.35	0.54
1:C:808:ARG:NH1	1:C:810:GLU:OE2	2.41	0.54
1:D:728:LYS:HA	1:F:235:ILE:HB	1.89	0.54
1:D:1017:LEU:O	1:D:1021:PHE:HB2	2.08	0.54
1:F:139:VAL:O	1:F:326:PRO:HD2	2.08	0.54
1:A:34:GLN:HA	1:A:333:VAL:HG13	1.90	0.54
1:B:66:GLU:OE2	1:B:818:ARG:HD3	2.08	0.54
1:B:172:VAL:HG13	1:B:291:ILE:HG23	1.90	0.54
1:B:294:ALA:O	1:B:296:GLY:N	2.40	0.54
1:B:600:THR:O	1:B:603:LYS:HB2	2.08	0.54
1:C:187:TRP:HB3	1:C:776:GLU:HG2	1.90	0.54
1:C:668:LEU:HB2	1:C:669:PRO:HD2	1.90	0.54
1:A:641:GLU:HB2	1:A:650:ARG:HH22	1.72	0.54
1:B:508:GLY:C	1:B:510:LYS:H	2.14	0.54
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.89	0.54
1:C:24:GLY:HA2	1:C:27:ILE:HG23	1.89	0.54
1:C:61:VAL:HG11	1:C:88:VAL:HG11	1.89	0.54
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.43	0.54
1:C:598:TYR:HB3	1:C:606:VAL:HG21	1.88	0.54
1:C:971:ARG:HB3	1:C:971:ARG:HH11	1.72	0.54
1:E:179:GLY:HA2	1:E:277:ILE:HD11	1.90	0.54
1:E:213:GLN:HA	1:E:237:GLN:O	2.08	0.54
1:E:776:GLU:HB3	1:E:779:TYR:CD1	2.42	0.54
1:F:249:ILE:HB	1:F:262:LEU:HB2	1.90	0.54
1:B:530:SER:OG	2:B:1101:LMT:H12	2.07	0.54
1:C:393:LEU:HD13	1:C:466:ILE:HA	1.88	0.54
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.42	0.54
1:E:165:ALA:HB3	1:E:313:MET:CE	2.38	0.54
1:A:401:ALA:O	1:A:405:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:ARG:NH2	1:A:722:GLU:OE1	2.37	0.54
1:B:553:ALA:O	1:B:557:VAL:HG23	2.08	0.54
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.43	0.54
1:E:121:GLU:O	1:E:125:GLN:HB2	2.08	0.54
1:E:351:VAL:HG22	1:E:981:ALA:HB1	1.90	0.54
1:F:428:LYS:O	1:F:432:ARG:HG3	2.08	0.54
1:A:434:SER:O	1:A:438:ILE:HG12	2.08	0.53
1:A:681:ASP:HB2	1:A:862:MET:HE3	1.89	0.53
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.37	0.53
1:B:448:VAL:O	1:B:452:VAL:HG13	2.08	0.53
1:B:596:HIS:O	1:B:600:THR:OG1	2.18	0.53
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.90	0.53
1:D:889:ALA:HA	1:D:894:SER:O	2.09	0.53
1:E:1041:GLU:HB3	1:E:1042:HIS:CB	2.39	0.53
1:F:145:THR:HA	1:F:284:GLN:NE2	2.22	0.53
1:B:174:ASP:HB3	1:B:292:LYS:HD2	1.90	0.53
1:C:587:THR:HA	1:C:590:VAL:HG23	1.91	0.53
1:D:225:VAL:O	1:D:228:GLN:HB2	2.09	0.53
1:D:359:LEU:O	1:D:361:ASN:N	2.41	0.53
1:F:941:ASN:CG	1:F:975:ILE:HG23	2.34	0.53
1:F:960:LEU:HD21	1:F:1027:VAL:HA	1.91	0.53
1:B:239:ARG:NH1	1:B:761:ASP:HB3	2.23	0.53
1:D:459:PHE:O	1:D:468:ARG:NH2	2.41	0.53
1:D:1038:GLU:OE1	1:D:1038:GLU:HA	2.09	0.53
1:E:7:ASP:OD2	1:E:432:ARG:NH2	2.41	0.53
1:F:355:MET:HB3	1:F:365:THR:HG23	1.90	0.53
1:A:888:LEU:HD22	1:A:892:TYR:CE2	2.43	0.53
1:C:948:PHE:CD2	1:C:970:MET:HE3	2.43	0.53
1:D:885:PHE:CE1	1:D:898:PRO:HB2	2.43	0.53
1:E:669:PRO:CB	1:E:674:LEU:HD12	2.38	0.53
1:F:368:PRO:O	1:F:371:ALA:HB3	2.08	0.53
1:A:186:ILE:HD13	1:A:262:LEU:HD21	1.91	0.53
1:B:398:MET:HG3	1:B:473:THR:HG22	1.91	0.53
1:B:652:THR:HG22	1:B:665:ALA:H	1.73	0.53
1:D:414:GLU:HG3	1:D:974:PRO:HG3	1.90	0.53
1:E:158:VAL:HG13	1:E:162:MET:HB2	1.91	0.53
1:E:559:LEU:HD12	1:E:923:ASN:HB2	1.90	0.53
1:F:187:TRP:CB	1:F:776:GLU:HG2	2.38	0.53
1:A:200:PRO:HA	1:A:203:VAL:HG23	1.91	0.53
1:B:307:ARG:HG2	1:B:325:TYR:OH	2.08	0.53
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:PHE:CE2	1:D:103:ALA:HB1	2.43	0.53
1:D:234:ILE:HD11	1:E:754:TRP:CE3	2.44	0.53
1:E:1041:GLU:HB3	1:E:1042:HIS:HB3	1.90	0.53
1:F:758:TYR:HB2	1:F:772:TYR:CZ	2.43	0.53
1:C:376:LEU:HD22	1:C:398:MET:SD	2.49	0.53
1:C:594:VAL:HG22	1:C:655:PHE:CE2	2.44	0.53
1:E:157:TYR:CE1	1:E:318:PRO:HD3	2.44	0.53
1:E:675:GLY:HA3	1:E:862:MET:SD	2.49	0.53
1:A:598:TYR:HB3	1:A:606:VAL:HG21	1.89	0.53
1:B:34:GLN:HG3	1:B:333:VAL:HG22	1.90	0.53
1:D:335:ILE:O	1:D:339:GLU:HG2	2.09	0.53
1:E:639:GLY:O	1:E:643:LYS:HG3	2.09	0.53
1:F:27:ILE:HA	1:F:30:LEU:HD22	1.91	0.53
1:A:43:VAL:HG23	1:A:94:PHE:HE1	1.74	0.53
1:B:751:GLY:O	1:B:753:ALA:N	2.42	0.53
1:C:3:ASN:O	1:C:6:ILE:N	2.41	0.53
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.44	0.53
1:D:194:ASN:HA	1:D:798:MET:HE2	1.90	0.53
1:D:556:PHE:HD1	1:D:913:LEU:HD21	1.72	0.53
1:D:754:TRP:HZ3	1:F:219:LEU:HD23	1.73	0.53
1:E:445:ILE:HD12	1:E:449:LEU:HG	1.91	0.53
1:E:1035:ARG:CZ	1:E:1035:ARG:HB3	2.39	0.53
1:F:186:ILE:HD13	1:F:262:LEU:HD21	1.90	0.53
1:F:378:GLY:HA3	1:F:480:LEU:HD11	1.91	0.53
1:C:298:ASN:HB3	1:C:301:ASP:HB2	1.91	0.53
1:D:355:MET:HE1	1:D:410:ILE:HD11	1.90	0.53
1:D:396:PHE:HE1	1:D:999:ALA:HB1	1.74	0.53
1:D:602:GLU:HB3	1:D:606:VAL:HG23	1.90	0.53
1:E:190:PRO:HB3	1:E:789:TRP:CE2	2.43	0.53
1:E:343:THR:HG21	1:E:399:VAL:HG13	1.91	0.53
1:F:152:GLU:HA	1:F:155:SER:HB2	1.90	0.53
1:F:352:PHE:HD2	1:F:353:LEU:HD23	1.73	0.53
1:F:378:GLY:O	1:F:382:VAL:HG23	2.08	0.53
1:F:643:LYS:HE2	1:F:645:GLU:CG	2.39	0.53
1:C:743:ILE:H	1:C:743:ILE:HD12	1.74	0.52
1:D:886:LEU:HD13	1:F:18:ILE:HG13	1.91	0.52
1:E:38:ILE:HG22	1:E:462:SER:HB3	1.92	0.52
1:A:952:LEU:O	1:A:956:GLU:HB2	2.09	0.52
1:A:1034:SER:HA	1:A:1035:ARG:HB2	1.91	0.52
1:B:36:PRO:HD3	1:B:391:ASN:OD1	2.09	0.52
1:B:516:PHE:HA	1:B:519:MET:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:VAL:HG22	1:B:655:PHE:CE2	2.44	0.52
1:C:944:LEU:C	1:C:971:ARG:HD2	2.34	0.52
1:D:412:VAL:HG22	1:D:438:ILE:CD1	2.39	0.52
1:D:442:LEU:O	1:D:445:ILE:HG13	2.10	0.52
1:D:744:ASN:O	1:D:748:THR:HG23	2.09	0.52
1:E:124:GLN:HE21	1:E:758:TYR:HD2	1.56	0.52
1:E:237:GLN:OE1	1:F:747:ASN:ND2	2.39	0.52
1:E:504:ASP:C	1:E:506:GLY:H	2.16	0.52
1:A:416:VAL:HG12	1:A:420:MET:HE2	1.91	0.52
1:A:712:MET:HG2	1:A:843:LEU:HG	1.91	0.52
1:A:955:LYS:O	1:A:956:GLU:HG2	2.10	0.52
1:C:396:PHE:O	1:C:400:LEU:HB2	2.08	0.52
1:C:449:LEU:HD11	1:C:937:LEU:HD21	1.91	0.52
1:C:694:LYS:HE3	1:C:694:LYS:H	1.74	0.52
1:C:968:VAL:HA	1:C:971:ARG:NH1	2.24	0.52
1:D:191:ASN:C	1:D:193:LEU:H	2.17	0.52
1:D:577:GLN:OE1	1:D:624:THR:HG23	2.09	0.52
1:E:111:LEU:O	1:E:115:MET:HG2	2.10	0.52
1:E:415:ASN:O	1:E:419:VAL:HG23	2.09	0.52
1:E:418:ARG:HD2	1:E:422:GLU:OE1	2.09	0.52
1:E:817:GLU:OE1	1:E:825:MET:HA	2.09	0.52
1:F:600:THR:C	1:F:602:GLU:H	2.18	0.52
1:B:600:THR:C	1:B:602:GLU:H	2.17	0.52
1:C:310:LEU:HD23	1:C:323:ILE:HG21	1.91	0.52
1:C:413:VAL:O	1:C:417:GLU:HG2	2.10	0.52
1:C:818:ARG:NH2	1:C:821:GLY:O	2.43	0.52
1:D:58:GLN:HA	1:D:62:THR:HB	1.92	0.52
1:E:897:ILE:O	1:E:900:SER:OG	2.27	0.52
1:E:960:LEU:HD21	1:E:1027:VAL:HA	1.90	0.52
1:F:351:VAL:HG12	1:F:355:MET:HE2	1.90	0.52
1:A:1020:PHE:CE2	2:A:1101:LMT:H22	2.44	0.52
1:C:393:LEU:HD11	1:C:466:ILE:HD13	1.92	0.52
1:C:456:MET:HB3	1:C:876:LEU:HD21	1.90	0.52
1:D:230:LEU:HD21	1:E:809:TRP:CH2	2.43	0.52
1:E:35:TYR:HD2	1:E:393:LEU:HG	1.74	0.52
1:E:535:LEU:O	1:E:536:ARG:C	2.51	0.52
1:F:764:ASP:OD1	1:F:765:ARG:HG3	2.09	0.52
1:F:947:GLU:HG3	1:F:948:PHE:N	2.24	0.52
1:A:451:ALA:HB1	1:A:883:VAL:HG12	1.92	0.52
1:A:781:MET:CE	1:C:225:VAL:H	2.23	0.52
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.89	0.52
1:E:987:MET:HB3	1:E:988:PRO:HD3	1.91	0.52
1:F:412:VAL:HG22	1:F:438:ILE:HD12	1.92	0.52
1:F:447:MET:SD	1:F:891:LEU:HD22	2.50	0.52
1:A:973:ARG:HG2	1:A:977:MET:HE2	1.90	0.52
1:B:415:ASN:O	1:B:419:VAL:HG23	2.09	0.52
1:E:536:ARG:CZ	2:E:1101:LMT:H4B	2.39	0.52
1:E:949:ALA:HB3	1:E:1026:PHE:CE2	2.45	0.52
1:F:379:THR:HG23	1:F:476:SER:OG	2.09	0.52
1:A:350:LEU:CD2	1:A:984:LEU:HB3	2.36	0.52
1:C:682:PHE:HE1	1:C:857:TYR:HB2	1.73	0.52
1:C:898:PRO:O	1:C:901:VAL:HG12	2.10	0.52
1:D:14:VAL:HG13	1:E:886:LEU:HG	1.91	0.52
1:E:371:ALA:O	1:E:375:VAL:HG23	2.09	0.52
1:A:168:ARG:NE	1:B:78:MET:HE2	2.25	0.52
1:A:768:VAL:HG12	1:B:63:GLN:NE2	2.24	0.52
1:B:149:MET:HB3	1:B:153:ASP:HB3	1.92	0.52
1:B:516:PHE:O	1:B:520:PHE:N	2.43	0.52
1:C:551:GLY:O	1:C:555:LEU:HB2	2.10	0.52
1:E:783:PRO:HA	1:E:786:ILE:HG12	1.91	0.52
1:F:743:ILE:H	1:F:743:ILE:HD12	1.74	0.52
1:A:375:VAL:HG21	1:A:481:SER:HA	1.92	0.52
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.44	0.52
1:A:743:ILE:H	1:A:743:ILE:HD12	1.75	0.52
1:B:641:GLU:O	1:B:650:ARG:NH2	2.24	0.52
1:D:355:MET:HB3	1:D:365:THR:OG1	2.10	0.52
1:D:540:ARG:O	1:D:543:VAL:HB	2.10	0.52
1:E:57:VAL:HG11	1:E:86:GLY:HA2	1.92	0.52
1:E:435:MET:SD	1:E:490:PRO:HB3	2.50	0.52
1:E:445:ILE:HB	1:E:940:LYS:HG3	1.92	0.52
1:E:576:VAL:HG22	1:E:663:VAL:HG22	1.91	0.52
1:E:588:GLN:O	1:E:592:ASN:ND2	2.42	0.52
1:E:846:GLN:O	1:E:850:LYS:HG2	2.11	0.52
1:F:63:GLN:OE1	1:F:67:GLN:NE2	2.43	0.52
1:F:407:ASP:OD1	1:F:978:THR:HG23	2.09	0.52
1:F:491:ALA:O	1:F:495:THR:HG23	2.10	0.52
1:F:925:VAL:HA	1:F:928:GLN:OE1	2.09	0.52
1:A:586:ARG:O	1:A:589:LYS:HB3	2.10	0.51
1:A:817:GLU:HB2	1:A:824:SER:O	2.10	0.51
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.92	0.51
1:D:13:TRP:CZ2	1:D:492:LEU:HD21	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:THR:HG23	1:D:469:GLN:HB3	1.92	0.51
1:D:445:ILE:HG12	1:D:940:LYS:HE3	1.92	0.51
1:E:347:ALA:CB	1:E:402:ILE:HG21	2.40	0.51
1:F:463:THR:HG23	1:F:925:VAL:HG22	1.92	0.51
1:F:531:VAL:O	1:F:535:LEU:HG	2.10	0.51
1:A:508:GLY:O	1:A:511:GLY:N	2.42	0.51
1:A:957:GLY:HA2	1:A:1042:HIS:CB	2.28	0.51
1:B:544:LEU:HA	1:B:547:ILE:HD12	1.91	0.51
1:B:654:ALA:O	1:B:658:ILE:HG12	2.10	0.51
1:D:587:THR:HB	1:D:613:ASN:HD21	1.74	0.51
1:E:691:GLY:N	1:E:694:LYS:HD3	2.25	0.51
1:E:743:ILE:H	1:E:743:ILE:HD12	1.75	0.51
1:E:762:PHE:CE1	1:E:764:ASP:HB2	2.45	0.51
1:F:165:ALA:HB3	1:F:313:MET:HE1	1.92	0.51
1:F:881:LEU:HD22	1:F:902:MET:HE1	1.92	0.51
1:F:888:LEU:HD11	1:F:943:ILE:HD11	1.91	0.51
1:F:1035:ARG:HB2	1:F:1038:GLU:HB2	1.92	0.51
1:A:47:ALA:O	1:A:87:THR:HA	2.11	0.51
1:A:58:GLN:NE2	1:A:63:GLN:HE21	2.08	0.51
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.91	0.51
1:D:360:GLN:NE2	1:D:513:PHE:HB3	2.25	0.51
1:F:412:VAL:CG2	1:F:442:LEU:HD11	2.41	0.51
1:A:238:THR:HG23	1:B:728:LYS:NZ	2.26	0.51
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.44	0.51
1:A:888:LEU:HD22	1:A:892:TYR:HE2	1.75	0.51
1:B:344:LEU:HD11	1:B:398:MET:HE3	1.93	0.51
1:C:504:ASP:C	1:C:506:GLY:H	2.17	0.51
1:C:742:SER:O	1:C:746:ILE:HG23	2.10	0.51
1:C:893:GLU:HG3	1:C:893:GLU:O	2.09	0.51
1:D:219:LEU:HD23	1:E:754:TRP:CZ3	2.35	0.51
1:E:527:TYR:O	1:E:530:SER:HB3	2.10	0.51
1:E:527:TYR:CE2	1:E:972:LEU:HG	2.46	0.51
1:F:192:GLU:HB3	1:F:265:VAL:HA	1.92	0.51
1:F:525:HIS:HA	1:F:528:THR:CG2	2.40	0.51
1:A:225:VAL:HG22	1:B:781:MET:HE2	1.93	0.51
1:A:958:LYS:HB3	1:A:963:ALA:HB2	1.92	0.51
1:B:65:ILE:O	1:B:69:MET:HG2	2.11	0.51
1:B:143:ILE:HG21	1:B:281:PHE:CD2	2.46	0.51
1:D:2:PRO:O	1:D:6:ILE:HG23	2.10	0.51
1:D:717:ARG:O	1:D:827:ILE:HG23	2.10	0.51
1:E:457:ALA:HB2	1:E:471:SER:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:594:VAL:HG22	1:F:655:PHE:CE2	2.45	0.51
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.92	0.51
1:C:736:ALA:HB1	1:C:741:VAL:HG23	1.92	0.51
1:D:559:LEU:HD23	1:D:560:PRO:HD2	1.92	0.51
1:F:162:MET:O	1:F:164:ASP:N	2.43	0.51
1:F:479:ALA:O	1:F:483:LEU:HD23	2.10	0.51
1:F:945:ILE:HA	1:F:971:ARG:NH1	2.25	0.51
1:F:1034:SER:OG	1:F:1035:ARG:N	2.43	0.51
1:B:575:MET:HB3	1:B:626:ILE:HG13	1.92	0.51
1:D:393:LEU:HD12	1:D:469:GLN:HG3	1.92	0.51
1:D:777:ALA:HB1	1:F:225:VAL:HG12	1.91	0.51
1:E:776:GLU:HB3	1:E:779:TYR:CE1	2.44	0.51
1:F:873:ALA:HB2	1:F:928:GLN:NE2	2.25	0.51
1:F:947:GLU:HG3	1:F:948:PHE:HD1	1.75	0.51
1:A:904:VAL:CG1	1:A:938:SER:HB2	2.40	0.51
1:C:82:SER:HB2	1:C:816:LEU:HB2	1.92	0.51
1:D:616:GLY:HA3	1:D:624:THR:HG22	1.93	0.51
1:E:696:THR:HG23	1:E:699:ARG:NH1	2.25	0.51
1:F:376:LEU:O	1:F:379:THR:N	2.44	0.51
1:F:400:LEU:HD11	1:F:1007:VAL:HG21	1.93	0.51
1:F:598:TYR:HB3	1:F:606:VAL:HG21	1.92	0.51
1:F:720:GLY:HA3	1:F:817:GLU:OE1	2.11	0.51
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.93	0.51
1:A:355:MET:HB3	1:A:365:THR:OG1	2.10	0.51
1:A:726:GLN:OE1	1:A:812:GLY:HA3	2.11	0.51
1:A:775:SER:HB2	1:A:789:TRP:CZ2	2.46	0.51
1:B:267:LYS:HD3	1:B:776:GLU:OE2	2.11	0.51
1:B:422:GLU:O	1:B:502:LYS:NZ	2.44	0.51
1:C:40:PRO:HG2	1:C:674:LEU:HD21	1.91	0.51
1:C:408:ASP:O	1:C:412:VAL:HG23	2.11	0.51
1:D:941:ASN:HB3	1:D:975:ILE:HD13	1.93	0.51
1:D:1026:PHE:CE2	1:D:1030:ARG:HG3	2.46	0.51
