



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:06 PM UTC

PDB ID : 4AV6 / pdb_00004av6
Title : Crystal structure of Thermotoga maritima sodium pumping membrane integral pyrophosphatase at 4 Å in complex with phosphate and magnesium
Authors : Kajander, T.; Kellosalo, J.; Kogan, K.; Pokharel, K.; Goldman, A.
Deposited on : 2012-05-23
Resolution : 4.00 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

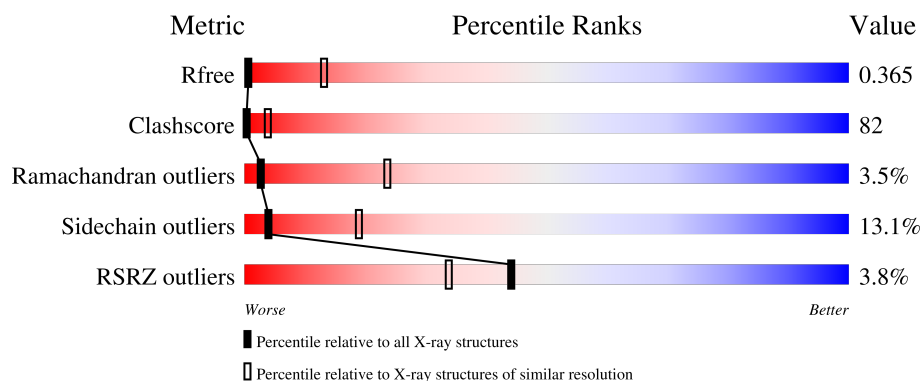
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	735	
1	B	735	

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	PO4	A	1728	-	-	X	-
2	PO4	B	1728	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9406 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called K(+)-STIMULATED PYROPHOSPHATE-ENERGIZED SODIUM PUMP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	0	0
			4771	3140	742	868	21			
1	B	642	Total	C	N	O	S	0	0	0
			4605	3025	718	842	20			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP Q9S5X0
A	-7	ARG	-	expression tag	UNP Q9S5X0
A	-6	GLY	-	expression tag	UNP Q9S5X0
A	-5	SER	-	expression tag	UNP Q9S5X0
A	-4	HIS	-	expression tag	UNP Q9S5X0
A	-3	HIS	-	expression tag	UNP Q9S5X0
A	-2	HIS	-	expression tag	UNP Q9S5X0
A	-1	HIS	-	expression tag	UNP Q9S5X0
A	0	HIS	-	expression tag	UNP Q9S5X0
A	1	HIS	-	expression tag	UNP Q9S5X0
A	353	LEU	VAL	engineered mutation	UNP Q9S5X0
A	395	GLY	SER	engineered mutation	UNP Q9S5X0
B	-8	MET	-	expression tag	UNP Q9S5X0
B	-7	ARG	-	expression tag	UNP Q9S5X0
B	-6	GLY	-	expression tag	UNP Q9S5X0
B	-5	SER	-	expression tag	UNP Q9S5X0
B	-4	HIS	-	expression tag	UNP Q9S5X0
B	-3	HIS	-	expression tag	UNP Q9S5X0
B	-2	HIS	-	expression tag	UNP Q9S5X0
B	-1	HIS	-	expression tag	UNP Q9S5X0
B	0	HIS	-	expression tag	UNP Q9S5X0
B	1	HIS	-	expression tag	UNP Q9S5X0
B	353	LEU	VAL	engineered mutation	UNP Q9S5X0
B	395	GLY	SER	engineered mutation	UNP Q9S5X0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		
3	B	4	Total	Mg	0	0
			4	4		

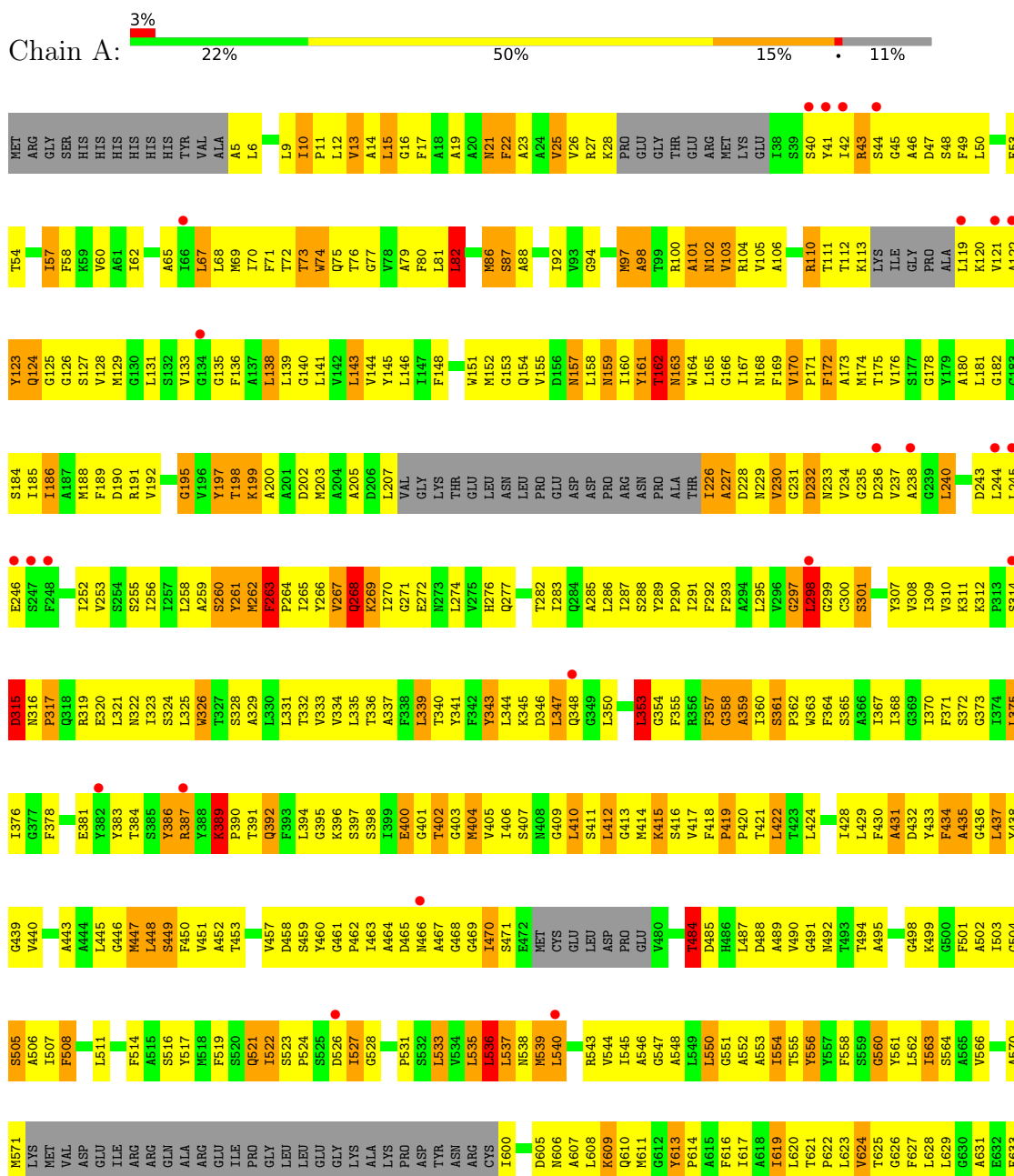
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

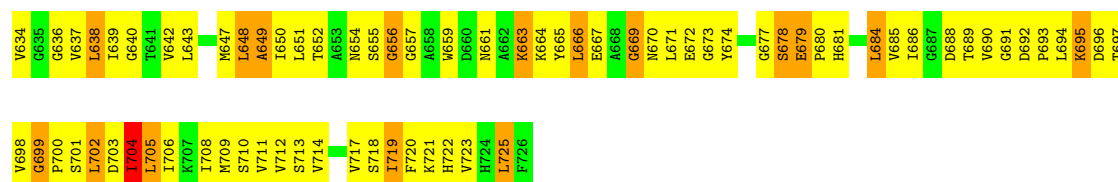
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		

3 Residue-property plots

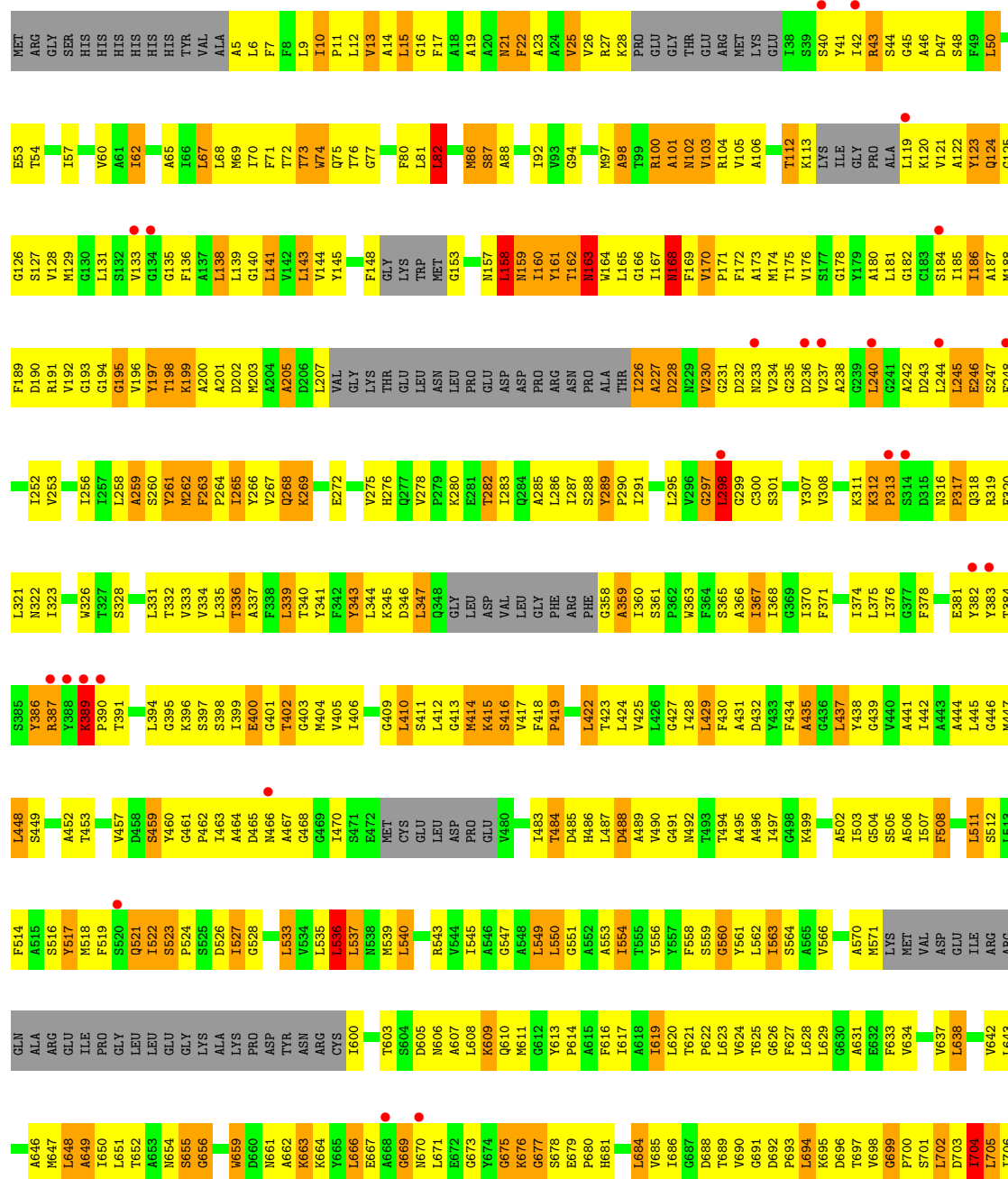
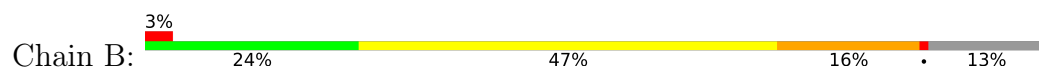
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: K(+)-STIMULATED PYROPHOSPHATE-ENERGIZED SODIUM PUMP





• Molecule 1: K(+)-STIMULATED PYROPHOSPHATE-ENERGIZED SODIUM PUMP



K707	V717
I708	S718
M709	I719
S710	F720
V711	K721
V712	H722
S713	V723
V714	H724
	L725
	F726

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.80Å 112.27Å 109.71Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	29.83 – 4.00 29.83 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.83-4.00) 98.6 (29.83-4.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 4.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.295 , 0.365 0.298 , 0.365	Depositor DCC
R_{free} test set	866 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	178.0	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 178.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9406	wwPDB-VP
Average B, all atoms (Å ²)	239.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, K, MG

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	0.72	0/4869	1.54	98/6629 (1.5%)
1	B	0.68	0/4692	1.56	99/6390 (1.5%)
All	All	0.70	0/9561	1.55	197/13019 (1.5%)

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	A	1	0

There are no bond length outliers.

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	LYS	N-CA-CB	15.94	137.44	110.49
1	B	669	GLY	N-CA-C	-15.93	97.01	111.67
1	B	470	ILE	N-CA-C	12.71	123.58	110.62
1	A	272	GLU	N-CA-C	11.62	127.11	112.24
1	B	261	TYR	CA-CB-CG	-11.27	93.62	113.90
1	A	170	VAL	CA-C-N	-11.24	105.79	119.84
1	A	170	VAL	C-N-CA	-11.24	105.79	119.84
1	B	698	VAL	N-CA-C	10.87	120.64	110.42
1	A	669	GLY	N-CA-C	-10.71	101.82	111.67
1	B	272	GLU	N-CA-C	10.12	125.02	112.47
1	A	656	GLY	N-CA-C	-10.08	100.63	112.73
1	B	170	VAL	CA-C-N	-10.04	107.30	119.84
1	B	170	VAL	C-N-CA	-10.04	107.30	119.84
1	A	268	GLN	N-CA-C	9.64	131.34	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	ILE	N-CA-C	9.59	120.41	110.72
1	A	261	TYR	CA-CB-CG	-9.44	96.91	113.90
1	B	161	TYR	N-CA-C	-9.37	95.89	110.42
1	B	677	GLY	N-CA-C	-9.22	101.73	112.79
1	B	170	VAL	N-CA-C	8.52	115.31	107.56
1	A	315	ASP	N-CA-C	8.44	123.88	113.50
1	A	698	VAL	N-CA-C	8.39	118.44	110.30
1	A	263	PHE	CA-C-N	-8.37	110.31	119.19
1	A	263	PHE	C-N-CA	-8.37	110.31	119.19
1	B	197	TYR	N-CA-C	-8.23	102.25	111.14
1	B	308	VAL	N-CA-C	8.02	118.83	110.72
1	A	161	TYR	N-CA-C	-7.96	98.09	110.42
1	B	198	THR	N-CA-C	7.96	120.66	111.11
1	B	346	ASP	N-CA-C	7.89	119.91	110.44
1	A	232	ASP	N-CA-C	7.86	119.84	111.28
1	B	432	ASP	N-CA-C	7.83	120.90	111.82
1	B	656	GLY	N-CA-C	-7.75	103.43	112.73
1	B	60	VAL	N-CA-C	7.62	118.42	110.72
1	A	60	VAL	N-CA-C	7.56	118.36	110.72
1	A	328	SER	N-CA-C	-7.54	103.04	111.71
1	B	312	LYS	CA-C-N	7.49	127.25	119.76
1	B	312	LYS	C-N-CA	7.49	127.25	119.76
1	B	101	ALA	N-CA-C	-7.47	103.22	111.36
1	B	263	PHE	N-CA-C	7.43	122.59	112.55
1	B	43	ARG	N-CA-C	-7.36	103.19	111.14
1	A	432	ASP	N-CA-C	7.34	120.34	111.82
1	B	62	ILE	N-CA-C	-7.34	103.38	110.42
1	A	307	TYR	N-CA-C	7.24	118.82	111.07
1	A	162	THR	N-CA-C	7.22	119.10	110.44
1	A	556	TYR	N-CA-C	-7.20	103.52	111.36
1	A	226	ILE	CA-C-N	7.19	130.23	120.38
1	A	226	ILE	C-N-CA	7.19	130.23	120.38
1	B	261	TYR	N-CA-C	7.15	124.76	114.39
1	A	43	ARG	N-CA-C	-7.13	103.44	111.14
1	B	386	TYR	N-CA-C	-7.12	100.67	110.35
1	A	419	PRO	CA-C-N	-7.09	111.12	118.85
1	A	419	PRO	C-N-CA	-7.09	111.12	118.85
1	B	694	LEU	N-CA-C	7.09	118.79	111.14
1	A	389	LYS	CA-C-N	-7.07	111.61	118.97
1	A	389	LYS	C-N-CA	-7.07	111.61	118.97
1	A	197	TYR	N-CA-C	-7.06	103.51	111.14
1	A	639	ILE	N-CA-C	7.05	117.19	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	LEU	N-CA-C	6.96	118.95	111.36
1	B	16	GLY	N-CA-C	-6.95	104.14	113.24
1	A	120	LYS	N-CA-C	-6.90	103.54	112.23
1	A	415	LYS	N-CA-C	-6.90	103.54	112.23
1	A	505	SER	N-CA-C	-6.88	103.56	112.23
1	A	312	LYS	N-CA-C	-6.81	100.99	109.64
1	A	157	ASN	N-CA-C	-6.80	102.47	111.24
1	B	120	LYS	N-CA-C	-6.79	103.68	112.23
1	B	82	LEU	N-CA-C	-6.79	103.89	111.28
1	B	282	THR	N-CA-C	-6.73	103.87	111.07
1	A	261	TYR	N-CA-C	6.67	124.79	114.64
1	A	301	SER	N-CA-C	6.65	118.61	111.36
1	B	21	ASN	N-CA-C	6.64	119.36	111.33
1	B	670	ASN	N-CA-C	6.63	120.95	112.86
1	B	486	HIS	N-CA-C	-6.61	104.00	111.14
1	A	353	LEU	N-CA-C	-6.59	104.18	111.82
1	A	101	ALA	N-CA-C	-6.58	104.19	111.36
1	A	82	LEU	N-CA-C	-6.55	104.14	111.28
1	B	263	PHE	CA-C-N	-6.52	112.28	119.19
1	B	263	PHE	C-N-CA	-6.52	112.28	119.19
1	A	172	PHE	N-CA-C	6.51	118.46	111.36
1	A	123	TYR	N-CA-C	6.47	118.33	111.28
1	B	488	ASP	N-CA-C	6.46	117.98	111.07
1	A	343	TYR	CA-CB-CG	-6.42	102.34	113.90
1	B	226	ILE	CA-C-N	6.38	129.13	120.38
1	B	226	ILE	C-N-CA	6.38	129.13	120.38
1	B	160	ILE	N-CA-C	-6.38	96.07	109.34
1	A	21	ASN	N-CA-C	6.38	119.05	111.33
1	B	673	GLY	N-CA-C	-6.31	106.53	115.30
1	A	516	SER	N-CA-C	-6.30	104.33	111.07
1	A	10	ILE	CA-C-N	6.25	125.81	119.19
1	A	10	ILE	C-N-CA	6.25	125.81	119.19
1	B	25	VAL	N-CA-C	6.23	116.86	110.82
1	B	259	ALA	N-CA-C	-6.22	104.42	111.07
1	B	245	LEU	N-CA-C	-6.20	104.43	111.07
1	B	517	TYR	N-CA-C	6.13	118.74	111.33
1	A	16	GLY	N-CA-C	-6.12	105.22	113.24
1	A	73	THR	N-CA-C	6.10	118.76	107.60
1	A	421	THR	N-CA-C	6.07	117.56	111.07
1	B	10	ILE	CA-C-N	6.07	125.62	119.19
1	B	10	ILE	C-N-CA	6.07	125.62	119.19
1	B	15	LEU	N-CA-C	6.07	117.97	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	389	LYS	CB-CG-CD	6.07	125.25	111.30
1	A	484	THR	N-CA-C	6.00	117.49	111.07
1	B	648	LEU	N-CA-C	6.00	118.78	111.82
1	B	511	LEU	N-CA-C	6.00	117.90	111.36
1	A	451	VAL	N-CA-C	5.97	119.41	111.17
1	A	309	ILE	N-CA-C	5.96	116.14	110.42
1	A	62	ILE	N-CA-C	-5.95	104.71	110.42
1	A	521	GLN	N-CA-C	-5.94	106.04	113.28
1	A	536	LEU	CA-CB-CG	5.92	137.04	116.30
1	A	648	LEU	N-CA-C	5.92	118.69	111.82
1	A	673	GLY	N-CA-C	-5.91	107.09	115.30
1	B	205	ALA	N-CA-C	5.90	117.38	111.07
1	B	141	LEU	N-CA-C	5.89	117.70	111.28
1	B	313	PRO	N-CA-C	5.89	120.43	111.19
1	A	431	ALA	N-CA-C	-5.87	104.07	111.11
1	B	195	GLY	N-CA-C	-5.86	105.70	112.73
1	B	444	ALA	N-CA-C	-5.83	104.28	111.33
1	A	111	THR	N-CA-C	-5.81	104.94	111.28
1	B	246	GLU	N-CA-C	5.81	117.29	111.07
1	A	361	SER	CA-C-N	-5.78	113.72	119.56
1	A	361	SER	C-N-CA	-5.78	113.72	119.56
1	B	280	LYS	N-CA-C	5.78	118.04	111.11
1	A	539	MET	N-CA-C	5.75	119.56	112.54
1	B	22	PHE	N-CA-CB	5.71	118.29	110.01
1	B	719	ILE	N-CA-C	-5.70	106.25	111.67
1	B	317	PRO	N-CA-C	5.68	120.96	113.86
1	B	649	ALA	N-CA-C	-5.68	105.00	111.07
1	B	389	LYS	CA-C-N	-5.67	113.07	118.97
1	B	389	LYS	C-N-CA	-5.67	113.07	118.97
1	A	22	PHE	N-CA-CB	5.66	118.22	110.01
1	A	508	PHE	CA-C-N	5.66	127.80	120.44
1	A	508	PHE	C-N-CA	5.66	127.80	120.44
1	B	73	THR	N-CA-C	5.65	117.94	107.60
1	A	704	ILE	N-CA-C	5.63	116.41	110.72
1	B	470	ILE	CB-CA-C	-5.63	104.54	112.14
1	A	97	MET	N-CA-C	5.62	117.09	111.07
1	B	416	SER	N-CA-C	-5.62	106.38	113.18
1	B	699	GLY	CA-C-N	5.62	125.14	119.19
1	B	699	GLY	C-N-CA	5.62	125.14	119.19
1	A	98	ALA	N-CA-C	-5.58	104.42	111.11
1	A	227	ALA	CA-C-N	5.57	127.74	120.28
1	A	227	ALA	C-N-CA	5.57	127.74	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	SER	N-CA-C	-5.56	105.36	111.82
1	A	725	LEU	N-CA-C	5.55	119.65	111.04
1	B	367	ILE	N-CA-C	5.53	115.73	110.42
1	A	447	MET	N-CA-C	-5.51	104.66	111.33
1	A	317	PRO	N-CA-C	5.50	120.74	113.86
1	A	560	GLY	N-CA-C	-5.50	106.12	112.50
1	B	483	ILE	N-CA-C	-5.48	105.03	110.62
1	B	560	GLY	N-CA-C	-5.47	105.77	112.77
1	B	100	ARG	N-CA-CB	5.44	118.28	110.40
1	A	699	GLY	CA-C-N	5.42	125.24	119.28
1	A	699	GLY	C-N-CA	5.42	125.24	119.28
1	B	415	LYS	N-CA-C	-5.36	105.48	112.23
1	B	172	PHE	N-CA-C	5.34	117.19	111.36
1	B	343	TYR	CA-CB-CG	-5.34	104.30	113.90
1	A	272	GLU	CB-CA-C	-5.33	103.09	111.51
1	B	459	SER	N-CA-C	-5.29	106.09	112.54
1	B	549	LEU	N-CA-C	-5.29	105.60	111.36
1	B	228	ASP	N-CA-C	5.28	117.03	111.28
1	A	25	VAL	N-CA-C	5.26	115.92	110.82
1	A	73	THR	CB-CA-C	-5.24	103.73	111.70
1	B	227	ALA	CA-C-N	5.22	127.27	120.28
1	B	227	ALA	C-N-CA	5.22	127.27	120.28
1	A	649	ALA	N-CA-C	-5.21	105.60	111.28
1	B	336	THR	N-CA-C	-5.21	105.60	111.28
1	A	386	TYR	N-CA-C	-5.20	103.28	110.35
1	B	285	ALA	N-CA-C	-5.20	105.30	111.69
1	B	289	TYR	CA-C-N	-5.19	113.69	119.19
1	B	289	TYR	C-N-CA	-5.19	113.69	119.19
1	A	49	PHE	N-CA-C	-5.18	105.71	111.36
1	B	98	ALA	N-CA-C	-5.18	105.06	111.33
1	B	123	TYR	N-CA-C	5.18	116.93	111.28
1	A	434	PHE	N-CA-C	5.18	118.46	112.97
1	A	308	VAL	CA-C-N	5.16	127.06	120.56
1	A	308	VAL	C-N-CA	5.16	127.06	120.56
1	B	659	TRP	N-CA-C	5.12	116.86	111.28
1	A	624	VAL	CB-CA-C	-5.12	105.41	111.81
1	B	419	PRO	CA-C-N	-5.12	113.37	119.05
1	B	419	PRO	C-N-CA	-5.12	113.37	119.05
1	A	198	THR	N-CA-C	5.11	117.25	111.11
1	A	719	ILE	N-CA-C	-5.11	106.81	111.67
1	B	400	GLU	N-CA-C	5.11	119.67	113.38
1	A	357	PHE	N-CA-C	5.11	119.05	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	725	LEU	N-CA-C	5.10	118.94	111.04
1	A	110	ARG	CA-CB-CG	5.09	124.28	114.10
1	B	25	VAL	CB-CA-C	-5.06	105.41	112.04
1	B	414	MET	N-CA-C	5.06	116.80	111.28
1	B	704	ILE	N-CA-C	5.06	115.83	110.72
1	B	518	MET	N-CA-C	-5.05	105.85	111.36
1	A	160	ILE	N-CA-C	-5.05	98.84	109.34
1	A	195	GLY	N-CA-C	-5.04	106.68	112.73
1	A	110	ARG	CA-C-N	5.04	127.03	120.28
1	A	110	ARG	C-N-CA	5.04	127.03	120.28
1	A	326	TRP	CA-C-N	5.04	127.03	120.28
1	A	326	TRP	C-N-CA	5.04	127.03	120.28
1	B	536	LEU	CA-CB-CG	5.03	133.91	116.30
1	A	400	GLU	N-CA-C	5.03	119.56	113.38
1	B	521	GLN	N-CA-C	-5.02	107.16	113.28