1:E:46:SER:OG	1:E:89:GLN:HG2	2.10	0.51
1:E:203:VAL:HG12	1:E:207:ILE:HD11	1.93	0.51
1:B:295:THR:O	1:B:295:THR:OG1	2.25	0.51
1:C:149:MET:HB2	1:C:153:ASP:HB3	1.91	0.51
1:E:1041:GLU:HB3	1:E:1042:HIS:C	2.36	0.51
1:F:27:ILE:HG22	1:F:380:PHE:HB3	1.93	0.51
1:C:576:VAL:HG21	1:C:591:LEU:HD23	1.93	0.50
1:C:751:GLY:O	1:C:754:TRP:N	2.44	0.50
1:C:888:LEU:HD11	1:C:943:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:GLY:O	1:D:536:ARG:HG3	2.11	0.50
1:E:167:SER:HB2	1:E:175:VAL:HG11	1.93	0.50
1:E:183:ALA:HB2	1:E:273:GLU:HG3	1.93	0.50
1:F:344:LEU:HA	1:F:399:VAL:HG22	1.93	0.50
1:B:158:VAL:HA	1:B:162:MET:HE2	1.92	0.50
1:C:139:VAL:O	1:C:326:PRO:HD2	2.11	0.50
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.94	0.50
1:C:683:GLU:HB3	1:C:685:ILE:HD11	1.94	0.50
1:D:775:SER:HB2	1:D:789:TRP:HZ2	1.76	0.50
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.93	0.50
1:A:72:ILE:HD13	1:A:107:VAL:HG22	1.93	0.50
1:A:144:ASN:HD22	1:A:321:LEU:HD23	1.76	0.50
1:A:467:TYR:HE2	1:A:925:VAL:HG13	1.76	0.50
1:B:36:PRO:HG3	1:B:469:GLN:HG3	1.93	0.50
1:B:877:TYR:HA	1:B:880:SER:HB3	1.93	0.50
1:B:966:ASP:O	1:B:970:MET:HG2	2.10	0.50
1:F:182:TYR:O	1:F:769:LYS:HD3	2.11	0.50
1:F:372:VAL:HG22	1:F:405:LEU:HD11	1.93	0.50
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.93	0.50
1:A:391:ASN:O	1:A:395:MET:HG2	2.10	0.50
1:A:781:MET:HE2	1:C:225:VAL:HG22	1.93	0.50
1:B:267:LYS:N	1:B:267:LYS:HD2	2.25	0.50
1:B:1026:PHE:CD2	1:B:1026:PHE:C	2.89	0.50
1:D:401:ALA:O	1:D:405:LEU:HG	2.12	0.50
1:D:453:PHE:O	1:D:471:SER:OG	2.21	0.50
1:D:892:TYR:CD2	1:D:897:ILE:HG22	2.47	0.50
1:E:102:ILE:O	1:E:106:GLN:HG3	2.11	0.50
1:E:190:PRO:HB3	1:E:789:TRP:CD2	2.46	0.50
1:F:431:THR:HG21	1:F:490:PRO:O	2.12	0.50
1:C:112:GLN:OE1	1:C:115:MET:HG3	2.12	0.50
1:C:203:VAL:O	1:C:207:ILE:HG13	2.12	0.50
1:C:519:MET:O	1:C:523:SER:OG	2.26	0.50
1:C:744:ASN:O	1:C:748:THR:HG23	2.12	0.50
1:D:634:TRP:CD1	1:D:634:TRP:N	2.80	0.50
1:E:362:PHE:O	1:E:365:THR:HG22	2.11	0.50
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.94	0.50
1:B:412:VAL:HG22	1:B:438:ILE:HD11	1.93	0.50
1:C:447:MET:HE2	1:C:887:CYS:SG	2.52	0.50
1:E:16:ALA:HB2	1:E:488:LEU:HD13	1.94	0.50
1:E:298:ASN:HB3	1:E:301:ASP:HB2	1.92	0.50
1:E:339:GLU:HA	1:E:342:LYS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:404:LEU:HB3	1:F:478:MET:SD	2.51	0.50
1:F:896:SER:HB3	1:F:1033:PHE:CE1	2.47	0.50
1:F:987:MET:HB3	1:F:988:PRO:HD3	1.93	0.50
1:A:878:ALA:O	1:A:882:ILE:HG12	2.12	0.50
1:A:896:SER:HB3	1:A:1033:PHE:CD1	2.47	0.50
1:B:273:GLU:CD	1:B:770:LYS:HD2	2.36	0.50
1:B:531:VAL:O	1:B:534:ILE:HG23	2.12	0.50
1:C:359:LEU:O	1:C:361:ASN:N	2.43	0.50
1:D:191:ASN:O	1:D:193:LEU:N	2.44	0.50
1:D:414:GLU:CD	1:D:974:PRO:HG3	2.36	0.50
1:F:5:PHE:CE2	1:F:8:ARG:HD2	2.46	0.50
1:F:372:VAL:HA	1:F:405:LEU:HD13	1.93	0.50
1:F:959:GLY:HA3	1:F:1042:HIS:O	2.12	0.50
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.46	0.50
1:D:563:PHE:O	1:D:564:LEU:HD12	2.11	0.50
1:D:598:TYR:HB3	1:D:606:VAL:HG11	1.93	0.50
1:A:985:GLY:O	1:A:988:PRO:HD2	2.12	0.50
1:C:343:THR:HA	1:C:346:GLU:OE1	2.12	0.50
1:C:597:TYR:CD1	1:C:601:LYS:HD2	2.47	0.50
1:D:441:ALA:HB2	1:D:947:GLU:CD	2.37	0.50
1:D:907:LEU:HD21	1:D:1021:PHE:CB	2.41	0.50
1:E:163:LYS:HG2	1:E:163:LYS:O	2.12	0.50
1:E:240:LEU:HB2	1:E:246:PHE:CE1	2.47	0.50
1:E:668:LEU:HD12	1:E:672:VAL:HG12	1.94	0.50
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.12	0.50
1:A:62:THR:OG1	1:A:88:VAL:HG21	2.12	0.49
1:B:383:LEU:HD11	1:B:473:THR:HG23	1.94	0.49
1:C:1020:PHE:CD1	2:C:1101:LMT:H41	2.47	0.49
1:D:162:MET:HA	1:D:313:MET:SD	2.52	0.49
1:D:414:GLU:CG	1:D:974:PRO:HG3	2.42	0.49
1:F:133:SER:OG	1:F:293:LEU:O	2.28	0.49
1:F:194:ASN:OD1	1:F:798:MET:HG3	2.12	0.49
1:B:478:MET:O	1:B:482:VAL:HG12	2.12	0.49
1:B:696:THR:HG23	1:B:699:ARG:NH1	2.27	0.49
1:B:948:PHE:CD2	1:B:970:MET:HE3	2.46	0.49
1:C:979:SER:CB	1:C:1015:THR:HG21	2.43	0.49
1:D:362:PHE:O	1:D:365:THR:HG22	2.11	0.49
1:E:3:ASN:HA	1:E:6:ILE:HD12	1.93	0.49
1:E:46:SER:HA	1:E:88:VAL:O	2.12	0.49
1:F:969:ARG:HH11	1:F:970:MET:HB3	1.77	0.49
1:A:17:ILE:CG2	1:B:886:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:HA	1:A:880:SER:OG	2.13	0.49
1:B:151:GLN:OE1	1:B:278:ILE:HA	2.12	0.49
1:B:184:MET:HB3	1:B:771:VAL:HA	1.94	0.49
1:B:425:LEU:HD13	1:B:429:GLU:HG3	1.93	0.49
1:B:544:LEU:O	1:B:547:ILE:HB	2.12	0.49
1:E:484:VAL:HG13	1:E:488:LEU:HB3	1.93	0.49
1:F:139:VAL:HA	1:F:289:LEU:O	2.12	0.49
1:F:435:MET:CE	1:F:490:PRO:HB3	2.43	0.49
1:A:228:GLN:HG3	1:A:229:GLN:N	2.27	0.49
1:B:47:ALA:HB2	1:B:127:VAL:HG13	1.94	0.49
1:B:155:SER:O	1:B:158:VAL:HB	2.12	0.49
1:C:144:ASN:HB3	1:C:148:THR:HG23	1.95	0.49
1:D:83:ASP:OD1	1:D:815:ARG:HD3	2.13	0.49
1:D:623:ASN:OD1	1:D:623:ASN:N	2.45	0.49
1:E:654:ALA:O	1:E:658:ILE:HG12	2.11	0.49
1:E:862:MET:HE2	1:E:862:MET:HA	1.95	0.49
1:F:344:LEU:CD2	1:F:402:ILE:HD11	2.42	0.49
1:A:1037:ASN:HA	1:A:1038:GLU:O	2.12	0.49
1:A:1040:ILE:HG12	1:A:1041:GLU:H	1.77	0.49
1:B:61:VAL:HG21	1:B:122:VAL:HG21	1.95	0.49
1:B:905:VAL:HG13	1:B:935:ILE:HG23	1.94	0.49
1:C:11:PHE:C	1:C:11:PHE:CD2	2.91	0.49
1:C:35:TYR:HB3	1:C:38:ILE:HD12	1.94	0.49
1:C:968:VAL:CA	1:C:971:ARG:HH12	2.26	0.49
1:E:343:THR:OG1	1:E:989:LEU:HD21	2.13	0.49
1:F:480:LEU:O	1:F:484:VAL:HG23	2.13	0.49
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.21	0.49
1:A:348:ILE:HG22	1:A:349:ILE:HD13	1.94	0.49
1:A:549:VAL:O	1:A:552:MET:HE2	2.11	0.49
1:A:644:VAL:HG11	1:A:667:ASN:HB2	1.94	0.49
1:C:534:ILE:HD12	1:C:535:LEU:HD23	1.94	0.49
1:D:156:ASP:OD1	1:D:765:ARG:NH2	2.45	0.49
1:D:236:ALA:O	1:E:728:LYS:NZ	2.38	0.49
1:E:42:ALA:O	1:E:132:SER:N	2.27	0.49
1:E:172:VAL:HG22	1:E:306:ILE:HD11	1.93	0.49
1:E:904:VAL:HG12	1:E:938:SER:OG	2.11	0.49
1:B:76:MET:HE3	1:B:95:GLU:HA	1.93	0.49
1:B:394:THR:O	1:B:473:THR:HG21	2.12	0.49
1:B:668:LEU:HD23	1:B:668:LEU:H	1.77	0.49
1:C:1033:PHE:N	1:C:1034:SER:OG	2.27	0.49
1:A:17:ILE:HG22	1:B:886:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:VAL:HG13	1:A:488:LEU:HB3	1.93	0.49
1:B:736:ALA:HB1	1:B:741:VAL:HG23	1.94	0.49
1:C:154:ILE:O	1:C:157:TYR:N	2.45	0.49
1:C:904:VAL:HG21	1:C:942:ALA:HB2	1.94	0.49
1:C:945:ILE:HG12	1:C:971:ARG:CZ	2.43	0.49
1:D:445:ILE:HD13	1:D:940:LYS:HE3	1.95	0.49
1:E:32:VAL:HA	1:E:390:ILE:O	2.13	0.49
1:E:979:SER:CB	1:E:1015:THR:HG21	2.42	0.49
1:E:1016:VAL:O	1:E:1016:VAL:HG12	2.11	0.49
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.94	0.49
1:A:534:ILE:HG22	1:A:541:TYR:OH	2.13	0.49
1:A:776:GLU:HG2	1:A:777:ALA:H	1.77	0.49
1:C:244:GLU:O	1:C:247:GLY:N	2.46	0.49
1:D:163:LYS:O	1:D:163:LYS:HG2	2.12	0.49
1:D:696:THR:HG23	1:D:699:ARG:NH1	2.28	0.49
1:E:507:GLU:OE1	1:E:518:ARG:HG2	2.13	0.49
1:E:600:THR:C	1:E:602:GLU:H	2.21	0.49
1:A:537:SER:O	1:A:537:SER:OG	2.23	0.49
1:C:152:GLU:CD	1:C:152:GLU:H	2.20	0.49
1:C:904:VAL:O	1:C:907:LEU:HB2	2.12	0.49
1:D:78:MET:HE1	1:F:168:ARG:CZ	2.43	0.49
1:F:163:LYS:O	1:F:163:LYS:HG2	2.13	0.49
1:F:968:VAL:O	1:F:972:LEU:HB2	2.13	0.49
1:B:76:MET:HB2	1:B:93:THR:O	2.13	0.48
1:D:531:VAL:O	1:D:534:ILE:HG13	2.13	0.48
1:D:643:LYS:HZ2	1:D:993:THR:HG23	1.77	0.48
1:D:754:TRP:CZ3	1:F:219:LEU:HD23	2.48	0.48
1:F:112:GLN:HA	1:F:115:MET:HB2	1.94	0.48
1:F:154:ILE:HG22	1:F:287:SER:HB3	1.94	0.48
1:F:459:PHE:CE1	1:F:876:LEU:HG	2.48	0.48
1:A:76:MET:HB2	1:A:93:THR:O	2.13	0.48
1:A:574:THR:HG21	1:A:598:TYR:CE2	2.43	0.48
1:B:199:THR:HB	1:B:749:THR:HG21	1.95	0.48
1:B:307:ARG:HG2	1:B:325:TYR:CZ	2.49	0.48
1:B:672:VAL:O	1:B:673:GLU:HB3	2.13	0.48
1:C:527:TYR:HE2	1:C:968:VAL:HG13	1.77	0.48
1:C:885:PHE:HD2	1:C:886:LEU:HD13	1.78	0.48
1:D:445:ILE:CD1	1:D:940:LYS:HE3	2.43	0.48
1:A:393:LEU:CD1	1:A:466:ILE:HA	2.43	0.48
1:A:752:ALA:O	1:A:774:MET:HA	2.13	0.48
1:B:532:GLY:O	1:B:536:ARG:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:TYR:HB2	1:B:772:TYR:CZ	2.48	0.48
1:D:504:ASP:C	1:D:506:GLY:H	2.22	0.48
1:E:733:GLN:HE22	1:E:743:ILE:HG21	1.78	0.48
1:E:744:ASN:O	1:E:748:THR:HG23	2.13	0.48
1:E:922:THR:O	1:E:924:ASP:N	2.43	0.48
1:F:358:PHE:O	1:F:973:ARG:NH2	2.45	0.48
1:A:220:GLY:HA2	1:B:781:MET:HE3	1.95	0.48
1:A:751:GLY:O	1:A:754:TRP:N	2.45	0.48
1:B:355:MET:HE1	1:B:410:ILE:HG12	1.96	0.48
1:B:383:LEU:HD13	1:B:388:PHE:CD1	2.44	0.48
1:C:380:PHE:CD2	1:C:383:LEU:HD12	2.48	0.48
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.95	0.48
1:D:445:ILE:CG1	1:D:940:LYS:HE3	2.44	0.48
1:E:261:LEU:HD12	1:E:263:ARG:NH1	2.24	0.48
1:E:776:GLU:HG2	1:E:777:ALA:H	1.78	0.48
1:E:982:PHE:CD2	1:E:1011:MET:HG3	2.49	0.48
1:A:184:MET:HE2	1:A:268:ILE:HG23	1.95	0.48
1:A:536:ARG:HD2	2:A:1101:LMT:O4'	2.13	0.48
1:B:24:GLY:O	1:B:27:ILE:HG22	2.14	0.48
1:B:110:LYS:HD3	1:B:113:LEU:HD12	1.96	0.48
1:D:470:PHE:CD2	1:D:929:VAL:HG21	2.48	0.48
1:D:911:GLY:HA3	1:D:1013:THR:OG1	2.13	0.48
1:F:504:ASP:C	1:F:506:GLY:N	2.71	0.48
1:F:733:GLN:OE1	1:F:743:ILE:HG12	2.14	0.48
1:A:141:GLY:O	1:A:323:ILE:HA	2.14	0.48
1:A:412:VAL:O	1:A:416:VAL:HG23	2.13	0.48
1:A:655:PHE:HB3	1:A:663:VAL:HB	1.95	0.48
1:B:76:MET:SD	1:B:864:TYR:HE2	2.37	0.48
1:B:423:GLU:O	1:B:502:LYS:HD2	2.14	0.48
1:C:58:GLN:HA	1:C:62:THR:HB	1.96	0.48
1:C:197:GLN:HA	1:C:798:MET:SD	2.53	0.48
1:D:191:ASN:C	1:D:193:LEU:N	2.69	0.48
1:D:279:ALA:HB3	1:D:286:ALA:O	2.14	0.48
1:D:348:ILE:HG22	1:D:349:ILE:HD12	1.94	0.48
1:E:902:MET:O	1:E:905:VAL:HG23	2.14	0.48
1:F:456:MET:HB3	1:F:876:LEU:HD21	1.96	0.48
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.49	0.48
1:A:279:ALA:HB3	1:A:286:ALA:O	2.14	0.48
1:C:58:GLN:HG3	1:C:82:SER:OG	2.14	0.48
1:D:647:ILE:HG12	1:D:650:ARG:NH1	2.29	0.48
1:E:26:ALA:O	1:E:30:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:VAL:HA	1:F:162:MET:HE2	1.96	0.48
1:F:602:GLU:HB3	1:F:606:VAL:HG23	1.95	0.48
1:A:887:CYS:O	1:A:890:ALA:HB3	2.14	0.48
1:B:11:PHE:HD2	1:B:11:PHE:O	1.97	0.48
1:B:136:PHE:CD2	1:B:290:GLY:HA3	2.49	0.48
1:B:527:TYR:O	1:B:530:SER:HB3	2.14	0.48
1:C:182:TYR:HD2	1:C:765:ARG:NH2	2.12	0.48
1:C:967:ALA:HA	1:C:970:MET:HE2	1.96	0.48
1:D:137:LEU:HB2	1:D:293:LEU:HB2	1.96	0.48
1:D:141:GLY:HA3	1:D:324:VAL:HG12	1.95	0.48
1:E:527:TYR:O	1:E:531:VAL:HG23	2.14	0.48
1:E:586:ARG:O	1:E:589:LYS:HB3	2.14	0.48
1:F:452:VAL:C	1:F:455:PRO:HD2	2.38	0.48
1:A:902:MET:O	1:A:905:VAL:HG23	2.13	0.48
1:B:208:LYS:HE3	1:B:759:VAL:HG22	1.95	0.48
1:B:501:ALA:O	1:B:504:ASP:HB2	2.14	0.48
1:B:985:GLY:O	1:B:988:PRO:HD2	2.14	0.48
1:C:901:VAL:HG23	1:C:942:ALA:CB	2.44	0.48
1:E:210:GLN:O	1:E:237:GLN:NE2	2.44	0.48
1:E:844:MET:HA	1:E:844:MET:CE	2.44	0.48
1:F:941:ASN:HA	1:F:944:LEU:HD12	1.94	0.48
1:A:110:LYS:HD3	1:A:110:LYS:HA	1.59	0.48
1:A:216:ALA:HB1	1:A:234:ILE:CG2	2.44	0.48
1:B:153:ASP:OD2	1:B:182:TYR:OH	2.26	0.48
1:B:888:LEU:HD21	1:B:943:ILE:HD11	1.95	0.48
1:C:375:VAL:HB	1:C:405:LEU:HD22	1.96	0.48
1:E:291:ILE:HG21	1:E:306:ILE:HD11	1.96	0.48
1:F:380:PHE:O	1:F:383:LEU:HB2	2.14	0.48
1:F:452:VAL:O	1:F:455:PRO:HD2	2.14	0.48
1:A:446:ALA:CB	1:A:482:VAL:HG21	2.36	0.47
1:B:69:MET:HE1	1:B:107:VAL:HG13	1.96	0.47
1:B:845:GLU:HG2	1:B:857:TYR:CE1	2.48	0.47
1:C:479:ALA:O	1:C:482:VAL:HG23	2.14	0.47
1:C:1032:ARG:O	1:C:1033:PHE:HD1	1.97	0.47
1:D:233:SER:O	1:E:726:GLN:HB2	2.14	0.47
1:E:414:GLU:HG3	1:E:974:PRO:HB3	1.96	0.47
1:E:699:ARG:NH1	1:E:825:MET:HE1	2.28	0.47
1:F:47:ALA:HB1	1:F:122:VAL:HG13	1.96	0.47
1:A:359:LEU:C	1:A:361:ASN:H	2.21	0.47
1:A:758:TYR:HB2	1:A:772:TYR:CZ	2.49	0.47
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:649:MET:SD	1:C:653:ARG:NH2	2.87	0.47
1:C:960:LEU:HB2	1:C:1040:ILE:HG13	1.95	0.47
1:D:49:TYR:CE1	1:D:60:THR:HG21	2.48	0.47
1:E:318:PRO:HG2	1:E:321:LEU:HB2	1.96	0.47
1:F:987:MET:O	1:F:990:VAL:HG23	2.14	0.47
1:C:400:LEU:HD23	1:C:474:ILE:HD11	1.95	0.47
1:C:953:MET:HE3	1:C:953:MET:HB2	1.68	0.47
1:C:992:SER:HB3	1:C:997:SER:HB2	1.96	0.47
1:D:340:VAL:HG12	1:D:395:MET:HE3	1.96	0.47
1:D:542:LEU:O	1:D:546:LEU:HG	2.14	0.47
1:D:644:VAL:HG12	1:D:645:GLU:N	2.30	0.47
1:F:659:LYS:HA	1:F:659:LYS:HD3	1.63	0.47
1:A:420:MET:HB3	1:A:500:ILE:HB	1.96	0.47
1:A:444:GLY:O	1:A:448:VAL:HG23	2.13	0.47
1:A:641:GLU:HB2	1:A:650:ARG:NH2	2.29	0.47
1:A:841:MET:HG2	1:A:859:TRP:CH2	2.49	0.47
1:B:189:ASN:OD1	1:B:190:PRO:HD2	2.14	0.47
1:B:541:TYR:HH	2:B:1101:LMT:H6'	1.63	0.47
1:B:789:TRP:O	1:B:801:PHE:HD2	1.97	0.47
1:B:960:LEU:O	1:B:964:THR:HG23	2.14	0.47
1:C:186:ILE:HG22	1:C:773:VAL:HG23	1.96	0.47
1:C:409:ALA:O	1:C:413:VAL:HG23	2.14	0.47
1:D:586:ARG:O	1:D:590:VAL:HG23	2.14	0.47
1:E:11:PHE:HE2	1:E:15:ILE:HD11	1.78	0.47
1:E:597:TYR:OH	1:E:650:ARG:HG3	2.14	0.47
1:F:343:THR:HG21	1:F:989:LEU:CD2	2.44	0.47
1:A:166:ILE:HD11	1:A:310:LEU:HD13	1.97	0.47
1:A:276:ASP:HA	1:C:222:THR:HG21	1.96	0.47
1:B:270:LEU:HA	1:B:270:LEU:HD12	1.67	0.47
1:B:516:PHE:N	1:B:519:MET:HE2	2.29	0.47
1:B:521:GLU:HA	1:B:524:THR:HG23	1.97	0.47
1:B:767:ARG:HG2	1:B:767:ARG:HH11	1.79	0.47
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.96	0.47
1:C:143:ILE:HG22	1:C:286:ALA:CB	2.43	0.47
1:C:447:MET:SD	1:C:891:LEU:HD22	2.54	0.47
1:D:355:MET:HG3	1:D:359:LEU:HD12	1.96	0.47
1:D:456:MET:HE3	1:D:471:SER:HA	1.97	0.47
1:E:542:LEU:O	1:E:545:TYR:HB3	2.15	0.47
1:E:961:ILE:HG13	1:E:962:GLU:N	2.28	0.47
1:F:727:PHE:CZ	1:F:807:SER:HB2	2.49	0.47
1:A:225:VAL:H	1:B:781:MET:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:GLU:O	1:A:569:GLN:HG3	2.14	0.47
1:A:728:LYS:HB2	1:A:810:GLU:OE1	2.15	0.47
1:B:682:PHE:N	1:B:827:ILE:O	2.47	0.47
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.45	0.47
1:C:382:VAL:HG12	1:C:472:ILE:HD11	1.95	0.47
1:D:100:ALA:HB1	1:D:131:LYS:HD2	1.96	0.47
1:D:508:GLY:H	1:D:518:ARG:HG3	1.79	0.47
1:D:984:LEU:HA	1:D:984:LEU:HD23	1.71	0.47
1:E:544:LEU:O	1:E:548:ILE:HG13	2.15	0.47
1:F:780:ARG:O	1:F:781:MET:HE2	2.14	0.47
1:F:901:VAL:HG22	1:F:942:ALA:HB1	1.96	0.47
1:A:414:GLU:HG3	1:A:977:MET:HE1	1.96	0.47
1:A:818:ARG:HH22	1:A:823:PRO:HD3	1.79	0.47
1:B:428:LYS:HE2	1:B:494:ALA:O	2.14	0.47
1:B:459:PHE:O	1:B:464:GLY:HA3	2.13	0.47
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.62	0.47
1:B:588:GLN:HB2	1:B:613:ASN:HD22	1.79	0.47
1:B:728:LYS:HB2	1:B:810:GLU:OE1	2.15	0.47
1:B:953:MET:HE2	1:B:963:ALA:HB3	1.96	0.47
1:C:137:LEU:HD22	1:C:293:LEU:HD23	1.97	0.47
1:C:177:LEU:HD23	1:C:178:PHE:N	2.29	0.47
1:C:329:THR:O	1:C:332:PHE:HB3	2.14	0.47
1:C:574:THR:HG21	1:C:598:TYR:HE2	1.80	0.47
1:C:647:ILE:HG12	1:C:650:ARG:HH12	1.80	0.47
1:D:137:LEU:HD13	1:D:293:LEU:HB2	1.97	0.47
1:D:582:ALA:HA	1:D:586:ARG:HH21	1.79	0.47
1:D:933:THR:O	1:D:936:GLY:N	2.47	0.47
1:D:1040:ILE:HG23	1:D:1041:GLU:N	2.30	0.47
1:E:104:GLN:OE1	1:E:131:LYS:HD3	2.14	0.47
1:E:350:LEU:HD21	1:E:984:LEU:HB2	1.95	0.47
1:E:478:MET:O	1:E:482:VAL:HG12	2.14	0.47
1:E:858:ASP:OD1	1:E:859:TRP:N	2.48	0.47
1:E:886:LEU:HD12	1:E:886:LEU:HA	1.72	0.47
1:E:911:GLY:HA2	1:E:914:LEU:HD22	1.96	0.47
1:F:509:LYS:HB3	1:F:514:GLY:HA3	1.96	0.47
1:F:904:VAL:HG21	1:F:1022:VAL:HG22	1.96	0.47
1:A:783:PRO:HA	1:A:786:ILE:HG12	1.97	0.47
1:B:317:PHE:HE2	1:B:323:ILE:HD11	1.79	0.47
1:B:520:PHE:O	1:B:524:THR:HG22	2.14	0.47
1:B:910:ILE:HG23	1:B:911:GLY:N	2.30	0.47
1:C:11:PHE:HD2	1:C:11:PHE:C	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:VAL:HG13	1:C:118:LEU:HD13	1.96	0.47
1:C:1037:ASN:O	1:C:1038:GLU:HB2	2.15	0.47
1:F:776:GLU:HB2	1:F:779:TYR:CD1	2.50	0.47
1:F:937:LEU:HD13	1:F:1011:MET:SD	2.54	0.47
1:A:47:ALA:HB3	1:A:88:VAL:CG1	2.44	0.47
1:A:394:THR:HG22	1:A:473:THR:OG1	2.15	0.47
1:B:46:SER:HA	1:B:88:VAL:O	2.15	0.47
1:C:990:VAL:HG13	1:C:1005:THR:OG1	2.14	0.47
1:D:250:LEU:HD13	1:D:261:LEU:HD23	1.95	0.47
1:D:728:LYS:HG2	1:D:808:ARG:CZ	2.45	0.47
1:E:588:GLN:NE2	1:E:592:ASN:OD1	2.47	0.47
1:F:858:ASP:OD2	1:F:859:TRP:N	2.48	0.47
1:A:225:VAL:HG12	1:B:777:ALA:HB1	1.97	0.47
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.50	0.47
1:C:358:PHE:CG	1:C:977:MET:HE2	2.49	0.47
1:C:407:ASP:OD2	1:C:940:LYS:HD2	2.15	0.47
1:D:317:PHE:HA	1:D:318:PRO:HD3	1.60	0.47
1:D:518:ARG:O	1:D:522:LYS:HG3	2.15	0.47
1:E:987:MET:CB	1:E:1008:MET:HE1	2.45	0.47
1:F:451:ALA:HB3	1:F:884:VAL:HG22	1.97	0.47
1:A:383:LEU:HD11	1:A:473:THR:HG23	1.97	0.46
1:A:892:TYR:OH	1:A:943:ILE:HA	2.15	0.46
1:B:194:ASN:HA	1:B:798:MET:HE2	1.96	0.46
1:C:142:VAL:HG21	1:C:162:MET:HE1	1.96	0.46
1:C:363:ARG:O	1:C:367:ILE:HG13	2.14	0.46
1:C:907:LEU:HD21	1:C:1021:PHE:CB	2.44	0.46
1:D:162:MET:O	1:D:164:ASP:N	2.48	0.46
1:D:199:THR:CG2	1:D:791:VAL:HA	2.45	0.46
1:D:719:ASN:HB3	1:D:826:GLU:HG2	1.97	0.46
1:E:1001:ASN:HD22	1:E:1001:ASN:N	2.12	0.46
1:F:13:TRP:CH2	1:F:370:ILE:HD13	2.48	0.46
1:F:214:VAL:HG23	1:F:237:GLN:HB2	1.97	0.46
1:F:273:GLU:CD	1:F:770:LYS:HD2	2.39	0.46
1:F:425:LEU:HD13	1:F:429:GLU:HG3	1.96	0.46
1:F:898:PRO:O	1:F:902:MET:HG2	2.15	0.46
1:F:986:VAL:HG11	1:F:1007:VAL:HG12	1.97	0.46
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.96	0.46
1:A:680:PHE:HB2	1:A:859:TRP:CZ3	2.48	0.46
1:B:164:ASP:HA	1:B:167:SER:HB3	1.96	0.46
1:B:182:TYR:O	1:B:769:LYS:HD3	2.14	0.46
1:B:254:ASN:HB2	1:B:258:SER:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ILE:O	1:B:406:VAL:HG23	2.15	0.46
1:D:168:ARG:HB3	1:E:75:LEU:HD22	1.97	0.46
1:D:587:THR:OG1	1:D:622:GLN:O	2.14	0.46
1:D:971:ARG:C	1:D:971:ARG:CZ	2.88	0.46
1:A:45:ILE:HD12	1:A:90:ILE:HD12	1.96	0.46
1:A:457:ALA:HB2	1:A:471:SER:OG	2.15	0.46
1:A:648:THR:HG21	1:A:666:PHE:HA	1.97	0.46
1:B:235:ILE:HB	1:C:728:LYS:HA	1.98	0.46
1:C:343:THR:HG21	1:C:989:LEU:HD21	1.97	0.46
1:C:364:ALA:O	1:C:368:PRO:HD3	2.15	0.46
1:C:527:TYR:O	1:C:531:VAL:HG23	2.15	0.46
1:D:841:MET:HG2	1:D:859:TRP:CH2	2.50	0.46
1:E:726:GLN:CD	1:E:812:GLY:HA3	2.40	0.46
1:E:844:MET:HA	1:E:844:MET:HE2	1.96	0.46
1:A:445:ILE:HD12	1:A:446:ALA:N	2.30	0.46
1:A:1027:VAL:O	1:A:1031:ARG:HG3	2.15	0.46
1:B:571:VAL:HG12	1:B:668:LEU:HD21	1.98	0.46
1:C:480:LEU:O	1:C:484:VAL:HG23	2.15	0.46
1:D:26:ALA:O	1:D:30:LEU:HB2	2.15	0.46
1:D:108:GLN:OE1	1:D:129:VAL:HB	2.15	0.46
1:D:900:SER:HA	1:D:1025:PHE:HB3	1.97	0.46
1:F:156:ASP:OD2	1:F:769:LYS:NZ	2.47	0.46
1:F:576:VAL:HG22	1:F:663:VAL:HG22	1.97	0.46
1:F:736:ALA:HB1	1:F:741:VAL:HG23	1.97	0.46
1:A:244:GLU:C	1:A:246:PHE:N	2.73	0.46
1:A:335:ILE:O	1:A:339:GLU:HG2	2.16	0.46
1:A:524:THR:O	1:A:527:TYR:HB3	2.16	0.46
1:A:525:HIS:HA	1:A:528:THR:HG22	1.96	0.46
1:A:1035:ARG:C	1:A:1037:ASN:H	2.23	0.46
1:B:57:VAL:HG11	1:B:86:GLY:O	2.15	0.46
1:B:140:VAL:HG11	1:B:310:LEU:HD21	1.96	0.46
1:B:261:LEU:HD12	1:B:263:ARG:NH1	2.31	0.46
1:B:536:ARG:NH1	2:B:1101:LMT:O4'	2.48	0.46
1:B:776:GLU:O	1:B:780:ARG:HG2	2.16	0.46
1:C:61:VAL:HG21	1:C:122:VAL:HG21	1.98	0.46
1:C:356:TYR:C	1:C:358:PHE:H	2.23	0.46
1:D:979:SER:CB	1:D:1015:THR:HG21	2.46	0.46
1:E:160:ALA:HA	1:E:767:ARG:NH2	2.31	0.46
1:E:987:MET:O	1:E:990:VAL:HG23	2.16	0.46
1:F:818:ARG:HH12	1:F:823:PRO:HG3	1.80	0.46
1:F:897:ILE:HG23	1:F:946:VAL:CG1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:MET:HA	1:A:313:MET:SD	2.56	0.46
1:A:538:THR:O	1:A:542:LEU:HD13	2.15	0.46
1:B:36:PRO:HD3	1:B:391:ASN:CG	2.39	0.46
1:B:753:ALA:O	1:B:775:SER:HB3	2.16	0.46
1:D:225:VAL:HG13	1:E:781:MET:SD	2.56	0.46
1:E:418:ARG:HD3	1:E:970:MET:HB2	1.98	0.46
1:F:311:ALA:HA	1:F:314:GLU:CD	2.41	0.46
1:F:751:GLY:O	1:F:753:ALA:N	2.49	0.46
1:A:906:PRO:HA	1:A:909:VAL:HB	1.96	0.46
1:B:597:TYR:OH	1:B:650:ARG:HG3	2.16	0.46
1:C:527:TYR:CE2	1:C:968:VAL:HG13	2.50	0.46
1:C:668:LEU:HA	1:C:677:ALA:HA	1.97	0.46
1:D:135:SER:HB3	1:D:672:VAL:HG11	1.98	0.46
1:D:965:LEU:HA	1:D:965:LEU:HD23	1.63	0.46
1:E:291:ILE:HG21	1:E:306:ILE:CD1	2.45	0.46
1:E:903:LEU:O	1:E:906:PRO:HD2	2.15	0.46
1:A:539:GLY:O	1:A:542:LEU:HB2	2.15	0.46
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.96	0.46
1:B:261:LEU:HD12	1:B:263:ARG:HH12	1.81	0.46
1:B:459:PHE:CD1	1:B:876:LEU:HD12	2.50	0.46
1:B:767:ARG:HG2	1:B:767:ARG:NH1	2.31	0.46
1:C:35:TYR:HE1	1:C:670:ALA:HB1	1.80	0.46
1:C:167:SER:HA	1:C:175:VAL:HG21	1.98	0.46
1:C:415:ASN:O	1:C:419:VAL:HG23	2.15	0.46
1:E:225:VAL:HG13	1:F:781:MET:SD	2.55	0.46
1:E:356:TYR:HE1	1:E:362:PHE:N	2.13	0.46
1:E:520:PHE:O	1:E:524:THR:HG23	2.16	0.46
1:E:978:THR:O	1:E:982:PHE:N	2.47	0.46
1:F:361:ASN:HB3	1:F:364:ALA:CB	2.46	0.46
1:F:415:ASN:O	1:F:419:VAL:HG23	2.16	0.46
1:F:435:MET:HE3	1:F:490:PRO:HB3	1.96	0.46
1:F:452:VAL:HG13	1:F:884:VAL:HG23	1.98	0.46
1:F:1020:PHE:CZ	2:F:1101:LMT:H31	2.51	0.46
1:A:504:ASP:O	1:A:506:GLY:N	2.49	0.46
1:B:412:VAL:O	1:B:416:VAL:HG23	2.15	0.46
1:B:415:ASN:HB3	1:B:434:SER:OG	2.16	0.46
1:C:144:ASN:O	1:C:148:THR:HG23	2.16	0.46
1:C:504:ASP:C	1:C:506:GLY:N	2.74	0.46
1:C:937:LEU:HA	1:C:937:LEU:HD23	1.50	0.46
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.97	0.46
1:E:200:PRO:HB2	1:E:749:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:HD12	1:B:27:ILE:HA	1.66	0.46
1:B:509:LYS:HE2	1:B:509:LYS:HB3	1.63	0.46
1:C:898:PRO:HA	1:C:901:VAL:HG12	1.98	0.46
1:E:589:LYS:O	1:E:592:ASN:HB2	2.15	0.46
1:F:80:SER:HB3	1:F:90:ILE:HG23	1.97	0.46
1:F:352:PHE:HA	1:F:355:MET:HE3	1.97	0.46
1:F:959:GLY:HA3	1:F:1043:SER:HA	1.98	0.46
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.46	0.45
1:A:523:SER:O	1:A:526:HIS:HB2	2.16	0.45
1:B:1032:ARG:O	1:B:1033:PHE:HB2	2.15	0.45
1:C:778:LYS:HG3	1:C:779:TYR:CE1	2.51	0.45
1:D:58:GLN:OE1	1:D:63:GLN:NE2	2.49	0.45
1:D:592:ASN:O	1:D:596:HIS:HB2	2.15	0.45
1:E:231:ASN:HB2	1:F:583:THR:HG22	1.97	0.45
1:E:348:ILE:HG12	1:E:372:VAL:HG21	1.97	0.45
1:E:594:VAL:HG22	1:E:655:PHE:CE2	2.52	0.45
1:F:445:ILE:HG23	1:F:940:LYS:HG3	1.98	0.45
1:A:174:ASP:HB3	1:A:292:LYS:HB2	1.99	0.45
1:B:562:SER:OG	1:B:563:PHE:N	2.46	0.45
1:B:1038:GLU:CG	1:B:1039:ASP:H	2.29	0.45
1:C:730:ASP:OD2	1:C:808:ARG:NH2	2.49	0.45
1:C:947:GLU:HG3	1:C:948:PHE:N	2.30	0.45
1:D:602:GLU:OE2	1:D:650:ARG:NH1	2.50	0.45
1:D:680:PHE:HB2	1:D:859:TRP:HZ3	1.82	0.45
1:A:30:LEU:HD11	1:A:384:ALA:HA	1.97	0.45
1:A:244:GLU:O	1:A:246:PHE:N	2.49	0.45
1:A:491:ALA:O	1:A:495:THR:OG1	2.22	0.45
1:B:139:VAL:HG13	1:B:178:PHE:CE1	2.52	0.45
1:B:953:MET:HE3	1:B:953:MET:HB2	1.49	0.45
1:C:493:CYS:O	1:C:497:LEU:HB2	2.17	0.45
1:D:74:ASN:HB3	1:D:95:GLU:CG	2.46	0.45
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.98	0.45
1:E:953:MET:HB2	1:E:953:MET:HE3	1.43	0.45
1:F:6:ILE:C	1:F:8:ARG:H	2.23	0.45
1:F:410:ILE:HD13	1:F:977:MET:HG2	1.99	0.45
1:A:281:PHE:HD1	1:A:610:PHE:HD1	1.63	0.45
1:A:650:ARG:O	1:A:653:ARG:HB3	2.16	0.45
1:B:181:GLN:HG2	1:B:182:TYR:N	2.30	0.45
1:B:277:ILE:H	1:B:277:ILE:HG13	1.68	0.45
1:B:435:MET:HE2	1:B:490:PRO:HG3	1.98	0.45
1:B:682:PHE:C	1:B:682:PHE:CD2	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:903:LEU:O	1:B:906:PRO:HD2	2.16	0.45
1:D:412:VAL:HG22	1:D:438:ILE:HD12	1.97	0.45
1:D:520:PHE:HE2	1:D:973:ARG:HG3	1.80	0.45
1:D:960:LEU:O	1:D:964:THR:HG23	2.16	0.45
1:E:105:VAL:HG23	1:F:109:ASN:OD1	2.16	0.45
1:E:412:VAL:O	1:E:416:VAL:HG23	2.16	0.45
1:E:613:ASN:HD22	1:E:614:GLY:H	1.64	0.45
1:F:2:PRO:HB2	1:F:3:ASN:H	1.59	0.45
1:F:380:PHE:CD2	1:F:383:LEU:HD12	2.42	0.45
1:F:1022:VAL:HA	1:F:1025:PHE:HD1	1.82	0.45
1:F:1025:PHE:O	1:F:1029:VAL:HG23	2.16	0.45
1:A:244:GLU:C	1:A:246:PHE:H	2.25	0.45
1:A:459:PHE:CE2	1:A:876:LEU:HD12	2.52	0.45
1:B:108:GLN:CD	1:C:112:GLN:HG3	2.42	0.45
1:B:198:LEU:HA	1:B:198:LEU:HD23	1.79	0.45
1:B:758:TYR:OH	1:B:761:ASP:OD1	2.35	0.45
1:C:368:PRO:HA	1:C:409:ALA:HB1	1.98	0.45
1:C:699:ARG:HD3	1:C:825:MET:SD	2.56	0.45
1:C:1011:MET:O	1:C:1015:THR:HG23	2.17	0.45
1:D:527:TYR:OH	1:D:1019:ILE:O	2.19	0.45
1:D:538:THR:HG21	1:D:1028:VAL:HG22	1.98	0.45
1:D:752:ALA:O	1:D:774:MET:HA	2.16	0.45
1:E:230:LEU:HG	1:E:231:ASN:N	2.30	0.45
1:F:30:LEU:HA	1:F:31:PRO:HD3	1.88	0.45
1:F:363:ARG:O	1:F:367:ILE:HG13	2.17	0.45
1:F:1018:ALA:O	1:F:1022:VAL:HG23	2.16	0.45
1:F:1030:ARG:HH11	1:F:1033:PHE:HD2	1.64	0.45
1:A:692:HIS:NE2	1:A:723:ASP:OD1	2.50	0.45
1:B:138:MET:HE3	1:B:138:MET:HB2	1.61	0.45
1:B:457:ALA:HB2	1:B:471:SER:CB	2.46	0.45
1:B:743:ILE:H	1:B:743:ILE:HG13	1.65	0.45