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	268	GLN	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4771	0	4805	833	0
1	B	4605	0	4619	764	0
2	A	10	0	0	3	0
2	B	10	0	0	4	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	9406	0	9424	1550	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 82.

All (1550) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:TYR:CD2	1:A:680:PRO:HG2	1.61	1.35
1:A:170:VAL:HG22	1:A:261:TYR:OH	1.32	1.28
1:B:326:TRP:NE1	1:B:378:PHE:HZ	1.38	1.21
1:A:674:TYR:CE2	1:A:680:PRO:HG2	1.75	1.19
1:B:170:VAL:HG22	1:B:261:TYR:OH	1.37	1.19
1:A:19:ALA:HA	1:A:22:PHE:CE1	1.79	1.17
1:B:19:ALA:HA	1:B:22:PHE:CE1	1.79	1.16
1:B:383:TYR:HA	1:B:390:PRO:HG2	1.22	1.15
1:A:263:PHE:HB3	1:A:283:ILE:CD1	1.75	1.14
1:A:158:LEU:O	1:A:263:PHE:CZ	2.01	1.14
1:A:326:TRP:NE1	1:A:378:PHE:HZ	1.48	1.12
1:A:717:VAL:O	1:A:721:LYS:HG3	1.50	1.12
1:B:521:GLN:HE22	1:B:631:ALA:HB1	1.13	1.12
1:A:321:LEU:HD23	1:A:457:VAL:HG13	1.13	1.11
1:A:263:PHE:CD1	1:A:264:PRO:HD3	1.86	1.10
1:A:383:TYR:HA	1:A:390:PRO:HG2	1.13	1.10
1:A:65:ALA:HB2	1:A:81:LEU:HD21	1.34	1.09
1:B:19:ALA:HA	1:B:22:PHE:HE1	1.07	1.09
1:A:170:VAL:HG22	1:A:261:TYR:CZ	1.86	1.09
1:B:561:TYR:HE2	1:B:614:PRO:HD3	1.18	1.09
1:B:717:VAL:O	1:B:721:LYS:HG3	1.53	1.08
1:B:321:LEU:HD23	1:B:457:VAL:HG13	1.29	1.07
1:B:337:ALA:HB2	1:B:363:TRP:CE2	1.90	1.07
1:A:19:ALA:HA	1:A:22:PHE:HE1	1.06	1.07
1:A:561:TYR:CE2	1:A:614:PRO:HD3	1.90	1.06
1:A:561:TYR:HE2	1:A:614:PRO:HD3	1.01	1.06
1:A:198:THR:HG21	1:A:235:GLY:N	1.71	1.05
1:A:263:PHE:CE1	1:A:264:PRO:HD3	1.91	1.05
1:B:461:GLY:CA	1:B:491:GLY:HA2	1.87	1.05
1:B:65:ALA:HB2	1:B:81:LEU:HD21	1.36	1.05
1:B:198:THR:HG21	1:B:235:GLY:N	1.71	1.05
1:A:619:ILE:HD11	1:A:708:ILE:HG12	1.39	1.04
1:B:233:ASN:O	1:B:237:VAL:HG22	1.57	1.04
1:B:246:GLU:OE1	1:B:704:ILE:HD12	1.57	1.04
1:A:655:SER:OG	1:A:659:TRP:CZ3	2.10	1.04
1:A:468:GLY:HA2	1:A:484:THR:HG23	1.39	1.03
1:B:468:GLY:CA	1:B:484:THR:HG23	1.89	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:GLY:HA2	1:A:484:THR:CG2	1.89	1.02
1:A:674:TYR:HD2	1:A:680:PRO:HG2	1.22	1.02
1:A:492:ASN:ND2	2:A:1728:PO4:O2	1.91	1.02
1:A:674:TYR:CE2	1:A:680:PRO:CG	2.42	1.02
1:A:65:ALA:CB	1:A:81:LEU:HD21	1.88	1.01
1:A:102:ASN:O	1:A:105:VAL:HG12	1.61	1.01
1:B:73:THR:HG21	1:B:169:PHE:CE2	1.96	1.00
1:B:468:GLY:HA2	1:B:484:THR:HG23	1.39	1.00
1:A:563:ILE:HG21	1:B:411:SER:HB2	1.44	1.00
1:A:536:LEU:HD21	1:B:536:LEU:HD21	1.42	1.00
1:A:332:THR:O	1:A:336:THR:OG1	1.79	1.00
1:A:674:TYR:CD2	1:A:680:PRO:CG	2.45	1.00
1:B:105:VAL:HG11	1:B:467:ALA:HB2	1.39	1.00
1:B:162:THR:HA	1:B:168:ASN:HA	1.42	1.00
1:A:357:PHE:CE2	1:A:361:SER:HA	1.96	0.99
1:A:514:PHE:HZ	1:A:537:LEU:HD12	1.23	0.99
1:B:188:MET:HB2	1:B:704:ILE:HG21	1.40	0.99
1:A:22:PHE:HA	1:A:97:MET:HE2	1.43	0.99
1:B:170:VAL:HG22	1:B:261:TYR:CZ	1.98	0.98
1:A:286:LEU:O	1:A:438:TYR:OH	1.79	0.98
1:A:563:ILE:CG2	1:B:411:SER:HB2	1.93	0.98
1:B:461:GLY:HA3	1:B:491:GLY:HA2	1.40	0.98
1:B:65:ALA:CB	1:B:81:LEU:HD21	1.94	0.97
1:B:185:ILE:HG12	1:B:708:ILE:HD11	1.44	0.97
1:A:73:THR:O	1:A:75:GLN:N	1.96	0.97
1:B:561:TYR:CE2	1:B:614:PRO:HD3	1.99	0.97
1:B:102:ASN:O	1:B:105:VAL:HG12	1.64	0.97
1:B:468:GLY:HA2	1:B:484:THR:CG2	1.94	0.97
1:B:169:PHE:HB2	1:B:174:MET:HE3	1.45	0.97
1:B:73:THR:O	1:B:75:GLN:N	1.97	0.96
1:B:543:ARG:NH1	1:B:629:LEU:O	1.98	0.96
1:A:233:ASN:O	1:A:237:VAL:HG22	1.65	0.96
1:B:556:TYR:CE1	1:B:648:LEU:HD11	2.01	0.96
1:A:464:ALA:HB1	1:A:487:LEU:HB3	1.45	0.95
1:A:711:VAL:O	1:A:714:VAL:HG22	1.64	0.95
1:A:357:PHE:CE2	1:A:364:PHE:HD2	1.84	0.95
1:A:236:ASP:HB2	1:A:462:PRO:HG3	1.47	0.95
1:B:332:THR:O	1:B:336:THR:OG1	1.85	0.94
1:A:411:SER:HB2	1:B:563:ILE:CG2	1.96	0.94
1:A:514:PHE:CZ	1:A:537:LEU:HD12	2.03	0.94
1:A:105:VAL:HG11	1:A:467:ALA:HB2	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:VAL:HG21	1:A:720:PHE:HE1	1.32	0.94
1:A:705:LEU:HD21	1:A:709:MET:HE3	1.49	0.94
1:A:129:MET:HE1	1:A:237:VAL:HB	1.50	0.93
1:B:424:LEU:HD21	1:B:447:MET:HE1	1.50	0.93
1:B:608:LEU:HD23	1:B:611:MET:HE2	1.48	0.93
1:B:10:ILE:O	1:B:13:VAL:HG13	1.69	0.93
1:A:297:GLY:O	1:A:299:GLY:N	2.01	0.93
1:B:677:GLY:O	1:B:678:SER:OG	1.87	0.93
1:A:188:MET:HB2	1:A:704:ILE:HG21	1.51	0.93
1:A:246:GLU:OE1	1:A:704:ILE:HD12	1.69	0.93
1:B:619:ILE:HD11	1:B:708:ILE:HG12	1.51	0.93
1:A:401:GLY:O	1:A:403:GLY:N	2.01	0.93
1:B:22:PHE:HA	1:B:97:MET:HE2	1.51	0.92
1:A:316:ASN:O	1:A:320:GLU:OE1	1.86	0.92
1:B:333:VAL:O	1:B:363:TRP:NE1	2.00	0.92
1:A:73:THR:HG21	1:A:169:PHE:CE2	2.04	0.92
1:A:411:SER:HB2	1:B:563:ILE:HG21	1.48	0.92
1:A:666:LEU:C	1:A:666:LEU:HD13	1.95	0.91
1:B:634:VAL:HG21	1:B:720:PHE:HE1	1.33	0.91
1:B:399:ILE:HA	1:B:680:PRO:HG3	1.50	0.91
1:A:72:THR:O	1:A:163:ASN:ND2	2.02	0.91
1:A:198:THR:HG21	1:A:235:GLY:H	1.32	0.91
1:B:326:TRP:NE1	1:B:378:PHE:CZ	2.26	0.90
1:A:169:PHE:HE1	1:A:171:PRO:HA	1.36	0.90
1:B:409:GLY:HA3	1:B:659:TRP:CZ2	2.07	0.90
1:B:462:PRO:HA	1:B:465:ASP:HB3	1.54	0.90
1:A:262:MET:HG2	1:A:353:LEU:HD22	1.52	0.90
1:A:720:PHE:HA	1:A:723:VAL:HG12	1.51	0.90
1:B:316:ASN:O	1:B:320:GLU:OE1	1.90	0.90
1:B:401:GLY:O	1:B:403:GLY:N	2.05	0.90
1:B:711:VAL:O	1:B:714:VAL:HG22	1.70	0.90
1:B:170:VAL:HG22	1:B:261:TYR:HH	1.32	0.90
1:B:170:VAL:HB	1:B:173:ALA:HB3	1.54	0.90
1:B:666:LEU:HD13	1:B:666:LEU:C	1.98	0.89
1:A:608:LEU:HD23	1:A:611:MET:HE2	1.54	0.89
1:A:499:LYS:HE2	1:A:695:LYS:O	1.72	0.89
1:B:68:LEU:HD21	1:B:76:THR:HB	1.54	0.89
1:A:170:VAL:CG2	1:A:261:TYR:CE2	2.54	0.89
1:A:638:LEU:O	1:A:642:VAL:HG23	1.71	0.89
1:A:656:GLY:CA	1:A:695:LYS:HD3	2.02	0.89
1:A:263:PHE:CD1	1:A:264:PRO:CD	2.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:PRO:HB3	1:A:713:SER:OG	1.74	0.88
1:B:170:VAL:HG21	1:B:261:TYR:CE2	2.08	0.88
1:A:461:GLY:CA	1:A:491:GLY:HA2	2.04	0.88
1:B:414:MET:HG3	1:B:651:LEU:HD21	1.55	0.88
1:B:363:TRP:CZ2	1:B:367:ILE:HD11	2.08	0.87
1:A:169:PHE:HB2	1:A:174:MET:HE3	1.56	0.87
1:A:468:GLY:CA	1:A:484:THR:HG23	2.05	0.86
1:B:622:PRO:HB3	1:B:713:SER:OG	1.76	0.86
1:A:10:ILE:O	1:A:13:VAL:HG13	1.75	0.86
1:A:86:MET:HE1	1:A:139:LEU:HD23	1.58	0.86
1:A:333:VAL:HG13	1:A:367:ILE:HD11	1.56	0.86
1:B:297:GLY:O	1:B:299:GLY:N	2.08	0.86
1:B:86:MET:HE1	1:B:139:LEU:HD23	1.56	0.86
1:B:705:LEU:HD21	1:B:709:MET:HE3	1.56	0.86
1:A:666:LEU:HB3	1:A:684:LEU:HD23	1.56	0.86
1:B:720:PHE:HA	1:B:723:VAL:HG12	1.56	0.86
1:B:180:ALA:HB2	1:B:253:VAL:HG21	1.57	0.85
1:B:464:ALA:HB1	1:B:487:LEU:HB3	1.56	0.85
1:B:521:GLN:NE2	1:B:631:ALA:HB1	1.90	0.85
1:B:25:VAL:HG21	1:B:124:GLN:HB3	1.59	0.85
1:B:170:VAL:CG2	1:B:261:TYR:CE2	2.59	0.85
1:A:68:LEU:HD21	1:A:76:THR:HB	1.57	0.85
1:A:489:ALA:HA	1:A:661:ASN:HD21	1.42	0.85
1:A:170:VAL:HG21	1:A:261:TYR:CE2	2.12	0.85
1:A:424:LEU:O	1:A:428:ILE:HD13	1.76	0.85
1:A:561:TYR:HE2	1:A:614:PRO:CD	1.89	0.85
1:A:656:GLY:HA3	1:A:695:LYS:CD	2.07	0.85
1:A:517:TYR:OH	1:A:634:VAL:HG23	1.77	0.84
1:B:161:TYR:CD2	1:B:169:PHE:CE2	2.65	0.84
1:A:503:ILE:O	1:A:507:ILE:HD12	1.77	0.84
1:A:161:TYR:CD2	1:A:169:PHE:CE2	2.65	0.84
1:B:169:PHE:HE1	1:B:171:PRO:HA	1.41	0.84
1:A:409:GLY:HA3	1:A:659:TRP:CZ2	2.13	0.84
1:B:492:ASN:ND2	2:B:1728:PO4:O2	2.11	0.84
1:A:227:ALA:O	1:A:230:VAL:HG22	1.76	0.83
1:A:263:PHE:HB3	1:A:283:ILE:HD11	1.59	0.83
1:A:326:TRP:HE1	1:A:378:PHE:HZ	0.98	0.83
1:B:129:MET:HE1	1:B:237:VAL:HB	1.61	0.83
1:B:268:GLN:CB	1:B:275:VAL:HB	2.07	0.83
1:A:263:PHE:HB3	1:A:283:ILE:HD13	1.59	0.83
1:B:395:GLY:O	1:B:398:SER:OG	1.97	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:HA	1:A:97:MET:CE	2.07	0.82
1:A:503:ILE:HG12	1:A:703:ASP:OD1	1.78	0.82
1:A:545:ILE:HG13	1:B:511:LEU:HD21	1.59	0.82
1:B:663:LYS:HA	1:B:684:LEU:HB3	1.62	0.82
1:A:25:VAL:HG21	1:A:124:GLN:HB3	1.60	0.81
1:B:526:ASP:O	1:B:528:GLY:N	2.13	0.81
1:A:198:THR:HG22	1:A:231:GLY:HA2	1.62	0.81
1:A:536:LEU:CD2	1:B:536:LEU:HD21	2.10	0.81
1:A:170:VAL:O	1:A:171:PRO:C	2.22	0.81
1:B:105:VAL:HA	1:B:121:VAL:HG11	1.62	0.81
1:A:167:ILE:HG23	1:A:718:SER:HB3	1.62	0.81
1:A:263:PHE:CZ	1:A:264:PRO:HD3	2.15	0.81
1:B:163:ASN:HD21	1:B:164:TRP:HD1	1.26	0.81
1:A:259:ALA:C	1:A:261:TYR:H	1.87	0.81
1:A:355:PHE:CE2	1:A:362:PRO:HD3	2.16	0.81
1:A:656:GLY:CA	1:A:695:LYS:CD	2.59	0.81
1:B:321:LEU:CD2	1:B:457:VAL:HG13	2.08	0.81
1:B:506:ALA:HB1	1:B:706:ILE:HD11	1.60	0.81
1:A:167:ILE:HG23	1:A:718:SER:CB	2.11	0.80
1:A:42:ILE:HD12	1:A:43:ARG:N	1.96	0.80
1:A:205:ALA:HB2	1:A:228:ASP:HB2	1.64	0.80
1:A:656:GLY:HA3	1:A:695:LYS:HB3	1.61	0.80
1:B:666:LEU:HB3	1:B:684:LEU:HD23	1.63	0.80
1:A:170:VAL:HG11	1:A:173:ALA:CB	2.12	0.80
1:B:244:LEU:CD2	1:B:502:ALA:HB2	2.12	0.80
1:A:105:VAL:HA	1:A:121:VAL:HG11	1.62	0.80
1:A:350:LEU:HD22	1:A:355:PHE:CD2	2.17	0.80
1:A:14:ALA:O	1:A:17:PHE:HB3	1.82	0.80
1:B:522:ILE:HG23	1:B:522:ILE:O	1.82	0.79
1:B:617:ILE:O	1:B:621:THR:OG1	2.00	0.79
1:A:162:THR:HA	1:A:168:ASN:HA	1.64	0.79
1:A:461:GLY:HA3	1:A:491:GLY:HA2	1.62	0.79
1:A:719:ILE:HG22	1:A:723:VAL:HG11	1.65	0.79
1:B:170:VAL:O	1:B:171:PRO:C	2.21	0.79
1:A:226:ILE:HG22	1:A:227:ALA:N	1.96	0.79
1:A:357:PHE:CZ	1:A:361:SER:HA	2.16	0.79
1:B:105:VAL:CG1	1:B:467:ALA:HB2	2.10	0.79
1:B:556:TYR:HE1	1:B:648:LEU:HD11	1.47	0.79
1:B:282:THR:HG23	1:B:347:LEU:HB3	1.64	0.79
1:A:321:LEU:CD2	1:A:457:VAL:HG13	2.06	0.79
1:A:414:MET:HG3	1:A:651:LEU:HD21	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:THR:HA	1:A:347:LEU:HD12	1.65	0.79
1:A:169:PHE:CE1	1:A:171:PRO:HA	2.17	0.79
1:B:42:ILE:HD12	1:B:43:ARG:N	1.98	0.79
1:B:397:SER:HB2	1:B:404:MET:HE3	1.64	0.79
1:A:550:LEU:HD13	1:A:554:ILE:HD11	1.66	0.78
1:A:73:THR:HG21	1:A:169:PHE:CD2	2.18	0.78
1:A:521:GLN:HE22	1:A:631:ALA:HB1	1.46	0.78
1:A:170:VAL:CG2	1:A:261:TYR:CZ	2.65	0.78
1:B:198:THR:HG21	1:B:235:GLY:CA	2.14	0.78
1:B:72:THR:O	1:B:163:ASN:ND2	2.16	0.78
1:B:73:THR:HG21	1:B:169:PHE:CD2	2.18	0.78
1:B:127:SER:O	1:B:131:LEU:HD13	1.83	0.78
1:A:69:MET:HE2	1:A:74:TRP:HB2	1.65	0.78
1:B:634:VAL:HG21	1:B:720:PHE:CE1	2.18	0.78
1:A:333:VAL:O	1:A:363:TRP:NE1	2.16	0.77
1:A:357:PHE:HE2	1:A:360:ILE:HG23	1.49	0.77
1:A:521:GLN:NE2	1:A:631:ALA:HB1	2.00	0.77
1:A:663:LYS:HA	1:A:684:LEU:HB3	1.65	0.77
1:A:161:TYR:HD2	1:A:169:PHE:CE2	2.01	0.77
1:B:289:TYR:HB2	1:B:344:LEU:HD21	1.65	0.77
1:B:460:TYR:O	1:B:463:ILE:HG22	1.84	0.77
1:B:244:LEU:HD23	1:B:502:ALA:HB2	1.65	0.77
1:B:424:LEU:O	1:B:428:ILE:HD13	1.84	0.77
1:A:226:ILE:HG22	1:A:227:ALA:H	1.50	0.77
1:B:22:PHE:HA	1:B:97:MET:CE	2.14	0.77
1:B:666:LEU:HD11	1:B:681:HIS:HB2	1.67	0.77
1:A:445:LEU:O	1:A:449:SER:N	2.18	0.77
1:B:170:VAL:CB	1:B:173:ALA:HB3	2.14	0.77
1:A:337:ALA:HB2	1:A:363:TRP:CE2	2.19	0.77
1:A:634:VAL:HG21	1:A:720:PHE:CE1	2.18	0.77
1:B:686:ILE:O	1:B:690:VAL:HG23	1.84	0.77
1:A:357:PHE:CE1	1:A:434:PHE:HB3	2.20	0.77
1:A:263:PHE:CG	1:A:264:PRO:HD3	2.20	0.76
1:A:357:PHE:CZ	1:A:364:PHE:HD2	2.02	0.76
1:A:547:GLY:O	1:A:637:VAL:HA	1.85	0.76
1:B:14:ALA:O	1:B:17:PHE:HB3	1.83	0.76
1:A:21:ASN:HB3	1:A:124:GLN:OE1	1.86	0.76
1:A:666:LEU:HD11	1:A:681:HIS:HB2	1.68	0.76
1:B:317:PRO:O	1:B:321:LEU:HD13	1.85	0.76
1:B:521:GLN:HE22	1:B:631:ALA:CB	1.97	0.76
1:A:556:TYR:CE1	1:A:648:LEU:HD11	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ALA:HA	1:B:661:ASN:HD21	1.50	0.76
1:A:237:VAL:HG23	1:A:238:ALA:N	1.99	0.76
1:A:289:TYR:HB2	1:A:344:LEU:HD21	1.66	0.76
1:A:236:ASP:HB2	1:A:462:PRO:CG	2.15	0.76
1:B:73:THR:HG21	1:B:169:PHE:CZ	2.21	0.75
1:B:169:PHE:CE1	1:B:171:PRO:HA	2.21	0.75
1:B:301:SER:HB2	1:B:452:ALA:HB3	1.66	0.75
1:A:298:LEU:HD12	1:A:299:GLY:N	2.01	0.75
1:A:357:PHE:CE2	1:A:360:ILE:HG23	2.22	0.75
1:B:259:ALA:C	1:B:261:TYR:H	1.93	0.75
1:B:396:LYS:HG2	1:B:671:LEU:CD2	2.16	0.75
1:A:259:ALA:O	1:A:261:TYR:N	2.20	0.75
1:A:647:MET:HE1	1:B:553:ALA:HA	1.67	0.75
1:B:236:ASP:HB2	1:B:462:PRO:CG	2.17	0.75
1:B:560:GLY:O	1:B:563:ILE:HG22	1.87	0.75
1:A:97:MET:CG	1:A:125:GLY:HA2	2.16	0.75
1:B:666:LEU:HD11	1:B:681:HIS:CB	2.17	0.75
1:A:288:SER:HA	1:A:291:ILE:HD12	1.67	0.75
1:A:394:LEU:HD21	1:A:659:TRP:CD1	2.22	0.75
1:B:237:VAL:HG23	1:B:238:ALA:N	2.02	0.75
1:B:719:ILE:HG22	1:B:723:VAL:HG11	1.67	0.75
1:A:127:SER:O	1:A:131:LEU:HD13	1.87	0.74
1:A:526:ASP:O	1:A:528:GLY:N	2.20	0.74
1:B:402:THR:O	1:B:405:VAL:HG22	1.86	0.74
1:B:236:ASP:HB2	1:B:462:PRO:HG3	1.67	0.74
1:A:326:TRP:NE1	1:A:378:PHE:CZ	2.33	0.74
1:A:464:ALA:O	1:A:467:ALA:HB3	1.87	0.74
1:A:121:VAL:HG13	1:A:122:ALA:H	1.53	0.74
1:B:161:TYR:HD2	1:B:169:PHE:CE2	2.04	0.74
1:B:400:GLU:HG3	1:B:404:MET:HE2	1.69	0.74
1:B:86:MET:HE2	1:B:140:GLY:N	2.02	0.74
1:B:561:TYR:HE2	1:B:614:PRO:CD	1.97	0.74
1:B:76:THR:HG23	1:B:174:MET:O	1.88	0.74
1:B:461:GLY:HA2	1:B:491:GLY:HA2	1.66	0.74
1:B:710:SER:O	1:B:714:VAL:HG13	1.86	0.74
1:B:268:GLN:O	1:B:269:LYS:CB	2.35	0.74
1:A:617:ILE:O	1:A:621:THR:OG1	2.04	0.74
1:B:22:PHE:HB3	1:B:128:VAL:HG21	1.69	0.74
1:B:97:MET:CG	1:B:125:GLY:HA2	2.17	0.74
1:B:247:SER:OG	1:B:707:LYS:NZ	2.16	0.73
1:A:22:PHE:HB3	1:A:128:VAL:HG21	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:PHE:CE2	1:A:364:PHE:CD2	2.73	0.73
1:A:386:TYR:O	1:A:387:ARG:CB	2.35	0.73
1:B:358:GLY:N	1:B:361:SER:HG	1.86	0.73
1:B:460:TYR:CE1	1:B:490:VAL:CG1	2.71	0.73
1:A:674:TYR:HE2	1:A:680:PRO:CG	1.94	0.73
1:A:460:TYR:O	1:A:463:ILE:HG22	1.88	0.73
1:A:710:SER:O	1:A:714:VAL:HG13	1.88	0.73
1:B:521:GLN:HG2	1:B:721:LYS:HG2	1.70	0.73
1:A:298:LEU:HD12	1:A:299:GLY:H	1.52	0.73
1:B:259:ALA:O	1:B:261:TYR:N	2.22	0.73
1:A:290:PRO:HD3	1:A:438:TYR:OH	1.88	0.73
1:A:553:ALA:HA	1:B:647:MET:HE1	1.69	0.73
1:B:429:LEU:N	1:B:429:LEU:HD23	2.03	0.73
1:A:297:GLY:O	1:A:300:CYS:N	2.19	0.73
1:B:170:VAL:HG21	1:B:261:TYR:HE2	1.51	0.73
1:B:170:VAL:CG2	1:B:261:TYR:CZ	2.70	0.73
1:B:461:GLY:CA	1:B:491:GLY:CA	2.66	0.73
1:B:233:ASN:HD21	1:B:466:ASN:HD22	1.37	0.72
1:A:666:LEU:HD11	1:A:681:HIS:CB	2.19	0.72
1:A:686:ILE:O	1:A:690:VAL:HG23	1.89	0.72
1:A:5:ALA:O	1:A:9:LEU:HD12	1.89	0.72
1:A:262:MET:HG3	1:A:266:TYR:CD2	2.25	0.72
1:A:102:ASN:HD21	1:A:466:ASN:ND2	1.87	0.72
1:A:700:PRO:O	1:A:703:ASP:HB2	1.90	0.72
1:B:514:PHE:HZ	1:B:537:LEU:HD12	1.53	0.72
1:A:489:ALA:HA	1:A:661:ASN:ND2	2.05	0.72
1:A:522:ILE:O	1:A:522:ILE:HG23	1.89	0.72
1:B:396:LYS:HG2	1:B:671:LEU:HD21	1.71	0.72
1:B:396:LYS:O	1:B:399:ILE:HG12	1.89	0.72
1:A:317:PRO:O	1:A:321:LEU:HD13	1.89	0.72
1:A:192:VAL:HG13	1:A:562:LEU:HD21	1.69	0.72
1:A:619:ILE:HG22	1:A:620:LEU:HD12	1.72	0.72
1:B:268:GLN:N	1:B:275:VAL:O	2.17	0.72
1:A:105:VAL:CG1	1:A:467:ALA:HB2	2.20	0.72
1:B:536:LEU:HD13	1:B:536:LEU:O	1.89	0.72
1:B:677:GLY:C	1:B:678:SER:HG	1.95	0.72
1:B:317:PRO:HA	1:B:320:GLU:CD	2.15	0.72
1:B:167:ILE:HG23	1:B:718:SER:CB	2.20	0.71
1:B:558:PHE:CE1	1:B:562:LEU:HD11	2.25	0.71
1:B:613:TYR:O	1:B:617:ILE:HG13	1.91	0.71
1:A:19:ALA:CA	1:A:22:PHE:CE1	2.69	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:LEU:HD21	1:B:545:ILE:HG13	1.72	0.71
1:B:322:ASN:ND2	1:B:381:GLU:OE1	2.21	0.71
1:B:621:THR:O	1:B:625:THR:OG1	2.05	0.71
1:A:45:GLY:HA2	1:A:600:ILE:HD13	1.73	0.71
1:A:357:PHE:HE1	1:A:434:PHE:HB3	1.55	0.71
1:A:647:MET:CE	1:B:553:ALA:HA	2.20	0.71
1:B:386:TYR:HB3	1:B:391:THR:HG21	1.73	0.71
1:A:129:MET:SD	1:A:459:SER:HB2	2.30	0.71
1:B:129:MET:SD	1:B:459:SER:HB2	2.30	0.71
1:B:198:THR:HG21	1:B:235:GLY:H	1.53	0.71
1:A:236:ASP:CB	1:A:462:PRO:HG3	2.21	0.70
1:B:700:PRO:O	1:B:703:ASP:HB2	1.91	0.70
1:A:170:VAL:HG21	1:A:261:TYR:HE2	1.55	0.70
1:B:307:TYR:O	1:B:311:LYS:CB	2.38	0.70
1:B:191:ARG:O	1:B:195:GLY:N	2.24	0.70
1:B:394:LEU:HD21	1:B:659:TRP:CD1	2.26	0.70
1:A:170:VAL:HG11	1:A:173:ALA:HB3	1.72	0.70
1:B:386:TYR:HB3	1:B:391:THR:CG2	2.22	0.70
1:B:492:ASN:ND2	2:B:1728:PO4:O4	2.24	0.70
1:A:22:PHE:CA	1:A:97:MET:HE2	2.21	0.70
1:B:97:MET:HG2	1:B:128:VAL:CG2	2.21	0.70
1:B:492:ASN:ND2	2:B:1728:PO4:P	2.64	0.70
1:A:461:GLY:HA2	1:A:491:GLY:HA2	1.72	0.70
1:B:188:MET:CB	1:B:704:ILE:HG21	2.17	0.70
1:B:448:LEU:HD22	1:B:505:SER:OG	1.92	0.70
1:A:68:LEU:HD23	1:A:72:THR:OG1	1.92	0.70
1:A:185:ILE:HG12	1:A:708:ILE:HD11	1.74	0.70
1:B:521:GLN:O	1:B:523:SER:N	2.19	0.70
1:A:424:LEU:HD21	1:A:447:MET:HE1	1.71	0.70
1:B:383:TYR:CA	1:B:390:PRO:HG2	2.12	0.70
1:A:170:VAL:CG1	1:A:173:ALA:HB3	2.20	0.69
1:B:194:GLY:O	1:B:198:THR:HG23	1.91	0.69
1:A:191:ARG:HH22	1:A:240:LEU:HD23	1.57	0.69
1:B:163:ASN:CG	1:B:164:TRP:N	2.50	0.69
1:A:158:LEU:O	1:A:263:PHE:CE2	2.44	0.69
1:A:170:VAL:CB	1:A:173:ALA:HB3	2.22	0.69
1:A:418:PHE:HB3	1:A:419:PRO:HD3	1.73	0.69
1:B:333:VAL:HG13	1:B:367:ILE:HD11	1.73	0.69
1:B:5:ALA:O	1:B:9:LEU:HD12	1.91	0.69
1:B:21:ASN:HB3	1:B:124:GLN:OE1	1.93	0.69
1:B:290:PRO:HD3	1:B:438:TYR:OH	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ALA:HB1	1:B:425:VAL:HG13	1.73	0.69
1:A:674:TYR:CE2	1:A:680:PRO:HG3	2.28	0.69
1:B:126:GLY:HA2	1:B:459:SER:OG	1.91	0.69
1:B:424:LEU:CD2	1:B:447:MET:HE1	2.23	0.69
1:B:468:GLY:HA2	1:B:484:THR:OG1	1.92	0.69
1:B:521:GLN:HG2	1:B:721:LYS:CD	2.22	0.69
1:A:334:VAL:HG13	1:A:335:LEU:N	2.07	0.69
1:A:606:ASN:O	1:A:610:GLN:HB3	1.93	0.69
1:A:717:VAL:HG22	1:A:721:LYS:CG	2.22	0.69
1:A:717:VAL:C	1:A:721:LYS:HE3	2.17	0.69
1:B:550:LEU:O	1:B:554:ILE:HD12	1.93	0.69
1:A:417:VAL:HG11	1:A:647:MET:HE3	1.75	0.69
1:A:261:TYR:CD1	1:A:519:PHE:CE1	2.81	0.69
1:A:656:GLY:HA3	1:A:695:LYS:CB	2.23	0.69
1:B:383:TYR:HA	1:B:390:PRO:CG	2.12	0.69
1:B:514:PHE:CZ	1:B:537:LEU:HD12	2.28	0.69
1:B:562:LEU:O	1:B:566:VAL:HG23	1.92	0.69
1:B:185:ILE:HG12	1:B:708:ILE:CD1	2.23	0.68
1:A:619:ILE:CD1	1:A:708:ILE:HG12	2.21	0.68
1:B:45:GLY:HA2	1:B:600:ILE:HD13	1.74	0.68
1:B:341:TYR:O	1:B:345:LYS:N	2.27	0.68
1:B:717:VAL:HG22	1:B:721:LYS:CG	2.24	0.68
1:A:202:ASP:HA	1:A:228:ASP:CG	2.18	0.68
1:A:521:GLN:HG2	1:A:721:LYS:HG2	1.75	0.68
1:B:19:ALA:CA	1:B:22:PHE:CE1	2.69	0.68
1:B:97:MET:HG3	1:B:125:GLY:HA2	1.74	0.68
1:B:460:TYR:CD1	1:B:460:TYR:C	2.72	0.68
1:B:203:MET:HE3	1:B:693:PRO:HG3	1.74	0.68
1:B:468:GLY:HA2	1:B:484:THR:CB	2.22	0.68
1:B:167:ILE:HG23	1:B:718:SER:HB3	1.75	0.68
1:B:517:TYR:OH	1:B:634:VAL:HG23	1.93	0.68
1:B:666:LEU:HD12	1:B:681:HIS:HD2	1.59	0.68
1:A:205:ALA:CB	1:A:228:ASP:HB2	2.24	0.68
1:B:148:PHE:HB3	1:B:175:THR:HG21	1.76	0.67
1:B:656:GLY:C	1:B:695:LYS:HD3	2.20	0.67
1:B:717:VAL:C	1:B:721:LYS:HE3	2.19	0.67
1:B:104:ARG:C	1:B:121:VAL:HG21	2.19	0.67
1:A:121:VAL:HG13	1:A:122:ALA:N	2.09	0.67
1:A:398:SER:HB3	1:A:684:LEU:HD13	1.76	0.67
1:B:12:LEU:HD11	1:B:139:LEU:HD13	1.76	0.67
1:B:261:TYR:CD1	1:B:519:PHE:HE2	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:MET:HG3	1:A:266:TYR:CE2	2.29	0.67
1:B:121:VAL:HG13	1:B:122:ALA:H	1.60	0.67
1:B:199:LYS:CG	1:B:696:ASP:HB2	2.24	0.67
1:A:363:TRP:CZ2	1:A:367:ILE:HD11	2.30	0.67
1:B:414:MET:CG	1:B:651:LEU:HD21	2.25	0.67
1:A:545:ILE:HG13	1:B:511:LEU:CD2	2.25	0.66
1:A:100:ARG:O	1:A:103:VAL:HG23	1.96	0.66
1:A:355:PHE:HA	1:A:435:ALA:HA	1.77	0.66
1:A:86:MET:CE	1:A:139:LEU:HB3	2.25	0.66
1:A:263:PHE:CD1	1:A:264:PRO:N	2.64	0.66
1:B:368:ILE:HG21	1:B:431:ALA:N	2.11	0.66
1:A:86:MET:HE2	1:A:140:GLY:N	2.11	0.66
1:B:261:TYR:CD1	1:B:519:PHE:CE2	2.84	0.66
1:A:104:ARG:C	1:A:121:VAL:HG21	2.21	0.66
1:A:198:THR:CG2	1:A:231:GLY:O	2.43	0.66
1:B:71:PHE:O	1:B:167:ILE:HD12	1.96	0.66
1:B:184:SER:OG	1:B:246:GLU:HG3	1.96	0.66
1:A:539:MET:HG2	1:B:539:MET:CG	2.25	0.66
1:A:666:LEU:HD12	1:A:681:HIS:HD2	1.61	0.66
1:B:227:ALA:O	1:B:230:VAL:HG22	1.96	0.66
1:A:406:ILE:HD11	1:A:686:ILE:HG22	1.78	0.66
1:A:119:LEU:N	1:A:121:VAL:HG12	2.11	0.65
1:A:259:ALA:HB3	1:A:287:ILE:HG12	1.76	0.65
1:A:354:GLY:HA3	1:A:436:GLY:CA	2.26	0.65
1:A:717:VAL:HG22	1:A:721:LYS:HG2	1.76	0.65
1:B:12:LEU:HD11	1:B:139:LEU:CD1	2.26	0.65
1:B:205:ALA:HB2	1:B:228:ASP:HB2	1.78	0.65
1:B:261:TYR:CG	1:B:519:PHE:CE2	2.84	0.65
1:B:521:GLN:HG2	1:B:721:LYS:HD3	1.77	0.65
1:A:88:ALA:O	1:A:92:ILE:HG13	1.96	0.65
1:B:68:LEU:HD23	1:B:72:THR:OG1	1.96	0.65
1:A:357:PHE:HE1	1:A:434:PHE:CB	2.10	0.65
1:A:616:PHE:CD2	1:A:620:LEU:HD22	2.31	0.65
1:B:556:TYR:CD1	1:B:648:LEU:HD11	2.31	0.65
1:A:263:PHE:CE1	1:A:264:PRO:CD	2.77	0.65
1:A:102:ASN:ND2	1:A:466:ASN:HD22	1.94	0.65
1:A:332:THR:HG21	1:A:449:SER:OG	1.96	0.65
1:A:666:LEU:HD23	1:A:671:LEU:HD12	1.78	0.65
1:A:691:GLY:O	1:A:695:LYS:HG2	1.96	0.65
1:A:65:ALA:HB2	1:A:81:LEU:CD2	2.21	0.65
1:A:198:THR:CG2	1:A:234:VAL:HB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:VAL:HG22	1:A:650:ILE:HB	1.79	0.65
1:A:619:ILE:HD11	1:A:708:ILE:CG1	2.24	0.65
1:B:376:ILE:HD11	1:B:424:LEU:HG	1.79	0.65
1:A:200:ALA:HA	1:A:570:ALA:HB2	1.78	0.65
1:B:199:LYS:HG3	1:B:696:ASP:HB2	1.78	0.65
1:B:317:PRO:HA	1:B:320:GLU:OE1	1.97	0.65
1:A:12:LEU:HD11	1:A:139:LEU:HD13	1.76	0.64
1:A:390:PRO:HB3	1:A:412:LEU:HG	1.78	0.64
1:B:386:TYR:O	1:B:387:ARG:CB	2.44	0.64
1:A:97:MET:HG3	1:A:125:GLY:HA2	1.79	0.64
1:A:154:GLN:HG2	1:A:171:PRO:HB3	1.78	0.64
1:A:199:LYS:HA	1:A:199:LYS:HE3	1.79	0.64
1:A:170:VAL:HB	1:A:173:ALA:HB3	1.78	0.64
1:A:198:THR:HG22	1:A:231:GLY:O	1.98	0.64
1:B:148:PHE:CB	1:B:175:THR:HG21	2.27	0.64
1:A:286:LEU:HD21	1:A:350:LEU:HD21	1.79	0.64
1:A:679:GLU:N	1:A:679:GLU:OE1	2.30	0.64
1:B:11:PRO:HG3	1:B:295:LEU:CD2	2.28	0.64
1:A:319:ARG:O	1:A:323:ILE:HD13	1.96	0.64
1:A:450:PHE:CZ	1:A:501:PHE:CE2	2.84	0.64
1:B:119:LEU:N	1:B:121:VAL:HG12	2.12	0.64
1:B:170:VAL:HG11	1:B:173:ALA:CB	2.28	0.64
1:B:261:TYR:HB3	1:B:519:PHE:CE2	2.32	0.64
1:B:298:LEU:HD12	1:B:299:GLY:N	2.12	0.64
1:A:341:TYR:O	1:A:345:LYS:N	2.30	0.64
1:B:365:SER:HB3	1:B:439:GLY:O	1.97	0.64
1:B:638:LEU:O	1:B:642:VAL:HG23	1.97	0.64
1:A:170:VAL:CG2	1:A:261:TYR:HE2	2.04	0.64
1:A:383:TYR:CA	1:A:390:PRO:HG2	2.08	0.64
1:A:550:LEU:HB3	1:A:637:VAL:HG22	1.79	0.64
1:B:11:PRO:HB3	1:B:138:LEU:HB3	1.80	0.64
1:B:121:VAL:HG13	1:B:122:ALA:N	2.13	0.64
1:B:719:ILE:O	1:B:723:VAL:HG12	1.98	0.64
1:B:158:LEU:HD23	1:B:158:LEU:O	1.98	0.64
1:A:237:VAL:CG2	1:A:238:ALA:N	2.61	0.64
1:A:705:LEU:O	1:A:705:LEU:HD22	1.97	0.64
1:B:521:GLN:HG2	1:B:721:LYS:CG	2.27	0.64
1:A:429:LEU:O	1:A:433:TYR:N	2.29	0.63
1:B:167:ILE:O	1:B:168:ASN:C	2.41	0.63
1:B:705:LEU:O	1:B:705:LEU:HD22	1.98	0.63
1:A:23:ALA:HA	1:A:26:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:TYR:CD1	1:B:416:SER:HB2	2.32	0.63
1:B:468:GLY:HA3	1:B:484:THR:HG23	1.78	0.63
1:A:488:ASP:OD2	1:A:664:LYS:HE3	1.98	0.63
1:A:511:LEU:HD11	1:B:545:ILE:HG21	1.81	0.63
1:A:521:GLN:HA	1:A:721:LYS:HD3	1.80	0.63
1:A:514:PHE:CE2	1:B:540:LEU:HD12	2.33	0.63
1:A:492:ASN:ND2	2:A:1728:PO4:P	2.72	0.63
1:B:402:THR:HG21	1:B:686:ILE:HD13	1.80	0.63
1:B:691:GLY:O	1:B:695:LYS:HG2	1.99	0.63
1:A:521:GLN:O	1:A:523:SER:N	2.22	0.63
1:B:521:GLN:NE2	1:B:631:ALA:CB	2.59	0.63
1:B:666:LEU:C	1:B:666:LEU:CD1	2.72	0.63
1:A:674:TYR:HD2	1:A:680:PRO:CG	2.00	0.62
1:B:243:ASP:CG	1:B:704:ILE:HD11	2.24	0.62
1:B:418:PHE:HB3	1:B:419:PRO:HD3	1.80	0.62
1:A:11:PRO:HG3	1:A:295:LEU:CD2	2.29	0.62
1:A:198:THR:HG22	1:A:231:GLY:CA	2.29	0.62
1:A:237:VAL:HG23	1:A:238:ALA:H	1.64	0.62
1:A:717:VAL:O	1:A:721:LYS:HE3	1.99	0.62
1:B:205:ALA:CB	1:B:228:ASP:HB2	2.29	0.62
1:B:298:LEU:HD12	1:B:299:GLY:H	1.64	0.62
1:B:697:THR:O	1:B:701:SER:OG	2.09	0.62
1:B:297:GLY:O	1:B:300:CYS:N	2.32	0.62
1:A:548:ALA:HB1	1:B:643:LEU:HD11	1.81	0.62
1:B:262:MET:HE2	1:B:262:MET:N	2.14	0.62
1:B:563:ILE:CG2	1:B:564:SER:N	2.63	0.62
1:A:192:VAL:HG13	1:A:562:LEU:CD2	2.29	0.62
1:B:88:ALA:O	1:B:92:ILE:HG13	1.99	0.62
1:B:521:GLN:HA	1:B:721:LYS:HD3	1.80	0.62
1:A:97:MET:HG2	1:A:128:VAL:CG2	2.29	0.62
1:B:68:LEU:HD22	1:B:77:GLY:N	2.14	0.62
1:B:429:LEU:HD23	1:B:429:LEU:H	1.64	0.62
1:A:226:ILE:CG2	1:A:227:ALA:H	2.09	0.62
1:A:237:VAL:CG2	1:A:238:ALA:H	2.13	0.62
1:A:270:ILE:CG2	1:A:270:ILE:O	2.47	0.62
1:B:73:THR:CG2	1:B:169:PHE:CE2	2.77	0.62
1:B:102:ASN:ND2	1:B:466:ASN:HD22	1.98	0.62
1:B:667:GLU:HG2	1:B:681:HIS:NE2	2.14	0.62
1:A:511:LEU:CD2	1:B:545:ILE:HG13	2.29	0.62
1:A:411:SER:CB	1:B:563:ILE:HG21	2.27	0.61
1:B:163:ASN:ND2	1:B:164:TRP:HD1	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:O	1:B:438:TYR:OH	2.05	0.61
1:A:68:LEU:HD21	1:A:76:THR:CB	2.29	0.61
1:A:396:LYS:HG2	1:A:671:LEU:HD21	1.81	0.61
1:A:402:THR:HG21	1:A:686:ILE:HD13	1.80	0.61
1:B:23:ALA:HA	1:B:26:VAL:HG22	1.82	0.61
1:B:717:VAL:HG22	1:B:721:LYS:HG2	1.83	0.61
1:A:203:MET:CE	1:A:693:PRO:HG3	2.30	0.61
1:A:511:LEU:HD21	1:B:545:ILE:HG21	1.81	0.61
1:A:556:TYR:HE1	1:A:648:LEU:HD11	1.65	0.61
1:B:334:VAL:HG13	1:B:335:LEU:N	2.15	0.61
1:B:506:ALA:CB	1:B:706:ILE:HD11	2.29	0.61
1:A:697:THR:O	1:A:701:SER:OG	2.09	0.61
1:A:719:ILE:O	1:A:723:VAL:HG12	2.00	0.61
1:B:163:ASN:HD21	1:B:164:TRP:CD1	2.15	0.61
1:B:453:THR:O	1:B:457:VAL:HG23	2.01	0.61
1:A:154:GLN:NE2	1:A:175:THR:OG1	2.26	0.61
1:B:489:ALA:HA	1:B:661:ASN:ND2	2.14	0.61
1:A:495:ALA:O	1:A:499:LYS:HG3	2.01	0.61
1:A:556:TYR:CD1	1:A:648:LEU:HD11	2.35	0.61
1:B:237:VAL:HG23	1:B:238:ALA:H	1.64	0.61
1:B:445:LEU:O	1:B:449:SER:N	2.34	0.61
1:B:705:LEU:CD2	1:B:709:MET:HE3	2.28	0.61
1:A:705:LEU:CD2	1:A:709:MET:HE3	2.28	0.61
1:B:358:GLY:N	1:B:361:SER:OG	2.32	0.61
1:A:357:PHE:CZ	1:A:364:PHE:CD2	2.88	0.61
1:A:543:ARG:NH1	1:A:629:LEU:O	2.33	0.61
1:B:100:ARG:O	1:B:103:VAL:HG23	2.00	0.60
1:B:550:LEU:HD13	1:B:554:ILE:HD11	1.83	0.60
1:B:717:VAL:O	1:B:721:LYS:HE3	2.01	0.60
1:A:540:LEU:HD12	1:B:514:PHE:CE2	2.36	0.60
1:A:563:ILE:HG22	1:A:564:SER:N	2.15	0.60
1:A:611:MET:O	1:A:614:PRO:HD2	2.01	0.60
1:B:340:THR:HG23	1:B:344:LEU:HD12	1.81	0.60
1:A:261:TYR:CD1	1:A:519:PHE:HE1	2.19	0.60
1:B:76:THR:HG22	1:B:178:GLY:HA3	1.83	0.60
1:B:333:VAL:HG22	1:B:367:ILE:HG12	1.83	0.60
1:A:265:ILE:CB	1:A:519:PHE:HE2	2.14	0.60
1:A:398:SER:HB3	1:A:684:LEU:CD1	2.30	0.60
1:A:434:PHE:O	1:A:435:ALA:HB2	2.00	0.60
1:B:144:VAL:HG11	1:B:176:VAL:HG12	1.84	0.60
1:B:611:MET:O	1:B:614:PRO:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD11	1:A:139:LEU:CD1	2.30	0.60
1:A:396:LYS:HG2	1:A:671:LEU:CD2	2.32	0.60
1:A:677:GLY:O	1:A:678:SER:HB3	2.00	0.60
1:B:68:LEU:CD2	1:B:76:THR:HB	2.29	0.60
1:B:340:THR:HG22	1:B:359:ALA:O	2.01	0.60
1:B:550:LEU:C	1:B:554:ILE:HD12	2.26	0.60
1:A:261:TYR:HB3	1:A:519:PHE:CZ	2.36	0.60
1:A:123:TYR:CD1	1:A:123:TYR:C	2.80	0.60
1:A:539:MET:HG2	1:B:539:MET:HG3	1.83	0.60
1:A:666:LEU:C	1:A:666:LEU:CD1	2.71	0.60
1:B:68:LEU:HD21	1:B:76:THR:CB	2.29	0.60
1:B:102:ASN:C	1:B:102:ASN:OD1	2.45	0.60
1:B:102:ASN:HD21	1:B:466:ASN:ND2	1.98	0.60
1:B:499:LYS:HE2	1:B:695:LYS:O	2.02	0.60
1:A:68:LEU:HD22	1:A:77:GLY:N	2.17	0.60
1:A:553:ALA:HA	1:B:647:MET:CE	2.31	0.60
1:A:678:SER:OG	1:A:679:GLU:N	2.33	0.60
1:B:468:GLY:CA	1:B:484:THR:CG2	2.66	0.60
1:A:102:ASN:ND2	1:A:466:ASN:ND2	2.50	0.60
1:A:322:ASN:ND2	1:A:381:GLU:OE1	2.33	0.60
1:B:86:MET:CE	1:B:139:LEU:HB3	2.32	0.60
1:B:261:TYR:HE1	1:B:264:PRO:HG3	1.67	0.60
1:A:170:VAL:HG11	1:A:173:ALA:HB2	1.83	0.59
1:A:539:MET:CG	1:B:539:MET:HG2	2.32	0.59
1:B:163:ASN:CG	1:B:164:TRP:H	2.09	0.59
1:B:170:VAL:HG11	1:B:173:ALA:HB2	1.84	0.59
1:B:187:ALA:CB	1:B:242:ALA:HB1	2.31	0.59
1:A:25:VAL:HG21	1:A:124:GLN:CB	2.30	0.59
1:B:26:VAL:HG11	1:B:100:ARG:HH11	1.67	0.59
1:B:170:VAL:CG2	1:B:261:TYR:HE2	2.09	0.59
1:B:226:ILE:HG22	1:B:227:ALA:N	2.16	0.59
1:B:237:VAL:CG2	1:B:238:ALA:H	2.15	0.59
1:A:25:VAL:HB	1:A:97:MET:HE1	1.84	0.59
1:A:40:SER:O	1:A:42:ILE:N	2.35	0.59
1:A:199:LYS:CG	1:A:696:ASP:HB2	2.33	0.59
1:A:286:LEU:HD13	1:A:353:LEU:CD1	2.32	0.59
1:B:384:THR:HG21	1:B:496:ALA:CB	2.32	0.59
1:B:460:TYR:CE1	1:B:490:VAL:HG12	2.38	0.59
1:B:619:ILE:HG22	1:B:620:LEU:HD12	1.84	0.59
1:B:666:LEU:HB3	1:B:684:LEU:CD2	2.33	0.59
1:A:70:ILE:O	1:A:164:TRP:NE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:HG23	1:A:371:PHE:CE2	2.37	0.59