1:B:919:ARG:HB3	1:B:921:LEU:CD2	2.46	0.45
1:C:149:MET:HB2	1:C:153:ASP:CB	2.47	0.45
1:C:1034:SER:O	1:C:1035:ARG:HG2	2.16	0.45
1:D:13:TRP:CE2	1:D:492:LEU:HD21	2.51	0.45
1:D:344:LEU:HD23	1:D:402:ILE:HD11	1.97	0.45
1:D:368:PRO:HG3	1:D:413:VAL:HG21	1.99	0.45
1:D:953:MET:HB2	1:D:953:MET:HE3	1.43	0.45
1:D:959:GLY:CA	1:D:1039:ASP:HA	2.47	0.45
1:E:225:VAL:HG12	1:F:777:ALA:HB1	1.98	0.45
1:E:574:THR:HG21	1:E:598:TYR:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:PHE:HE2	1:F:15:ILE:HD11	1.81	0.45
1:F:34:GLN:CG	1:F:333:VAL:HG22	2.47	0.45
1:F:38:ILE:CG2	1:F:462:SER:HB2	2.43	0.45
1:F:497:LEU:HA	1:F:497:LEU:HD12	1.50	0.45
1:F:507:GLU:HG2	1:F:518:ARG:HG3	1.99	0.45
1:F:893:GLU:O	1:F:893:GLU:HG3	2.16	0.45
1:B:519:MET:O	1:B:523:SER:OG	2.33	0.45
1:B:764:ASP:OD1	1:B:765:ARG:HG3	2.17	0.45
1:B:799:VAL:HG12	1:B:800:PRO:O	2.16	0.45
1:C:733:GLN:OE1	1:C:743:ILE:HG21	2.16	0.45
1:C:1044:HIS:HB2	1:C:1045:THR:H	1.45	0.45
1:E:36:PRO:HD3	1:E:391:ASN:CG	2.42	0.45
1:E:457:ALA:HB2	1:E:471:SER:OG	2.17	0.45
1:E:1008:MET:HE3	1:E:1008:MET:HB2	1.85	0.45
1:F:11:PHE:CE2	1:F:15:ILE:HD11	2.51	0.45
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.52	0.45
1:F:595:THR:HG23	1:F:609:VAL:HB	1.98	0.45
1:A:75:LEU:HD11	1:A:92:LEU:HB3	1.99	0.45
1:A:393:LEU:HD13	1:A:466:ILE:HA	1.99	0.45
1:A:424:GLY:HA3	1:A:502:LYS:CG	2.37	0.45
1:A:449:LEU:HB3	1:A:478:MET:SD	2.57	0.45
1:A:902:MET:HE3	1:A:902:MET:HB2	1.84	0.45
1:B:13:TRP:HA	1:B:13:TRP:CE3	2.52	0.45
1:B:300:LEU:CD2	1:B:334:LYS:HG3	2.47	0.45
1:C:189:ASN:O	1:C:193:LEU:N	2.49	0.45
1:C:872:GLN:C	1:C:874:PRO:HD2	2.41	0.45
1:E:834:GLY:C	1:E:835:LYS:HE2	2.42	0.45
1:F:375:VAL:HG11	1:F:405:LEU:HB3	1.99	0.45
1:A:200:PRO:HB2	1:A:749:THR:HG22	1.99	0.45
1:A:542:LEU:HD11	1:A:1028:VAL:HG21	1.98	0.45
1:A:1034:SER:HA	1:A:1035:ARG:CB	2.46	0.45
1:B:344:LEU:HD11	1:B:398:MET:CE	2.47	0.45
1:B:767:ARG:NH2	1:C:67:GLN:HE22	2.14	0.45
1:D:184:MET:HE2	1:D:268:ILE:HG23	1.99	0.45
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.99	0.45
1:E:361:ASN:O	1:E:365:THR:HB	2.17	0.45
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.52	0.45
1:E:1021:PHE:HA	1:E:1024:VAL:HG23	1.98	0.45
1:F:789:TRP:O	1:F:801:PHE:HD2	2.00	0.45
1:F:885:PHE:HE1	1:F:899:PHE:CE2	2.35	0.45
1:F:910:ILE:O	1:F:914:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:O	1:A:112:GLN:HG2	2.17	0.45
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.83	0.45
1:A:703:LEU:CD2	1:A:718:PRO:HD3	2.46	0.45
1:B:682:PHE:CD2	1:B:827:ILE:HD12	2.52	0.45
1:C:684:LEU:HD11	1:C:851:LEU:HD11	1.99	0.45
1:C:686:ASP:HB3	1:C:823:PRO:O	2.17	0.45
1:C:717:ARG:NH2	1:C:828:LEU:HD13	2.32	0.45
1:D:223:PRO:HD3	1:E:275:TYR:CD1	2.52	0.45
1:E:310:LEU:CD1	1:E:323:ILE:HG12	2.46	0.45
1:E:440:GLY:C	1:E:891:LEU:HD11	2.42	0.45
1:E:687:GLN:HG3	1:E:822:LEU:HD13	1.99	0.45
1:F:371:ALA:O	1:F:375:VAL:HG23	2.17	0.45
1:F:486:LEU:O	1:F:490:PRO:HG2	2.17	0.45
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.53	0.44
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.99	0.44
1:B:145:THR:HA	1:B:284:GLN:OE1	2.17	0.44
1:B:185:ARG:HD3	1:B:772:TYR:HB2	1.98	0.44
1:D:239:ARG:HD2	1:D:761:ASP:O	2.16	0.44
1:E:47:ALA:O	1:E:87:THR:HA	2.18	0.44
1:F:746:ILE:HG22	1:F:791:VAL:HG21	1.99	0.44
1:A:712:MET:HE3	1:A:843:LEU:HG	1.98	0.44
1:A:785:ASP:O	1:A:789:TRP:HD1	2.00	0.44
1:A:793:ALA:HB3	1:A:795:ASP:OD2	2.17	0.44
1:B:507:GLU:O	1:B:509:LYS:N	2.50	0.44
1:C:200:PRO:CG	1:C:749:THR:HG22	2.47	0.44
1:C:453:PHE:CD2	1:C:456:MET:HE2	2.52	0.44
1:D:460:GLY:H	1:D:872:GLN:HE22	1.65	0.44
1:D:487:ILE:C	1:D:490:PRO:HD2	2.42	0.44
1:D:498:LYS:HG3	1:D:499:PRO:HD2	1.99	0.44
1:F:121:GLU:O	1:F:124:GLN:HG2	2.17	0.44
1:F:850:LYS:HG3	1:F:850:LYS:O	2.17	0.44
1:B:843:LEU:HD13	1:B:847:LEU:HG	2.00	0.44
1:B:904:VAL:O	1:B:907:LEU:HB2	2.18	0.44
1:C:841:MET:HG2	1:C:859:TRP:CH2	2.51	0.44
1:C:1041:GLU:HB3	1:C:1042:HIS:CB	2.36	0.44
1:D:212:ALA:HA	1:D:239:ARG:HD3	1.99	0.44
1:E:417:GLU:HG2	1:E:497:LEU:HD21	2.00	0.44
1:E:542:LEU:HA	1:E:542:LEU:HD23	1.68	0.44
1:E:659:LYS:HB3	1:E:659:LYS:HE3	1.60	0.44
1:F:587:THR:HG21	1:F:623:ASN:HA	1.98	0.44
1:A:66:GLU:OE1	1:A:821:GLY:HA2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.98	0.44
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.74	0.44
1:A:400:LEU:HG	1:A:933:THR:OG1	2.18	0.44
1:A:442:LEU:O	1:A:445:ILE:HG13	2.17	0.44
1:A:776:GLU:HB3	1:A:779:TYR:CD1	2.53	0.44
1:A:971:ARG:O	1:A:975:ILE:HG13	2.17	0.44
1:B:143:ILE:HG22	1:B:286:ALA:HB2	2.00	0.44
1:B:228:GLN:HG3	1:B:229:GLN:H	1.82	0.44
1:B:417:GLU:HA	1:B:420:MET:HE3	1.98	0.44
1:B:686:ASP:OD1	1:B:690:LEU:HG	2.17	0.44
1:B:996:GLY:O	1:B:1000:GLN:HG3	2.17	0.44
1:C:696:THR:HG23	1:C:825:MET:HE1	1.98	0.44
1:D:915:ALA:HB2	1:D:1009:GLY:HA3	1.99	0.44
1:D:982:PHE:HD2	1:D:1011:MET:HG3	1.82	0.44
1:E:327:TYR:HB2	1:E:628:PHE:CE2	2.53	0.44
1:E:607:GLU:HG3	1:E:607:GLU:O	2.17	0.44
1:E:892:TYR:O	1:E:893:GLU:HB2	2.16	0.44
1:E:950:LYS:HZ3	1:E:1030:ARG:HE	1.64	0.44
1:F:479:ALA:O	1:F:482:VAL:HG23	2.17	0.44
1:A:34:GLN:HB2	1:A:333:VAL:HG22	1.98	0.44
1:A:274:ASN:OD1	1:A:276:ASP:HB2	2.17	0.44
1:A:352:PHE:HD2	1:A:353:LEU:HD23	1.82	0.44
1:A:579:PRO:HD3	1:A:661:ALA:HB2	2.00	0.44
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.52	0.44
1:B:211:ASN:ND2	1:B:760:ASN:HD22	2.16	0.44
1:B:228:GLN:HG3	1:B:229:GLN:N	2.32	0.44
1:B:1045:THR:HB	1:B:1047:ASP:H	1.82	0.44
1:D:242:SER:O	1:D:246:PHE:HD1	2.00	0.44
1:E:674:LEU:HB3	1:E:675:GLY:H	1.40	0.44
1:E:1034:SER:HB3	1:E:1035:ARG:H	1.59	0.44
1:F:892:TYR:CD1	1:F:897:ILE:HG21	2.53	0.44
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.63	0.44
1:A:960:LEU:HD21	1:A:1027:VAL:HG13	1.99	0.44
1:B:119:PRO:O	1:B:123:GLN:HG3	2.18	0.44
1:B:211:ASN:O	1:B:760:ASN:ND2	2.44	0.44
1:B:293:LEU:HG	1:B:299:ALA:HA	1.99	0.44
1:B:545:TYR:HB2	1:B:1021:PHE:CE2	2.53	0.44
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.82	0.44
1:B:982:PHE:O	1:B:985:GLY:N	2.50	0.44
1:B:1044:HIS:CE1	1:B:1045:THR:HG1	2.36	0.44
1:C:188:MET:SD	1:C:200:PRO:HG3	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:VAL:HG12	1:C:355:MET:HE2	1.99	0.44
1:C:713:LEU:HD11	1:C:843:LEU:HD12	1.99	0.44
1:D:55:LYS:NZ	1:F:238:THR:OG1	2.23	0.44
1:D:168:ARG:C	1:E:75:LEU:HD22	2.42	0.44
1:D:456:MET:HE3	1:D:471:SER:CA	2.48	0.44
1:E:448:VAL:HG13	1:E:884:VAL:HG13	2.00	0.44
1:E:762:PHE:HD2	1:E:771:VAL:HG22	1.83	0.44
1:F:54:ALA:HB1	1:F:816:LEU:HG	2.00	0.44
1:F:908:GLY:O	1:F:1010:GLY:HA2	2.18	0.44
1:A:47:ALA:HB3	1:A:88:VAL:HG13	1.99	0.44
1:A:177:LEU:HD23	1:A:178:PHE:N	2.32	0.44
1:A:216:ALA:HB3	1:A:234:ILE:O	2.17	0.44
1:A:536:ARG:NH1	2:A:1101:LMT:O3B	2.51	0.44
1:A:818:ARG:NH1	1:A:823:PRO:HG3	2.25	0.44
1:D:193:LEU:HD13	1:D:200:PRO:HD3	2.00	0.44
1:D:438:ILE:O	1:D:441:ALA:HB3	2.17	0.44
1:D:877:TYR:O	1:D:881:LEU:HB2	2.17	0.44
1:E:246:PHE:O	1:E:249:ILE:HG23	2.18	0.44
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.99	0.44
1:E:428:LYS:HG2	1:E:494:ALA:HB1	1.99	0.44
1:E:727:PHE:CZ	1:E:807:SER:HB2	2.53	0.44
1:F:964:THR:O	1:F:968:VAL:HB	2.17	0.44
1:F:971:ARG:C	1:F:974:PRO:HD2	2.43	0.44
2:F:1101:LMT:H72	2:F:1101:LMT:H101	1.40	0.44
1:A:708:LYS:HB3	1:A:708:LYS:HE3	1.73	0.44
1:B:204:ILE:HG23	1:B:759:VAL:HG21	2.00	0.44
1:B:300:LEU:HD23	1:B:334:LYS:HG3	2.00	0.44
1:B:643:LYS:O	1:B:645:GLU:N	2.51	0.44
1:C:307:ARG:NH2	1:C:311:ALA:HB2	2.32	0.44
1:C:344:LEU:HD11	1:C:376:LEU:HD11	1.98	0.44
1:C:647:ILE:HG12	1:C:650:ARG:NH1	2.33	0.44
1:C:746:ILE:HG13	1:C:747:ASN:H	1.81	0.44
1:D:60:THR:HG23	1:D:61:VAL:HG23	2.00	0.44
1:E:166:ILE:HG12	1:E:306:ILE:HG23	1.99	0.44
1:E:327:TYR:HB2	1:E:628:PHE:CZ	2.53	0.44
1:E:515:TRP:O	1:E:519:MET:HG3	2.17	0.44
1:E:637:ARG:HD2	1:E:642:ASN:O	2.18	0.44
1:E:952:LEU:HB2	1:E:963:ALA:HB1	2.00	0.44
1:F:200:PRO:HB2	1:F:749:THR:HG22	2.00	0.44
1:F:492:LEU:O	1:F:496:MET:HG2	2.18	0.44
1:F:521:GLU:O	1:F:524:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:603:LYS:HE3	1:F:603:LYS:HB2	1.80	0.44
1:A:21:LEU:HA	1:A:21:LEU:HD13	1.71	0.44
2:A:1101:LMT:H21	2:A:1101:LMT:H51	1.66	0.44
1:B:143:ILE:HG12	1:B:322:LYS:O	2.18	0.44
1:B:190:PRO:HG3	1:B:779:TYR:HB3	2.00	0.44
1:B:787:GLY:C	1:B:789:TRP:H	2.26	0.44
1:B:952:LEU:HD13	1:B:966:ASP:HB3	2.00	0.44
1:C:472:ILE:O	1:C:476:SER:HB3	2.18	0.44
1:D:139:VAL:HA	1:D:289:LEU:O	2.18	0.44
1:D:805:SER:O	1:D:805:SER:OG	2.35	0.44
1:E:343:THR:HA	1:E:346:GLU:OE1	2.18	0.44
1:F:355:MET:HE3	1:F:355:MET:HB2	1.75	0.44
1:A:184:MET:HB3	1:A:771:VAL:HG13	2.00	0.43
1:A:622:GLN:NE2	1:C:222:THR:HG22	2.33	0.43
1:A:659:LYS:HA	1:A:659:LYS:HD3	1.48	0.43
1:A:726:GLN:CD	1:C:235:ILE:HD11	2.43	0.43
1:A:986:VAL:HG12	1:A:1008:MET:HE3	1.99	0.43
1:B:361:ASN:OD1	1:B:498:LYS:HD2	2.17	0.43
1:B:726:GLN:CD	1:B:812:GLY:HA3	2.43	0.43
1:B:958:LYS:HB3	1:B:963:ALA:HB2	2.00	0.43
1:B:1040:ILE:HG23	1:B:1041:GLU:H	1.83	0.43
1:C:144:ASN:O	1:C:284:GLN:NE2	2.50	0.43
1:C:524:THR:O	1:C:527:TYR:HB3	2.18	0.43
1:C:580:ALA:HB1	1:C:724:THR:HG22	2.00	0.43
1:D:228:GLN:HG3	1:D:229:GLN:N	2.33	0.43
1:D:413:VAL:O	1:D:417:GLU:HG2	2.18	0.43
1:E:47:ALA:HB3	1:E:88:VAL:HB	1.98	0.43
1:E:61:VAL:HG21	1:E:122:VAL:HG21	2.00	0.43
1:E:178:PHE:HD1	1:E:288:GLY:HA3	1.82	0.43
1:E:182:TYR:O	1:E:769:LYS:HD3	2.17	0.43
1:E:459:PHE:HD1	1:E:467:TYR:CG	2.36	0.43
1:A:7:ASP:O	1:A:8:ARG:HG3	2.18	0.43
1:A:166:ILE:HD13	1:A:166:ILE:HA	1.65	0.43
1:A:346:GLU:O	1:A:349:ILE:N	2.51	0.43
1:A:870:GLY:O	1:A:871:ASN:HB2	2.18	0.43
1:C:694:LYS:HA	1:C:697:GLN:OE1	2.18	0.43
1:D:108:GLN:NE2	1:E:109:ASN:HB3	2.32	0.43
1:D:259:ARG:NH1	1:E:734:GLU:OE2	2.51	0.43
1:D:460:GLY:N	1:D:872:GLN:HE22	2.15	0.43
1:E:147:GLY:C	1:E:149:MET:H	2.26	0.43
1:E:162:MET:C	1:E:164:ASP:N	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.47	0.43
1:E:578:LEU:HB2	1:E:623:ASN:O	2.18	0.43
1:F:667:ASN:O	1:F:678:THR:OG1	2.22	0.43
1:A:66:GLU:OE2	1:A:80:SER:OG	2.30	0.43
1:A:225:VAL:H	1:B:781:MET:CE	2.31	0.43
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.72	0.43
1:A:534:ILE:HG22	1:A:541:TYR:CZ	2.53	0.43
1:B:76:MET:HG2	1:B:864:TYR:OH	2.18	0.43
1:B:112:GLN:HA	1:B:115:MET:HG2	2.00	0.43
1:B:706:ALA:CB	1:B:716:VAL:HG11	2.46	0.43
1:B:805:SER:O	1:B:805:SER:OG	2.32	0.43
1:C:509:LYS:HD2	1:C:509:LYS:HA	1.70	0.43
1:C:690:LEU:O	1:C:694:LYS:HB2	2.19	0.43
1:C:698:ALA:O	1:C:701:GLN:HB3	2.18	0.43
1:C:888:LEU:HD23	1:C:888:LEU:HA	1.75	0.43
1:C:944:LEU:HB3	1:C:971:ARG:CD	2.45	0.43
1:C:1034:SER:OG	1:C:1035:ARG:N	2.48	0.43
1:D:138:MET:HE1	1:D:303:ALA:HA	2.01	0.43
1:D:449:LEU:O	1:D:453:PHE:HD1	2.02	0.43
1:E:132:SER:O	1:E:132:SER:OG	2.27	0.43
1:E:241:THR:N	1:E:245:GLU:OE1	2.52	0.43
1:F:2:PRO:O	1:F:5:PHE:HB3	2.18	0.43
1:F:42:ALA:HA	1:F:92:LEU:O	2.17	0.43
1:F:376:LEU:O	1:F:377:LEU:C	2.61	0.43
1:B:184:MET:HA	1:B:184:MET:HE3	1.99	0.43
1:B:715:SER:O	1:B:715:SER:OG	2.29	0.43
1:C:492:LEU:HA	1:C:495:THR:OG1	2.18	0.43
1:C:559:LEU:HD11	1:C:916:ALA:HB1	1.99	0.43
1:C:757:SER:O	1:C:772:TYR:HA	2.17	0.43
1:D:247:GLY:O	1:D:261:LEU:HB3	2.19	0.43
1:D:904:VAL:HG21	1:D:942:ALA:CB	2.47	0.43
1:E:690:LEU:HB2	1:E:694:LYS:HB2	2.00	0.43
1:A:448:VAL:O	1:A:451:ALA:HB3	2.19	0.43
1:A:459:PHE:CE1	1:A:876:LEU:HD12	2.53	0.43
1:A:818:ARG:NH2	1:A:823:PRO:HD3	2.33	0.43
1:B:211:ASN:ND2	1:B:246:PHE:HZ	2.17	0.43
1:B:424:GLY:HA3	1:B:502:LYS:HB2	2.01	0.43
1:B:520:PHE:O	1:B:523:SER:OG	2.36	0.43
1:B:1033:PHE:HA	1:B:1034:SER:HA	1.78	0.43
1:C:163:LYS:O	1:C:163:LYS:HG2	2.17	0.43
1:D:217:GLY:HA2	1:E:755:GLY:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:GLY:N	1:D:275:TYR:OH	2.50	0.43
1:D:393:LEU:HD22	1:D:470:PHE:HE1	1.84	0.43
1:D:698:ALA:O	1:D:701:GLN:HB3	2.18	0.43
1:D:743:ILE:H	1:D:743:ILE:HD12	1.83	0.43
1:E:166:ILE:O	1:E:169:THR:HB	2.19	0.43
1:E:686:ASP:HB2	1:E:695:LEU:HD21	1.99	0.43
1:F:135:SER:CB	1:F:673:GLU:HB3	2.35	0.43
1:F:379:THR:O	1:F:382:VAL:HB	2.18	0.43
1:F:560:PRO:HB2	1:F:836:SER:OG	2.18	0.43
1:F:671:ILE:CG2	1:F:674:LEU:HB2	2.48	0.43
1:A:75:LEU:CD1	1:A:92:LEU:HB3	2.49	0.43
1:A:250:LEU:HD11	1:A:259:ARG:HD2	2.00	0.43
1:A:485:ALA:O	1:A:490:PRO:HD3	2.18	0.43
1:A:508:GLY:O	1:A:509:LYS:C	2.61	0.43
1:A:900:SER:HB3	1:A:1029:VAL:HG21	2.01	0.43
1:A:903:LEU:HA	1:A:903:LEU:HD23	1.65	0.43
1:A:926:TYR:HE1	1:A:999:ALA:HB1	1.83	0.43
1:B:480:LEU:O	1:B:484:VAL:HG23	2.18	0.43
1:C:1032:ARG:O	1:C:1033:PHE:CD1	2.71	0.43
1:D:904:VAL:O	1:D:907:LEU:HB2	2.18	0.43
1:D:925:VAL:HA	1:D:928:GLN:OE1	2.17	0.43
1:E:52:ALA:HB3	1:E:57:VAL:HG12	2.01	0.43
1:E:525:HIS:O	1:E:526:HIS:C	2.60	0.43
1:F:565:PRO:O	1:F:567:GLU:HG2	2.19	0.43
1:A:634:TRP:CD1	1:A:634:TRP:N	2.77	0.43
1:A:757:SER:O	1:A:772:TYR:HA	2.19	0.43
1:A:862:MET:HG3	1:A:863:SER:H	1.84	0.43
1:B:136:PHE:HD2	1:B:290:GLY:HA3	1.82	0.43
1:B:194:ASN:OD1	1:B:798:MET:HE2	2.19	0.43
1:C:363:ARG:CZ	1:C:363:ARG:H	2.32	0.43
1:C:523:SER:HA	1:C:526:HIS:HB2	2.00	0.43
1:C:549:VAL:O	1:C:552:MET:HB3	2.18	0.43
1:C:955:LYS:O	1:C:956:GLU:HG2	2.18	0.43
1:C:1027:VAL:O	1:C:1031:ARG:HG3	2.19	0.43
1:D:971:ARG:NH1	1:D:971:ARG:N	2.64	0.43
1:E:455:PRO:O	1:E:876:LEU:HD13	2.18	0.43
1:E:743:ILE:O	1:E:746:ILE:HB	2.19	0.43
1:F:54:ALA:HB3	1:F:813:SER:O	2.18	0.43
1:F:140:VAL:HG11	1:F:310:LEU:CD2	2.49	0.43
1:F:405:LEU:HD12	1:F:406:VAL:N	2.34	0.43
1:A:668:LEU:HD23	1:A:668:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:ASP:OD1	1:A:689:GLY:N	2.48	0.43
1:A:1040:ILE:HG23	1:A:1041:GLU:N	2.33	0.43
1:B:193:LEU:HA	1:B:193:LEU:HD23	1.71	0.43
1:B:350:LEU:HD13	1:B:984:LEU:O	2.18	0.43
1:B:709:HIS:CE1	1:B:847:LEU:HD21	2.54	0.43
1:D:203:VAL:O	1:D:207:ILE:HG13	2.19	0.43
1:D:343:THR:O	1:D:344:LEU:C	2.61	0.43
1:D:678:THR:HA	1:D:837:THR:OG1	2.19	0.43
1:E:177:LEU:HA	1:E:289:LEU:HD23	2.00	0.43
1:E:702:LEU:HD12	1:E:702:LEU:HA	1.81	0.43
1:E:885:PHE:HD1	1:E:902:MET:HE1	1.83	0.43
1:E:888:LEU:HA	1:E:888:LEU:HD23	1.70	0.43
1:E:948:PHE:CD2	1:E:970:MET:HE2	2.53	0.43
1:F:270:LEU:HD12	1:F:270:LEU:HA	1.89	0.43
1:F:396:PHE:O	1:F:400:LEU:HB2	2.19	0.43
1:A:156:ASP:OD2	1:A:182:TYR:HB2	2.19	0.43
1:A:355:MET:HE1	1:A:410:ILE:HD11	2.01	0.43
1:A:641:GLU:HA	1:A:646:ALA:HB3	1.99	0.43
1:B:214:VAL:HG23	1:B:237:GLN:HB3	2.00	0.43
1:B:331:PRO:O	1:B:335:ILE:HD13	2.19	0.43
1:B:423:GLU:HA	1:B:502:LYS:HZ3	1.84	0.43
1:B:641:GLU:HA	1:B:646:ALA:HB3	2.01	0.43
1:B:704:ALA:O	1:B:708:LYS:HE3	2.19	0.43
1:C:102:ILE:HD13	1:C:102:ILE:HA	1.89	0.43
1:E:571:VAL:HG13	1:E:628:PHE:HE1	1.83	0.43
1:E:583:THR:HG22	1:E:584:GLN:N	2.33	0.43
1:E:880:SER:O	1:E:884:VAL:HG23	2.19	0.43
1:F:3:ASN:ND2	1:F:486:LEU:HD22	2.33	0.43
1:F:157:TYR:O	1:F:161:ASN:HB2	2.18	0.43
1:F:239:ARG:CZ	1:F:761:ASP:HB2	2.49	0.43
1:F:343:THR:HG21	1:F:989:LEU:HD23	2.00	0.43
1:F:598:TYR:CE2	1:F:629:VAL:HG21	2.53	0.43
1:A:259:ARG:NH2	1:A:261:LEU:HD11	2.34	0.43
1:A:906:PRO:C	1:A:908:GLY:N	2.76	0.43
1:B:187:TRP:HA	1:B:774:MET:O	2.19	0.43
1:B:310:LEU:HA	1:B:313:MET:HE3	2.01	0.43
1:B:523:SER:O	1:B:526:HIS:HB2	2.19	0.43
1:C:634:TRP:C	1:C:636:ASP:H	2.26	0.43
1:C:907:LEU:HD21	1:C:1021:PHE:HB3	2.01	0.43
1:D:49:TYR:HE1	1:D:60:THR:HG21	1.84	0.43
1:D:973:ARG:HB3	1:D:974:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1040:ILE:HG12	1:D:1041:GLU:H	1.84	0.43
1:E:180:SER:OG	1:E:273:GLU:N	2.52	0.43
1:F:188:MET:HA	1:F:266:ALA:HB2	1.99	0.43
1:F:361:ASN:HB3	1:F:364:ALA:HB3	2.00	0.43
1:F:511:GLY:O	1:F:512:PHE:CD2	2.72	0.43
1:F:534:ILE:HG22	2:F:1101:LMT:H5'	1.99	0.43
1:F:583:THR:O	1:F:587:THR:HG23	2.19	0.43
1:F:752:ALA:O	1:F:774:MET:HA	2.19	0.43
1:A:167:SER:O	1:B:70:ASN:HB2	2.19	0.42
1:A:225:VAL:HG11	1:B:778:LYS:HA	2.01	0.42
1:C:110:LYS:HA	1:C:110:LYS:HD3	1.86	0.42
1:C:659:LYS:HD3	1:C:659:LYS:HA	1.39	0.42
1:C:943:ILE:O	1:C:947:GLU:HB3	2.19	0.42
1:D:75:LEU:HD23	1:F:168:ARG:HB3	2.01	0.42
1:D:76:MET:HE3	1:D:95:GLU:HA	2.00	0.42
1:D:351:VAL:HG22	1:D:981:ALA:HB1	2.01	0.42
1:D:654:ALA:O	1:D:658:ILE:HG12	2.18	0.42
1:E:43:VAL:HA	1:E:130:GLU:O	2.19	0.42
1:E:652:THR:OG1	1:E:665:ALA:HB3	2.18	0.42
1:E:869:SER:HB2	1:E:872:GLN:NE2	2.33	0.42
1:F:15:ILE:O	1:F:19:ILE:HG13	2.19	0.42
1:F:463:THR:HG22	1:F:467:TYR:CZ	2.55	0.42
1:F:751:GLY:O	1:F:754:TRP:N	2.52	0.42
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.59	0.42
1:A:58:GLN:O	1:A:63:GLN:HG3	2.19	0.42
1:A:699:ARG:NH1	1:A:825:MET:SD	2.91	0.42
1:A:712:MET:O	1:A:832:ALA:N	2.50	0.42
1:A:953:MET:HE3	1:A:953:MET:HB2	1.78	0.42
1:B:10:ILE:HB	1:C:893:GLU:CD	2.44	0.42
1:B:277:ILE:HD12	1:B:277:ILE:O	2.18	0.42
1:B:668:LEU:H	1:B:668:LEU:CD2	2.33	0.42
1:B:790:TYR:HB3	1:B:798:MET:HE3	2.02	0.42
1:C:777:ALA:O	1:C:781:MET:HE3	2.19	0.42
1:C:851:LEU:HB3	1:C:852:PRO:HD2	2.00	0.42
1:C:904:VAL:O	1:C:904:VAL:HG12	2.18	0.42
1:D:655:PHE:HB3	1:D:663:VAL:HB	2.01	0.42
1:D:768:VAL:HG12	1:E:63:GLN:OE1	2.19	0.42
1:D:919:ARG:HG2	1:D:920:GLY:H	1.83	0.42
1:D:949:ALA:HA	1:D:967:ALA:HB2	2.01	0.42
1:E:53:ASP:O	1:E:57:VAL:HG13	2.18	0.42
1:E:187:TRP:HA	1:E:774:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:965:LEU:HD23	1:E:965:LEU:HA	1.86	0.42
1:F:39:ALA:HA	1:F:40:PRO:HD2	1.87	0.42
1:F:311:ALA:HA	1:F:314:GLU:HG3	2.01	0.42
1:A:633:ASP:OD1	1:A:635:ALA:HB3	2.19	0.42
1:B:13:TRP:HA	1:B:13:TRP:HE3	1.83	0.42
1:B:453:PHE:CD2	1:B:456:MET:HE2	2.54	0.42
1:B:455:PRO:HG2	1:B:880:SER:HB2	2.01	0.42
1:B:1016:VAL:HG13	2:B:1101:LMT:H102	2.01	0.42
1:C:101:ASP:O	1:C:105:VAL:HG23	2.19	0.42
1:C:133:SER:O	1:C:134:SER:HB2	2.19	0.42
1:C:182:TYR:HD2	1:C:765:ARG:HH22	1.67	0.42
1:C:213:GLN:HG2	1:C:239:ARG:HG3	2.02	0.42
1:C:274:ASN:OD1	1:C:276:ASP:HB2	2.20	0.42
1:C:897:ILE:HB	1:C:898:PRO:HD3	2.01	0.42
1:D:367:ILE:HD13	1:D:493:CYS:HA	2.01	0.42
1:D:690:LEU:HD11	1:D:853:THR:O	2.18	0.42
1:D:858:ASP:OD2	1:D:859:TRP:N	2.50	0.42
1:E:30:LEU:HD12	1:E:30:LEU:HA	1.83	0.42
1:E:102:ILE:HD12	1:E:102:ILE:HA	1.73	0.42
1:E:728:LYS:HB2	1:E:810:GLU:OE1	2.19	0.42
1:F:247:GLY:O	1:F:261:LEU:HB3	2.19	0.42
1:F:261:LEU:HD12	1:F:263:ARG:NH1	2.33	0.42
1:F:588:GLN:OE1	1:F:592:ASN:ND2	2.42	0.42
1:F:634:TRP:CD1	1:F:634:TRP:N	2.82	0.42
1:F:731:ILE:O	1:F:731:ILE:HG13	2.19	0.42
1:F:991:ILE:O	1:F:991:ILE:HG23	2.19	0.42
1:F:1022:VAL:N	1:F:1023:PRO:HD2	2.34	0.42
1:A:242:SER:OG	1:A:245:GLU:HG2	2.19	0.42
1:A:622:GLN:HE21	1:C:222:THR:HG22	1.84	0.42
1:B:368:PRO:HA	1:B:371:ALA:HB3	2.00	0.42
1:B:448:VAL:HG13	1:B:884:VAL:HG22	2.01	0.42
1:D:152:GLU:CD	1:D:152:GLU:H	2.28	0.42
1:E:61:VAL:CG2	1:E:122:VAL:HG21	2.49	0.42
1:E:434:SER:O	1:E:438:ILE:HG12	2.20	0.42
1:E:1010:GLY:O	1:E:1014:ALA:HB2	2.20	0.42
1:F:189:ASN:OD1	1:F:190:PRO:HD2	2.20	0.42
1:F:525:HIS:O	1:F:526:HIS:C	2.62	0.42
1:A:41:PRO:HG2	1:A:94:PHE:CB	2.41	0.42
1:A:889:ALA:N	1:A:898:PRO:HG3	2.34	0.42
1:B:575:MET:HB3	1:B:626:ILE:CG1	2.49	0.42
1:B:576:VAL:HG22	1:B:663:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.76	0.42
1:C:364:ALA:HA	1:C:367:ILE:CD1	2.49	0.42
1:C:492:LEU:O	1:C:496:MET:HG2	2.19	0.42
1:C:536:ARG:NH2	2:C:1101:LMT:H3O1	2.09	0.42
1:C:762:PHE:CE1	1:C:764:ASP:HB2	2.54	0.42
1:C:923:ASN:HA	1:C:927:PHE:CD2	2.55	0.42
1:D:151:GLN:H	1:D:151:GLN:NE2	2.17	0.42
1:D:186:ILE:HG12	1:D:268:ILE:HG12	2.02	0.42
1:D:751:GLY:O	1:D:754:TRP:N	2.53	0.42
1:D:838:GLY:O	1:D:841:MET:HB2	2.20	0.42
1:F:348:ILE:HG13	1:F:402:ILE:HD13	2.01	0.42
1:F:355:MET:SD	1:F:368:PRO:HB2	2.60	0.42
1:F:863:SER:HA	1:F:866:GLU:HB3	2.01	0.42
1:F:905:VAL:HG13	1:F:935:ILE:HG12	2.01	0.42
1:A:151:GLN:HG2	1:A:152:GLU:N	2.34	0.42
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.50	0.42
1:B:66:GLU:OE1	1:B:821:GLY:HA2	2.18	0.42
1:D:225:VAL:HG12	1:E:777:ALA:HB1	2.01	0.42
1:E:448:VAL:HG13	1:E:884:VAL:HG22	2.01	0.42
1:E:460:GLY:O	1:E:463:THR:OG1	2.38	0.42
1:F:134:SER:H	1:F:292:LYS:HD3	1.84	0.42
1:F:753:ALA:HA	1:F:775:SER:HB3	2.02	0.42
1:A:75:LEU:CD2	1:C:168:ARG:HD3	2.50	0.42
1:A:831:ALA:HB1	1:A:835:LYS:HB3	2.02	0.42
1:B:61:VAL:CG2	1:B:122:VAL:HG21	2.50	0.42
1:B:139:VAL:HG13	1:B:178:PHE:HE1	1.85	0.42
1:B:281:PHE:O	1:B:284:GLN:HB2	2.20	0.42
1:B:504:ASP:C	1:B:506:GLY:H	2.27	0.42
1:B:675:GLY:C	1:B:677:ALA:H	2.28	0.42
1:C:958:LYS:CB	1:C:963:ALA:HB2	2.50	0.42
1:D:76:MET:HB2	1:D:93:THR:O	2.20	0.42
1:D:344:LEU:HD13	1:D:376:LEU:CD1	2.46	0.42
1:D:505:HIS:HD2	1:D:521:GLU:CD	2.28	0.42
1:D:563:PHE:CE2	1:D:674:LEU:HD22	2.55	0.42
1:E:189:ASN:ND2	1:E:192:GLU:OE2	2.53	0.42
1:E:514:GLY:C	1:E:516:PHE:N	2.74	0.42
1:E:649:MET:O	1:E:653:ARG:HB2	2.20	0.42
1:E:758:TYR:HB2	1:E:772:TYR:CZ	2.54	0.42
1:F:163:LYS:HD2	1:F:177:LEU:HD12	2.02	0.42
1:A:30:LEU:HA	1:A:31:PRO:HD3	1.89	0.42
1:A:457:ALA:HB1	1:A:468:ARG:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:TRP:HH2	1:C:230:LEU:HD21	1.85	0.42
1:B:300:LEU:HD11	1:B:333:VAL:HG12	2.01	0.42
1:B:355:MET:HG3	1:B:359:LEU:HD12	2.01	0.42
1:C:252:LYS:O	1:C:260:VAL:HG23	2.20	0.42
1:C:356:TYR:HD1	1:C:365:THR:HG21	1.85	0.42
1:C:379:THR:HG23	1:C:476:SER:OG	2.19	0.42
1:E:324:VAL:HG12	1:E:326:PRO:HD3	2.01	0.42
1:F:249:ILE:O	1:F:262:LEU:N	2.52	0.42
1:F:588:GLN:HB2	1:F:613:ASN:HD22	1.85	0.42
1:F:892:TYR:HD1	1:F:897:ILE:HG21	1.84	0.42
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.96	0.42
1:B:231:ASN:ND2	1:C:622:GLN:CD	2.77	0.42
1:B:911:GLY:O	1:B:914:LEU:HB3	2.20	0.42
1:C:447:MET:O	1:C:451:ALA:HB2	2.20	0.42
1:C:567:GLU:OE1	1:C:996:GLY:HA2	2.19	0.42
1:C:587:THR:HG21	1:C:623:ASN:HA	2.02	0.42
1:D:138:MET:HG2	1:D:291:ILE:HB	2.01	0.42
1:D:489:THR:O	1:D:493:CYS:HB2	2.19	0.42
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.61	0.42
1:E:536:ARG:NH1	2:E:1101:LMT:H4B	2.35	0.42
1:E:751:GLY:C	1:E:753:ALA:N	2.77	0.42
1:E:960:LEU:O	1:E:964:THR:HG23	2.19	0.42
1:F:778:LYS:HG3	1:F:779:TYR:CE1	2.55	0.42
1:A:937:LEU:HD23	1:A:937:LEU:HA	1.53	0.42
1:B:634:TRP:CD1	1:B:634:TRP:N	2.79	0.42
1:C:445:ILE:HG23	1:C:940:LYS:HG3	2.01	0.42
1:C:940:LYS:O	1:C:943:ILE:HB	2.19	0.42
1:D:453:PHE:CE2	1:D:474:ILE:HG21	2.54	0.42
1:D:534:ILE:HG13	1:D:534:ILE:H	1.66	0.42
1:D:818:ARG:HH12	1:D:823:PRO:HG3	1.85	0.42
1:D:1037:ASN:HA	1:D:1038:GLU:C	2.44	0.42
1:E:270:LEU:HD12	1:E:270:LEU:HA	1.87	0.42
1:E:508:GLY:N	1:E:518:ARG:HG3	2.35	0.42
1:E:834:GLY:O	1:E:835:LYS:HE2	2.20	0.42
1:E:851:LEU:HB3	1:E:852:PRO:HD2	2.01	0.42
1:F:36:PRO:HD3	1:F:391:ASN:CG	2.44	0.42
1:F:36:PRO:HD3	1:F:391:ASN:ND2	2.35	0.42
1:F:973:ARG:NE	1:F:977:MET:HE1	2.35	0.42
1:A:300:LEU:HD11	1:A:333:VAL:HG11	2.02	0.41
1:A:471:SER:O	1:A:475:VAL:HG23	2.20	0.41
1:B:445:ILE:HG21	1:B:940:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:885:PHE:CD1	1:C:898:PRO:HB3	2.55	0.41
1:D:520:PHE:O	1:D:524:THR:HG22	2.20	0.41
1:D:556:PHE:CD1	1:D:913:LEU:HD21	2.54	0.41
1:D:764:ASP:HB3	1:D:769:LYS:HD2	2.02	0.41
1:D:862:MET:HG3	1:D:863:SER:H	1.85	0.41
1:E:267:LYS:HD3	1:E:776:GLU:OE2	2.20	0.41
1:E:281:PHE:CE1	1:E:608:SER:HB2	2.54	0.41
1:E:564:LEU:CD1	1:E:671:ILE:HD12	2.50	0.41
1:E:790:TYR:CE1	1:E:800:PRO:HB3	2.55	0.41
1:E:892:TYR:CD2	1:E:897:ILE:HG22	2.55	0.41
1:E:1041:GLU:HB3	1:E:1042:HIS:CA	2.50	0.41
1:F:49:TYR:N	1:F:86:GLY:O	2.41	0.41
1:F:182:TYR:HD1	1:F:182:TYR:HA	1.73	0.41
1:F:777:ALA:O	1:F:781:MET:HG2	2.20	0.41
1:A:102:ILE:HD12	1:C:101:ASP:HB3	2.02	0.41
1:A:138:MET:HE2	1:A:138:MET:HB3	1.88	0.41
1:B:177:LEU:HD23	1:B:178:PHE:N	2.36	0.41
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.51	0.41
1:B:420:MET:HB3	1:B:500:ILE:HB	2.02	0.41
1:C:15:ILE:O	1:C:19:ILE:HG13	2.20	0.41
1:C:30:LEU:HD13	1:C:384:ALA:HB2	2.02	0.41
1:C:75:LEU:HA	1:C:94:PHE:HD2	1.85	0.41
1:C:159:ALA:HB2	1:C:177:LEU:HD11	2.02	0.41
1:C:211:ASN:ND2	1:C:246:PHE:HZ	2.18	0.41
1:C:228:GLN:HG3	1:C:229:GLN:N	2.36	0.41
1:C:280:GLU:OE2	1:C:588:GLN:NE2	2.49	0.41
1:C:360:GLN:HB3	1:C:513:PHE:CE2	2.55	0.41
1:D:219:LEU:HD12	1:D:232:ALA:HB3	2.02	0.41
1:E:58:GLN:O	1:E:62:THR:HB	2.19	0.41
1:E:147:GLY:C	1:E:149:MET:N	2.77	0.41
1:E:451:ALA:O	1:E:880:SER:OG	2.34	0.41
1:F:23:GLY:O	1:F:27:ILE:HG23	2.19	0.41
1:F:193:LEU:HD23	1:F:193:LEU:HA	1.76	0.41
1:F:987:MET:HB3	1:F:987:MET:HE2	1.88	0.41