1:A:368:ILE:HG21	1:A:431:ALA:N	2.18	0.59
1:B:237:VAL:CG2	1:B:238:ALA:N	2.64	0.59
1:B:705:LEU:HD21	1:B:709:MET:CE	2.31	0.59
1:A:233:ASN:HD21	1:A:466:ASN:HD22	1.51	0.59
1:A:548:ALA:O	1:A:640:GLY:HA3	2.01	0.59
1:B:246:GLU:OE2	1:B:704:ILE:HG23	2.03	0.59
1:B:492:ASN:HD21	2:B:1728:PO4:P	2.25	0.59
1:B:620:LEU:O	1:B:624:VAL:HG23	2.02	0.59
1:A:340:THR:HG22	1:A:359:ALA:O	2.01	0.59
1:A:681:HIS:O	1:A:685:VAL:HG23	2.02	0.59
1:B:198:THR:HG22	1:B:234:VAL:HB	1.83	0.59
1:B:263:PHE:CZ	1:B:276:HIS:CE1	2.91	0.59
1:B:536:LEU:O	1:B:536:LEU:CD1	2.51	0.59
1:B:429:LEU:N	1:B:429:LEU:CD2	2.65	0.59
1:A:71:PHE:O	1:A:167:ILE:HD12	2.02	0.59
1:A:371:PHE:O	1:A:375:LEU:HD13	2.02	0.59
1:A:679:GLU:N	1:A:680:PRO:CD	2.65	0.59
1:A:704:ILE:HD13	1:A:704:ILE:N	2.18	0.59
1:B:191:ARG:NH2	1:B:700:PRO:HB3	2.18	0.59
1:B:70:ILE:O	1:B:164:TRP:NE1	2.35	0.59
1:A:519:PHE:O	1:A:522:ILE:HB	2.02	0.58
1:A:705:LEU:CD2	1:A:709:MET:HB2	2.33	0.58
1:B:457:VAL:O	1:B:460:TYR:HB3	2.03	0.58
1:B:606:ASN:O	1:B:610:GLN:CB	2.51	0.58
1:A:198:THR:HG21	1:A:235:GLY:CA	2.33	0.58
1:B:191:ARG:CZ	1:B:700:PRO:HB3	2.33	0.58
1:B:199:LYS:HG3	1:B:692:ASP:O	2.02	0.58
1:B:265:ILE:CB	1:B:519:PHE:HE1	2.15	0.58
1:B:460:TYR:CE1	1:B:490:VAL:HG11	2.38	0.58
1:A:717:VAL:O	1:A:721:LYS:CG	2.39	0.58
1:B:102:ASN:ND2	1:B:466:ASN:ND2	2.51	0.58
1:A:263:PHE:CG	1:A:264:PRO:CD	2.85	0.58
1:A:461:GLY:CA	1:A:491:GLY:CA	2.81	0.58
1:A:656:GLY:HA2	1:A:695:LYS:HD3	1.85	0.58
1:B:25:VAL:HB	1:B:97:MET:HE1	1.85	0.58
1:B:666:LEU:HD23	1:B:671:LEU:HD12	1.86	0.58
1:A:449:SER:OG	1:A:449:SER:O	2.19	0.58
1:B:123:TYR:CD1	1:B:123:TYR:C	2.81	0.58
1:A:126:GLY:HA2	1:A:459:SER:OG	2.01	0.58
1:A:395:GLY:O	1:A:398:SER:OG	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:TYR:CD1	1:A:460:TYR:C	2.82	0.58
1:A:533:LEU:O	1:A:533:LEU:HD23	2.02	0.58
1:A:667:GLU:HG2	1:A:681:HIS:NE2	2.19	0.58
1:B:101:ALA:HB1	1:B:121:VAL:O	2.04	0.58
1:B:616:PHE:CD2	1:B:620:LEU:HD22	2.37	0.58
1:A:556:TYR:OH	1:B:556:TYR:OH	2.22	0.58
1:B:283:ILE:O	1:B:287:ILE:HG13	2.04	0.58
1:A:65:ALA:CB	1:A:81:LEU:CD2	2.74	0.58
1:A:67:LEU:HD12	1:A:71:PHE:HE2	1.68	0.58
1:A:263:PHE:CD2	1:A:264:PRO:HD3	2.39	0.58
1:B:25:VAL:HG21	1:B:124:GLN:CB	2.32	0.58
1:B:461:GLY:HA3	1:B:491:GLY:CA	2.24	0.58
1:B:462:PRO:CA	1:B:465:ASP:HB3	2.31	0.58
1:B:563:ILE:HG22	1:B:564:SER:N	2.18	0.58
1:A:76:THR:HG22	1:A:178:GLY:HA3	1.86	0.57
1:A:297:GLY:O	1:A:298:LEU:C	2.47	0.57
1:A:285:ALA:HB3	1:A:347:LEU:HD11	1.85	0.57
1:A:298:LEU:CD1	1:A:299:GLY:N	2.67	0.57
1:A:457:VAL:HG12	1:A:494:THR:HB	1.84	0.57
1:B:717:VAL:HG22	1:B:721:LYS:HG3	1.87	0.57
1:A:620:LEU:O	1:A:624:VAL:N	2.23	0.57
1:B:261:TYR:HB3	1:B:519:PHE:CZ	2.38	0.57
1:B:367:ILE:HG23	1:B:371:PHE:CE2	2.39	0.57
1:A:333:VAL:HG13	1:A:367:ILE:CD1	2.33	0.57
1:A:563:ILE:HG22	1:B:411:SER:HB2	1.83	0.57
1:B:394:LEU:HD11	1:B:405:VAL:O	2.04	0.57
1:A:102:ASN:OD1	1:A:102:ASN:C	2.47	0.57
1:A:288:SER:HG	1:A:292:PHE:HE2	1.50	0.57
1:A:410:LEU:O	1:A:414:MET:HB2	2.05	0.57
1:A:270:ILE:O	1:A:270:ILE:HG23	2.03	0.57
1:A:506:ALA:HB1	1:A:706:ILE:HD11	1.86	0.57
1:B:383:TYR:CZ	1:B:416:SER:HA	2.39	0.57
1:A:22:PHE:O	1:A:26:VAL:HG13	2.05	0.57
1:A:105:VAL:N	1:A:121:VAL:HG21	2.19	0.57
1:A:266:TYR:CE1	1:A:531:PRO:HG2	2.40	0.57
1:A:301:SER:HB2	1:A:452:ALA:HB3	1.87	0.57
1:A:412:LEU:C	1:A:412:LEU:HD23	2.29	0.57
1:B:200:ALA:HA	1:B:570:ALA:HB2	1.86	0.57
1:A:536:LEU:HD13	1:A:536:LEU:O	2.05	0.57
1:B:191:ARG:CZ	1:B:700:PRO:CB	2.83	0.57
1:B:556:TYR:HE1	1:B:648:LEU:CD1	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLY:C	1:A:299:GLY:N	2.62	0.57
1:A:550:LEU:HD13	1:A:554:ILE:CD1	2.34	0.57
1:B:634:VAL:CG2	1:B:720:PHE:HE1	2.12	0.57
1:A:263:PHE:CB	1:A:283:ILE:HD11	2.34	0.57
1:A:286:LEU:O	1:A:438:TYR:CZ	2.58	0.57
1:A:402:THR:O	1:A:405:VAL:HG22	2.04	0.57
1:A:606:ASN:O	1:A:610:GLN:CB	2.52	0.57
1:A:68:LEU:CD2	1:A:76:THR:HB	2.31	0.56
1:A:448:LEU:HD22	1:A:505:SER:OG	2.05	0.56
1:B:258:LEU:HD23	1:B:516:SER:OG	2.05	0.56
1:A:263:PHE:CE2	1:A:264:PRO:HD3	2.40	0.56
1:A:293:PHE:CZ	1:A:336:THR:HG21	2.40	0.56
1:A:666:LEU:HD13	1:A:667:GLU:N	2.19	0.56
1:B:191:ARG:HH22	1:B:240:LEU:CD2	2.17	0.56
1:B:464:ALA:O	1:B:467:ALA:HB3	2.05	0.56
1:A:67:LEU:HD12	1:A:71:PHE:CE2	2.40	0.56
1:A:73:THR:HG21	1:A:169:PHE:CZ	2.40	0.56
1:A:76:THR:HG23	1:A:174:MET:O	2.04	0.56
1:A:259:ALA:C	1:A:261:TYR:N	2.54	0.56
1:B:73:THR:CG2	1:B:169:PHE:CD2	2.87	0.56
1:B:382:TYR:HE1	1:B:389:LYS:HB3	1.69	0.56
1:B:517:TYR:HE1	1:B:717:VAL:HB	1.69	0.56
1:B:188:MET:HB2	1:B:704:ILE:CG2	2.26	0.56
1:B:667:GLU:CG	1:B:681:HIS:NE2	2.67	0.56
1:B:723:VAL:O	1:B:723:VAL:HG22	2.05	0.56
1:A:11:PRO:HB3	1:A:138:LEU:HB3	1.87	0.56
1:A:82:LEU:O	1:A:86:MET:HB2	2.06	0.56
1:A:184:SER:HA	1:A:246:GLU:HG3	1.88	0.56
1:B:105:VAL:N	1:B:121:VAL:HG21	2.21	0.56
1:B:170:VAL:CG1	1:B:173:ALA:HB3	2.34	0.56
1:B:382:TYR:CD1	1:B:382:TYR:C	2.84	0.56
1:B:547:GLY:O	1:B:637:VAL:HA	2.05	0.56
1:A:340:THR:HG23	1:A:344:LEU:HD12	1.88	0.56
1:A:552:ALA:C	1:B:647:MET:HE2	2.31	0.56
1:B:40:SER:O	1:B:42:ILE:N	2.38	0.56
1:B:105:VAL:CG1	1:B:467:ALA:CB	2.82	0.56
1:B:441:ALA:HB2	1:B:512:SER:CB	2.36	0.56
1:B:622:PRO:HG3	1:B:709:MET:HG2	1.87	0.56
1:B:719:ILE:C	1:B:723:VAL:HG12	2.31	0.56
1:A:86:MET:HE2	1:A:140:GLY:H	1.69	0.56
1:B:6:LEU:H	1:B:6:LEU:HD12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:SER:HA	1:B:246:GLU:HG3	1.88	0.56
1:A:386:TYR:O	1:A:387:ARG:HB2	2.04	0.56
1:A:80:PHE:HD2	1:A:81:LEU:HD22	1.70	0.56
1:A:347:LEU:O	1:A:348:GLN:HB2	2.05	0.56
1:B:605:ASP:O	1:B:609:LYS:HB2	2.06	0.56
1:A:73:THR:CG2	1:A:169:PHE:CD2	2.88	0.55
1:A:73:THR:CG2	1:A:169:PHE:CE2	2.86	0.55
1:A:560:GLY:HA3	1:B:415:LYS:HG3	1.89	0.55
1:A:667:GLU:CG	1:A:681:HIS:NE2	2.69	0.55
1:A:268:GLN:HG3	1:A:277:GLN:OE1	2.06	0.55
1:A:343:TYR:CD1	1:A:343:TYR:N	2.74	0.55
1:A:622:PRO:HG3	1:A:709:MET:HG2	1.88	0.55
1:A:634:VAL:CG2	1:A:720:PHE:HE1	2.13	0.55
1:B:22:PHE:O	1:B:26:VAL:HG13	2.05	0.55
1:A:354:GLY:HA3	1:A:436:GLY:HA3	1.89	0.55
1:A:550:LEU:O	1:A:554:ILE:HD12	2.07	0.55
1:A:232:ASP:O	1:A:462:PRO:HB3	2.06	0.55
1:A:556:TYR:CE2	1:B:647:MET:HB3	2.41	0.55
1:B:261:TYR:CG	1:B:519:PHE:HE2	2.24	0.55
1:B:666:LEU:CD1	1:B:681:HIS:CD2	2.89	0.55
1:B:252:ILE:O	1:B:256:ILE:HD13	2.07	0.55
1:B:666:LEU:HD13	1:B:667:GLU:N	2.21	0.55
1:A:415:LYS:HG3	1:B:560:GLY:HA3	1.88	0.55
1:A:554:ILE:HD13	1:A:621:THR:HG21	1.89	0.55
1:A:695:LYS:HE2	1:A:696:ASP:OD2	2.06	0.55
1:B:297:GLY:O	1:B:298:LEU:C	2.49	0.55
1:B:318:GLN:OE1	1:B:490:VAL:HG22	2.07	0.55
1:B:358:GLY:O	1:B:359:ALA:HB3	2.06	0.55
1:B:460:TYR:HE1	1:B:490:VAL:CG1	2.19	0.55
1:A:392:GLN:NE2	1:A:665:TYR:CZ	2.75	0.55
1:A:607:ALA:O	1:A:611:MET:HB2	2.06	0.55
1:B:334:VAL:HG13	1:B:335:LEU:H	1.72	0.55
1:B:629:LEU:HD13	1:B:633:PHE:CD2	2.42	0.55
1:A:315:ASP:OD1	1:A:315:ASP:N	2.40	0.55
1:A:621:THR:O	1:A:625:THR:OG1	2.11	0.55
1:B:176:VAL:HG23	1:B:253:VAL:HG13	1.89	0.55
1:B:428:ILE:HD12	1:B:508:PHE:CE2	2.41	0.55
1:A:386:TYR:O	1:A:387:ARG:HB3	2.06	0.55
1:A:200:ALA:CA	1:A:570:ALA:HB2	2.36	0.55
1:A:267:VAL:HG13	1:A:276:HIS:HA	1.89	0.55
1:A:321:LEU:HG	1:A:457:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:PHE:CZ	1:A:501:PHE:HE2	2.24	0.55
1:A:626:GLY:HA2	1:A:634:VAL:HG13	1.88	0.55
1:B:243:ASP:O	1:B:246:GLU:HB3	2.07	0.55
1:B:263:PHE:HB3	1:B:264:PRO:CD	2.37	0.55
1:A:98:ALA:HA	1:A:463:ILE:HD12	1.89	0.54
1:A:172:PHE:O	1:A:176:VAL:HG22	2.07	0.54
1:A:386:TYR:HB3	1:A:391:THR:CG2	2.37	0.54
1:A:417:VAL:O	1:A:420:PRO:HG2	2.06	0.54
1:A:719:ILE:C	1:A:723:VAL:HG12	2.31	0.54
1:A:102:ASN:O	1:A:105:VAL:CG1	2.46	0.54
1:A:334:VAL:O	1:A:337:ALA:HB3	2.07	0.54
1:A:384:THR:HG22	1:A:657:GLY:HA3	1.90	0.54
1:A:397:SER:HB2	1:A:404:MET:HE3	1.88	0.54
1:B:82:LEU:CD1	1:B:144:VAL:HG23	2.36	0.54
1:B:289:TYR:HE1	1:B:339:LEU:HD12	1.72	0.54
1:B:434:PHE:O	1:B:435:ALA:HB2	2.08	0.54
1:A:129:MET:CE	1:A:237:VAL:HB	2.31	0.54
1:A:167:ILE:O	1:A:168:ASN:C	2.50	0.54
1:B:261:TYR:CE1	1:B:264:PRO:HG3	2.43	0.54
1:B:86:MET:HE3	1:B:139:LEU:HB3	1.89	0.54
1:B:126:GLY:O	1:B:129:MET:HG2	2.08	0.54
1:B:607:ALA:O	1:B:611:MET:HB2	2.07	0.54
1:B:620:LEU:O	1:B:624:VAL:N	2.25	0.54
1:A:129:MET:O	1:A:133:VAL:HG23	2.08	0.54
1:A:153:GLY:O	1:A:157:ASN:N	2.39	0.54
1:A:365:SER:HB3	1:A:439:GLY:O	2.08	0.54
1:B:287:ILE:O	1:B:291:ILE:HD12	2.07	0.54
1:B:390:PRO:HB3	1:B:412:LEU:HG	1.90	0.54
1:B:503:ILE:HG12	1:B:703:ASP:OD1	2.07	0.54
1:A:424:LEU:HD11	1:A:504:GLY:HA2	1.90	0.54
1:A:499:LYS:O	1:A:503:ILE:HG13	2.08	0.54
1:A:605:ASP:O	1:A:609:LYS:HB2	2.07	0.54
1:B:65:ALA:HB2	1:B:81:LEU:CD2	2.25	0.54
1:B:717:VAL:O	1:B:721:LYS:CG	2.41	0.54
1:A:65:ALA:HB1	1:A:81:LEU:HD21	1.81	0.54
1:A:188:MET:CB	1:A:704:ILE:HG21	2.33	0.54
1:A:334:VAL:HG13	1:A:335:LEU:H	1.71	0.54
1:A:546:ALA:HB2	1:B:429:LEU:HD21	1.89	0.54
1:A:717:VAL:HG22	1:A:721:LYS:HG3	1.90	0.54
1:B:704:ILE:N	1:B:704:ILE:HD13	2.23	0.54
1:B:97:MET:HG2	1:B:128:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:LEU:HD23	1:B:457:VAL:CG1	2.20	0.54
1:B:326:TRP:CE2	1:B:378:PHE:HZ	2.18	0.54
1:B:416:SER:OG	1:B:654:ASN:ND2	2.39	0.54
1:B:718:SER:HA	1:B:721:LYS:HE3	1.89	0.54
1:A:539:MET:HG2	1:B:539:MET:HG2	1.88	0.54
1:B:384:THR:HG21	1:B:496:ALA:HB1	1.89	0.54
1:A:170:VAL:CG1	1:A:173:ALA:CB	2.84	0.54
1:A:720:PHE:HA	1:A:723:VAL:CG1	2.32	0.54
1:B:67:LEU:HD12	1:B:71:PHE:HE2	1.72	0.54
1:B:198:THR:CG2	1:B:234:VAL:HB	2.38	0.54
1:B:159:ASN:HA	1:B:263:PHE:HE2	1.73	0.53
1:A:289:TYR:CD1	1:A:344:LEU:HD11	2.43	0.53
1:A:358:GLY:O	1:A:360:ILE:N	2.39	0.53
1:B:526:ASP:C	1:B:528:GLY:H	2.16	0.53
1:A:101:ALA:HB1	1:A:121:VAL:O	2.08	0.53
1:A:191:ARG:HH22	1:A:240:LEU:CD2	2.21	0.53
1:A:199:LYS:HG2	1:A:696:ASP:HB2	1.89	0.53
1:B:170:VAL:HG12	1:B:173:ALA:H	1.73	0.53
1:A:145:TYR:CE1	1:A:291:ILE:HD13	2.43	0.53
1:A:244:LEU:CD2	1:A:502:ALA:HB2	2.38	0.53
1:A:629:LEU:HD13	1:A:633:PHE:CD2	2.42	0.53
1:B:656:GLY:O	1:B:695:LYS:HD3	2.08	0.53
1:A:80:PHE:CE1	1:A:182:GLY:HA2	2.44	0.53
1:A:354:GLY:O	1:A:435:ALA:C	2.51	0.53
1:A:613:TYR:O	1:A:617:ILE:HG13	2.08	0.53
1:B:102:ASN:O	1:B:105:VAL:CG1	2.48	0.53
1:B:266:TYR:CB	1:B:278:VAL:HG23	2.38	0.53
1:B:337:ALA:HB2	1:B:363:TRP:CD2	2.43	0.53
1:B:495:ALA:O	1:B:499:LYS:HG3	2.09	0.53
1:A:105:VAL:O	1:A:106:ALA:C	2.50	0.53
1:B:80:PHE:HD2	1:B:81:LEU:HD22	1.73	0.53
1:B:82:LEU:O	1:B:86:MET:HB2	2.09	0.53
1:B:202:ASP:HA	1:B:228:ASP:CG	2.34	0.53
1:B:337:ALA:HB2	1:B:363:TRP:CZ2	2.39	0.53
1:A:286:LEU:HD13	1:A:353:LEU:HD11	1.91	0.53
1:A:468:GLY:HA2	1:A:484:THR:HG21	1.87	0.53
1:B:163:ASN:HB2	1:B:169:PHE:CD2	2.43	0.53
1:B:666:LEU:CD1	1:B:681:HIS:HD2	2.20	0.53
1:A:26:VAL:HG11	1:A:100:ARG:HH11	1.73	0.53
1:A:81:LEU:HD22	1:A:81:LEU:N	2.24	0.53
1:A:470:ILE:O	1:A:471:SER:C	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:GLN:HA	1:A:721:LYS:CE	2.39	0.53
1:B:26:VAL:C	1:B:28:LYS:H	2.17	0.53
1:A:674:TYR:HE2	1:A:680:PRO:HG3	1.65	0.53
1:B:81:LEU:HD22	1:B:81:LEU:N	2.24	0.53
1:B:464:ALA:HB1	1:B:487:LEU:CB	2.32	0.53
1:B:133:VAL:HG13	1:B:245:LEU:HD12	1.90	0.53
1:A:723:VAL:HG22	1:A:723:VAL:O	2.08	0.52
1:B:76:THR:CG2	1:B:174:MET:O	2.57	0.52
1:A:400:GLU:HB2	1:A:404:MET:HE2	1.91	0.52
1:A:402:THR:O	1:A:406:ILE:HG12	2.09	0.52
1:B:461:GLY:HA2	1:B:491:GLY:CA	2.36	0.52
1:B:608:LEU:HD23	1:B:611:MET:CE	2.32	0.52
1:A:82:LEU:CD1	1:A:144:VAL:HG23	2.39	0.52
1:A:259:ALA:O	1:A:283:ILE:HG23	2.09	0.52
1:A:259:ALA:HB3	1:A:287:ILE:CG1	2.40	0.52
1:A:545:ILE:HG21	1:B:511:LEU:HD21	1.92	0.52
1:A:656:GLY:C	1:A:695:LYS:HD2	2.35	0.52
1:B:233:ASN:O	1:B:234:VAL:C	2.53	0.52
1:B:638:LEU:HD11	1:B:713:SER:OG	2.08	0.52
1:A:26:VAL:C	1:A:28:LYS:H	2.16	0.52
1:B:460:TYR:OH	1:B:487:LEU:HD23	2.10	0.52
1:B:606:ASN:O	1:B:610:GLN:HB3	2.09	0.52
1:A:172:PHE:CE2	1:A:256:ILE:HG21	2.45	0.52
1:B:69:MET:HE2	1:B:74:TRP:CB	2.39	0.52
1:B:489:ALA:CA	1:B:661:ASN:HD21	2.20	0.52
1:B:718:SER:CA	1:B:721:LYS:HE3	2.38	0.52
1:A:321:LEU:N	1:A:321:LEU:HD12	2.25	0.52
1:A:718:SER:CA	1:A:721:LYS:HE3	2.40	0.52
1:B:233:ASN:ND2	1:B:466:ASN:HD22	2.05	0.52
1:B:382:TYR:HD1	1:B:382:TYR:O	1.91	0.52
1:A:252:ILE:O	1:A:256:ILE:HD13	2.09	0.52
1:A:563:ILE:CG2	1:A:564:SER:N	2.73	0.52
1:B:337:ALA:HB2	1:B:363:TRP:NE1	2.22	0.52
1:A:197:TYR:HE2	1:A:230:VAL:HG23	1.75	0.52
1:A:317:PRO:HA	1:A:320:GLU:OE1	2.10	0.52
1:B:184:SER:CB	1:B:246:GLU:HG3	2.40	0.52
1:B:191:ARG:HH22	1:B:240:LEU:HD23	1.74	0.52
1:B:507:ILE:HD11	1:B:646:ALA:CB	2.39	0.52
1:A:555:THR:HG23	1:A:702:LEU:HD11	1.92	0.52
1:A:679:GLU:OE1	1:A:679:GLU:CA	2.57	0.52
1:A:718:SER:HA	1:A:721:LYS:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:MET:CB	1:B:128:VAL:HB	2.40	0.52
1:A:10:ILE:N	1:A:11:PRO:CD	2.72	0.51
1:A:245:LEU:HD23	1:A:245:LEU:C	2.34	0.51
1:B:619:ILE:CD1	1:B:708:ILE:HG12	2.33	0.51
1:A:97:MET:O	1:A:98:ALA:C	2.53	0.51
1:A:200:ALA:HB1	1:A:570:ALA:CA	2.41	0.51
1:B:186:ILE:HG12	1:B:186:ILE:O	2.11	0.51
1:B:233:ASN:ND2	1:B:466:ASN:ND2	2.59	0.51
1:B:244:LEU:HD21	1:B:502:ALA:HB2	1.88	0.51
1:A:6:LEU:O	1:A:10:ILE:HD13	2.09	0.51
1:B:298:LEU:CD1	1:B:299:GLY:N	2.73	0.51
1:A:261:TYR:CG	1:A:519:PHE:CE1	2.98	0.51
1:A:334:VAL:CG1	1:A:335:LEU:N	2.71	0.51
1:B:105:VAL:O	1:B:106:ALA:C	2.52	0.51
1:B:705:LEU:CD2	1:B:709:MET:HB2	2.39	0.51
1:B:621:THR:HB	1:B:622:PRO:HD3	1.92	0.51
1:A:656:GLY:HA3	1:A:695:LYS:CG	2.40	0.51
1:A:666:LEU:CD1	1:A:681:HIS:CD2	2.93	0.51
1:B:67:LEU:HD12	1:B:71:PHE:CE2	2.46	0.51
1:B:158:LEU:O	1:B:263:PHE:CD2	2.63	0.51
1:B:297:GLY:C	1:B:299:GLY:N	2.68	0.51
1:A:154:GLN:HE21	1:A:172:PHE:HA	1.76	0.51
1:A:226:ILE:CG2	1:A:227:ALA:N	2.63	0.51
1:A:262:MET:O	1:A:266:TYR:HD2	1.94	0.51
1:A:562:LEU:O	1:A:566:VAL:HG23	2.11	0.51
1:B:243:ASP:OD1	1:B:704:ILE:CD1	2.59	0.51
1:B:442:ILE:O	1:B:445:LEU:HB3	2.10	0.51
1:A:126:GLY:O	1:A:129:MET:HG2	2.11	0.51
1:A:170:VAL:CG1	1:A:261:TYR:HE2	2.23	0.51
1:A:621:THR:HB	1:A:622:PRO:HD3	1.93	0.51
1:B:138:LEU:HD12	1:B:141:LEU:HD12	1.93	0.51
1:B:360:ILE:O	1:B:363:TRP:HB3	2.11	0.51
1:B:367:ILE:CG2	1:B:371:PHE:CE2	2.94	0.51
1:B:666:LEU:HD12	1:B:681:HIS:CD2	2.44	0.51
1:A:331:LEU:O	1:A:334:VAL:HG12	2.11	0.51
1:A:468:GLY:CA	1:A:484:THR:CG2	2.73	0.51
1:A:262:MET:HG2	1:A:353:LEU:CD2	2.33	0.51
1:B:53:GLU:OE2	1:B:190:ASP:OD1	2.29	0.51
1:B:370:ILE:O	1:B:374:ILE:HG13	2.11	0.51
1:A:154:GLN:NE2	1:A:171:PRO:O	2.45	0.50
1:A:157:ASN:C	1:A:159:ASN:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:SER:HB3	1:A:290:PRO:HG3	1.93	0.50
1:A:286:LEU:CD1	1:A:353:LEU:HG	2.40	0.50
1:A:536:LEU:O	1:A:536:LEU:CD1	2.59	0.50
1:B:97:MET:HG3	1:B:125:GLY:CA	2.41	0.50
1:A:263:PHE:CD1	1:A:263:PHE:C	2.88	0.50
1:A:321:LEU:HD23	1:A:457:VAL:CG1	2.08	0.50
1:A:623:LEU:HD13	1:A:712:VAL:CG1	2.42	0.50
1:B:261:TYR:CB	1:B:519:PHE:CE2	2.93	0.50
1:A:162:THR:O	1:A:163:ASN:O	2.28	0.50
1:A:186:ILE:O	1:A:186:ILE:HG12	2.11	0.50
1:A:656:GLY:C	1:A:695:LYS:CD	2.83	0.50
1:B:343:TYR:CD1	1:B:343:TYR:N	2.80	0.50
1:B:718:SER:N	1:B:721:LYS:HE3	2.26	0.50
1:A:261:TYR:CE1	1:A:264:PRO:HG3	2.47	0.50
1:A:666:LEU:CD1	1:A:681:HIS:HA	2.42	0.50
1:B:112:THR:O	1:B:113:LYS:HG2	2.12	0.50
1:B:267:VAL:O	1:B:268:GLN:O	2.30	0.50
1:B:447:MET:SD	1:B:504:GLY:C	2.95	0.50
1:B:623:LEU:HD13	1:B:712:VAL:CG1	2.42	0.50
1:A:164:TRP:CH2	1:A:165:LEU:HD21	2.46	0.50
1:A:350:LEU:O	1:A:355:PHE:HB2	2.11	0.50
1:A:705:LEU:HD22	1:A:705:LEU:C	2.36	0.50
1:A:123:TYR:CD1	1:A:123:TYR:O	2.64	0.50
1:A:718:SER:N	1:A:721:LYS:HE3	2.26	0.50
1:B:236:ASP:HB2	1:B:462:PRO:HG2	1.91	0.50
1:B:462:PRO:HA	1:B:465:ASP:CB	2.35	0.50
1:A:15:LEU:HG	1:A:135:GLY:HA3	1.94	0.50
1:A:392:GLN:NE2	1:A:665:TYR:CE1	2.80	0.50
1:B:10:ILE:N	1:B:11:PRO:CD	2.74	0.50
1:B:144:VAL:HA	1:B:148:PHE:HD2	1.77	0.50
1:A:460:TYR:OH	1:A:487:LEU:CD2	2.60	0.50
1:A:638:LEU:HD11	1:A:713:SER:OG	2.12	0.50
1:B:123:TYR:CD1	1:B:123:TYR:O	2.65	0.50
1:A:167:ILE:O	1:A:167:ILE:HG22	2.12	0.50
1:A:260:SER:HA	1:A:287:ILE:HD11	1.93	0.50
1:A:519:PHE:CD1	1:A:519:PHE:C	2.90	0.50
1:B:424:LEU:HD11	1:B:504:GLY:HA2	1.94	0.50
1:B:521:GLN:C	1:B:523:SER:H	2.14	0.50
1:B:666:LEU:HD11	1:B:681:HIS:HA	1.93	0.50
1:A:26:VAL:C	1:A:28:LYS:N	2.69	0.49
1:A:708:ILE:HA	1:A:711:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LEU:C	1:B:159:ASN:O	2.53	0.49
1:B:170:VAL:CG1	1:B:173:ALA:CB	2.89	0.49
1:B:666:LEU:CD1	1:B:681:HIS:HA	2.42	0.49
1:A:236:ASP:CB	1:A:462:PRO:CG	2.86	0.49
1:A:288:SER:HB2	1:A:292:PHE:CE2	2.47	0.49
1:B:321:LEU:CD1	1:B:321:LEU:N	2.75	0.49
1:B:363:TRP:CE2	1:B:367:ILE:HD11	2.46	0.49
1:A:465:ASP:OD2	1:A:488:ASP:OD1	2.29	0.49
1:A:489:ALA:CA	1:A:661:ASN:HD21	2.20	0.49
1:B:22:PHE:CA	1:B:97:MET:HE2	2.34	0.49
1:B:94:GLY:HA3	1:B:129:MET:CB	2.42	0.49
1:B:289:TYR:CD1	1:B:344:LEU:HD11	2.47	0.49
1:A:97:MET:CB	1:A:128:VAL:HB	2.42	0.49
1:A:180:ALA:HB2	1:A:253:VAL:HG21	1.94	0.49
1:A:199:LYS:HG3	1:A:692:ASP:O	2.11	0.49
1:B:65:ALA:CB	1:B:81:LEU:CD2	2.80	0.49
1:B:101:ALA:CB	1:B:125:GLY:HA3	2.43	0.49
1:B:321:LEU:HG	1:B:457:VAL:HG22	1.93	0.49
1:A:22:PHE:CB	1:A:97:MET:HE2	2.43	0.49
1:A:163:ASN:HB2	1:A:169:PHE:HD2	1.76	0.49
1:A:185:ILE:CG1	1:A:708:ILE:HD11	2.42	0.49
1:A:357:PHE:CZ	1:A:434:PHE:HB3	2.48	0.49
1:A:466:ASN:O	1:A:467:ALA:C	2.54	0.49
1:A:553:ALA:CA	1:B:647:MET:HE1	2.40	0.49
1:B:11:PRO:HG3	1:B:295:LEU:HD21	1.93	0.49
1:B:464:ALA:CB	1:B:487:LEU:HB3	2.37	0.49
1:A:97:MET:HG2	1:A:125:GLY:HA2	1.92	0.49
1:A:203:MET:HE2	1:A:693:PRO:HG3	1.94	0.49
1:A:453:THR:O	1:A:457:VAL:HG23	2.13	0.49
1:B:514:PHE:O	1:B:517:TYR:HB3	2.13	0.49
1:B:162:THR:O	1:B:163:ASN:O	2.31	0.49
1:B:339:LEU:O	1:B:343:TYR:HB2	2.13	0.49
1:B:705:LEU:HD22	1:B:705:LEU:C	2.36	0.49
1:A:87:SER:O	1:A:88:ALA:C	2.56	0.49
1:A:98:ALA:HA	1:A:463:ILE:CD1	2.43	0.49
1:A:105:VAL:CG1	1:A:467:ALA:CB	2.90	0.49
1:A:339:LEU:HD13	1:A:339:LEU:C	2.38	0.49
1:A:461:GLY:HA2	1:A:491:GLY:CA	2.43	0.49
1:A:652:THR:HG22	1:A:694:LEU:HB3	1.95	0.49
1:A:674:TYR:CD2	1:A:680:PRO:CB	2.95	0.49
1:B:423:THR:O	1:B:427:GLY:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:ILE:HA	1:B:711:VAL:HG22	1.94	0.49
1:A:82:LEU:HD11	1:A:140:GLY:O	2.13	0.49
1:A:94:GLY:HA3	1:A:129:MET:CB	2.43	0.49
1:A:170:VAL:HG11	1:A:261:TYR:HE2	1.78	0.49
1:A:233:ASN:O	1:A:234:VAL:C	2.53	0.49
1:B:161:TYR:CD2	1:B:169:PHE:HE2	2.24	0.49
1:B:192:VAL:O	1:B:196:VAL:CG2	2.61	0.49
1:B:233:ASN:C	1:B:237:VAL:HG22	2.33	0.49
1:B:236:ASP:CB	1:B:462:PRO:HG3	2.40	0.49
1:B:312:LYS:HA	1:B:313:PRO:HD3	1.63	0.49
1:B:341:TYR:O	1:B:345:LYS:CA	2.61	0.49
1:B:626:GLY:HA2	1:B:634:VAL:HG13	1.95	0.49
1:A:121:VAL:CG1	1:A:122:ALA:H	2.24	0.48
1:B:15:LEU:HD11	1:B:136:PHE:HD1	1.78	0.48
1:B:86:MET:HE2	1:B:140:GLY:H	1.77	0.48
1:B:198:THR:CG2	1:B:235:GLY:N	2.62	0.48
1:B:463:ILE:CG2	1:B:464:ALA:N	2.76	0.48
1:A:138:LEU:HD12	1:A:141:LEU:HD12	1.95	0.48
1:A:229:ASN:HD21	1:A:469:GLY:HA3	1.78	0.48
1:A:548:ALA:HA	1:A:636:GLY:O	2.13	0.48
1:A:643:LEU:HD12	1:B:643:LEU:HD12	1.95	0.48
1:B:26:VAL:C	1:B:28:LYS:N	2.70	0.48
1:A:97:MET:HE2	1:A:128:VAL:HG21	1.95	0.48
1:A:97:MET:HG3	1:A:125:GLY:CA	2.44	0.48
1:A:202:ASP:OD2	1:A:692:ASP:OD2	2.31	0.48
1:A:6:LEU:HD12	1:A:6:LEU:H	1.77	0.48
1:A:158:LEU:O	1:A:263:PHE:HZ	1.84	0.48
1:A:158:LEU:HG	1:A:263:PHE:CE2	2.49	0.48
1:A:170:VAL:HG22	1:A:261:TYR:CE2	2.20	0.48
1:A:170:VAL:CG1	1:A:261:TYR:CE2	2.96	0.48
1:A:357:PHE:CD2	1:A:360:ILE:CG2	2.96	0.48
1:A:539:MET:CG	1:B:539:MET:CG	2.90	0.48
1:B:263:PHE:HB2	1:B:283:ILE:HD13	1.95	0.48
1:A:514:PHE:O	1:A:517:TYR:HB3	2.13	0.48
1:B:72:THR:C	1:B:73:THR:HG23	2.38	0.48
1:B:391:THR:HG23	1:B:662:ALA:CA	2.42	0.48
1:A:144:VAL:HA	1:A:148:PHE:HD2	1.79	0.48
1:A:270:ILE:O	1:A:271:GLY:C	2.57	0.48
1:A:503:ILE:HD13	1:A:649:ALA:CB	2.43	0.48
1:B:153:GLY:O	1:B:157:ASN:N	2.42	0.48
1:B:161:TYR:CE2	1:B:169:PHE:HE2	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ILE:O	1:B:167:ILE:HG22	2.13	0.48
1:B:191:ARG:CZ	1:B:700:PRO:HB2	2.44	0.48
1:B:259:ALA:HB3	1:B:287:ILE:HG12	1.94	0.48
1:B:391:THR:HG23	1:B:662:ALA:HA	1.96	0.48
1:A:11:PRO:HG3	1:A:295:LEU:HD22	1.93	0.48
1:A:97:MET:HB2	1:A:128:VAL:HG11	1.96	0.48
1:A:666:LEU:CD1	1:A:681:HIS:HD2	2.25	0.48
1:A:139:LEU:O	1:A:143:LEU:HD12	2.13	0.48
1:A:164:TRP:CZ2	1:A:165:LEU:HD21	2.49	0.48
1:A:191:ARG:HH21	1:A:243:ASP:HB2	1.78	0.48
1:A:656:GLY:HA3	1:A:695:LYS:HD2	1.91	0.48
1:A:667:GLU:HG3	1:A:681:HIS:CD2	2.49	0.48
1:B:65:ALA:HB1	1:B:81:LEU:HD21	1.87	0.48
1:B:205:ALA:C	1:B:207:LEU:H	2.21	0.48
1:A:655:SER:OG	1:A:659:TRP:CE3	2.56	0.48
1:B:76:THR:CG2	1:B:178:GLY:HA3	2.43	0.48
1:B:98:ALA:HB2	1:B:129:MET:CE	2.43	0.48
1:B:263:PHE:HB3	1:B:264:PRO:HD3	1.95	0.48
1:B:368:ILE:HG21	1:B:431:ALA:H	1.77	0.48
1:A:76:THR:CG2	1:A:178:GLY:HA3	2.44	0.48
1:B:82:LEU:HD11	1:B:140:GLY:O	2.14	0.48
1:B:97:MET:O	1:B:98:ALA:C	2.55	0.48
1:B:158:LEU:HD23	1:B:158:LEU:C	2.39	0.48
1:B:158:LEU:HD23	1:B:263:PHE:CD2	2.49	0.48
1:B:232:ASP:OD2	1:B:465:ASP:OD1	2.32	0.48
1:B:461:GLY:O	1:B:465:ASP:HB2	2.13	0.48
1:B:551:GLY:CA	1:B:637:VAL:HG13	2.43	0.48
1:A:264:PRO:O	1:A:267:VAL:HG23	2.14	0.47
1:A:402:THR:HG21	1:A:686:ILE:CD1	2.43	0.47
1:B:386:TYR:O	1:B:387:ARG:HB3	2.14	0.47
1:A:97:MET:HG2	1:A:128:VAL:HG21	1.96	0.47
1:A:666:LEU:HD11	1:A:681:HIS:HA	1.96	0.47
1:B:258:LEU:CD2	1:B:516:SER:OG	2.61	0.47
1:B:390:PRO:CB	1:B:412:LEU:HD11	2.45	0.47
1:A:620:LEU:O	1:A:624:VAL:HG23	2.14	0.47
1:B:86:MET:HE2	1:B:140:GLY:CA	2.45	0.47
1:B:144:VAL:HA	1:B:148:PHE:CD2	2.49	0.47
1:B:316:ASN:C	1:B:316:ASN:OD1	2.57	0.47
1:B:519:PHE:O	1:B:522:ILE:HB	2.15	0.47
1:A:262:MET:SD	1:A:266:TYR:HE2	2.38	0.47
1:A:521:GLN:HG2	1:A:721:LYS:CG	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ASP:OD2	1:B:488:ASP:OD1	2.33	0.47
1:B:667:GLU:HG3	1:B:681:HIS:CD2	2.50	0.47
1:A:72:THR:C	1:A:73:THR:HG23	2.40	0.47
1:A:144:VAL:O	1:A:148:PHE:HB2	2.15	0.47
1:A:656:GLY:CA	1:A:695:LYS:HD2	2.42	0.47
1:B:321:LEU:N	1:B:321:LEU:HD12	2.29	0.47
1:A:15:LEU:HD11	1:A:136:PHE:HD1	1.79	0.47
1:A:334:VAL:CG1	1:A:335:LEU:H	2.27	0.47
1:B:667:GLU:CG	1:B:681:HIS:CD2	2.97	0.47
1:A:161:TYR:CD2	1:A:169:PHE:HE2	2.26	0.47
1:A:360:ILE:O	1:A:363:TRP:HB3	2.14	0.47
1:A:383:TYR:CD1	1:A:416:SER:HB2	2.50	0.47
1:A:463:ILE:CG2	1:A:464:ALA:N	2.78	0.47
1:B:80:PHE:CE1	1:B:182:GLY:HA2	2.50	0.47
1:B:101:ALA:HB3	1:B:463:ILE:HD11	1.97	0.47
1:B:139:LEU:O	1:B:143:LEU:HD12	2.15	0.47
1:B:144:VAL:O	1:B:148:PHE:HB2	2.14	0.47
1:B:522:ILE:O	1:B:522:ILE:CG2	2.54	0.47
1:B:686:ILE:HA	1:B:689:THR:HG22	1.97	0.47
1:A:325:LEU:HD22	1:A:450:PHE:HE2	1.80	0.47
1:A:434:PHE:O	1:A:435:ALA:CB	2.63	0.47
1:A:521:GLN:CB	1:A:721:LYS:HD3	2.44	0.47
1:B:675:GLY:O	1:B:676:LYS:CB	2.63	0.47
1:A:155:VAL:HA	1:A:158:LEU:HD13	1.97	0.47
1:A:244:LEU:HD23	1:A:502:ALA:HB2	1.97	0.47
1:A:521:GLN:HA	1:A:721:LYS:CD	2.43	0.47
1:B:236:ASP:CB	1:B:462:PRO:CG	2.91	0.47
1:B:533:LEU:HD23	1:B:533:LEU:O	2.14	0.47
1:B:711:VAL:HG23	1:B:712:VAL:N	2.30	0.47
1:A:68:LEU:HD21	1:A:76:THR:CG2	2.44	0.47
1:B:72:THR:C	1:B:73:THR:CG2	2.88	0.47
1:B:321:LEU:CG	1:B:457:VAL:HG13	2.44	0.47
1:B:488:ASP:OD2	1:B:664:LYS:HE3	2.14	0.47
1:B:619:ILE:HD11	1:B:708:ILE:CG1	2.33	0.47
1:B:720:PHE:HA	1:B:723:VAL:CG1	2.37	0.47
1:A:86:MET:HE2	1:A:139:LEU:HB3	1.96	0.46
1:A:121:VAL:CG1	1:A:122:ALA:N	2.78	0.46
1:A:608:LEU:HA	1:A:611:MET:HB2	1.97	0.46
1:A:616:PHE:CD1	1:A:616:PHE:C	2.93	0.46
1:A:633:PHE:CE1	1:A:637:VAL:CG2	2.97	0.46
1:B:699:GLY:N	1:B:700:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:HA	1:A:148:PHE:CD2	2.50	0.46
1:A:154:GLN:NE2	1:A:172:PHE:HA	2.30	0.46
1:A:288:SER:OG	1:A:292:PHE:HE2	1.98	0.46
1:A:503:ILE:CD1	1:A:649:ALA:HB1	2.44	0.46
1:A:526:ASP:C	1:A:528:GLY:H	2.24	0.46
1:B:164:TRP:CZ2	1:B:165:LEU:HD21	2.51	0.46
1:B:191:ARG:HH21	1:B:243:ASP:HB2	1.81	0.46
1:B:301:SER:CB	1:B:452:ALA:HB3	2.42	0.46
1:A:69:MET:CE	1:A:74:TRP:HB2	2.38	0.46
1:A:98:ALA:HB2	1:A:129:MET:CE	2.45	0.46
1:A:101:ALA:CB	1:A:125:GLY:HA3	2.46	0.46
1:A:154:GLN:CG	1:A:171:PRO:HB3	2.43	0.46
1:B:187:ALA:HB1	1:B:242:ALA:HB1	1.96	0.46
1:B:266:TYR:O	1:B:267:VAL:C	2.57	0.46
1:B:390:PRO:HB3	1:B:412:LEU:CG	2.45	0.46
1:B:616:PHE:CD1	1:B:616:PHE:C	2.93	0.46
1:A:129:MET:SD	1:A:459:SER:CB	3.01	0.46
1:A:170:VAL:HG12	1:A:173:ALA:H	1.79	0.46
1:A:233:ASN:C	1:A:237:VAL:HG22	2.39	0.46
1:A:462:PRO:HA	1:A:465:ASP:HB3	1.98	0.46
1:A:511:LEU:HD21	1:B:545:ILE:CG1	2.43	0.46
1:B:71:PHE:O	1:B:167:ILE:CD1	2.64	0.46
1:B:197:TYR:HE2	1:B:230:VAL:HG23	1.81	0.46
1:B:230:VAL:CG2	1:B:231:GLY:N	2.78	0.46
1:B:339:LEU:C	1:B:339:LEU:CD1	2.88	0.46
1:B:447:MET:SD	1:B:505:SER:N	2.89	0.46
1:A:188:MET:O	1:A:192:VAL:HG23	2.16	0.46
1:A:240:LEU:HD12	1:A:458:ASP:HB3	1.97	0.46
1:A:416:SER:OG	1:A:654:ASN:ND2	2.47	0.46
1:A:623:LEU:O	1:A:627:PHE:HD2	1.98	0.46
1:A:666:LEU:HD12	1:A:681:HIS:CD2	2.45	0.46
1:B:12:LEU:CD1	1:B:139:LEU:HD13	2.43	0.46
1:B:122:ALA:O	1:B:463:ILE:HD13	2.15	0.46
1:B:193:GLY:O	1:B:197:TYR:N	2.48	0.46
1:B:200:ALA:CA	1:B:570:ALA:HB2	2.46	0.46
1:B:441:ALA:HB2	1:B:512:SER:HB2	1.96	0.46
1:A:53:GLU:HA	1:A:608:LEU:CD1	2.46	0.46
1:A:458:ASP:OD2	1:A:498:GLY:HA3	2.16	0.46
1:A:663:LYS:HD3	1:A:688:ASP:CB	2.44	0.46
1:A:172:PHE:CE2	1:A:256:ILE:CG2	2.98	0.46
1:A:176:VAL:HG23	1:A:253:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:MET:HE2	1:B:262:MET:CA	2.46	0.46
1:B:386:TYR:O	1:B:387:ARG:HB2	2.14	0.46
1:B:619:ILE:HD12	1:B:712:VAL:HG21	1.98	0.46
1:A:368:ILE:HG21	1:A:431:ALA:H	1.81	0.46
1:A:448:LEU:C	1:A:450:PHE:H	2.23	0.46
1:B:396:LYS:HA	1:B:671:LEU:HD21	1.98	0.46
1:B:681:HIS:O	1:B:685:VAL:HG23	2.15	0.46
1:A:72:THR:C	1:A:73:THR:CG2	2.89	0.46
1:A:390:PRO:HB3	1:A:412:LEU:CG	2.46	0.46
1:A:460:TYR:OH	1:A:487:LEU:HD23	2.16	0.46
1:A:517:TYR:OH	1:A:634:VAL:CG2	2.56	0.46
1:A:521:GLN:HG2	1:A:721:LYS:CD	2.46	0.46
1:A:372:SER:O	1:A:376:ILE:HG13	2.15	0.46
1:A:522:ILE:O	1:A:522:ILE:CG2	2.61	0.46
1:A:666:LEU:HD11	1:A:681:HIS:CA	2.46	0.46
1:B:202:ASP:OD2	1:B:692:ASP:OD2	2.34	0.46
1:B:298:LEU:HA	1:B:301:SER:OG	2.15	0.46
1:B:319:ARG:O	1:B:323:ILE:HD13	2.15	0.46
1:B:363:TRP:CZ2	1:B:367:ILE:CD1	2.92	0.46
1:A:12:LEU:CD1	1:A:139:LEU:HD13	2.43	0.45
1:A:138:LEU:HD22	1:A:298:LEU:HD23	1.97	0.45
1:A:154:GLN:NE2	1:A:171:PRO:C	2.74	0.45
1:A:261:TYR:HE1	1:A:264:PRO:HG3	1.81	0.45
1:A:263:PHE:O	1:A:267:VAL:HG22	2.16	0.45
1:A:357:PHE:CE2	1:A:360:ILE:CG2	2.97	0.45
1:A:383:TYR:CD1	1:A:390:PRO:HG3	2.51	0.45
1:B:87:SER:O	1:B:88:ALA:C	2.58	0.45
1:B:97:MET:HB2	1:B:128:VAL:HG11	1.98	0.45
1:B:406:ILE:HD11	1:B:686:ILE:HG22	1.98	0.45
1:A:198:THR:HG22	1:A:231:GLY:C	2.41	0.45
1:A:256:ILE:HD12	1:A:290:PRO:HG2	1.97	0.45
1:A:357:PHE:CE2	1:A:361:SER:CA	2.84	0.45
1:A:431:ALA:HB1	1:A:443:ALA:HB2	1.98	0.45
1:B:170:VAL:HG11	1:B:261:TYR:HE2	1.81	0.45
1:B:383:TYR:CD1	1:B:390:PRO:HG3	2.50	0.45
1:B:503:ILE:CD1	1:B:649:ALA:HB1	2.46	0.45
1:A:287:ILE:O	1:A:290:PRO:HD2	2.16	0.45
1:A:317:PRO:HA	1:A:320:GLU:CD	2.41	0.45
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.58	0.45
1:A:652:THR:HB	1:A:694:LEU:C	2.42	0.45
1:A:666:LEU:CB	1:A:684:LEU:HD23	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:LEU:HD22	1:A:709:MET:HB2	1.98	0.45
1:B:321:LEU:CD1	1:B:321:LEU:H	2.28	0.45
1:B:484:THR:HG22	1:B:485:ASP:N	2.31	0.45
1:A:386:TYR:HB3	1:A:391:THR:HG22	1.98	0.45
1:A:460:TYR:CE1	1:A:490:VAL:CG1	2.99	0.45
1:A:663:LYS:HD3	1:A:688:ASP:HB3	1.98	0.45
1:B:76:THR:OG1	1:B:174:MET:HG3	2.15	0.45
1:B:289:TYR:CG	1:B:344:LEU:HD11	2.52	0.45
1:B:333:VAL:HG13	1:B:363:TRP:CZ2	2.51	0.45
1:B:334:VAL:CG1	1:B:335:LEU:N	2.80	0.45
1:B:666:LEU:HD11	1:B:681:HIS:CA	2.45	0.45
1:A:148:PHE:HB3	1:A:175:THR:HG21	1.97	0.45
1:A:386:TYR:CD1	1:A:386:TYR:C	2.93	0.45