1:A:141:GLY:O	1:A:323:ILE:HG23	2.20	0.41
1:A:456:MET:HB3	1:A:877:TYR:OH	2.20	0.41
1:A:992:SER:O	1:A:997:SER:HB2	2.20	0.41
1:B:251:LEU:HD21	1:B:262:LEU:HD13	2.02	0.41
1:B:420:MET:HG2	1:B:425:LEU:O	2.21	0.41
1:B:888:LEU:HA	1:B:888:LEU:HD23	1.71	0.41
1:C:931:LEU:HD23	1:C:931:LEU:HA	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:LYS:HG3	1:D:289:LEU:HD21	2.01	0.41
1:D:700:ASN:HA	1:D:703:LEU:HD12	2.02	0.41
1:D:775:SER:HB2	1:D:789:TRP:CZ2	2.54	0.41
1:F:208:LYS:HE3	1:F:759:VAL:HG13	2.02	0.41
1:A:457:ALA:O	1:A:468:ARG:NE	2.28	0.41
1:A:782:LEU:HA	1:A:783:PRO:HD3	1.85	0.41
1:A:905:VAL:HG13	1:A:935:ILE:HD13	2.01	0.41
1:A:946:VAL:HG22	1:A:1026:PHE:HB2	2.03	0.41
1:B:249:ILE:HD13	1:B:249:ILE:HG21	1.83	0.41
1:B:390:ILE:HG23	1:B:395:MET:CG	2.51	0.41
1:B:1038:GLU:HG3	1:B:1039:ASP:H	1.85	0.41
1:C:151:GLN:OE1	1:C:151:GLN:N	2.54	0.41
1:C:189:ASN:O	1:C:193:LEU:HG	2.21	0.41
1:C:273:GLU:CD	1:C:770:LYS:HD2	2.45	0.41
1:D:190:PRO:HB3	1:D:789:TRP:CZ2	2.54	0.41
1:D:340:VAL:CG1	1:D:395:MET:HE3	2.50	0.41
1:D:602:GLU:OE1	1:D:647:ILE:HG23	2.20	0.41
1:D:618:ALA:O	1:D:815:ARG:NH2	2.54	0.41
1:D:781:MET:CE	1:F:225:VAL:H	2.33	0.41
1:E:148:THR:HG21	1:E:319:SER:OG	2.20	0.41
1:E:402:ILE:HG22	1:E:406:VAL:HG23	2.01	0.41
1:E:482:VAL:O	1:E:485:ALA:HB3	2.20	0.41
1:E:907:LEU:HD21	1:E:1021:PHE:HB3	2.02	0.41
1:F:418:ARG:O	1:F:422:GLU:HB2	2.20	0.41
1:A:3:ASN:O	1:A:6:ILE:HG13	2.20	0.41
1:A:188:MET:HB2	1:A:188:MET:HE3	1.79	0.41
1:A:463:THR:O	1:A:466:ILE:HB	2.20	0.41
1:A:480:LEU:HA	1:A:480:LEU:HD23	1.73	0.41
1:A:575:MET:O	1:A:575:MET:HG3	2.18	0.41
1:A:678:THR:O	1:A:678:THR:OG1	2.36	0.41
1:B:407:ASP:O	1:B:411:VAL:HG23	2.20	0.41
1:B:662:MET:HE3	1:B:664:PHE:CE2	2.55	0.41
1:C:121:GLU:OE1	1:C:121:GLU:N	2.49	0.41
1:D:5:PHE:HD2	1:D:12:ALA:HB2	1.85	0.41
1:D:26:ALA:HB1	1:D:384:ALA:CB	2.50	0.41
1:D:74:ASN:HB3	1:D:95:GLU:HG3	2.03	0.41
1:D:235:ILE:HD11	1:E:726:GLN:CD	2.45	0.41
1:E:184:MET:HB2	1:E:762:PHE:CE2	2.56	0.41
1:E:327:TYR:CD2	1:E:327:TYR:C	2.99	0.41
1:E:364:ALA:HB2	1:E:497:LEU:HD11	2.01	0.41
1:E:578:LEU:HD13	1:E:661:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:783:PRO:O	1:E:786:ILE:HB	2.20	0.41
1:E:841:MET:O	1:E:845:GLU:HG3	2.20	0.41
1:F:352:PHE:CD2	1:F:353:LEU:HD23	2.53	0.41
1:F:602:GLU:OE2	1:F:650:ARG:HD2	2.20	0.41
1:F:666:PHE:N	1:F:666:PHE:CD1	2.88	0.41
1:F:900:SER:OG	1:F:1026:PHE:HD1	2.04	0.41
1:A:58:GLN:NE2	1:A:818:ARG:NH1	2.69	0.41
1:A:576:VAL:HG22	1:A:663:VAL:HG22	2.02	0.41
1:B:255:GLN:H	1:B:255:GLN:HG3	1.29	0.41
1:B:343:THR:O	1:B:344:LEU:C	2.64	0.41
1:C:1011:MET:HE3	1:C:1015:THR:CG2	2.51	0.41
1:D:27:ILE:HD11	1:D:380:PHE:CD1	2.56	0.41
1:D:393:LEU:HB3	1:D:470:PHE:CE1	2.55	0.41
1:D:603:LYS:HE2	1:D:603:LYS:HB3	1.91	0.41
1:D:921:LEU:HA	1:D:921:LEU:HD13	1.84	0.41
1:F:982:PHE:CD2	1:F:1011:MET:HG2	2.52	0.41
1:A:143:ILE:HG22	1:A:286:ALA:HB2	2.02	0.41
1:A:182:TYR:HD1	1:A:182:TYR:HA	1.66	0.41
1:A:714:THR:HB	1:A:830:GLN:HB2	2.03	0.41
1:B:373:PRO:O	1:B:376:LEU:HB2	2.20	0.41
1:B:524:THR:O	1:B:527:TYR:HB3	2.20	0.41
1:C:53:ASP:OD1	1:C:56:THR:OG1	2.35	0.41
1:C:725:PRO:HG3	1:C:811:TYR:HE1	1.85	0.41
1:D:61:VAL:CG2	1:D:122:VAL:HG21	2.42	0.41
1:D:822:LEU:HA	1:D:823:PRO:HD3	1.95	0.41
1:D:932:LEU:HD23	1:D:932:LEU:HA	1.75	0.41
1:E:108:GLN:HA	1:E:129:VAL:HG21	2.03	0.41
1:E:357:LEU:O	1:E:358:PHE:HD1	2.04	0.41
1:E:868:LEU:HD23	1:E:868:LEU:HA	1.73	0.41
1:E:1034:SER:O	1:E:1035:ARG:HB2	2.19	0.41
1:F:45:ILE:H	1:F:45:ILE:HG13	1.54	0.41
1:F:967:ALA:HA	1:F:970:MET:HE2	2.02	0.41
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	2.03	0.41
1:B:80:SER:HB3	1:B:818:ARG:HB2	2.03	0.41
1:B:166:ILE:CD1	1:B:310:LEU:HD13	2.51	0.41
1:B:551:GLY:O	1:B:552:MET:C	2.64	0.41
1:B:682:PHE:HB3	1:B:827:ILE:HB	2.02	0.41
1:B:1038:GLU:HG3	1:B:1040:ILE:HB	2.01	0.41
1:C:587:THR:H	1:C:587:THR:HG23	1.62	0.41
1:C:944:LEU:HD13	1:C:975:ILE:HG12	2.03	0.41
1:D:225:VAL:H	1:E:781:MET:CE	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:531:VAL:HB	1:D:965:LEU:HD21	2.02	0.41
1:D:659:LYS:HD3	1:D:659:LYS:HA	1.76	0.41
1:D:754:TRP:CE3	1:F:234:ILE:HD11	2.56	0.41
1:D:888:LEU:HD13	1:D:898:PRO:O	2.21	0.41
1:D:959:GLY:HA2	1:D:1039:ASP:HA	2.02	0.41
1:E:6:ILE:HG23	1:E:494:ALA:HB2	2.03	0.41
1:F:11:PHE:C	1:F:11:PHE:CD2	2.99	0.41
1:F:559:LEU:HA	1:F:560:PRO:HD2	1.80	0.41
1:F:1041:GLU:OE1	1:F:1044:HIS:ND1	2.54	0.41
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.53	0.41
1:A:81:ASN:O	1:A:88:VAL:HA	2.21	0.41
1:A:375:VAL:CG2	1:A:481:SER:HA	2.51	0.41
1:A:728:LYS:HE3	1:A:730:ASP:HB2	2.03	0.41
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	2.02	0.41
1:A:957:GLY:O	1:A:1041:GLU:HA	2.21	0.41
1:B:3:ASN:O	1:B:6:ILE:HB	2.21	0.41
1:B:108:GLN:HE22	1:C:112:GLN:CB	2.29	0.41
1:B:375:VAL:HG22	1:B:484:VAL:HG21	2.02	0.41
1:B:448:VAL:HG13	1:B:884:VAL:HG13	2.03	0.41
1:B:751:GLY:C	1:B:753:ALA:N	2.78	0.41
1:B:1041:GLU:HB2	1:B:1042:HIS:H	1.71	0.41
1:C:373:PRO:O	1:C:377:LEU:N	2.49	0.41
1:C:563:PHE:HB2	1:C:866:GLU:CG	2.50	0.41
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.55	0.41
1:C:850:LYS:O	1:C:850:LYS:HG3	2.21	0.41
1:C:882:ILE:HG22	1:C:886:LEU:HD22	2.02	0.41
1:D:84:SER:HB3	1:D:814:PRO:HA	2.03	0.41
1:D:185:ARG:HD3	1:D:185:ARG:HA	1.95	0.41
1:D:189:ASN:OD1	1:D:190:PRO:HD2	2.21	0.41
1:D:209:ALA:O	1:D:237:GLN:NE2	2.53	0.41
1:D:340:VAL:HG22	1:D:396:PHE:CE2	2.56	0.41
1:D:405:LEU:HD22	1:D:481:SER:HB2	2.02	0.41
1:D:800:PRO:HG2	1:D:803:ALA:HB2	2.02	0.41
1:D:878:ALA:O	1:D:882:ILE:HG12	2.19	0.41
1:E:43:VAL:HG13	1:E:130:GLU:O	2.21	0.41
1:E:162:MET:CE	1:E:323:ILE:HD11	2.51	0.41
1:E:249:ILE:HD13	1:E:262:LEU:HD22	2.03	0.41
1:E:352:PHE:CD2	1:E:352:PHE:C	2.99	0.41
1:E:407:ASP:OD2	1:E:940:LYS:HD3	2.20	0.41
1:E:682:PHE:CE1	1:E:857:TYR:HB2	2.56	0.41
1:E:949:ALA:CB	1:E:1026:PHE:HE2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:393:LEU:HD12	1:F:469:GLN:HG3	2.02	0.41
1:F:462:SER:O	1:F:466:ILE:HG12	2.21	0.41
1:F:463:THR:HG23	1:F:925:VAL:CG2	2.50	0.41
1:F:746:ILE:HG13	1:F:747:ASN:H	1.86	0.41
1:F:905:VAL:CG1	1:F:935:ILE:HG12	2.50	0.41
1:A:188:MET:HA	1:A:266:ALA:HB2	2.03	0.41
1:A:393:LEU:HB3	1:A:470:PHE:CE1	2.56	0.41
1:A:1042:HIS:HB3	1:A:1043:SER:H	1.75	0.41
1:B:415:ASN:HD22	1:B:434:SER:CB	2.33	0.41
1:B:552:MET:HE2	1:B:552:MET:HB3	1.97	0.41
1:B:656:SER:HA	1:B:662:MET:HE1	2.03	0.41
1:B:695:LEU:HD12	1:B:825:MET:HG3	2.02	0.41
1:B:982:PHE:O	1:B:983:ILE:C	2.63	0.41
1:C:68:ASN:CG	1:C:113:LEU:HB2	2.46	0.41
1:C:188:MET:HB3	1:C:193:LEU:HD11	2.02	0.41
1:C:418:ARG:HH11	1:C:422:GLU:CD	2.29	0.41
1:C:449:LEU:HD11	1:C:937:LEU:CD2	2.50	0.41
1:D:325:TYR:HA	1:D:326:PRO:HD2	1.88	0.41
1:D:361:ASN:HD21	1:D:363:ARG:HG2	1.85	0.41
1:D:451:ALA:O	1:D:880:SER:OG	2.32	0.41
1:D:455:PRO:HG2	1:D:880:SER:CB	2.47	0.41
1:D:575:MET:HE1	1:D:617:ALA:HB3	2.03	0.41
1:D:687:GLN:HA	1:D:822:LEU:HD13	2.03	0.41
1:E:445:ILE:HG13	1:E:446:ALA:N	2.35	0.41
1:E:605:ASN:O	1:E:632:LYS:HG3	2.21	0.41
1:F:732:ASP:HB3	1:F:735:LYS:HG3	2.02	0.41
1:F:776:GLU:HB2	1:F:779:TYR:HD1	1.84	0.41
1:F:1041:GLU:HB3	1:F:1042:HIS:CB	2.39	0.41
1:A:525:HIS:CD2	1:A:525:HIS:O	2.74	0.40
1:B:166:ILE:HD12	1:B:166:ILE:HA	1.71	0.40
1:B:207:ILE:HG12	1:B:249:ILE:CD1	2.50	0.40
1:B:905:VAL:HB	1:B:906:PRO:HD3	2.03	0.40
1:B:987:MET:HG3	1:B:1008:MET:HE1	2.03	0.40
1:C:407:ASP:O	1:C:411:VAL:HG23	2.21	0.40
1:C:454:VAL:HB	1:C:455:PRO:HD3	2.03	0.40
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.87	0.40
1:D:150:THR:HB	1:D:151:GLN:NE2	2.36	0.40
1:D:188:MET:HB2	1:D:188:MET:HE3	1.72	0.40
1:D:309:GLU:O	1:D:312:LYS:HB2	2.21	0.40
1:D:645:GLU:O	1:D:648:THR:OG1	2.30	0.40
1:E:47:ALA:N	1:E:88:VAL:O	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:SER:O	1:E:246:PHE:HD1	2.04	0.40
1:E:252:LYS:HB3	1:E:252:LYS:HE2	1.83	0.40
1:F:146:ASP:O	1:F:148:THR:OG1	2.33	0.40
1:F:172:VAL:HG13	1:F:291:ILE:HG23	2.03	0.40
1:F:445:ILE:HG12	1:F:940:LYS:HG3	2.03	0.40
1:A:564:LEU:CD2	1:A:565:PRO:HD2	2.47	0.40
1:A:781:MET:SD	1:C:225:VAL:HG13	2.61	0.40
1:B:360:GLN:HB3	1:B:513:PHE:CZ	2.56	0.40
1:C:61:VAL:HG22	1:C:119:PRO:HD2	2.01	0.40
1:C:344:LEU:HA	1:C:399:VAL:HG22	2.02	0.40
1:C:932:LEU:HD23	1:C:932:LEU:HA	1.81	0.40
1:C:991:ILE:HD13	1:C:991:ILE:C	2.46	0.40
1:D:5:PHE:CD2	1:D:487:ILE:HG23	2.56	0.40
1:D:6:ILE:CD1	1:D:432:ARG:HE	2.34	0.40
1:D:149:MET:HB2	1:D:153:ASP:HB3	2.04	0.40
1:D:210:GLN:OE1	1:D:249:ILE:HG23	2.20	0.40
1:D:913:LEU:HD23	1:D:913:LEU:HA	1.96	0.40
1:E:214:VAL:HG21	1:F:747:ASN:CG	2.46	0.40
1:E:756:GLY:HA2	1:E:774:MET:HG3	2.03	0.40
1:F:120:GLN:HA	1:F:123:GLN:HB2	2.03	0.40
1:F:412:VAL:O	1:F:416:VAL:HG23	2.21	0.40
1:F:453:PHE:N	1:F:453:PHE:CD1	2.89	0.40
1:F:453:PHE:N	1:F:453:PHE:HD1	2.19	0.40
1:A:154:ILE:O	1:A:155:SER:C	2.64	0.40
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.53	0.40
1:A:538:THR:HG23	1:A:542:LEU:HD13	2.03	0.40
1:A:1040:ILE:HG23	1:A:1041:GLU:H	1.86	0.40
1:B:58:GLN:HG2	1:B:59:ASP:OD1	2.21	0.40
1:B:307:ARG:NH1	1:B:328:ASP:OD2	2.50	0.40
1:B:717:ARG:HD2	1:B:828:LEU:HB2	2.04	0.40
1:B:841:MET:O	1:B:845:GLU:HG3	2.21	0.40
1:C:189:ASN:OD1	1:C:190:PRO:HD2	2.21	0.40
1:C:201:VAL:O	1:C:204:ILE:HB	2.21	0.40
1:C:488:LEU:O	1:C:491:ALA:HB3	2.21	0.40
1:C:567:GLU:CD	1:C:996:GLY:HA2	2.47	0.40
1:C:671:ILE:HG21	1:C:674:LEU:HD12	2.03	0.40
1:D:47:ALA:HB3	1:D:88:VAL:CG1	2.52	0.40
1:D:372:VAL:O	1:D:373:PRO:C	2.64	0.40
1:D:409:ALA:O	1:D:413:VAL:HG23	2.22	0.40
1:D:429:GLU:H	1:D:429:GLU:HG2	1.44	0.40
1:D:551:GLY:O	1:D:555:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:650:ARG:O	1:D:653:ARG:HB3	2.21	0.40
1:D:888:LEU:CB	1:D:898:PRO:HB3	2.51	0.40
1:D:950:LYS:HZ1	1:D:1030:ARG:NE	2.20	0.40
1:E:24:GLY:O	1:E:28:LEU:HB2	2.20	0.40
1:E:167:SER:OG	1:E:175:VAL:HG21	2.22	0.40
1:E:189:ASN:HB3	1:E:192:GLU:CB	2.47	0.40
1:E:680:PHE:HB2	1:E:863:SER:OG	2.21	0.40
1:E:992:SER:O	1:E:997:SER:HB2	2.22	0.40
1:F:138:MET:HE3	1:F:138:MET:HB2	1.87	0.40
1:F:746:ILE:HG22	1:F:791:VAL:HG11	2.03	0.40
1:A:74:ASN:O	1:A:94:PHE:HD2	2.04	0.40
1:A:492:LEU:HD22	1:A:496:MET:SD	2.62	0.40
1:A:906:PRO:C	1:A:908:GLY:H	2.30	0.40
1:B:492:LEU:O	1:B:496:MET:HG2	2.21	0.40
1:B:781:MET:HE3	1:B:781:MET:HB3	1.89	0.40
1:C:725:PRO:HG3	1:C:811:TYR:CE1	2.57	0.40
1:D:199:THR:HG21	1:D:791:VAL:HA	2.03	0.40
1:E:383:LEU:HD23	1:E:383:LEU:HA	1.83	0.40
1:E:504:ASP:C	1:E:506:GLY:N	2.80	0.40
1:E:507:GLU:CD	1:E:518:ARG:HG2	2.47	0.40
1:E:588:GLN:HG3	1:E:592:ASN:HD21	1.86	0.40
1:E:602:GLU:OE1	1:E:650:ARG:HD2	2.22	0.40
1:E:805:SER:O	1:E:805:SER:OG	2.37	0.40
1:F:58:GLN:HG3	1:F:82:SER:OG	2.21	0.40
1:F:674:LEU:CD2	1:F:861:GLY:HA2	2.51	0.40
1:F:1044:HIS:O	1:F:1045:THR:C	2.64	0.40
1:A:682:PHE:CD2	1:A:682:PHE:C	3.00	0.40
1:A:909:VAL:HG22	1:A:931:LEU:HD21	2.04	0.40
1:A:1018:ALA:C	1:A:1020:PHE:N	2.79	0.40
1:B:356:TYR:C	1:B:358:PHE:N	2.76	0.40
1:B:427:PRO:CD	1:B:499:PRO:HB3	2.52	0.40
1:C:165:ALA:HB3	1:C:313:MET:CE	2.50	0.40
1:C:246:PHE:O	1:C:249:ILE:HG13	2.22	0.40
1:C:501:ALA:O	1:C:504:ASP:HB2	2.20	0.40
1:C:926:TYR:HE1	1:C:999:ALA:HA	1.87	0.40
1:C:948:PHE:HB3	1:C:970:MET:CE	2.52	0.40
1:C:991:ILE:HD13	1:C:991:ILE:O	2.21	0.40
1:D:287:SER:OG	1:D:288:GLY:N	2.50	0.40
1:D:712:MET:O	1:D:832:ALA:N	2.46	0.40
1:D:730:ASP:HB2	1:D:808:ARG:NH2	2.37	0.40
1:D:964:THR:O	1:D:967:ALA:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:ILE:O	1:E:157:TYR:N	2.55	0.40
1:E:353:LEU:C	1:E:355:MET:N	2.72	0.40
1:E:396:PHE:O	1:E:400:LEU:HB2	2.20	0.40
1:E:415:ASN:ND2	1:E:437:GLN:OE1	2.47	0.40
1:E:445:ILE:CG1	1:E:940:LYS:HE3	2.48	0.40
1:E:453:PHE:HB3	1:E:475:VAL:HG22	2.02	0.40
1:E:792:ARG:HB2	1:E:798:MET:SD	2.61	0.40
1:E:1017:LEU:HD12	1:E:1017:LEU:HA	1.70	0.40
1:F:194:ASN:HA	1:F:798:MET:HE2	2.04	0.40
1:F:222:THR:HA	1:F:223:PRO:HA	1.90	0.40
1:F:522:LYS:O	1:F:525:HIS:N	2.54	0.40
1:F:535:LEU:HD23	1:F:535:LEU:HA	1.72	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:529:ASP:OD1	1:F:529:ASP:OD2[2_555]	2.08	0.12