1:A:465:ASP:OD2	2:A:1727:PO4:O1	2.35	0.45
1:B:25:VAL:O	1:B:28:LYS:CB	2.65	0.45
1:B:97:MET:HE2	1:B:128:VAL:HG21	1.99	0.45
1:B:460:TYR:C	1:B:463:ILE:HG22	2.40	0.45
1:B:663:LYS:HZ3	1:B:664:LYS:HE2	1.81	0.45
1:A:80:PHE:CD2	1:A:81:LEU:HD22	2.49	0.45
1:A:266:TYR:CD1	1:A:531:PRO:HG2	2.52	0.45
1:A:626:GLY:CA	1:A:634:VAL:HG13	2.47	0.45
1:B:428:ILE:HD12	1:B:508:PHE:CZ	2.51	0.45
1:B:517:TYR:HB2	1:B:714:VAL:HG12	1.99	0.45
1:B:608:LEU:HA	1:B:611:MET:HB2	1.99	0.45
1:A:161:TYR:CE2	1:A:169:PHE:HE2	2.34	0.45
1:A:350:LEU:HD22	1:A:355:PHE:CE2	2.51	0.45
1:A:386:TYR:HB3	1:A:391:THR:HG21	1.97	0.45
1:A:608:LEU:CD2	1:A:611:MET:HE2	2.35	0.45
1:B:145:TYR:CE1	1:B:291:ILE:HD13	2.52	0.45
1:B:157:ASN:O	1:B:159:ASN:N	2.50	0.45
1:B:164:TRP:CH2	1:B:165:LEU:HD21	2.52	0.45
1:B:198:THR:CG2	1:B:235:GLY:H	2.27	0.45
1:B:317:PRO:HA	1:B:320:GLU:OE2	2.16	0.45
1:B:521:GLN:C	1:B:523:SER:N	2.73	0.45
1:B:606:ASN:O	1:B:610:GLN:HB2	2.17	0.45
1:A:357:PHE:CE1	1:A:434:PHE:CD1	3.04	0.45
1:A:667:GLU:CG	1:A:681:HIS:CD2	3.00	0.45
1:A:53:GLU:OE2	1:A:190:ASP:OD1	2.34	0.45
1:A:192:VAL:CG1	1:A:562:LEU:HD21	2.44	0.45
1:A:546:ALA:CB	1:B:429:LEU:HD21	2.47	0.45
1:A:610:GLN:HG3	1:A:610:GLN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:HD11	1:B:136:PHE:CD1	2.52	0.45
1:A:112:THR:O	1:A:113:LYS:HG2	2.17	0.45
1:A:181:LEU:HD13	1:A:711:VAL:CG2	2.46	0.45
1:A:506:ALA:CB	1:A:706:ILE:HD11	2.46	0.45
1:A:430:PHE:O	1:A:431:ALA:C	2.58	0.44
1:A:470:ILE:HG22	1:A:471:SER:N	2.31	0.44
1:A:484:THR:HG22	1:A:485:ASP:N	2.31	0.44
1:A:507:ILE:HG21	1:B:549:LEU:HD11	1.99	0.44
1:A:686:ILE:HA	1:A:689:THR:HG22	1.99	0.44
1:A:711:VAL:HG23	1:A:712:VAL:N	2.32	0.44
1:B:382:TYR:C	1:B:382:TYR:HD1	2.25	0.44
1:B:623:LEU:O	1:B:627:PHE:HD2	2.00	0.44
1:A:535:LEU:HB3	1:B:540:LEU:HD23	2.00	0.44
1:B:395:GLY:O	1:B:398:SER:CB	2.65	0.44
1:B:708:ILE:HA	1:B:711:VAL:CG2	2.48	0.44
1:A:154:GLN:HB3	1:A:171:PRO:HB2	1.99	0.44
1:A:185:ILE:O	1:A:189:PHE:HD1	2.01	0.44
1:A:347:LEU:HD13	1:A:347:LEU:HA	1.80	0.44
1:A:397:SER:HB2	1:A:404:MET:CE	2.48	0.44
1:B:80:PHE:CD2	1:B:81:LEU:HD22	2.52	0.44
1:B:288:SER:O	1:B:291:ILE:HB	2.17	0.44
1:B:663:LYS:HD3	1:B:688:ASP:CB	2.48	0.44
1:B:666:LEU:O	1:B:669:GLY:N	2.48	0.44
1:B:705:LEU:CD2	1:B:705:LEU:C	2.91	0.44
1:A:42:ILE:HD12	1:A:42:ILE:C	2.42	0.44
1:A:419:PRO:N	1:A:420:PRO:HD2	2.32	0.44
1:B:181:LEU:HD13	1:B:711:VAL:CG2	2.48	0.44
1:A:25:VAL:O	1:A:28:LYS:CB	2.65	0.44
1:A:167:ILE:O	1:A:167:ILE:CG2	2.65	0.44
1:A:292:PHE:HB3	1:A:339:LEU:HD21	2.00	0.44
1:A:398:SER:HB2	1:A:680:PRO:O	2.18	0.44
1:B:138:LEU:HD22	1:B:298:LEU:HD23	1.99	0.44
1:B:163:ASN:HB2	1:B:169:PHE:HD2	1.81	0.44
1:B:261:TYR:C	1:B:263:PHE:N	2.73	0.44
1:B:341:TYR:O	1:B:345:LYS:CB	2.66	0.44
1:A:138:LEU:HD12	1:A:138:LEU:HA	1.61	0.44
1:A:321:LEU:N	1:A:321:LEU:CD1	2.80	0.44
1:A:341:TYR:O	1:A:345:LYS:CA	2.65	0.44
1:A:424:LEU:O	1:A:428:ILE:CD1	2.59	0.44
1:A:558:PHE:HE1	1:A:701:SER:HB3	1.83	0.44
1:B:62:ILE:O	1:B:65:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:GLY:CA	1:B:129:MET:HA	2.48	0.44
1:B:307:TYR:O	1:B:311:LYS:N	2.49	0.44
1:B:662:ALA:O	1:B:684:LEU:HD23	2.18	0.44
1:A:499:LYS:CE	1:A:695:LYS:O	2.57	0.44
1:A:521:GLN:CA	1:A:721:LYS:HD3	2.47	0.44
1:A:545:ILE:CG1	1:B:511:LEU:HD21	2.39	0.44
1:A:719:ILE:HG22	1:A:723:VAL:CG1	2.42	0.44
1:B:386:TYR:HB3	1:B:391:THR:HG22	1.97	0.44
1:B:430:PHE:O	1:B:431:ALA:C	2.59	0.44
1:B:711:VAL:C	1:B:714:VAL:HG22	2.41	0.44
1:A:711:VAL:C	1:A:714:VAL:HG22	2.39	0.44
1:B:261:TYR:CD1	1:B:264:PRO:CG	3.01	0.44
1:B:347:LEU:HD13	1:B:347:LEU:HA	1.77	0.44
1:B:559:SER:OG	1:B:702:LEU:HD21	2.17	0.44
1:B:129:MET:CE	1:B:237:VAL:HB	2.40	0.44
1:B:129:MET:O	1:B:133:VAL:HG23	2.17	0.44
1:A:15:LEU:HD11	1:A:136:PHE:CD1	2.53	0.43
1:A:702:LEU:HD12	1:A:702:LEU:HA	1.69	0.43
1:A:705:LEU:CD2	1:A:705:LEU:C	2.90	0.43
1:B:82:LEU:HD21	1:B:140:GLY:HA2	1.99	0.43
1:B:184:SER:CA	1:B:246:GLU:HG3	2.47	0.43
1:B:185:ILE:O	1:B:189:PHE:HD1	2.01	0.43
1:B:243:ASP:CG	1:B:704:ILE:CD1	2.90	0.43
1:B:263:PHE:CE1	1:B:276:HIS:CE1	3.06	0.43
1:B:339:LEU:C	1:B:339:LEU:HD13	2.43	0.43
1:B:526:ASP:O	1:B:527:ILE:C	2.60	0.43
1:A:623:LEU:O	1:A:627:PHE:CD2	2.71	0.43
1:B:633:PHE:CE1	1:B:637:VAL:CG2	3.02	0.43
1:A:82:LEU:HD21	1:A:140:GLY:HA2	2.00	0.43
1:A:122:ALA:O	1:A:463:ILE:HG21	2.17	0.43
1:A:205:ALA:C	1:A:207:LEU:H	2.26	0.43
1:A:285:ALA:CB	1:A:347:LEU:HD11	2.48	0.43
1:A:411:SER:CB	1:B:563:ILE:CG2	2.83	0.43
1:A:708:ILE:HA	1:A:711:VAL:CG2	2.47	0.43
1:B:138:LEU:HD12	1:B:138:LEU:HA	1.68	0.43
1:A:246:GLU:OE2	1:A:704:ILE:HG23	2.18	0.43
1:A:295:LEU:O	1:A:298:LEU:HD12	2.17	0.43
1:A:316:ASN:OD1	1:A:316:ASN:C	2.60	0.43
1:A:539:MET:HG3	1:B:539:MET:HG2	1.98	0.43
1:B:248:PHE:CE1	1:B:252:ILE:HD11	2.53	0.43
1:B:334:VAL:CG1	1:B:335:LEU:H	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:VAL:HG13	1:B:721:LYS:HE2	1.99	0.43
1:A:158:LEU:HD21	1:A:283:ILE:HG21	1.98	0.43
1:B:15:LEU:HG	1:B:135:GLY:HA3	2.00	0.43
1:B:382:TYR:CE1	1:B:389:LYS:HB3	2.52	0.43
1:A:325:LEU:HD22	1:A:450:PHE:CE2	2.53	0.43
1:A:398:SER:HA	1:A:405:VAL:CG1	2.48	0.43
1:B:68:LEU:HD22	1:B:77:GLY:CA	2.49	0.43
1:A:389:LYS:O	1:A:390:PRO:C	2.60	0.43
1:A:411:SER:HB2	1:B:563:ILE:HG23	1.94	0.43
1:A:551:GLY:HA2	1:A:637:VAL:HG13	2.01	0.43
1:B:167:ILE:O	1:B:167:ILE:CG2	2.67	0.43
1:B:199:LYS:CG	1:B:696:ASP:CB	2.96	0.43
1:B:337:ALA:N	1:B:363:TRP:CD1	2.87	0.43
1:B:437:LEU:HD13	1:B:437:LEU:HA	1.59	0.43
1:A:145:TYR:CD1	1:A:291:ILE:HD13	2.54	0.43
1:A:297:GLY:C	1:A:299:GLY:H	2.25	0.43
1:A:373:GLY:HA3	1:A:447:MET:HG3	2.01	0.43
1:B:326:TRP:CE2	1:B:378:PHE:CZ	3.00	0.43
1:B:448:LEU:HA	1:B:448:LEU:HD12	1.81	0.43
1:A:101:ALA:HB3	1:A:125:GLY:HA3	2.00	0.43
1:A:169:PHE:CB	1:A:174:MET:HE3	2.38	0.43
1:A:264:PRO:HG2	1:A:519:PHE:HZ	1.84	0.43
1:B:197:TYR:HE2	1:B:230:VAL:CG2	2.30	0.43
1:B:664:LYS:HD3	1:B:664:LYS:HA	1.80	0.43
1:A:261:TYR:O	1:A:264:PRO:HD2	2.19	0.43
1:B:121:VAL:CG1	1:B:122:ALA:H	2.31	0.43
1:B:170:VAL:CG1	1:B:261:TYR:HE2	2.32	0.43
1:B:401:GLY:O	1:B:402:THR:C	2.60	0.43
1:B:526:ASP:C	1:B:528:GLY:N	2.71	0.43
1:A:65:ALA:HB1	1:A:81:LEU:CD2	2.47	0.42
1:A:81:LEU:HD13	1:A:81:LEU:HA	1.72	0.42
1:A:191:ARG:O	1:A:195:GLY:N	2.47	0.42
1:A:446:GLY:O	1:A:447:MET:C	2.62	0.42
1:A:457:VAL:O	1:A:460:TYR:HB3	2.19	0.42
1:A:720:PHE:CA	1:A:723:VAL:HG12	2.35	0.42
1:B:46:ALA:O	1:B:47:ASP:C	2.60	0.42
1:B:144:VAL:CG1	1:B:176:VAL:HG12	2.49	0.42
1:B:289:TYR:CE1	1:B:339:LEU:HD12	2.53	0.42
1:B:331:LEU:O	1:B:334:VAL:HG12	2.19	0.42
1:B:562:LEU:HD13	1:B:701:SER:CB	2.49	0.42
1:A:148:PHE:CB	1:A:175:THR:HG21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ALA:HB1	1:A:570:ALA:HA	2.00	0.42
1:A:289:TYR:CE2	1:A:362:PRO:HB2	2.53	0.42
1:A:571:MET:HE2	1:A:571:MET:HB3	1.78	0.42
1:B:42:ILE:HD12	1:B:42:ILE:C	2.44	0.42
1:B:200:ALA:HB1	1:B:570:ALA:CA	2.48	0.42
1:A:22:PHE:O	1:A:26:VAL:N	2.40	0.42
1:A:301:SER:CB	1:A:452:ALA:HB3	2.50	0.42
1:A:684:LEU:HA	1:A:684:LEU:HD12	1.41	0.42
1:B:68:LEU:HD21	1:B:76:THR:CG2	2.49	0.42
1:B:77:GLY:O	1:B:80:PHE:HB3	2.20	0.42
1:B:261:TYR:HD1	1:B:264:PRO:HD2	1.84	0.42
1:B:263:PHE:O	1:B:267:VAL:HG23	2.19	0.42
1:B:410:LEU:HA	1:B:410:LEU:HD12	1.59	0.42
1:B:517:TYR:OH	1:B:634:VAL:CG2	2.62	0.42
1:B:684:LEU:HA	1:B:684:LEU:HD12	1.46	0.42
1:A:57:ILE:O	1:A:58:PHE:C	2.63	0.42
1:A:123:TYR:C	1:A:123:TYR:HD1	2.25	0.42
1:A:138:LEU:HD23	1:A:298:LEU:CD2	2.50	0.42
1:A:261:TYR:CD1	1:A:519:PHE:CZ	3.07	0.42
1:B:623:LEU:O	1:B:627:PHE:CD2	2.72	0.42
1:A:322:ASN:O	1:A:326:TRP:CD1	2.73	0.42
1:A:540:LEU:HD23	1:B:535:LEU:HD23	2.01	0.42
1:B:72:THR:O	1:B:73:THR:HG22	2.19	0.42
1:B:86:MET:HE3	1:B:136:PHE:O	2.19	0.42
1:B:101:ALA:HB3	1:B:125:GLY:HA3	2.01	0.42
1:B:262:MET:HE2	1:B:262:MET:H	1.84	0.42
1:B:558:PHE:O	1:B:562:LEU:HG	2.20	0.42
1:A:321:LEU:CD1	1:A:321:LEU:H	2.33	0.42
1:A:431:ALA:HB1	1:A:443:ALA:CB	2.49	0.42
1:A:521:GLN:C	1:A:523:SER:H	2.22	0.42
1:B:261:TYR:CD1	1:B:264:PRO:HD2	2.54	0.42
1:A:10:ILE:N	1:A:11:PRO:HD3	2.34	0.42
1:A:343:TYR:O	1:A:344:LEU:HD23	2.20	0.42
1:A:699:GLY:N	1:A:700:PRO:CD	2.81	0.42
1:B:358:GLY:O	1:B:359:ALA:CB	2.67	0.42
1:B:417:VAL:HG22	1:B:650:ILE:HB	2.02	0.42
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.87	0.42
1:A:289:TYR:CG	1:A:344:LEU:HD11	2.54	0.42
1:A:526:ASP:C	1:A:528:GLY:N	2.78	0.42
1:A:666:LEU:O	1:A:669:GLY:N	2.50	0.42
1:A:669:GLY:O	1:A:670:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LEU:O	1:B:259:ALA:C	2.60	0.42
1:B:263:PHE:HB2	1:B:283:ILE:CD1	2.49	0.42
1:B:461:GLY:O	1:B:465:ASP:CB	2.68	0.42
1:B:563:ILE:HG22	1:B:564:SER:H	1.85	0.42
1:B:667:GLU:HG2	1:B:681:HIS:CD2	2.55	0.42
1:B:677:GLY:O	1:B:678:SER:CB	2.66	0.42
1:A:6:LEU:O	1:A:10:ILE:CD1	2.68	0.42
1:A:282:THR:HA	1:A:347:LEU:CD1	2.45	0.42
1:A:337:ALA:HB2	1:A:363:TRP:NE1	2.34	0.42
1:A:422:LEU:HD22	1:A:422:LEU:O	2.20	0.42
1:B:7:PHE:HA	1:B:10:ILE:HD13	2.02	0.42
1:B:15:LEU:CD2	1:B:135:GLY:HA3	2.49	0.42
1:B:398:SER:OG	1:B:684:LEU:CD2	2.68	0.42
1:B:422:LEU:O	1:B:422:LEU:HD22	2.20	0.42
1:B:652:THR:HB	1:B:694:LEU:C	2.44	0.42
1:A:71:PHE:O	1:A:167:ILE:CD1	2.68	0.42
1:A:286:LEU:HD13	1:A:353:LEU:HG	2.01	0.41
1:A:329:ALA:O	1:A:333:VAL:HG23	2.20	0.41
1:A:705:LEU:O	1:A:705:LEU:CD2	2.68	0.41
1:B:72:THR:O	1:B:73:THR:CG2	2.68	0.41
1:B:189:PHE:CD2	1:B:611:MET:SD	3.13	0.41
1:A:192:VAL:HG11	1:A:614:PRO:HG2	2.00	0.41
1:A:200:ALA:CB	1:A:570:ALA:HB2	2.50	0.41
1:A:363:TRP:CZ2	1:A:367:ILE:CD1	3.02	0.41
1:A:129:MET:HE2	1:A:129:MET:HB3	1.83	0.41
1:A:370:ILE:HG12	1:A:446:GLY:O	2.21	0.41
1:B:123:TYR:C	1:B:123:TYR:HD1	2.27	0.41
1:B:366:ALA:O	1:B:370:ILE:HG13	2.20	0.41
1:A:46:ALA:O	1:A:47:ASP:C	2.60	0.41
1:A:259:ALA:CB	1:A:287:ILE:CG1	2.99	0.41
1:A:627:PHE:CD1	1:A:720:PHE:HB3	2.56	0.41
1:A:647:MET:HE1	1:B:553:ALA:CA	2.46	0.41
1:B:198:THR:O	1:B:201:ALA:HB3	2.20	0.41
1:B:608:LEU:CD2	1:B:611:MET:HE2	2.35	0.41
1:B:663:LYS:HD3	1:B:688:ASP:HB3	2.02	0.41
1:A:79:ALA:O	1:A:82:LEU:HB3	2.20	0.41
1:A:151:TRP:CE3	1:A:152:MET:HG2	2.55	0.41
1:A:337:ALA:HA	1:A:363:TRP:CD1	2.56	0.41
1:B:140:GLY:O	1:B:143:LEU:HB2	2.21	0.41
1:B:168:ASN:C	1:B:168:ASN:HD22	2.27	0.41
1:B:261:TYR:CE1	1:B:264:PRO:CG	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:TYR:CD1	1:B:382:TYR:O	2.73	0.41
1:A:74:TRP:O	1:A:75:GLN:C	2.64	0.41
1:A:157:ASN:C	1:A:159:ASN:N	2.79	0.41
1:A:447:MET:HE3	1:A:447:MET:HB2	1.96	0.41
1:A:613:TYR:HB3	1:A:614:PRO:HD3	2.02	0.41
1:B:86:MET:HE1	1:B:139:LEU:CD2	2.40	0.41
1:B:282:THR:HA	1:B:347:LEU:HD12	2.03	0.41
1:B:389:LYS:HB3	1:B:390:PRO:HD3	2.03	0.41
1:A:158:LEU:C	1:A:159:ASN:O	2.63	0.41
1:A:300:CYS:SG	1:A:332:THR:HA	2.60	0.41
1:A:373:GLY:CA	1:A:447:MET:HG3	2.50	0.41
1:B:81:LEU:HD13	1:B:81:LEU:HA	1.65	0.41
1:B:170:VAL:CG1	1:B:261:TYR:CE2	3.03	0.41
1:A:185:ILE:HG23	1:A:189:PHE:CE1	2.55	0.41
1:A:259:ALA:HB1	1:A:287:ILE:HG13	2.01	0.41
1:A:310:VAL:O	1:A:311:LYS:C	2.63	0.41
1:A:413:GLY:O	1:A:416:SER:HB3	2.21	0.41
1:A:526:ASP:O	1:A:527:ILE:C	2.63	0.41
1:A:717:VAL:HG13	1:A:721:LYS:HE2	2.03	0.41
1:B:460:TYR:OH	1:B:487:LEU:HA	2.20	0.41
1:A:67:LEU:CD1	1:A:71:PHE:HE2	2.32	0.41
1:A:72:THR:O	1:A:73:THR:HG22	2.21	0.41
1:A:72:THR:O	1:A:73:THR:CG2	2.69	0.41
1:A:77:GLY:O	1:A:80:PHE:HB3	2.21	0.41
1:A:138:LEU:HD23	1:A:298:LEU:HD21	2.03	0.41
1:A:138:LEU:CD2	1:A:298:LEU:HD23	2.51	0.41
1:A:282:THR:O	1:A:286:LEU:HG	2.21	0.41
1:A:288:SER:CB	1:A:292:PHE:CE2	3.04	0.41
1:A:370:ILE:CG1	1:A:446:GLY:O	2.69	0.41
1:A:410:LEU:HD12	1:A:410:LEU:HA	1.81	0.41
1:A:538:ASN:O	1:A:544:VAL:HG21	2.20	0.41
1:B:25:VAL:CG2	1:B:124:GLN:CD	2.94	0.41
1:B:44:SER:O	1:B:45:GLY:C	2.64	0.41
1:B:413:GLY:O	1:B:417:VAL:HG23	2.21	0.41
1:B:494:THR:HA	1:B:497:ILE:HD12	2.03	0.41
1:B:619:ILE:O	1:B:622:PRO:HD2	2.21	0.41
1:B:649:ALA:HA	1:B:699:GLY:CA	2.51	0.41
1:A:44:SER:O	1:A:45:GLY:C	2.63	0.41
1:A:68:LEU:HD22	1:A:77:GLY:CA	2.51	0.41
1:A:341:TYR:O	1:A:345:LYS:CB	2.68	0.41
1:A:523:SER:HB3	1:A:524:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:TYR:CE2	1:A:613:TYR:HB3	2.56	0.41
1:A:605:ASP:OD1	1:A:609:LYS:HD2	2.21	0.41
1:A:619:ILE:HD12	1:A:712:VAL:HG21	2.03	0.41
1:B:129:MET:SD	1:B:459:SER:CB	3.06	0.41
1:B:168:ASN:O	1:B:168:ASN:ND2	2.42	0.41
1:B:332:THR:O	1:B:336:THR:CB	2.69	0.41
1:B:651:LEU:O	1:B:655:SER:HB3	2.20	0.41
1:A:337:ALA:HB2	1:A:363:TRP:CZ2	2.55	0.40
1:A:357:PHE:CE1	1:A:434:PHE:HD1	2.39	0.40
1:A:404:MET:HE3	1:A:404:MET:HB3	1.74	0.40
1:A:448:LEU:HA	1:A:448:LEU:HD12	1.77	0.40
1:B:163:ASN:ND2	1:B:164:TRP:H	2.19	0.40
1:B:446:GLY:O	1:B:447:MET:C	2.63	0.40
1:A:53:GLU:HA	1:A:608:LEU:HD11	2.04	0.40
1:A:401:GLY:O	1:A:402:THR:C	2.62	0.40
1:A:553:ALA:HB1	1:B:418:PHE:CD1	2.56	0.40
1:A:563:ILE:HG21	1:A:563:ILE:HD13	1.91	0.40
1:A:624:VAL:O	1:A:628:LEU:HD13	2.21	0.40
1:B:400:GLU:CG	1:B:404:MET:HE2	2.46	0.40
1:B:679:GLU:N	1:B:680:PRO:CD	2.84	0.40
1:A:258:LEU:O	1:A:259:ALA:C	2.62	0.40
1:A:310:VAL:O	1:A:310:VAL:CG1	2.69	0.40
1:A:339:LEU:O	1:A:343:TYR:HB2	2.21	0.40
1:A:357:PHE:HZ	1:A:364:PHE:HB2	1.85	0.40
1:A:437:LEU:O	1:A:440:VAL:HB	2.21	0.40
1:A:503:ILE:HD13	1:A:649:ALA:HB1	2.01	0.40
1:B:603:THR:HA	1:B:606:ASN:HB3	2.04	0.40
1:B:626:GLY:CA	1:B:634:VAL:HG13	2.51	0.40
1:B:719:ILE:HG22	1:B:723:VAL:CG1	2.45	0.40
1:B:50:LEU:HD13	1:B:50:LEU:HA	1.91	0.40
1:B:87:SER:OG	1:B:186:ILE:HG21	2.21	0.40
1:A:354:GLY:O	1:A:435:ALA:CA	2.69	0.40
1:A:450:PHE:HZ	1:A:501:PHE:CE2	2.35	0.40
1:B:122:ALA:O	1:B:463:ILE:HG21	2.21	0.40
1:B:517:TYR:CE1	1:B:717:VAL:HG11	2.56	0.40
1:B:523:SER:HB3	1:B:524:PRO:HD2	2.03	0.40
1:B:622:PRO:HG3	1:B:709:MET:CG	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	643/735 (88%)	579 (90%)	42 (6%)	22 (3%)	3	24
1	B	626/735 (85%)	566 (90%)	37 (6%)	23 (4%)	2	22
All	All	1269/1470 (86%)	1145 (90%)	79 (6%)	45 (4%)	3	23

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	TYR
1	A	74	TRP
1	A	163	ASN
1	A	260	SER
1	A	269	LYS
1	A	298	LEU
1	A	359	ALA
1	A	402	THR
1	A	522	ILE
1	A	527	ILE
1	A	672	GLU
1	B	41	TYR
1	B	74	TRP
1	B	158	LEU
1	B	163	ASN
1	B	268	GLN
1	B	269	LYS
1	B	298	LEU
1	B	402	THR
1	B	522	ILE
1	B	527	ILE
1	A	159	ASN
1	A	297	GLY
1	A	358	GLY
1	A	387	ARG

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Mol	Chain	Res	Type
1	A	435	ALA
1	B	159	ASN
1	B	260	SER
1	B	297	GLY
1	B	359	ALA
1	B	387	ARG
1	B	435	ALA
1	B	676	LYS
1	A	449	SER
1	B	166	GLY
1	A	27	ARG
1	A	166	GLY
1	A	678	SER
1	B	168	ASN
1	A	389	LYS
1	A	470	ILE
1	B	27	ARG
1	B	389	LYS
1	B	523	SER
1	B	675	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	482/575 (84%)	415 (86%)	67 (14%)	3	17
1	B	460/575 (80%)	404 (88%)	56 (12%)	5	21
All	All	942/1150 (82%)	819 (87%)	123 (13%)	4	19