3.3 Torsion angles

3.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1040/1049 (99%)	939 (90%)	82 (8%)	19 (2%)	6	29
1	B	1044/1049 (100%)	925 (89%)	92 (9%)	27 (3%)	4	21
1	C	1042/1049 (99%)	931 (89%)	91 (9%)	20 (2%)	6	28
1	D	1040/1049 (99%)	941 (90%)	83 (8%)	16 (2%)	8	33
1	E	1040/1049 (99%)	919 (88%)	97 (9%)	24 (2%)	5	24
1	F	1044/1049 (100%)	936 (90%)	87 (8%)	21 (2%)	6	27
All	All	6250/6294 (99%)	5591 (90%)	532 (8%)	127 (2%)	6	27

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	675	GLY
1	A	1038	GLU
1	B	163	LYS
1	B	360	GLN
1	B	509	LYS
1	B	516	PHE
1	B	644	VAL
1	B	673	GLU
1	B	677	ALA
1	B	1033	PHE
1	B	1038	GLU
1	B	1040	ILE
1	B	1041	GLU
1	B	1046	VAL
1	C	134	SER
1	C	147	GLY
1	C	163	LYS
1	C	360	GLN
1	C	509	LYS
1	C	691	GLY
1	C	1034	SER
1	C	1038	GLU
1	D	163	LYS
1	D	360	GLN
1	D	508	GLY
1	D	511	GLY
1	D	644	VAL
1	D	1035	ARG
1	D	1037	ASN
1	E	163	LYS
1	E	354	VAL
1	E	360	GLN
1	E	536	ARG
1	E	632	LYS
1	E	644	VAL
1	E	673	GLU
1	E	674	LEU
1	E	893	GLU
1	E	1035	ARG
1	F	134	SER
1	F	147	GLY

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Mol	Chain	Res	Type
1	F	360	GLN
1	F	644	VAL
1	F	691	GLY
1	F	1039	ASP
1	F	1042	HIS
1	F	1045	THR
1	F	1046	VAL
1	A	507	GLU
1	A	644	VAL
1	A	677	ALA
1	A	751	GLY
1	A	1040	ILE
1	B	295	THR
1	B	508	GLY
1	B	751	GLY
1	B	1037	ASN
1	C	133	SER
1	C	644	VAL
1	C	689	GLY
1	C	751	GLY
1	C	752	ALA
1	C	893	GLU
1	C	1042	HIS
1	D	675	GLY
1	D	751	GLY
1	D	752	ALA
1	D	992	SER
1	D	1033	PHE
1	D	1040	ILE
1	E	132	SER
1	E	508	GLY
1	E	672	VAL
1	E	751	GLY
1	E	1040	ILE
1	F	6	ILE
1	F	163	LYS
1	F	751	GLY
1	F	1043	SER
1	A	37	THR
1	A	752	ALA
1	A	907	LEU
1	A	1035	ARG

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Mol	Chain	Res	Type
1	B	41	PRO
1	B	358	PHE
1	B	638	PRO
1	B	672	VAL
1	B	833	PRO
1	B	960	LEU
1	C	1033	PHE
1	C	1037	ASN
1	C	1041	GLU
1	D	960	LEU
1	E	752	ALA
1	E	907	LEU
1	E	993	THR
1	F	133	SER
1	F	146	ASP
1	F	148	THR
1	A	163	LYS
1	A	505	HIS
1	A	688	ALA
1	A	1033	PHE
1	B	1044	HIS
1	D	907	LEU
1	E	195	LYS
1	E	1042	HIS
1	F	638	PRO
1	F	907	LEU
1	B	40	PRO
1	B	752	ALA
1	E	638	PRO
1	E	1037	ASN
1	F	960	LEU
1	A	195	LYS
1	A	418	ARG
1	A	638	PRO
1	B	907	LEU
1	E	353	LEU
1	F	923	ASN
1	B	870	GLY
1	C	511	GLY
1	E	833	PRO
1	C	217	GLY
1	D	638	PRO

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Mol	Chain	Res	Type
1	F	511	GLY

3.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	845/852 (99%)	769 (91%)	76 (9%)	9	30
1	B	849/852 (100%)	717 (84%)	132 (16%)	2	12
1	C	847/852 (99%)	753 (89%)	94 (11%)	6	22
1	D	845/852 (99%)	767 (91%)	78 (9%)	8	30
1	E	845/852 (99%)	715 (85%)	130 (15%)	2	12
1	F	849/852 (100%)	759 (89%)	90 (11%)	6	24
All	All	5080/5112 (99%)	4480 (88%)	600 (12%)	5	20

All (600) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	21	LEU
1	A	25	LEU
1	A	27	ILE
1	A	38	ILE
1	A	44	THR
1	A	45	ILE
1	A	60	THR
1	A	88	VAL
1	A	101	ASP
1	A	146	ASP
1	A	152	GLU
1	A	166	ILE
1	A	169	THR
1	A	185	ARG
1	A	203	VAL
1	A	205	THR

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Mol	Chain	Res	Type
1	A	253	VAL
1	A	255	GLN
1	A	267	LYS
1	A	270	LEU
1	A	280	GLU
1	A	293	LEU
1	A	336	SER
1	A	343	THR
1	A	349	ILE
1	A	350	LEU
1	A	353	LEU
1	A	355	MET
1	A	360	GLN
1	A	362	PHE
1	A	429	GLU
1	A	434	SER
1	A	437	GLN
1	A	452	VAL
1	A	472	ILE
1	A	493	CYS
1	A	502	LYS
1	A	523	SER
1	A	528	THR
1	A	530	SER
1	A	538	THR
1	A	540	ARG
1	A	559	LEU
1	A	561	SER
1	A	564	LEU
1	A	578	LEU
1	A	590	VAL
1	A	602	GLU
1	A	603	LYS
1	A	612	VAL
1	A	623	ASN
1	A	634	TRP
1	A	644	VAL
1	A	659	LYS
1	A	662	MET
1	A	673	GLU
1	A	682	PHE
1	A	716	VAL

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Mol	Chain	Res	Type
1	A	741	VAL
1	A	768	VAL
1	A	802	SER
1	A	901	VAL
1	A	921	LEU
1	A	922	THR
1	A	931	LEU
1	A	940	LYS
1	A	947	GLU
1	A	961	ILE
1	A	970	MET
1	A	975	ILE
1	A	986	VAL
1	A	1036	LYS
1	A	1038	GLU
1	A	1039	ASP
1	A	1041	GLU
1	B	3	ASN
1	B	6	ILE
1	B	13	TRP
1	B	17	ILE
1	B	27	ILE
1	B	28	LEU
1	B	32	VAL
1	B	43	VAL
1	B	48	SER
1	B	53	ASP
1	B	58	GLN
1	B	72	ILE
1	B	79	SER
1	B	105	VAL
1	B	127	VAL
1	B	128	SER
1	B	166	ILE
1	B	175	VAL
1	B	180	SER
1	B	203	VAL
1	B	213	GLN
1	B	255	GLN
1	B	259	ARG
1	B	270	LEU
1	B	277	ILE

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Mol	Chain	Res	Type
1	B	278	ILE
1	B	280	GLU
1	B	289	LEU
1	B	293	LEU
1	B	295	THR
1	B	298	ASN
1	B	310	LEU
1	B	314	GLU
1	B	322	LYS
1	B	329	THR
1	B	330	THR
1	B	336	SER
1	B	348	ILE
1	B	349	ILE
1	B	350	LEU
1	B	352	PHE
1	B	353	LEU
1	B	355	MET
1	B	358	PHE
1	B	360	GLN
1	B	365	THR
1	B	374	VAL
1	B	383	LEU
1	B	398	MET
1	B	400	LEU
1	B	404	LEU
1	B	472	ILE
1	B	473	THR
1	B	475	VAL
1	B	480	LEU
1	B	482	VAL
1	B	489	THR
1	B	507	GLU
1	B	523	SER
1	B	524	THR
1	B	534	ILE
1	B	543	VAL
1	B	555	LEU
1	B	558	ARG
1	B	559	LEU
1	B	561	SER
1	B	563	PHE

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Mol	Chain	Res	Type
1	B	564	LEU
1	B	569	GLN
1	B	578	LEU
1	B	590	VAL
1	B	599	LEU
1	B	612	VAL
1	B	626	ILE
1	B	629	VAL
1	B	634	TRP
1	B	644	VAL
1	B	662	MET
1	B	667	ASN
1	B	668	LEU
1	B	672	VAL
1	B	682	PHE
1	B	683	GLU
1	B	687	GLN
1	B	690	LEU
1	B	695	LEU
1	B	703	LEU
1	B	708	LYS
1	B	717	ARG
1	B	741	VAL
1	B	743	ILE
1	B	759	VAL
1	B	761	ASP
1	B	767	ARG
1	B	768	VAL
1	B	775	SER
1	B	788	ASP
1	B	806	SER
1	B	808	ARG
1	B	835	LYS
1	B	843	LEU
1	B	853	THR
1	B	862	MET
1	B	869	SER
1	B	871	ASN
1	B	886	LEU
1	B	901	VAL
1	B	919	ARG
1	B	921	LEU