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	48	SER
1	A	50	LEU

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Mol	Chain	Res	Type
1	A	54	THR
1	A	57	ILE
1	A	67	LEU
1	A	82	LEU
1	A	86	MET
1	A	87	SER
1	A	102	ASN
1	A	103	VAL
1	A	110	ARG
1	A	124	GLN
1	A	138	LEU
1	A	143	LEU
1	A	162	THR
1	A	186	ILE
1	A	199	LYS
1	A	230	VAL
1	A	240	LEU
1	A	262	MET
1	A	263	PHE
1	A	267	VAL
1	A	268	GLN
1	A	274	LEU
1	A	298	LEU
1	A	314	SER
1	A	315	ASP
1	A	324	SER
1	A	339	LEU
1	A	346	ASP
1	A	347	LEU
1	A	353	LEU
1	A	375	LEU
1	A	389	LYS
1	A	392	GLN
1	A	404	MET
1	A	407	SER
1	A	410	LEU
1	A	412	LEU
1	A	422	LEU
1	A	437	LEU
1	A	448	LEU
1	A	484	THR
1	A	508	PHE

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Mol	Chain	Res	Type
1	A	533	LEU
1	A	535	LEU
1	A	536	LEU
1	A	537	LEU
1	A	540	LEU
1	A	550	LEU
1	A	554	ILE
1	A	563	ILE
1	A	609	LYS
1	A	613	TYR
1	A	619	ILE
1	A	638	LEU
1	A	663	LYS
1	A	666	LEU
1	A	679	GLU
1	A	684	LEU
1	A	695	LYS
1	A	702	LEU
1	A	704	ILE
1	A	705	LEU
1	A	722	HIS
1	A	725	LEU
1	B	13	VAL
1	B	48	SER
1	B	50	LEU
1	B	54	THR
1	B	57	ILE
1	B	67	LEU
1	B	82	LEU
1	B	86	MET
1	B	87	SER
1	B	102	ASN
1	B	103	VAL
1	B	112	THR
1	B	124	GLN
1	B	138	LEU
1	B	143	LEU
1	B	158	LEU
1	B	160	ILE
1	B	162	THR
1	B	163	ASN
1	B	168	ASN

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Mol	Chain	Res	Type
1	B	186	ILE
1	B	199	LYS
1	B	230	VAL
1	B	240	LEU
1	B	262	MET
1	B	298	LEU
1	B	339	LEU
1	B	347	LEU
1	B	375	LEU
1	B	410	LEU
1	B	422	LEU
1	B	429	LEU
1	B	437	LEU
1	B	448	LEU
1	B	484	THR
1	B	508	PHE
1	B	533	LEU
1	B	536	LEU
1	B	537	LEU
1	B	540	LEU
1	B	550	LEU
1	B	554	ILE
1	B	563	ILE
1	B	571	MET
1	B	609	LYS
1	B	619	ILE
1	B	628	LEU
1	B	638	LEU
1	B	655	SER
1	B	663	LYS
1	B	666	LEU
1	B	684	LEU
1	B	702	LEU
1	B	704	ILE
1	B	705	LEU
1	B	722	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	229	ASN

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Mol	Chain	Res	Type
1	A	233	ASN
1	A	276	HIS
1	A	318	GLN
1	A	466	ASN
1	A	486	HIS
1	A	521	GLN
1	A	606	ASN
1	A	661	ASN
1	B	233	ASN
1	B	466	ASN
1	B	521	GLN
1	B	661	ASN
1	B	670	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	B	1727	3	4,4,4	0.98	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	B	1728	4,3	4,4,4	0.97	0	6,6,6	0.43	0
2	PO4	A	1727	3	4,4,4	0.97	0	6,6,6	0.43	0
2	PO4	A	1728	4,3	4,4,4	0.98	0	6,6,6	0.52	0

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.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1728	PO4	4	0
2	A	1727	PO4	1	0
2	A	1728	PO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	655/735 (89%)	0.06	24 (3%) 45 34	92, 214, 365, 540	0
1	B	642/735 (87%)	0.09	25 (3%) 43 33	77, 244, 418, 583	0
All	All	1297/1470 (88%)	0.07	49 (3%) 44 34	77, 228, 390, 583	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	668	ALA	5.7
1	A	540	LEU	4.9
1	B	119	LEU	4.9
1	B	387	ARG	4.9
1	B	236	ASP	4.7
1	A	44	SER	4.7
1	A	245	LEU	4.2
1	B	314	SER	4.1
1	A	119	LEU	4.1
1	B	244	LEU	4.1
1	B	248	PHE	4.1
1	A	387	ARG	4.0
1	A	348	GLN	4.0
1	A	248	PHE	3.9
1	A	526	ASP	3.4
1	A	246	GLU	3.2
1	A	247	SER	3.2
1	B	382	TYR	3.0
1	A	314	SER	3.0
1	B	237	VAL	2.9
1	B	670	ASN	2.7
1	B	520	SER	2.7
1	A	236	ASP	2.6
1	A	298	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	233	ASN	2.6
1	B	383	TYR	2.5
1	B	313	PRO	2.5
1	A	41	TYR	2.5
1	A	40	SER	2.5
1	B	134	GLY	2.5
1	A	122	ALA	2.5
1	B	40	SER	2.4
1	B	240	LEU	2.4
1	A	238	ALA	2.4
1	A	244	LEU	2.4
1	A	66	ILE	2.3
1	B	133	VAL	2.3
1	B	42	ILE	2.3
1	B	388	TYR	2.3
1	B	298	LEU	2.2
1	B	184	SER	2.2
1	B	389	LYS	2.2
1	A	134	GLY	2.1
1	A	121	VAL	2.1
1	A	382	TYR	2.1
1	A	466	ASN	2.1
1	B	466	ASN	2.1
1	A	42	ILE	2.0
1	B	390	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	1730	1/1	0.73	0.12	194,194,194,194	0
2	PO4	B	1727	5/5	0.77	0.15	294,296,296,296	0
4	K	A	1733	1/1	0.79	0.17	151,151,151,151	0
3	MG	B	1730	1/1	0.80	0.23	124,124,124,124	0
2	PO4	A	1727	5/5	0.80	0.10	348,350,350,352	0
2	PO4	B	1728	5/5	0.81	0.12	209,217,220,220	0
3	MG	A	1729	1/1	0.83	0.14	170,170,170,170	0
3	MG	B	1731	1/1	0.84	0.12	269,269,269,269	0
2	PO4	A	1728	5/5	0.85	0.09	184,205,210,217	0
3	MG	A	1732	1/1	0.89	0.09	220,220,220,220	0
4	K	B	1733	1/1	0.93	0.14	151,151,151,151	0
3	MG	A	1731	1/1	0.94	0.09	213,213,213,213	0
3	MG	B	1729	1/1	0.95	0.14	133,133,133,133	0
3	MG	B	1732	1/1	0.96	0.05	184,184,184,184	0

6.5 Other polymers [i](#)

There are no such residues in this entry.