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Mol	Chain	Res	Type
1	B	953	MET
1	B	956	GLU
1	B	965	LEU
1	B	968	VAL
1	B	970	MET
1	B	975	ILE
1	B	978	THR
1	B	980	LEU
1	B	986	VAL
1	B	1015	THR
1	B	1017	LEU
1	B	1024	VAL
1	B	1032	ARG
1	B	1035	ARG
1	B	1036	LYS
1	B	1038	GLU
1	B	1039	ASP
1	B	1040	ILE
1	B	1041	GLU
1	B	1042	HIS
1	B	1044	HIS
1	B	1045	THR
1	B	1046	VAL
1	C	3	ASN
1	C	6	ILE
1	C	27	ILE
1	C	28	LEU
1	C	48	SER
1	C	55	LYS
1	C	88	VAL
1	C	92	LEU
1	C	102	ILE
1	C	108	GLN
1	C	120	GLN
1	C	145	THR
1	C	148	THR
1	C	151	GLN
1	C	203	VAL
1	C	239	ARG
1	C	249	ILE
1	C	253	VAL
1	C	255	GLN

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Mol	Chain	Res	Type
1	C	270	LEU
1	C	280	GLU
1	C	293	LEU
1	C	300	LEU
1	C	330	THR
1	C	337	ILE
1	C	343	THR
1	C	349	ILE
1	C	353	LEU
1	C	358	PHE
1	C	360	GLN
1	C	363	ARG
1	C	392	THR
1	C	405	LEU
1	C	432	ARG
1	C	447	MET
1	C	452	VAL
1	C	463	THR
1	C	472	ILE
1	C	482	VAL
1	C	513	PHE
1	C	523	SER
1	C	526	HIS
1	C	538	THR
1	C	540	ARG
1	C	550	VAL
1	C	555	LEU
1	C	559	LEU
1	C	564	LEU
1	C	590	VAL
1	C	602	GLU
1	C	603	LYS
1	C	608	SER
1	C	612	VAL
1	C	623	ASN
1	C	624	THR
1	C	634	TRP
1	C	644	VAL
1	C	649	MET
1	C	659	LYS
1	C	662	MET
1	C	666	PHE

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Mol	Chain	Res	Type
1	C	673	GLU
1	C	678	THR
1	C	694	LYS
1	C	695	LEU
1	C	696	THR
1	C	721	LEU
1	C	734	GLU
1	C	741	VAL
1	C	746	ILE
1	C	748	THR
1	C	808	ARG
1	C	843	LEU
1	C	847	LEU
1	C	860	THR
1	C	865	GLN
1	C	868	LEU
1	C	876	LEU
1	C	886	LEU
1	C	887	CYS
1	C	914	LEU
1	C	940	LYS
1	C	947	GLU
1	C	950	LYS
1	C	961	ILE
1	C	968	VAL
1	C	971	ARG
1	C	975	ILE
1	C	980	LEU
1	C	986	VAL
1	C	991	ILE
1	C	1033	PHE
1	C	1040	ILE
1	C	1041	GLU
1	D	3	ASN
1	D	21	LEU
1	D	27	ILE
1	D	101	ASP
1	D	102	ILE
1	D	146	ASP
1	D	151	GLN
1	D	152	GLU
1	D	203	VAL

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Mol	Chain	Res	Type
1	D	229	GLN
1	D	253	VAL
1	D	270	LEU
1	D	276	ASP
1	D	280	GLU
1	D	293	LEU
1	D	330	THR
1	D	336	SER
1	D	343	THR
1	D	353	LEU
1	D	355	MET
1	D	362	PHE
1	D	400	LEU
1	D	429	GLU
1	D	434	SER
1	D	452	VAL
1	D	462	SER
1	D	472	ILE
1	D	483	LEU
1	D	493	CYS
1	D	502	LYS
1	D	505	HIS
1	D	523	SER
1	D	526	HIS
1	D	534	ILE
1	D	538	THR
1	D	542	LEU
1	D	550	VAL
1	D	559	LEU
1	D	561	SER
1	D	563	PHE
1	D	578	LEU
1	D	590	VAL
1	D	602	GLU
1	D	603	LYS
1	D	608	SER
1	D	623	ASN
1	D	624	THR
1	D	634	TRP
1	D	644	VAL
1	D	657	GLN
1	D	662	MET

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Mol	Chain	Res	Type
1	D	671	ILE
1	D	673	GLU
1	D	697	GLN
1	D	717	ARG
1	D	733	GLN
1	D	741	VAL
1	D	743	ILE
1	D	748	THR
1	D	768	VAL
1	D	797	GLN
1	D	843	LEU
1	D	881	LEU
1	D	901	VAL
1	D	921	LEU
1	D	931	LEU
1	D	943	ILE
1	D	951	ASP
1	D	961	ILE
1	D	968	VAL
1	D	970	MET
1	D	971	ARG
1	D	975	ILE
1	D	980	LEU
1	D	986	VAL
1	D	1035	ARG
1	D	1036	LYS
1	D	1038	GLU
1	E	3	ASN
1	E	10	ILE
1	E	17	ILE
1	E	28	LEU
1	E	45	ILE
1	E	57	VAL
1	E	58	GLN
1	E	60	THR
1	E	76	MET
1	E	82	SER
1	E	87	THR
1	E	91	THR
1	E	93	THR
1	E	102	ILE
1	E	105	VAL

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Mol	Chain	Res	Type
1	E	110	LYS
1	E	113	LEU
1	E	117	LEU
1	E	128	SER
1	E	146	ASP
1	E	153	ASP
1	E	156	ASP
1	E	166	ILE
1	E	174	ASP
1	E	175	VAL
1	E	203	VAL
1	E	205	THR
1	E	213	GLN
1	E	218	GLN
1	E	229	GLN
1	E	233	SER
1	E	238	THR
1	E	249	ILE
1	E	250	LEU
1	E	253	VAL
1	E	255	GLN
1	E	259	ARG
1	E	268	ILE
1	E	270	LEU
1	E	276	ASP
1	E	280	GLU
1	E	293	LEU
1	E	295	THR
1	E	298	ASN
1	E	300	LEU
1	E	310	LEU
1	E	321	LEU
1	E	323	ILE
1	E	324	VAL
1	E	329	THR
1	E	330	THR
1	E	340	VAL
1	E	345	VAL
1	E	349	ILE
1	E	352	PHE
1	E	353	LEU
1	E	355	MET

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Mol	Chain	Res	Type
1	E	365	THR
1	E	372	VAL
1	E	400	LEU
1	E	404	LEU
1	E	410	ILE
1	E	418	ARG
1	E	420	MET
1	E	445	ILE
1	E	449	LEU
1	E	450	SER
1	E	452	VAL
1	E	456	MET
1	E	472	ILE
1	E	480	LEU
1	E	482	VAL
1	E	507	GLU
1	E	512	PHE
1	E	523	SER
1	E	540	ARG
1	E	550	VAL
1	E	558	ARG
1	E	563	PHE
1	E	564	LEU
1	E	590	VAL
1	E	593	GLU
1	E	607	GLU
1	E	608	SER
1	E	612	VAL
1	E	634	TRP
1	E	644	VAL
1	E	653	ARG
1	E	659	LYS
1	E	673	GLU
1	E	683	GLU
1	E	687	GLN
1	E	690	LEU
1	E	694	LYS
1	E	703	LEU
1	E	708	LYS
1	E	714	THR
1	E	716	VAL
1	E	717	ARG

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Mol	Chain	Res	Type
1	E	741	VAL
1	E	748	THR
1	E	767	ARG
1	E	768	VAL
1	E	804	PHE
1	E	806	SER
1	E	817	GLU
1	E	835	LYS
1	E	844	MET
1	E	857	TYR
1	E	865	GLN
1	E	871	ASN
1	E	886	LEU
1	E	901	VAL
1	E	907	LEU
1	E	914	LEU
1	E	917	THR
1	E	931	LEU
1	E	937	LEU
1	E	947	GLU
1	E	953	MET
1	E	958	LYS
1	E	961	ILE
1	E	980	LEU
1	E	986	VAL
1	E	987	MET
1	E	1001	ASN
1	E	1017	LEU
1	E	1021	PHE
1	E	1032	ARG
1	E	1042	HIS
1	F	3	ASN
1	F	6	ILE
1	F	25	LEU
1	F	27	ILE
1	F	28	LEU
1	F	34	GLN
1	F	45	ILE
1	F	48	SER
1	F	55	LYS
1	F	60	THR
1	F	88	VAL

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Mol	Chain	Res	Type
1	F	104	GLN
1	F	112	GLN
1	F	120	GLN
1	F	148	THR
1	F	151	GLN
1	F	203	VAL
1	F	205	THR
1	F	243	THR
1	F	249	ILE
1	F	270	LEU
1	F	278	ILE
1	F	280	GLU
1	F	293	LEU
1	F	330	THR
1	F	335	ILE
1	F	337	ILE
1	F	340	VAL
1	F	349	ILE
1	F	353	LEU
1	F	360	GLN
1	F	392	THR
1	F	405	LEU
1	F	429	GLU
1	F	432	ARG
1	F	434	SER
1	F	439	GLN
1	F	452	VAL
1	F	456	MET
1	F	472	ILE
1	F	481	SER
1	F	482	VAL
1	F	493	CYS
1	F	512	PHE
1	F	526	HIS
1	F	534	ILE
1	F	540	ARG
1	F	550	VAL
1	F	559	LEU
1	F	571	VAL
1	F	578	LEU
1	F	590	VAL
1	F	604	ASN

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Mol	Chain	Res	Type
1	F	612	VAL
1	F	623	ASN
1	F	626	ILE
1	F	634	TRP
1	F	643	LYS
1	F	644	VAL
1	F	649	MET
1	F	666	PHE
1	F	673	GLU
1	F	674	LEU
1	F	703	LEU
1	F	734	GLU
1	F	743	ILE
1	F	808	ARG
1	F	843	LEU
1	F	847	LEU
1	F	860	THR
1	F	864	TYR
1	F	865	GLN
1	F	867	ARG
1	F	868	LEU
1	F	876	LEU
1	F	887	CYS
1	F	895	TRP
1	F	918	PHE
1	F	947	GLU
1	F	950	LYS
1	F	953	MET
1	F	961	ILE
1	F	968	VAL
1	F	980	LEU
1	F	986	VAL
1	F	990	VAL
1	F	991	ILE
1	F	1011	MET
1	F	1015	THR
1	F	1042	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN

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Mol	Chain	Res	Type
1	A	112	GLN
1	A	123	GLN
1	A	124	GLN
1	A	161	ASN
1	A	231	ASN
1	A	298	ASN
1	A	584	GLN
1	A	588	GLN
1	A	592	ASN
1	A	846	GLN
1	A	1001	ASN
1	B	63	GLN
1	B	74	ASN
1	B	106	GLN
1	B	108	GLN
1	B	120	GLN
1	B	161	ASN
1	B	189	ASN
1	B	213	GLN
1	B	231	ASN
1	B	525	HIS
1	B	623	ASN
1	B	709	HIS
1	B	760	ASN
1	B	865	GLN
1	C	67	GLN
1	C	70	ASN
1	C	125	GLN
1	C	361	ASN
1	C	592	ASN
1	C	872	GLN
1	C	923	ASN
1	C	1000	GLN
1	D	34	GLN
1	D	74	ASN
1	D	109	ASN
1	D	151	GLN
1	D	439	GLN
1	D	469	GLN
1	D	505	HIS
1	D	525	HIS
1	E	70	ASN

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Mol	Chain	Res	Type
1	E	123	GLN
1	E	189	ASN
1	E	439	GLN
1	E	588	GLN
1	E	592	ASN
1	E	613	ASN
1	E	623	ASN
1	E	642	ASN
1	E	747	ASN
1	F	63	GLN
1	F	67	GLN
1	F	68	ASN
1	F	104	GLN
1	F	108	GLN
1	F	231	ASN
1	F	846	GLN

3.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

3.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

3.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 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	1042/1049 (99%)	0.14	33 (3%)	50	30	28, 63, 113, 139	0
1	B	1046/1049 (99%)	-0.14	21 (2%)	65	44	26, 57, 100, 161	0
1	C	1044/1049 (99%)	-0.00	38 (3%)	46	27	17, 56, 98, 173	0
1	D	1042/1049 (99%)	0.19	38 (3%)	46	27	21, 81, 133, 168	0
1	E	1042/1049 (99%)	0.24	37 (3%)	46	27	38, 77, 119, 154	0
1	F	1046/1049 (99%)	0.32	57 (5%)	31	18	29, 73, 120, 143	0
All	All	6262/6294 (99%)	0.12	224 (3%)	46	27	17, 68, 116, 173	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	291	ILE	7.5
1	F	856	GLY	7.3
1	C	69	MET	7.3
1	C	856	GLY	7.0
1	C	838	GLY	6.9
1	E	164	ASP	6.3
1	D	869	SER	6.3
1	B	869	SER	6.0
1	D	337	ILE	5.9
1	F	69	MET	5.7
1	F	836	SER	5.3
1	F	442	LEU	5.3
1	C	871	ASN	5.3
1	F	837	THR	5.1
1	E	290	GLY	5.1
1	C	837	THR	5.1
1	E	869	SER	5.0
1	B	715	SER	5.0
1	D	59	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	396	PHE	4.8
1	D	306	ILE	4.4
1	A	383	LEU	4.3
1	C	122	VAL	4.1
1	F	410	ILE	4.1
1	E	678	THR	4.1
1	C	97	GLY	4.0
1	A	35	TYR	4.0
1	D	461	GLY	4.0
1	C	494	ALA	4.0
1	D	875	SER	3.9
1	F	874	PRO	3.8
1	F	107	VAL	3.8
1	C	79	SER	3.8
1	F	3	ASN	3.7
1	F	481	SER	3.7
1	F	117	LEU	3.7
1	F	501	ALA	3.7
1	D	678	THR	3.6
1	D	715	SER	3.6
1	F	406	VAL	3.5
1	F	49	TYR	3.5
1	D	400	LEU	3.5
1	D	334	LYS	3.4
1	E	488	LEU	3.4
1	E	177	LEU	3.4
1	F	892	TYR	3.3
1	F	335	ILE	3.3
1	F	96	SER	3.3
1	A	376	LEU	3.3
1	D	866	GLU	3.3
1	C	65	ILE	3.2
1	C	403	GLY	3.2
1	F	417	GLU	3.2
1	A	310	LEU	3.2
1	E	137	LEU	3.2
1	F	122	VAL	3.1
1	F	503	GLY	3.1
1	A	386	PHE	3.1
1	F	59	ASP	3.1
1	F	127	VAL	3.1
1	A	677	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	465	ALA	3.0
1	F	873	ALA	3.0
1	D	32	VAL	3.0
1	E	487	ILE	3.0
1	F	441	ALA	3.0
1	F	706	ALA	3.0
1	D	677	ALA	3.0
1	D	71	GLY	3.0
1	C	166	ILE	3.0
1	E	2	PRO	2.9
1	C	9	PRO	2.9
1	F	888	LEU	2.9
1	F	866	GLU	2.9
1	C	68	ASN	2.9
1	E	105	VAL	2.9
1	A	330	THR	2.9
1	F	402	ILE	2.9
1	C	511	GLY	2.8
1	B	703	LEU	2.8
1	F	10	ILE	2.8
1	D	721	LEU	2.8
1	F	827	ILE	2.8
1	A	71	GLY	2.8
1	C	96	SER	2.8
1	D	714	THR	2.8
1	E	6	ILE	2.8
1	C	847	LEU	2.7
1	E	25	LEU	2.7
1	A	372	VAL	2.7
1	C	8	ARG	2.7
1	D	60	THR	2.7
1	B	59	ASP	2.7
1	B	884	VAL	2.7
1	A	337	ILE	2.7
1	A	299	ALA	2.7
1	F	306	ILE	2.6
1	E	292	LYS	2.6
1	A	493	CYS	2.6
1	D	681	ASP	2.6
1	F	60	THR	2.6
1	C	686	ASP	2.6
1	A	411	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	813	SER	2.6
1	F	109	ASN	2.6
1	E	158	VAL	2.6
1	E	71	GLY	2.5
1	F	111	LEU	2.5
1	A	935	ILE	2.5
1	B	6	ILE	2.5
1	D	837	THR	2.5
1	F	72	ILE	2.5
1	A	413	VAL	2.5
1	A	16	ALA	2.5
1	A	27	ILE	2.5
1	F	55	LYS	2.5
1	C	49	TYR	2.5
1	D	865	GLN	2.5
1	F	855	VAL	2.5
1	A	92	LEU	2.5
1	A	321	LEU	2.5
1	B	1035	ARG	2.5
1	F	118	LEU	2.5
1	D	333	VAL	2.5
1	C	501	ALA	2.4
1	C	890	ALA	2.4
1	E	541	TYR	2.4
1	A	679	GLY	2.4
1	F	434	SER	2.4
1	B	177	LEU	2.4
1	C	822	LEU	2.4
1	D	463	THR	2.4
1	D	870	GLY	2.4
1	E	995	ALA	2.4
1	B	292	LYS	2.4
1	F	869	SER	2.4
1	B	678	THR	2.4
1	E	406	VAL	2.4
1	D	51	GLY	2.4
1	E	86	GLY	2.4
1	F	97	GLY	2.4
1	A	445	ILE	2.4
1	B	472	ILE	2.4
1	A	509	LYS	2.4
1	B	895	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	175	VAL	2.4
1	E	129	VAL	2.4
1	D	460	GLY	2.4
1	D	335	ILE	2.4
1	B	515	TRP	2.4
1	A	569	GLN	2.3
1	D	137	LEU	2.3
1	A	515	TRP	2.3
1	E	862	MET	2.3
1	F	871	ASN	2.3
1	D	112	GLN	2.3
1	D	859	TRP	2.3
1	E	33	ALA	2.3
1	F	61	VAL	2.3
1	F	494	ALA	2.3
1	A	334	LYS	2.3
1	C	33	ALA	2.2
1	F	54	ALA	2.2
1	E	599	LEU	2.2
1	A	327	TYR	2.2
1	C	127	VAL	2.2
1	C	129	VAL	2.2
1	C	855	VAL	2.2
1	B	886	LEU	2.2
1	A	678	THR	2.2
1	F	169	THR	2.2
1	B	1043	SER	2.2
1	C	776	GLU	2.2
1	B	870	GLY	2.2
1	C	28	LEU	2.2
1	C	433	LYS	2.2
1	F	57	VAL	2.2
1	B	866	GLU	2.2
1	B	871	ASN	2.2
1	C	25	LEU	2.2
1	D	674	LEU	2.2
1	B	939	ALA	2.2
1	E	679	GLY	2.2
1	F	773	VAL	2.2
1	E	166	ILE	2.2
1	E	293	LEU	2.2
1	C	451	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	2	PRO	2.2
1	A	825	MET	2.1
1	C	417	GLU	2.1
1	C	874	PRO	2.1
1	D	179	GLY	2.1
1	D	675	GLY	2.1
1	A	470	PHE	2.1
1	D	515	TRP	2.1
1	D	716	VAL	2.1
1	A	473	THR	2.1
1	F	822	LEU	2.1
1	F	848	ALA	2.1
1	E	14	VAL	2.1
1	C	395	MET	2.1
1	E	398	MET	2.1
1	F	170	SER	2.1
1	C	835	LYS	2.1
1	E	515	TRP	2.1
1	F	854	GLY	2.1
1	C	80	SER	2.1
1	E	306	ILE	2.1
1	E	712	MET	2.1
1	C	2	PRO	2.1
1	A	410	ILE	2.0
1	E	72	ILE	2.0
1	E	405	LEU	2.0
1	A	494	ALA	2.0
1	B	174	ASP	2.0
1	E	495	THR	2.0
1	D	141	GLY	2.0
1	F	502	LYS	2.0
1	D	72	ILE	2.0
1	D	336	SER	2.0
1	F	698	ALA	2.0
1	F	857	TYR	2.0
1	E	556	PHE	2.0
1	F	474	ILE	2.0

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

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

4.3 Carbohydrates

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

4.4 Other polymers

There are no such residues in this entry.